

Network-based Drug Ranking and Repositioning with respect to DrugBank Therapeutic Categories: Supplemental Material

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The supplemental material reports additional results, tables and figures that could not be included, but that are referenced by the main paper.

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TABLE 1

DrugBank Therapeutic Categories (TC) with more than 15 drugs considered in the experiments. The first column reports the abbreviated name, the second the full DrugBank name and the third the cardinality of the TC.

Therapeutic categories with more than 15 drugs		
Abbreviated name	Full DrugBank name name	Card.
Adren.A.	Adrenergic_Agents	26
Adren.In.	Adrenergic_Uptake_Inhibitors	20
Adren.a.	Strategic_alpha.Agonists	23
Adren.b.	Adrenergic_beta.Antagonists	25
Analges.	Analgesics	40
Analg.Op.	Analgesics_Opioid	24
Anti.Aller.	Anti.Allergic_Agents	35
Anti.Arrh.	Anti.Arrhythmia_Agents	42
Anti.Bact.	Anti.Bacterial_Agents	103
Anti.HIV	Anti.HIV_Agents	22
Anti.Inf.A.	Anti.Infective_Agents	29
Anti.Inf.	Anti.Infectives	19
Anti.Ulcer	Anti.Ulcer_Agents	19
Anti.anx.	Anti.anxiety_Agents	35
Anti.infl.	Anti.inflammatory_Agents	49
Antiarr.A.	Antiarrhythmic_Agents	29
Anticonv.	Anticonvulsants	46
Antidysk.	Antidyskinetics	23
Antiemetics	Antiemetics	34
Antifungal	Antifungal_Agents	22
Antihist.	Antihistamines	24
Antihypert.	Antihypertensive_Agents	105
Antimetab.	Antimetabolites	26
Antineopl.	Antineoplastic_Agents	86
Antineopl.H.	Antineoplastic_Agents_Hormonal	18
Antipark.	Antiparkinson_Agents	27
Antipsyc.A.	Antipsychotic_Agents	39
Antipsyc.	Antipsychotics	27
Antiviral	Antiviral_Agents	25
Bronchodil.	Bronchodilator_Agents	33
Ca.Ch.Block.	Calcium_Channel_Blockers	22
Cephalosp.	Cephalosporins	30
Cycloox.Inh.	Cyclooxygenase_Inhibitors	24
Dietary.sup.	Dietary_supplement	47
Diuretics	Diuretics	23
Dopam..Ant.	Dopamine_Antagonists	29
Enzyme.Inh.	Enzyme_Inhibitors	64
GABA.Mod.	GABA_Modulators	26
Glucocort.	Glucocorticoids	21
Hist.H1.Ant.	Histamine_H1_Antagonists	28
Hypnot.Sed.	Hypnotics_and_Sedatives	41
Hypoglyc.	Hypoglycemic_Agents	22
Immunosup.	Immunosuppressive_Agents	20
Micronutr.	Micronutrient	45
Musc.Ant.	Muscarinic_Antagonists	23
Narcotics	Narcotics	22
Penicillins	Penicillins	20
Sympathol.	Sympatholytics	24
Sympathomim.	Sympathomimetics	32
Vasoconstr.	Vasoconstrictor_Agents	25
Vasodilator	Vasodilator_Agents	55

TABLE 2

The 10 best and the 10 worst AUC values of DrugBank Therapeutic Categories achieved by the S_{AV} score with 3 steps random walk kernel. The last three columns report the precision at 10, 20 and 40 % recall.

The 10 best ranked TCs				
TC	AUC	P10R	P20R	P40R
Penicillins	0.9999	1.0000	1.0000	1.0000
Cephalosporins	0.9995	1.0000	1.0000	1.0000
Hypoglycemic_Agents	0.9990	1.0000	1.0000	1.0000
Analgesics._Opioid	0.9979	1.0000	1.0000	0.8333
Narcotics	0.9977	1.0000	1.0000	1.0000
GABA_Modulators	0.9966	1.0000	1.0000	0.9166
Cyclooxygenase_Inhibitors	0.9950	0.7500	0.8333	0.9090
Diuretics	0.9948	0.6000	0.6250	0.6923
Glucocorticoids	0.9948	1.0000	1.0000	0.7692
Dopamine_Antagonists	0.9940	1.0000	1.0000	0.7500
The 10 worst ranked TCs				
TC	AUC	P10R	P20R	P40R
Vasoconstrictor_Agents	0.8975	0.7500	0.8333	0.6666
Anti.Infectives	0.8776	0.4000	0.5000	0.3478
Antiarrhythmic_Agents	0.8719	0.1363	0.0895	0.1428
Antiviral_Agents	0.8681	1.0000	1.0000	0.5555
Antineoplastic_Agents	0.8657	0.6923	0.6428	0.4605
Antifungal_Agents	0.8616	0.7500	0.8333	0.9000
Immunosuppressive_Agents	0.8428	0.6666	0.5714	0.4705
Analgesics	0.8402	0.1600	0.2285	0.2758
Anti.Ulcer_Agents	0.8001	1.0000	1.0000	1.0000
Enzyme_Inhibitors	0.7701	0.6363	0.5909	0.4000

TABLE 3

DrugBank Therapeutic Categories (TC) with less than 15 drugs considered in the experiments. The first column reports the abbreviated name, the second the full DrugBank name and the third the cardinality of the TC.

Therapeutic categories with less than 15 drugs		
Abbr. name	Full DrugBank name	Card.
Antipyr.	Antipyretics	7
Antigl.A.	Antiglaucomic_Agents	5
Antirh.A.	Antirheumatic_Agents	7
Antitub.A.	Antitubercular_Agents	7
Ang.Rec.Ant.	Angiotensin_II_Receptor_Antagonists	5
Antithr.A.	Antithrombotic_Agents	5
Osteopor.Pr.	Osteoporosis_Prophylactic	5
Antidotes	Antidotes	5
Nasal.Dec.	Nasal_Decongestants	7
Corticost.	Corticosteroids	5
Antichol.A.	Anticholesteremic_Agents	11
Dermat.A.	Dermatologic_Agents	11
Gastroint.A.	Gastrointestinal_Agents	10
Sulfonamides	Sulfonamides	10
Antid.Tric.	Antidepressive_Agents._Tricyclic	10
Muscle.Rela.	Muscle_Relaxants._Central	11
Anti.Asth.A.	Anti.Asthmatic_Agents	9
Fibrin.A.	Fibrinolytic_Agents	11
Nootropic.A.	Nootropic_Agents	9
Phenothiaz.	Phenothiazines	11
Antibiotics	Antibiotics	14
Anticoag.	Anticoagulants	15
Antid.IIGen.	Antidepressive_Agents._Second.Generation	14
Antihypoc.A.	Antihypocalcemic_Agents	13
AntiInf.Ur.	Anti.Infective_Agents._Urinary	14
CNS.Stim.	Central_Nervous_System_Stimulants	14
Neuroprot.A.	Neuroprotective_Agents	13
NSAIAs	Nonsteroidal_Anti.inflammatory_Agents_.NSAIAs.	14
Seroton.Inh.	Serotonin_Uptake_Inhibitors	13
Ang.Enz.In.	Angiotensin.converting_Enzyme_Inhibitors	13

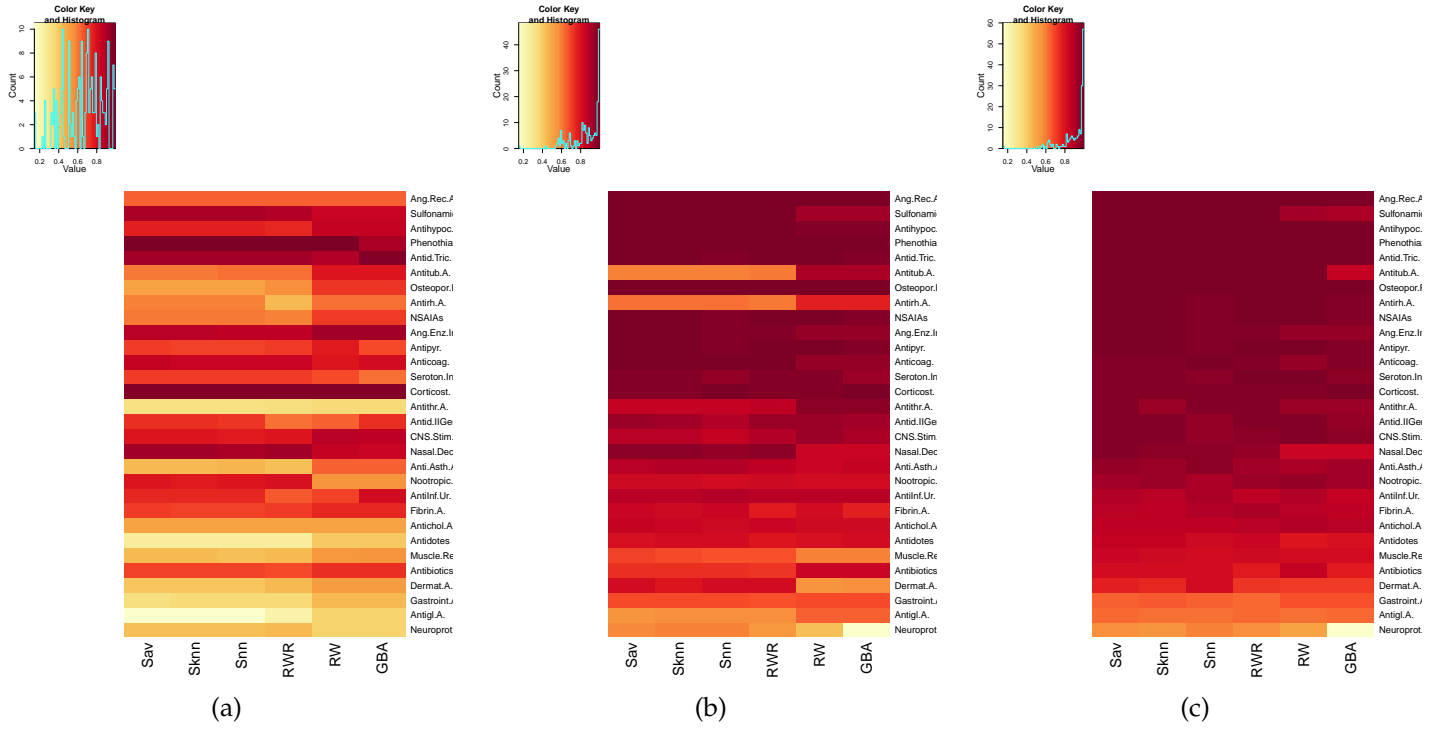


Fig. 1. TCs with less than 15 drugs: per class AUC scores compared across methods. Yellow corresponds to the lowest AUC values, while red to the highest AUC values. (a) W_1 , (b) W_2 and (c) W_3 pharmacological networks.

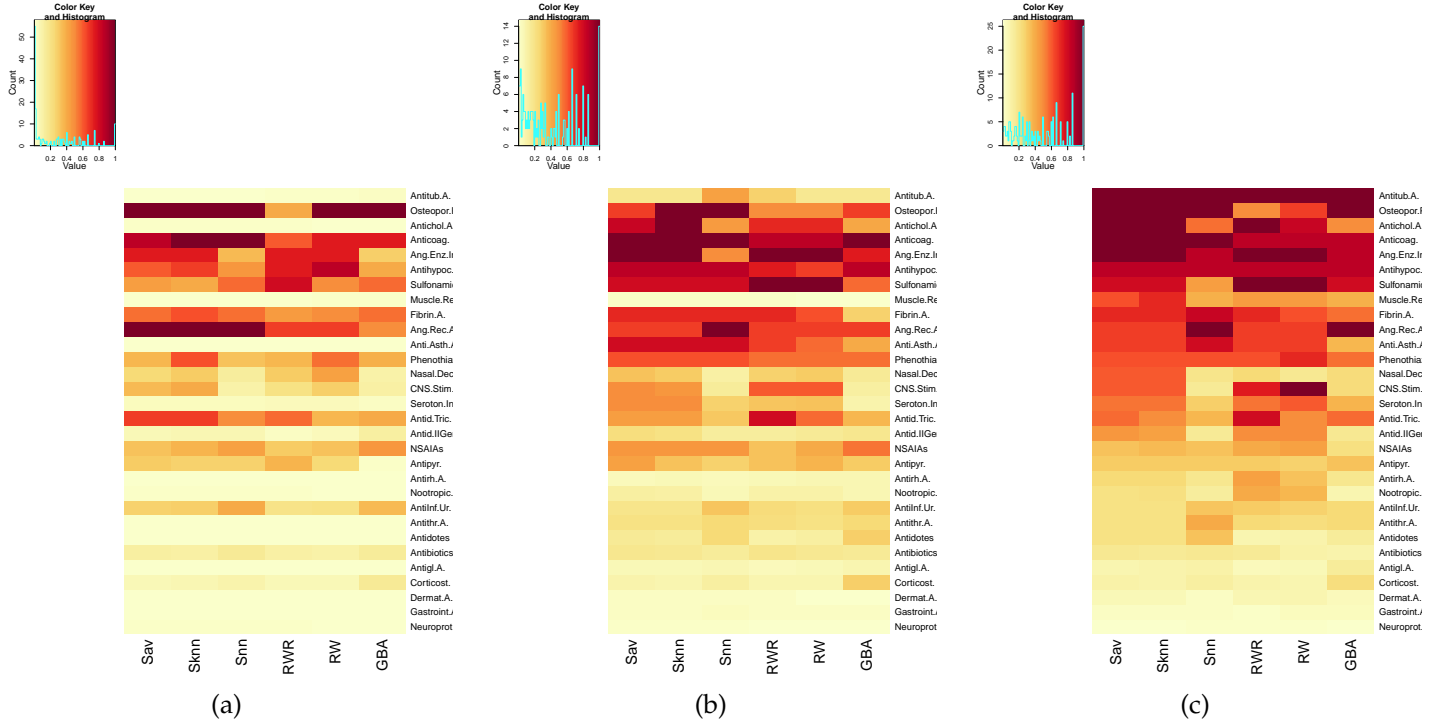


Fig. 2. TC with less than 15 drugs: per class precision at 40% recall scores compared across methods. Yellow corresponds to the lowest precision values, while red to the highest values. (a) W_1 , (b) W_2 and (c) W_3 pharmacological networks.