

Generalized Read-Across (GenRA): A Workflow Implemented into the EPA CompTox Chemicals Dashboard

EPA United States Environmental Protection Agency

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Fluconazole

86386-73-4 | DTXSID3020627
Searched by DSSTox Substance Id.

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV FATE/TRANSPORT

HAZARD

ADME

EXPOSURE

BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

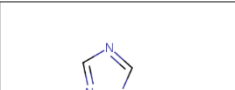
RELATED SUBSTANCES

SYNONYMS

LITERATURE

LINKS

COMMENTS



Wikipedia

Fluconazole is an antifungal medication used for a number of fungal infections. This includes candidiasis, blastomycosis, coccidioidomycosis, cryptococcosis, histoplasmosis, dermatophytoses, and pharyngitis vesicosa. It is also used to prevent candidiasis in those who are at high risk such as following organ transplantation, low birth weight babies, and those with low blood neutrophil counts. It is given either by mouth or by injection into a vein.

Common side effects include vomiting.

[Read more](#)

Intrinsic Properties

- Molecular Formula: $C_{12}H_8F_2N_4O$ [Mol File](#) [Find All Chemicals](#)
- Average Mass: 306.277 g/mol [Isotopic Mass Distribution](#)
- Monoisotopic Mass: 306.104065 g/mol

Structural Identifiers

Linked Substances

Presence in Lists

Record information

Quality Control Notes

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Step One: Analog Identification and Evaluation

Neighbors by: Chem Morgan Fgprats Filter by: In vivo data

of Analogs: 10 Find

Chemical Name	Morgan	Fgprats	In vivo data
Telaprevir			
Flutazone			
Cyproheptadine			
Pyrazole m.			
Mycophenolate			
Ergonovine			
Telenorin			
Metoprolol			
Isoproterenol			
Bromocriptine			

doi:10.14573/altex.1811292s

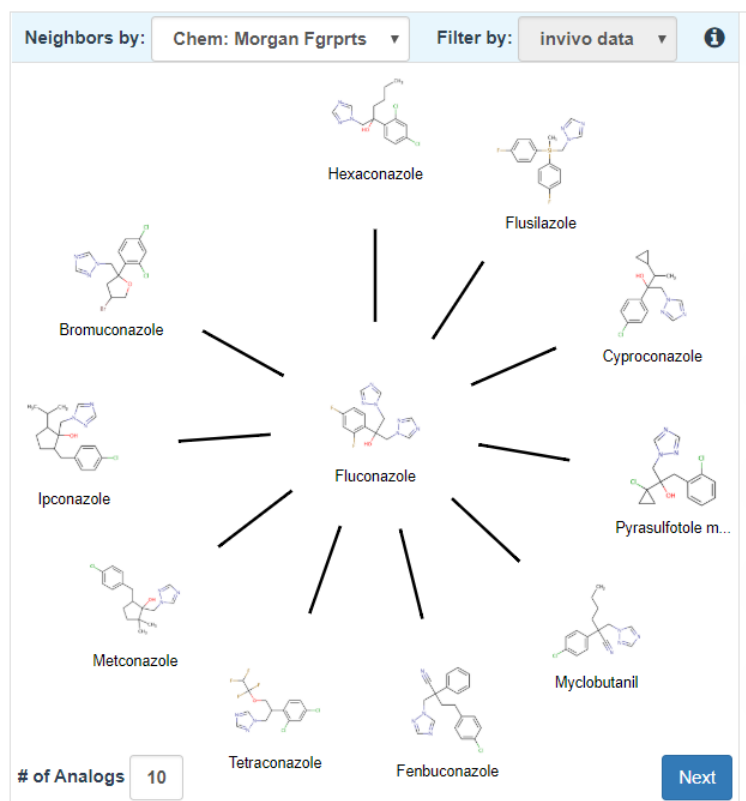


Fig. S3: Analogue identification view in GenRA

Summary Data Gap Analysis

	bio tx21	bio txct	chm ct	tox txrf
Fluconazole	3	714	15	0
Hexaconazole	43	819	18	345
Flusilazole	28	819	9	345
Cyproconazole	14	819	16	408
Pyrasulfotole metabolite ...	0	0	18	234
Myclobutanil	15	818	15	345
Fenbuconazole	34	819	17	345
Tetraconazole	35	819	20	345
Metconazole	35	215	15	82
Ipconazole	46	232	16	180
Bromuconazole	24	277	13	345

Fig. S4: Summary data gap analysis view

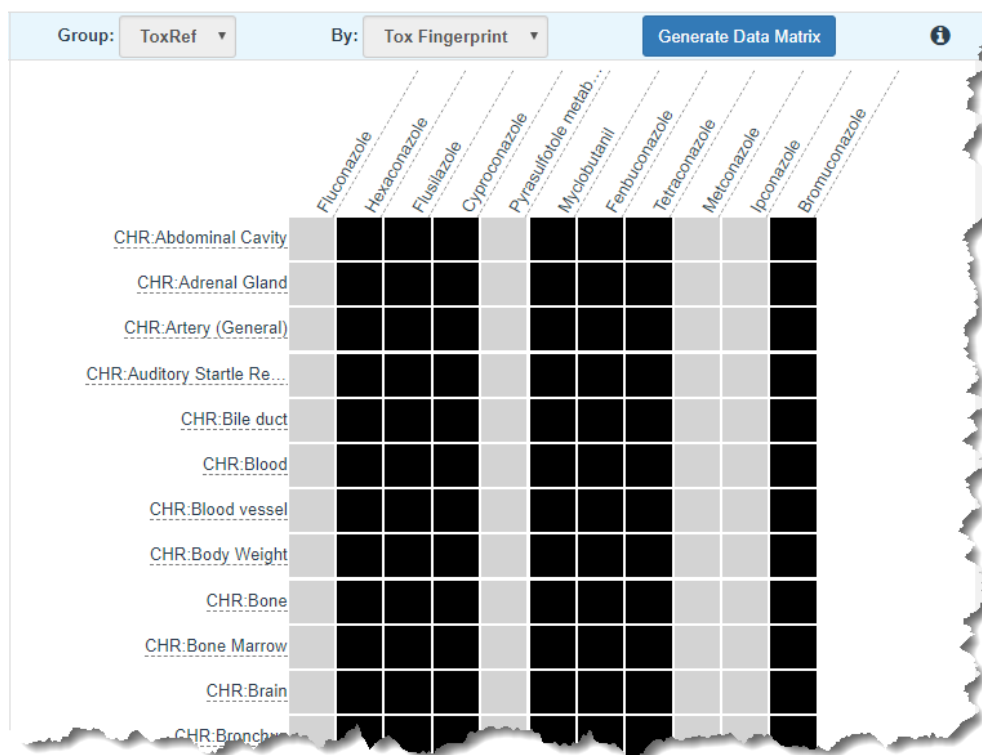


Fig. S5: Summary data gap matrix view

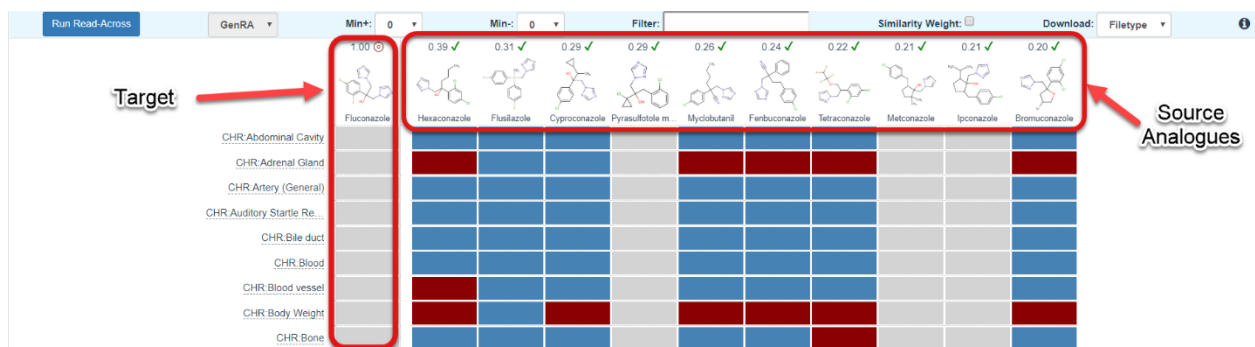


Fig. S6: Data matrix view

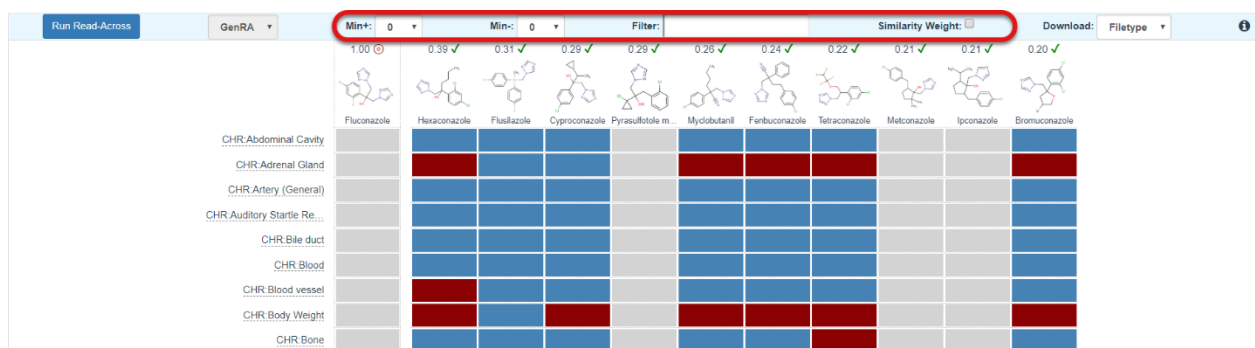


Fig. S7: Filtering options in the GenRA data matrix view

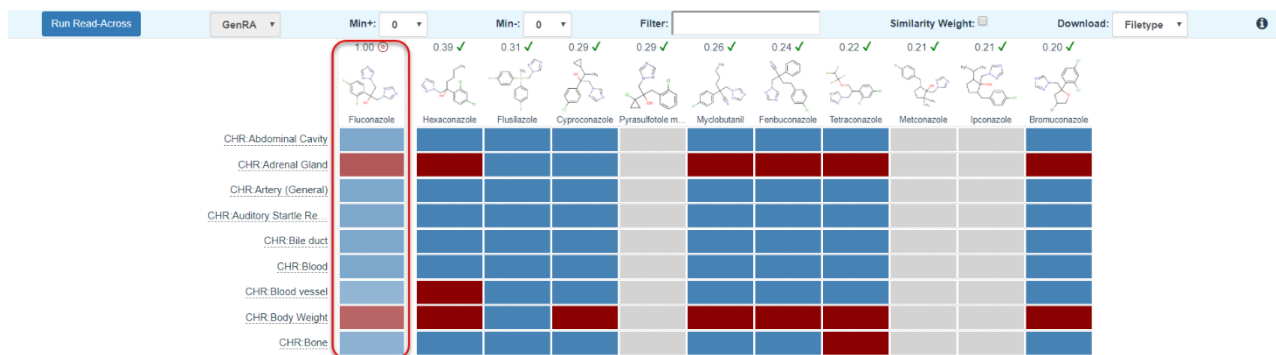


Fig. S8: GenRA predictions

cls	target	analog	analog	analog	analog	analog	analog	analog	analog	analog	analog	analog
label	Fluconazole	Hexaconazole	Flusilazole	Cyproconazole	Pyrasulfotole metabolite (SXX	Myclobutanil	Fenbuconazole	Tetraconazole	Metconazole	Ipconazole	Bromuconazole	
dsstox_cid	DTXCID10627	DTXCID2014653	DTXCID704235	DTXCID8012601	DTXCID1024338	DTXCID304315	DTXCID6012548	DTXCID6014956	DTXCID2014497	DTXCID5014674	DTXCID701253	
casrn	86386-73-4	79983-71-4	85509-19-9	94361-06-5	120983-64-4	88671-89-0	114369-43-6	112281-77-3	125116-23-6	125225-28-7	116255-48-2	
jaccard	1	0.38888889	0.3125	0.289473684	0.285714286	0.256410256	0.238095238	0.223529412	0.211764706	0.206896552	0.19767441	
CHR:Abdominal Cavity	GenRA Neg Act=0 (0) AUC=0	no_effect 4.700	no_effect	no_effect	no_data	no_effect 70.200	no_effect 30.000	no_effect 27.700	no_data	no_data	no_effect 25.000	
CHR:Adrenal Gland	Act=1 (0.684)	mg/kg/day	no_effect	no_effect	no_data	mg/kg/day	mg/kg/day	mg/kg/day	no_data	no_data	mg/kg/day	
CHR:Artery (General)	GenRA Neg Act=0 (0) AUC=0	no_effect	no_effect	no_effect	no_data	no_effect	no_effect	no_effect	no_data	no_data	no_effect	
CHR:Auditory Startle Reflex	GenRA Neg Act=0 (0) AUC=0	no_effect	no_effect	no_effect	no_data	no_effect	no_effect	no_effect	no_data	no_data	no_effect	
CHR:Bile duct	GenRA Neg Act=0 (0) AUC=0	no_effect	no_effect	no_effect	no_data	no_effect	no_effect	no_effect	no_data	no_data	no_effect	
CHR:Blood	GenRA Neg Act=0 (0) AUC=0	no_effect 50.000	no_effect	no_effect	no_data	no_effect	no_effect	no_effect	no_data	no_data	no_effect	
CHR:Blood vessel	GenRA Neg Act=0 (0.204)	mg/kg/day	no_effect	no_effect	no_data	no_effect	no_effect	no_effect	no_data	no_data	no_effect	
CHR:Body Weight	GenRA Pos Act=1 (0.836)	6.100 mg/kg/day	3.200	mg/kg/day	no_data	6.250 mg/kg/day	3.750 mg/kg/day	12.970 mg/kg/day	no_data	no_data	55.600 mg/kg/day	
CHR:Bone	GenRA Neg Act=0 (0.117)	no_effect	no_effect	no_effect	no_data	no_effect	no_effect	27.700 mg/kg/day	no_data	no_data	no_effect	
CHR:Bone Marrow	GenRA Neg Act=0 (0) AUC=0	no_effect	no_effect	no_effect	no_data	no_effect	no_effect	no_effect	no_data	no_data	no_effect	
CHR:Brain	GenRA Neg Act=0 (0.355)	no_effect	no_effect	no_effect	no_data	393.500 mg/kg/day	59.000 mg/kg/day	59.000 mg/kg/day	no_data	no_data	134.500 mg/kg/day	
CHR:Bronchus	GenRA Neg Act=0 (0) AUC=0	no_effect	no_effect	no_effect	no_data	no_effect	no_effect	no_effect	no_data	no_data	no_effect	
CHR:Cervix	GenRA Neg Act=0 (0) AUC=0	no_effect	no_effect	no_effect	no_data	no_effect	no_effect	no_effect	no_data	no_data	no_effect	
CHR:Clinical Chemistry	GenRA Pos Act=1 (1) AUC=0	4.700 mg/kg/day	13.000	2.730 mg/kg/day	no_data	10.060 mg/kg/day	30.000 mg/kg/day	12.970 mg/kg/day	no_data	no_data	0.880 mg/kg/day	

Fig. S9: Partial view of export file of predictions