Helman et al.:

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

Supplementary Data

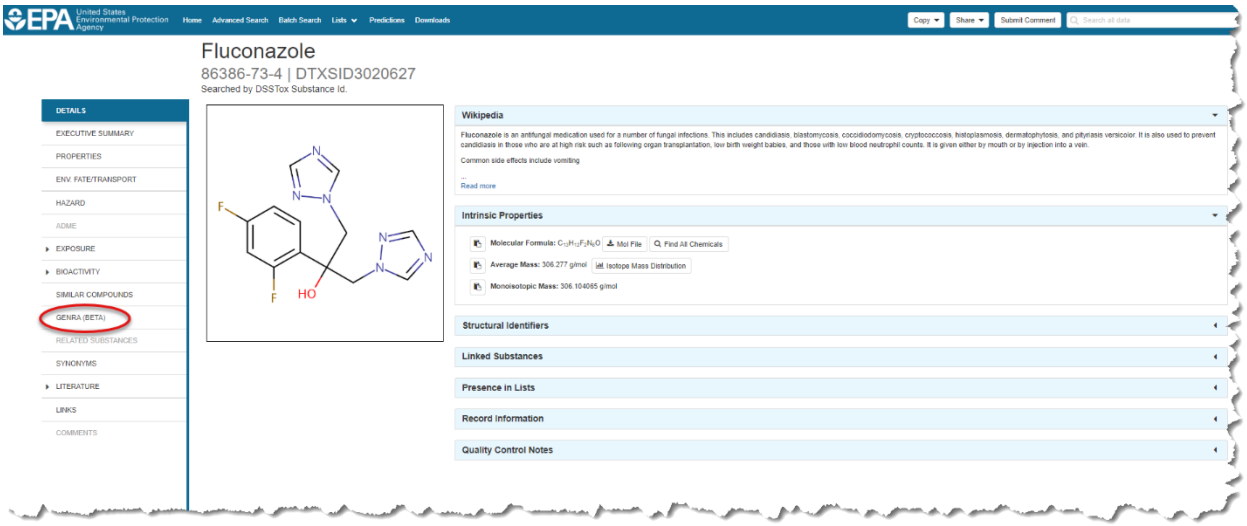

Fig. S1: Chemical results page for example substance fluconazole

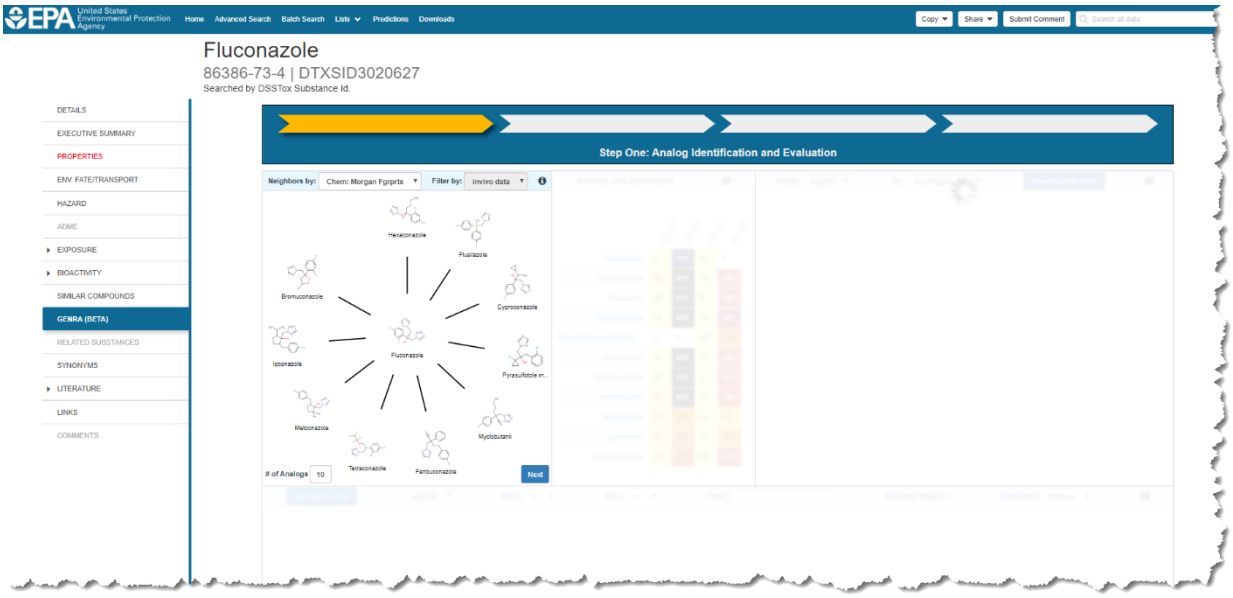

Fig. S2: Working interface of GenRA

doi:10.14573/altex.1811292s

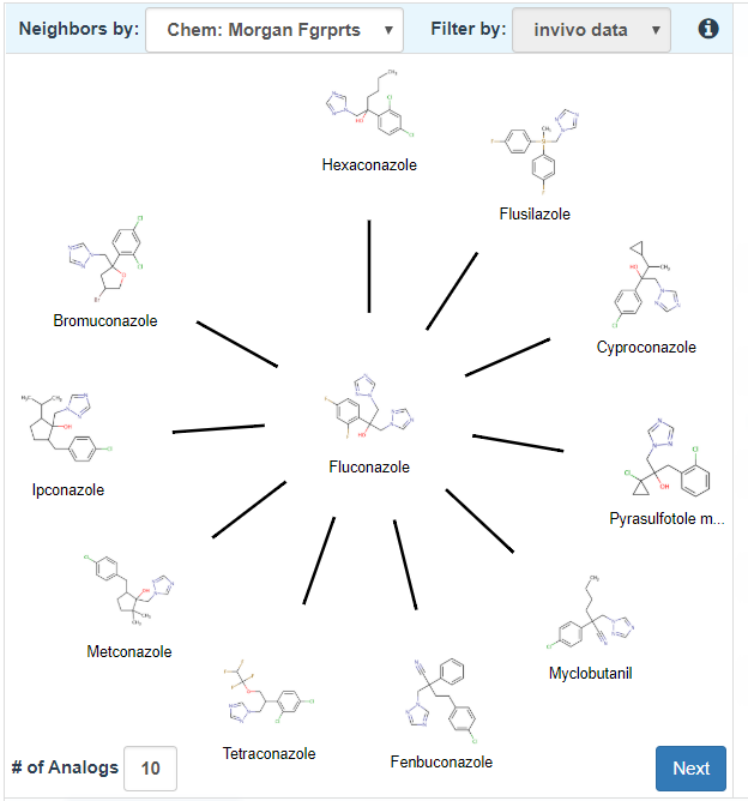

Fig. S3: Analogue identification view in GenRA

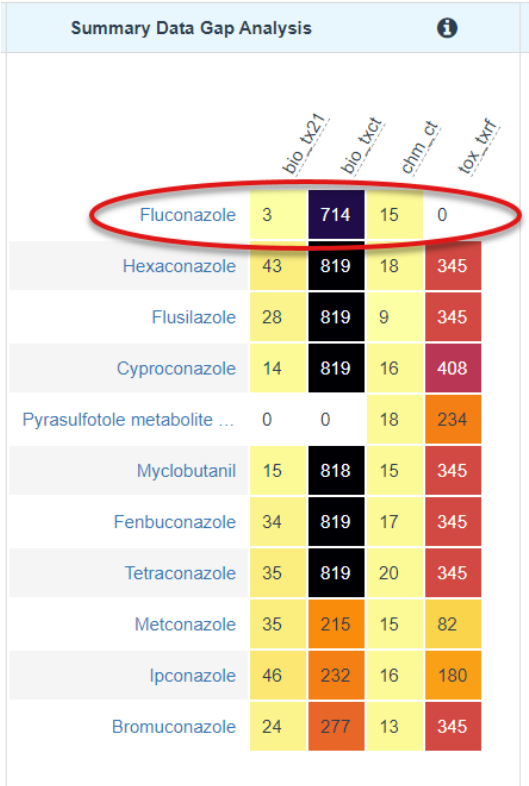

Fig. S4: Summary data gap analysis view

Fig. S5: Summary data gap matrix view

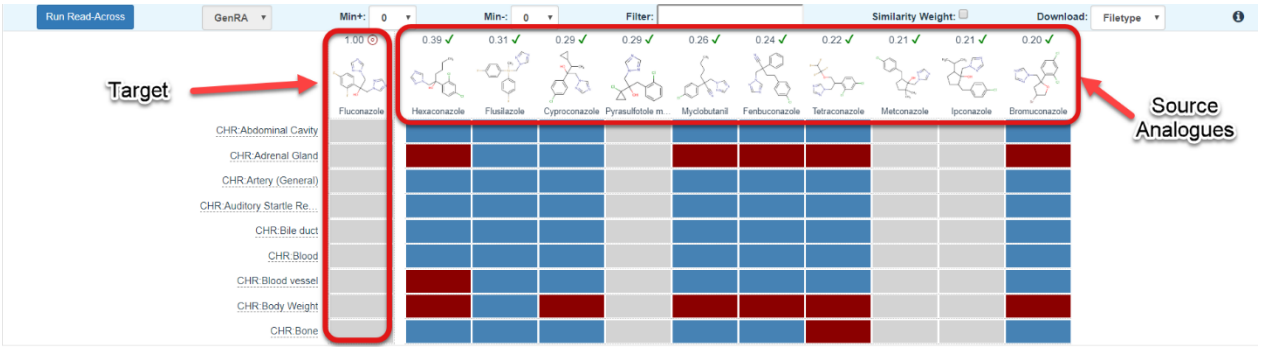

Fig. S6: Data matrix view

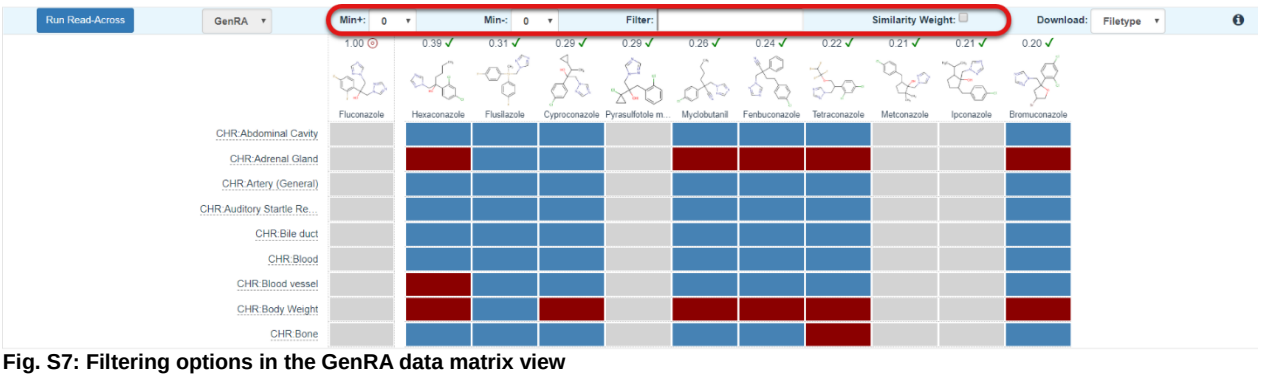

Fig. S7: Filtering options in the GenRA data matrix view

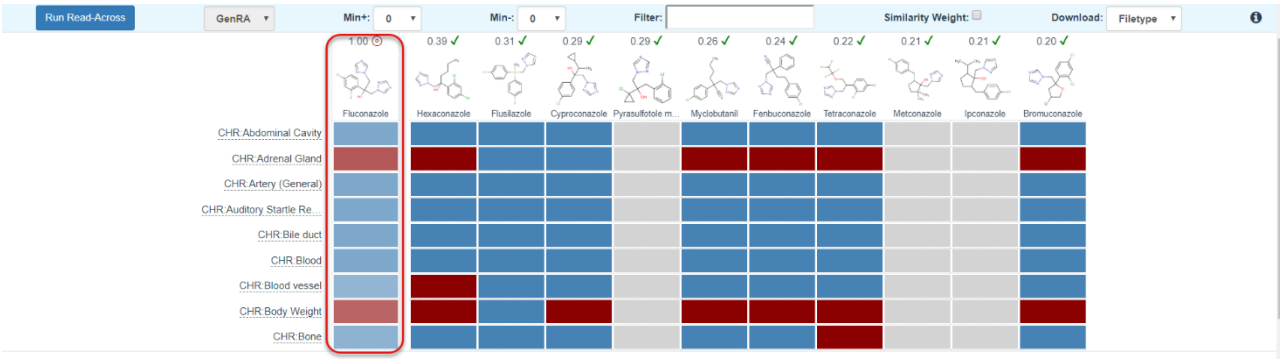

Fig. S8: GenRA predictions

cls	target	analog	analog	analog	analog	analog	analog	analog	analog	analog	analog
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	0.388888889	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	no_effect	no_effect	no_data	no_effect	no_effect	no_effect	no_data	no_data	no_effect
CHR:Adrenal Gland	GenRA Pos Act=1 (0.684)	4.700 mg/kg/day	no_effect	no_effect	no_data	70.200 mg/kg/day	30.000 mg/kg/day	27.700 mg/kg/day	no_data	no_data	25.000 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	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)	50.000 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	no_effect	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	no_effect	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)	4.700	13.000	2.730		10.060	30.000	12.970			0.880

Fig. S9: Partial view of export file of predictions