Table 1: Results For Models
--- Baseline (Grayscale only) ---

precision recall f1-score support

1-octanol	0.00	0.00	0.00	2
2,5-furandimethano				
2-Oleoylglycerol				2
4-CMTB	0.00	0.00	0.00	2
4-methylhistamine				
7-hydroxystaurospori				00 2
A205804	0.00	0.00	0.00	1
AC-710	0.00	0.00	0.00	2
			0.00	2
ANR-94	0.00	0.00	0.00	1
AR-12	1.00	1.00	1.00	1
AVL-292		0.00	0.00	2
AZ191	0.00	0.00	0.00	2
AZD7762	0.00		0.00	3
AZD9668	0.00	0.00	0.00	2
BAM7	0.00	0.00	0.00	2
BAN-ORL-24				
BAX-channel-block				00 2
BAY-87-2243	0.00			2
BI-2536	0.00	0.00	0.00	3
BMS-536924	0.00			1
BQ-788	0.20	1.00	0.33	1
BRL-50481	0.00	0.00	0.00	2
BVT-948	0.00	0.00	0.00	2
CC-401	0.00	0.00	0.00	2
CCG-50014		0.00	0.00	2
CCG-63802			0.00	1
CGP-53353	0.00	0.00	0.00	1
CP-724714	0.00	0.00	0.00	2
CVT-10216	0.00	0.00	0.00	2
CYM-50260	0.00			2
CYM-50358	0.00			2
CYM-5442			0.00	1
CYM-5520	0.00	0.00	0.00	2
CYT-997	0.00	0.00	0.00	3
DDR1-IN-1	0.00	0.00	0.00	2
DG-172	0.00	0.00	0.00	1
DMSO	0.23	0.56	0.32	102
		.00 0		2
FK-866	0.00	0.00	0.00	3
FPS-ZM1	0.00	0.00	0.00	2
GK921	0.00	0.00	0.00	2

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GNF-5
                              0.00
                                     0.00
                                             0.00
                                                      2
                 GNF-5837
                                0.00
                                       0.00
                                               00.0
                                                        2
                                                         2
                 GSK-37647
                                0.00
                                        0.00
                                               0.00
                 GSK1070916
                                 0.00
                                         0.00
                                                0.00
                                                          2
                 GSK2110183
                                 0.00
                                         0.00
                                                0.00
                                                          3
                  GSK3787
                                0.00
                                       0.00
                                               0.00
                                                        2
                                                         2
                 GW-311616
                                0.00
                                        0.00
                                                0.00
                                                         2
                                 0.00
                                         0.00
                                                0.00
                H2L-5765834
                  IRL-2500
                               0.00
                                      0.00
                                              0.00
                                                       2
                                                       2
                   IWP-L6
                              0.00
                                      0.00
                                             0.00
                                                       2
                  JTE-607
                              0.00
                                      0.00
                                             0.00
                    KG-5
                             0.00
                                     0.00
                                            0.00
                                                      2
                  KH-CB19
                                00.0
                                       0.00
                                               00.0
                                                        2
                                                        2
                  KU-55933
                                       0.00
                                0.00
                                               0.00
                  KU-60019
                                                        2
                                0.00
                                       0.00
                                               0.00
                 L-proline
                              0.00
                                     0.00
                                             0.00
                                                      2
                                 0.33
                                         0.50
                                                0.40
                                                         2
                 LDN-212854
                                        0.00
                                                         2
                 LDN-27219
                                0.00
                                               0.00
                  LGK-974
                               0.00
                                       0.00
                                              0.00
                                                        2
                 LOXO-101
                                0.00
                                        0.00
                                               0.00
                                                         2
                                                         2
                 LY2109761
                                0.00
                                        0.00
                                               0.00
                                                      2
                    M-25
                             0.00
                                     0.00
                                            0.00
                   MCOPPB
                                0.00
                                        0.00
                                                         2
                                               0.00
                                       0.00
                  ME-0328
                               0.00
                                              0.00
                                                        2
                                                       2
                   ME0328
                               0.00
                                      0.00
                                              0.00
                                                       2
                   ML-193
                              00.0
                                      00.0
                                              00.0
                   ML-228
                              0.00
                                      0.00
                                              0.00
                                                       2
                                                       2
                   ML-323
                                              0.00
                              0.00
                                      0.00
N-alpha-Methylhistamine-dihydrochloride
                                                          0.00
                                                                    2
                                           0.00
                                                   0.00
                                            0.00
                                                    0.00
                                                             2
         N6-cyclopentyladenosine
                                     0.00
                NNC-55-0396
                                 00.0
                                         0.00
                                                0.00
                                                          2
                                                       2
                   NODI-1
                              0.00
                                      0.00
                                              0.00
                  NS-11021
                               0.00
                                       0.00
                                              0.00
                                                        1
                                     0.00
                                             0.00
                                                      2
                   NS-309
                              0.00
                NSC-625987
                                 0.00
                                        0.00
                                                0.00
                                                         2
                                                         2
                NSC-632839
                                 0.00
                                        0.00
                                                0.00
                NSC-663284
                                 0.00
                                        0.00
                                                0.00
                                                         2
                                        0.00
                                               0.00
                 NSC-95397
                                0.00
                                                           2
                NVP-ADW742
                                   0.00
                                          0.00
                                                  00.0
                 NVP-AEW541
                                   0.00
                                          0.00
                                                  0.00
                                                           1
                                                          2
                NVP-HSP990
                                  0.00
                                         0.00
                                                 0.00
                  PD-98059
                               0.00
                                       0.00
                                              0.00
                                                        2
                               0.00
                                       0.00
                                              0.00
                                                        2
                   PETCM
                PF-03758309
                                0.00
                                        0.00
                                                0.00
                                                         1
                PF-04217903
                                0.00
                                        0.00
                                                0.00
                                                         2
                PF-05190457
                                0.00
                                        0.00
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PF-431396
                      0.00
                              0.00
                                     0.00
                                               2
          PFI-1
                   0.00
                           0.00
                                   0.00
                                            2
                                                 3
       PHA-793887
                        0.25
                               0.33
                                       0.29
          PP-1
                   0.00
                           0.00
                                  0.00
                                             2
         PP-121
                    0.00
                            0.00
                                    0.00
          PP-2
                   00.0
                           0.00
                                  0.00
                                            1
       RGB-286638
                        0.00
                               0.00
                                       0.00
                                                 2
        RGFP966
                      0.00
                              0.00
                                      0.00
                                               2
        RKI-1447
                      0.00
                              0.00
                                     0.00
                                               2
                                                2
       RX-821002
                       0.00
                              0.00
                                      0.00
                                                2
       Ro-1138452
                       0.00
                              0.00
                                      0.00
       SB-202190
                      0.00
                              0.00
                                      0.00
                                               1
       SB-203580
                      0.00
                              0.00
                                      0.00
                                               2
         SGX523
                      00.0
                             00.0
                                     00.0
                                               2
SRC-kinase-inhibitor-I
                                 0.00
                                                   2
                         0.00
                                         0.00
         SU3327
                     0.25
                             1.00
                                     0.40
                                              1
                                    0.00
                                              1
       SirReal-2
                     0.00
                            0.00
       TC-S-7004
                                               2
                      0.00
                              0.00
                                      0.00
         TCN201
                     0.00
                             0.00
                                     0.00
                                               2
                                              2
        TFC-007
                     0.00
                             0.00
                                     0.00
                                              2
         TG-003
                     0.00
                            0.00
                                    0.00
          TG-02
                    0.00
                            0.00
                                    0.00
                                             2
       TG-101348
                      0.67
                              1.00
                                      0.80
                                               2
        TUG-891
                      0.00
                              0.00
                                     0.00
                                               2
                                               2
        UNC1999
                       1.00
                              0.50
                                      0.67
                                               2
        UNC2025
                      0.00
                              0.00
                                      0.00
          VU591
                     0.00
                            0.00
                                    0.00
                                              2
                                               2
        WH-4-023
                       1.00
                              0.50
                                      0.67
          YC-1
                   0.00
                           0.00
                                   0.00
                                             2
        ZK-93423
                              0.00
                                               3
                      0.00
                                     0.00
        ZK811752
                      0.00
                              0.00
                                      0.00
                                               2
                                                2
       ZM-336372
                       0.00
                               0.00
                                      0.00
     acalabrutinib
                     0.00
                             0.00
                                     0.00
                                               2
                                                2
     acetohexamide
                       0.00
                               0.00
                                       0.00
    acetylcysteine
                      0.00
                              0.00
                                     0.00
                                               2
                                               2
      afimoxifene
                      0.00
                             0.00
                                     0.00
         alda-1
                   0.00
                           0.00
                                   0.00
                                            2
      aloxistatin
                    0.00
                            0.00
                                    0.00
                                             1
                    0.00
                           0.00
                                   0.00
                                             2
       alrestatin
                     0.00
                                              2
       amiloride
                            0.00
                                    0.00
  aminopurvalanol-a
                         0.00
                                0.00
                                        0.00
                                                  1
                      0.00
                              0.00
                                     0.00
                                               2
       amlexanox
       amlodipine
                     0.00
                             0.00
                                     0.00
                                               2
       anandamide
                                               2
                      0.00
                              0.00
                                      0.00
       anisomycin
                      0.00
                              0.00
                                     0.00
                                               1
        apatinib
                    0.00
                           00.0
                                   0.00
                                             2
```

arcyriaflavin-a	0.00	0.00	0.00	2
arundic-acid	0.00	0.00	0.00	2 2
ascorbic-acid	0.00	0.00	0.00	2
azacitidine	0.00	0.00	0.00	3
azathioprine	0.00	0.00	0.00	2
azeliragon	0.00	0.00	0.00	2
baclofen	0.00	0.00	0.00	2
batimastat	0.00	0.00	0.00	2
benzamil	0.00	0.00	0.00	2 2
bepridil	0.00	0.00	0.00	2
briciclib	0.33		0.40	2
brinzolamide	0.00	0.00	0.00	1
bufexamac	0.00	0.00	0.00	2
buparlisib	0.00	0.00	0.00	3
carzenide	0.00	0.00	0.00	2
castanospermine				2
cediranib	0.33	0.50	0.40	2
			0.00	2
citric-acid	0.00	0.00	0.00	2
colchicine	0.00	0.00	0.00	2 2 2 2 2
conivaptan	0.00	0.00	0.00	2
conivapian	0.00	0.00	0.00	2
				2
cycloheximide				
cyclosporine	0.00	0.00	0.00	2 1
dalbavancin	0.00	0.00	0.00	
dalfampridine	0.00	0.00	0.00	2
danusertib	0.00	0.00	0.00	2
deferasirox	0.00	0.00	0.00	2
delanzomib	0.00	0.00	0.00	1
desonide	0.00	0.00	0.00	2
dexamethason				2
diacerein			0.00	2
dilazep	0.00	0.00	0.00	2
droxinostat	0.00	0.00	0.00	2 2 2 2 2
dyphylline	0.00	0.00	0.00	2
edoxaban	0.00	0.00	0.00	2
efaproxiral	0.00	0.00	0.00	2
enflurane	0.00	0.00	0.00	
enilconazole	0.00	0.00	0.00	2
epoprostenol	0.00	0.00	0.00	2 2
epothilone-b	0.00	0.00	0.00	2
ethoxzolamide				2
ethyl-pyruvate	0.00	0.00	0.00	2
felodipine	0.00	0.00	0.00	2
filgotinib	0.00	0.00	0.00	2
flindokalner	0.00	0.00	0.00	2

fludarabine	0.00	0.00	0.00	2
flufenamic-acid				2
flupirtine	0.00	0.00	0.00	2
fomepizole	0.00	0.00	0.00	1
formononetin	0.00	0.00	0.00	2
gabapentin-enacarl	oil 0.	00 0.	0.0	0 2
ganetespib	0.00	0.00	0.00	3
geldanamycin	0.00	0.00	0.00	2
glutamine-(l)	0.00	0.00	0.00	2
glyburide	0.00	0.00	0.00	2
guanidine	0.00	0.00	0.00	1
halopemide	0.00	0.00	0.00	1
hexestrol	0.00	0.00	0.00	2
ibudilast	0.00	0.00	0.00	2
ibutamoren	0.00	0.00	0.00	2
ibutilide	0.00	0.00	0.00	1
ilomastat	0.00	0.00	0.00	2
ingenol-mebutat				2
isoflurane	0.00	0.00	0.00	2
ixabepilone	0.00	0.00	0.00	1
leflunomide	0.00	0.00	0.00	2
lercanidipine	0.00	0.00	0.00	2
lonafarnib	0.00	0.00	0.00	3
meclofenamic-ac			0.0	0 2
		.00	0.0	_
			0.00	
menadione	0.00	0.00	0.00	2 2
menadione methoxsalen	0.00	0.00	0.00	2 2
menadione methoxsalen miglitol	0.00 0.00 0.00	0.00 0.00 0.00	0.00 0.00 0.00	2 2 2
menadione methoxsalen miglitol minocycline	0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00	2 2 2 2
menadione methoxsalen miglitol minocycline misoprostol	0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00	2 2 2 2 2
menadione methoxsalen miglitol minocycline misoprostol motesanib	0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00	2 2 2 2 2 1
menadione methoxsalen miglitol minocycline misoprostol motesanib nafamostat	0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00	2 2 2 2 2 1 1
menadione methoxsalen miglitol minocycline misoprostol motesanib nafamostat nialamide	0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00	2 2 2 2 2 1 1 2
menadione methoxsalen miglitol minocycline misoprostol motesanib nafamostat nialamide nilvadipine	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	2 2 2 2 2 1 1 2 1
menadione methoxsalen miglitol minocycline misoprostol motesanib nafamostat nialamide nilvadipine octreotide	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	2 2 2 2 1 1 2 1 2
menadione methoxsalen miglitol minocycline misoprostol motesanib nafamostat nialamide nilvadipine octreotide olopatadine	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	2 2 2 2 2 1 1 2 1 2 2
menadione methoxsalen miglitol minocycline misoprostol motesanib nafamostat nialamide nilvadipine octreotide olopatadine oxibendazole	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	2 2 2 2 1 1 2 1 2 2 2
menadione methoxsalen miglitol minocycline misoprostol motesanib nafamostat nialamide nilvadipine octreotide olopatadine oxibendazole oxytocin	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	2 2 2 2 1 1 2 1 2 2 1
menadione methoxsalen miglitol minocycline misoprostol motesanib nafamostat nialamide nilvadipine octreotide olopatadine oxibendazole oxytocin ozagrel	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	2 2 2 2 1 1 2 1 2 2 1 2
menadione methoxsalen miglitol minocycline misoprostol motesanib nafamostat nialamide nilvadipine octreotide olopatadine oxibendazole oxytocin ozagrel paliperidone	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	2 2 2 2 1 1 2 1 2 2 1 2 1 2
menadione methoxsalen miglitol minocycline misoprostol motesanib nafamostat nialamide nilvadipine octreotide olopatadine oxibendazole oxytocin ozagrel paliperidone pazopanib	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	2 2 2 2 1 1 2 1 2 2 1 2 1 2 1 2
menadione methoxsalen miglitol minocycline misoprostol motesanib nafamostat nialamide nilvadipine octreotide olopatadine oxibendazole oxytocin ozagrel paliperidone pazopanib phenylbutazone	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	2 2 2 2 1 1 2 1 2 2 1 2 1 2 1 2
menadione methoxsalen miglitol minocycline misoprostol motesanib nafamostat nialamide nilvadipine octreotide olopatadine oxibendazole oxytocin ozagrel paliperidone pazopanib phenylbutazone picrotin	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	2 2 2 2 1 1 2 1 2 2 1 2 1 2 1 2 1 2
menadione methoxsalen miglitol minocycline misoprostol motesanib nafamostat nialamide nilvadipine octreotide olopatadine oxibendazole oxytocin ozagrel paliperidone pazopanib phenylbutazone picrotin polydatin	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	2 2 2 2 1 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1
menadione methoxsalen miglitol minocycline misoprostol motesanib nafamostat nialamide nilvadipine octreotide olopatadine oxibendazole oxytocin ozagrel paliperidone pazopanib phenylbutazone picrotin polydatin ponatinib	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	2 2 2 2 1 1 2 1 2 2 1 2 1 2 1 2 1 2 1 2
menadione methoxsalen miglitol minocycline misoprostol motesanib nafamostat nialamide nilvadipine octreotide olopatadine oxibendazole oxytocin ozagrel paliperidone pazopanib phenylbutazone picrotin polydatin	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	2 2 2 2 1 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1

quinidine	0.00	0.00	0.00	2
quinine	0.00	0.00	0.00	2
racecadotril	0.00	0.00	0.00	2
rifamycin	0.00	0.00	0.00	2
riociguat	0.00	0.00	0.00	2
ruxolitinib	0.00	0.00	0.00	1
ryuvidine	0.00	0.00	0.00	1
saclofen	0.00	0.00	0.00	2
sacubitril	0.00	0.00	0.00	1
somatostatin	0.00	0.00	0.00	2
sorbinil	0.00	0.00	0.00	2
sotrastaurin	0.00	0.00	0.00	2
spiroxatrine	0.00	0.00	0.00	2
sulfasalazine	1.00	1.00	1.00	1
sulfinpyrazone	0.00	0.00	0.00	2
taladegib	0.00	0.00	0.00	2
thioguanine	0.00	0.00	0.00	3
thiostrepton	0.33	0.33	0.33	3
torcitabine	0.00	0.00	0.00	2
tranilast	0.00	0.00	0.00	2
trazodone	0.00	0.00	0.00	1
trihexyphenidyl	0.00	0.0	0.00	2
vitamin-E	0.00	0.00	0.00	2
vitamin-E zamifenacin		0.00	0.00	2 2
zamifenacin	0.00	0.00	0.00	2
zamifenacin accuracy	0.00	0.00	0.00	2
zamifenacin	0.00	0.00 0.03	0.00 .12 57 0.03	2

--- With Cellpose features --precision recall f1-score support

1-octanol	0.00	0.00	0.00	2	
2,5-furandimethan	ol 0	.00 0	.00 0.	00	2
2-Oleoylglycerol	0.0	0.0	0.0	0 2	2
4-CMTB	0.00	0.00	0.00	2	
4-methylhistamin	e 0.0	00 0.	0.0	00	2
7-hydroxystaurospor	rine	0.50	0.50	0.50	2
A205804	0.00	0.00	0.00	1	
AC-710	0.17	0.50	0.25	2	
AK-7	0.00	0.00	0.00	2	
ANR-94	0.00	0.00	0.00	1	
AR-12	0.00	0.00	0.00	1	
AVL-292	0.50	0.50	0.50	2	
AZ191	0.50	0.50	0.50	2	

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AZD7762
                    00.0
                           0.00
                                  0.00
                                            3
      AZD9668
                    0.00
                           0.00
                                  0.00
                                            2
        BAM7
                  0.00
                          0.00
                                 0.00
                                           2
     BAN-ORL-24
                      0.00
                             0.00
                                              1
                                     0.00
BAX-channel-blocker
                        0.00
                               0.00
                                       0.00
                                                2
                            0.00
                                             2
    BAY-87-2243
                     0.00
                                    0.00
       BI-2536
                  0.75
                          1.00
                                 0.86
                                          3
                             0.00
     BMS-536924
                     0.00
                                    0.00
                                             1
       BQ-788
                  0.00
                          0.00
                                 0.00
                                           1
     BRL-50481
                            0.00
                                            2
                    0.00
                                   0.00
      BVT-948
                   0.00
                          0.00
                                  0.00
                                           2
       CC-401
                  0.00
                          0.00
                                 0.00
                                          2
     CCG-50014
                    0.00
                            0.00
                                   0.00
                                             2
     CCG-63802
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                            0.00
                                   0.00
                                             1
     CGP-53353
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                            0.00
                                   0.00
                                            1
     CP-724714
                    0.00
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                                   0.00
                                            2
                                            2
     CVT-10216
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                            0.00
                                   0.00
                                             2
     CYM-50260
                     0.00
                            0.00
                                    0.00
     CYM-50358
                                             2
                     0.00
                            0.00
                                    0.00
      CYM-5442
                    0.00
                            0.00
                                   0.00
                                             1
                                             2
      CYM-5520
                    0.00
                            0.00
                                   0.00
      CYT-997
                   0.40
                          0.67
                                  0.50
                                           3
     DDR1-IN-1
                                            2
                    0.00
                            0.00
                                   0.00
       DG-172
                  0.00
                          0.00
                                 0.00
                                           1
        DMSO
                   0.23
                          0.70
                                  0.34
                                          102
                       0.00
                               0.00
         EI1
                0.00
                                        2
       FK-866
                  0.00
                          0.00
                                          3
                                 0.00
      FPS-ZM1
                                            2
                    0.00
                           0.00
                                  0.00
                                 0.00
                                          2
       GK921
                  0.00
                          0.00
                         0.00
                                 0.00
                                          2
       GNF-5
                  0.00
      GNF-5837
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                    0.00
                           0.00
                                   0.00
     GSK-37647
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                                             2
     GSK1070916
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                                    0.00
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     GSK2110183
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                             0.00
                                    0.00
      GSK3787
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                                             2
     GW-311616
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                                   0.00
                             0.00
                                             2
    H2L-5765834
                     0.00
                                    0.00
                                           2
      IRL-2500
                   0.00
                          0.00
                                  0.00
                                           2
       IWP-L6
                  0.00
                          0.00
                                 0.00
                                          2
      JTE-607
                  0.00
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                                 0.00
                         0.00
                                0.00
        KG-5
                 0.00
                           0.00
                                            2
      KH-CB19
                    0.00
                                   0.00
      KU-55933
                    0.00
                           0.00
                                   0.00
                                            2
                                            2
      KU-60019
                    0.67
                           1.00
                                   0.80
     L-proline
                  0.00
                         0.00
                                 0.00
                                          2
     LDN-212854
                     0.00
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LDN-27219
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                  LGK-974
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                                                        2
                 LOXO-101
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                                                0.00
                                                         2
                 LY2109761
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                                        0.00
                                               0.00
                                                         2
                    M-25
                             0.00
                                     0.00
                                            0.00
                                                      2
                                                         2
                   MCOPPB
                                0.50
                                        0.50
                                               0.50
                                                        2
                  ME-0328
                               0.00
                                       0.00
                                              0.00
                                              0.00
                                                        2
                   ME0328
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                                       0.00
                                                       2
                   ML-193
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                                      0.00
                                              00.0
                                                       2
                   ML-228
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                                      0.00
                                              0.00
                   ML-323
                                                       2
                              0.00
                                      0.00
                                              0.00
N-alpha-Methylhistamine-dihydrochloride
                                           0.00
                                                   0.00
                                                           0.00
                                                                    2
         N6-cyclopentyladenosine
                                            0.00
                                                    0.00
                                                             2
                                     0.00
                NNC-55-0396
                                 0.00
                                         0.00
                                                 0.00
                                                          2
                   NQDI-1
                              0.00
                                                       2
                                      0.00
                                              0.00
                  NS-11021
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                                       0.00
                                              0.00
                                                        1
                                                       2
                   NS-309
                              0.00
                                      0.00
                                             0.00
                                                         2
                NSC-625987
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                                        0.00
                                                0.00
                                 0.00
                                        0.00
                                                0.00
                                                          2
                NSC-632839
                NSC-663284
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                                                         2
                 NSC-95397
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                                        0.00
                                               0.00
                NVP-ADW742
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                                           0.00
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                                                            2
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                                          0.00
                                                           1
                NVP-AEW541
                                                  0.00
                NVP-HSP990
                                  0.00
                                         0.00
                                                 0.00
                                                          2
                                                        2
                 PD-98059
                               0.00
                                       0.00
                                              0.00
                   PETCM
                               00.0
                                       0.00
                                              0.00
                                                        2
                PF-03758309
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                                                         1
                                        0.00
                                                0.00
                                                         2
                                                0.00
                PF-04217903
                                 0.00
                                        0.00
                PF-05190457
                                                         2
                                 0.00
                                        0.00
                                                0.00
                 PF-431396
                               0.50
                                       0.50
                                                        2
                                               0.50
                   PFI-1
                             0.00
                                    0.00
                                            0.00
                                                     2
                                                          3
                PHA-793887
                                 0.00
                                         0.00
                                                0.00
                    PP-1
                            0.33
                                    0.50
                                            0.40
                                                     2
                   PP-121
                                                      2
                              0.50
                                     0.50
                                             0.50
                    PP-2
                            0.33
                                    1.00
                                            0.50
                                                     1
                                                          2
                RGB-286638
                                 0.00
                                         0.00
                                                0.00
                  RGFP966
                                0.00
                                       0.00
                                               00.0
                                                        2
                  RKI-1447
                               0.00
                                       0.00
                                              0.00
                                                        2
                                                         2
                 RX-821002
                                0.00
                                        0.00
                                               0.00
                                                         2
                 Ro-1138452
                                0.00
                                        0.00
                                               0.00
                                0.00
                                       0.00
                                               0.00
                 SB-202190
                                                        1
                 SB-203580
                                0.33
                                       1.00
                                               0.50
                                                        2
                   SGX523
                               0.00
                                       0.00
                                              0.00
                                                        2
                                                  0.00
                                                            2
         SRC-kinase-inhibitor-I
                                   0.00
                                          0.00
                   SU3327
                              0.00
                                      0.00
                                              0.00
                                                       1
                 SirReal-2
                              0.00
                                      0.00
                                             00.0
                                                       1
```

TC-S-7004	0.00	0.00	0.00	2	
TCN201	0.00	0.00	0.00		
TFC-007	0.00	0.00	0.00	2 2	
TG-003	0.00	0.00	0.00	2	
TG-02	0.00	0.00	0.00	2	
TG-101348	0.50			2	
TUG-891	0.00	0.00	0.00	2	
UNC1999	0.00			2	
UNC2025	0.00	0.00	0.00	2	
VU591	0.00	0.00	0.00	2	
WH-4-023	0.00	0.00	0.00	2	
YC-1	0.00	0.00	0.00	2	
ZK-93423	0.00	0.00	0.00	3	
ZK811752	0.00			2	
ZM-336372			0.00	2	
acalabrutinib	0.00	0.00	0.00	2	
acetohexamide	0.00	0.00	0.00	2	
acetylcysteine	0.00	0.00	0.00	2	
afimoxifene	0.00	0.00	0.00	2	
alda-1	0.00	0.00	0.00	2	
aloxistatin	0.00	0.00	0.00	1	
alrestatin	0.00	0.00	0.00	2	
amiloride	0.00	0.00	0.00	2	
aminopurvalanol	. 0.	00 00	0.00	1	
animopurvaianor	-a 0.	0.0	0.0) 1	
aminopur varanor amlexanox	-a 0.0	0.00	0.00	2	
amlexanox					
-	0.00	0.00	0.00	2	
amlexanox amlodipine	0.00	0.00	0.00	2 2	
amlexanox amlodipine anandamide anisomycin	0.00 0.00 0.00	0.00 0.00 0.00	0.00 0.00 0.00	2 2 2	
amlexanox amlodipine anandamide	0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00	2 2 2 1	
amlexanox amlodipine anandamide anisomycin apatinib	0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00	2 2 2 1 2 2	
amlexanox amlodipine anandamide anisomycin apatinib arcyriaflavin-a arundic-acid	0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00	2 2 2 1 2	
amlexanox amlodipine anandamide anisomycin apatinib arcyriaflavin-a arundic-acid ascorbic-acid	0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00	2 2 2 1 2 2 2	
amlexanox amlodipine anandamide anisomycin apatinib arcyriaflavin-a arundic-acid ascorbic-acid azacitidine	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.25	0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00	2 2 1 2 2 2 2 2 3	
amlexanox amlodipine anandamide anisomycin apatinib arcyriaflavin-a arundic-acid ascorbic-acid azacitidine azathioprine	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.25 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.33 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	2 2 1 2 2 2 2 2 3 2	
amlexanox amlodipine anandamide anisomycin apatinib arcyriaflavin-a arundic-acid ascorbic-acid azacitidine azathioprine azeliragon	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.25 0.00 0.50	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.33 0.00 0.50	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.29 0.00 0.50	2 2 1 2 2 2 2 2 3 2 2	
amlexanox amlodipine anandamide anisomycin apatinib arcyriaflavin-a arundic-acid ascorbic-acid azacitidine azathioprine azeliragon baclofen	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.25 0.00 0.50 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.33 0.00 0.50 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.29 0.00 0.50 0.00	2 2 1 2 2 2 2 2 3 2 2 2 2	
amlexanox amlodipine anandamide anisomycin apatinib arcyriaflavin-a arundic-acid ascorbic-acid azacitidine azathioprine azeliragon baclofen batimastat	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.25 0.00 0.50 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.33 0.00 0.50 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.29 0.00 0.50 0.00 0.00	2 2 1 2 2 2 2 2 3 2 2 2 2 2 2 2 2 2 2 2	
amlexanox amlodipine anandamide anisomycin apatinib arcyriaflavin-a arundic-acid ascorbic-acid azacitidine azathioprine azeliragon baclofen batimastat benzamil	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.25 0.00 0.50 0.00 0.0	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.33 0.00 0.50 0.00 0.0	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.29 0.00 0.50 0.00 0.00	2 2 1 2 2 2 2 2 3 2 2 2 2 2 2 2 2 2 2 2	
amlexanox amlodipine anandamide anisomycin apatinib arcyriaflavin-a arundic-acid ascorbic-acid azacitidine azathioprine azeliragon baclofen batimastat benzamil	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.25 0.00 0.50 0.00 0.0	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.33 0.00 0.50 0.00 0.0	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.29 0.00 0.50 0.00 0.00 0.00	2 2 1 2 2 2 2 2 3 2 2 2 2 2 2 2 2 2 2 2	
amlexanox amlodipine anandamide anisomycin apatinib arcyriaflavin-a arundic-acid ascorbic-acid azacitidine azathioprine azeliragon baclofen batimastat benzamil bepridil briciclib	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.25 0.00 0.50 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.33 0.00 0.50 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.29 0.00 0.50 0.00 0.00 0.00 0.00	2 2 1 2 2 2 2 2 3 2 2 2 2 2 2 2 2 2 2 2	
amlexanox amlodipine anandamide anisomycin apatinib arcyriaflavin-a arundic-acid ascorbic-acid azacitidine azathioprine azeliragon baclofen batimastat benzamil bepridil briciclib	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.25 0.00 0.50 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.33 0.00 0.50 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.29 0.00 0.50 0.00 0.00 0.00 0.00	2 2 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	
amlexanox amlodipine anandamide anisomycin apatinib arcyriaflavin-a arundic-acid ascorbic-acid azacitidine azathioprine azeliragon baclofen batimastat benzamil bepridil briciclib brinzolamide bufexamac	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.25 0.00 0.50 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.33 0.00 0.50 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.29 0.00 0.50 0.00 0.00 0.00 0.00 0.00	2 2 2 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	
amlexanox amlodipine anandamide anisomycin apatinib arcyriaflavin-a arundic-acid ascorbic-acid azacitidine azathioprine azeliragon baclofen batimastat benzamil bepridil briciclib brinzolamide bufexamac buparlisib	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.25 0.00 0.50 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.33 0.00 0.50 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.29 0.00 0.50 0.00 0.00 0.00 0.00 0.00 0.00	2 2 2 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	
amlexanox amlodipine anandamide anisomycin apatinib arcyriaflavin-a arundic-acid ascorbic-acid azacitidine azathioprine azeliragon baclofen batimastat benzamil bepridil briciclib brinzolamide bufexamac buparlisib carzenide	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.25 0.00 0.50 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.33 0.00 0.50 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.29 0.00 0.50 0.00 0.00 0.00 0.00 0.00 0.00 0.00	2 2 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	
amlexanox amlodipine anandamide anisomycin apatinib arcyriaflavin-a arundic-acid ascorbic-acid azacitidine azathioprine azeliragon baclofen batimastat benzamil bepridil briciclib brinzolamide bufexamac buparlisib	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.25 0.00 0.50 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.33 0.00 0.50 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.29 0.00 0.50 0.00 0.00 0.00 0.00 0.00 0.00 0.00	2 2 2 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	

cetilistat	0.00	0.00	0.00	2
citric-acid	0.00	0.00	0.00	2
colchicine	0.33	0.50	0.40	2
conivaptan	0.00	0.00	0.00	2
coumarin	0.00	0.00	0.00	2
cycloheximide	0.00			2
cyclosporine	0.00	0.00	0.00	2
dalbavancin	0.00	0.00	0.00	1
dalfampridine	0.00			2
danusertib	0.00	0.00	0.00	2
deferasirox	0.00	0.00	0.00	2
delanzomib	0.00	0.00	0.00	1
desonide	0.00	0.00	0.00	2
dexamethason				
diacerein	0.00	0.00	0.00	2
dilazep	0.00	0.00	0.00	2
droxinostat	0.00	0.00	0.00	2
dyphylline	0.00	0.00	0.00	
edoxaban	0.00	0.00	0.00	2 2
efaproxiral	0.00	0.00	0.00	2
enflurane	0.00	0.00	0.00	2
enilconazole	0.00	0.00	0.00	2
epoprostenol	0.00	0.00	0.00	2
epothilone-b	0.00	0.00	0.00	2
ethoxzolamide				2
ethyl-pyruvate	0.00	0.00		2
felodipine	0.00	0.00	0.00	2
filgotinib	0.00	0.00	0.00	2
flindokalner	0.00	0.00	0.00	2
fludarabine	0.00	0.00	0.00	$\overset{2}{2}$
flufenamic-acid				2
		0.00	0.00	2
fomepizole	0.00		0.00	1
formononetin				2
gabapentin-enacarl			0.0 0.0	
ganetespib	0.00	0.00	0.00	3
geldanamycin				2
glutamine-(l)	0.00	0.00	0.00	2
glyburide	0.00	0.00	0.00	2
guanidine	0.00	0.00	0.00	1
halopemide	0.00	0.00	0.00	1
hexestrol	0.00	0.00	0.00	2
ibudilast	0.00	0.00	0.00	$\overset{2}{2}$
ibutamoren	0.00	0.00	0.00	2
ibutilide	0.00	0.00	0.00	1
ilomastat	0.00	0.00	0.00	2
Homastat	0.00	0.00	0.00	2

ingenol-mebutat	te 0.0	0.0	0.00		2
isoflurane	0.00	0.00	0.00	2	
ixabepilone	0.25	1.00	0.40	1	
leflunomide	0.00	0.00	0.00	2	
lercanidipine	0.00	0.00	0.00	2	
lonafarnib	0.00	0.00	0.00	3	
meclofenamic-ad	cid 0.	00 0.	0.0	0	2
menadione	0.00	0.00	0.00	2	
methoxsalen	0.00	0.00	0.00	2	
miglitol	0.00	0.00	0.00	2	
minocycline	0.00	0.00	0.00	2	
misoprostol	0.00	0.00	0.00	2	
motesanib	0.00	0.00	0.00	1	
nafamostat	0.00	0.00	0.00	1	
nialamide	0.00	0.00	0.00	2	
nilvadipine	0.00	0.00	0.00	1	
octreotide	0.00	0.00	0.00	2	
olopatadine	0.00	0.00	0.00	2	
oxibendazole	0.00	0.00	0.00	2	
oxytocin	0.00	0.00	0.00	1	
ozagrel	0.00	0.00	0.00	2	
paliperidone	0.00	0.00	0.00	1	
pazopanib	0.00	0.00	0.00	2	
phenylbutazon			0.00		1
picrotin				•	
picionii	0.00	0.00	0.00	2	
			0.00	2	
polydatin	0.00	0.00	0.00	2	
polydatin ponatinib	0.00 0.50	0.00 1.00	0.00 0.67	2 2	
polydatin ponatinib puromycin	0.00 0.50 1.00	0.00 1.00 0.50	0.00 0.67 0.67	2 2 2	
polydatin ponatinib puromycin purvalanol-a	0.00 0.50 1.00 0.00	0.00 1.00 0.50 0.00	0.00 0.67 0.67 0.00	2 2 2 2	
polydatin ponatinib puromycin purvalanol-a quinidine	0.00 0.50 1.00	0.00 1.00 0.50	0.00 0.67 0.67	2 2 2	
polydatin ponatinib puromycin purvalanol-a	0.00 0.50 1.00 0.00 0.00 0.00	0.00 1.00 0.50 0.00 0.00 0.00	0.00 0.67 0.67 0.00 0.00	2 2 2 2 2	
polydatin ponatinib puromycin purvalanol-a quinidine quinine racecadotril	0.00 0.50 1.00 0.00 0.00 0.00 0.00	0.00 1.00 0.50 0.00 0.00	0.00 0.67 0.67 0.00 0.00 0.00 0.00	2 2 2 2 2 2 2	
polydatin ponatinib puromycin purvalanol-a quinidine quinine racecadotril rifamycin	0.00 0.50 1.00 0.00 0.00 0.00 0.00 0.00	0.00 1.00 0.50 0.00 0.00 0.00 0.00 0.00	0.00 0.67 0.67 0.00 0.00 0.00 0.00 0.00	2 2 2 2 2 2 2 2	
polydatin ponatinib puromycin purvalanol-a quinidine quinine racecadotril rifamycin riociguat	0.00 0.50 1.00 0.00 0.00 0.00 0.00 0.00	0.00 1.00 0.50 0.00 0.00 0.00 0.00 0.00	0.00 0.67 0.67 0.00 0.00 0.00 0.00 0.00	2 2 2 2 2 2 2 2 2 2	
polydatin ponatinib puromycin purvalanol-a quinidine quinine racecadotril rifamycin riociguat ruxolitinib	0.00 0.50 1.00 0.00 0.00 0.00 0.00 0.00	0.00 1.00 0.50 0.00 0.00 0.00 0.00 0.00	0.00 0.67 0.67 0.00 0.00 0.00 0.00 0.00	2 2 2 2 2 2 2 2	
polydatin ponatinib puromycin purvalanol-a quinidine quinine racecadotril rifamycin riociguat ruxolitinib ryuvidine	0.00 0.50 1.00 0.00 0.00 0.00 0.00 0.00	0.00 1.00 0.50 0.00 0.00 0.00 0.00 0.00	0.00 0.67 0.67 0.00 0.00 0.00 0.00 0.00	2 2 2 2 2 2 2 2 2 2 1 1	
polydatin ponatinib puromycin purvalanol-a quinidine quinine racecadotril rifamycin riociguat ruxolitinib ryuvidine saclofen	0.00 0.50 1.00 0.00 0.00 0.00 0.00 0.00	0.00 1.00 0.50 0.00 0.00 0.00 0.00 0.00	0.00 0.67 0.67 0.00 0.00 0.00 0.00 0.00	2 2 2 2 2 2 2 2 2 2 1	
polydatin ponatinib puromycin purvalanol-a quinidine quinine racecadotril rifamycin riociguat ruxolitinib ryuvidine saclofen sacubitril	0.00 0.50 1.00 0.00 0.00 0.00 0.00 0.00	0.00 1.00 0.50 0.00 0.00 0.00 0.00 0.00	0.00 0.67 0.67 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	2 2 2 2 2 2 2 2 2 2 1 1 2 1	
polydatin ponatinib puromycin purvalanol-a quinidine quinine racecadotril rifamycin riociguat ruxolitinib ryuvidine saclofen sacubitril somatostatin	0.00 0.50 1.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 1.00 0.50 0.00 0.00 0.00 0.00 0.00	0.00 0.67 0.67 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	2 2 2 2 2 2 2 2 2 1 1 2 1 2	
polydatin ponatinib puromycin purvalanol-a quinidine quinine racecadotril rifamycin riociguat ruxolitinib ryuvidine saclofen sacubitril somatostatin sorbinil	0.00 0.50 1.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 1.00 0.50 0.00 0.00 0.00 0.00 0.00	0.00 0.67 0.67 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	2 2 2 2 2 2 2 2 2 1 1 2 1 2 2	
polydatin ponatinib puromycin purvalanol-a quinidine quinine racecadotril rifamycin riociguat ruxolitinib ryuvidine saclofen sacubitril somatostatin sorbinil	0.00 0.50 1.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 1.00 0.50 0.00 0.00 0.00 0.00 0.00	0.00 0.67 0.67 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	2 2 2 2 2 2 2 2 2 1 1 2 1 2 2 2 2	
polydatin ponatinib puromycin purvalanol-a quinidine quinine racecadotril rifamycin riociguat ruxolitinib ryuvidine saclofen sacubitril somatostatin sorbinil sotrastaurin spiroxatrine	0.00 0.50 1.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 1.00 0.50 0.00 0.00 0.00 0.00 0.00	0.00 0.67 0.67 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	2 2 2 2 2 2 2 2 2 1 1 2 1 2 2 2 2 2 2 2	
polydatin ponatinib puromycin purvalanol-a quinidine quinine racecadotril rifamycin riociguat ruxolitinib ryuvidine saclofen sacubitril somatostatin sorbinil sotrastaurin spiroxatrine sulfasalazine	0.00 0.50 1.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 1.00 0.50 0.00 0.00 0.00 0.00 0.00	0.00 0.67 0.67 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	2 2 2 2 2 2 2 2 1 1 2 1 2 2 2 1 2 1 2 1	
polydatin ponatinib puromycin purvalanol-a quinidine quinine racecadotril rifamycin riociguat ruxolitinib ryuvidine saclofen sacubitril somatostatin sorbinil sotrastaurin spiroxatrine sulfasalazine sulfinpyrazone	0.00 0.50 1.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 1.00 0.50 0.00 0.00 0.00 0.00 0.00	0.00 0.67 0.67 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	2 2 2 2 2 2 2 2 1 1 2 2 2 2 2 2 2 2 2 2	
polydatin ponatinib puromycin purvalanol-a quinidine quinine racecadotril rifamycin riociguat ruxolitinib ryuvidine saclofen sacubitril somatostatin sorbinil sotrastaurin spiroxatrine sulfasalazine	0.00 0.50 1.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 1.00 0.50 0.00 0.00 0.00 0.00 0.00	0.00 0.67 0.67 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	2 2 2 2 2 2 2 2 1 1 2 1 2 2 2 1 2 1 2 1	

thiostrepton 0.00 0.00 0.00 3 torcitabine 0.00 0.00 0.00 2 tranilast 0.00 0.00 0.00 2 0.00 0.00 1 trazodone 0.00 trihexyphenidyl 0.00 0.00 0.00 2 2 vitamin-E 0.00 0.00 0.00 zamifenacin 0.00 2 0.00 0.00 accuracy 0.18 574 0.05 0.06 0.05 574 macro avg weighted avg 0.08 0.18 0.11 574

--- CNN Baseline (Grayscale Only) [Final Test Evaluation] --- precision recall f1-score support

0.00 0.00 0.00 1-octanol 2,5-furandimethanol 0.00 0.00 0.00 1 2-Oleoylglycerol 0.00 0.00 0.00 4 3 4-CMTB 0.00 0.00 0.00 4-methylhistamine 0.00 0.00 0.00 1 A205804 0.00 0.00 0.00 1 AC-710 0.00 0.00 0.00 1 AK-7 0.00 0.00 0.00 2 ANR-94 0.000.0000.0 4 0.00 0.00 0.00 1 AR-12 0.00AVL-292 0.00 0.00 1 0.00 0.00 0.00 AZ191 1 2 AZD7762 0.00 0.00 0.00 AZD9668 0.00 0.00 0.00 2 BAM7 0.00 0.00 0.00 1 0.00BAN-ORL-24 0.00 0.00 2 0.00 3 BAX-channel-blocker 0.00 0.00 BAY-87-2243 0.00 0.00 0.00 1 BI-2536 0.00 0.00 0.00 3 BMS-536924 0.000.00 3 0.00 3 BQ-788 0.00 0.00 0.00 BVT-948 3 0.00 0.00 0.00 3 CC-401 0.00 0.00 0.00 0.00 CCG-50014 0.00 0.00 1 0.00 0.00 3 CCG-63802 0.00 0.00 0.00 0.00 CP-724714 1 CVT-10216 3 0.00 0.00 0.00 2 CYM-50260 0.00 0.00 0.00 CYM-50358 0.00 0.000.002

```
CYM-5442
                                0.00
                                        0.00
                                               0.00
                                                         1
                  CYM-5520
                                0.00
                                        0.00
                                               0.00
                                                         1
                  CYT-997
                               0.00
                                      0.00
                                              0.00
                                                       2
                                0.00
                                                         3
                 DDR1-IN-1
                                        0.00
                                               0.00
                   DG-172
                              0.00
                                      0.00
                                             0.00
                                                       1
                                                       78
                    DMSO
                               0.18
                                      1.00
                                              0.31
                                   0.00
                                           0.00
                    EI1
                            0.00
                              0.00
                                     0.00
                                             0.00
                   FK-866
                                                       4
                  FPS-ZM1
                                0.00
                                       0.00
                                               0.00
                                                        1
                GSK1070916
                                 0.00
                                         0.00
                                                0.00
                                                          1
                GSK2110183
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                                                          6
                  GSK3787
                                0.00
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                 GW-311616
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                                                         3
                H2L-5765834
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                                         0.00
                                                0.00
                                                          1
                  IRL-2500
                               0.00
                                      0.00
                                              0.00
                                                       1
                   IWP-L6
                              0.00
                                      0.00
                                             0.00
                                                       1
                    KG-5
                             0.00
                                     0.00
                                            0.00
                                                      2
                  KU-55933
                                                        2
                                0.00
                                       0.00
                                               0.00
                  KU-60019
                                       0.00
                                                        1
                                0.00
                                               0.00
                 L-proline
                              0.00
                                     0.00
                                             0.00
                                                      2
                 LDN-27219
                                0.00
                                        0.00
                                                         2
                                               0.00
                 LY2109761
                                0.00
                                        0.00
                                               0.00
                                                         2
                   MCOPPB
                                        0.00
                                               0.00
                                                         1
                                0.00
                  ME-0328
                               0.00
                                       0.00
                                              0.00
                                                        2
                   ME0328
                               0.00
                                      0.00
                                              0.00
                                                       1
                   ML-323
                               00.0
                                      0.00
                                              0.00
                                                       1
N-alpha-Methylhistamine-dihydrochloride
                                           0.00
                                                          0.00
                                                                    1
                                                   0.00
                NNC-55-0396
                                 00.0
                                                0.00
                                         0.00
                                                          1
                              0.00
                   NQDI-1
                                      0.00
                                             0.00
                                                       3
                   NS-309
                              0.00
                                     0.00
                                             0.00
                                                       1
                NSC-625987
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                                        0.00
                                                0.00
                                                         1
                NSC-632839
                                 0.00
                                        0.00
                                                0.00
                                                         2
                 NSC-95397
                                0.00
                                        0.00
                                               0.00
                                                         1
                 NVP-ADW742
                                   0.00
                                          0.00
                                                  0.00
                                                           1
                NVP-AEW541
                                   0.00
                                          0.00
                                                  0.00
                                                           2
                                                          2
                NVP-HSP990
                                  0.00
                                         0.00
                                                 0.00
                 PD-98059
                               0.00
                                       0.00
                                              0.00
                                                        1
                   PETCM
                               0.00
                                       0.00
                                              0.00
                                                        2
                                 00.0
                                        0.00
                                                         2
                PHA-793887
                                                0.00
                    PP-1
                            0.00
                                    0.00
                                           0.00
                                                     1
                   PP-121
                                     0.00
                                             0.00
                                                      1
                             0.00
                    PP-2
                            0.00
                                    0.00
                                           0.00
                                                     2
                  RKI-1447
                               0.00
                                                        3
                                       0.00
                                              0.00
                                                        2
                 SB-203580
                                0.00
                                       0.00
                                               0.00
                   SGX523
                               0.00
                                       0.00
                                              0.00
                                                        1
         SRC-kinase-inhibitor-I
                                   0.00
                                          0.00
                                                  0.00
                                                           2
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G' D 12 000 000 000 2
SirReal-2 0.00 0.00 0.00 2
TC-S-7004 0.00 0.00 0.00 1
TCN201 0.00 0.00 0.00 1
TG-02 0.00 0.00 0.00 2
TUG-891 0.00 0.00 0.00 2
UNC1999 0.00 0.00 0.00 2
VU591 0.00 0.00 0.00 1
YC-1 0.00 0.00 0.00 3
ZK-93423 0.00 0.00 0.00 3
ZK811752 0.00 0.00 0.00 1
ZM-336372 0.00 0.00 0.00 1
acalabrutinib 0.00 0.00 0.00 1
acetohexamide 0.00 0.00 0.00 1
acetylcysteine 0.00 0.00 0.00 2
afimoxifene 0.00 0.00 0.00 2
alda-1 0.00 0.00 0.00 1
alrestatin 0.00 0.00 0.00 1
amiloride 0.00 0.00 0.00 2
aminopurvalanol-a 0.00 0.00 0.00 1
amlexanox 0.00 0.00 0.00 1
amlodipine 0.00 0.00 0.00 3
anandamide 0.00 0.00 0.00 1
anisomycin 0.00 0.00 0.00 3
arcyriaflavin-a 0.00 0.00 0.00 2
arundic-acid 0.00 0.00 0.00 4
ascorbic-acid 0.00 0.00 0.00 3
azacitidine 0.00 0.00 0.00 3
azathioprine 0.00 0.00 0.00 2
baclofen 0.00 0.00 0.00 5
batimastat 0.00 0.00 0.00 1
benzamil 0.00 0.00 0.00 2
bepridil 0.00 0.00 0.00 2
brinzolamide 0.00 0.00 0.00 2
buparlisib 0.00 0.00 0.00 1
carzenide 0.00 0.00 0.00 1
castanospermine 0.00 0.00 0.00 2
cetilistat 0.00 0.00 0.00 1
colchicine 0.00 0.00 0.00 1
1
cyclosporine 0.00 0.00 0.00 4 dalbavancin 0.00 0.00 0.00 3
dalfampridine 0.00 0.00 0.00 1
danusertib 0.00 0.00 0.00 2
delanzomib 0.00 0.00 0.00 1
dexamethasone 0.00 0.00 0.00 3

1	0.00	0.00	0.00	4	
diacerein	0.00	0.00	0.00	1	
dilazep	0.00	0.00	0.00	1	
droxinostat	0.00	0.00	0.00	4	
edoxaban	0.00	0.00	0.00	3	
efaproxiral	0.00	0.00	0.00	2	
enflurane	0.00	0.00	0.00	3	
enilconazole	0.00	0.00	0.00	1	
epoprostenol	0.00	0.00	0.00	1	
ethoxzolamide					
ethyl-pyruvate	0.00			1	
felodipine	0.00	0.00	0.00	2	
filgotinib	0.00	0.00	0.00	3	
flindokalner	0.00	0.00	0.00	2	
fludarabine	0.00	0.00	0.00	2	
flupirtine	0.00	0.00	0.00	1	
fomepizole	0.00	0.00	0.00	2	
formononetin	0.00	0.00	0.00	1	
ganetespib	0.00	0.00	0.00	2	
geldanamycin	0.00	0.00	0.00	3	
glutamine-(l)	0.00	0.00	0.00	2	
glyburide	0.00	0.00	0.00	3	
halopemide	0.00	0.00	0.00	2	
ibudilast	0.00	0.00	0.00	1	
ibutamoren	0.00	0.00	0.00	3	
ingenol-mebutat	e 0.0	0.0	0.00) 1	
isoflurane	0.00	0.00	0.00	1	
ixabepilone	0.00	0.00	0.00	1	
leflunomide	0.00	0.00	0.00	1	
lonafarnib	0.00	0.00	0.00	5	
meclofenamic-ac	id 0.	.00 0	0.0	00 1	
menadione	0.00	0.00	0.00	2	
methoxsalen	0.00	0.00	0.00	2	
miglitol	0.00	0.00	0.00	2	
minocycline	0.00	0.00	0.00	1	
misoprostol	0.00	0.00	0.00	1	
nafamostat	0.00	0.00	0.00	1	
nialamide	0.00	0.00	0.00	2	
nilvadipine	0.00	0.00	0.00	3	
octreotide	0.00	0.00	0.00	1	
olopatadine	0.00	0.00	0.00	2	
oxibendazole	0.00			4	
oxytocin	0.00	0.00	0.00	2	
ozagrel	0.00	0.00	0.00	3	
paliperidone	0.00	0.00	0.00	1	
pazopanib	0.00	0.00	0.00	1	
phenylbutazon					
phonyrodiazon	0.0	0.0	0.00	<i>-</i>	

. ,.	0.00	0.00	0.00	1
picrotin	0.00	0.00	0.00	1
polydatin	0.00	0.00	0.00	1
ponatinib	0.00	0.00	0.00	1
purvalanol-a	0.00	0.00	0.00	2
quinidine	0.00	0.00	0.00	1
quinine	0.00	0.00	0.00	3
riociguat	0.00	0.00	0.00	3
ruxolitinib	0.00	0.00	0.00	2
saclofen	0.00	0.00	0.00	1
somatostatin	0.00	0.00	0.00	1
sotrastaurin	0.00	0.00	0.00	3
spiroxatrine	0.00	0.00	0.00	1
taladegib	0.00	0.00	0.00	2
thioguanine	0.00	0.00	0.00	4
thiostrepton	0.00	0.00	0.00	7
torcitabine	0.00	0.00	0.00	1
tranilast	0.00	0.00	0.00	2
trazodone	0.00	0.00	0.00	1
vitamin-E	0.00	0.00	0.00	1
zamifenacin	0.00	0.00	0.00	1
		0	10 4	2.1
accuracy				31
macro avg	0.00	0.01	0.00	431
weighted avg	0.03	0.18	0.06	431

--- CNN With Cellpose Mask [Final Test Evaluation] --- precision recall f1-score support

1-octanol	0.00	0.00	0.00	4	
4-CMTB	0.00	0.00	0.00	1	
4-methylhistamir	ne 0.0	0.0	0.0	00 1	
7-hydroxystaurospo	rine	0.00	0.00	0.00	3
A205804	0.00	0.00	0.00	1	
AC-710	0.00	0.00	0.00	4	
AK-7	0.00	0.00	0.00	1	
ANR-94	0.00	0.00	0.00	1	
AR-12	0.00	0.00	0.00	4	
AVL-292	0.00	0.00	0.00	1	
AZ191	0.00	0.00	0.00	2	
AZD7762	0.00	0.00	0.00	4	
AZD9668	0.00	0.00	0.00	2	
BAM7	0.00	0.00	0.00	1	
BAN-ORL-2	24 0.0	0.0	0.0	00 2	
BAY-87-2243	0.0	0.0	0.00) 1	
BI-2536	0.00	0.00	0.00	4	

```
2
                   BQ-788
                               00.0
                                      0.00
                                              0.00
                 BRL-50481
                                0.00
                                        0.00
                                               0.00
                                                         1
                                                        3
                  BVT-948
                               0.00
                                       0.00
                                              0.00
                   CC-401
                              0.00
                                      0.00
                                              0.00
                                                       1
                 CCG-50014
                                0.00
                                        0.00
                                                0.00
                                                         2
                                                         3
                 CCG-63802
                                0.00
                                        0.00
                                                0.00
                                                         2
                 CGP-53353
                                0.00
                                        0.00
                                                0.00
                                               0.00
                                                        2
                 CP-724714
                                0.00
                                       0.00
                 CVT-10216
                                0.00
                                        0.00
                                               0.00
                                                         1
                                                          2
                 CYM-50358
                                                0.00
                                 0.00
                                         0.00
                  CYT-997
                               0.00
                                       0.00
                                              0.00
                                                        4
                 DDR1-IN-1
                                0.00
                                        0.00
                                                0.00
                                                         4
                   DG-172
                               0.00
                                      0.00
                                              0.00
                                                       1
                                              0.27
                    DMSO
                               0.16
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                                                       68
                     EI1
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                   FK-866
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                                                       5
                  FPS-ZM1
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                   GNF-5
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                GSK1070916
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                GSK2110183
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                  GSK3787
                 GW-311616
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                  IRL-2500
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                  JTE-607
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                    KG-5
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                  KH-CB19
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                  KU-55933
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                 L-proline
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                LDN-212854
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                                                        2
                  LGK-974
                               0.00
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                                        0.00
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                                                         3
                  LOXO-101
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                 LY2109761
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                                        0.00
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                                                         2
                    M-25
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                                     0.00
                                            0.00
                                                      2
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                   MCOPPB
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                                        0.00
                                                0.00
                  ME-0328
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                   ML-193
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                   ML-228
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                               0.00
                   ML-323
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                                                                    2
N-alpha-Methylhistamine-dihydrochloride
                                           0.00
                                                   0.00
                                                    0.00
         N6-cyclopentyladenosine
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                                            0.00
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                                                 00.0
                NNC-55-0396
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                                                        3
                  NS-11021
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                   NS-309
                NSC-625987
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                NSC-632839
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                NSC-663284
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NVP-ADW742
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    NVP-AEW541
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    NVP-HSP990
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   PF-03758309
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                                    0.00
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   PF-04217903
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    PF-431396
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       PFI-1
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    PHA-793887
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      PP-121
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    RGB-286638
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      RGFP966
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     RKI-1447
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    Ro-1138452
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                                   0.00
                           0.00
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    SB-202190
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                                   0.00
    SB-203580
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      SGX523
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                          0.00
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      SU3327
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                  0.00
    SirReal-2
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    TC-S-7004
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                                             3
      TCN201
                   0.00
                          0.00
                                  0.00
                                            1
      TFC-007
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                          0.00
                                  0.00
                                            1
      TG-003
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                                  0.00
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    TG-101348
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      TUG-891
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                           0.00
                                   0.00
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      UNC1999
                    00.0
                           0.00
                                   0.00
      UNC2025
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                                   0.00
                                             1
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                         0.00
       YC-1
     ZK-93423
                   0.00
                           0.00
                                   0.00
                                             3
    ZM-336372
                    0.00
                            0.00
                                    0.00
                                              1
  acalabrutinib
                   0.00
                          0.00
                                  0.00
                                            2
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                     0.00
                            0.00
                                    0.00
  acetohexamide
 acetylcysteine
                   0.00
                           0.00
                                   0.00
                                             1
   afimoxifene
                   0.00
                           0.00
                                  0.00
                                            3
      alda-1
                0.00
                        0.00
                                0.00
                                          2
                 0.00
                                           1
   aloxistatin
                         0.00
                                 0.00
                      0.00
                              0.00
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                                               1
aminopurvalanol-a
                                            3
                           0.00
                                  0.00
    amlodipine
                   0.00
                           0.00
                                   0.00
                                             3
    anandamide
                   0.00
                           0.00
                                   0.00
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    anisomycin
                   0.00
                   00.0
 arcyriaflavin-a
                           0.00
                                   0.00
                                            1
                  0.00
                         0.00
                                 0.00
   azacitidine
                                           1
                  0.00
                          0.00
                                  0.00
                                            1
   azathioprine
                                           2
    azeliragon
                  0.00
                          0.00
                                  0.00
     baclofen
                 0.00
                         0.00
                                 0.00
                                           1
    batimastat
                  0.00
                          0.00
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                                           3
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briciclib	0.00	0.00	0.00	3			
brinzolamide	0.00	0.00	0.00	1			
bufexamac	0.00	0.00	0.00	1			
buparlisib	0.00	0.00	0.00	3			
carzenide	0.00	0.00	0.00	1			
castanospermine 0.00 0.00 0.00 1							
cediranib	0.00	0.00	0.00	2			
citric-acid	0.00	0.00	0.00	1			
colchicine	0.00	0.00	0.00	1			
coumarin	0.00	0.00	0.00	1			
cycloheximide	0.00	0.00		3			
cyclosporine	0.00	0.00	0.00	2			
danusertib	0.00	0.00	0.00	1			
deferasirox	0.00	0.00	0.00	1			
desonide	0.00	0.00	0.00	2			
diacerein	0.00	0.00	0.00	2			
dilazep	0.00	0.00	0.00	1			
droxinostat	0.00	0.00	0.00	1			
dyphylline	0.00	0.00	0.00	2			
edoxaban	0.00	0.00	0.00	1			
efaproxiral	0.00	0.00	0.00	2			
enflurane	0.00	0.00	0.00	1			
enilconazole	0.00	0.00	0.00	1			
epothilone-b	0.00	0.00	0.00	1			
ethoxzolamide				2			
ethyl-pyruvate	0.00	0.00	0.00	1			
felodipine	0.00	0.00	0.00	2			
filgotinib	0.00	0.00	0.00	1			
fludarabine	0.00	0.00	0.00	1			
flufenamic-acid	0.00	0.00	0.00	1			
flupirtine	0.00	0.00	0.00	2			
fomepizole	0.00	0.00	0.00	2			
formononetin		0.00	0.00	1			
gabapentin-enacarbil 0.00 0.00 0.00 5							
ganetespib	0.00	0.00	0.00	1			
glutamine-(1)	0.00	0.00	0.00	1			
glyburide	0.00	0.00	0.00	2			
guanidine	0.00	0.00	0.00	1			
halopemide	0.00	0.00	0.00	2			
ibudilast	0.00	0.00	0.00	2			
ibutamoren	0.00	0.00	0.00	2			
ibutilide	0.00	0.00	0.00	2			
ilomastat	0.00	0.00	0.00	2			
ingenol-mebutate 0.00 0.00 0.00 1							
isoflurane	0.00	0.00	0.00	1			
ixabepilone	0.00	0.00	0.00	4			

leflunomide	0.00	0.00	0.00	1		
meclofenamic-ac			0.0			
menadione	0.00	0.00	0.00	3		
methoxsalen	0.00	0.00	0.00	1		
miglitol	0.00	0.00	0.00	2		
minocycline	0.00	0.00	0.00	2		
misoprostol	0.00	0.00	0.00	1		
motesanib	0.00	0.00	0.00	2		
nialamide	0.00	0.00	0.00	1		
nilvadipine	0.00	0.00	0.00	2		
octreotide	0.00	0.00	0.00	2		
olopatadine	0.00	0.00	0.00	2		
oxibendazole	0.00	0.00	0.00	3		
oxytocin	0.00	0.00	0.00	1		
ozagrel	0.00	0.00	0.00	1		
paliperidone	0.00	0.00	0.00	2		
pazopanib	0.00	0.00	0.00	2		
phenylbutazone 0.00 0.00 0.00 1						
picrotin	0.00	0.00	0.00	1		
polydatin	0.00	0.00	0.00	2		
purvalanol-a	0.00	0.00	0.00	3		
quinidine	0.00	0.00	0.00	3		
quinine	0.00	0.00	0.00	1		
racecadotril	0.00	0.00	0.00	2		
rifamycin	0.00	0.00	0.00	1		
ryuvidine	0.00	0.00	0.00	5		
sacubitril	0.00	0.00	0.00	2		
somatostatin	0.00	0.00	0.00	1		
sorbinil	0.00	0.00	0.00	2		
sotrastaurin	0.00	0.00	0.00	3		
spiroxatrine	0.00	0.00	0.00	1		
sulfasalazine	0.00	0.00	0.00	3		
sulfinpyrazone	0.00	0.00	0.00	1		
taladegib	0.00	0.00	0.00	1		
thioguanine	0.00	0.00	0.00	3		
thiostrepton	0.00	0.00	0.00	3		
torcitabine	0.00	0.00	0.00	2		
tranilast	0.00	0.00	0.00	2		
trihexyphenidyl	0.00	0.00	0.00	2		
accuracy 0.16 431						
macro avg	0.00	0.01	0.00	431		
weighted avg	0.00		0.04	431		
8 8						