COMPUTATIONAL WORKFLOW FOR PREDICTING DRUG METABOLISM BY GUT MICROBIOTA

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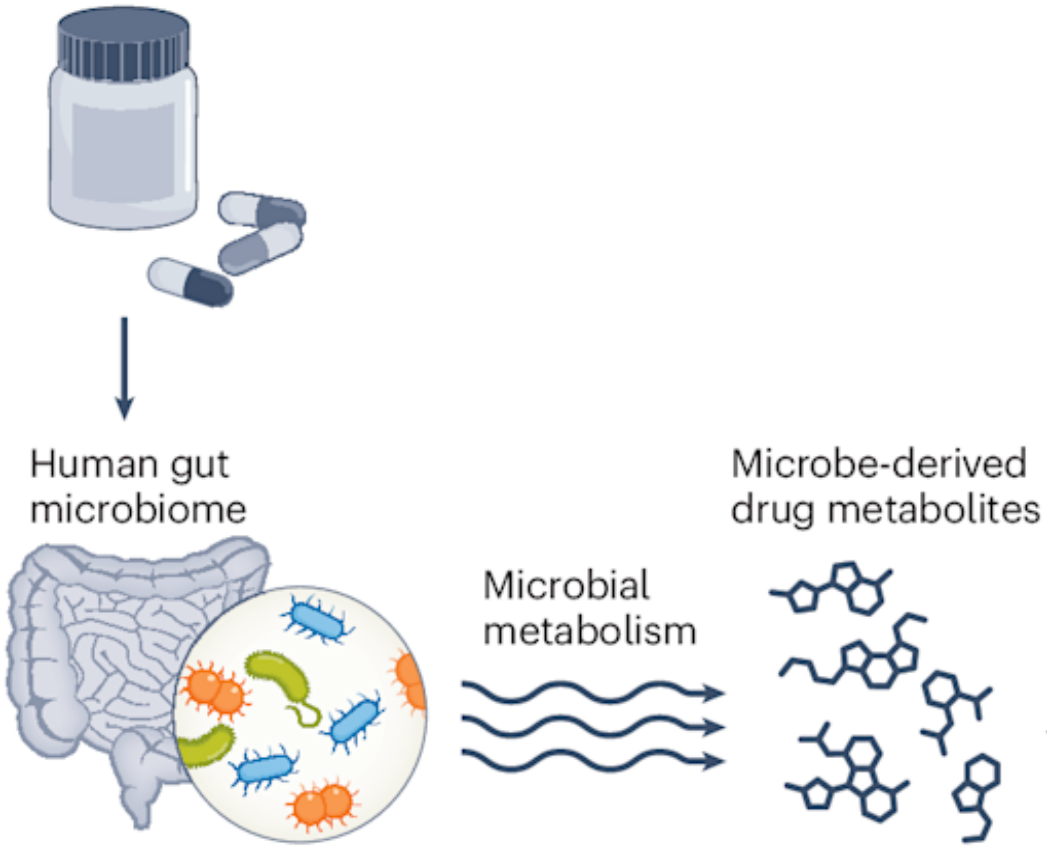
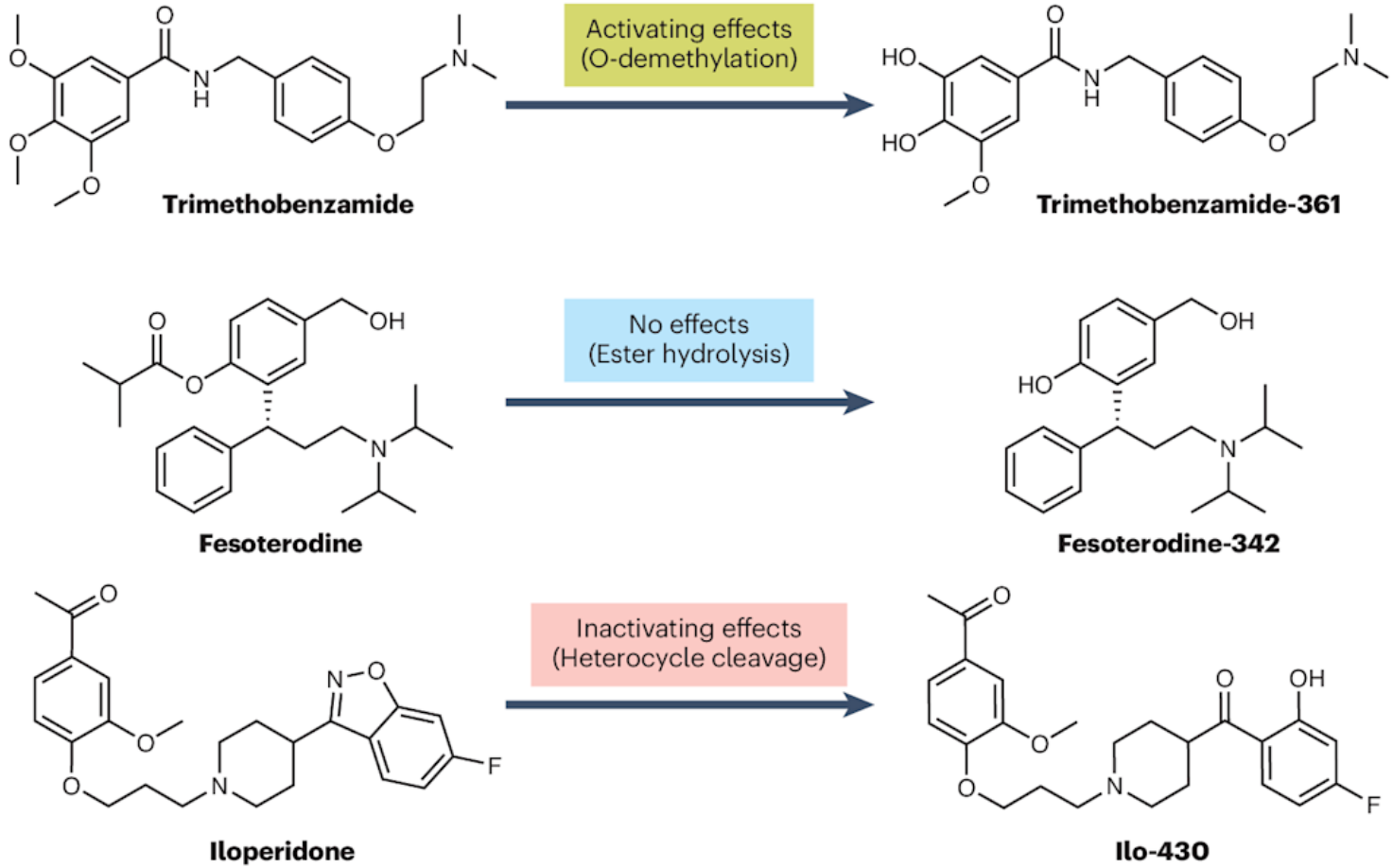
Dmitry A. Filimonov, Vladimir. V. Poroikov

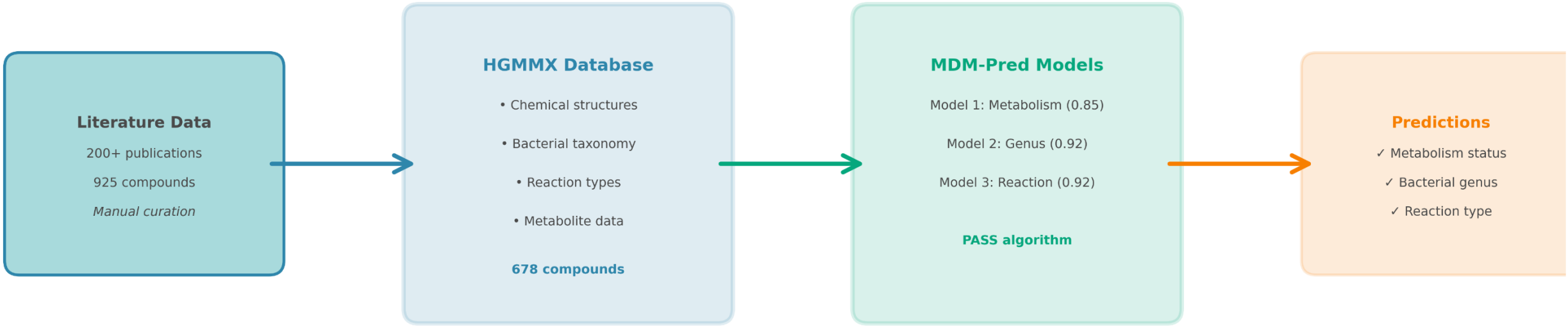
Virtual, 21.10.2025

RELEVANCE

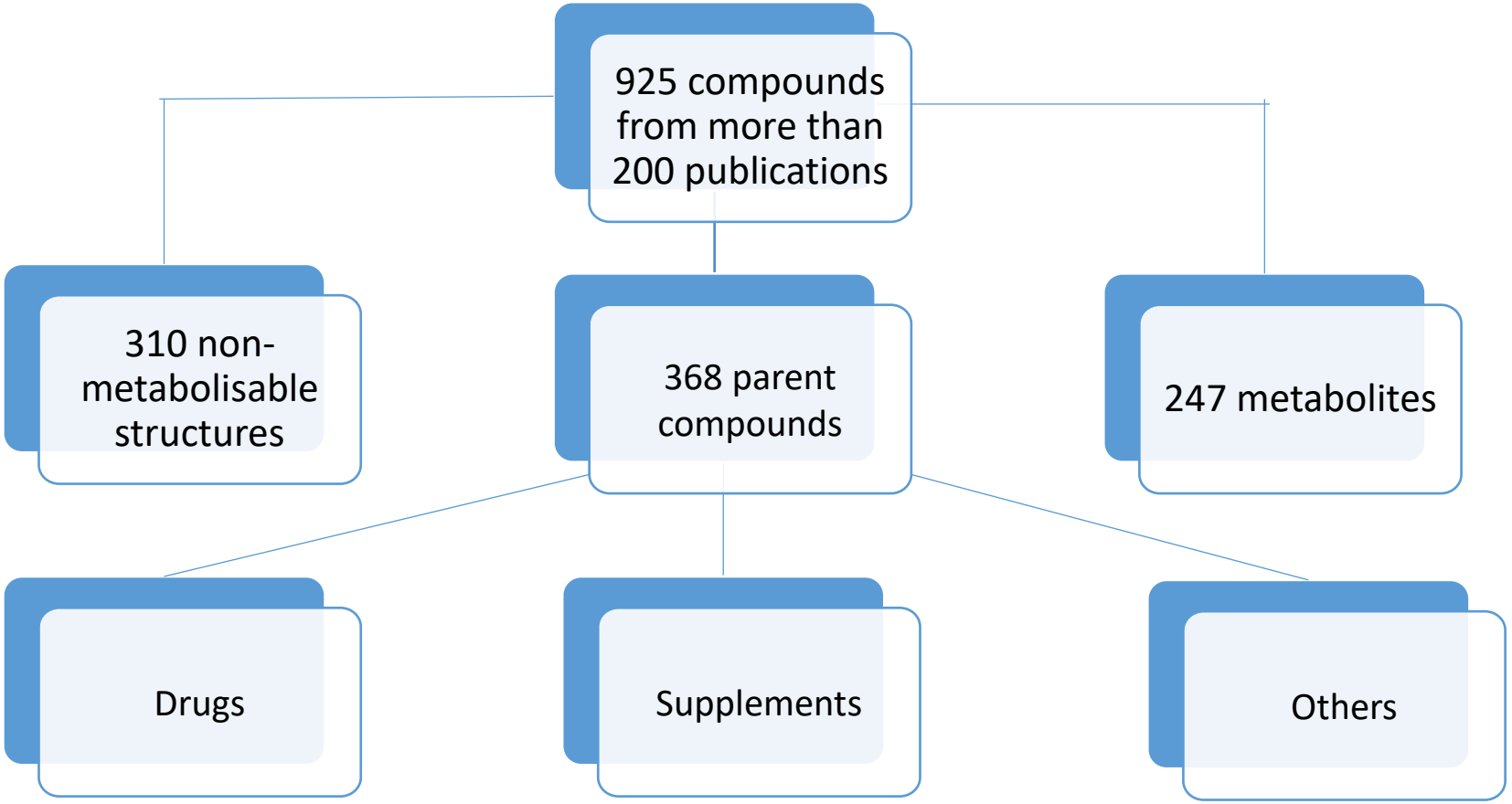

Human gut
microbiome
Microbial
metabolism
Microbe-derived
drug metabolites


Activating effects
(O-demethylation)
Trimethobenzamide
Trimethobenzamide-361
No effects
(Ester hydrolysis)
Fesoterodine
Fesoterodine-342
Inactivating effects
(Heterocycle cleavage)
Iloperidone
Ilo-430

Computational workflow



Database content



Web-service

Parent compounds | Metabolites | Similarity search | Download

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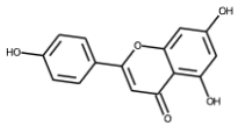
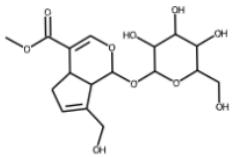
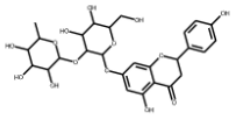
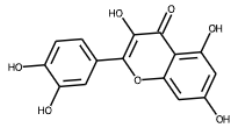
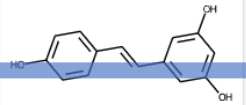
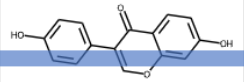
Dietary supplement

Apigenin

Dietary supplement

Geniposide

Dietary supplement

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

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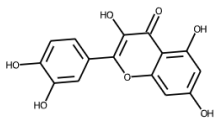
Quercetin



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

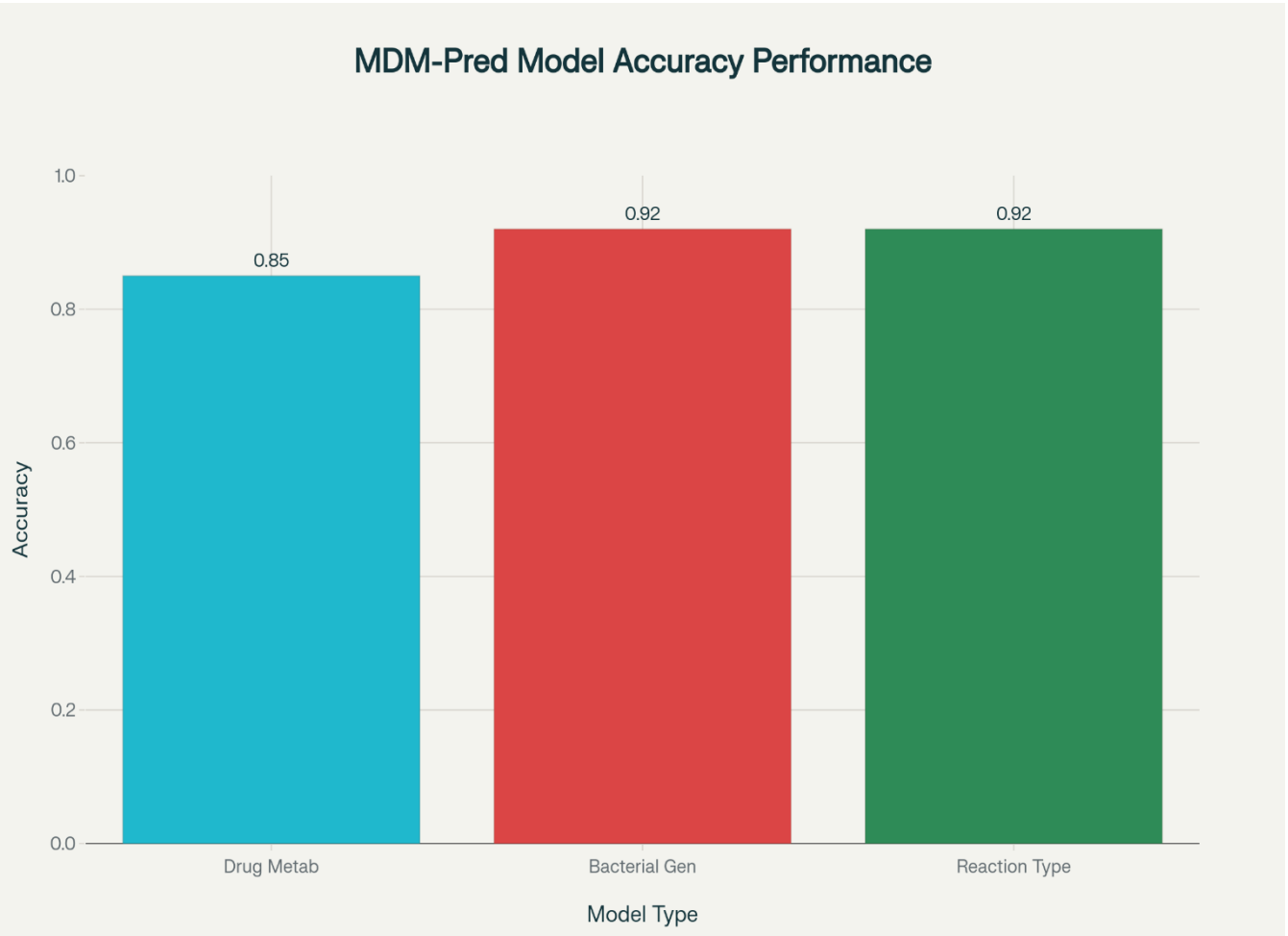
Metabolites

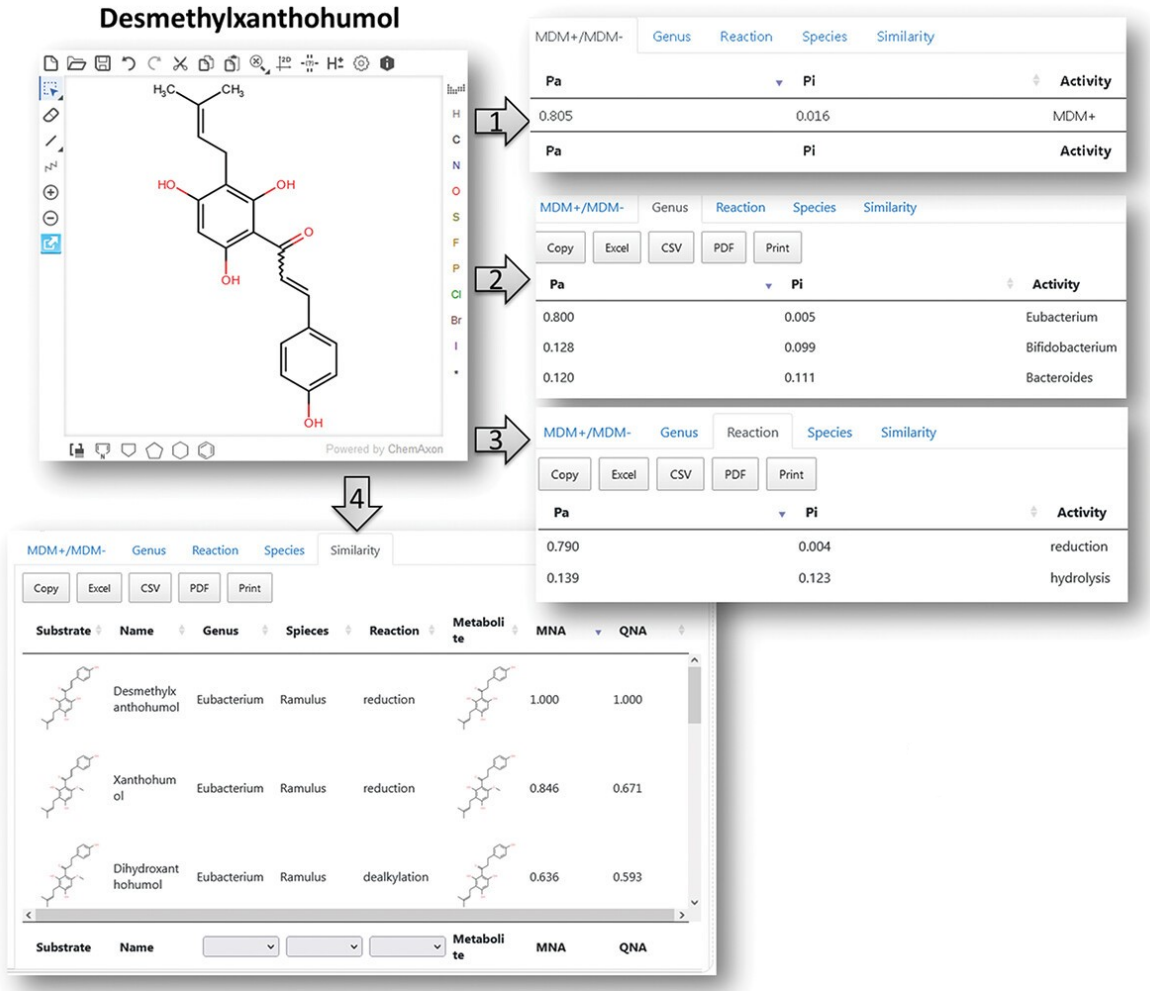
Show 50 entries

Search:

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

MDM-pred models





Thanks for your attention

Acknowledgements

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Ionov Nikita
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Alexey Lagunin
Vladimir Poroikov