Anticancer Screening Library

Search for chemotherapeutic cancer treatment is one of the most acute problems of modern pharmacology. To pursue this issue Life Chemicals has prepared its Anticancer Library using similarity search within its proprietary stock collection of HTS compounds against publicly available databases (ChEMBL and BindingDB) of the compounds possessing antitumor activity.

The Life Chemicals HTS Compound Collection was screened against 12,000 reference compounds with assigned activity values lower than 10 mM. Similarity search and 80 % similarity cut-off (Tanimoto) and PAINS / reactive group filtration gave over **1,500** compounds with potential inhibitory activity against the following cell lines*:

3LL
A253
A-375
A549
AGS
B16-F10
BC1
Bel-7402
BGC-823
CCRF-CEM
CHRC5
DU-145
Fibrosarcoma cell line
HBL-100
HCC 2998
HCT-116
HeLa
Hepatoblastoma cell line
HepG2
HL-60
HNO 97
HONE1
HT-29
Human T-cell line
Jurkat
K562
KB
KU812
KYSE-150
KYSE-70
Leukemia 60 cell line
Lewis lung carcinoma cell line
LNCaP
LoVo
LOX IMVI
Lung cancer cell line
LXF-289
M14
MCF7
MDA-MB-231
Melanoma tumor cell line
MOLT-4
NCI/ADR-RES
NCI-H157
NCI-H2009
NCI-H460
NUGC-3
P388
Panel leukemia (Carcinoma cell lines)
Panel NCI-60 (60 carcinoma cell lines)
PC-3
SF-268
SF-295
SH-SY5Y
SK-MEL-5
SK-OV-3
T-24
T98G
THP-1
TK-10
U-937
UO-31

Also was searched for compounds similar to each of the known compounds related to different targets using the 80 % similarity cut-off (Tanimoto) on MDL public keys fingerprints reducing their variety. As a result, around **4,800** compounds, of the following Anticancer Screening Library targets* were produced:

- Anoctamin-1
- ATP-binding cassette sub-family G member 2
- Beta-hexosaminidase subunit beta
- Breast cancer type 1 susceptibility protein
- Bromodomain testis-specific protein
- Cyclin-dependent kinase 2-associated protein 1
- L-type amino acid transporter 3
- Lysine-specific demethylase 5B
- MAP kinase p38 alpha
- Mitogen-activated protein kinase kinase kinase 8
- Mixed lineage kinase 7
- Nuclear receptor coactivator 3
- PDZ-binding kinase
- Serine/threonine-protein kinase WNK2

All PAINS, toxic and reactive compounds are excluded from the library, Ro5 compliance is indicated.

**The results could be traced back to the specific cell lines or single targets (indicated in the column "Target type" within the corresponding sdf file).*

References

1. Ackova DG, Smilkov K, Bosnakovski D.Contemporary Formulations for Drug Delivery of Anticancer Bioactive Compounds // Recent Pat Anticancer Drug Discov. 2019;14(1):19-31.
2. Geromichalos GD, Alifieris CE, Geromichalou EG, Trafalis DT. Overview on the current status of virtual high-throughput screening and combinatorial chemistry approaches in multi-target anticancer drug discovery; Part I // J BUON. 2016 Jul-Aug;21(4):764-779; Part II //J BUON. 2016;21(6):1337-1358.
3. Hameed R, Khan A, Khan S, Perveen S. Computational Approaches Towards Kinases as Attractive Targets for Anticancer Drug Discovery and Development // Anticancer Agents Med Chem. 2019;19(5):592-598.