

**Supplementary Material II.** The number of drug samples in each category for dataset  $DS_2$ .

Tag	Disease	Number of drugs
$D_1$	Antihypertensive	127
$D_2$	Uterine stimulant	7
$D_3$	Antithrombotic	47
$D_4$	Radioactive agent	7
$D_5$	Pharmaceutic aid	19
$D_6$	Antiarrhythmic	30
$D_7$	Vasodilator	47
$D_8$	Laxative	9
$D_9$	Diagnostic aid	15
$D_{10}$	Antiviral	46
$D_{11}$	Nutrient	14
$D_{12}$	Antineoplastic	193
$D_{13}$	Antipsoriatic	17
$D_{14}$	Vasoconstrictor	13
$D_{15}$	Anthelmintic	22
$D_{16}$	Antimalarial	14
$D_{17}$	Antifungal	44
$D_{18}$	Hypolipidemic	37
$D_{19}$	Antibacterial	86
$D_{20}$	Antibiotic	108

$D_{21}$	Choleretic	9
$D_{22}$	Antiinflammatory	107
$D_{23}$	Immunomodulator	19
$D_{24}$	Muscle relaxant	24
$D_{25}$	Analgesic	131
$D_{26}$	Disinfectant	22
$D_{27}$	Diuretic	23
$D_{28}$	Anticonvulsant	31
$D_{29}$	Antidepressant	91
$D_{30}$	Antioxidant	13
$D_{31}$	Antiparkinsonian	34
$D_{32}$	Antiulcerative	14
$D_{33}$	CNS stimulant	16
$D_{34}$	Antipsychotic	92
$D_{35}$	Antianginal	20
$D_{36}$	Cognition enhancer	10
$D_{37}$	Antidiabetic	46
$D_{38}$	Psychodysleptic	9
$D_{39}$	Anxiolytic	59
$D_{40}$	Anti-Alzheimer's Disease	17
$D_{41}$	Antiemetic	27
$D_{42}$	Antihistamine	44

$D_{43}$	Cardiotonic	23
$D_{44}$	Antiglaucoma	13
$D_{45}$	Antiallergic/Antiasthmatic	70
$D_{46}$	Hypocholesterolemic	12
$D_{47}$	Uricosuric	9
$D_{48}$	Sedative/Hypnotic	16
$D_{49}$	Anesthetic	13
$D_{50}$	Antiamoebic	7
$D_{51}$	Spasmolytic	29
$D_{52}$	Antianorexic	11
$D_{53}$	Antiatherosclerotic	13
$D_{54}$	Antisecretory (gastric)	8
$D_{55}$	Antiobesity	14
$D_{56}$	Narcotic antagonist	7
Total	---	2,005