Electronic Supplementary Material (ESI) for RSC Advances.

DiaNat-DB: A Molecular Database of Antidiabetic Compounds from Medicinal Plants

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Supplementary Information

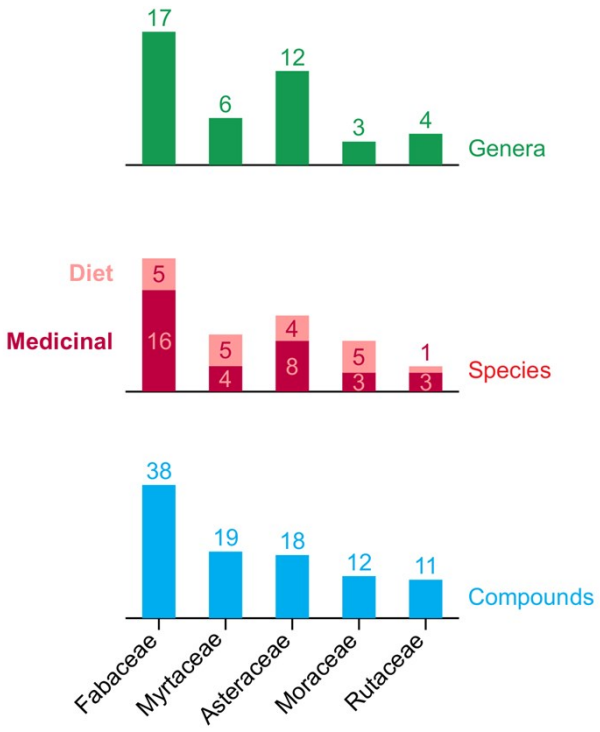


Figure S1. The taxonomic diversity and use of the most representative families in DiaNat-DB.

Table S1. Exemplary DiaNat-DB compounds similar to antidiabetic drugs (DM-ref).

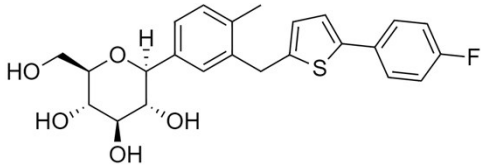
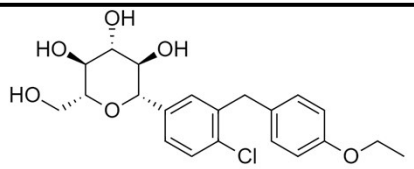
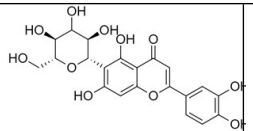
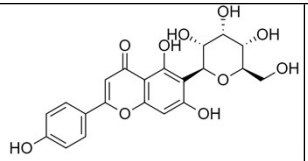
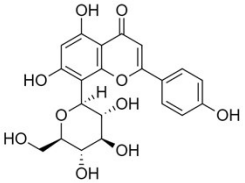
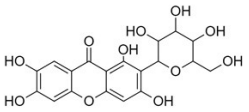
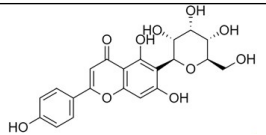
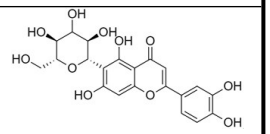
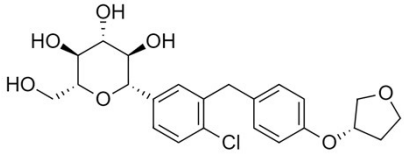
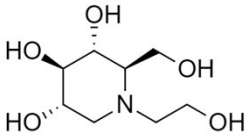
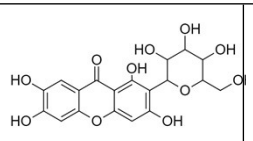
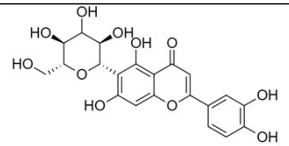
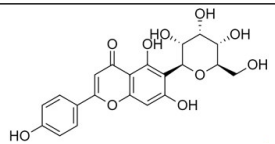
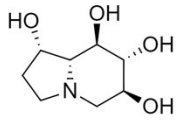
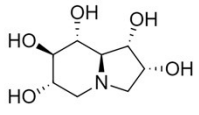
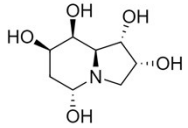
Compound in DM-ref	 Canagliflozin			 Dapagliflozin:		
Similar in DiaNat-DB	 DiaNatDB-22 Similarity: 0.80	 DiaNatDB-290 Similarity: 0.80	 DiaNatDB-20 Similarity: 0.79	 DiaNatDB-18 Similarity: 0.83	 DiaNatDB-290 Similarity: 0.80	 DiaNatDB-22 Similarity: 0.80
Compund in DM-ref	 Empagliflozin			 Miglitol		
Similar in DiaNat-DB	 DiaNatDB-18 Similarity: 0.81	 DiaNatDB-22 Similarity: 0.78	 DiaNatDB-290 Similarity: 0.78	 DiaNatDB-120 Similarity: 0.94	 DiaNatDB-221 Similarity: 0.94	 DiaNatDB-222 Similarity: 0.92

Table S2. Some of the most similar scaffolds between DiaNat-DB and FDA.

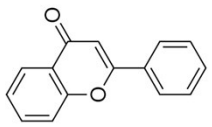
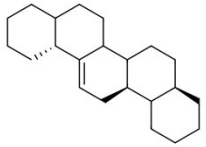
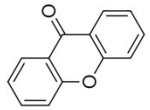
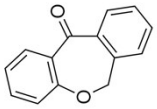
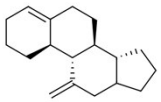
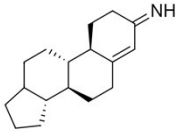
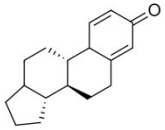
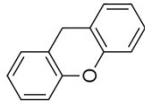
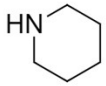
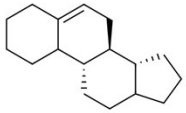
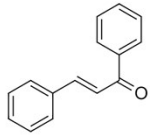
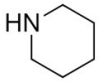
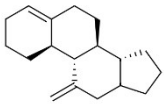
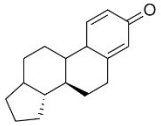
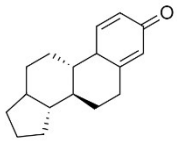
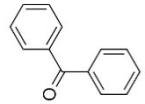
Scaffold in DiaNat-DB			
Most similar scaffold in FDA	 Similarity: 0.75 Antidepressants, antihistaminic	   Similarity: 0.96 Similarity: 0.89 Similarity: 0.86 Progestin medications, antidepressants.	 Similarity: 0.76 Hyperhidrosis, stomach spasms
Scaffold in DiaNat-DB			
Most similar scaffold in FDA	 FDA Similarity: 1.0 Miglitol: **antidiabetic**	   FDA FDA FDA Similarity: 0.97 Similarity: 0.87 Similarity: 0.87 Progestin medications, antidepressants, treatment of adrenogenital syndrome and adrenal insufficiency	 FDA Similarity: 0.76 Analgesic, anti-inflammatory, **reduces risk of diabetic retinopathy**, Parkinson's disease

Table S3. List of FDA-approved antidiabetic small molecules (DM-ref) from DrugBank.

Drug	Mechanism of action / Target
Acarbose	Alpha-glucosidase inhibitor that impairs digestion and absortion of carbohydrates in the small bowel.
Alogliptin	Dipeptidil peptidase 4 (DPP4) inhibitor.
Canagliflozin	Inhibitor of the kidney sodium-glucose transporter 2 (SGLT2).
Clorpropamide	Inhibitor of potassium ATP channel in pancreatic β-cells (KATP).
Dapagliflozin	SGLT2 inhibitor.
Empagliflozin	SGLT2 inhibitor.
Ertugliflozin	SGLT2 inhibitor.
Glibenclamide / glyburide	KATP inhibitor.
Gliclazide	KATP inhibitor.
Glimepiride	KATP inhibitor.
Glipizide	KATP inhibitor.
Linagliptin	DPP4 inhibitor.
Metformin	AMPK activator (insulin sensitizer).
Miglitol	Alpha glucosidase inhibitor.
Nateglinide	KATP inhibitor.
Pioglitazone	PPAR-gamma inhibitor (insulin sensitizer).

Repaglinide	KATP inhibitor.
Rosiglitazone	PPAR-gamma inhibitor.
Saxagliptin	DPP4 inhibitor.
Sitagliptin	DPP4 inhibitor.
Tolazamide	KATP inhibitor.
Tolbutamide	KATP inhibitor.
Vildagliptin	DPP4 inhibitor.