**Drug Synergy data curation: Rules**

**How to find papers**

* Enter pubmed ID in http://www.ncbi.nlm.nih.gov/pubmed
* First read the abstract, then read the full text
* To get the full text: iupui library

<http://www.ulib.iupui.edu/resources/databases>

Note: sometimes you can directly get html full text in google scholar. (https://scholar.google.com/)

* No full text via iupui: indicate in “SPECIAL NOTES BY YOU” column.

I will find the full text and deposit it in your box folder

**Rules**

1. Copy and paste from the paper as much as possible.

* For columns 3 to 14: only copy words or phrases.
* For the last 8 columns you can copy entire sentences (marked as Copy and paste the sentences.)
* Try to avoid unnecessary spaces.

2. No entry for a column: put “na” (lower case)

3. One row for each combination and each concentration, each cell line

i.e. You will have >1 row for the papers testing different combinations and concentrations

e.g.

paper1 tamoxifen ibuprofen 1\_mol 5\_mol H3255

paper1 tamoxifen ibuprofen 1\_mol 10\_mol H3255

paper1 tamoxifen naproxen 1\_mol 10\_mol H3255

paper1 tamoxifen ibuprofen 1\_mol 5\_mol MDMB235

4. Measurements and units, target and activity, drug1 and drug 2 carriers: separate by underscore “\_”

5. More than 1 entry in 1 cell: separate by “comma(,)”

KRAS\_inhibiting,KRAS\_modulator,HRAS\_inhibiting

6. Individual drug effects: DONOT record

**Column descriptions**

**1. PUBMED ID**: I’ll give you the IDs. No entry by you.

**2. TITLE**: Copy and paste the title of the paper

**3. CELL LINE**: cell line used, copy and paste. If they specifically mutate a gene in a cell line indicate that after “underscore”.

E.g. H3255\_EGFRmutation

**4. DRUG1**: name of the first drug, as given in the paper

**5. DRUG1 TARGET\_ACTIVITY**: Target gene of drug1 and how does the drug1 interact with the gene, separated by underscore

e.g. KRAS\_inhibiting

If more than 1 target gene, separate them by comma

e.g.

KRAS\_inhibiting

KRAS\_modulator

HRAS\_inhibiting

PAR1\_antagonist of proteinase-activated receptor 1 (PAR1)

Tyrosine kinase\_inhibitor

* No specific gene: just write the action after underscore.

E.g. \_apoptosis

**6. DRUG1 CONCENTRATION\_UNIT**: copy and paste concentration and units of the concentration separated by underscore

E.g. 10\_micromolar

**7. DRUG2**: name of the second drug, as given in the paper

**8. DRUG1 TARGET\_ACTIVITY**: Target gene of drug2 and how does the drug2 interact with the gene, separated by underscore

e.g. KRAS\_inhibiting

If more than 1 target gene, separate them by comma

e.g.

KRAS\_inhibiting

KRAS\_modulator

HRAS\_inhibiting

PAR1\_antagonist of proteinase-activated receptor 1 (PAR1)

Tyrosine kinase\_inhibitor

**9. DRUG2 CONCENTRATION\_UNIT**: copy and paste concentration and units of the concentration separated by underscore

**10. CARRIER (OR VEHICLE)**: what is used to prepare the drug solution, other than water. Drug 1 carrier and drug 2 carrier separated by underscore.

* Make sure that Drug 1 and Drug 2 agrees with what you entered in columns 4 and 7

e.g.

DMSO\_DMSO

NACL,DMSO\_DMSO

**10. CONTROL**: What is used in the Control experiment, instead of the drug.

Most of the time same as the carrier.

DMSO

DMSO,NACL

**11. FIRST DRUG TO ADMINISTER**: name of the first drug added to the cell line

Copy and paste the drug name. **DO NOT PUT** “Drug1” or “Drug2”

**12. SECOND DRUG TO ADMINISTER**: name of the second drug added to the cell line

Copy and paste the drug name. **DO NOT PUT** “Drug1” or “Drug2”

**13. TIME BETWEEN ADMINISTERING DRUG 1 AND DRUG 2:** How much time between adding drug 1 and adding drug 2 to the cells. If both drugs added at the same time, this will be zero. Time and unit separate by underscore.

e.g.

1\_hr 30\_min

**14. INCUBATION TIME BEFORE MEASURING SYNERGY**: After adding both drugs, did they measure the synergy right away or incubated them for some time. Time and unit separate by underscore.

e.g.

2\_hrs 2\_days

**15. SYNERGYSTIC/ANTAGONISTIC/ADDITIVE/NO INTERACTION**: If they specify the combination as synergistic, antagonistic, additive, no interaction or ANY OTHER TERM that they used to describe the interaction. Copy and paste the sentences.

* Different assays used to test the same combination (D1,D2,concentration, cell line): separate the synergy description with comma.

E.g.

Synergy, synergy

Accordingly, the different assays should be entered in column 18, separated by comma.

E.g.

MTT assay, colony forming assay

**16. SYNERGY VALUE**: if they give a numerical value for synergy, copy and paste it.

If CI(combination index) given, record the CI value directly as the synergy value

**17. DEFINITION OF SYNERGY**: copy and paste how they defined synergy.

Copy and paste the sentences.

e.g.

Interactions between erlotinib and pemetrexed were expressed as the combination index by the CalcuSyn software. 1 represents synergistic cytotoxicity; 1 represents addictive: 1 represents antagonistic cytotoxicity

**18. ASSY USED TO MEASURE SYNERGY**: copy and paste the assay they used to measure synergy. Copy and paste the sentences.

E.g.

Exponentially growing cells were seeded in 96-well plastic plates and exposed to serial dilutions of erlotinib, pemetrexed, or the combination at a constant concentration ratio of 4:1 in triplicates for 72 h. Cell viability was assayed by cell count and the 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide assay (31). Growth inhibition was expressed as the percentage of surviving cells in drug-treated versus PBS-treated control cells (which was considered as 100% viability). The IC50 value was the concentration resulting in 50% cell growth inhibition by a 72-h exposure to drug(s) compared with untreated control cells and was calculated by the CalcuSyn software (Biosoft, Inc.).

* If >1 assay used: separate them by comma

**19. INSTRUMENT/S USED**: Instruments used in the assay they to measure the synergy. This corresponds to the **ASSY USED TO MEASURE SYNERGY** column.

You can copy and paste the sentences if there are multiple instruments used..

E.g.

Acumen Explorer

**20. OTHER PHARMACOLOGICAL INFO**: IC50, AUC of the drugs. You can copy and paste the sentences.

**21. SPECIAL NOTES BY YOU**: Things that help me to understand what you have recoded.

You can copy and paste the sentences.

e.g.

Synonyms for drug 1 and drug 2,

Issues with the experiment (if you read the full text)

No full text? (very few cases)

**22. YOUR NAME:** first names please ☺