static conventional workflow



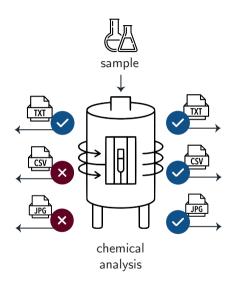
specific input format & specific spectra type



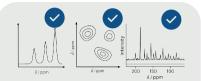
fixed output format



molecule SMILES



dynamic GPM generated workflow



flexible intput format & variable spectra type



flexible output format



products

analysis of



plots



summary report