A COMPREHENSIVE DATABASE FOR PREDICTING METABOLISM OF XENOBIOTICS BY HUMAN MICROBIOME

Anton Kolodnitsky

Virtual, 19.09.2023

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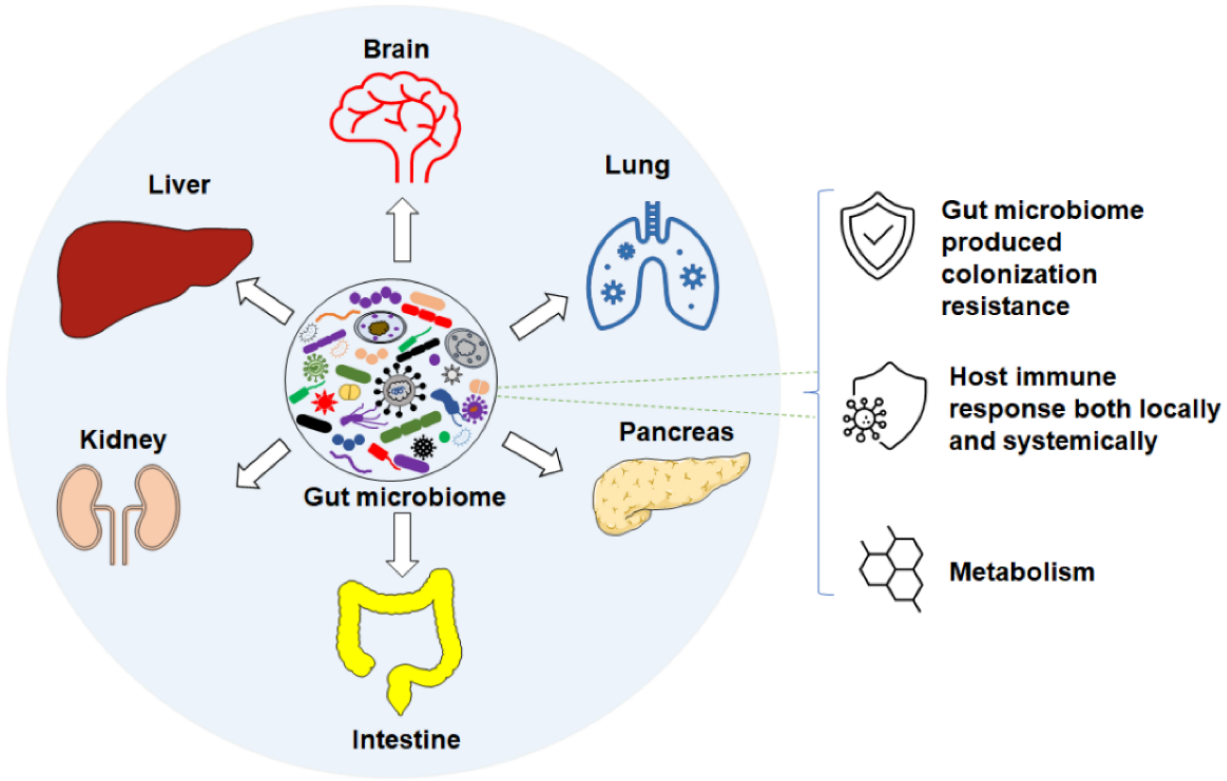
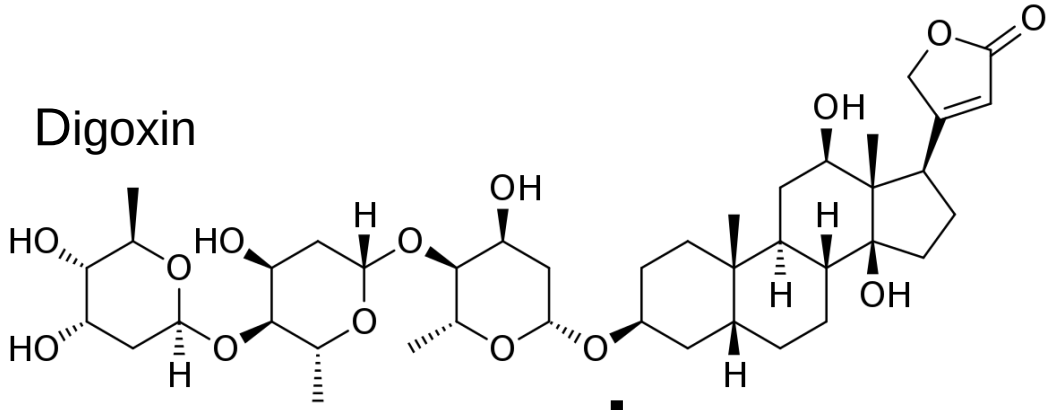
RELEVANCE



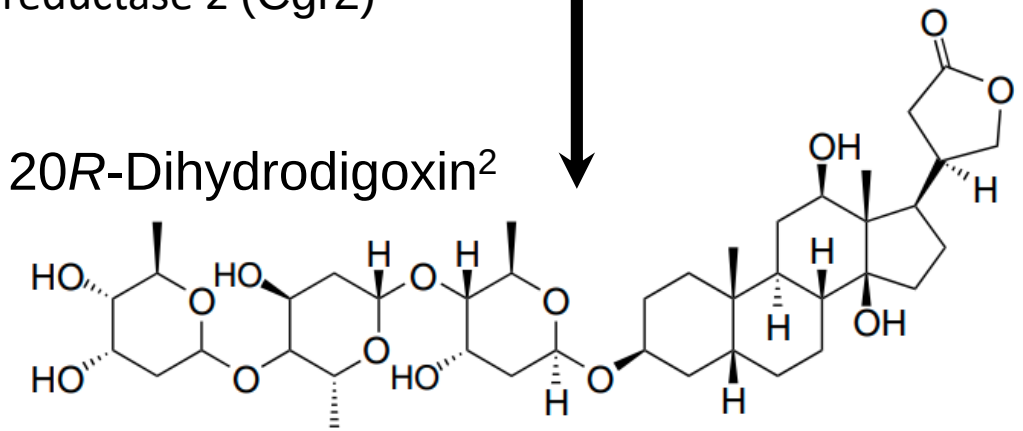
Digoxin



cardiac glycoside reductase 2 (Cgr2)

Eubacterium lentum

20*R*-Dihydrodigoxin[2]



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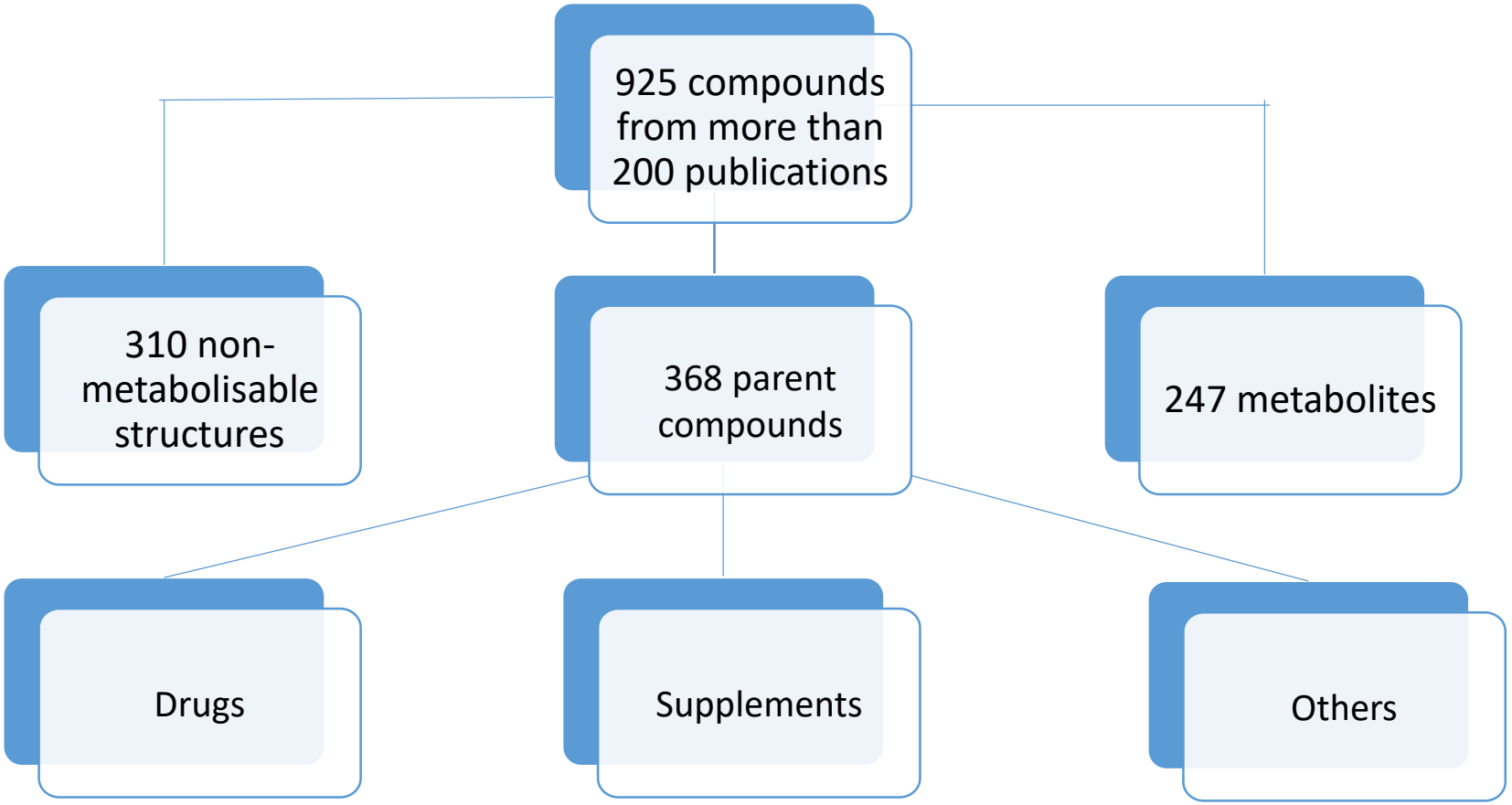

Web-service

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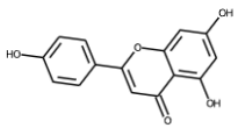
Apigenin

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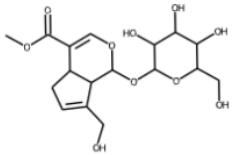
Geniposide

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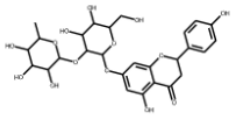
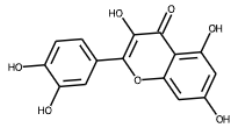
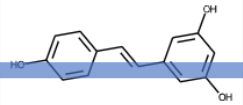
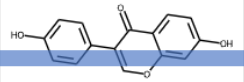

Naringin

Dietary supplement

Quercetin

Dietary supplement

Trans-resveratrol

Dietary supplement

Daidzein

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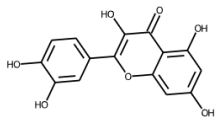
Search:

Compounds's name	IUPAC	PubChem CID	InChi Key	SMILES
2,3-Dinitrotoluene	1-methyl-2,3-dinitrobenzene	11761	DYSXLQBUUOPLBB-UHFFFAOYSA-N	CC1=CC=CC([N+](=O)[O-])=C1[N+](=O)[O-]
2,4,5-Trichlorobiphenyl	1,2,4-trichloro-5-phenylbenzene	27514	VGVIKVCCUATMNG-UHFFFAOYSA-N	ClC1=CC(Cl)=C(C2=CC=CC=C2)C=C1Cl
2,4-Dinitrotoluene	1-methyl-2,4-dinitrobenzene	8461	RMBFBMJGBANMMK-UHFFFAOYSA-N	CC1=CC=C([N+](=O)[O-])C=C1[N+](=O)[O-]
2-Amino-3-methylimidazo-(4,5-f)quinoline N-glucuronide	(2S,3S,4S,5R,6R)-3,4,5-trihydroxy-6-[(3-methyl-2-imidazo[4,5-f]quinolinyl)amino]-2-oxanecarboxylic acid	3035934	YLRCRCCBJUCMKF-SBJFKYEJSA-N	CN1C(NC2OC(C(=O)O)C(O)C(O)C2O)=NC2=C3C=CC=NC3=CC=C21
2-Chloro-5-nitro-N-	2-chloro-5-nitro-N-	644213	DNTSIBUQMRRYIU-	O=C(NC1=CC=CC=C1)C1=CC([N+](=O)[O-])=CC=C1Cl

Showing 1 to 10 of 368 entries

Previous 1 2 3 4 5 ... 37 Next

Quercetin



Type:	Dietary supplement
PubChem:	5280343
DrugBank:	DB04216
IUPAC:	2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-1-benzopyran-4-one
Standard InChI:	InChI=1S/C15H10O7/c16-7-4-10(19)12-11(5-7)22-15(14(21)13(12)20)6-1-2-8(17)9(18)3-6/h1-5,16-19,21H
Standard InChIKey:	REFJWTPEDVJJIY-UHFFFAOYSA-N
SMILES:	O=C1C(O)=C(C2=CC=C(O)C(O)=C2)OC2=CC(O)=CC(O)=C12
Metabolism-related information:	Increase activity and absorption
Reference:	10.1155/2015/905215

Metabolites

Show 10 entries

Search:

Chemical Structure	Metabolite's name	Reaction name	Genus	Species	Reference
	3-(3,4-Dihydroxyphenyl)propionic acid	Cleavage	Eubacterium	ramulus	10.1155/2015/905215

Data usability

Research Article

MDM-Pred: a freely available web application for predicting the metabolism of drug-like compounds by the gut microbiota

A.S. Kolodnitsky, N.S. Ionov, A.V. Rudik, A.A. Lagunin, D.A. Filimonov & V.V. Poroikov

Pages 383-393 | Received 01 Mar 2023, Accepted 11 May 2023, Published online: 25 May 2023

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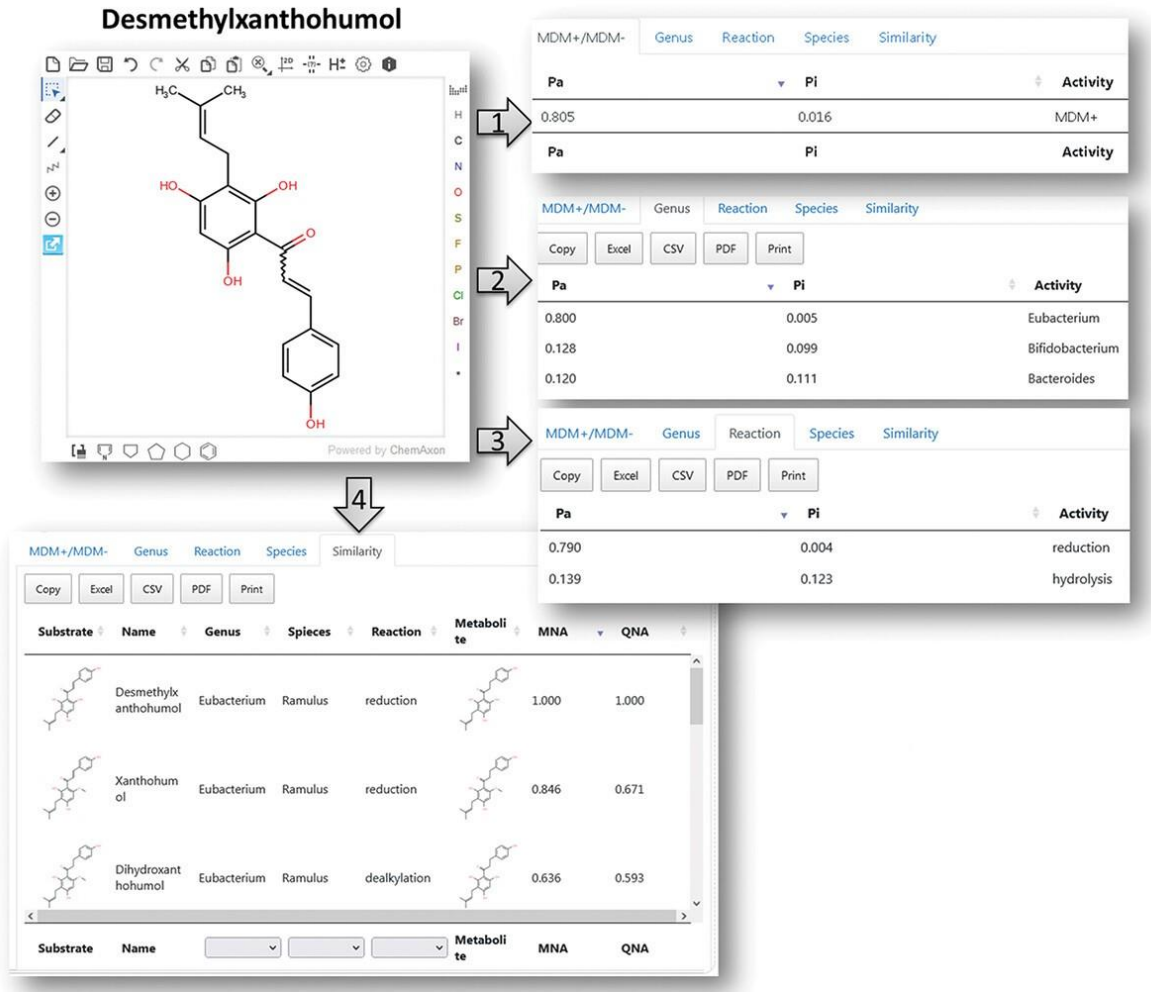
1. The first model with an accuracy of prediction 0.85 estimates whether compounds will be metabolized by human gut microbiota
2. The second model with an average accuracy of prediction 0.92 estimates which bacterial genera are responsible for the drug metabolism.
3. The third model with an average accuracy of prediction 0.92 estimates the biotransformation reactions during metabolism.



Thanks for your attention

Acknowledgements

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Alexey Lagunin
Vladimir Poroikov

Web-service

MDM-pred