

Supplementary Material II: The dataset $S_{\text{ex-te}}$ consisting of 110 drug samples, classified into 14 main ATC-class.

(1) 23 drug samples in class “Alimentary tract and metabolism”

DB00030	DB00129	DB00146	DB00147	DB00163	DB00360
DB00377	DB00505	DB00536	DB00769	DB00836	DB01164
DB01294	DB01345	DB01370	DB01373	DB01378	DB01593
DB02329	DB02659	DB02901	DB04876	DB08907	

(2) 12 drug samples in class “Blood and blood forming organs”

DB00407	DB00682	DB00775	DB01088	DB01109	DB01164
DB01225	DB01345	DB01373	DB01378	DB01592	DB01593

(3) 21 drug samples in class “Cardiovascular system”

DB00147	DB00148	DB00159	DB00325	DB00373	DB00375
DB00464	DB00509	DB00542	DB00686	DB00769	DB01109
DB01116	DB01345	DB01370	DB01373	DB01378	DB01412
DB01592	DB01593	DB04840			

(4) 15 drug samples in class “Dermatologicals”

DB00129	DB00337	DB00596	DB00626	DB00764	DB00769
DB00856	DB00971	DB01123	DB01130	DB01345	DB01370
DB01373	DB01378	DB01593			

(5) 9 drug samples in class “Genito urinary system and sex hormones”

DB00957	DB01152	DB01164	DB01373	DB01378	DB02901
DB04938	DB06713	DB06730			

(6) 5 drug samples in class “Systemic hormonal preparations, excluding sex hormones and insulins”

DB00509	DB01345	DB02638	DB04630	DB08869	
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(7) 10 drug samples in class “Antiinfectives for systemic use”

DB00260	DB00369	DB00626	DB00955	DB01373	DB01601
DB01604	DB03615	DB04835	DB08795		

(8) 10 drug samples in class “Antineoplastic and immunomodulating agents”

DB00290	DB00539	DB00570	DB00642	DB00707	DB04106
DB05109	DB08881	DB08889	DB08910		

(9) 7 drug samples in class “Musculo-skeletal system”

DB00141	DB00416	DB00732	DB00825	DB01337	DB01339
DB01370					

(10) 13 drug samples in class "Nervous system"

DB00122	DB00176	DB00234	DB00647	DB00837	DB01063
DB01273	DB01345	DB01354	DB01373	DB01440	DB01592
DB04948					

(11) 7 drug samples in class "Antiparasitic products, insecticides and repellents"

DB00129	DB00738	DB01131	DB01345	DB02640	DB04786
DB06708					

(12) 16 drug samples in class "Respiratory system"

DB00122	DB00151	DB00332	DB00397	DB00626	DB00764
DB00768	DB00825	DB00985	DB01274	DB01345	DB01373
DB01409	DB01411	DB01412	DB04819		

(13) 9 drug samples in class "Sensory organs"

DB00122	DB00151	DB00373	DB00768	DB00955	DB01109
DB01345	DB01370	DB01593			

(14) 11 drug samples in class "Various"

DB00122	DB00151	DB00638	DB00733	DB00743	DB01130
DB01345	DB01373	DB01378	DB01592	DB04173	