

Table S1. Unique drugs of each cluster from rank3

Drugs in cluster1	Drugs in cluster2	Drugs in cluster3
15-deltaprostaglandinJ2	deferoxamine	alpha-estradiol
17-allylamino-geldanamycin	fisetin	butein
celecoxib	genistein	butirosin
coppersulfate	Valproic acid	dimethyloxalylglycine
diclofenac	4,5-dianilinophthalimide	docosahexaenoicacidethylester
fasudil		estradiol
imatinib		fulvestrant
indometacin		mercaptopurine
LY-294002		monastrol
monorden		resveratrol
novobiocin		splitomicin
pirinixicacid		U0125
rofecoxib		HNMPA-(AM)3
rosiglitazone		
sodiumphenylbutyrate		
tetraethylenepentamine		
tretinoin		
trichostatinA		
trogglitazone		
TTNPB		
Valproic acid		

Table S2 drug interaction in cluster2 in page9

	alpha-estradiol	diclofenac	estradiol	fulvestrant	genistein	imatinib	mercaptopurine
alpha-estradiol(ethinylestradiol)							
diclofenac	–						
estradiol	+	–					
fulvestrant	+	–					
genistein	–		–				
imatinib	–	–	–		–		
mercaptopurine		–	–			+	
resveratrol							+
rosiglitazone		–			–	–	
tetraethylenepentamine(colestipol)		–	–				
tretinoin		+	–			+	
valproicacid	+	–	+	–	–	+	–