

**Table S4.** Details of class label assignments at each iterative optimization and data splitting

T2PK products name	Initial class label	Class label A	Class label B	Class label C	Class label D	Class label E	Class label F	Final class label	Dataset splitting	
									5 class labels	9 class labels
A-74528-Hex	13	II	IV	V	VI	VII	VIII	IX	train	train
Abx	13	II	IV	V	VI	VII	VIII	IX	test	test
+ABXA-BE-24566B	13	II	IV	V	VI	VII	VIII	IX	train	train
Accramycin	13	II	IV	V	VI	VII	VIII	IX	test	test
Aclacinomycin-Pr	10	III	III	III	III	III	III	VI	test	test
Aclacinomycin-Pr	10	III	III	III	III	III	IV	VI	train	train
Actinorhodin	8	I	I	I	I	I	I	I	test	test
Alloclonine	10	III	III	IV	IV	V	VI	VII	train	train
Alnumycin-Bu	8	I	I	I	I	I	I	I	train	train
Anthrabenzoquinone	13	II	IV	V	VI	VII	VIII	IX	train	train
AQ-256	8	II	IV	V	VI	VII	VIII	IX	train	train
Aranciamycin	10	III	III	III	III	III	IV	VI	train	train
Arenimycin	12	II	IV	V	VI	VII	VIII	IX	test	test
Arenimycin'	12	II	IV	V	VI	VII	VIII	IX	train	train
Arimetamycin	10	III	III	III	III	III	IV	VI	train	train
Arixanthomycin	13	II	IV	V	VI	VII	VIII	IX	train	train
Auricin	10	III	III	IV	IV	V	VI	VII	train	train
Azceemicin-aziridine	10	III	III	IV	IV	V	III	IV	train	train
Azceemicin-aziridine	10	III	III	IV	IV	V	III	IV	train	train
Baikalomycin	10	III	III	III	III	III	IV	VI	train	train
BE-7585A	10	III	IV	V	VI	VII	VIII	IX	train	train
Benastatin-Hex	12	II	III	IV	IV	IV	V	VI	train	train
Bipentamycin	10	III	III	IV	IV	V	III	IV	test	test
Brasiliquinone-Pr	10	III	III	IV	IV	V	III	IV	test	test
Calixanthomycin	12	III	IV	V	VI	VII	VIII	IX	train	train
Cervimycin-malonoamyl	9	II	IV	V	VI	VII	VIII	IX	train	train
Chartreusin	10	III	III	III	III	III	IV	VI	test	test
Chartreusin'	10	III	III	III	III	III	IV	VI	train	train
Chartreusin'	10	III	III	IV	IV	V	III	IV	train	train
Chattamycin	10	III	III	III	III	III	IV	V	train	train
Chelocardin	10	III	III	III	III	III	IV	VI	train	train
Chlortetracycline	10	III	III	III	III	III	IV	VI	train	train
Chromomycin	10	III	III	III	III	III	IV	VI	train	train
Chrysomycin-Pr	10	III	III	III	III	III	IV	VI	train	train
Cinerubin-Pr	10	III	III	IV	IV	IV	V	II	test	test
Clostrubin	10	III	III	IV	IV	IV	V	II	train	train
Clostrubin'	10	III	III	IV	IV	V	III	IV	train	train
Collinone	13	III	IV	V	VI	VII	VIII	IX	train	train
CosmomycinC-Pr	10	III	III	III	III	III	IV	V	train	train
Cosmomycin-Pr	10	III	III	III	III	III	IV	V	test	test
Cur	12	III	IV	V	VI	VII	VIII	IX	test	test
Cysgriseusin	10	II	III	III	III	III	IV	VI	train	train
Cytorhodin-Pr	10	III	III	III	III	III	IV	V	train	train
Dactylocycline	10	III	III	III	III	III	IV	VI	train	train
Damnorubcin-Pr	10	III	III	III	III	III	IV	VI	train	train
Dendrubin	9	III	IV	V	VI	VII	VIII	IX	test	test
Doxorubicin-Pr	10	II	III	III	III	III	IV	VI	test	test
Dotomycin	10	III	III	III	III	III	IV	VI	train	train
Elloramycin	10	III	III	III	III	III	IV	VI	train	train
Elloramycin	10	III	III	III	III	III	IV	VI	train	train
Enduracynone	13	III	IV	V	VI	VII	VIII	IX	train	train
Enterocin-Bn	8	I	I	I	I	I	I	I	train	train
Erdacin	8	I	I	I	I	I	I	I	train	train
FD-594-Bu	13	I	IV	V	VI	VII	VIII	IX	train	train
Fluostatin	10	II	III	IV	IV	V	III	IV	train	train
FluostatinM	10	III	III	IV	IV	V	III	IV	train	train
FluostatinMQ	10	III	III	IV	IV	V	III	IV	train	train
Fogacin	8	III	I	I	I	I	I	I	test	test
FogacinC-HCS	8	I	I	I	I	I	I	I	train	train
Formicamycin	13	I	IV	V	VI	VII	VIII	IX	train	train
Frankiamycin	12	II	IV	V	V	VI	VII	IX	train	train
FredericamycinC	13	II	IV	V	VI	VII	VIII	IX	test	test
Fredericamycin-Hex	13	II	IV	V	VI	VII	VIII	IX	train	train
Frenolicin-Bu	8	II	I	I	I	I	I	I	train	train
Frigocyclinone	10	I	III	IV	IV	V	VI	VII	test	test
Gaulimycin	10	III	III	IV	IV	V	VI	VII	train	train
Gilvocarcin-Pr	10	III	III	IV	IV	IV	V	VI	test	test
Granaticin	8	III	I	I	I	I	I	I	train	train
Granaticin'	8	I	I	I	I	I	I	I	train	train
Granaticin''	8	I	I	I	I	I	I	I	train	train
Gricamycin	10	I	III	IV	IV	V	III	IV	test	test
Grisorhodin	13	III	IV	V	VI	VII	VIII	IX	train	train
Grisorhodin'	13	II	IV	V	VI	VII	VIII	IX	test	test
Griseusin	10	II	III	III	III	III	IV	VI	train	train
Hatamarubigin	10	III	III	IV	IV	V	VI	VII	train	train
Hedlamycin-Hex	10	III	III	III	III	III	IV	VI	train	train
Heliquinomycin	13	III	IV	V	VI	VII	VIII	IX	train	train
Hexaricin	13	II	IV	V	VI	VII	VIII	IX	train	train
Hiroshidine	8	II	I	I	I	I	I	I	train	train
Huanglongmycin	9	I	II	II	II	II	II	III	train	train
Hyaluromycin	13	II	IV	V	VI	VII	VIII	IX	train	train
Hydroxyfujiamycin	10	III	III	IV	IV	V	III	IV	train	train
IFOs	8	III	I	I	I	I	I	I	train	train
Isatropolone-Bu	8	I	I	I	I	I	I	I	test	test
Isoindolinomycin-Gly	8	I	I	I	I	I	I	I	train	train
Jadomycin	10	I	III	IV	IV	V	III	IV	train	train
JBIR-76	8	III	I	I	I	I	I	I	train	train
Julkchrome	9	I	II	II	II	II	II	III	train	train
Julkchrome'	9	II	II	II	II	II	II	III	train	train
Keycin	10	II	III	III	III	III	IV	VI	train	train
Kiamycin	9	III	II	II	II	II	III	IV	train	train
Kinamycin	10	II	III	IV	IV	V	III	IV	train	train
kinanthraquinone	9	III	II	II	II	II	III	IV	test	test
Komodoquinone	10	II	III	III	III	III	IV	VI	test	test
Komodoquinone'	10	III	III	III	III	III	IV	VI	train	train
Kosinostatin	10	III	III	III	III	III	IV	VI	train	train
Lactonomycin-Gly	10	III	III	III	III	III	IV	VI	train	train
LactonomycinZ-Gly	10	III	III	III	III	III	IV	VI	train	train
Landomycin	10	III	III	IV	IV	V	VI	VII	test	test
LandomycinE	10	III	III	IV	IV	V	VI	VII	train	train
LandomycinE'	10	III	III	IV	IV	V	VI	VII	train	train
LL-D49194etl-Ile	10	III	III	III	III	III	IV	VI	train	train
Lomaiviticin-Pr	10	III	III	III	III	III	IV	V	train	train
Lomaiviticin'-Pr	10	III	III	III	III	III	IV	V	test	test
Lomaiviticin''-Pr	10	III	III	III	III	III	IV	V	train	train
Lugduromycin	10	III	III	IV	IV	V	III	IV	train	train
Lysolipin	12	III	IV	V	VI	VII	VIII	IX	test	test
Maduralactomycin	10	II	III	III	III	III	IV	VI	train	train
Mayamycin	10	III	III	IV	IV	V	III	IV	train	train
Medermycin	8	III	I	I	I	I	I	I	train	train
Mensacarin	10	I	III	III	III	III	IV	VI	test	test
Metathramycin	10	III	III	IV	IV	V	III	IV	train	train
Methyketangomycin	10	III	III	IV	IV	V	III	IV	train	train
Mithramycin	10	III	III	III	III	III	IV	VI	train	train
Murayaquinone	10	III	III	III	III	III	IV	VI	train	train
Naphthocyclinone	8	I	I	I	I	I	I	I	train	train
Nenestatin-Pr	10	III	III	III	III	III	IV	V	train	train
Nivetetracyclate-Pr	10	III	III	III	III	III	IV	VI	train	train
Nocardiopeptin-Pr	10	III	III	IV	IV	V	III	IV	train	train
Nogalamycin	10	III	III	III	III	III	IV	VI	train	train

Ovidomycin	10	III	III	IV	IV	V	III	IV	train	train
Metamycin-iPr	9	I	IV	V	V	VI	VII	II	test	test
Oxytetracycline	10	III	III	III	III	III	IV	VI	train	train
Piloquinone-Leu	9	III	IV	V	VI	VII	VIII	IX	train	train
Paramagnetoquinone	12	II	III	IV	IV	V	VI	VII	train	train
PD116740	10	III	III	IV	IV	V	III	IV	train	train
Persiamycin	10	III	III	IV	IV	V	III	IV	train	train
Poliketomycin	10	III	III	III	III	III	IV	VI	test	test
Pradimicin	12	II	IV	V	VI	VII	VIII	IX	train	train
Pyxidicycline	9	I	IV	V	V	VI	VII	II	train	train
Qimimycin	8	I	I	I	I	I	I	I	test	test
R1128-Leu	8	III	I	I	I	I	I	I	train	train
Ravidomycin-Pr	10	III	III	IV	IV	V	III	IV	train	train
Resistomycin	10	III	III	IV	IV	IV	V	VI	train	train
Rhodomycin-Pr	10	I	III	III	III	III	IV	V	train	train
Rishirilde-Leu	9	I	I	I	I	I	I	I	train	train
Rishirilde-Leu	9	I	I	I	I	I	I	I	test	test
Rubrolone-Bu	8	II	I	I	I	I	I	I	train	train
Rubromycin	13	II	IV	V	VI	VII	VIII	IX	test	test
Rubromycin'	13	III	IV	V	VI	VII	VIII	IX	train	train
Saprolmycin	10	III	III	IV	IV	V	III	IV	train	train
SaaguayamycinA	10	III	III	IV	IV	V	III	IV	test	test
SaaguayamycinZ	10	II	III	IV	IV	V	III	IV	train	train
Sch	12	III	IV	V	V	VI	VII	VIII	train	train
Sch47554	10	II	III	IV	IV	V	III	IV	train	train
Setomimycin	9	III	II	II	II	II	II	III	test	test
SF2575	10	III	III	IV	IV	V	VI	VII	train	train
Simocyclinone	10	III	III	IV	IV	V	III	IV	test	test
Simocyclinone'	10	III	III	IV	IV	V	III	IV	train	train
Steffmycin	10	III	III	III	III	III	IV	VI	train	train
Streptoketide-Pr	10	III	III	III	III	III	IV	VI	train	train
Tetarimycin	10	III	III	III	III	III	IV	VI	train	train
Tetracenomylin	10	III	III	III	III	III	IV	VI	train	train
Thioangucycline	10	II	III	IV	IV	V	III	IV	train	train
TLN-05220-Ile	13	III	IV	V	VI	VII	VIII	IX	train	train
Trioxacarcin-Ile	10	II	III	III	III	III	IV	VI	train	train
Turbimycin	13	III	IV	V	VI	VII	VIII	IX	train	train
Urdamycin	10	III	III	IV	IV	V	III	IV	train	train
UT-X26-F129	10	III	III	III	III	III	IV	VI	test	test
Warkmycin	10	II	III	III	III	III	IV	VI	train	train
Wexrubicin	10	II	III	IV	IV	IV	V	II	train	train
WhE	12	III	IV	V	V	VI	VII	VIII	train	train
WS79089D	13	II	IV	V	VI	VII	VIII	IX	train	train
X26	10	II	III	III	III	III	IV	VI	train	train
Xantholipin	13	II	IV	V	VI	VII	VIII	IX	train	train
ZHMpentangular	13	II	IV	V	V	VI	VII	VIII	train	train