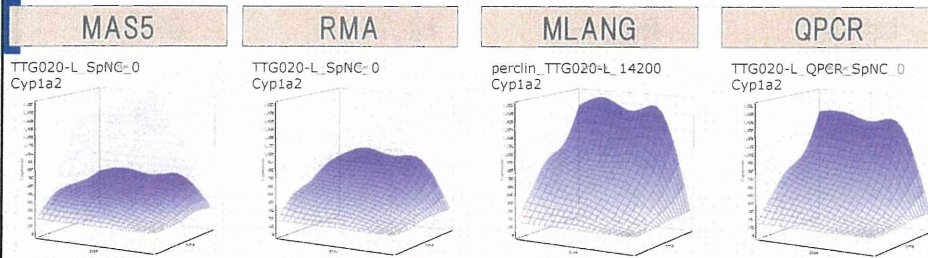


補正結果 TCDD Cyp1a2

Cyp(Cytochrome P450)は、ダイオキシン類によって誘導されることが知られている。



TCDDIによって強く誘導され、マイクロアレイでは飽和現象が見え始めており、MAS5では飽和を処理しきれない。RMAでは、一部解消されている。MLANGではかなり飽和がキャンセルされている。

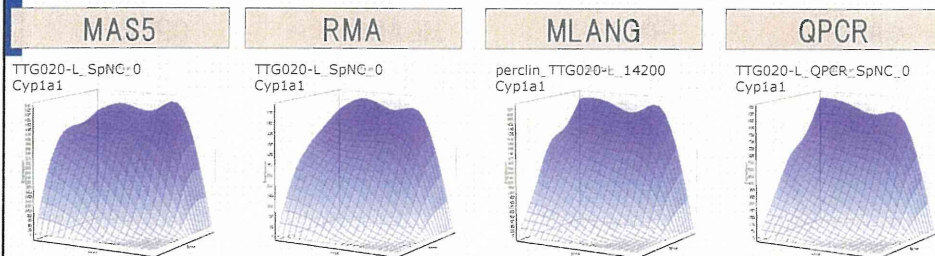
11

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TERADATA THE BEST DECISION POSSIBLE

補正結果 TCDD Cyp1a1

Cyp(Cytochrome P450)は、ダイオキシン類によって誘導されることが知られている。



TCDDIによって強く誘導され、マイクロアレイでは飽和現象が見え始めており、MAS5では飽和を処理しきれない。RMAでは、一部解消されている。MLANGではかなり飽和がキャンセルされている。

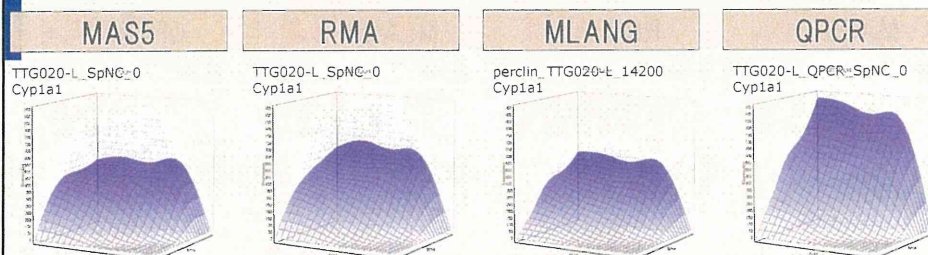
11

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TERADATA THE BEST DECISION POSSIBLE

補正結果 TCDD Cyp1a1

Cyp(Cytochrome P450)は、ダイオキシン類によって誘導されることが知られている。



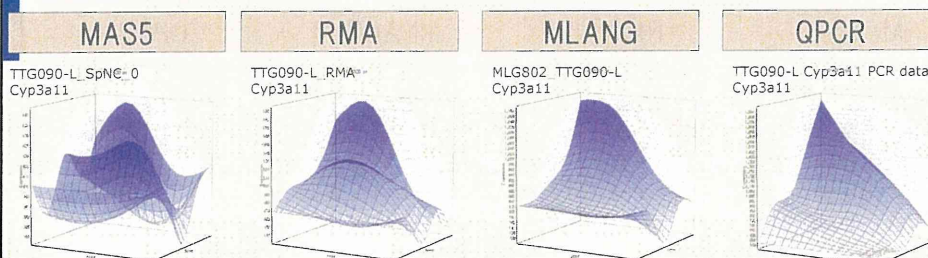
TCDDによって強く誘導され、マイクロアレイでは飽和現象が見え始めており、MAS5では飽和を処理しきれない。RMAでは、一部解消されている。MLANGではかなり飽和がキャンセルされている。

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TERADATA THE BEST DECISION POSSIBLE

補正結果 Pregnenolone Carbonitrile Cyp3a11

本化合物は、Cyp3a11を誘導するが、マイクロアレイでは測定できないものと看做されてきた。



MAS5では、非常に大きく動き、意味のある動きをではない。RMAでは誘導されているかのような動きを見せているが不明瞭である。MLANGでは飽和がキャンセルされ、誘導されていることがわかる

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TERADATA THE BEST DECISION POSSIBLE

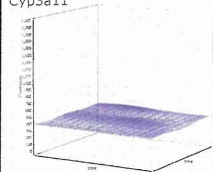
補正結果

Pregnenolone Carbonitrile Cyp3a11

本化合物は、Cyp3a11を誘導するが、マイクロアレイでは測定できないものと看做されてきた。

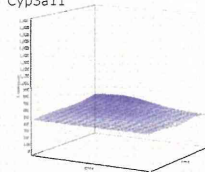
MAS5

TTG090-L_SpNC-0
Cyp3a11



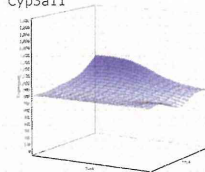
RMA

TTG090-L_RMA⁺
Cyp3a11



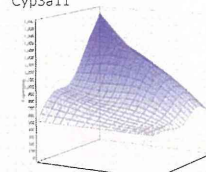
MLANG

MLG802_TTG090-L
Cyp3a11



QPCR

TTG090-L Cyp3a11 PCR data
Cyp3a11



MAS5では、非常に大きく動き、意味のある動きをではない。RMAでは誘導されているかのような動きを見せているが不明瞭である。MLANGでは飽和がキャンセルされ、誘導されていることがわかる

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(資料 4)

Percellome Database

-Percellome Explorer 解析結果-

Percellome Database

Project List

(gavage, Liver only)

2012/03

| Name | Condition | Total Num |
|-------------|---|-----------|
| TTG010-L | Acetaminophen | 910 |
| TTG011-L | Isoniazid | 470 |
| TTG014-L | "2,4-dinitrophenol" | 208 |
| TTG015-L | "4-amino-2,6-dichlorophenol" | 208 |
| TTG016-L | Pentachlorophenol | 1396 |
| TTG016-L(C) | Pentachlorophenol | 3357 |
| TTG019-L | 2-Vinylpyridine | 676 |
| TTG020-L | "TCDD(2,3,7,8-Tetrachlorodibenzo-p-Dioxin)" | 910 |
| TTG023-L | Transplatin | 216 |
| TTG026-L | "TCDF(2,3,7,8-Tetrachlorodibenzofuran)" | 175 |
| TTG027-L | "1,2,3-Triazole" | 613 |
| TTG028-L | "1,2,4-Triazole" | 423 |
| TTG029-L | 2-Aminomethylpyridine | 169 |
| TTG030-L | N-Methylaniline | 443 |
| TTG031-L | "2-Chloro-4,6-dimethylaniline" | 1537 |
| TTG032-L | "3-Amino-1H-1,2,4-triazole" | 1283 |
| TTG033-L | "1,2-Dichloro-3-nitrobenzene" | 371 |
| TTG034-L | 4-Ethylnitrobenzene | 358 |
| TTG035-L | Acetaminophen | 1341 |
| TTG037-L | Phenobarbital | 3580 |
| TTG038-L | Hydroxycitric Acid | 346 |
| TTG039-L | Citric acid-calcium salt | 211 |
| TTG040-L | Cisplatin | 821 |
| TTG041-L | Valproic Acid | 2557 |
| TTG042-L | Ethinyl estradiol (PLD) | 437 |
| TTG043-L | Testosterone propionate | 266 |
| TTG044-L | Clofibrate | 2111 |
| TTG045-L | Troglitazone | 1210 |
| TTG046-L | Tributyltin | 2071 |
| TTG047-L | Bisphenol A (PLD) | 303 |
| TTG048-L | Genistein (PLD) | 634 |
| TTG049-L | Tributyltin | 234 |
| TTG051-L | 9-cis retinoic acid | 379 |
| TTG052-L | All trans retinoic acid | 770 |
| TTG053-L | Ethinyl estradiol (PLD) | 1703 |
| TTG054-L | Diethylnitrosamine (C57BL/6) | 1204 |
| TTG055-L | N-ethyl-N-nitrosourea | 336 |
| TTG056-L | 3-methylcholanthrene | 747 |
| TTG057-L | Indigo | 235 |
| TTG058-L | Diethylnitrosamine (C3H) | 955 |
| TTG059-L | Caffeine | 652 |
| TTG060-L | Forskolin | 402 |
| TTG061-L | Paraquat | 818 |
| TTG062-L(C) | Dexamethasone | 920 |
| TTG063-L | Sodium Arsenite | 297 |
| TTG066-L | Methoprene | 1183 |
| TTG067-L | Acephate | 554 |
| TTG068-L | Carbaryl | 308 |
| TTG070-L | Formaldehyde | 113 |
| TTG071-L | Acetaldehyde | 303 |
| TTG073-L | Toluene | 1850 |
| TTG074-L | Bromobenzene | 742 |
| TTG075-L | Carbon tetrachloride | 530 |
| TTG077-L | Monocrotaline | 313 |
| TTG078-L | Ethanol | 372 |
| TTG079-L | Methanol | 422 |
| TTG080-L | DMSO | 303 |

| | | |
|-----------|---|------|
| TTG081-L | Warfarin | 380 |
| TTG083-L | Diethylstilbestrol | 599 |
| TTG084-L | Tamoxifen | 275 |
| TTG085-L | Trybutyltin | 443 |
| TTG086-L | Coenzyme Q10 | 420 |
| TTG087-L | Pyriproxyfen | 1640 |
| TTG088-L | Tebufenozide | 134 |
| TTG089-L | Rifampicin | 962 |
| TTG090-L | Pregnenolone Carbonitrile | 893 |
| TTG091-L | Azacytidine | 202 |
| TTG092-L | Deet | 440 |
| TTG093-L | AraC | 222 |
| TTG094-L | Aspirin | 1430 |
| TTG095-L | Ibuprofen (dl-p-isobutylhydratropic acid) | 468 |
| TTG096-L | Omeprazole | 1416 |
| TTG097-L | Permethrin | 350 |
| TTG098-L | DEHP | 3154 |
| TTG099-L | Paclitaxel (Taxol) | 247 |
| TTG100-L | Phenytoin | 660 |
| TTG104-L | MEHP | 3299 |
| TTG109-L | Acephate | 1631 |
| TTG110-L | Glycyrrhizin | 485 |
| TTG112-L | FK506 | 339 |
| TTG114-L | Benzene | 488 |
| TTG115-L | Kanamycin monosulfate | 224 |
| TTG116-L | Agaricine | 483 |
| TTG117-L | Digitoxin | 174 |
| TTG118-L | Clofibrate x Clofibrate | 1960 |
| TTG119-L | Carbon tetrachloride | 575 |
| TTG120-L | Clofibrate x PCN | 1135 |
| TTG121-L | Clofibrate x ATRA | 1023 |
| TTG122-L | CoenzymeQ10(14day) | 1736 |
| TTG123-L | Caffeine | 487 |
| TTG124-L | Vat Red I | 131 |
| TTG126-L | Thalidomide | 664 |
| TTG128-L | alpha-Lipoic Acid | 256 |
| TTG129-L | CCl4 x Clofibrate | 1559 |
| TTG130-L | CCl4 x CCl4 | 342 |
| TTG131B-L | CCl4 x Phenobarbital | 964 |
| TTG132-L | Curcumin | 1147 |
| TTG133-L | Maltol | 434 |
| TTG134-L | Nerolidol | 327 |
| TTG135-L | Methyl dihydro jasmonate | 455 |
| TTG136-L | Phytol | 1461 |
| TTG137-L | alpha-Lipoic Acid | 366 |
| TTG139-L | Indigo Carmine | 506 |
| TTG140-L | Food Red No.40 | 405 |
| TTG141-L | Tributyltin x Clofibrate | 2711 |
| TTG144-L | Tributyltin x Phenobarbital | 1449 |
| TTG145-L | Tributyltin x Tributyltin | 842 |
| TTG146-L | Forskolin | 609 |
| TTG147-L | Estragole | 707 |
| TTG148-L | Verbenone | 381 |
| TTG149-L | Valproic acid sodium salt x Aspirin | 1470 |
| TTG150-L | Valproic acid sodium salt x Thalidomide | 510 |
| TTG151-L | Valproic acid sodium salt x Valproic acid sodium salt | 1413 |
| TTG152-L | FD&C Blue No.1 | 516 |
| TTG154-L | Sodium Dehydroacetate | 2948 |
| TTG155-L | Aluminum ammonium sulfate | 329 |

| | | |
|----------|---|------|
| TTG156-L | Food Red No.104 | 977 |
| TTG157-L | Valproic acid sodium salt | 2314 |
| TTG158-L | Deet x Permethrin | 576 |
| TTG159-L | Deet x Deet | 1028 |
| TTG160-L | 5-fluorouracil | 1703 |
| TTG161-L | Food Yellow No.4 | 1042 |
| TTG162-L | Sesame seed oil unsaponified matter | 1310 |
| TTG163-L | Aluminum lactate | 621 |
| TTG165-L | Chlorpyrifos | 958 |
| TTG166-L | Carbaryl | 606 |
| TTG167-L | Aloe arborescens extract | 227 |
| TTG168-L | Mastic | 968 |
| TTG169-L | Houttuynia extract | 438 |
| TTG170-L | 3-methylcholanthrene/AhRKO | 371 |
| TTG173-L | TCDD/AhRKO | 5813 |
| TTG176-L | Green No.204 (Pyranine Conc) | 243 |
| TTG177-L | Red No.102 | 438 |
| TTG178-L | Aluminum sulfate | 303 |
| TTG180-L | Red No.105 | 269 |
| TTG183-L | Bisphenol A (corn oil) | 636 |
| TTG184-L | Bisphenol A/ERaKO(Chambon) (corn oil) | 364 |
| TTG185-L | Ethynyl estradiol (corn oil) | 304 |
| TTG186-L | Ethynyl estradiol/ERaKO(Chambon) (corn oil) | 485 |
| TTG187-L | Violet No.201 | 228 |

Percellome Database

PDBEx-PCA

(gavage, Liver only)

2012/03

Percellome Explorer ver. 0.4.8

DataSet: PDBEx_RSort101008_Std-Av

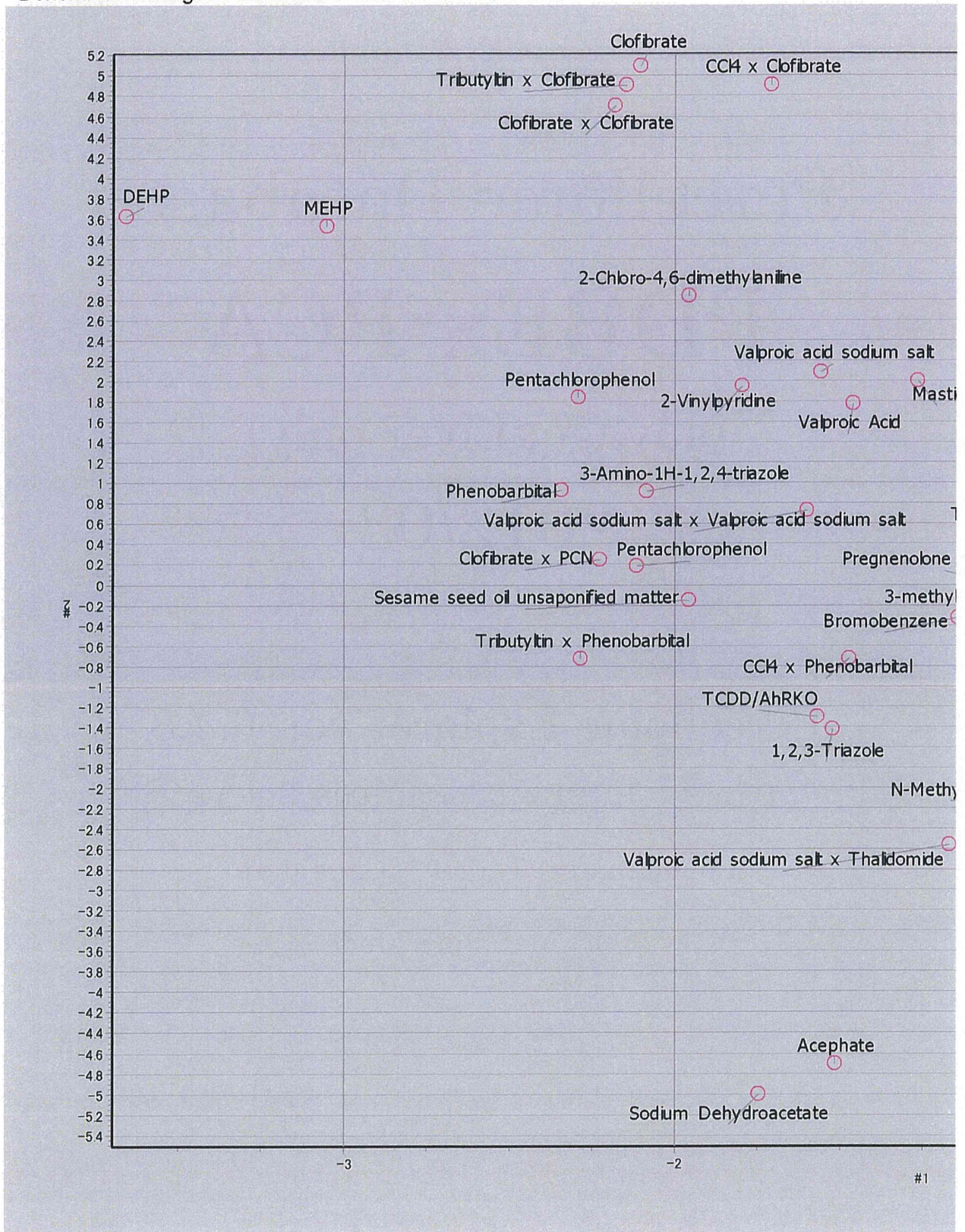
Denominator: Target * Candidate

Strict Matching Mode

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

Percellome Explorer ver. 0.4.8 : PDBEx_RSort101008_Std-Av

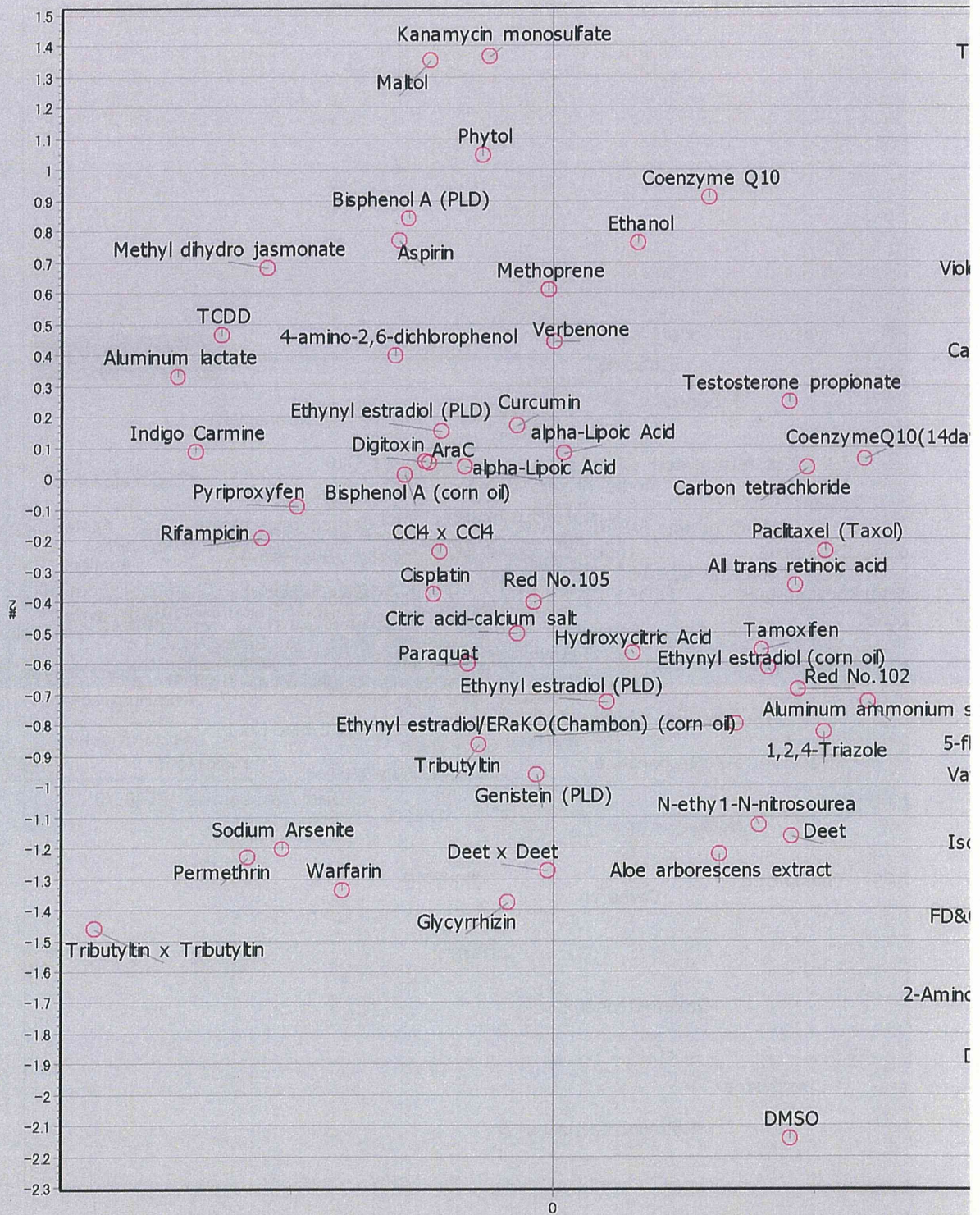
Denominator: Target * Candidate

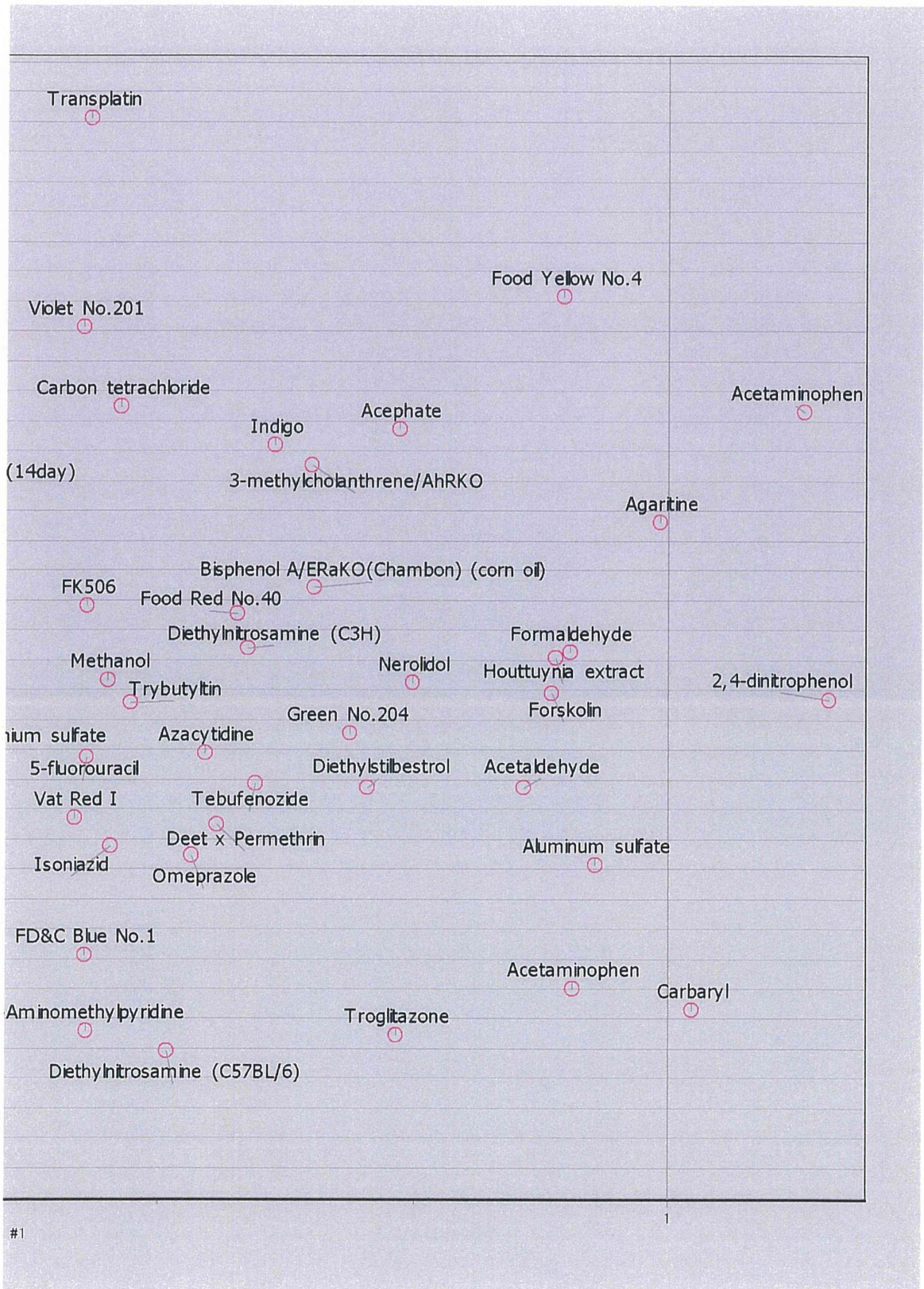


PDBEx-PCA (#1 vs #2) : origin view

Percellome Explorer ver. 0.4.8 : PDBEx_RSort101008_Std-Av

Denominator: Target * Candidate





#1

1

Percellome Database

Matching List

(gavage, Liver only)

2012/03

Percellome Explorer ver. 0.4.8

DataSet: PDBEx_RSort101008_Std-Av

Denominator: Target * Candidate

Strict Matching Mode

Name : Surface ID

Condition : Chemical

Num : Size of Gene list

Cor : correlation index

;Percellome Explorer ver. 0.4.8 : PDBEx_RSort101008_Std-Av

;Target Prj: vs TTG010-L // Acetaminophen

;Denominator: Target * Candidate

| Name | Condition | Num | Cor |
|-------------|---|-----|--------|
| TTG010-L | Acetaminophen | 910 | 10.989 |
| TTG019-L | 2-Vinylpyridine | 102 | 1.658 |
| TTG030-L | N-Methylaniline | 50 | 1.24 |
| TTG031-L | 2-Chloro-4,6-dimethylaniline | 144 | 1.03 |
| TTG077-L | Monocrotaline | 22 | 0.772 |
| TTG027-L | 1,2,3-Triazole | 42 | 0.753 |
| TTG034-L | 4-Ethylnitrobenzene | 24 | 0.737 |
| TTG114-L | Benzene | 27 | 0.608 |
| TTG078-L | Ethanol | 20 | 0.591 |
| TTG028-L | 1,2,4-Triazole | 22 | 0.572 |
| TTG062-L(C) | Dexamethasone | 46 | 0.549 |
| TTG023-L | Transplatin | 10 | 0.509 |
| TTG042-L | Ethynyl estradiol (PLD) | 19 | 0.478 |
| TTG109-L | Acephate | 71 | 0.478 |
| TTG075-L | Carbon tetrachloride | 23 | 0.477 |
| TTG150-L | Valproic acid sodium salt x Thalidomide | 22 | 0.474 |
| TTG166-L | Carbaryl | 26 | 0.471 |
| TTG029-L | 2-Aminomethylpyridine | 7 | 0.455 |
| TTG177-L | Red No.102 | 17 | 0.427 |
| TTG096-L | Omeprazole | 54 | 0.419 |
| TTG160-L | 5-fluorouracil | 63 | 0.407 |
| TTG093-L | AraC | 8 | 0.396 |
| TTG115-L | Kanamycin monosulfate | 8 | 0.392 |
| TTG131B-L | CCl4 x Phenobarbital | 34 | 0.388 |
| TTG154-L | Sodium Dehydroacetate | 102 | 0.38 |
| TTG059-L | Caffeine | 22 | 0.371 |
| TTG014-L | 2,4-dinitrophenol | 7 | 0.37 |
| TTG165-L | Chlorpyrifos | 32 | 0.367 |
| TTG126-L | Thalidomide | 22 | 0.364 |
| TTG033-L | 1,2-Dichloro-3-nitrobenzene | 12 | 0.355 |
| TTG056-L | 3-methylcholanthrene | 24 | 0.353 |
| TTG011-L | Isoniazid | 15 | 0.351 |
| TTG128-L | alpha-Lipoic Acid | 8 | 0.343 |
| TTG100-L | Phenytoin | 20 | 0.333 |
| TTG060-L | Forskolin | 12 | 0.328 |
| TTG057-L | Indigo | 7 | 0.327 |
| TTG016-L | Pentachlorophenol | 41 | 0.323 |
| TTG051-L | 9-cis retinoic acid | 11 | 0.319 |
| TTG117-L | Digitoxin | 5 | 0.316 |
| TTG026-L | TCDF(2,3,7,8-Tetrachlorodibenzofuran) | 5 | 0.314 |
| TTG137-L | alpha-Lipoic Acid | 10 | 0.3 |
| TTG116-L | Agaricine | 13 | 0.296 |
| TTG170-L | 3-methylcholanthrene/AhRKO | 10 | 0.296 |
| TTG032-L | 3-Amino-1H-1,2,4-triazole | 34 | 0.291 |
| TTG104-L | MEHP | 87 | 0.29 |
| TTG167-L | Aloe arborescens extract | 6 | 0.29 |
| TTG041-L | Valproic Acid | 67 | 0.288 |
| TTG084-L | Tamoxifen | 7 | 0.28 |
| TTG162-L | Sesame seed oil unsaponified matter | 33 | 0.277 |
| TTG183-L | Bisphenol A (corn oil) | 16 | 0.276 |
| TTG091-L | Azacytidine | 5 | 0.272 |
| TTG098-L | DEHP | 76 | 0.265 |
| TTG163-L | Aluminum lactate | 15 | 0.265 |
| TTG055-L | N-ethyl-N-nitrosourea | 8 | 0.262 |
| TTG039-L | Citric acid-calcium salt | 5 | 0.26 |

;Percellome Explorer ver. 0.4.8 : PDBEx_RSort101008_Std-Av

;Target Prj: vs TTG011-L // Isoniazid

;Denominator: Target * Candidate

| Name | Condition | Num | Cor |
|-------------|---|-----|--------|
| TTG011-L | Isoniazid | 470 | 21.277 |
| TTG030-L | N-Methylaniline | 15 | 0.72 |
| TTG062-L(C) | Dexamethasone | 26 | 0.601 |
| TTG059-L | Caffeine | 18 | 0.587 |
| TTG028-L | 1,2,4-Triazole | 11 | 0.553 |
| TTG034-L | 4-Ethylnitrobenzene | 9 | 0.535 |
| TTG166-L | Carbaryl | 15 | 0.527 |
| TTG014-L | 2,4-dinitrophenol | 5 | 0.511 |
| TTG029-L | 2-Aminomethylpyridine | 4 | 0.504 |
| TTG128-L | alpha-Lipoic Acid | 6 | 0.499 |
| TTG124-L | Vat Red I | 3 | 0.487 |
| TTG114-L | Benzene | 11 | 0.48 |
| TTG019-L | 2-Vinylpyridine | 14 | 0.441 |
| TTG154-L | Sodium Dehydroacetate | 59 | 0.426 |
| TTG027-L | 1,2,3-Triazole | 12 | 0.417 |
| TTG048-L | Genistein (PLD) | 12 | 0.403 |
| TTG023-L | Transplatin | 4 | 0.394 |
| TTG100-L | Phenytoin | 12 | 0.387 |
| TTG109-L | Acephate | 29 | 0.378 |
| TTG165-L | Chlorpyrifos | 17 | 0.378 |
| TTG117-L | Digitoxin | 3 | 0.367 |
| TTG063-L | Sodium Arsenite | 5 | 0.358 |
| TTG010-L | Acetaminophen | 15 | 0.351 |
| TTG068-L | Carbaryl | 5 | 0.345 |
| TTG081-L | Warfarin | 6 | 0.336 |
| TTG150-L | Valproic acid sodium salt x Thalidomide | 8 | 0.334 |
| TTG083-L | Diethylstilbestrol | 9 | 0.32 |
| TTG088-L | Tebufenozide | 2 | 0.318 |
| TTG091-L | Azacytidine | 3 | 0.316 |
| TTG180-L | Red No.105 | 4 | 0.316 |
| TTG038-L | Hydroxycitric Acid | 5 | 0.307 |
| TTG123-L | Caffeine | 7 | 0.306 |
| TTG039-L | Citric acid-calcium salt | 3 | 0.303 |
| TTG137-L | alpha-Lipoic Acid | 5 | 0.291 |
| TTG177-L | Red No.102 | 6 | 0.291 |
| TTG093-L | AraC | 3 | 0.288 |
| TTG185-L | Ethynyl estradiol (corn oil) | 4 | 0.28 |
| TTG163-L | Aluminum lactate | 8 | 0.274 |
| TTG031-L | 2-Chloro-4,6-dimethylaniline | 19 | 0.263 |
| TTG176-L | Green No.204 (Pyranine Conc) | 3 | 0.263 |
| TTG186-L | Ethynyl estradiol/ERaKO(Chambon) (corn oil) | 6 | 0.263 |
| TTG056-L | 3-methylcholanthrene | 9 | 0.256 |
| TTG126-L | Thalidomide | 8 | 0.256 |
| TTG152-L | FD&C Blue No.1 | 6 | 0.247 |
| TTG151-L | Valproic acid sodium salt x Valproic acid sodium salt | 16 | 0.241 |
| TTG043-L | Testosterone propionate | 3 | 0.24 |
| TTG085-L | Trybutyltin | 5 | 0.24 |
| TTG090-L | Pregnenolone Carbonitrile | 10 | 0.238 |
| TTG084-L | Tamoxifen | 3 | 0.232 |
| TTG067-L | Acephate | 6 | 0.23 |
| TTG078-L | Ethanol | 4 | 0.229 |
| TTG121-L | Clofibrate x ATRA | 11 | 0.229 |
| TTG095-L | Ibuprofen (dl-p-isobutylhydratropic acid) | 5 | 0.227 |
| TTG094-L | Aspirin | 15 | 0.223 |
| TTG052-L | All trans retinoic acid | 8 | 0.221 |

;Percellome Explorer ver. 0.4.8 : PDBEx_RSort101008_Std-Av

;Target Prj: vs TTG014-L // "2,4-dinitrophenol"

;Denominator: Target * Candidate

| Name | Condition | Num | Cor |
|-------------|---|-----|--------|
| TTG014-L | 2,4-dinitrophenol | 208 | 48.077 |
| TTG029-L | 2-Aminomethylpyridine | 3 | 0.853 |
| TTG116-L | Agaridine | 8 | 0.796 |
| TTG068-L | Carbaryl | 5 | 0.78 |
| TTG091-L | Azacytidine | 3 | 0.714 |
| TTG034-L | 4-Ethylnitrobenzene | 5 | 0.671 |
| TTG019-L | 2-Vinylpyridine | 9 | 0.64 |
| TTG167-L | Aloe arborescens extract | 3 | 0.635 |
| TTG178-L | Aluminum sulfate | 4 | 0.635 |
| TTG028-L | 1,2,4-Triazole | 5 | 0.568 |
| TTG184-L | Bisphenol A/ERaKO(Chambon) (corn oil) | 4 | 0.528 |
| TTG062-L(C) | Dexamethasone | 10 | 0.523 |
| TTG011-L | Isoniazid | 5 | 0.511 |
| TTG158-L | Deet x Permethrin | 6 | 0.501 |
| TTG083-L | Diethylstilbestrol | 6 | 0.482 |
| TTG071-L | Acetaldehyde | 3 | 0.476 |
| TTG159-L | Deet x Deet | 10 | 0.468 |
| TTG079-L | Methanol | 4 | 0.456 |
| TTG075-L | Carbon tetrachloride | 5 | 0.454 |
| TTG183-L | Bisphenol A (corn oil) | 6 | 0.454 |
| TTG092-L | Deet | 4 | 0.437 |
| TTG100-L | Phenytoin | 6 | 0.437 |
| TTG093-L | AraC | 2 | 0.433 |
| TTG109-L | Acephate | 14 | 0.413 |
| TTG049-L | Tributyltin | 2 | 0.411 |
| TTG095-L | Ibuprofen (dl-p-isobutylhydratropic acid) | 4 | 0.411 |
| TTG031-L | 2-Chloro-4,6-dimethylaniline | 13 | 0.407 |
| TTG160-L | 5-fluorouracil | 14 | 0.395 |
| TTG035-L | Acetaminophen | 11 | 0.394 |
| TTG152-L | FD&C Blue No.1 | 4 | 0.373 |
| TTG010-L | Acetaminophen | 7 | 0.37 |
| TTG059-L | Caffeine | 5 | 0.369 |
| TTG126-L | Thalidomide | 5 | 0.362 |
| TTG180-L | Red No.105 | 2 | 0.357 |
| TTG177-L | Red No.102 | 3 | 0.329 |
| TTG030-L | N-Methylaniline | 3 | 0.326 |
| TTG154-L | Sodium Dehydroacetate | 20 | 0.326 |
| TTG077-L | Monocrotaline | 2 | 0.307 |
| TTG096-L | Omeprazole | 9 | 0.306 |
| TTG110-L | Glycyrrhizin | 3 | 0.297 |
| TTG123-L | Caffeine | 3 | 0.296 |
| TTG040-L | Cisplatin | 5 | 0.293 |
| TTG090-L | Pregnenolone Carbonitrile | 5 | 0.269 |
| TTG137-L | alpha-Lipoic Acid | 2 | 0.263 |
| TTG032-L | 3-Amino-1H-1,2,4-triazole | 7 | 0.262 |
| TTG067-L | Acephate | 3 | 0.26 |
| TTG033-L | 1,2-Dichloro-3-nitrobenzene | 2 | 0.259 |
| TTG170-L | 3-methylcholanthrene/AhRKO | 2 | 0.259 |
| TTG016-L(C) | Pentachlorophenol | 18 | 0.258 |
| TTG016-L | Pentachlorophenol | 7 | 0.241 |
| TTG060-L | Forskolin | 2 | 0.239 |
| TTG045-L | Troglitazone | 6 | 0.238 |
| TTG146-L | Forskolin | 3 | 0.237 |
| TTG027-L | 1,2,3-Triazole | 3 | 0.235 |
| TTG144-L | Tributyltin x Phenobarbital | 7 | 0.232 |

;Percellome Explorer ver. 0.4.8 : PDBEx_RSort101008_Std-Av

;Target Prj: vs TTG015-L // "4-amino-2,6-dichlorophenol"

;Denominator: Target * Candidate

| Name | Condition | Num | Cor |
|-------------|---|-----|--------|
| TTG015-L | 4-amino-2,6-dichlorophenol | 208 | 48.077 |
| TTG026-L | TCDF(2,3,7,8-Tetrachlorodibenzofuran) | 4 | 1.099 |
| TTG060-L | Forskolin | 8 | 0.957 |
| TTG019-L | 2-Vinylpyridine | 13 | 0.925 |
| TTG120-L | Clofibrate x PCN | 19 | 0.805 |
| TTG046-L | Tributyltin | 32 | 0.743 |
| TTG020-L | TCDD(2,3,7,8-Tetrachlorodibenzo-p-Dioxin) | 14 | 0.74 |
| TTG032-L | 3-Amino-1H-1,2,4-triazole | 19 | 0.712 |
| TTG098-L | DEHP | 46 | 0.701 |
| TTG104-L | MEHP | 46 | 0.67 |
| TTG162-L | Sesame seed oil unsaponified matter | 17 | 0.624 |
| TTG168-L | Mastic | 12 | 0.596 |
| TTG123-L | Caffeine | 6 | 0.592 |
| TTG016-L | Pentachlorophenol | 17 | 0.585 |
| TTG144-L | Tributyltin x Phenobarbital | 15 | 0.498 |
| TTG141-L | Tributyltin x Clofibrate | 25 | 0.443 |
| TTG155-L | Aluminum ammonium sulfate | 3 | 0.438 |
| TTG090-L | Pregnenolone Carbonitrile | 8 | 0.431 |
| TTG062-L(C) | Dexamethasone | 8 | 0.418 |
| TTG119-L | Carbon tetrachloride | 5 | 0.418 |
| TTG073-L | Toluene | 16 | 0.416 |
| TTG066-L | Methoprene | 10 | 0.406 |
| TTG027-L | 1,2,3-Triazole | 5 | 0.392 |
| TTG033-L | 1,2-Dichloro-3-nitrobenzene | 3 | 0.389 |
| TTG037-L | Phenobarbital | 29 | 0.389 |
| TTG099-L | Paclitaxel (Taxol) | 2 | 0.389 |
| TTG183-L | Bisphenol A (corn oil) | 5 | 0.378 |
| TTG128-L | alpha-Lipoic Acid | 2 | 0.376 |
| TTG151-L | Valproic acid sodium salt x Valproic acid sodium salt | 11 | 0.374 |
| TTG140-L | Food Red No.40 | 3 | 0.356 |
| TTG131B-L | CCl4 x Phenobarbital | 7 | 0.349 |
| TTG031-L | 2-Chloro-4,6-dimethylaniline | 11 | 0.344 |
| TTG129-L | CCl4 x Clofibrate | 11 | 0.339 |
| TTG132-L | Curcumin | 8 | 0.335 |
| TTG157-L | Valproic acid sodium salt | 16 | 0.332 |
| TTG016-L(C) | Pentachlorophenol | 23 | 0.329 |
| TTG030-L | N-Methylaniline | 3 | 0.326 |
| TTG063-L | Sodium Arsenite | 2 | 0.324 |
| TTG109-L | Acephate | 11 | 0.324 |
| TTG056-L | 3-methylcholanthrene | 5 | 0.322 |
| TTG094-L | Aspirin | 9 | 0.303 |
| TTG156-L | Food Red No.104 | 6 | 0.295 |
| TTG134-L | Nerolidol | 2 | 0.294 |
| TTG154-L | Sodium Dehydroacetate | 18 | 0.294 |
| TTG087-L | Pyriproxyfen | 10 | 0.293 |
| TTG150-L | Valproic acid sodium salt x Thalidomide | 3 | 0.283 |
| TTG130-L | CCl4 x CCl4 | 2 | 0.281 |
| TTG038-L | Hydroxycitric Acid | 2 | 0.278 |
| TTG147-L | Estragole | 4 | 0.272 |
| TTG118-L | Clofibrate x Clofibrate | 11 | 0.27 |
| TTG137-L | alpha-Lipoic Acid | 2 | 0.263 |
| TTG149-L | Valproic acid sodium salt x Aspirin | 8 | 0.262 |
| TTG074-L | Bromobenzene | 4 | 0.259 |
| TTG148-L | Verbenone | 2 | 0.252 |
| TTG083-L | Diethylstilbestrol | 3 | 0.241 |

;Percellome Explorer ver. 0.4.8 : PDBEx_RSort101008_Std-Av

;Target Prj: vs TTG016-L // Pentachlorophenol

;Denominator: Target * Candidate

| Name | Condition | Num | Cor |
|-------------|---|------|-------|
| TTG016-L | Pentachlorophenol | 1396 | 7.163 |
| TTG026-L | TCDF(2,3,7,8-Tetrachlorodibenzofuran) | 31 | 1.269 |
| TTG019-L | 2-Vinylpyridine | 104 | 1.102 |
| TTG032-L | 3-Amino-1H-1,2,4-triazole | 176 | 0.983 |
| TTG098-L | DEHP | 412 | 0.936 |
| TTG120-L | Clofibrate x PCN | 148 | 0.934 |
| TTG144-L | Tributyltin x Phenobarbital | 188 | 0.929 |
| TTG033-L | 1,2-Dichloro-3-nitrobenzene | 46 | 0.888 |
| TTG027-L | 1,2,3-Triazole | 73 | 0.853 |
| TTG150-L | Valproic acid sodium salt x Thalidomide | 58 | 0.815 |
| TTG016-L(C) | Pentachlorophenol | 374 | 0.798 |
| TTG168-L | Mastic | 107 | 0.792 |
| TTG104-L | MEHP | 352 | 0.764 |
| TTG074-L | Bromobenzene | 78 | 0.753 |
| TTG162-L | Sesame seed oil unsaponified matter | 135 | 0.738 |
| TTG028-L | 1,2,4-Triazole | 42 | 0.711 |
| TTG141-L | Tributyltin x Clofibrate | 230 | 0.608 |
| TTG020-L | TCDD(2,3,7,8-Tetrachlorodibenzo-p-Dioxin) | 77 | 0.606 |
| TTG118-L | Clofibrate x Clofibrate | 165 | 0.603 |
| TTG044-L | Clofibrate | 175 | 0.594 |
| TTG015-L | 4-amino-2,6-dichlorophenol | 17 | 0.585 |
| TTG129-L | CCl4 x Clofibrate | 124 | 0.57 |
| TTG031-L | 2-Chloro-4,6-dimethylaniline | 121 | 0.564 |
| TTG056-L | 3-methylcholanthrene | 58 | 0.556 |
| TTG090-L | Pregnenolone Carbonitrile | 69 | 0.553 |
| TTG131B-L | CCl4 x Phenobarbital | 74 | 0.55 |
| TTG151-L | Valproic acid sodium salt x Valproic acid sodium salt | 108 | 0.548 |
| TTG137-L | alpha-Lipoic Acid | 25 | 0.489 |
| TTG077-L | Monocrotaline | 21 | 0.481 |
| TTG037-L | Phenobarbital | 239 | 0.478 |
| TTG051-L | 9-cis retinoic acid | 24 | 0.454 |
| TTG139-L | Indigo Carmine | 32 | 0.453 |
| TTG047-L | Bisphenol A (PLD) | 19 | 0.449 |
| TTG080-L | DMSO | 19 | 0.449 |
| TTG149-L | Valproic acid sodium salt x Aspirin | 91 | 0.443 |
| TTG126-L | Thalidomide | 41 | 0.442 |
| TTG034-L | 4-Ethylnitrobenzene | 22 | 0.44 |
| TTG046-L | Tributyltin | 126 | 0.436 |
| TTG093-L | AraC | 13 | 0.419 |
| TTG059-L | Caffeine | 38 | 0.417 |
| TTG183-L | Bisphenol A (corn oil) | 36 | 0.405 |
| TTG062-L(C) | Dexamethasone | 49 | 0.382 |
| TTG154-L | Sodium Dehydroacetate | 153 | 0.372 |
| TTG095-L | Ibuprofen (dl-p-isobutylhydratropic acid) | 24 | 0.367 |
| TTG114-L | Benzene | 25 | 0.367 |
| TTG109-L | Acephate | 83 | 0.365 |
| TTG147-L | Estragole | 35 | 0.355 |
| TTG073-L | Toluene | 91 | 0.352 |
| TTG132-L | Curcumin | 56 | 0.35 |
| TTG010-L | Acetaminophen | 41 | 0.323 |
| TTG041-L | Valproic Acid | 115 | 0.322 |
| TTG135-L | Methyl dihydro jasmonate | 20 | 0.315 |
| TTG063-L | Sodium Arsenite | 13 | 0.314 |
| TTG130-L | CCl4 x CCl4 | 15 | 0.314 |
| TTG136-L | Phytol | 64 | 0.314 |

;Percellome Explorer ver. 0.4.8 : PDBEx_RSort101008_Std-Av

;Target Prj: vs TTG016-L(C) // Pentachlorophenol

;Denominator: Target * Candidate

| Name | Condition | Num | Cor |
|-------------|---|------|-------|
| TTG016-L(C) | Pentachlorophenol | 3357 | 2.979 |
| TTG016-L | Pentachlorophenol | 374 | 0.798 |
| TTG028-L | 1,2,4-Triazole | 86 | 0.606 |
| TTG077-L | Monocrotaline | 58 | 0.552 |
| TTG032-L | 3-Amino-1H-1,2,4-triazole | 218 | 0.506 |
| TTG027-L | 1,2,3-Triazole | 104 | 0.505 |
| TTG144-L | Tributyltin x Phenobarbital | 244 | 0.502 |
| TTG150-L | Valproic acid sodium salt x Thalidomide | 84 | 0.491 |
| TTG074-L | Bromobenzene | 119 | 0.478 |
| TTG033-L | 1,2-Dichloro-3-nitrobenzene | 58 | 0.466 |
| TTG098-L | DEHP | 487 | 0.46 |
| TTG019-L | 2-Vinylpyridine | 104 | 0.458 |
| TTG168-L | Mastic | 138 | 0.425 |
| TTG026-L | TCDF(2,3,7,8-Tetrachlorodibenzofuran) | 24 | 0.409 |
| TTG031-L | 2-Chloro-4,6-dimethylaniline | 209 | 0.405 |
| TTG120-L | Clofibrate x PCN | 152 | 0.399 |
| TTG118-L | Clofibrate x Clofibrate | 251 | 0.381 |
| TTG104-L | MEHP | 413 | 0.373 |
| TTG157-L | Valproic acid sodium salt | 277 | 0.357 |
| TTG149-L | Valproic acid sodium salt x Aspirin | 174 | 0.353 |
| TTG131B-L | CCl4 x Phenobarbital | 112 | 0.346 |
| TTG151-L | Valproic acid sodium salt x Valproic acid sodium salt | 163 | 0.344 |
| TTG137-L | alpha-Lipoic Acid | 42 | 0.342 |
| TTG037-L | Phenobarbital | 408 | 0.339 |
| TTG091-L | Azacytidine | 23 | 0.339 |
| TTG141-L | Tributyltin x Clofibrate | 303 | 0.333 |
| TTG154-L | Sodium Dehydroacetate | 330 | 0.333 |
| TTG056-L | 3-methylcholanthrene | 83 | 0.331 |
| TTG162-L | Sesame seed oil unsaponified matter | 145 | 0.33 |
| TTG015-L | 4-amino-2,6-dichlorophenol | 23 | 0.329 |
| TTG059-L | Caffeine | 72 | 0.329 |
| TTG051-L | 9-cis retinoic acid | 41 | 0.322 |
| TTG063-L | Sodium Arsenite | 32 | 0.321 |
| TTG090-L | Pregnenolone Carbonitrile | 95 | 0.317 |
| TTG129-L | CCl4 x Clofibrate | 166 | 0.317 |
| TTG062-L(C) | Dexamethasone | 97 | 0.314 |
| TTG044-L | Clofibrate | 222 | 0.313 |
| TTG020-L | TCDD(2,3,7,8-Tetrachlorodibenzo-p-Dioxin) | 95 | 0.311 |
| TTG041-L | Valproic Acid | 266 | 0.31 |
| TTG126-L | Thalidomide | 69 | 0.31 |
| TTG095-L | Ibuprofen (dl-p-isobutylhydratropic acid) | 48 | 0.306 |
| TTG183-L | Bisphenol A (corn oil) | 65 | 0.304 |
| TTG040-L | Cisplatin | 78 | 0.283 |
| TTG123-L | Caffeine | 46 | 0.281 |
| TTG147-L | Estragole | 66 | 0.278 |
| TTG166-L | Carbaryl | 56 | 0.275 |
| TTG060-L | Forskolin | 36 | 0.267 |
| TTG034-L | 4-Ethylnitrobenzene | 32 | 0.266 |
| TTG042-L | Ethynyl estradiol (PLD) | 39 | 0.266 |
| TTG014-L | 2,4-dinitrophenol | 18 | 0.258 |
| TTG109-L | Acephate | 138 | 0.252 |
| TTG177-L | Red No.102 | 37 | 0.252 |
| TTG097-L | Permethrin | 29 | 0.247 |
| TTG047-L | Bisphenol A (PLD) | 25 | 0.246 |
| TTG061-L | Paraquat | 67 | 0.244 |