# 1 Semi-empirical methods

• GFN2-xTB<sup>1</sup>

# 2 Density Functional Theory

- $B97D3^2$
- PBE0<sup>3</sup>

#### 3 Basis sets

• def2-family<sup>4</sup>

# 4 Quantum-chemical programs

 $\bullet$  Gaussian  $16^5$ 

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