

Table 1: Results For Models

--- Baseline (Grayscale only) ---

	precision	recall	f1-score	support
1-octanol	0.00	0.00	0.00	2
2,5-furandimethanol	0.00	0.00	0.00	2
2-Oleoylglycerol	0.00	0.00	0.00	2
4-CMTB	0.00	0.00	0.00	2
4-methylhistamine	0.00	0.00	0.00	2
7-hydroxystaurosporine	0.00	0.00	0.00	2
A205804	0.00	0.00	0.00	1
AC-710	0.00	0.00	0.00	2
AK-7	0.00	0.00	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	0.00	2
AZ191	0.00	0.00	0.00	2
AZD7762	0.00	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	0.00	1
BAX-channel-blocker	0.00	0.00	0.00	2
BAY-87-2243	0.00	0.00	0.00	2
BI-2536	0.00	0.00	0.00	3
BMS-536924	0.00	0.00	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	0.00	2
CCG-63802	0.00	0.00	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	0.00	0.00	2
CYM-50358	0.00	0.00	0.00	2
CYM-5442	0.00	0.00	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
EI1	0.00	0.00	0.00	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

GNF-5	0.00	0.00	0.00	2	
GNF-5837	0.00	0.00	0.00	2	
GSK-37647	0.00	0.00	0.00	2	
GSK1070916	0.00	0.00	0.00	2	
GSK2110183	0.00	0.00	0.00	3	
GSK3787	0.00	0.00	0.00	2	
GW-311616	0.00	0.00	0.00	2	
H2L-5765834	0.00	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	0.00	0.00	2	
KG-5	0.00	0.00	0.00	2	
KH-CB19	0.00	0.00	0.00	2	
KU-55933	0.00	0.00	0.00	2	
KU-60019	0.00	0.00	0.00	2	
L-proline	0.00	0.00	0.00	2	
LDN-212854	0.33	0.50	0.40	2	
LDN-27219	0.00	0.00	0.00	2	
LGK-974	0.00	0.00	0.00	2	
LOXO-101	0.00	0.00	0.00	2	
LY2109761	0.00	0.00	0.00	2	
M-25	0.00	0.00	0.00	2	
MCOPPB	0.00	0.00	0.00	2	
ME-0328	0.00	0.00	0.00	2	
ME0328	0.00	0.00	0.00	2	
ML-193	0.00	0.00	0.00	2	
ML-228	0.00	0.00	0.00	2	
ML-323	0.00	0.00	0.00	2	
N-alpha-Methylhistamine-dihydrochloride		0.00	0.00	0.00	2
N6-cyclopentyladenosine	0.00	0.00	0.00	2	
NNC-55-0396	0.00	0.00	0.00	2	
NQDI-1	0.00	0.00	0.00	2	
NS-11021	0.00	0.00	0.00	1	
NS-309	0.00	0.00	0.00	2	
NSC-625987	0.00	0.00	0.00	2	
NSC-632839	0.00	0.00	0.00	2	
NSC-663284	0.00	0.00	0.00	2	
NSC-95397	0.00	0.00	0.00	2	
NVP-ADW742	0.00	0.00	0.00	2	
NVP-AEW541	0.00	0.00	0.00	1	
NVP-HSP990	0.00	0.00	0.00	2	
PD-98059	0.00	0.00	0.00	2	
PETCM	0.00	0.00	0.00	2	
PF-03758309	0.00	0.00	0.00	1	
PF-04217903	0.00	0.00	0.00	2	
PF-05190457	0.00	0.00	0.00	2	

PF-431396	0.00	0.00	0.00	2
PFI-1	0.00	0.00	0.00	2
PHA-793887	0.25	0.33	0.29	3
PP-1	0.00	0.00	0.00	2
PP-121	0.00	0.00	0.00	2
PP-2	0.00	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
RX-821002	0.00	0.00	0.00	2
Ro-1138452	0.00	0.00	0.00	2
SB-202190	0.00	0.00	0.00	1
SB-203580	0.00	0.00	0.00	2
SGX523	0.00	0.00	0.00	2
SRC-kinase-inhibitor-I	0.00	0.00	0.00	2
SU3327	0.25	1.00	0.40	1
SirReal-2	0.00	0.00	0.00	1
TC-S-7004	0.00	0.00	0.00	2
TCN201	0.00	0.00	0.00	2
TFC-007	0.00	0.00	0.00	2
TG-003	0.00	0.00	0.00	2
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
UNC1999	1.00	0.50	0.67	2
UNC2025	0.00	0.00	0.00	2
VU591	0.00	0.00	0.00	2
WH-4-023	1.00	0.50	0.67	2
YC-1	0.00	0.00	0.00	2
ZK-93423	0.00	0.00	0.00	3
ZK811752	0.00	0.00	0.00	2
ZM-336372	0.00	0.00	0.00	2
acalabrutinib	0.00	0.00	0.00	2
acetoexamide	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-a	0.00	0.00	0.00	1
amlexanox	0.00	0.00	0.00	2
amlodipine	0.00	0.00	0.00	2
anandamide	0.00	0.00	0.00	2
anisomycin	0.00	0.00	0.00	1
apatinib	0.00	0.00	0.00	2

arcyriaflavin-a	0.00	0.00	0.00	2
arundic-acid	0.00	0.00	0.00	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
bepriidil	0.00	0.00	0.00	2
briciclib	0.33	0.50	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	0.00	0.00	0.00	2
cediranib	0.33	0.50	0.40	2
cetilistat	0.00	0.00	0.00	2
citric-acid	0.00	0.00	0.00	2
colchicine	0.00	0.00	0.00	2
conivaptan	0.00	0.00	0.00	2
coumarin	0.00	0.00	0.00	2
cycloheximide	0.00	0.00	0.00	2
cyclosporine	0.00	0.00	0.00	2
dalbavancin	0.00	0.00	0.00	1
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
dexamethasone	0.00	0.00	0.00	2
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	2
edoxaban	0.00	0.00	0.00	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	0.00	0.00	0.00	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	0.00	0.00	0.00	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-enacarbil	0.00	0.00	0.00	2
ganetespib	0.00	0.00	0.00	3
geldanamycin	0.00	0.00	0.00	2
glutamine-(1)	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-mebutate	0.00	0.00	0.00	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-acid	0.00	0.00	0.00	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
phenylbutazone	0.00	0.00	0.00	1
picrotin	0.00	0.00	0.00	2
polydatin	0.00	0.00	0.00	2
ponatinib	0.00	0.00	0.00	2
puromycin	0.00	0.00	0.00	2
purvalanol-a	0.00	0.00	0.00	2

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
ryuvudine	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	0.00	0.00	2
vitamin-E	0.00	0.00	0.00	2
zamifenacin	0.00	0.00	0.00	2
accuracy		0.12		574
macro avg	0.03	0.03	0.03	574
weighted avg	0.06	0.12	0.08	574

--- With Cellpose features ---

	precision	recall	f1-score	support
1-octanol	0.00	0.00	0.00	2
2,5-furandimethanol	0.00	0.00	0.00	2
2-Oleoylglycerol	0.00	0.00	0.00	2
4-CMTB	0.00	0.00	0.00	2
4-methylhistamine	0.00	0.00	0.00	2
7-hydroxystaurosporine	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

AZD7762	0.00	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	0.00	1
BAX-channel-blocker	0.00	0.00	0.00	2
BAY-87-2243	0.00	0.00	0.00	2
BI-2536	0.75	1.00	0.86	3
BMS-536924	0.00	0.00	0.00	1
BQ-788	0.00	0.00	0.00	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	0.00	2
CCG-63802	0.00	0.00	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	0.00	0.00	2
CYM-50358	0.00	0.00	0.00	2
CYM-5442	0.00	0.00	0.00	1
CYM-5520	0.00	0.00	0.00	2
CYT-997	0.40	0.67	0.50	3
DDR1-IN-1	0.00	0.00	0.00	2
DG-172	0.00	0.00	0.00	1
DMSO	0.23	0.70	0.34	102
EI1	0.00	0.00	0.00	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
GNF-5	0.00	0.00	0.00	2
GNF-5837	0.00	0.00	0.00	2
GSK-37647	0.00	0.00	0.00	2
GSK1070916	0.00	0.00	0.00	2
GSK2110183	0.00	0.00	0.00	3
GSK3787	0.00	0.00	0.00	2
GW-311616	0.00	0.00	0.00	2
H2L-5765834	0.00	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	0.00	0.00	2
KG-5	0.00	0.00	0.00	2
KH-CB19	0.00	0.00	0.00	2
KU-55933	0.00	0.00	0.00	2
KU-60019	0.67	1.00	0.80	2
L-proline	0.00	0.00	0.00	2
LDN-212854	0.00	0.00	0.00	2

LDN-27219	0.00	0.00	0.00	2	
LGK-974	0.00	0.00	0.00	2	
LOXO-101	0.00	0.00	0.00	2	
LY2109761	0.00	0.00	0.00	2	
M-25	0.00	0.00	0.00	2	
MCOPPB	0.50	0.50	0.50	2	
ME-0328	0.00	0.00	0.00	2	
ME0328	0.00	0.00	0.00	2	
ML-193	0.00	0.00	0.00	2	
ML-228	0.00	0.00	0.00	2	
ML-323	0.00	0.00	0.00	2	
N-alpha-Methylhistamine-dihydrochloride		0.00	0.00	0.00	2
N6-cyclopentyladenosine	0.00	0.00	0.00	2	
NNC-55-0396	0.00	0.00	0.00	2	
NQDI-1	0.00	0.00	0.00	2	
NS-11021	0.00	0.00	0.00	1	
NS-309	0.00	0.00	0.00	2	
NSC-625987	0.00	0.00	0.00	2	
NSC-632839	0.00	0.00	0.00	2	
NSC-663284	0.00	0.00	0.00	2	
NSC-95397	0.00	0.00	0.00	2	
NVP-ADW742	0.00	0.00	0.00	2	
NVP-AEW541	0.00	0.00	0.00	1	
NVP-HSP990	0.00	0.00	0.00	2	
PD-98059	0.00	0.00	0.00	2	
PETCM	0.00	0.00	0.00	2	
PF-03758309	0.00	0.00	0.00	1	
PF-04217903	0.00	0.00	0.00	2	
PF-05190457	0.00	0.00	0.00	2	
PF-431396	0.50	0.50	0.50	2	
PFI-1	0.00	0.00	0.00	2	
PHA-793887	0.00	0.00	0.00	3	
PP-1	0.33	0.50	0.40	2	
PP-121	0.50	0.50	0.50	2	
PP-2	0.33	1.00	0.50	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	
RX-821002	0.00	0.00	0.00	2	
Ro-1138452	0.00	0.00	0.00	2	
SB-202190	0.00	0.00	0.00	1	
SB-203580	0.33	1.00	0.50	2	
SGX523	0.00	0.00	0.00	2	
SRC-kinase-inhibitor-I	0.00	0.00	0.00	2	
SU3327	0.00	0.00	0.00	1	
SirReal-2	0.00	0.00	0.00	1	



TC-S-7004	0.00	0.00	0.00	2
TCN201	0.00	0.00	0.00	2
TFC-007	0.00	0.00	0.00	2
TG-003	0.00	0.00	0.00	2
TG-02	0.00	0.00	0.00	2
TG-101348	0.50	0.50	0.50	2
TUG-891	0.00	0.00	0.00	2
UNC1999	0.00	0.00	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	0.00	0.00	2
ZM-336372	0.00	0.00	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-a	0.00	0.00	0.00	1
amlexanox	0.00	0.00	0.00	2
amlodipine	0.00	0.00	0.00	2
anandamide	0.00	0.00	0.00	2
anisomycin	0.00	0.00	0.00	1
apatinib	0.00	0.00	0.00	2
arcyriaflavin-a	0.00	0.00	0.00	2
arundic-acid	0.00	0.00	0.00	2
ascorbic-acid	0.00	0.00	0.00	2
azacitidine	0.25	0.33	0.29	3
azathioprine	0.00	0.00	0.00	2
azeliragon	0.50	0.50	0.50	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
bepriidil	0.00	0.00	0.00	2
briciclib	0.50	0.50	0.50	2
brinzolamide	0.00	0.00	0.00	1
bufexamac	0.00	0.00	0.00	2
buparlisib	1.00	0.67	0.80	3
carzenide	0.00	0.00	0.00	2
castanospermine	0.00	0.00	0.00	2
cediranib	0.50	0.50	0.50	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	0.00	0.00	2
cyclosporine	0.00	0.00	0.00	2
dalbavancin	0.00	0.00	0.00	1
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
dexamethasone	0.00	0.00	0.00	2
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	2
edoxaban	0.00	0.00	0.00	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	0.00	0.00	0.00	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	0.00	0.00	0.00	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-enacarbil	0.00	0.00	0.00	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-mebutate	0.00	0.00	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-acid	0.00	0.00	0.00	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
phenylbutazone	0.00	0.00	0.00	1
picrotin	0.00	0.00	0.00	2
polydatin	0.00	0.00	0.00	2
ponatinib	0.50	1.00	0.67	2
puromycin	1.00	0.50	0.67	2
purvalanol-a	0.00	0.00	0.00	2
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	0.00	0.00	0.00	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	0.00	0.00	0.00	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	0.00	0.00	2
vitamin-E	0.00	0.00	0.00	2
zamifenacin	0.00	0.00	0.00	2
accuracy		0.18		574
macro avg	0.05	0.06	0.05	574
weighted avg	0.08	0.18	0.11	574

--- CNN Baseline (Grayscale Only) [Final Test Evaluation] ---

	precision	recall	f1-score	support
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1-octanol	0.00	0.00	0.00	2
2,5-furandimethanol	0.00	0.00	0.00	1
2-Oleoylglycerol	0.00	0.00	0.00	4
4-CMTB	0.00	0.00	0.00	3
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	0.00	0.00	0.00	4
AR-12	0.00	0.00	0.00	1
AVL-292	0.00	0.00	0.00	1
AZ191	0.00	0.00	0.00	1
AZD7762	0.00	0.00	0.00	2
AZD9668	0.00	0.00	0.00	2
BAM7	0.00	0.00	0.00	1
BAN-ORL-24	0.00	0.00	0.00	2
BAX-channel-blocker	0.00	0.00	0.00	3
BAY-87-2243	0.00	0.00	0.00	1
BI-2536	0.00	0.00	0.00	3
BMS-536924	0.00	0.00	0.00	3
BQ-788	0.00	0.00	0.00	3
BVT-948	0.00	0.00	0.00	3
CC-401	0.00	0.00	0.00	3
CCG-50014	0.00	0.00	0.00	1
CCG-63802	0.00	0.00	0.00	3
CP-724714	0.00	0.00	0.00	1
CVT-10216	0.00	0.00	0.00	3
CYM-50260	0.00	0.00	0.00	2
CYM-50358	0.00	0.00	0.00	2

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	
DDR1-IN-1	0.00	0.00	0.00	3	
DG-172	0.00	0.00	0.00	1	
DMSO	0.18	1.00	0.31	78	
EI1	0.00	0.00	0.00	2	
FK-866	0.00	0.00	0.00	4	
FPS-ZM1	0.00	0.00	0.00	1	
GSK1070916	0.00	0.00	0.00	1	
GSK2110183	0.00	0.00	0.00	6	
GSK3787	0.00	0.00	0.00	1	
GW-311616	0.00	0.00	0.00	3	
H2L-5765834	0.00	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	0.00	0.00	0.00	2	
KU-60019	0.00	0.00	0.00	1	
L-proline	0.00	0.00	0.00	2	
LDN-27219	0.00	0.00	0.00	2	
LY2109761	0.00	0.00	0.00	2	
MCOPPB	0.00	0.00	0.00	1	
ME-0328	0.00	0.00	0.00	2	
ME0328	0.00	0.00	0.00	1	
ML-323	0.00	0.00	0.00	1	
N-alpha-Methylhistamine-dihydrochloride	0.00	0.00	0.00	1	
NNC-55-0396	0.00	0.00	0.00	1	
NQDI-1	0.00	0.00	0.00	3	
NS-309	0.00	0.00	0.00	1	
NSC-625987	0.00	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	
NVP-HSP990	0.00	0.00	0.00	2	
PD-98059	0.00	0.00	0.00	1	
PETCM	0.00	0.00	0.00	2	
PHA-793887	0.00	0.00	0.00	2	
PP-1	0.00	0.00	0.00	1	
PP-121	0.00	0.00	0.00	1	
PP-2	0.00	0.00	0.00	2	
RKI-1447	0.00	0.00	0.00	3	
SB-203580	0.00	0.00	0.00	2	
SGX523	0.00	0.00	0.00	1	
SRC-kinase-inhibitor-I	0.00	0.00	0.00	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
acetoexamide	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
bepiridil	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
conivaptan	0.00	0.00	0.00	2
coumarin	0.00	0.00	0.00	3
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

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
ethoxzalamide	0.00	0.00	0.00	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	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-mebutate	0.00	0.00	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-acid	0.00	0.00	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	0.00	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
phenylbutazone	0.00	0.00	0.00	2

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
accuracy		0.18		431
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-methylhistamine	0.00	0.00	0.00	1
7-hydroxystaurosporine	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-24	0.00	0.00	0.00	2
BAY-87-2243	0.00	0.00	0.00	1
BI-2536	0.00	0.00	0.00	4



BQ-788	0.00	0.00	0.00	2	
BRL-50481	0.00	0.00	0.00	1	
BVT-948	0.00	0.00	0.00	3	
CC-401	0.00	0.00	0.00	1	
CCG-50014	0.00	0.00	0.00	2	
CCG-63802	0.00	0.00	0.00	3	
CGP-53353	0.00	0.00	0.00	2	
CP-724714	0.00	0.00	0.00	2	
CVT-10216	0.00	0.00	0.00	1	
CYM-50358	0.00	0.00	0.00	2	
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	
DMSO	0.16	1.00	0.27	68	
EI1	0.00	0.00	0.00	1	
FK-866	0.00	0.00	0.00	5	
FPS-ZM1	0.00	0.00	0.00	1	
GNF-5	0.00	0.00	0.00	1	
GSK1070916	0.00	0.00	0.00	2	
GSK2110183	0.00	0.00	0.00	1	
GSK3787	0.00	0.00	0.00	1	
GW-311616	0.00	0.00	0.00	1	
IRL-2500	0.00	0.00	0.00	4	
JTE-607	0.00	0.00	0.00	4	
KG-5	0.00	0.00	0.00	1	
KH-CB19	0.00	0.00	0.00	1	
KU-55933	0.00	0.00	0.00	4	
L-proline	0.00	0.00	0.00	2	
LDN-212854	0.00	0.00	0.00	2	
LGK-974	0.00	0.00	0.00	2	
LOXO-101	0.00	0.00	0.00	3	
LY2109761	0.00	0.00	0.00	2	
M-25	0.00	0.00	0.00	2	
MCOPPB	0.00	0.00	0.00	3	
ME-0328	0.00	0.00	0.00	1	
ML-193	0.00	0.00	0.00	1	
ML-228	0.00	0.00	0.00	1	
ML-323	0.00	0.00	0.00	1	
N-alpha-Methylhistamine-dihydrochloride		0.00	0.00	0.00	2
N6-cyclopentyladenosine		0.00	0.00	0.00	2
NNC-55-0396	0.00	0.00	0.00	1	
NS-11021	0.00	0.00	0.00	3	
NS-309	0.00	0.00	0.00	4	
NSC-625987	0.00	0.00	0.00	1	
NSC-632839	0.00	0.00	0.00	2	
NSC-663284	0.00	0.00	0.00	2	

NVP-ADW742	0.00	0.00	0.00	1
NVP-AEW541	0.00	0.00	0.00	2
NVP-HSP990	0.00	0.00	0.00	1
PF-03758309	0.00	0.00	0.00	3
PF-04217903	0.00	0.00	0.00	3
PF-431396	0.00	0.00	0.00	1
PFI-1	0.00	0.00	0.00	4
PHA-793887	0.00	0.00	0.00	2
PP-1	0.00	0.00	0.00	2
PP-121	0.00	0.00	0.00	3
RGB-286638	0.00	0.00	0.00	1
RGFP966	0.00	0.00	0.00	1
RKI-1447	0.00	0.00	0.00	1
Ro-1138452	0.00	0.00	0.00	4
SB-202190	0.00	0.00	0.00	2
SB-203580	0.00	0.00	0.00	2
SGX523	0.00	0.00	0.00	2
SU3327	0.00	0.00	0.00	1
SirReal-2	0.00	0.00	0.00	1
TC-S-7004	0.00	0.00	0.00	3
TCN201	0.00	0.00	0.00	1
TFC-007	0.00	0.00	0.00	1
TG-003	0.00	0.00	0.00	1
TG-101348	0.00	0.00	0.00	1
TUG-891	0.00	0.00	0.00	2
UNC1999	0.00	0.00	0.00	3
UNC2025	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
ZM-336372	0.00	0.00	0.00	1
acalabrutinib	0.00	0.00	0.00	2
acetohexamide	0.00	0.00	0.00	2
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
aloxistatin	0.00	0.00	0.00	1
aminopurvalanol-a	0.00	0.00	0.00	1
amlodipine	0.00	0.00	0.00	3
anandamide	0.00	0.00	0.00	3
anisomycin	0.00	0.00	0.00	1
arcyriaflavin-a	0.00	0.00	0.00	1
azacitidine	0.00	0.00	0.00	1
azathioprine	0.00	0.00	0.00	1
azeliragon	0.00	0.00	0.00	2
baclofen	0.00	0.00	0.00	1
batimastat	0.00	0.00	0.00	3

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	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	0.00	0.00	0.00	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	0.00	1
gabapentin-enacarbil	0.00	0.00	0.00	5
ganetespib	0.00	0.00	0.00	1
glutamine-(l)	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-acid	0.00	0.00	0.00	1
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	0.02	0.16	0.04	431