

I. Properties databases

- 1) Follow the link below, look for Chlorpyrifos, what kind of information can we find on that website?**

<https://www.reaxys.com/#/structure-editor> :

- 2) With the same link, go to “draw” and draw a Methane molecule (CH₄) with apparent bonds in 2D and in 3D**

<https://www.reaxys.com/#/structure-editor> :

- 3) Follow the link below and look for physico-chemical properties information on Fonofos (pesticide) using EpiSuite values, if experimental value exist give experimental, if not, give predicted values**

<http://www.chemspider.com/>

Give information for:

- Vapor pressure:
- log K_{ow}:
- Solubility in water:
- Half life in air:

II. Compounds and spectra database

- 4) Look for Spectra for D-glucose, using only the number of atoms: $C_6H_{12}O_6$; Copy/paste the spectra below and indicate the associated InChI of the molecule

https://sdfs.db.aist.go.jp/sdfs/cgi-bin/cre_index.cgi

III. Biological database

5) Follow the link below,

Let's use BLAST to see if we can identify 20 unknown uncultured bacteriums

<https://blast.ncbi.nlm.nih.gov/Blast.cgi>

Link to get to the data (20 unknown sequences):

<https://go.usa.gov/xUEX4>

*(just in case computer is very slow, **do not click on it otherwise**, link to results:*

<https://blast.ncbi.nlm.nih.gov/Blast.cgi?CMD=Get&RID=NH1S873K015>)

MOLE-BLAST

<https://blast.ncbi.nlm.nih.gov/moleblast/moleblast.cgi>

Copy/paste the 3 sequences

KU524801.1

AB759680.1

GQ158974.1

Run with 16s database

IV. Registration Database:

6) Find authorization status for the following compound at the EU level, using the following link

<https://go.drugbank.com/> (Drug database)

https://ec.europa.eu/food/plants/pesticides/eu-pesticides-database_en (EU pesticide database)

<https://www.echemportal.org/echemportal/> (EU chemical portal)

<https://risctox.istas.net/en/> (Toxic substance database)

<https://echa.europa.eu/home> (ECHA website)

For these compounds:

Dicloxacillin – Epoxiconazole – Decachlorobiphenyl