

# Delta score calculation tutorial

Bhagwan Yadav

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This is tutorial to compute delta score using R. First, we have to load required libraries in r programming

```
# Load libraries required
library(drc)
library(kriging)
library(reshape2)
library(compiler)
options(warn=-1)
```

Set the working directory to the folder where finction.R file is kept.

```
# Set working directory
setwd("/home/bhagwan/Dropbox/PhD_Projects/Project-5_VBS/Manuscript/r_codes")
```

Source the function file

```
# Source the functions file
source(paste(getwd(), "/functions.R", sep=""))
```

Read response data as well as metadata files

```
# Read response and metadata
response<-read.csv("/home/bhagwan/Dropbox/PhD_Projects/Project-5_VBS/data/Griner_et_al/241/responses.csv")
metadata<-read.csv("/home/bhagwan/Dropbox/PhD_Projects/Project-5_VBS/data/Griner_et_al/241/metadata.csv")
```

Get the unique block IDs

```
# get unique bolck ids
blockId<-unique(response$BlockId)
```

Make matrix to store delta score

```
# Make matrix to store delta score
delta_score<-matrix(NA,length(blockId),4)
colnames(delta_score)<-c("blockId", "Drug1", "Drug2", "Delta")
```

Compute delta score for each block store in above variable.

```
# Loop to compute delta for each combination
#set.seed(0)
suppressWarnings(
for(i in 1:length(blockId)){
```

```

blockIndex<-which(response$BlockId %in% blockId[i])
dataM<-response[blockIndex,c(2,3,4)]

##### Preparing Input Files start #####
# Making plate matrix file
plate.file<-acast(dataM,Col~Row,value.var="Value")
plate.file<-apply(t(apply(t(plate.file),2,rev)),2,rev)
plate.mat <- 100-plate.file
plate.mat<-apply(plate.mat,2,as.numeric)

# Mapping concentration range file
meta.blockIndex<-which(metadata$BlockId %in% blockId[i])

drug1name<-as.character(as.matrix(metadata$RowName[meta.blockIndex]))
drug2name<-"Ibrutinib"
colnames(plate.file)<-rep(drug1name,ncol(plate.file))
rownames(plate.file)<-rep(drug2name,nrow(plate.file))

drug1conc<-as.character(as.matrix(metadata$RowConcs[meta.blockIndex]))
drug1conc<-rev(as.numeric(unlist(strsplit(drug1conc,","))))*2
drug2conc<-as.character(as.matrix(metadata$ColConcs[meta.blockIndex]))
drug2conc<-rev(as.numeric(unlist(strsplit(drug2conc,","))))*2

conc.file<-rbind(drug1conc,drug2conc)
conc.file<-cbind(rbind(drug1name,drug2name),conc.file)
conc.range <-conc.file
conc.range[1,2:ncol(conc.range)]<-as.character(round(
as.numeric(conc.range[1,2:ncol(conc.range)]),digits=1))
conc.range[2,2:ncol(conc.range)]<-as.character(
round(as.numeric(conc.range[2,2:ncol(conc.range)]),digits=1))
# Add col names and row names to plate mat
colnames(plate.mat)<-colnames(plate.file)
rownames(plate.mat)<-rownames(plate.file)

# Making drug combination file
pairs.file<-matrix(NA,1,5)
pairs.file[1,]<-c(1,drug1name,drug2name,"cellline",1)
pairs.file <- as.data.frame(pairs.file)
pair.list <- pairs.file
colnames(pair.list)<-c("index","drug1","drug2","cell.line","plate")

##### Preparing Input Files End #####

##### Baseline correction #####

output_baseline= c.SDbaselineCor(plate.mat,conc.range,pair.list)

##### Two Way Fitting #####
# Single plate analysis

# raw_matrix=output_baseline[[1]] # raw matrix
cor_matrix=output_baseline[[2]] # matrix after baseline correction

```

```

drug_pair=output_baseline[[3]] # drug names

output = c.twowayfitting(cor_matrix,drug_pair)

delta_score[i,1] = blockId[i]
delta_score[i,2] = unique(colnames(plate.mat))
delta_score[i,3] = unique(rownames(plate.mat))
delta_score[i,4] = round(output,digits=4)

})

```

```

# print delta score
print(delta_score)

```

##		blockId	Drug1	Drug2	Delta
##	[1,]	"1"	"Bendamustine"	"Ibrutinib"	"-6.3468"
##	[2,]	"2"	"Lonidamine"	"Ibrutinib"	"-1.9388"
##	[3,]	"3"	"Lenalidomide"	"Ibrutinib"	"6.2456"
##	[4,]	"4"	"Cladribine"	"Ibrutinib"	"4.0013"
##	[5,]	"5"	"Pentostatin"	"Ibrutinib"	"-3.9636"
##	[6,]	"6"	"6-mercaptopurine"	"Ibrutinib"	"-2.1205"
##	[7,]	"7"	"Everolimus"	"Ibrutinib"	"11.1983"
##	[8,]	"8"	"Aminoglutethimide"	"Ibrutinib"	"-1.9985"
##	[9,]	"9"	"Formestane"	"Ibrutinib"	"-0.8742"
##	[10,]	"10"	"Letrozole"	"Ibrutinib"	"-0.2915"
##	[11,]	"11"	"Pemetrexed disodium"	"Ibrutinib"	"-0.4784"
##	[12,]	"12"	"Gemcitabine"	"Ibrutinib"	"1.2103"
##	[13,]	"13"	"Tamoxifen"	"Ibrutinib"	"4.0054"
##	[14,]	"14"	"Vincristine sulfate"	"Ibrutinib"	"4.8455"
##	[15,]	"15"	"Combretastatin A-4"	"Ibrutinib"	"0.4951"
##	[16,]	"16"	"Plinabulin"	"Ibrutinib"	"5.9503"
##	[17,]	"17"	"Docetaxel"	"Ibrutinib"	"14.4558"
##	[18,]	"18"	"Blebbistatin"	"Ibrutinib"	"2.8375"
##	[19,]	"19"	"Ispinesib"	"Ibrutinib"	"17.5966"
##	[20,]	"20"	"Doxorubicin"	"Ibrutinib"	"5.3546"
##	[21,]	"21"	"Topotecan hydrochloride"	"Ibrutinib"	"6.7647"
##	[22,]	"22"	"Cyclophosphamide"	"Ibrutinib"	"-4.7014"
##	[23,]	"23"	"5-Azacitidine"	"Ibrutinib"	"-3.2309"
##	[24,]	"24"	"Actinomycin D"	"Ibrutinib"	"0.7481"
##	[25,]	"25"	"Mithramycin"	"Ibrutinib"	"4.1517"
##	[26,]	"26"	"Itraconazole"	"Ibrutinib"	"3.1795"
##	[27,]	"27"	"Hydroxychloroquine sulfate"	"Ibrutinib"	"-0.9994"
##	[28,]	"28"	"Mifepristone"	"Ibrutinib"	"1.4239"
##	[29,]	"29"	"Metformin HCl"	"Ibrutinib"	"-2.2858"
##	[30,]	"30"	"Acadesine"	"Ibrutinib"	"2.9887"
##	[31,]	"31"	"A-769662"	"Ibrutinib"	"1.9776"
##	[32,]	"32"	"Imatinib"	"Ibrutinib"	"1.2214"
##	[33,]	"33"	"Nilotinib"	"Ibrutinib"	"6.2084"
##	[34,]	"34"	"Ponatinib"	"Ibrutinib"	"8.374"
##	[35,]	"35"	"DCC-2036"	"Ibrutinib"	"4.1032"
##	[36,]	"36"	"Dasatinib"	"Ibrutinib"	"3.1478"
##	[37,]	"37"	"Bosutinib"	"Ibrutinib"	"0.5349"
##	[38,]	"38"	"Saracatinib"	"Ibrutinib"	"5.4986"

##	[39,]	"39"	"PD-166285"	"Ibrutinib"	"5.5027"
##	[40,]	"40"	"Vandetanib"	"Ibrutinib"	"-2.7533"
##	[41,]	"41"	"Erlotinib hydrochloride"	"Ibrutinib"	"0.9148"
##	[42,]	"42"	"Gefitinib"	"Ibrutinib"	"-0.3579"
##	[43,]	"43"	"Lapatinib"	"Ibrutinib"	"0.2124"
##	[44,]	"44"	"Neratinib"	"Ibrutinib"	"-2.0381"
##	[45,]	"45"	"Canertinib"	"Ibrutinib"	"-14.0386"
##	[46,]	"46"	"AV-412"	"Ibrutinib"	"-6.8827"
##	[47,]	"47"	"Dacomitinib"	"Ibrutinib"	"-5.2818"
##	[48,]	"48"	"CP-724714"	"Ibrutinib"	"-5.0341"
##	[49,]	"49"	"Afatinib"	"Ibrutinib"	"-2.6713"
##	[50,]	"50"	"AEE-788"	"Ibrutinib"	"-0.504"
##	[51,]	"51"	"CUDC-101"	"Ibrutinib"	"3.268"
##	[52,]	"52"	"Pelitinib"	"Ibrutinib"	"-6.0806"
##	[53,]	"53"	"WZ-4002"	"Ibrutinib"	"-9.6184"
##	[54,]	"54"	"Linifanib"	"Ibrutinib"	"-6.2503"
##	[55,]	"55"	"Axitinib"	"Ibrutinib"	"-11.7996"
##	[56,]	"56"	"Sorafenib"	"Ibrutinib"	"-0.2569"
##	[57,]	"57"	"Vatalanib"	"Ibrutinib"	"-5.9609"
##	[58,]	"58"	"Motesanib"	"Ibrutinib"	"-3.674"
##	[59,]	"59"	"Tivozanib"	"Ibrutinib"	"-3.5885"
##	[60,]	"60"	"Vargatef"	"Ibrutinib"	"6.94"
##	[61,]	"61"	"Brivanib"	"Ibrutinib"	"1.0834"
##	[62,]	"62"	"Telatinib"	"Ibrutinib"	"-5.7898"
##	[63,]	"63"	"Cabozantinib"	"Ibrutinib"	"-3.16"
##	[64,]	"64"	"Cediranib"	"Ibrutinib"	"1.9473"
##	[65,]	"65"	"BMS-794833"	"Ibrutinib"	"-6.2111"
##	[66,]	"66"	"Lenvatinib"	"Ibrutinib"	"7.0859"
##	[67,]	"67"	"OSI-632"	"Ibrutinib"	"-5.42"
##	[68,]	"68"	"Foretinib"	"Ibrutinib"	"3.4648"
##	[69,]	"69"	"Regorafenib"	"Ibrutinib"	"-1.9613"
##	[70,]	"70"	"Dovitinib"	"Ibrutinib"	"-0.4967"
##	[71,]	"71"	"Masitinib"	"Ibrutinib"	"3.1735"
##	[72,]	"72"	"PD-173074"	"Ibrutinib"	"-3.1279"
##	[73,]	"73"	"SG-00529"	"Ibrutinib"	"5.5659"
##	[74,]	"74"	"Amuvatinib"	"Ibrutinib"	"-0.9104"
##	[75,]	"75"	"OSI-930"	"Ibrutinib"	"4.1966"
##	[76,]	"76"	"Crizotinib"	"Ibrutinib"	"3.8533"
##	[77,]	"77"	"PHA-665752"	"Ibrutinib"	"0.9738"
##	[78,]	"78"	"BMS-777607"	"Ibrutinib"	"0.671"
##	[79,]	"79"	"PF-04217903"	"Ibrutinib"	"-1.3699"
##	[80,]	"80"	"JNJ-38877605"	"Ibrutinib"	"0.0382"
##	[81,]	"81"	"SGX-523"	"Ibrutinib"	"4.1568"
##	[82,]	"82"	"AMG-51"	"Ibrutinib"	"0.428"
##	[83,]	"83"	"Podofilox"	"Ibrutinib"	"3.8533"
##	[84,]	"84"	"Linsitinib"	"Ibrutinib"	"1.622"
##	[85,]	"85"	"GSK-1904529A"	"Ibrutinib"	"-6.2493"
##	[86,]	"86"	"Dorsomorphin"	"Ibrutinib"	"-1.1126"
##	[87,]	"87"	"LY2157299"	"Ibrutinib"	"-1.0503"
##	[88,]	"88"	"LY2109761"	"Ibrutinib"	"-2.5351"
##	[89,]	"89"	"A 83-01"	"Ibrutinib"	"-0.2188"
##	[90,]	"90"	"SJN 2511"	"Ibrutinib"	"-0.3455"
##	[91,]	"91"	"SD-208"	"Ibrutinib"	"3.3713"

##	[92,]	"92"	"TAE-684"	"Ibrutinib"	"1.1458"
##	[93,]	"93"	"SB-525334"	"Ibrutinib"	"-1.9296"
##	[94,]	"94"	"SB-431542"	"Ibrutinib"	"-3.8038"
##	[95,]	"95"	"Tandutinib"	"Ibrutinib"	"-5.8832"
##	[96,]	"96"	"Quizartinib"	"Ibrutinib"	"0.3518"
##	[97,]	"97"	"AZ-23"	"Ibrutinib"	"3.4151"
##	[98,]	"98"	"LDN-193189"	"Ibrutinib"	"-3.3286"
##	[99,]	"99"	"PRT-060318"	"Ibrutinib"	"2.6408"
##	[100,]	"100"	"R406"	"Ibrutinib"	"2.9619"
##	[101,]	"101"	"Perifosine"	"Ibrutinib"	"4.0698"
##	[102,]	"102"	"GDC-0941"	"Ibrutinib"	"2.8008"
##	[103,]	"103"	"GSK-2126458"	"Ibrutinib"	"1.9257"
##	[104,]	"104"	"IC-87114"	"Ibrutinib"	"7.3593"
##	[105,]	"105"	"PIK-90"	"Ibrutinib"	"6.4427"
##	[106,]	"106"	"BKM-120"	"Ibrutinib"	"0.9764"
##	[107,]	"107"	"CAL-101"	"Ibrutinib"	"10.8295"
##	[108,]	"108"	"BAG-956"	"Ibrutinib"	"5.4527"
##	[109,]	"109"	"AZD-6482"	"Ibrutinib"	"4.7657"
##	[110,]	"110"	"CAY10626"	"Ibrutinib"	"5.8777"
##	[111,]	"111"	"PI-103"	"Ibrutinib"	"3.9729"
##	[112,]	"112"	"17_-hydroxy Wortmannin"	"Ibrutinib"	"10.3078"
##	[113,]	"113"	"Deguelin"	"Ibrutinib"	"4.0447"
##	[114,]	"114"	"MK-2206"	"Ibrutinib"	"11.2472"
##	[115,]	"115"	"A-674563"	"Ibrutinib"	"-0.1616"
##	[116,]	"116"	"GSK-690693"	"Ibrutinib"	"3.9824"
##	[117,]	"117"	"BEZ-235"	"Ibrutinib"	"6.6094"
##	[118,]	"118"	"PF-05212384"	"Ibrutinib"	"6.6506"
##	[119,]	"119"	"GDC-0980"	"Ibrutinib"	"4.1276"
##	[120,]	"120"	"Torin-1"	"Ibrutinib"	"6.072"
##	[121,]	"121"	"Torin-2"	"Ibrutinib"	"8.3212"
##	[122,]	"122"	"AZD-8055"	"Ibrutinib"	"3.4301"
##	[123,]	"123"	"OSI-027"	"Ibrutinib"	"3.2355"
##	[124,]	"124"	"KU-0063794"	"Ibrutinib"	"-0.2222"
##	[125,]	"125"	"WYE-354"	"Ibrutinib"	"3.3161"
##	[126,]	"126"	"Salirasib"	"Ibrutinib"	"3.6518"
##	[127,]	"127"	"NU-7441"	"Ibrutinib"	"7.3682"
##	[128,]	"128"	"KU 0060648"	"Ibrutinib"	"5.9441"
##	[129,]	"129"	"NSC 23766"	"Ibrutinib"	"0.5056"
##	[130,]	"130"	"NCGC00188866-01"	"Ibrutinib"	"1.3509"
##	[131,]	"131"	"VX-702"	"Ibrutinib"	"1.526"
##	[132,]	"132"	"SB-203580"	"Ibrutinib"	"0.9049"
##	[133,]	"133"	"VX-745"	"Ibrutinib"	"2.2659"
##	[134,]	"134"	"Doramapimod"	"Ibrutinib"	"4.3496"
##	[135,]	"135"	"PH-797804"	"Ibrutinib"	"-0.1161"
##	[136,]	"136"	"RWJ-67657"	"Ibrutinib"	"0.9253"
##	[137,]	"137"	"Talmapimod"	"Ibrutinib"	"3.541"
##	[138,]	"138"	"FMK"	"Ibrutinib"	"5.3827"
##	[139,]	"139"	"BI-D1870"	"Ibrutinib"	"4.2654"
##	[140,]	"140"	"NCGC00253463-01"	"Ibrutinib"	"5.8137"
##	[141,]	"141"	"PHA-408"	"Ibrutinib"	"2.1371"
##	[142,]	"142"	"Withaferin A"	"Ibrutinib"	"4.6917"
##	[143,]	"143"	"BX-795"	"Ibrutinib"	"9.8416"
##	[144,]	"144"	"Bardoxolone methyl"	"Ibrutinib"	"6.6851"

## [145,]	"145"	"IKK16"	"Ibrutinib"	"4.0977"
## [146,]	"146"	"PF-184"	"Ibrutinib"	"0.6804"
## [147,]	"147"	"IMD-0354"	"Ibrutinib"	"-0.0515"
## [148,]	"148"	"PS-1145"	"Ibrutinib"	"1.0353"
## [149,]	"149"	"MLN-120B"	"Ibrutinib"	"2.3123"
## [150,]	"150"	"cycloheximide"	"Ibrutinib"	"-0.0464"
## [151,]	"151"	"CT-99021"	"Ibrutinib"	"-6.72"
## [152,]	"152"	"SB-216763"	"Ibrutinib"	"-12.6769"
## [153,]	"153"	"NCGC00161703"	"Ibrutinib"	"10.4519"
## [154,]	"154"	"WAY-204688"	"Ibrutinib"	"3.3684"
## [155,]	"155"	"Sulfasalazine"	"Ibrutinib"	"-0.883"
## [156,]	"156"	"NCGC00263020-01"	"Ibrutinib"	"4.3433"
## [157,]	"157"	"BX-795"	"Ibrutinib"	"-2.2567"
## [158,]	"158"	"KU-60019"	"Ibrutinib"	"1.2964"
## [159,]	"159"	"KU-0064"	"Ibrutinib"	"3.5376"
## [160,]	"160"	"CP-466722"	"Ibrutinib"	"0.4825"
## [161,]	"161"	"SM-164"	"Ibrutinib"	"-7.164"
## [162,]	"162"	"TW-37"	"Ibrutinib"	"-0.3849"
## [163,]	"163"	"(-)-Gossypol"	"Ibrutinib"	"-0.7108"
## [164,]	"164"	"Chelerythrine chloride"	"Ibrutinib"	"3.174"
## [165,]	"165"	"Obatoclox"	"Ibrutinib"	"-3.3754"
## [166,]	"166"	"Navitoclox"	"Ibrutinib"	"13.2502"
## [167,]	"167"	"Nutlin-3"	"Ibrutinib"	"6.466"
## [168,]	"168"	"Ac-SAH-p53-8"	"Ibrutinib"	"-0.2576"
## [169,]	"169"	"Serdemetan"	"Ibrutinib"	"3.6526"
## [170,]	"170"	"HLI-373989"	"Ibrutinib"	"-3.4475"
## [171,]	"171"	"SJ-172550"	"Ibrutinib"	"2.3218"
## [172,]	"172"	"AZD-7762"	"Ibrutinib"	"6.9659"
## [173,]	"173"	"PF-477736"	"Ibrutinib"	"6.4006"
## [174,]	"174"	"Flavopiridol???"	"Ibrutinib"	"3.8065"
## [175,]	"175"	"Purvalanol B"	"Ibrutinib"	"-1.7598"
## [176,]	"176"	"Seliciclib"	"Ibrutinib"	"2.809"
## [177,]	"177"	"PHA-690509"	"Ibrutinib"	"6.6421"
## [178,]	"178"	"AT7519"	"Ibrutinib"	"2.1474"
## [179,]	"179"	"AT7519"	"Ibrutinib"	"1.4255"
## [180,]	"180"	"SNS-032"	"Ibrutinib"	"2.362"
## [181,]	"181"	"PHA-793887"	"Ibrutinib"	"2.2839"
## [182,]	"182"	"PD-0332991"	"Ibrutinib"	"8.2939"
## [183,]	"183"	"DA-3003-1"	"Ibrutinib"	"0.396"
## [184,]	"184"	"JNJ-7706621"	"Ibrutinib"	"-0.7994"
## [185,]	"185"	"SNS-314"	"Ibrutinib"	"2.6661"
## [186,]	"186"	"Tozasertib"	"Ibrutinib"	"3.9173"
## [187,]	"187"	"Alisertib"	"Ibrutinib"	"1.7995"
## [188,]	"188"	"Danusertib"	"Ibrutinib"	"1.6745"
## [189,]	"189"	"CYC-116"	"Ibrutinib"	"0.3857"
## [190,]	"190"	"AZD-1152-HQPA"	"Ibrutinib"	"1.7661"
## [191,]	"191"	"AMG-900"	"Ibrutinib"	"0.1407"
## [192,]	"192"	"ENMD-981693"	"Ibrutinib"	"0.6939"
## [193,]	"193"	"CHIR-265"	"Ibrutinib"	"2.9094"
## [194,]	"194"	"AZ-628"	"Ibrutinib"	"-0.3608"
## [195,]	"195"	"Vemurafenib"	"Ibrutinib"	"-1.7404"
## [196,]	"196"	"PLX-4720"	"Ibrutinib"	"0.8676"
## [197,]	"197"	"AR-00341677"	"Ibrutinib"	"-8.6081"

## [198,]	"198"	"RDEA-119"	"Ibrutinib"	"-3.7577"
## [199,]	"199"	"Selumetinib"	"Ibrutinib"	"2.0339"
## [200,]	"200"	"PD-0325901"	"Ibrutinib"	"6.848"
## [201,]	"201"	"Trametinib"	"Ibrutinib"	"8.5621"
## [202,]	"202"	"TAK-733"	"Ibrutinib"	"1.3587"
## [203,]	"203"	"XMD8-92"	"Ibrutinib"	"-1.2673"
## [204,]	"204"	"NCGC00242487"	"Ibrutinib"	"-5.7912"
## [205,]	"205"	"S6K-18"	"Ibrutinib"	"-2.3854"
## [206,]	"206"	"PF-4708671"	"Ibrutinib"	"3.5897"
## [207,]	"207"	"PF-431396"	"Ibrutinib"	"-0.8793"
## [208,]	"208"	"PF-573228"	"Ibrutinib"	"6.0946"
## [209,]	"209"	"PCI-32765"	"Ibrutinib"	"-3.3197"
## [210,]	"210"	"NCGC00188382-01"	"Ibrutinib"	"7.2905"
## [211,]	"211"	"BMS-509744"	"Ibrutinib"	"4.4802"
## [212,]	"212"	"Midostaurin"	"Ibrutinib"	"2.6752"
## [213,]	"213"	"Enzastaurin"	"Ibrutinib"	"2.0163"
## [214,]	"214"	"Sotrastaurin"	"Ibrutinib"	"-2.4207"
## [215,]	"215"	"Ruboxistaurin mesilate"	"Ibrutinib"	"6.2243"
## [216,]	"216"	"NCGC00263018-01"	"Ibrutinib"	"-1.7551"
## [217,]	"217"	"GW 843682X"	"Ibrutinib"	"-0.1172"
## [218,]	"218"	"BI-2536"	"Ibrutinib"	"8.3663"
## [219,]	"219"	"Volasertib"	"Ibrutinib"	"4.3044"
## [220,]	"220"	"GSK-461364A"	"Ibrutinib"	"12.8113"
## [221,]	"221"	"KN-93"	"Ibrutinib"	"2.4081"
## [222,]	"222"	"KN-62"	"Ibrutinib"	"-3.8864"
## [223,]	"223"	"GSK-269962A"	"Ibrutinib"	"2.2392"
## [224,]	"224"	"Y-27632"	"Ibrutinib"	"-5.0092"
## [225,]	"225"	"GSK-650394"	"Ibrutinib"	"2.768"
## [226,]	"226"	"AZD-1480"	"Ibrutinib"	"3.9775"
## [227,]	"227"	"Tofacitinib"	"Ibrutinib"	"-3.3457"
## [228,]	"228"	"Ruxolitinib"	"Ibrutinib"	"-1.2363"
## [229,]	"229"	"CYT387"	"Ibrutinib"	"0.5113"
## [230,]	"230"	"Lestaurtinib???"	"Ibrutinib"	"8.3604"
## [231,]	"231"	"SB1518"	"Ibrutinib"	"7.0246"
## [232,]	"232"	"Leflunomide"	"Ibrutinib"	"-4.9537"
## [233,]	"233"	"NVP-BSK805"	"Ibrutinib"	"1.8655"
## [234,]	"234"	"Degrasyn"	"Ibrutinib"	"2.0821"
## [235,]	"235"	"R0495"	"Ibrutinib"	"2.1487"
## [236,]	"236"	"NCGC00244250-01"	"Ibrutinib"	"5.9113"
## [237,]	"237"	"NCGC00244250-01"	"Ibrutinib"	"1.5557"
## [238,]	"238"	"ICG-001"	"Ibrutinib"	"3.1328"
## [239,]	"239"	"Wnt-C59"	"Ibrutinib"	"-5.9843"
## [240,]	"240"	"D-4476"	"Ibrutinib"	"-4.369"
## [241,]	"241"	"Silmitasertib"	"Ibrutinib"	"9.2125"
## [242,]	"242"	"NVP-LDE-225"	"Ibrutinib"	"-3.2522"
## [243,]	"243"	"Cyclopamine"	"Ibrutinib"	"0.3075"
## [244,]	"244"	"LY-2940680??"	"Ibrutinib"	"-1.5425"
## [245,]	"245"	"SANT-2"	"Ibrutinib"	"3.7299"
## [246,]	"246"	"Hh-Ag1.5"	"Ibrutinib"	"4.9584"
## [247,]	"247"	"Vismodegib"	"Ibrutinib"	"-2.5658"
## [248,]	"248"	"R0-4929097"	"Ibrutinib"	"-3.9081"
## [249,]	"249"	"MK-0752"	"Ibrutinib"	"0.6312"
## [250,]	"250"	"Y0-01027"	"Ibrutinib"	"-1.466"

## [251,]	"251"	"GSI-9"	"Ibrutinib"	"0.1532"
## [252,]	"252"	"NVP-XAV-939"	"Ibrutinib"	"-3.6868"
## [253,]	"253"	"NCGC00263015-01"	"Ibrutinib"	"1.407"
## [254,]	"254"	"CPG-52364"	"Ibrutinib"	"0.3165"
## [255,]	"255"	"IRAK-1-4 Inhibitor I"	"Ibrutinib"	"-6.1298"
## [256,]	"256"	"NCGC00241410-01"	"Ibrutinib"	"-4.037"
## [257,]	"257"	"NCGC00241411-01"	"Ibrutinib"	"-4.7634"
## [258,]	"258"	"BI-78D3"	"Ibrutinib"	"-1.1909"
## [259,]	"259"	"SR-3306"	"Ibrutinib"	"3.8395"
## [260,]	"260"	"STF-083010"	"Ibrutinib"	"-0.0302"
## [261,]	"261"	"Irestatin 9389"	"Ibrutinib"	"0.854"
## [262,]	"262"	"SB-265610"	"Ibrutinib"	"-0.1963"
## [263,]	"263"	"Apilimod"	"Ibrutinib"	"-2.4141"
## [264,]	"264"	"PD-0220245"	"Ibrutinib"	"3.589"
## [265,]	"265"	"KRP 203"	"Ibrutinib"	"0.9584"
## [266,]	"266"	"AMG-47a"	"Ibrutinib"	"2.5703"
## [267,]	"267"	"Pim 1 inhibitor 2"	"Ibrutinib"	"-6.9234"
## [268,]	"268"	"SGI-1776"	"Ibrutinib"	"2.9402"
## [269,]	"269"	"KI-20227"	"Ibrutinib"	"0.8618"
## [270,]	"270"	"ABT-702"	"Ibrutinib"	"-6.545"
## [271,]	"271"	"AZ-3146"	"Ibrutinib"	"4.5631"
## [272,]	"272"	"MK-1775"	"Ibrutinib"	"2.8493"
## [273,]	"273"	"BMS-5"	"Ibrutinib"	"-2.4721"
## [274,]	"274"	"AMG-Tie2-1"	"Ibrutinib"	"4.9118"
## [275,]	"275"	"NVP231"	"Ibrutinib"	"3.1704"
## [276,]	"276"	"D-NMAPPD"	"Ibrutinib"	"4.2715"
## [277,]	"277"	"Pazopanib"	"Ibrutinib"	"-0.8906"
## [278,]	"278"	"TG-101348"	"Ibrutinib"	"1.7072"
## [279,]	"279"	"Alvespimycin hydrochloride"	"Ibrutinib"	"2.0508"
## [280,]	"280"	"CCT-018159"	"Ibrutinib"	"-4.962"
## [281,]	"281"	"CNF-2024"	"Ibrutinib"	"2.0949"
## [282,]	"282"	"NVP-AUY922"	"Ibrutinib"	"2.8594"
## [283,]	"283"	"Elesclomol"	"Ibrutinib"	"8.6765"
## [284,]	"284"	"VER-155008"	"Ibrutinib"	"-0.66"
## [285,]	"285"	"ISOX"	"Ibrutinib"	"6.0767"
## [286,]	"286"	"Vorinostat"	"Ibrutinib"	"1.4428"
## [287,]	"287"	"AR-42"	"Ibrutinib"	"3.779"
## [288,]	"288"	"Belinostat"	"Ibrutinib"	"8.2978"
## [289,]	"289"	"Mocetinostat"	"Ibrutinib"	"-3.5319"
## [290,]	"290"	"Panobinostat"	"Ibrutinib"	"3.2171"
## [291,]	"291"	"Pracinostat"	"Ibrutinib"	"2.5123"
## [292,]	"292"	"Romidepsin"	"Ibrutinib"	"0.9377"
## [293,]	"293"	"SRT1720"	"Ibrutinib"	"-0.2566"
## [294,]	"294"	"EX-527"	"Ibrutinib"	"0.577"
## [295,]	"295"	"Entinostat"	"Ibrutinib"	"-1.1256"
## [296,]	"296"	"MG-149"	"Ibrutinib"	"-2.413"
## [297,]	"297"	"Veliparib"	"Ibrutinib"	"-3.4708"
## [298,]	"298"	"Olaparib"	"Ibrutinib"	"-2.0275"
## [299,]	"299"	"AG-14361"	"Ibrutinib"	"-2.3848"
## [300,]	"300"	"Rucaparib"	"Ibrutinib"	"-0.7533"
## [301,]	"301"	"Iniparib"	"Ibrutinib"	"2.3941"
## [302,]	"302"	"MLN-2238??"	"Ibrutinib"	"-1.792"
## [303,]	"303"	"Carfilzomib"	"Ibrutinib"	"5.2159"



## [304,]	"304"	"Bortezomib"	"Ibrutinib"	"0.972"
## [305,]	"305"	"Tosedostat"	"Ibrutinib"	"-3.7345"
## [306,]	"306"	"Teriflunomide"	"Ibrutinib"	"0.0655"
## [307,]	"307"	"PD-166793"	"Ibrutinib"	"-5.3921"
## [308,]	"308"	"SSR-69071"	"Ibrutinib"	"-0.2588"
## [309,]	"309"	"RG-108"	"Ibrutinib"	"-1.2989"
## [310,]	"310"	"BIX-01294"	"Ibrutinib"	"0.2473"
## [311,]	"311"	"JQ1"	"Ibrutinib"	"6.1719"
## [312,]	"312"	"NCGC00185090-04"	"Ibrutinib"	"-1.9086"
## [313,]	"313"	"NCGC00189393-02"	"Ibrutinib"	"0.3327"
## [314,]	"314"	"NCGC00247866-02"	"Ibrutinib"	"2.1733"
## [315,]	"315"	"NCGC00241036-01"	"Ibrutinib"	"-0.875"
## [316,]	"316"	"NCGC00183808-01"	"Ibrutinib"	"0.7783"
## [317,]	"317"	"Tipifarnib"	"Ibrutinib"	"9.9156"
## [318,]	"318"	"LG100268"	"Ibrutinib"	"-1.6015"
## [319,]	"319"	"AHPN"	"Ibrutinib"	"0.1237"
## [320,]	"320"	"AC-261066"	"Ibrutinib"	"-4.7539"
## [321,]	"321"	"Fenretinide"	"Ibrutinib"	"6.0443"
## [322,]	"322"	"Hydrocortisone"	"Ibrutinib"	"10.2627"
## [323,]	"323"	"Dexamethasone"	"Ibrutinib"	"11.5539"
## [324,]	"324"	"Cortivazol"	"Ibrutinib"	"11.1809"
## [325,]	"325"	"Deacetyl cortivazol"	"Ibrutinib"	"7.8513"
## [326,]	"326"	"Abiraterone"	"Ibrutinib"	"8.0934"
## [327,]	"327"	"2-Methoxyestradiol"	"Ibrutinib"	"2.4975"
## [328,]	"328"	"Quercetine"	"Ibrutinib"	"-2.7979"
## [329,]	"329"	"Doxercalciferol"	"Ibrutinib"	"-0.7968"
## [330,]	"330"	"Seocalcitol"	"Ibrutinib"	"3.7612"
## [331,]	"331"	"methyl jasmonate"	"Ibrutinib"	"2.8518"
## [332,]	"332"	"Bicalutamide"	"Ibrutinib"	"-6.2474"
## [333,]	"333"	"Andarine"	"Ibrutinib"	"-2.2026"
## [334,]	"334"	"MDV-3100"	"Ibrutinib"	"-3.5389"
## [335,]	"335"	"RD-162"	"Ibrutinib"	"-1.6821"
## [336,]	"336"	"CITC0"	"Ibrutinib"	"2.5567"
## [337,]	"337"	"PK-11195"	"Ibrutinib"	"-5.393"
## [338,]	"338"	"Pioglitazone HCl"	"Ibrutinib"	"-3.2065"
## [339,]	"339"	"GW-7647"	"Ibrutinib"	"-5.1003"
## [340,]	"340"	"GW-0742"	"Ibrutinib"	"-1.578"
## [341,]	"341"	"GW-501516"	"Ibrutinib"	"2.0511"
## [342,]	"342"	"Troglitazone"	"Ibrutinib"	"-5.9511"
## [343,]	"343"	"Telmisartan"	"Ibrutinib"	"-8.6714"
## [344,]	"344"	"GSK-3787"	"Ibrutinib"	"-0.1895"
## [345,]	"345"	"MK-767"	"Ibrutinib"	"-0.5208"
## [346,]	"346"	"SID 7969543"	"Ibrutinib"	"9.056"
## [347,]	"347"	"Bazedoxifene"	"Ibrutinib"	"-2.8463"
## [348,]	"348"	"Triptolide"	"Ibrutinib"	"6.637"
## [349,]	"349"	"Apratastat"	"Ibrutinib"	"0.0233"
## [350,]	"350"	"HC-067047"	"Ibrutinib"	"-0.2501"
## [351,]	"351"	"DE-096"	"Ibrutinib"	"8.3289"
## [352,]	"352"	"GSK-3965"	"Ibrutinib"	"-2.2712"
## [353,]	"353"	"Omeprazole"	"Ibrutinib"	"4.6107"
## [354,]	"354"	"Elacridar"	"Ibrutinib"	"-0.3537"
## [355,]	"355"	"Secin H3"	"Ibrutinib"	"0.0463"
## [356,]	"356"	"CDIBA"	"Ibrutinib"	"9.2589"

## [357,]	"357"	"U-73122??"	"Ibrutinib"	"4.6077"
## [358,]	"358"	"BAY-60-7550"	"Ibrutinib"	"-9.1944"
## [359,]	"359"	"anagrelide"	"Ibrutinib"	"-7.7538"
## [360,]	"360"	"Olprinone"	"Ibrutinib"	"-2.2559"
## [361,]	"361"	"NCGC00168459-01"	"Ibrutinib"	"2.1073"
## [362,]	"362"	"NCGC00249759-01"	"Ibrutinib"	"-4.5155"
## [363,]	"363"	"NVP-ABE171"	"Ibrutinib"	"-2.8188"
## [364,]	"364"	"Lirimilast"	"Ibrutinib"	"-1.961"
## [365,]	"365"	"Sildenafil citrate"	"Ibrutinib"	"0.9777"
## [366,]	"366"	"Alacepril"	"Ibrutinib"	"2.1223"
## [367,]	"367"	"Ubenimex"	"Ibrutinib"	"-1.4994"
## [368,]	"368"	"BAY-41-8543"	"Ibrutinib"	"-1.0795"
## [369,]	"369"	"Vinpocetine"	"Ibrutinib"	"-2.9691"
## [370,]	"370"	"Verapamil"	"Ibrutinib"	"0.7655"
## [371,]	"371"	"(S)-(+)-Niguldipine"	"Ibrutinib"	"0.3308"
## [372,]	"372"	"SR 33805"	"Ibrutinib"	"2.6059"
## [373,]	"373"	"Zaldaride maleate"	"Ibrutinib"	"-0.2416"
## [374,]	"374"	"Riluzole"	"Ibrutinib"	"-5.0337"
## [375,]	"375"	"SSR-504734"	"Ibrutinib"	"-1.7259"
## [376,]	"376"	"SCH-900435"	"Ibrutinib"	"3.9508"
## [377,]	"377"	"Ivacaftor"	"Ibrutinib"	"-1.5649"
## [378,]	"378"	"Ivabradine hydrochloride"	"Ibrutinib"	"-2.1055"
## [379,]	"379"	"ICI-D7288"	"Ibrutinib"	"-1.9585"
## [380,]	"380"	"GSK-1016790A"	"Ibrutinib"	"-0.4923"
## [381,]	"381"	"Fenobam"	"Ibrutinib"	"1.473"
## [382,]	"382"	"MPEP"	"Ibrutinib"	"-4.0393"
## [383,]	"383"	"Piboserod hydrochloride"	"Ibrutinib"	"1.9556"
## [384,]	"384"	"SB-224289"	"Ibrutinib"	"6.5923"
## [385,]	"385"	"SB-206553"	"Ibrutinib"	"-4.9748"
## [386,]	"386"	"Meclinetant"	"Ibrutinib"	"1.6796"
## [387,]	"387"	"Zibotentan"	"Ibrutinib"	"-0.9321"
## [388,]	"388"	"GW-4064X"	"Ibrutinib"	"-3.4697"
## [389,]	"389"	"Turofexorate isopropyl"	"Ibrutinib"	"-1.1582"
## [390,]	"390"	"GW-9508"	"Ibrutinib"	"-2.1943"
## [391,]	"391"	"AG-041R"	"Ibrutinib"	"5.2175"
## [392,]	"392"	"MK-0354"	"Ibrutinib"	"-5.3955"
## [393,]	"393"	"PB-28"	"Ibrutinib"	"0.7069"
## [394,]	"394"	"Cutamesine hydrochloride"	"Ibrutinib"	"-0.0496"
## [395,]	"395"	"BD-1047"	"Ibrutinib"	"-0.0756"
## [396,]	"396"	"SCH-79797"	"Ibrutinib"	"2.2604"
## [397,]	"397"	"Vorapaxar"	"Ibrutinib"	"0.882"
## [398,]	"398"	"GB 83"	"Ibrutinib"	"0.3567"
## [399,]	"399"	"Aprepitant"	"Ibrutinib"	"4.3963"
## [400,]	"400"	"GR-159897"	"Ibrutinib"	"-1.0661"
## [401,]	"401"	"Osanetant"	"Ibrutinib"	"-0.0306"
## [402,]	"402"	"Rolofylline"	"Ibrutinib"	"-3.9131"
## [403,]	"403"	"Maraviroc"	"Ibrutinib"	"-5.8541"
## [404,]	"404"	"LY-320135"	"Ibrutinib"	"-5.4082"
## [405,]	"405"	"ACPA"	"Ibrutinib"	"-8.9368"
## [406,]	"406"	"MK-886"	"Ibrutinib"	"-0.0876"
## [407,]	"407"	"Veliflapon"	"Ibrutinib"	"-5.5199"
## [408,]	"408"	"Licofelone"	"Ibrutinib"	"-6.338"
## [409,]	"409"	"Zileuton"	"Ibrutinib"	"1.0959"

## [410,]	"410"	"NCGC00185053"	"Ibrutinib"	"1.8018"
## [411,]	"411"	"Celecoxib"	"Ibrutinib"	"0.628"
## [412,]	"412"	"Pravadoline"	"Ibrutinib"	"-2.4313"
## [413,]	"413"	"PF-3845"	"Ibrutinib"	"-5.4409"
## [414,]	"414"	"Fluvastatin"	"Ibrutinib"	"-1.3686"
## [415,]	"415"	"Simvastatin"	"Ibrutinib"	"-6.5355"
## [416,]	"416"	"Dalcetrapib"	"Ibrutinib"	"1.0539"
## [417,]	"417"	"JK 184"	"Ibrutinib"	"4.3315"
## [418,]	"418"	"NCGC00037850"	"Ibrutinib"	"-2.3021"
## [419,]	"419"	"CAY10581"	"Ibrutinib"	"2.8465"
## [420,]	"420"	"EBPC"	"Ibrutinib"	"-3.3191"
## [421,]	"421"	"Piraxostat"	"Ibrutinib"	"5.9882"
## [422,]	"422"	"JZL-184"	"Ibrutinib"	"-2.9316"
## [423,]	"423"	"GW 4869"	"Ibrutinib"	"-5.0537"
## [424,]	"424"	"Ezatiostat"	"Ibrutinib"	"0.3211"
## [425,]	"425"	"Vapiprost hydrochloride"	"Ibrutinib"	"-0.0533"
## [426,]	"426"	"Ezetimibe"	"Ibrutinib"	"-0.8794"
## [427,]	"427"	"GSK-1995010"	"Ibrutinib"	"0.9241"
## [428,]	"428"	"FASN BI"	"Ibrutinib"	"1.6052"
## [429,]	"429"	"GSK837149A"	"Ibrutinib"	"6.0655"
## [430,]	"430"	"FASN MRK"	"Ibrutinib"	"-0.0071"
## [431,]	"431"	"Daporinad"	"Ibrutinib"	"-2.8081"
## [432,]	"432"	"cPEPCK inhibitor"	"Ibrutinib"	"0.9414"
## [433,]	"433"	"GLS968"	"Ibrutinib"	"-0.0824"
## [434,]	"434"	"IPFK2"	"Ibrutinib"	"4.9532"
## [435,]	"435"	"NCGC00186528"	"Ibrutinib"	"-3.1249"
## [436,]	"436"	"NCGC00185916"	"Ibrutinib"	"1.8846"
## [437,]	"437"	"AZD-7545"	"Ibrutinib"	"-1.9476"
## [438,]	"438"	"PDHK RIKEN"	"Ibrutinib"	"-0.6746"
## [439,]	"439"	"NCGC00262689"	"Ibrutinib"	"-0.8472"
## [440,]	"440"	"IDH-001"	"Ibrutinib"	"-1.5858"
## [441,]	"441"	"AR-C155858"	"Ibrutinib"	"5.8313"
## [442,]	"442"	"CAP-232"	"Ibrutinib"	"0.5516"
## [443,]	"443"	"NCGC00238624"	"Ibrutinib"	"0.5642"
## [444,]	"444"	"ACC1 BMS"	"Ibrutinib"	"-2.1855"
## [445,]	"445"	"Ibutamoren mesilate"	"Ibrutinib"	"-1.0902"
## [446,]	"446"	"ML 141"	"Ibrutinib"	"3.1015"
## [447,]	"447"	"QS11"	"Ibrutinib"	"-5.7021"
## [448,]	"448"	"Gavestinel sodium"	"Ibrutinib"	"-0.5013"
## [449,]	"449"	"Eliprodil"	"Ibrutinib"	"0.7497"
## [450,]	"450"	"Caroverine hydrochloride"	"Ibrutinib"	"2.8002"
## [451,]	"451"	"GYKI-53655"	"Ibrutinib"	"5.3415"
## [452,]	"452"	"Dapagliflozin"	"Ibrutinib"	"-0.2877"
## [453,]	"453"	"GSK-4112"	"Ibrutinib"	"-1.966"
## [454,]	"454"	"Sepantronium bromide"	"Ibrutinib"	"1.723"
## [455,]	"455"	"BIBR 1532"	"Ibrutinib"	"0.8965"
## [456,]	"456"	"ITX3"	"Ibrutinib"	"4.5565"
## [457,]	"457"	"Salinomycin"	"Ibrutinib"	"6.1848"
## [458,]	"458"	"Efavirenz"	"Ibrutinib"	"-3.7459"
## [459,]	"459"	"Ivachtin"	"Ibrutinib"	"-0.7658"
## [460,]	"460"	"PAC-1"	"Ibrutinib"	"2.345"
## [461,]	"461"	"Necrostatin-1"	"Ibrutinib"	"5.0675"
## [462,]	"462"	"NCGC00262398"	"Ibrutinib"	"-0.31"

```
## [463,] "463"      "Tiplasinin"           "Ibrutinib" "-2.0905"
## [464,] "464"      "ASR-isobudimer-SO2Ph-4-CH2OC(=O)NMe2" "Ibrutinib" "0.0207"
## [465,] "465"      "BTM-2C-dimer ketone"  "Ibrutinib" "11.1432"
## [466,] "466"      "BTM-2C-dimer allyl oxime" "Ibrutinib" "1.0771"
```

### Compiling dynamic reporting file

```
#library(knitr)
#library("tools")
#texi2pdf(knit("Delta_calculation_dynamic_report.Rnw"))
```