

NASKAH TUTORIAL

GENERATE DECOY MENGUNAKAN DECOYFINDER

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DOWNLOAD DECOYFINDER



[https://github.com/URV-
cheminformatics/DecoyFinder/releases/tag/v2.0](https://github.com/URV-cheminformatics/DecoyFinder/releases/tag/v2.0)

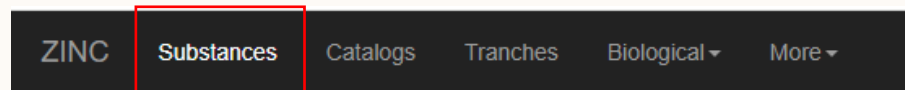
DATABASE YANG PERLU DISIAPKAN

- Database molekul dari Zink (<https://zinc.docking.org>)
- File-file ligan aktif format .mol2 atau .sdf dari DUDE (<https://dude.docking.org/>) atau BindingDB (<https://www.bindingdb.org/rwd/bind/index.jsp>)

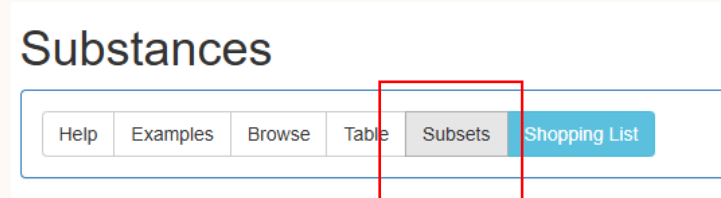
CARA MENDOWNLOAD DATABASE MOLEKUL DARI ZINC

1. Buka website <https://zinc.docking.org>

2. Pilih Substances

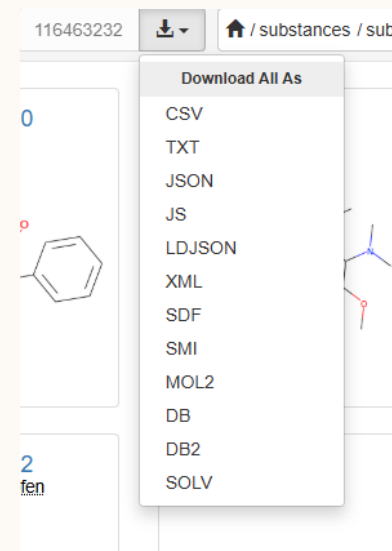


3. Pilih Subsets



4. Pilih wait-ok dan/atau for-sale (sesuai kebutuhan)

5. Download format .sdf

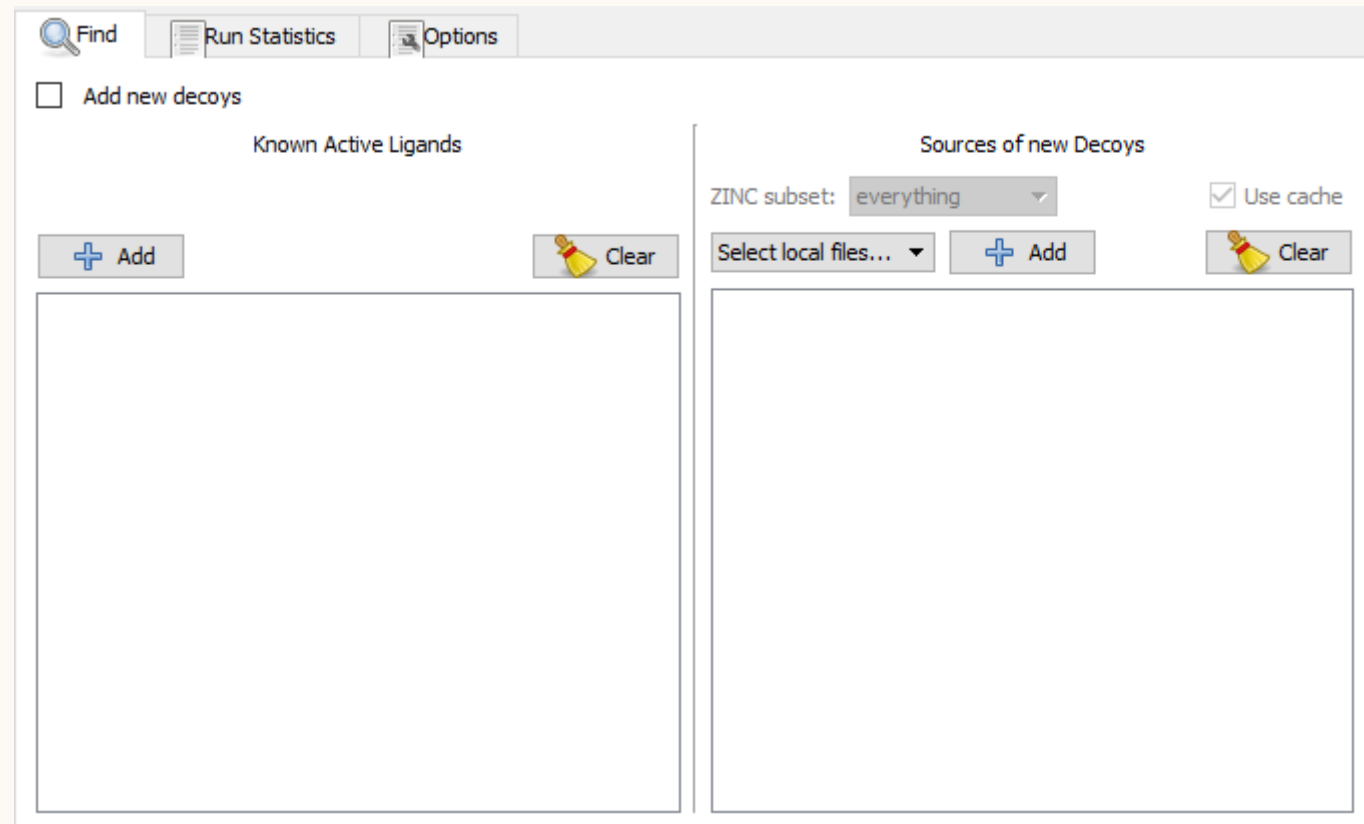


Name	Availability	Estimated Size (purchasable)
bb	Available in preparative quantities, typically at least 250 mg	42908449 (42908449)
in-stock	Compounds purchased direct from manufacturer, already made, sitting on a shelf, ready to ship to you.	12084317 (12084317)
agent	All substances that are available in stock, via procurement agents	3010821 (3010821)
on-demand	All substances that are for sale	95008076 (95008076)
boutique	Boutique substances are generally much more expensive than \$100/sample, often made to order, yet still cheaper than making it yourself.	12949291 (12949291)
now	Immediate delivery, includes in-stock and agent	21455156 (21455156)
wait-ok	Compounds you can get in 8-10 weeks at modest prices, includes in-stock, agent and on-demand	116463232 (116463232)
for-sale	All substances that are for sale, includes in-stock, on-demand, and boutique	389000000 (389000000)
not-for-sale	All substances that cannot be bought as far as we know - tell us if we are mistaken	2100644 (0)

TAHAP GENERATE DECOY

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1. Buka aplikasi DecoyFinder
2. Klik Find → Know Active Ligands → Add → Pilih file-file ligan aktif .mol2/ .sdf
3. Klik Find → Sources of new decoys → Add → Pilih database molekul dari Zink yang telah didownload



TAHAP GENERATE DECOY

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4. Klik Options → pilih Molecular weight based decoys → Isi data sesuai pada gambar → Isi Cache directory (folder untuk hasil download decoys yang telah di-generate) → klik Find decoys → tunggu hingga proses generasi selesai

The screenshot shows the 'Options' dialog box with the following settings:

- Options** (selected tab)
- ☒ Molecular weight based decoys
- ☐ Molecular descriptor based decoys
- Maximum standard deviations away from active: 1,00
- Maximum decoys per active ligand: 50
- Minimum decoys per active ligand: 50
- Cache directory: c:\users\asus\AppData\Local\temp
- Buttons: Find, Run Statistics, Options, Load Defaults, Clear all, Stop, Find decoys
- Status: 0 decoys found

5. Hasil berada di folder yang diisikan pada Cache directory dengan format .sdf

**THANK
YOU**