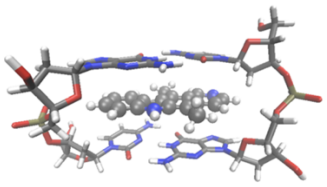
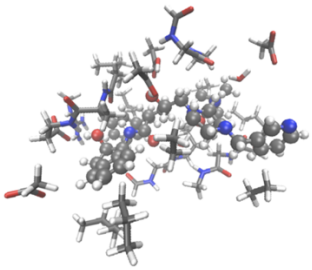
Q-CHEM™
A Quantum Leap Into the Future of Chemistry

Extended Symmetry-Adapted Perturbation Theory (XSAPT)



DNA / ellipticine



HIV / indinavir

Method		E_{int} (kcal/mol) DNA/ellipticine	HIV/indinavir
B97M-V (+counterpoise)[a]		−41.3	—
ωB97M-V (+counterpoise)[a]		−43.7	—
HF-3c		−41.7	−132.8
PBEh-3c		−37.3	−119.1
XSAPT+*ai*D3 (CM5)[b]		−36.7	−106.2
XSAPT+MBD (CM5)[b]		−41.7	−125.4
XSAPT Energy Decomposition			
E_{elst}		−22.2	−114.9
E_{exch}		59.2	190.0
E_{ind}		−8.0	−65.9
E_{disp}	*ai*D3+ATM	−65.7	−115.4
	MBD+esDQ	−70.7	−134.6

[a]def2-TZVPPD basis set. [b]def2-hpTZVPP basis set

XSAPT+aiD Interaction Energies and Energy Decomposition Analysis

- Benchmark-quality intermolecular interaction energies;
- Energy decomposition analysis provides a powerful interpretive utility;
- Unfolds interaction energies into contributions from electrostatics, Pauli repulsion, polarization, and London dispersion;
- A fully many-body interaction energy protocol:
  - Accounts for many-body polarization effects via charge embedding;
  - Includes many-body dispersion interactions (MBD+esDQ potential).
- Cost scales with monomer size; no need for supersystem calculations;
- Faster than supersystem DFT for the DNA complex shown above (4,651 basis functions);
- Trivially parallelizable across fragments;
- Capable of high-accuracy interaction energies in systems larger than 10,000 basis functions.

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