Supplemental data

S1: Relationship between inhibited reactions and predecessors of C00022 in N_1 and N_2 in Dataset 1.

Node	Predecessors		IP-FVS1	IP-FVS2	IP-EM
R00200	N_1	N_2	-	-	-
R00703	N_1	N_2	-	-	-
R05605	N_1	-	-	-	ko
R04779	-	-	-	ko	ko
R01541	-	-	-	ko	-
size	3	2	no solution	2	2

S2: Relationship between inhibited reactions and predecessors of C00074 in N_1 and N_2 in Dataset 1.

Node	Predecessors		IP-FVS1	IP-FVS2	IP-EM
R00658	N_1	N_2	-	-	-
R04779	-	-	-	ko	ko
R01541	-	-	-	ko	-
size	1	1	no solution	2	1

S3: Relationship between knocked-out nodes and predecessors of all the above 5 compounds are targets in Data1

Node	Predecessors		IP-FVS1	IP-FVS2	IP-EM
R00200	N_1	N_2	-	-	-
R00658	N_1	N_2	-	-	-
R00703	N_1	N_2	-	-	-
R00710	N_1	N_2	-	-	-
R05605	N_1	-	-	-	ko
R00351	-	N_2	-	-	-
R04779	-	-	-	-	ko
size	5	5	no solution	no solution	2

S4: Relationship among inhibited reactions and predecessors of C00022 in Dataset 2

Node	Predecessors		IP-FVS1	IP-FVS2	IP-EM
R00200	N_1	N_2	ko	ko	-
R00220	N_1	N_2	-	-	-
R00214	N_1	-	ko	ko	ko
R00216	N_1	-	ko	ko	ko
R01196	N_1	-	ko	ko	-
R05605	N_1	-	ko	ko	ko
R00586	-	-	ko	-	-
R00945	-	-	ko	-	-
R01512	-	-	-	-	ko
size	6	2	7	5	4

S5: Relationship among inhibited reactions and predecessors of C00024 in Dataset 2

Node	Predecessors		IP-FVS1	IP-FVS2	IP-EM
R00230	N_1	N_2	ko	-	-
R00238	N_1	-	ko	-	-
R01196	N_1	-	ko	ko	ko
R00209	-	N_2	-	-	-
R00351	-	N_2	-	-	-
R00352	-	N_2	-	-	-
size	3	4	3	1	1

S6: Relationship among inhibited reactions and predecessors of C00033 in Dataset 2

Node	Predecessors		IP-FVS1	IP-FVS2	IP-EM
R00315	N_1	N_2	-	-	-
R01196	-	-	-	ko	ko
size	1	1	no solution	1	1

S7: Relationship among inhibited reactions and predecessors of C00036 in Dataset 2

Node	Predecessors		IP-FVS1	IP-FVS2	IP-EM
R00345	N_1	N_2	-	-	ko
R00355	N_1	-	-	-	-
R00351	-	N_2	-	-	-
R00352	-	N_2	-	-	-
size	2	3	no solution	no solution	1

S8: Relationship among inhibited reactions and predecessors of C00074 in Dataset 2

Node	Predecessors		IP-FVS1	IP-FVS2	IP-EM
R00658	N_1	N_2	-	-	-
R00199	N_1	-	-	-	ko
R00206	N_1	-	-	-	ko
R01015	-	-	-	-	ko
R01829	-	-	-	-	ko
R04533	-	-	-	-	ko
size	3	1	no solution	no solution	5

S9: Relationship among inhibited reactions and predecessors of all the above 5 compounds are targets in Dataset 2

Node	Predecessors		IP-FVS1	IP-FVS2	IP-EM
R00200	N_1	N_2	-	-	-
R00220	N_1	N_2	-	-	-
R00230	N_1	N_2	-	-	-
R00315	N_1	N_2	-	-	-
R00345	N_1	N_2	-	-	-
R00658	N_1	N_2	-	-	-
R00199	N_1	-	-	-	-
R00206	N_1	-	-	-	-
R00214	N_1	-	-	-	ko
R00216	N_1	-	-	-	ko
R00238	N_1	-	-	-	-
R00355	N_1	-	-	-	-
R01196	N_1	-	-	-	-
R05605	N_1	-	-	-	ko
R00209	-	N_2	-	-	-
R00351	-	N_2	-	-	-
R00352	-	N_2	-	-	-
R01512	-	-	-	-	ko
size	14	9	no solution	no solution	4

S10: Relationship among inhibited reactions and predecessors of C00022 in Dataset 3

Node	Predecessors		IP-FVS1	IP-FVS1-approx(10)	IP-FVS2	IP-FVS2-approx(10)
R00200	N_1	N_2	ko	ko	-	ko
R00212	N_1	N_2	ko	ko	-	-
R00220	N_1	N_2	ko	ko	-	-
R00703	N_1	N_2	ko	ko	-	-
R00782	N_1	N_2	ko	ko	-	-
R02320	N_1	N_2	ko	ko	-	-
R05636	N_1	N_2	ko	ko	-	-
R00214	N_1	-	ko	ko	-	-
R00470	N_1	-	ko	ko	-	ko
R00704	N_1	-	ko	ko	-	-
R03105	N_1	-	-	ko	-	-
R05605	N_1	-	ko	ko	-	-
R00258	-	N_2	-	-	-	-
R00896	-	-	ko	-	-	-
R01220	-	-	-	-	-	ko
size	12	8	12	12	NA	3

S11: Relationship among inhibited reactions and predecessors of C00024 in Dataset 3

Node	Predecessors		IP-FVS1	IP-FVS1-approx(10)	IP-FVS2	IP-FVS2-approx(10)
R00212	N_1	N_2	ko	ko	-	ko
R00228	N_1	N_2	ko	ko	-	-
R00230	N_1	N_2	ko	ko	-	-
R05351	N_1	N_2	ko	ko	-	ko
R00238	N_1	-	ko	ko	-	-
R01177	N_1	-	ko	ko	-	-
R04386	N_1	-	ko	ko	-	-
R00351	-	N_2	-	-	-	-
R03026	-	-	-	-	-	ko
size	7	5	7	7	NA	3

S12: Relationship among inhibited reactions and predecessors of C00033 in Dataset 3

Node	Predecessors		IP-FVS1	IP-FVS-1-approx(10)	IP-FVS2	IP-FVS2-approx(10)
R00315	N_1	N_2	-	-	-	-
R00317	N_1	N_2	-	-	-	-
R00710	N_1	N_2	-	-	-	-
R00212	-	-	-	-	-	ko
R00238	-	-	-	-	-	ko
R05351	-	-	-	-	-	ko
size	3	3	no solution	no solution	NA	3

S13: Relationship among inhibited reactions and predecessors of C00036 in Dataset 3

Node	Predecessors		IP-FVS1	IP-FVS1-approx(10)	IP-FVS2	IP-FVS2-approx(10)
R00345	N_1	N_2	ko	ko	-	ko
R00355	N_1	N_2	ko	ko	-	-
R00357	N_1	N_2	-	ko	-	-
R00351	-	N_2	-	-	-	-
R00483	-	-	ko	-	-	-
R00485	-	-	-	-	-	ko
size	3	4	3	3	NA	2