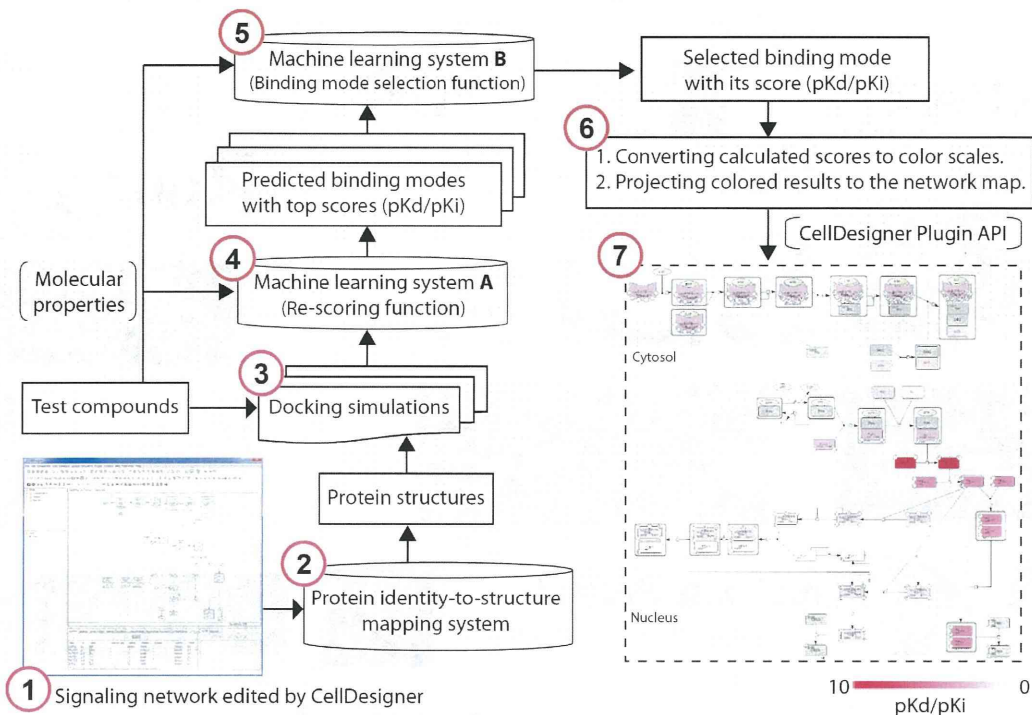
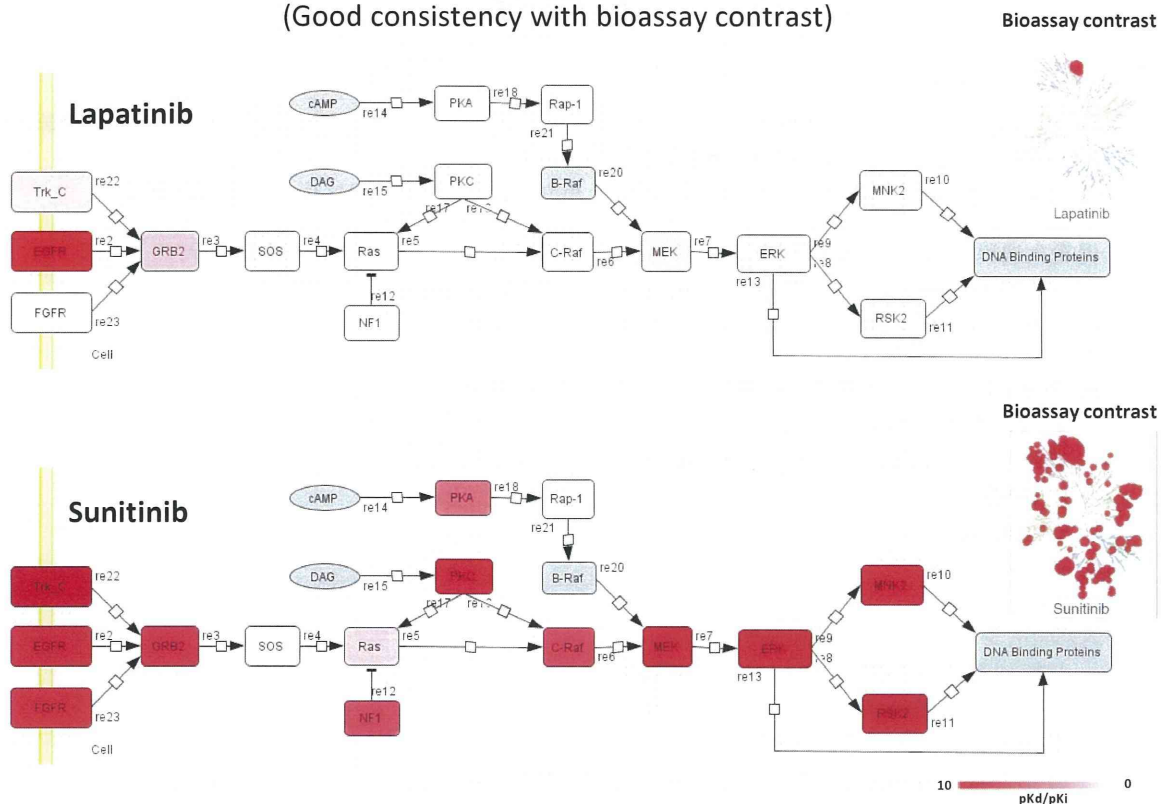


## Network-based screening pipeline



61

## Case Study Using Our Method over MAPK Pathway (Good consistency with bioassay contrast)



62

# Garuda Alliance (snapshot May 2013)



63

## まとめ

- 新型反復暴露解析:
  - 過渡反応と基線反応の基本的な関連性を見いだした。毒性学的に新規性が高くエピジェネティクス等の機序の関与が示唆される。上流にEif2、RICTORなどが想定された。
  - 反復毒性の分子毒性学的理解の促進、及び、単回暴露データからの反復毒性予測に重要。
- 胎児発生過程におけるマスター遺伝子を基軸とした遺伝子発現ネットワークの網羅的解析:
  - 微分解析手法により、網羅的・効率的に発生マスター遺伝子の解析に成功した。
  - 未報告の上流制御系が抽出される可能性が見いだされた。
- Percellome 3次元データ等の為の専用解析ソフトウェアの開発研究
  - 異種動物データの統合技術
  - 絶対量化されていない非Percellomeデータの絶対量推定技術
  - RSort改良
  - WebAPI改良
  - その他
- システムトキシコロジー解析基盤の研究開発:
  - 状態制御遺伝子群推定アルゴリズムAGCT
  - オルソログ制御領域分析ソフトウェアSHOE
  - 遺伝子制御関係推定アルゴリズム
  - Web公開/Garuda Platform実装/AOP適合/Networkによるスクリーニングパイプライン
  - 次世代Computational Tox Screening Systemの創出

64

(資料 2)

Percellome Database  
-PercellomeExplorer 解析結果-

Percellome Database

# Project List

(gavage, Liver only)

2015/03

Name	Condition	Total Num
TTG010-L	Acetaminophen	3251
TTG011-L	Isoniazid	1871
TTG014-L	"2,4-dinitrophenol"	1092
TTG015-L	"4-amino-2,6-dichlorophenol"	980
TTG016-L(C)	Pentachlorophenol	4420
TTG019-L	2-Vinylpyridine	2065
TTG020-L	"TCDD(2,3,7,8-Tetrachlorodibenzo-p-Dioxin)"	2988
TTG023-L	Transplatin	849
TTG026-L	"TCDF(2,3,7,8-Tetrachlorodibenzofuran)"	2793
TTG027-L	"1,2,3-Triazole"	1669
TTG028-L	"1,2,4-Triazole"	1692
TTG029-L	2-Aminomethylpyridine	790
TTG030-L	N-Methylaniline	2509
TTG031-L	"2-Chloro-4,6-dimethylaniline"	2884
TTG032-L	"3-Amino-1H-1,2,4-triazole"	6628
TTG033-L	"1,2-Dichloro-3-nitrobenzene"	1561
TTG034-L	4-Ethylnitrobenzene	1453
TTG035-L	Acetaminophen	3140
TTG037-L	Phenobarbital	5580
TTG038-L	Hydroxycitric Acid	1681
TTG039-L	Citric acid-calcium salt	1229
TTG040-L	Cisplatin	2538
TTG041-L	Valproic acid sodium salt	5706
TTG042-L	Ethynyl estradiol (PLD)	1646
TTG043-L	Testosterone propionate	1639
TTG044-L	Clofibrate	3317
TTG045-L	Troglitazone	3171
TTG046-L	Levothyroxine	2953
TTG047-L	Bisphenol A (PLD)	1575
TTG048-L	Genistein (PLD)	2445
TTG049-L	Tributyltin chloride	1228
TTG051-L	9-cis retinoic acid	1592
TTG052-L	All trans retinoic acid	5388
TTG053-L	Ethynyl estradiol (PLD)	4203
TTG054-L	Diethylnitrosamine (C57BL/6)	3699
TTG055-L	N-ethy1-N-nitrosourea	1359
TTG056-L	3-methylcholanthrene	3012
TTG057-L	Indigo	1067
TTG058-L	Diethylnitrosamine (C3H)	1368
TTG059-L	Caffeine	2307
TTG060-L	Forskolin	1351
TTG061-L	Paraquat dichloride	2592
TTG062-L(C)	Dexamethasone	3080
TTG063-L	Sodium Arsenite	1774
TTG066-L	Methoprene	1893
TTG067-L	Acephate	1465
TTG068-L	Carbaryl	2190
TTG070-L	Formaldehyde	764
TTG071-L	Acetaldehyde	2137
TTG073-L	Toluene	2981
TTG074-L	Bromobenzene	4605
TTG075-L	Carbon tetrachloride	1993
TTG077-L	Monocrotaline	1230
TTG078-L	Ethanol	1484
TTG079-L	Methanol	1968
TTG080-L	DMSO	1325
TTG081-L	Warfarin	1043
TTG083-L	Diethylstilbestrol	1978
TTG084-L	Tamoxifen	1824
TTG085-L	Trybutyltin	1968
TTG086-L	Coenzyme Q10	3750
TTG087-L	Pyriproxyfen	2210
TTG088-L	Tebufenozide	994
TTG089-L	Rifampicin	1659
TTG090-L	Pregnenolone Carbonitrile	2960

TTG091-L	Azacytidine	1693
TTG092-L	Deet	2076
TTG093-L	AraC	2163
TTG094-L	Aspirin	2922
TTG095-L	Ibuprofen (dl-p-isobutylhydratropic acid)	2088
TTG096-L	Omeprazole	2844
TTG097-L	Permethrin	1061
TTG098-L	DEHP	5677
TTG099-L	Paclitaxel (Taxol)	1330
TTG100-L	Phenytoin	2753
TTG104-L	MEHP	5444
TTG109-L	Acephate	3384
TTG110-L	Glycyrrhizin	4107
TTG112-L	FK506	1407
TTG114-L	Benzene	2955
TTG115-L	Kanamycin monosulfate	1333
TTG116-L	Agaricine	1614
TTG117-L	Digitoxin	2017
TTG118-L	Clofibrate x Clofibrate	3527
TTG119-L	Carbon tetrachloride	1724
TTG120-L	Clofibrate x PCN	2847
TTG121-L	Clofibrate x ATRA	2227
TTG122-L	CoenzymeQ10(14day)	3068
TTG123-L	Caffeine	1761
TTG124-L	Vat Red I	1849
TTG126-L	Thalidomide	1807
TTG128-L	alpha-Lipoic Acid	1532
TTG129-L	CCl4 x Clofibrate	2935
TTG130-L	CCl4 x CCl4	1206
TTG131B-L	CCl4 x Phenobarbital	2878
TTG132-L	Curcumin	3832
TTG133-L	Maltol	1393
TTG134-L	Nerolidol	1234
TTG135-L	Methyl dihydro jasmonate	1274
TTG136-L	Phytol	4729
TTG137-L	alpha-Lipoic Acid	1910
TTG139-L	Indigo Carmine	2443
TTG140-L	Food Red No.40	1860
TTG141-L	Tributyltin chloride x Clofibrate	4392
TTG144-L	Tributyltin chloride x Phenobarbital	2900
TTG145-L	Tributyltin chloride x Tributyltin chloride	1801
TTG146-L	Forskolin	2515
TTG147-L	Estragole	1869
TTG148-L	Verbenone	1326
TTG149-L	Valproic acid sodium salt x Aspirin	2765
TTG150-L	Valproic acid sodium salt x Thalidomide	2990
TTG151-L	Valproic acid sodium salt x Valproic acid sodium salt	3622
TTG152-L	FD&C Blue No.1	2908
TTG154-L	Sodium Dehydroacetate	3953
TTG155-L	Aluminum ammonium sulfate	2215
TTG156-L	Food Red No.104	3344
TTG157-L	Valproic acid sodium salt	4741
TTG158-L	Deet x Permethrin	2031
TTG159-L	Deet x Deet	2881
TTG160-L	5-fluorouracil	3974
TTG161-L	Food Yellow No.4	2725
TTG162-L	Sesame seed oil unsaponified matter	3143
TTG163-L	Aluminum lactate	2266
TTG165-L	Chlorpyrifos	2007
TTG166-L	Carbaryl	2901
TTG167-L	Aloe arborescens extract	1487
TTG168-L	Mastic	2642
TTG169-L	Houttuynia extract	1425
TTG170-L	3-methylcholanthrene/AhRKO	1619

TTG170-L	3-methylcholanthrene/AhRKO	1619
TTG173-L	TCDD/AhRKO	6384
TTG176-L	Green No.204 (Pyranine Conc)	1453
TTG177-L	Red No.102	1750
TTG178-L	Aluminum sulfate	2231
TTG180-L	Red No.105	2176
TTG182-L	Imidacloprid	3359
TTG183-L	Bisphenol A (corn oil)	2065
TTG184-L	Bisphenol A/ERaKO(Chambon) (corn oil)	1781
TTG185-L(B)	Ethynyl estradiol (corn oil)	1725
TTG186-L	Ethynyl estradiol/ERaKO(Chambon) (corn oil)	1632
TTG187-L	Violet No.201	2093
TTG188-L	Violet No.401	1426
TTG190-L	TTG4: A) CCl4, B) Ccl4 (TTG4(2+1))	1228
TTG191-L	TTG4: A) CCl4, B) Ccl4 (TTG4(4+1))	1451
TTG189-L	TTG4: A) CCl4, B) Ccl4 (TTG4(1+1))	2628
TTG193-L	TTG4: A) Valproic acid sodium salt, B) Valproic acid sodium salt (TTG4(1+1))	3387
TTG194-L	TTG4: A) Valproic acid sodium salt, B) Valproic acid sodium salt (TTG4(2+1))	5057
TTG195-L	TTG4: A) Valproic acid sodium salt, B) Valproic acid sodium salt (TTG4(4+1))	4246
TTG199-L	Black No.401	1582
TTG202-L	TTG4: A) Clofibrate, B) Clofibrate (TTG4(4+1))	1936
TTG200-L	TTG4: A) Clofibrate, B) Clofibrate (TTG4(1+1))	2028
TTG201-L	TTG4: A) Clofibrate, B) Clofibrate (TTG4(2+1))	2152
TTG204-L	Red No.225	4199
TTG205-L	BTAZ3846(CoCAM 1)	12257
TTG206-L	BTAZ3864(CoCAM 2)	9318

# Percellome Database

## PDBEx-PCA

(gavage, Liver only)

2015/03

Percellome Explorer ver. 0.5.0

DataSet: PDBEx\_RSort\_Expand\_H\_G2\_AP\_Std-Av@

Denominator: Target \* Candidate

Strict Matching Mode



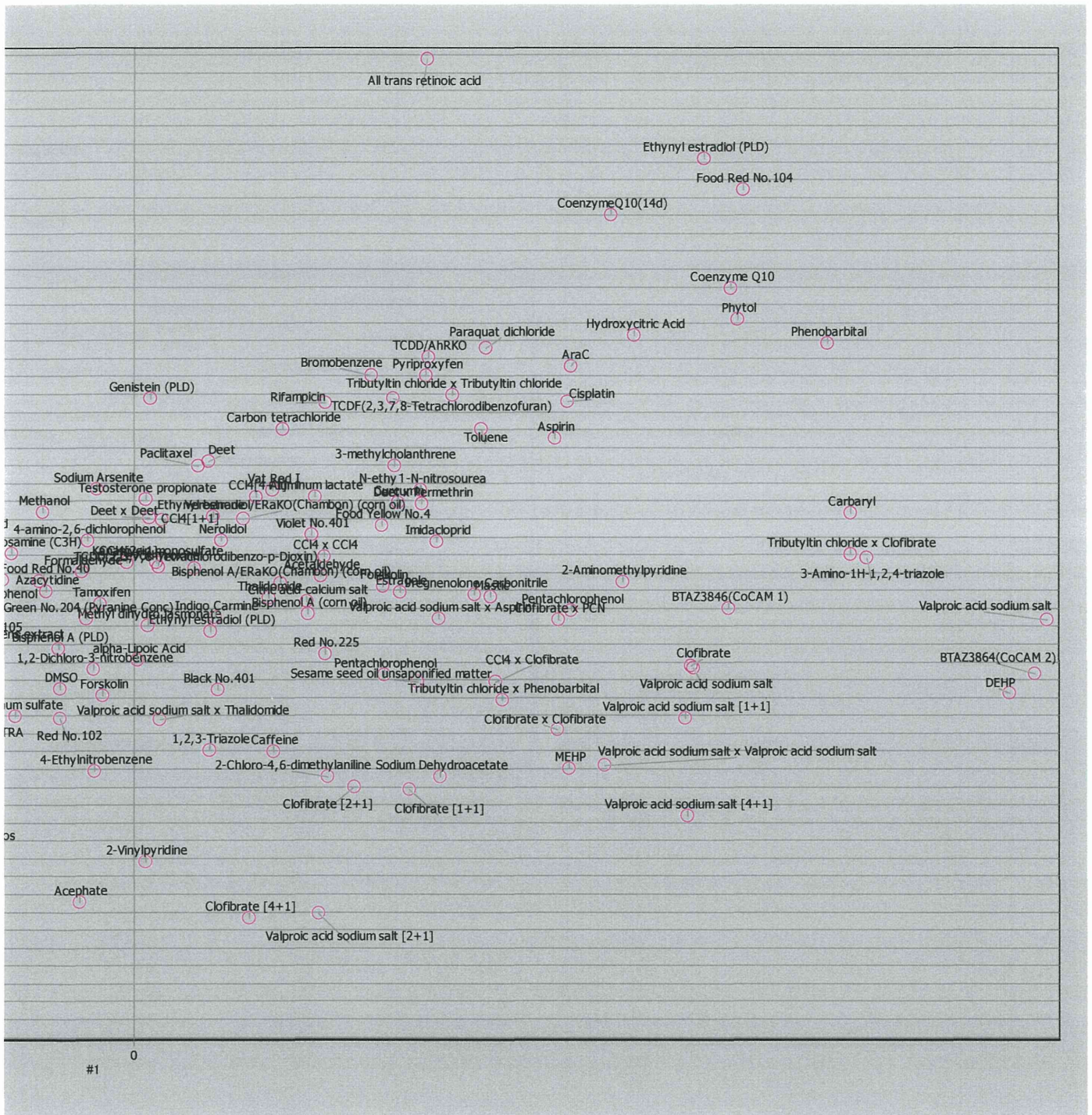
# PDBEx-PCA (#1 vs #2) : whole view

Percellome Explorer ver. 0.5.0 : PDBEx\_RSort\_Expand\_H\_G2\_AP\_Std-Av@

Denominator: Target \* Candidate







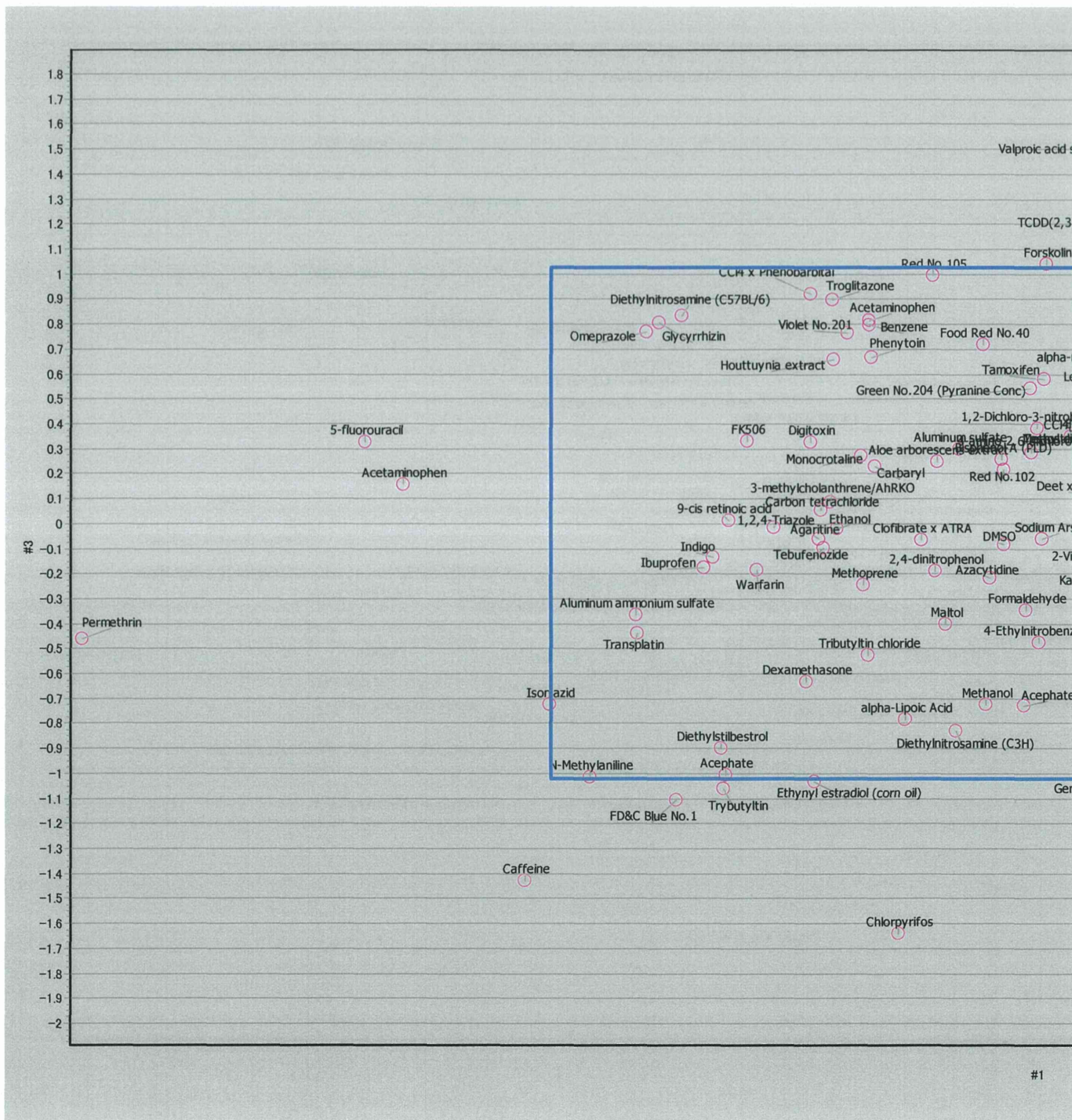
→ #1成分と#2成分が比較的強い正の相関を示しているため、#3成分も検討する



# PDBEx-PCA (#1 vs #3) : whole view

Percellome Explorer ver. 0.5.0 : PDBEx\_RSort\_Expand\_H\_G2\_AP\_Std-Av@

Denominator: Target \* Candidate





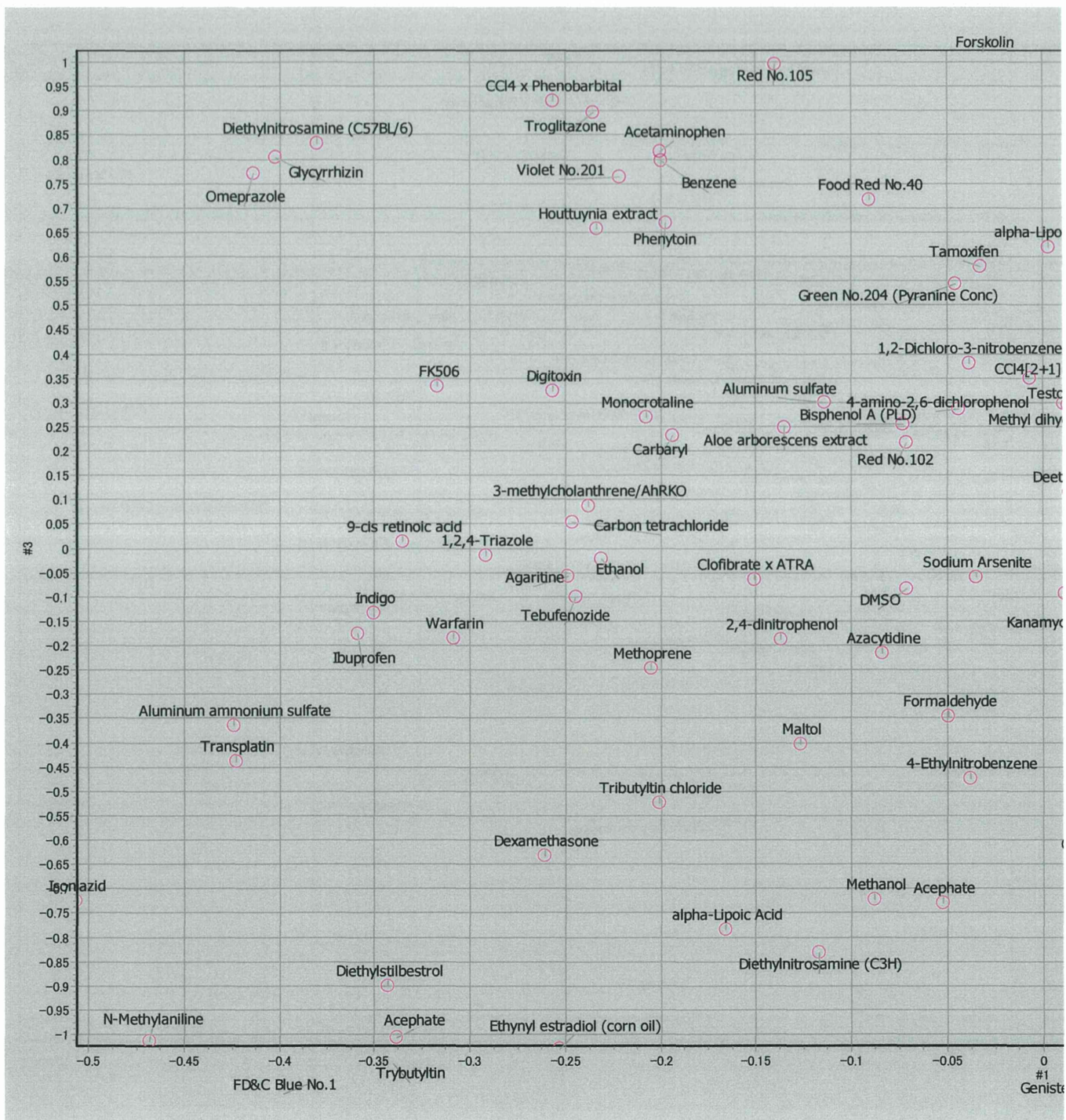




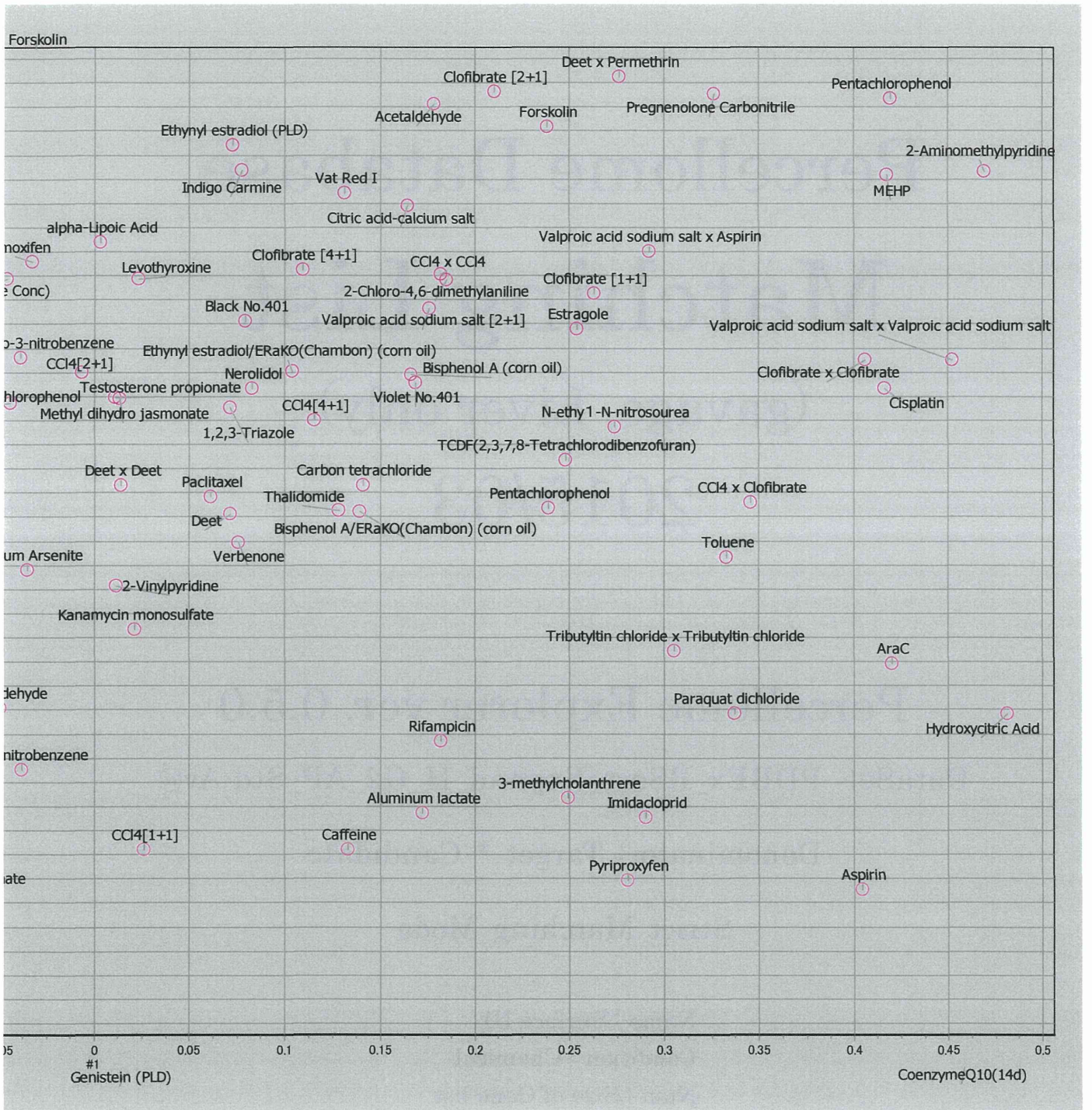
# PDBEx-PCA (#1 vs #3) : origin view

Percellome Explorer ver. 0.5.0 : PDBEx\_RSort\_Expand\_H\_G2\_AP\_Std-Av@

Denominator: Target \* Candidate







# Percellome Database

# Matching List

(gavage, Liver only)

2015/03

Percellome Explorer ver. 0.5.0

DataSet: PDBEx\_RSort\_Expand\_H\_G2\_AP\_Std-Av@

Denominator: Target \* Candidate

Strict Matching Mode

Name : Surface ID

Condition : Chemical

Num : Size of Gene list

Cor : correlation index

Name	Condition	Num	Cor
TTG010-L	Acetaminophen	3251	3.076
TTG027-L	1,2,3-Triazole	241	0.444
TTG019-L	2-Vinylpyridine	264	0.393
TTG011-L	Isoniazid	238	0.391
TTG078-L	Ethanol	188	0.39
TTG160-L	5-fluorouracil	496	0.384
TTG028-L	1,2,4-Triazole	195	0.355
TTG096-L	Omeprazole	325	0.352
TTG029-L	2-Aminomethylpyridine	90	0.35
TTG068-L	Carbaryl	247	0.347
TTG077-L	Monocrotaline	137	0.343
TTG031-L	2-Chloro-4,6-dimethylaniline	316	0.337
TTG071-L	Acetaldehyde	234	0.337
TTG034-L	4-Ethylnitrobenzene	158	0.334
TTG100-L	Phenytoin	294	0.328
TTG030-L	N-Methylaniline	264	0.324
TTG186-L	Ethynyl estradiol/ERaKO(Chambon) (corn oil)	171	0.322
TTG084-L	Tamoxifen	190	0.32
TTG150-L	Valproic acid sodium salt x Thalidomide	307	0.316
TTG130-L	CCl4 x CCl4	123	0.314
TTG014-L	2,4-dinitrophenol	109	0.307
TTG095-L	Ibuprofen (dl-p-isobutylhydratropic acid)	206	0.303
TTG097-L	Permethrin	104	0.302
TTG114-L	Benzene	289	0.301
TTG062-L(C)	Dexamethasone	299	0.299
TTG146-L	Forskolin	241	0.295
TTG167-L	Aloe arborescens extract	142	0.294
TTG109-L	Acephate	315	0.286
TTG177-L	Red No.102	162	0.285
TTG112-L	FK506	130	0.284
TTG035-L	Acetaminophen	289	0.283
TTG054-L	Diethylnitrosamine (C57BL/6)	339	0.282
TTG202-L	TTG4: A) Clofibrate, B) Clofibrate (TTG4(4+1))	176	0.28
TTG178-L	Aluminum sulfate	202	0.279
TTG057-L	Indigo	94	0.271
TTG059-L	Caffeine	203	0.271
TTG075-L	Carbon tetrachloride	175	0.27
TTG083-L	Diethylstilbestrol	171	0.266
TTG039-L	Citric acid-calcium salt	105	0.263
TTG170-L	3-methylcholanthrene/AhRKO	138	0.262
TTG116-L	Agaritin	136	0.259
TTG121-L	Clofibrate x ATRA	187	0.258
TTG023-L	Transplatin	71	0.257
TTG042-L	Ethynyl estradiol (PLD)	137	0.256
TTG080-L	DMSO	110	0.255
TTG169-L	Houttuynia extract	117	0.253
TTG131B-L	CCl4 x Phenobarbital	233	0.249
TTG081-L	Warfarin	84	0.248
TTG110-L	Glycyrrhizin	331	0.248
TTG152-L	FD&C Blue No.1	234	0.248
TTG085-L	Trybutyltin	156	0.244
TTG051-L	9-cis retinoic acid	122	0.236
TTG126-L	Thalidomide	138	0.235
TTG154-L	Sodium Dehydroacetate	300	0.233
TTG060-L	Forskolin	101	0.23
TTG145-L	Tributyltin chloride x Tributyltin chloride	132	0.225
TTG033-L	1,2-Dichloro-3-nitrobenzene	113	0.223
TTG067-L	Acephate	106	0.223
TTG115-L	Kanamycin monosulfate	96	0.222
TTG049-L	Tributyltin chloride	87	0.218
TTG180-L	Red No.105	154	0.218
TTG148-L	Verbenone	93	0.216
TTG163-L	Aluminum lactate	157	0.213



Name	Condition	Num	Cor
TTG011-L	Isoniazid	1871	5.345
TTG010-L	Acetaminophen	238	0.391
TTG014-L	2,4-dinitrophenol	78	0.382
TTG019-L	2-Vinylpyridine	119	0.308
TTG083-L	Diethylstilbestrol	112	0.303
TTG027-L	1,2,3-Triazole	92	0.295
TTG160-L	5-fluorouracil	214	0.288
TTG078-L	Ethanol	79	0.285
TTG085-L	Trybutyltin	103	0.28
TTG081-L	Warfarin	54	0.277
TTG096-L	Omeprazole	147	0.276
TTG186-L	Ethynyl estradiol/ERaKO(Chambon) (corn oil)	84	0.275
TTG068-L	Carbaryl	112	0.273
TTG028-L	1,2,4-Triazole	85	0.269
TTG034-L	4-Ethylnitrobenzene	73	0.269
TTG116-L	Agaritin	81	0.268
TTG133-L	Maltol	69	0.265
TTG177-L	Red No.102	84	0.257
TTG059-L	Caffeine	110	0.255
TTG080-L	DMSO	63	0.254
TTG146-L	Forskolin	119	0.253
TTG202-L	TTG4: A) Clofibrate, B) Clofibrate (TTG4(4+1))	91	0.251
TTG029-L	2-Aminomethylpyridine	37	0.25
TTG084-L	Tamoxifen	85	0.249
TTG134-L	Nerolidol	56	0.243
TTG152-L	FD&C Blue No.1	132	0.243
TTG163-L	Aluminum lactate	102	0.241
TTG100-L	Phenytoin	122	0.237
TTG062-L(C)	Dexamethasone	136	0.236
TTG015-L	4-amino-2,6-dichlorophenol	43	0.235
TTG165-L	Chlorpyrifos	88	0.234
TTG167-L	Aloe arborescens extract	65	0.234
TTG126-L	Thalidomide	77	0.228
TTG030-L	N-Methylaniline	105	0.224
TTG130-L	CCl4 x CCl4	50	0.222
TTG042-L	Ethynyl estradiol (PLD)	68	0.221
TTG067-L	Acephate	60	0.219
TTG114-L	Benzene	121	0.219
TTG154-L	Sodium Dehydroacetate	162	0.219
TTG051-L	9-cis retinoic acid	65	0.218
TTG040-L	Cisplatin	103	0.217
TTG121-L	Clofibrate x ATRA	90	0.216
TTG128-L	alpha-Lipoic Acid	62	0.216
TTG057-L	Indigo	43	0.215
TTG109-L	Acephate	136	0.215
TTG150-L	Valproic acid sodium salt x Thalidomide	119	0.213
TTG178-L	Aluminum sulfate	89	0.213
TTG097-L	Permethrin	42	0.212
TTG095-L	Ibuprofen (dl-p-isobutylhydratropic acid)	81	0.207
TTG122-L	CoenzymeQ10(14day)	119	0.207
TTG200-L	TTG4: A) Clofibrate, B) Clofibrate (TTG4(1+1))	77	0.203
TTG166-L	Carbaryl	108	0.199
TTG075-L	Carbon tetrachloride	74	0.198
TTG170-L	3-methylcholanthrene/AhRKO	60	0.198
TTG185-L(B)	Ethynyl estradiol (corn oil)	64	0.198
TTG061-L	Paraquat dichloride	95	0.196
TTG079-L	Methanol	72	0.196
TTG145-L	Tributyltin chloride x Tributyltin chloride	66	0.196
TTG048-L	Genistein (PLD)	89	0.195
TTG058-L	Diethylnitrosamine (C3H)	49	0.191
TTG056-L	3-methylcholanthrene	107	0.19
TTG071-L	Acetaldehyde	76	0.19
TTG089-L	Rifampicin	59	0.19

Name	Condition	Num	Cor
TTG014-L	2,4-dinitrophenol	1092	9.158
TTG029-L	2-Aminomethylpyridine	33	0.383
TTG011-L	Isoniazid	78	0.382
TTG019-L	2-Vinylpyridine	77	0.341
TTG028-L	1,2,4-Triazole	63	0.341
TTG080-L	DMSO	46	0.318
TTG010-L	Acetaminophen	109	0.307
TTG016-L	Pentachlorophenol	98	0.3
TTG015-L	4-amino-2,6-dichlorophenol	32	0.299
TTG034-L	4-Ethylnitrobenzene	47	0.296
TTG202-L	TTG4: A) Clofibrate, B) Clofibrate (TTG4(4+1))	62	0.293
TTG100-L	Phenytoin	87	0.289
TTG187-L	Violet No.201	65	0.284
TTG055-L	N-ethyl-N-nitrosourea	42	0.283
TTG166-L	Carbaryl	88	0.278
TTG062-L(C)	Dexamethasone	93	0.277
TTG123-L	Caffeine	53	0.276
TTG109-L	Acephate	101	0.273
TTG114-L	Benzene	88	0.273
TTG160-L	5-fluorouracil	117	0.27
TTG135-L	Methyl dihydro jasmonate	37	0.266
TTG158-L	Deet x Permethrin	59	0.266
TTG200-L	TTG4: A) Clofibrate, B) Clofibrate (TTG4(1+1))	59	0.266
TTG169-L	Houttuynia extract	41	0.263
TTG116-L	Agaritin	46	0.261
TTG097-L	Permethrin	30	0.259
TTG167-L	Aloe arborescens extract	42	0.259
TTG057-L	Indigo	30	0.257
TTG085-L	Trybutyltin	55	0.256
TTG201-L	TTG4: A) Clofibrate, B) Clofibrate (TTG4(2+1))	60	0.255
TTG051-L	9-cis retinoic acid	44	0.253
TTG068-L	Carbaryl	60	0.251
TTG059-L	Caffeine	63	0.25
TTG083-L	Diethylstilbestrol	54	0.25
TTG145-L	Tributyltin chloride x Tributyltin chloride	49	0.249
TTG063-L	Sodium Arsenite	48	0.248
TTG079-L	Methanol	53	0.247
TTG129-L	CCl4 x Clofibrate	78	0.243
TTG078-L	Ethanol	39	0.241
TTG090-L	Pregnenolone Carbonitrile	78	0.241
TTG155-L	Aluminum ammonium sulfate	58	0.24
TTG185-L(B)	Ethynyl estradiol (corn oil)	45	0.239
TTG165-L	Chlorpyrifos	52	0.237
TTG027-L	1,2,3-Triazole	43	0.236
TTG071-L	Acetaldehyde	55	0.236
TTG016-L(C)	Pentachlorophenol	112	0.232
TTG031-L	2-Chloro-4,6-dimethylaniline	73	0.232
TTG095-L	Ibuprofen (dl-p-isobutylhydratropic acid)	53	0.232
TTG096-L	Omeprazole	72	0.232
TTG088-L	Tebufenozide	25	0.23
TTG186-L	Ethynyl estradiol/ERaKO(Chambon) (corn oil)	41	0.23
TTG204-L	Red No.225	105	0.229
TTG128-L	alpha-Lipoic Acid	38	0.227
TTG154-L	Sodium Dehydroacetate	98	0.227
TTG163-L	Aluminum lactate	56	0.226
TTG183-L	Bisphenol A (corn oil)	51	0.226
TTG177-L	Red No.102	43	0.225
TTG121-L	Clofibrate x ATRA	54	0.222
TTG146-L	Forskolin	61	0.222
TTG130-L	CCl4 x CCl4	29	0.22
TTG067-L	Acephate	35	0.219
TTG033-L	1,2-Dichloro-3-nitrobenzene	37	0.217
TTG070-L	Formaldehyde	18	0.216

Name	Condition	Num	Cor
TTG015-L	4-amino-2,6-dichlorophenol	980	10.204
TTG019-L	2-Vinylpyridine	92	0.455
TTG120-L	Clofibrate x PCN	118	0.423
TTG046-L	Levothyroxine	122	0.422
TTG139-L	Indigo Carmine	96	0.401
TTG016-L	Pentachlorophenol	113	0.386
TTG162-L	Sesame seed oil unsaponified matter	118	0.383
TTG043-L	Testosterone propionate	61	0.38
TTG098-L	DEHP	211	0.379
TTG132-L	Curcumin	139	0.37
TTG204-L	Red No.225	151	0.367
TTG060-L	Forskolin	48	0.363
TTG029-L	2-Aminomethylpyridine	28	0.362
TTG104-L	MEHP	187	0.351
TTG168-L	Mastic	90	0.348
TTG020-L	TCDD(2,3,7,8-Tetrachlorodibenzo-p-Dioxin)	101	0.345
TTG124-L	Vat Red I	62	0.342
TTG066-L	Methoprene	63	0.34
TTG206-L	BTAZ3864(CoCAM 2)	297	0.325
TTG187-L	Violet No.201	66	0.322
TTG151-L	Valproic acid sodium salt x Valproic acid sodium salt	113	0.318
TTG144-L	Tributyltin chloride x Phenobarbital	90	0.317
TTG070-L	Formaldehyde	23	0.307
TTG090-L	Pregnenolone Carbonitrile	88	0.303
TTG140-L	Food Red No.40	55	0.302
TTG041-L	Valproic acid sodium salt	168	0.3
TTG014-L	2,4-dinitrophenol	32	0.299
TTG058-L	Diethylnitrosamine (C3H)	40	0.298
TTG129-L	CCl4 x Clofibrate	85	0.296
TTG205-L	BTAZ3846(CoCAM 1)	355	0.296
TTG062-L(C)	Dexamethasone	89	0.295
TTG118-L	Clofibrate x Clofibrate	102	0.295
TTG182-L	Imidacloprid	96	0.292
TTG044-L	Clofibrate	94	0.289
TTG200-L	TTG4: A) Clofibrate, B) Clofibrate (TTG4(1+1))	57	0.287
TTG037-L	Phenobarbital	154	0.282
TTG163-L	Aluminum lactate	62	0.279
TTG188-L	Violet No.401	39	0.279
TTG026-L	TCDF(2,3,7,8-Tetrachlorodibenzofuran)	76	0.278
TTG056-L	3-methylcholanthrene	82	0.278
TTG032-L	3-Amino-1H-1,2,4-triazole	180	0.277
TTG161-L	Food Yellow No.4	74	0.277
TTG136-L	Phytol	127	0.274
TTG047-L	Bisphenol A (PLD)	42	0.272
TTG119-L	Carbon tetrachloride	46	0.272
TTG141-L	Tributyltin chloride x Clofibrate	117	0.272
TTG183-L	Bisphenol A (corn oil)	55	0.272
TTG109-L	Acephate	89	0.268
TTG123-L	Caffeine	46	0.267
TTG023-L	Transplatin	22	0.264
TTG122-L	CoenzymeQ10(14day)	79	0.263
TTG154-L	Sodium Dehydroacetate	102	0.263
TTG155-L	Aluminum ammonium sulfate	57	0.263
TTG147-L	Estragole	48	0.262
TTG195-L	TTG4: A) Valproic acid sodium salt, B) Valproic acid sodium salt (TTG4(4+1))	109	0.262
TTG016-L(C)	Pentachlorophenol	112	0.259
TTG057-L	Indigo	27	0.258
TTG078-L	Ethanol	37	0.254
TTG112-L	FK506	35	0.254
TTG059-L	Caffeine	57	0.252
TTG087-L	Pyriproxyfen	54	0.249
TTG134-L	Nerolidol	30	0.248
TTG089-L	Rifampicin	40	0.246

Name	Condition	Num	Cor
TTG016-L(C)	Pentachlorophenol	4420	2.262
TTG016-L	Pentachlorophenol	744	0.563
TTG144-L	Tributyltin chloride x Phenobarbital	578	0.451
TTG098-L	DEHP	1128	0.45
TTG195-L	TTG4: A) Valproic acid sodium salt, B) Valproic acid sodium salt (TTG4(4+1))	793	0.423
TTG031-L	2-Chloro-4,6-dimethylaniline	528	0.414
TTG028-L	1,2,4-Triazole	306	0.409
TTG044-L	Clofibrate	592	0.404
TTG193-L	TTG4: A) Valproic acid sodium salt, B) Valproic acid sodium salt (TTG4(1+1))	603	0.403
TTG118-L	Clofibrate x Clofibrate	626	0.402
TTG204-L	Red No.225	747	0.402
TTG206-L	BTAZ3864(CoCAM 2)	1627	0.395
TTG151-L	Valproic acid sodium salt x Valproic acid sodium salt	626	0.391
TTG154-L	Sodium Dehydroacetate	674	0.386
TTG200-L	TTG4: A) Clofibrate, B) Clofibrate (TTG4(1+1))	344	0.384
TTG032-L	3-Amino-1H-1,2,4-triazole	1122	0.383
TTG120-L	Clofibrate x PCN	481	0.382
TTG157-L	Valproic acid sodium salt	801	0.382
TTG141-L	Tributyltin chloride x Clofibrate	738	0.38
TTG074-L	Bromobenzene	767	0.377
TTG077-L	Monocrotaline	204	0.375
TTG019-L	2-Vinylpyridine	340	0.373
TTG037-L	Phenobarbital	905	0.367
TTG165-L	Chlorpyrifos	326	0.367
TTG162-L	Sesame seed oil unsaponified matter	507	0.365
TTG104-L	MEHP	875	0.364
TTG205-L	BTAZ3846(CoCAM 1)	1968	0.363
TTG199-L	Black No.401	252	0.36
TTG059-L	Caffeine	364	0.357
TTG060-L	Forskolin	213	0.357
TTG168-L	Mastic	412	0.353
TTG183-L	Bisphenol A (corn oil)	321	0.352
TTG027-L	1,2,3-Triazole	259	0.351
TTG123-L	Caffeine	270	0.347
TTG129-L	CCl4 x Clofibrate	450	0.347
TTG033-L	1,2-Dichloro-3-nitrobenzene	237	0.343
TTG089-L	Rifampicin	251	0.342
TTG137-L	alpha-Lipoic Acid	288	0.341
TTG041-L	Valproic acid sodium salt	856	0.339
TTG056-L	3-methylcholanthrene	445	0.334
TTG202-L	TTG4: A) Clofibrate, B) Clofibrate (TTG4(4+1))	286	0.334
TTG090-L	Pregnenolone Carbonitrile	435	0.332
TTG149-L	Valproic acid sodium salt x Aspirin	406	0.332
TTG091-L	Azacytidine	247	0.33
TTG047-L	Bisphenol A (PLD)	228	0.328
TTG061-L	Paraquat dichloride	375	0.327
TTG189-L	TTG4: A) CCl4, B) Ccl4 (TTG4(1+1))	376	0.324
TTG062-L(C)	Dexamethasone	440	0.323
TTG094-L	Aspirin	417	0.323
TTG087-L	Pyriproxyfen	312	0.319
TTG147-L	Estragole	263	0.318
TTG043-L	Testosterone propionate	228	0.315
TTG182-L	Imidacloprid	467	0.315
TTG073-L	Toluene	414	0.314
TTG194-L	TTG4: A) Valproic acid sodium salt, B) Valproic acid sodium salt (TTG4(2+1))	700	0.313
TTG093-L	AraC	298	0.312
TTG163-L	Aluminum lactate	311	0.311
TTG136-L	Phytol	646	0.309
TTG066-L	Methoprene	258	0.308
TTG088-L	Tebufenozide	134	0.305
TTG155-L	Aluminum ammonium sulfate	298	0.304
TTG026-L	TCDF(2,3,7,8-Tetrachlorodibenzofuran)	374	0.303
TTG048-L	Genistein (PLD)	327	0.303