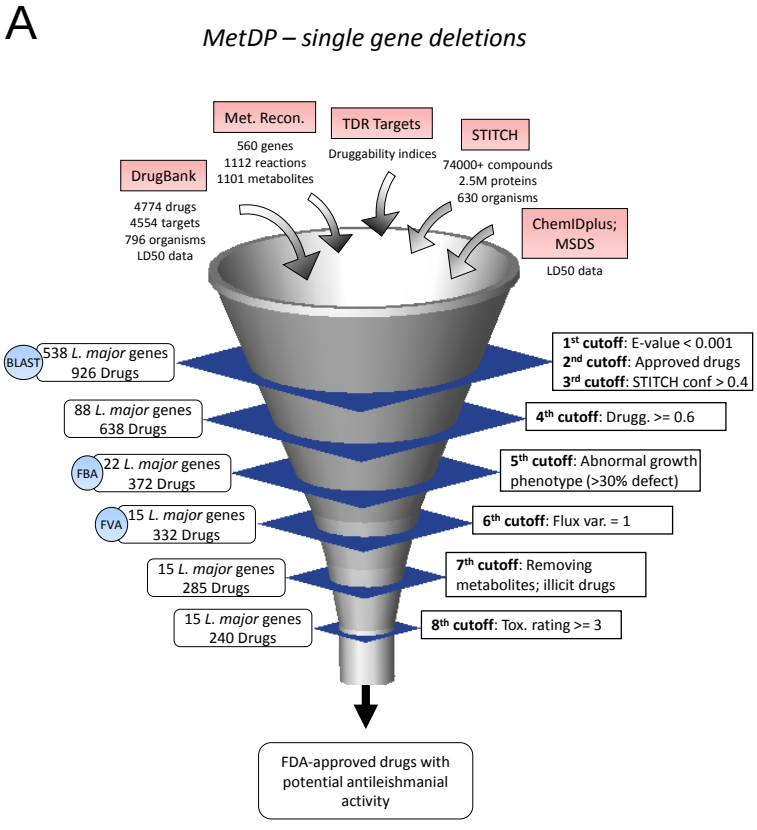
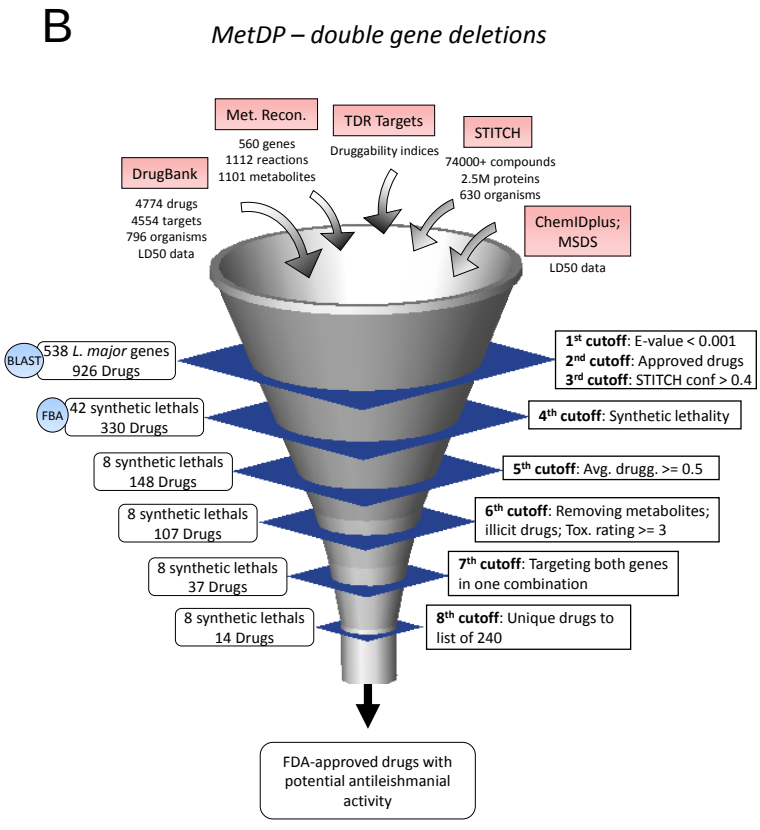

A
MetDP – single gene deletions
Met. Recon.
560 genes
1112 reactions
1101 metabolites
TDR Targets
Druggability indices
STITCH
74000+ compounds
2.5M proteins
630 organisms
DrugBank
4774 drugs
4554 targets
796 organisms
LD50 data
ChemIDplus; MSDS
LD50 data
BLAST
538 L. major genes
926 Drugs
88 L. major genes
638 Drugs
FBA
22 L. major genes
372 Drugs
FVA
15 L. major genes
332 Drugs
15 L. major genes
285 Drugs
15 L. major genes
240 Drugs
1st cutoff: E-value < 0.001
2nd cutoff: Approved drugs
3rd cutoff: STITCH conf > 0.4
4th cutoff: Drugg. >= 0.6
5th cutoff: Abnormal growth phenotype (>30% defect)
6th cutoff: Flux var. = 1
7th cutoff: Removing metabolites; illicit drugs
8th cutoff: Tox. rating >= 3
FDA-approved drugs with potential antileishmanial activity


B
MetDP – double gene deletions
Met. Recon.
560 genes
1112 reactions
1101 metabolites
TDR Targets
Druggability indices
STITCH
74000+ compounds
2.5M proteins
630 organisms
DrugBank
4774 drugs
4554 targets
796 organisms
LD50 data
ChemIDplus; MSDS
LD50 data
BLAST
538 L. major genes
926 Drugs
FBA
42 synthetic lethals
330 Drugs
8 synthetic lethals
148 Drugs
8 synthetic lethals
107 Drugs
8 synthetic lethals
37 Drugs
8 synthetic lethals
14 Drugs
1st cutoff: E-value < 0.001
2nd cutoff: Approved drugs
3rd cutoff: STITCH conf > 0.4
4th cutoff: Synthetic lethality
5th cutoff: Avg. drugg. >= 0.5
6th cutoff: Removing metabolites; illicit drugs; Tox. rating >= 3
7th cutoff: Targeting both genes in one combination
8th cutoff: Unique drugs to list of 240
FDA-approved drugs with potential antileishmanial activity