I preparatory :
- folder structure on laptop / HPC
- molecular structure generation

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II calculations:
- ADF, DIRAC
- can by via pyadf

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III data analysis :
- collecting numerical results
- exporting real-space data on grids
- using more advanced tools (adding visualization, statistics, etc.)

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IV data summarization :
- plots
- tables
- text

→ toolbox
→ recipes

FAIR
→ Findable
→ Accessible
→ Interoperable
→ Reproducible