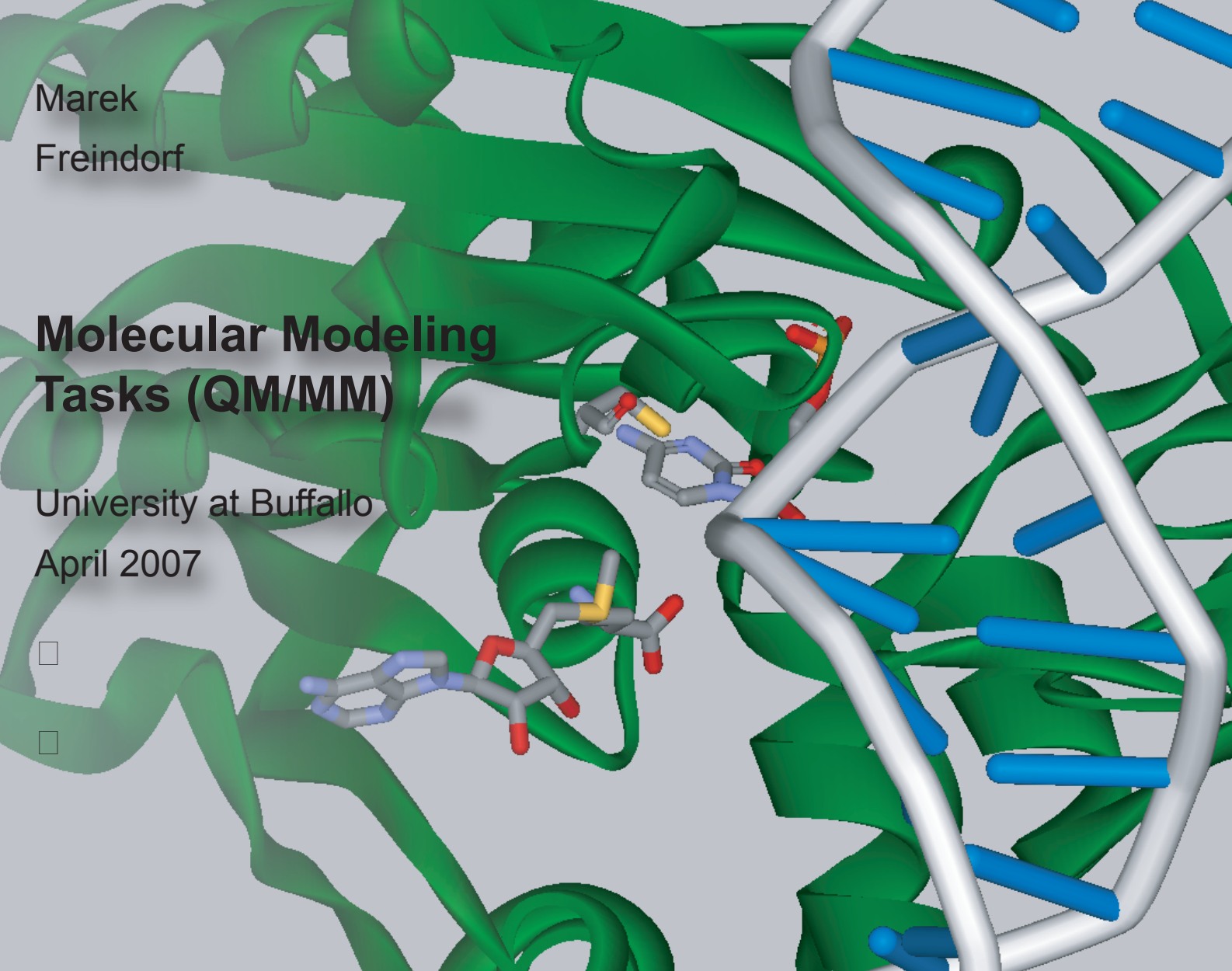
Marek
Freindorf

Molecular Modeling Tasks (QM/MM)

University at Buffalo

April 2007



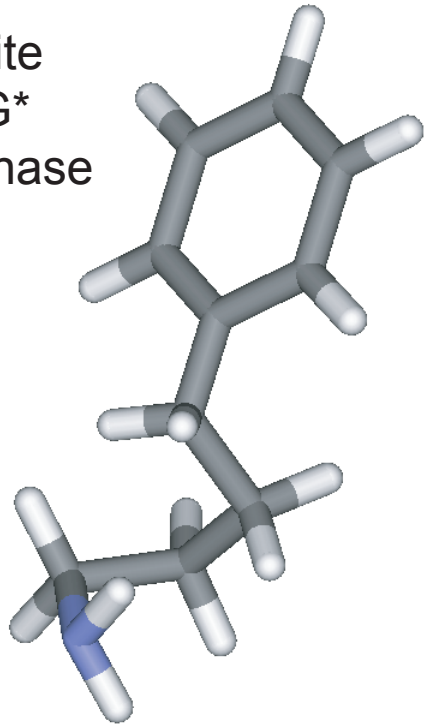
QM/MM geometry optimization (QM/MM-1)

1. Calculate an optimal geometry of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase

2. Report in a table atomic charges of all atoms

3. Report in a table interatomic distances and angles between bonds of the ring

4. Report in a figure a value and an orientation of a molecular dipole moment



5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM/MM geometry optimization (QM/MM-2)

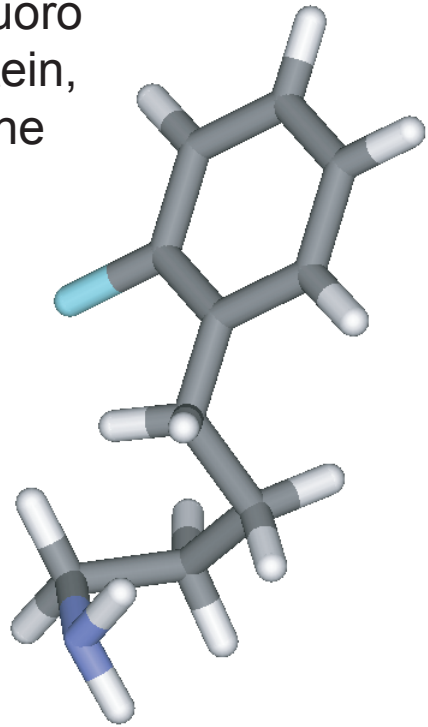
1. Calculate an optimal geometry of the ortho fluoro compound of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase

2. Report in a table atomic charges of all atoms

3. Report in a table interatomic distances and angles between bonds of the ring

4. Report in a figure a value and an orientation of a molecular dipole moment

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



QM/MM geometry optimization (QM/MM-3)

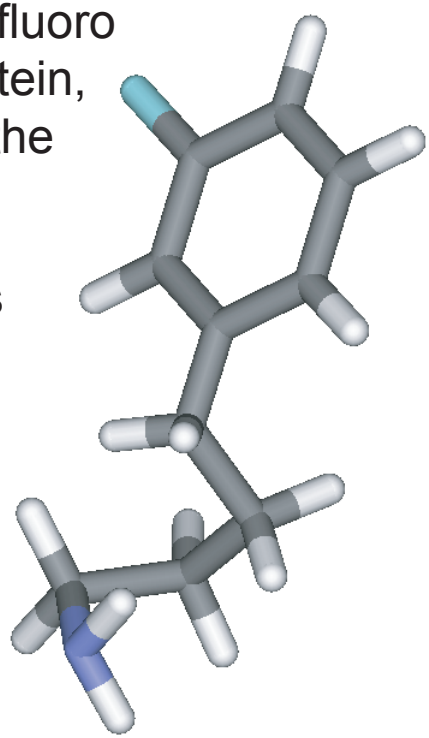
1. Calculate an optimal geometry of the metha fluoro compound of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase

2. Report in a table atomic charges of all atoms

3. Report in a table interatomic distances and angles between bonds of the ring

4. Report in a figure a value and an orientation of a molecular dipole moment

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



QM/MM geometry optimization (QM/MM-4)

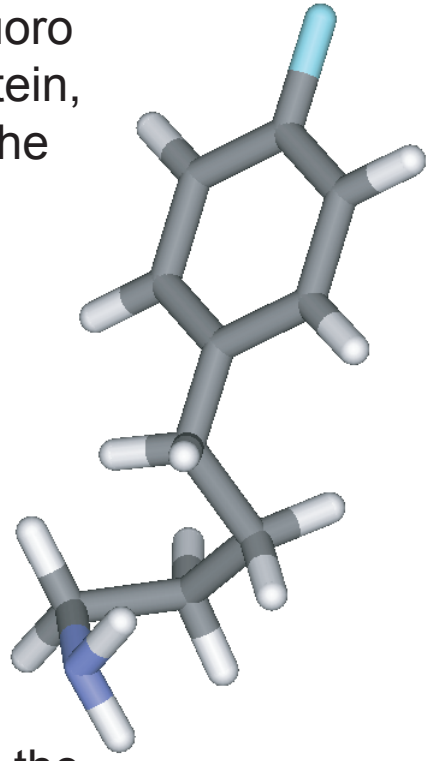
1. Calculate an optimal geometry of the para fluoro compound of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase

2. Report in a table atomic charges of all atoms

3. Report in a table interatomic distances and angles between bonds of the ring

4. Report in a figure a value and an orientation of a molecular dipole moment

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



QM/MM geometry optimization (QM/MM-5)

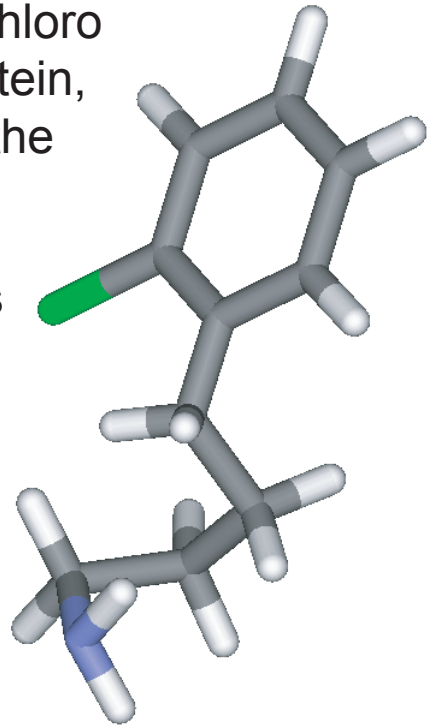
1. Calculate an optimal geometry of the ortho chloro compound of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase

2. Report in a table atomic charges of all atoms

3. Report in a table interatomic distances and angles between bonds of the ring

4. Report in a figure a value and an orientation of a molecular dipole moment

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



QM/MM geometry optimization (QM/MM-6)

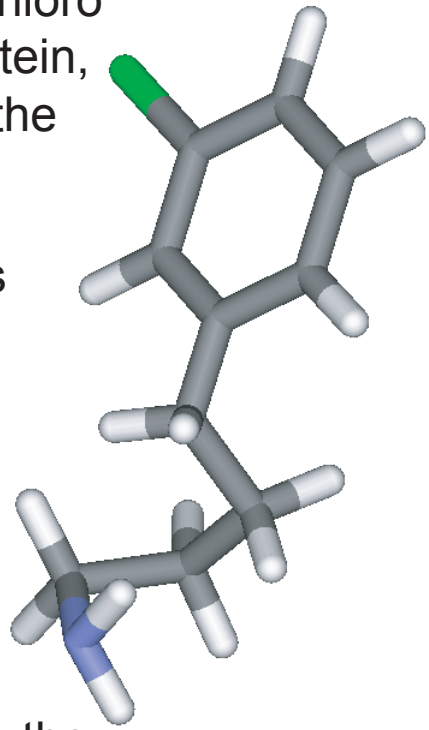
1. Calculate an optimal geometry of the meta chloro compound of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase

2. Report in a table atomic charges of all atoms

3. Report in a table interatomic distances and angles between bonds of the ring

4. Report in a figure a value and an orientation of a molecular dipole moment

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



QM/MM geometry optimization (QM/MM-7)

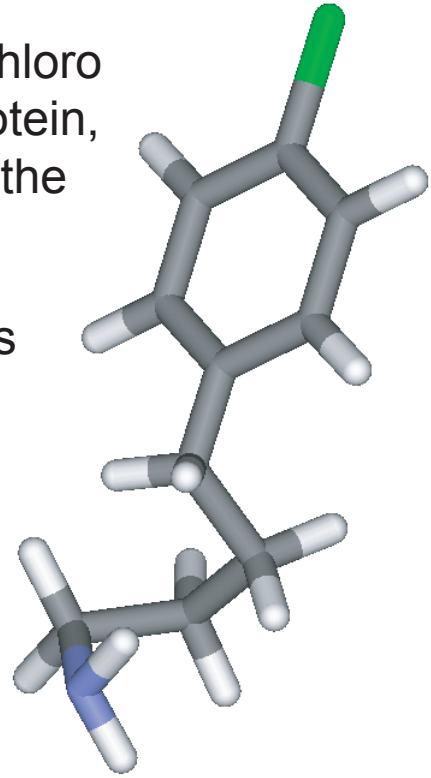
1. Calculate an optimal geometry of the para chloro compound of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase

2. Report in a table atomic charges of all atoms

3. Report in a table interatomic distances and angles between bonds of the ring

4. Report in a figure a value and an orientation of a molecular dipole moment

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



QM/MM molecular vibrations (QM/MM-8)

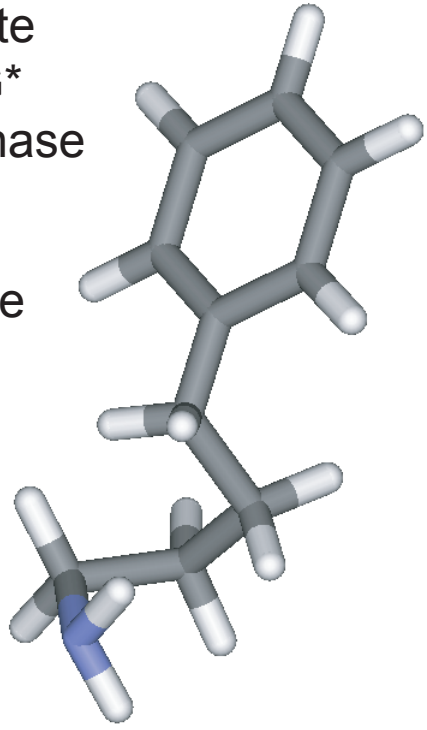
1. Calculate an optimal geometry of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase

2. For the optimal geometry, calculate molecular oscillations, in the protein and in the gas phase

3. Report in a table frequencies of the oscillations of the phenyl ring

4. Repeat frequency calculations for the system where carbons of the phenyl ring have been substituted by their isotopes

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



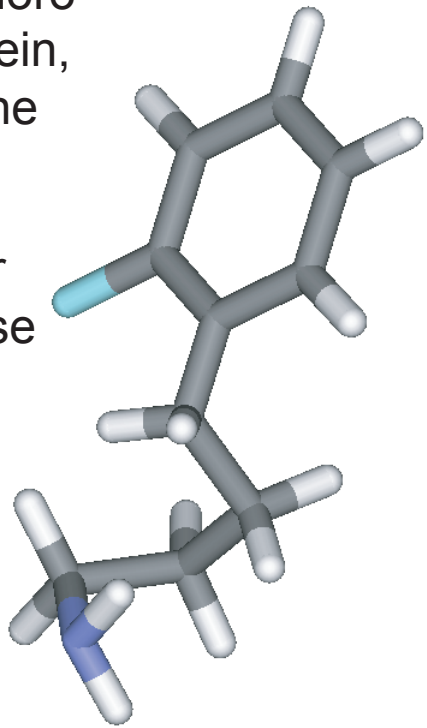
QM/MM molecular vibrations (QM/MM-9)

1. Calculate an optimal geometry of the ortho fluoro compound of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase

2. For the optimal geometry, calculate molecular oscillations, in the protein and in the gas phase

3. Report in a table frequencies of the oscillations of the phenyl ring

4. Repeat frequency calculations for the system where the heteroatom of the phenyl ring has been substituted by its isotope



5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

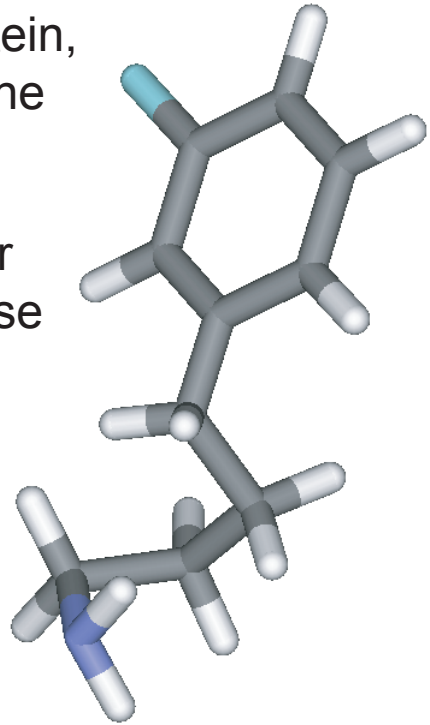
QM/MM molecular vibrations (QM/MM-10)

1. Calculate an optimal geometry of the meta fluoro compound of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase

2. For the optimal geometry, calculate molecular oscillations, in the protein and in the gas phase

3. Report in a table frequencies of the oscillations of the phenyl ring

4. Repeat frequency calculations for the system where the heteroatom of the phenyl ring has been substituted by its isotope



5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM/MM molecular vibrations (QM/MM-11)

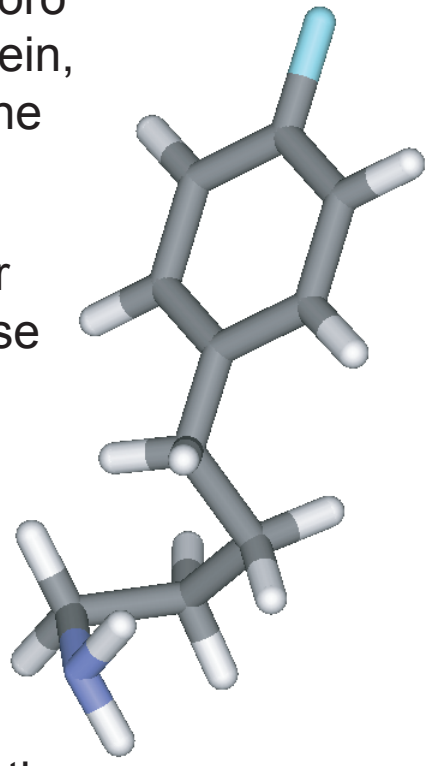
1. Calculate an optimal geometry of the para fluoro compound of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase

2. For the optimal geometry, calculate molecular oscillations, in the protein and in the gas phase

3. Report in a table frequencies of the oscillations of the phenyl ring

4. Repeat frequency calculations for the system where the heteroatom of the phenyl ring has been substituted by its isotope

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



QM/MM molecular vibrations (QM/MM-12)

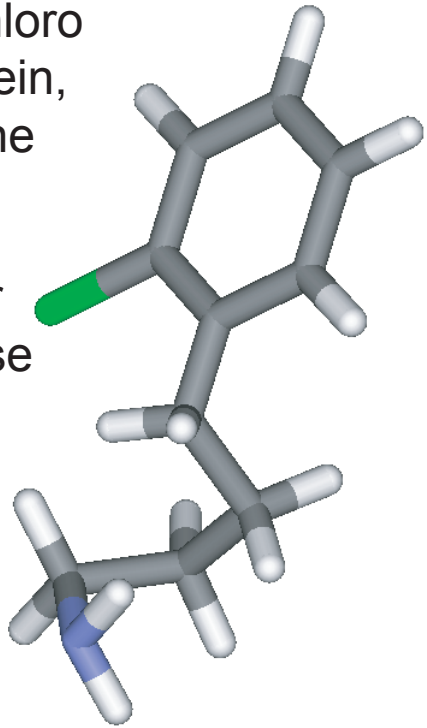
1. Calculate an optimal geometry of the ortho chloro compound of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase

2. For the optimal geometry, calculate molecular oscillations, in the protein and in the gas phase

3. Report in a table frequencies of the oscillations of the phenyl ring

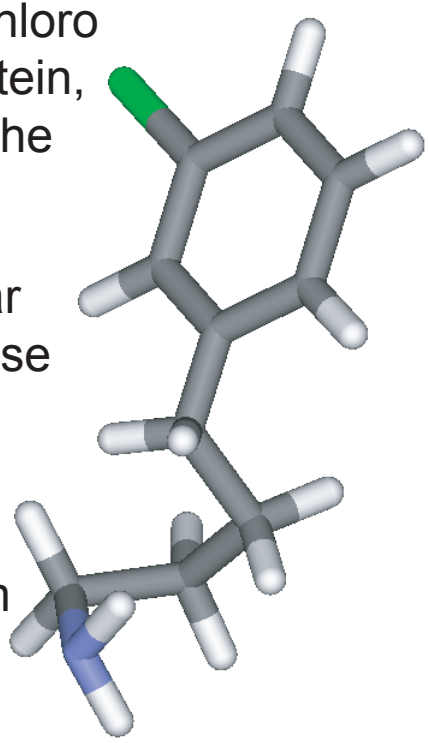
4. Repeat frequency calculations for the system where the heteroatom of the phenyl ring has been substituted by its isotope

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



QM/MM molecular vibrations (QM/MM-13)

1. Calculate an optimal geometry of the meta chloro compound of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase
2. For the optimal geometry, calculate molecular oscillations, in the protein and in the gas phase
3. Report in a table frequencies of the oscillations of the phenyl ring
4. Repeat frequency calculations for the system where the heteroatom of the phenyl ring has been substituted by its isotope
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



QM/MM molecular vibrations (QM/MM-14)

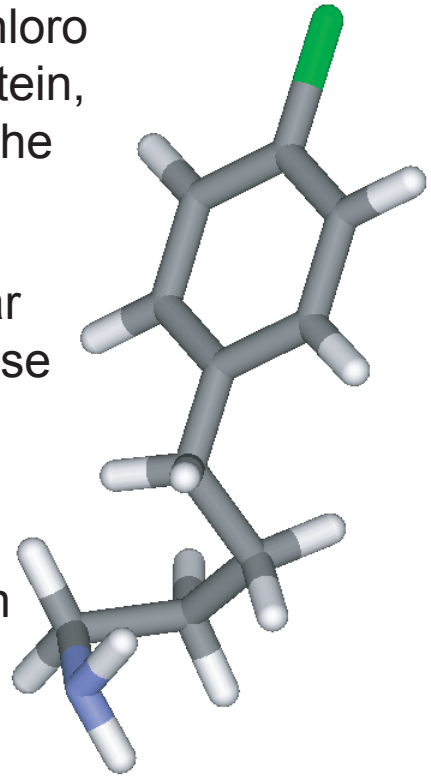
1. Calculate an optimal geometry of the para chloro compound of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase

2. For the optimal geometry, calculate molecular oscillations, in the protein and in the gas phase

3. Report in a table frequencies of the oscillations of the phenyl ring

4. Repeat frequency calculations for the system where the heteroatom of the phenyl ring has been substituted by its isotope

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

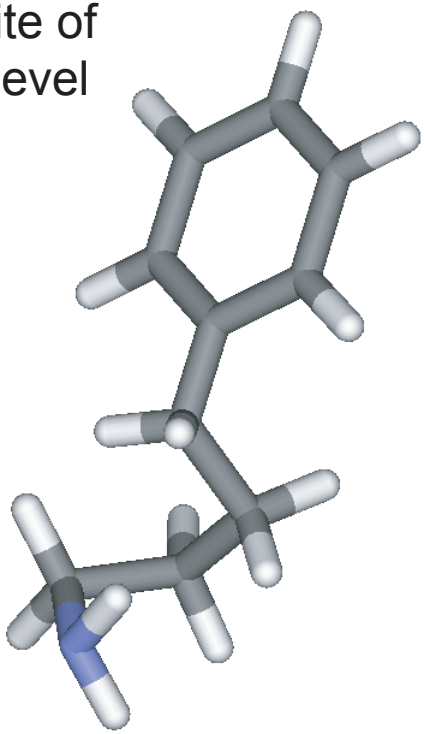


QM/MM electrostatic potential (QM/MM-15)

1. Calculate an optimal geometry of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase

2. For the optimal geometry, calculate the electrostatic potential in the ring plane, in the protein and in the gas phase

3. For the optimal geometry, calculate the electrostatic potential in the perpendicular plane, in the protein and in the gas phase



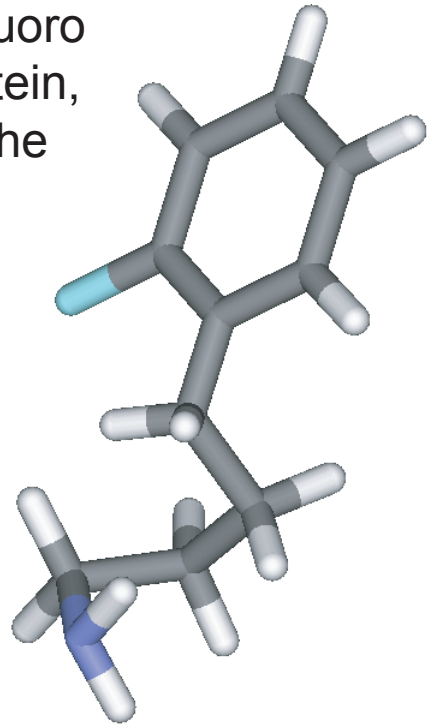
4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM/MM electrostatic potential (QM/MM-16)

1. Calculate an optimal geometry of the ortho fluoro compound of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase

2. For the optimal geometry, calculate the electrostatic potential in the ring plane, in the protein and in the gas phase

3. For the optimal geometry, calculate the electrostatic potential in the perpendicular plane, in the protein and in the gas phase



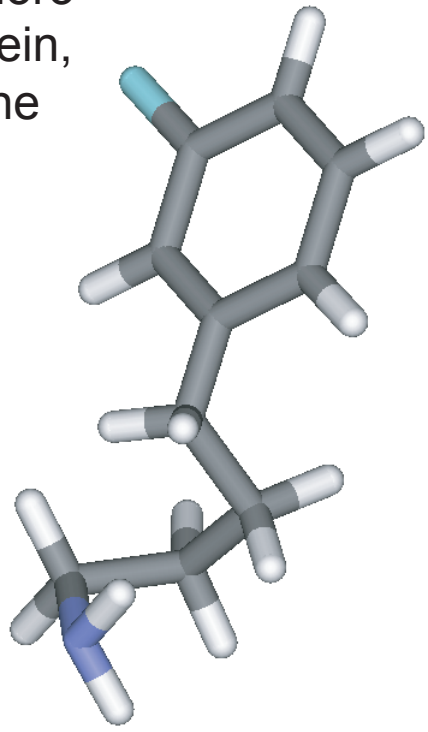
4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM/MM electrostatic potential (QM/MM-17)

1. Calculate an optimal geometry of the meta fluoro compound of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase

2. For the optimal geometry, calculate the electrostatic potential in the ring plane, in the protein and in the gas phase

3. For the optimal geometry, calculate the electrostatic potential in the perpendicular plane, in the protein and in the gas phase



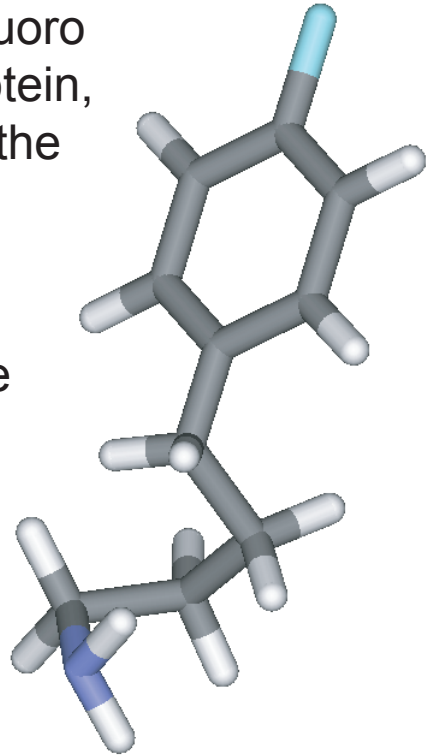
4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM/MM electrostatic potential (QM/MM-18)

1. Calculate an optimal geometry of the para fluoro compound of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase

2. For the optimal geometry, calculate the electrostatic potential in the ring plane, in the protein and in the gas phase

3. For the optimal geometry, calculate the electrostatic potential in the perpendicular plane, in the protein and in the gas phase



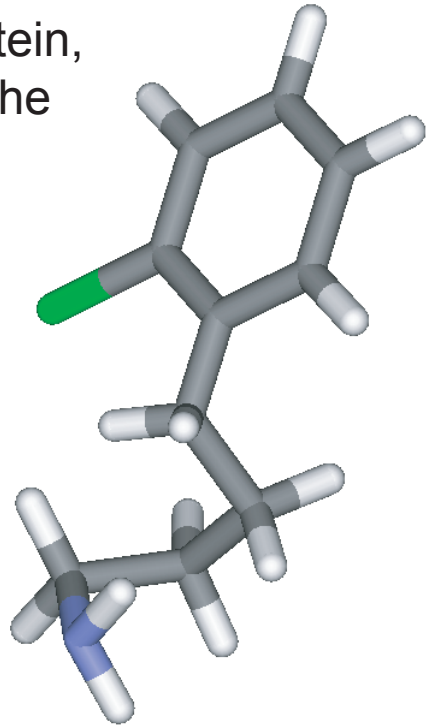
4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM/MM electrostatic potential (QM/MM-19)

1. Calculate an optimal geometry of the ortho chloro compound of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase

2. For the optimal geometry, calculate the electrostatic potential in the ring plane, in the protein and in the gas phase

3. For the optimal geometry, calculate the electrostatic potential in the perpendicular plane, in the protein and in the gas phase



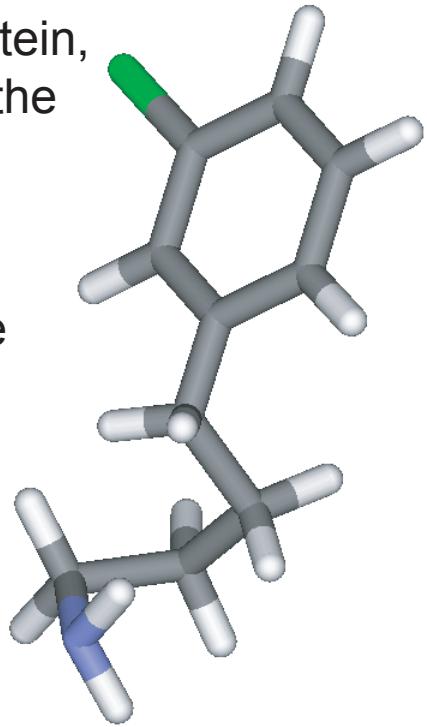
4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM/MM electrostatic potential (QM/MM-20)

1. Calculate an optimal geometry of the meta chloro compound of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase

2. For the optimal geometry, calculate the electrostatic potential in the ring plane, in the protein and in the gas phase

3. For the optimal geometry, calculate the electrostatic potential in the perpendicular plane, in the protein and in the gas phase



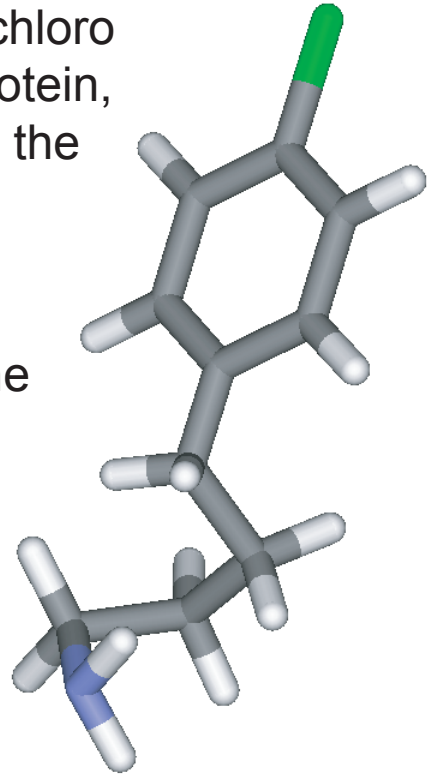
4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM/MM electrostatic potential (QM/MM-21)

1. Calculate an optimal geometry of the para chloro compound of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase

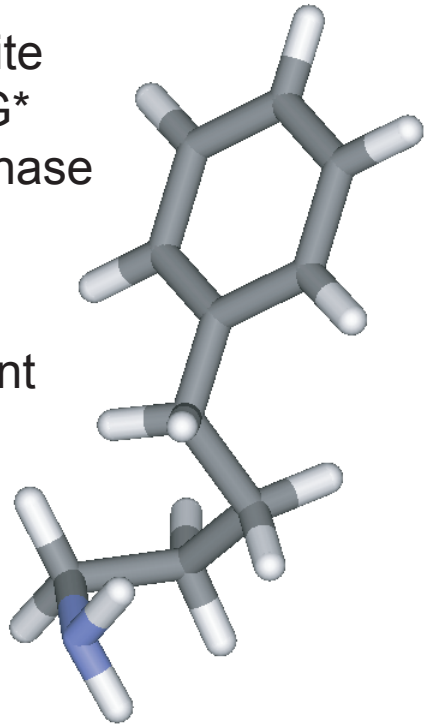
2. For the optimal geometry, calculate the electrostatic potential in the ring plane, in the protein and in the gas phase

3. For the optimal geometry, calculate the electrostatic potential in the perpendicular plane, in the protein and in the gas phase



4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

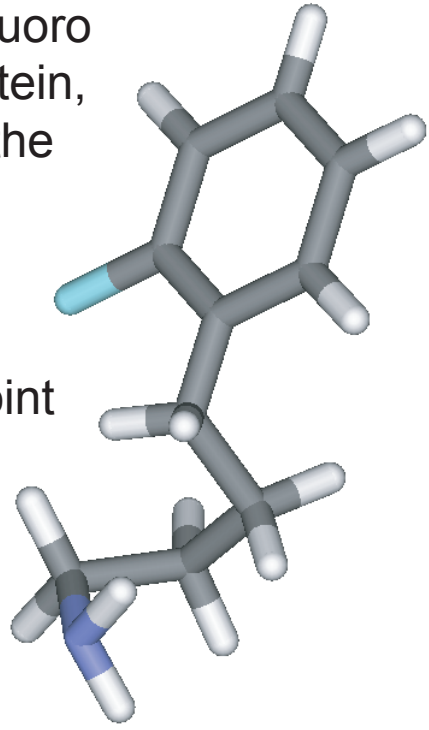
QM/MM internal rotation (QM/MM-22)



1. Calculate an optimal geometry of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase
2. For the optimal geometry, change the orientation of the phenyl ring relative to the rest of the ligand, and calculate the single point energy
3. Repeat the calculations for different ring positions in the protein and in the gas phase, and report the energy as a function of the torsional angle
4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM/MM internal rotation (QM/MM-23)

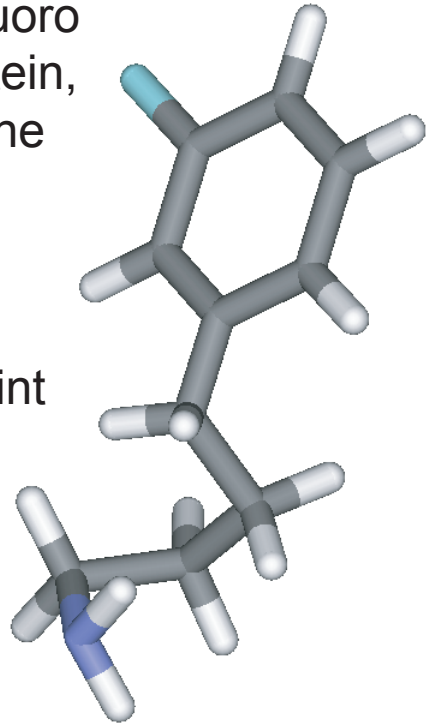
1. Calculate an optimal geometry of the ortho fluoro compound of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase
2. For the optimal geometry, change the orientation of the phenyl ring relative to the rest of the ligand, and calculate the single point energy
3. Repeat the calculations for different ring positions in the protein and in the gas phase, and report the energy as a function of the torsional angle



4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

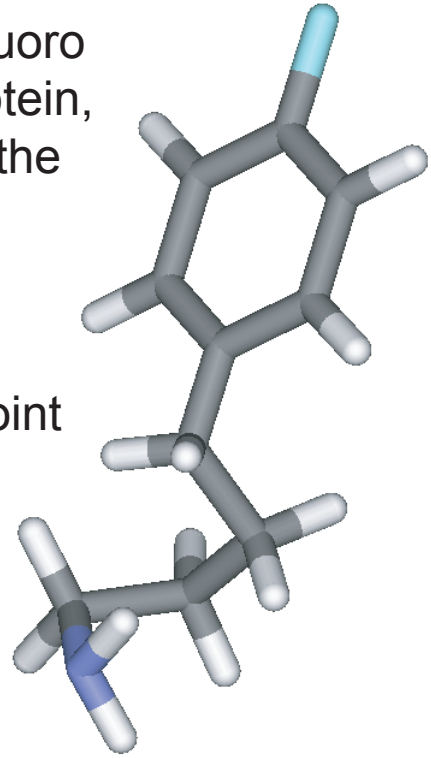
QM/MM internal rotation (QM/MM-24)

1. Calculate an optimal geometry of the meta fluoro compound of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase
2. For the optimal geometry, change the orientation of the phenyl ring relative to the rest of the ligand, and calculate the single point energy
3. Repeat the calculations for different ring positions in the protein and in the gas phase, and report the energy as a function of the torsional angle
4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



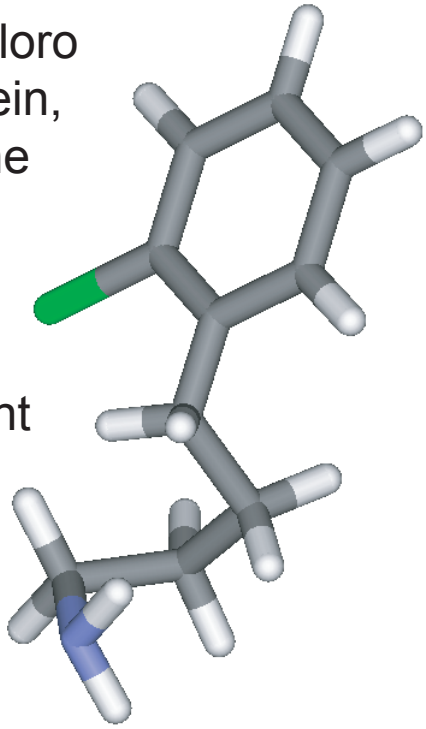
QM/MM internal rotation (QM/MM-25)

1. Calculate an optimal geometry of the para fluoro compound of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase
2. For the optimal geometry, change the orientation of the phenyl ring relative to the rest of the ligand, and calculate the single point energy
3. Repeat the calculations for different ring positions in the protein and in the gas phase, and report the energy as a function of the torsional angle
4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



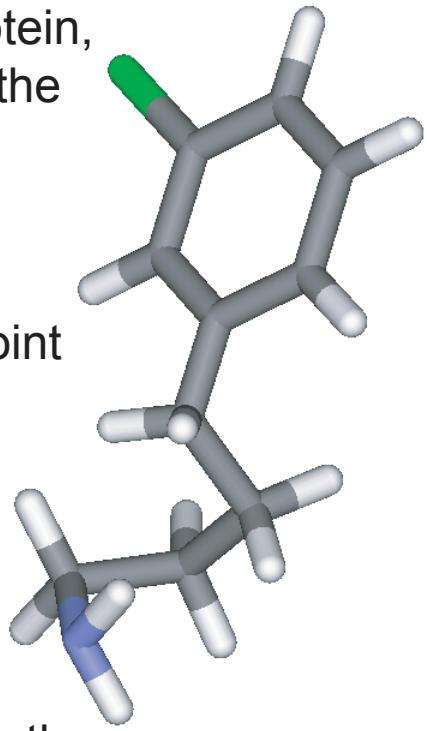
QM/MM internal rotation (QM/MM-26)

1. Calculate an optimal geometry of the ortho chloro compound of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase
2. For the optimal geometry, change the orientation of the phenyl ring relative to the rest of the ligand, and calculate the single point energy
3. Repeat the calculations for different ring positions in the protein and in the gas phase, and report the energy as a function of the torsional angle
4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



QM/MM internal rotation (QM/MM-27)

1. Calculate an optimal geometry of the meta chloro compound of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase
2. For the optimal geometry, change the orientation of the phenyl ring relative to the rest of the ligand, and calculate the single point energy
3. Repeat the calculations for different ring positions in the protein and in the gas phase, and report the energy as a function of the torsional angle
4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



QM/MM internal rotation (QM/MM-28)

1. Calculate an optimal geometry of the para chloro compound of the active site of the PCAF protein, using the B3LYP/6-31+G* level of theory, in the protein and in the gas phase
2. For the optimal geometry, change the orientation of the phenyl ring relative to the rest of the ligand, and calculate the single point energy
3. Repeat the calculations for different ring positions in the protein and in the gas phase, and report the energy as a function of the torsional angle
4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory