HerbalCDB integrates carbohydrate information from GlyTouCan 1and CSD2, along with eight global pharmacopoeias. This information encompasses basic data such as the IUPAC, CID, molecular weight, molecular formula, InChIKey, and structural representation for carbohydrate, accompanied by corresponding species information. For each acquired carbohydrate, we designed and implemented a set of processes (shown in Figure S4). These processes have been uploaded to GitHub (https://github.com/GreatChenLab/GNDC/tree/main/CDB).

1 Aoki-Kinoshita, K. *et al.* GlyTouCan 1.0 – The international glycan structure repository. *Nucleic acids research* **44**, D1237-D1242, doi:10.1093/nar/gkv1041 (2016).

2 Toukach, P. V. & Egorova, K. S. Carbohydrate structure database merged from bacterial, archaeal, plant and fungal parts. *Nucleic acids research* **44**, D1229-D1236, doi:10.1093/nar/gkv840 (2016).