Supplementary Materials for: Simulating Absorption Spectra of Flavonoids in Aqueous Solution: a Polarizable QM/MM Study

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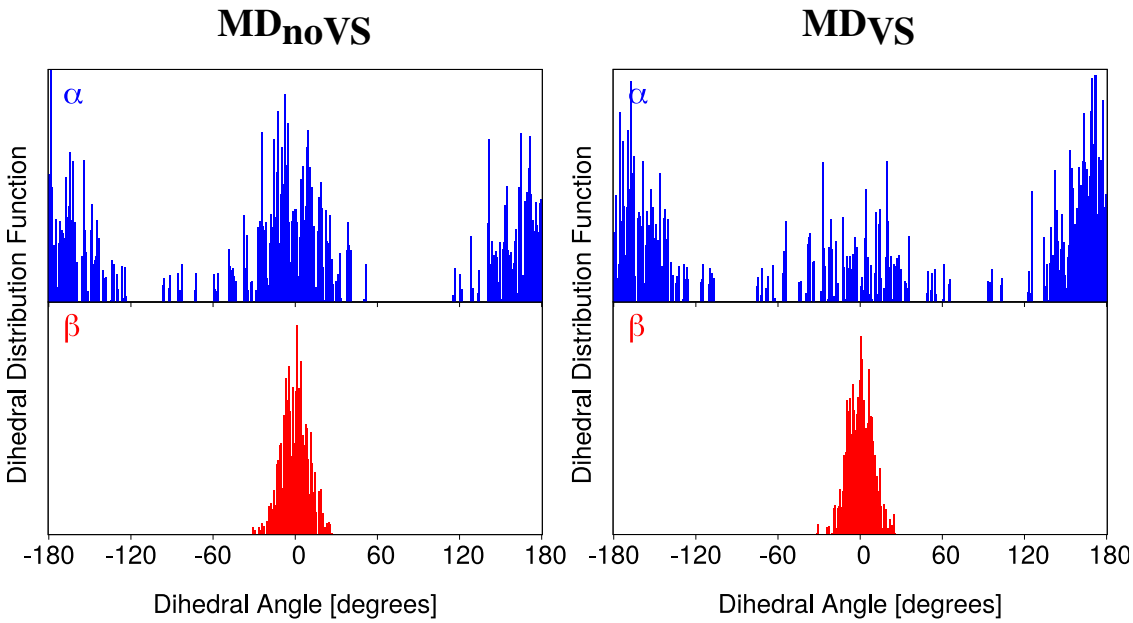

Figure S1: Dihedral distribution functions of α (top,blue), β (bottom,red) dihedral angles of Luteolin (**L**) as obtained from $\mathrm{MD_{noVS}}$ (left) and $\mathrm{MD_{VS}}$ (right).

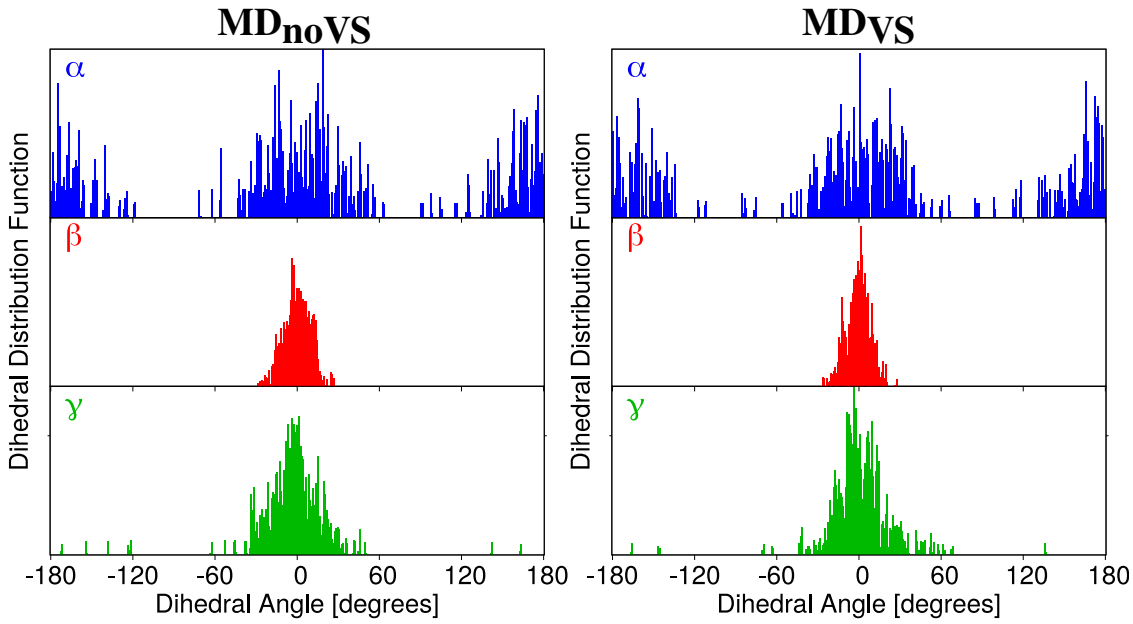

Figure S2: Dihedral distribution functions of α (top,blue), β (middle,red) and γ (bottom,green) dihedral angles of Kaempferol (**K**) as obtained from $\mathrm{MD_{noVS}}$ (left) and $\mathrm{MD_{VS}}$ (right).

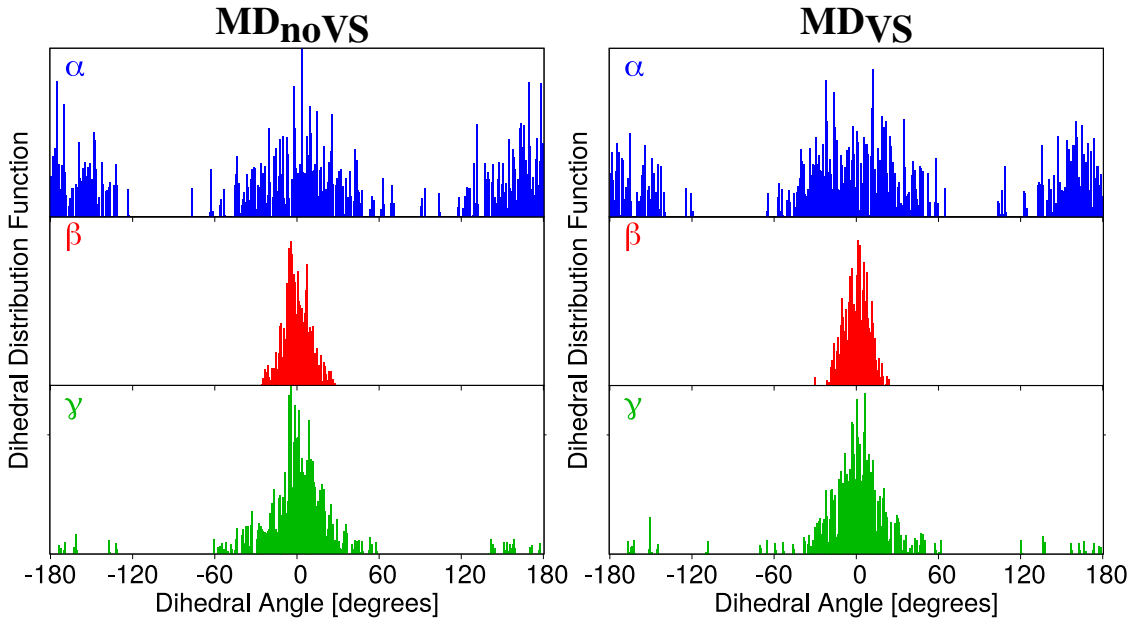

Figure S3: Dihedral distribution functions of α (top,blue), β (middle,red) and γ (bottom,green) dihedral angles of Quercetin (**Q**) as obtained from MD_{noVS} (left) and MD_{VS} (right).

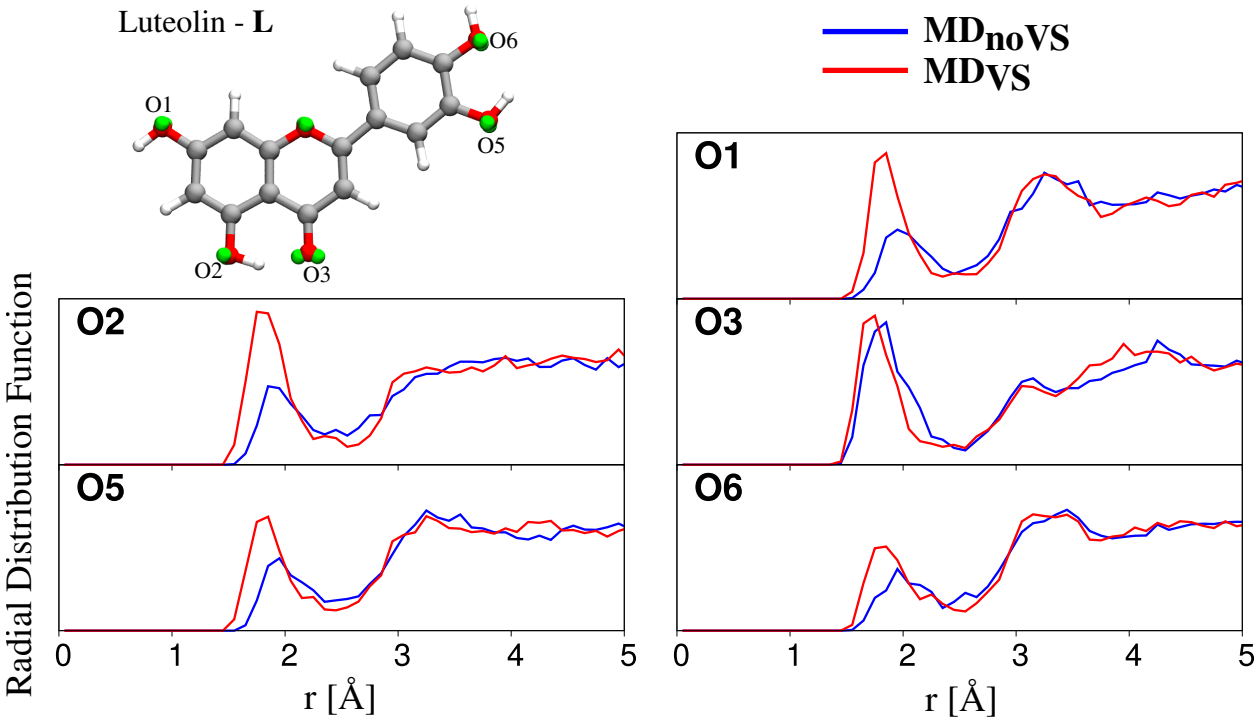

Figure S4: Radial distribution functions between selected Oxygen atoms of Luteolin and water Hydrogen atoms as obtained from MD_{noVS} (blue) and MD_{VS} (red).

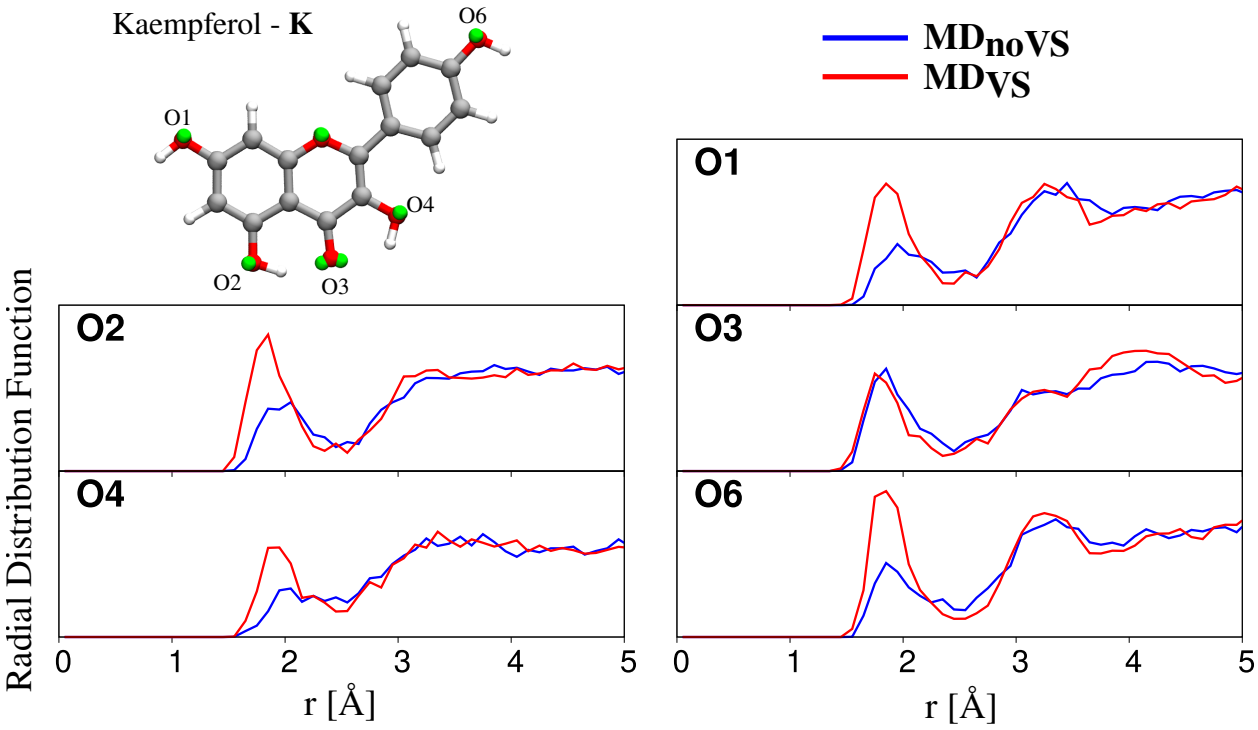

Figure S5: Radial distribution functions between selected Oxygen atoms of Kaempferol and water Hydrogen atoms as obtained from MD_{noVS} (blue) and MD_{VS} (red).

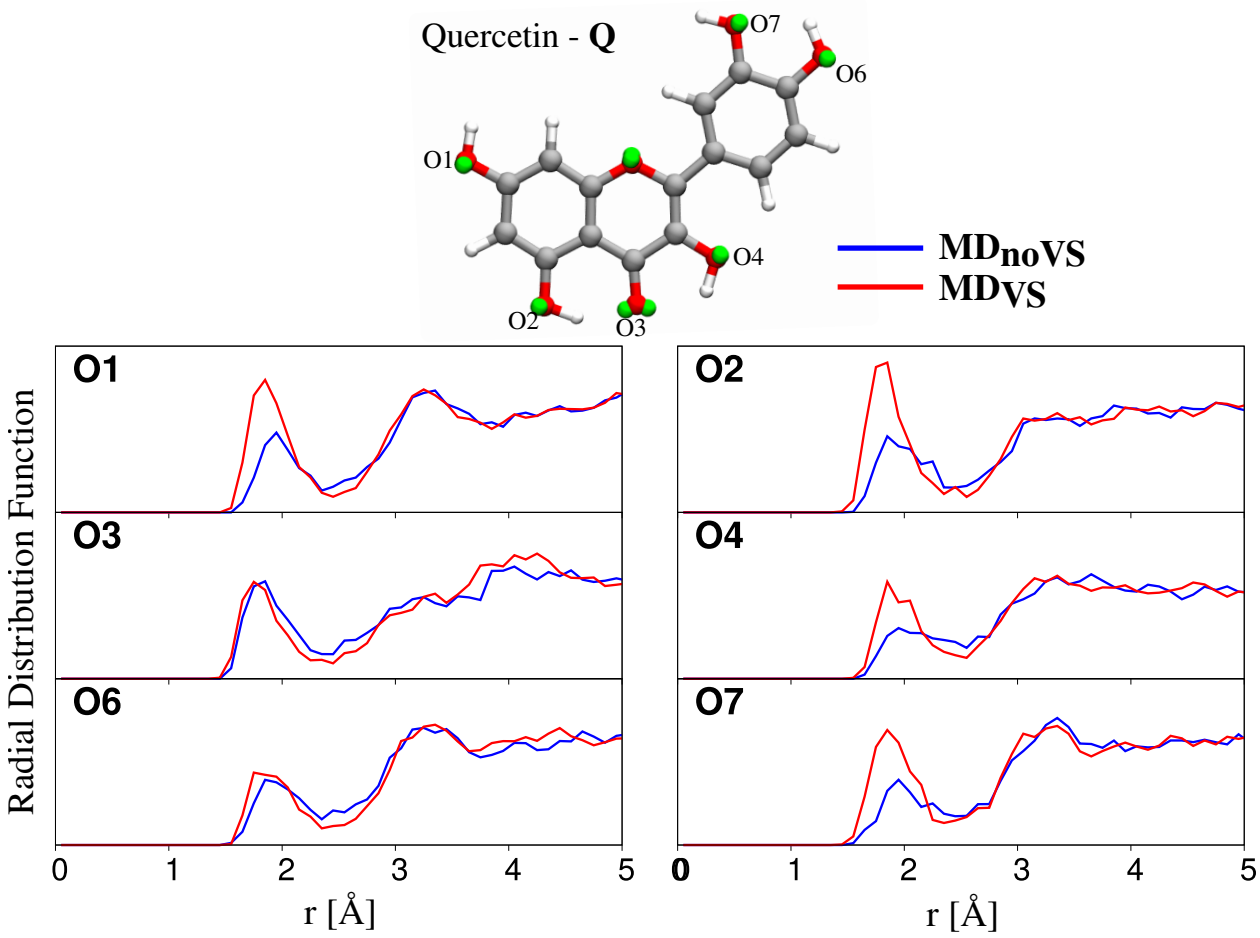

Figure S6: Radial distribution functions between selected Oxygen atoms of Quercetin and water Hydrogen atoms as obtained from MD_{noVS} (blue) and MD_{VS} (red).

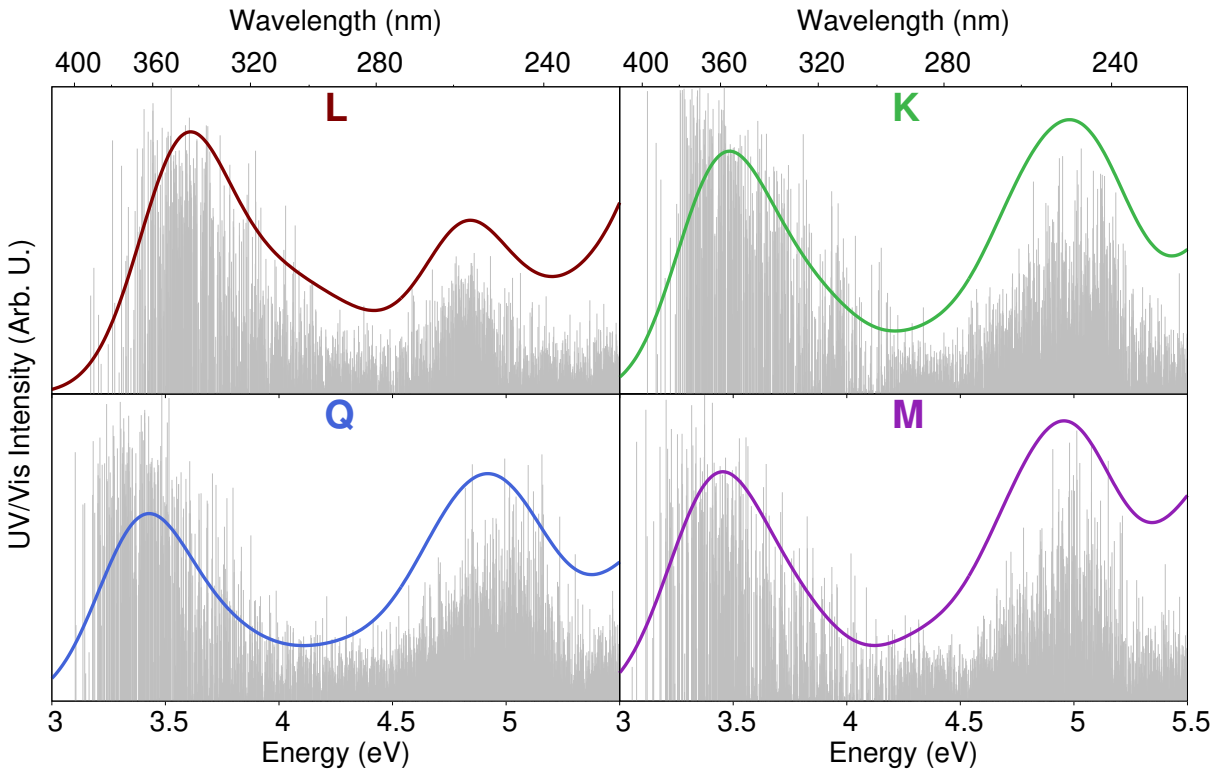

Figure S7: QM/FQ UV/Vis stick spectra computed on the snapshots extracted from MD_{VS}. The convoluted QM/FQ spectra are also plotted.

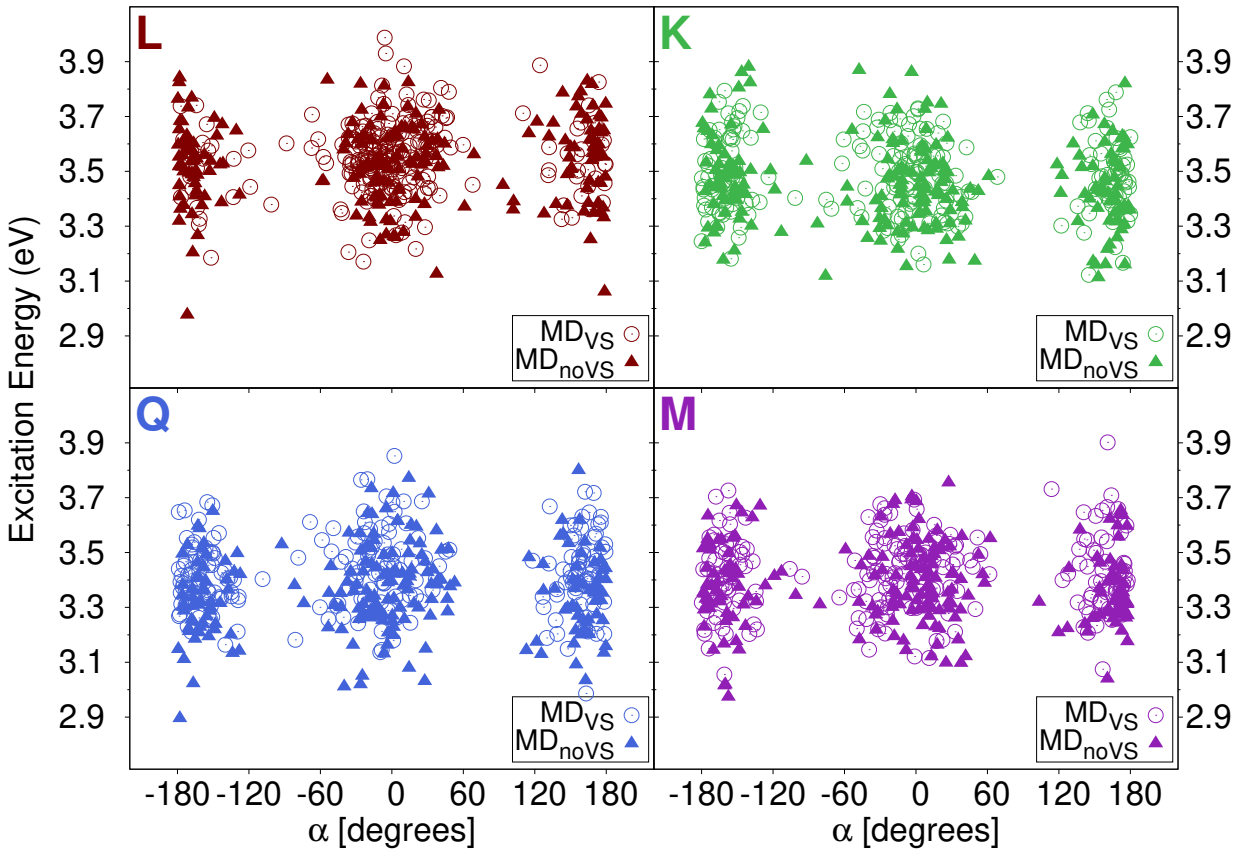

Figure S8: QM/FQ Excitation Energies of the first electronic transition as a function of α dihedral angle.

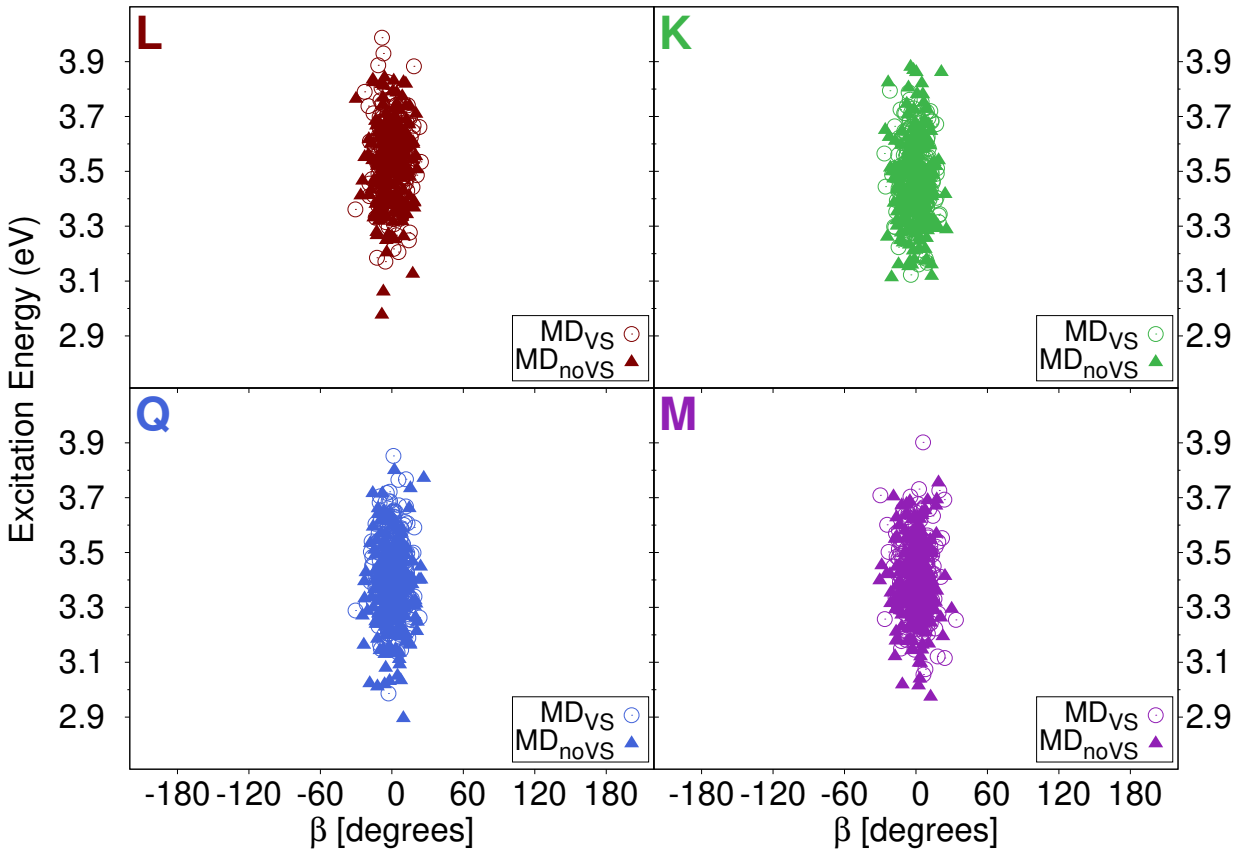

Figure S9: QM/FQ Excitation Energies of the first electronic transition as a function of β dihedral angle.

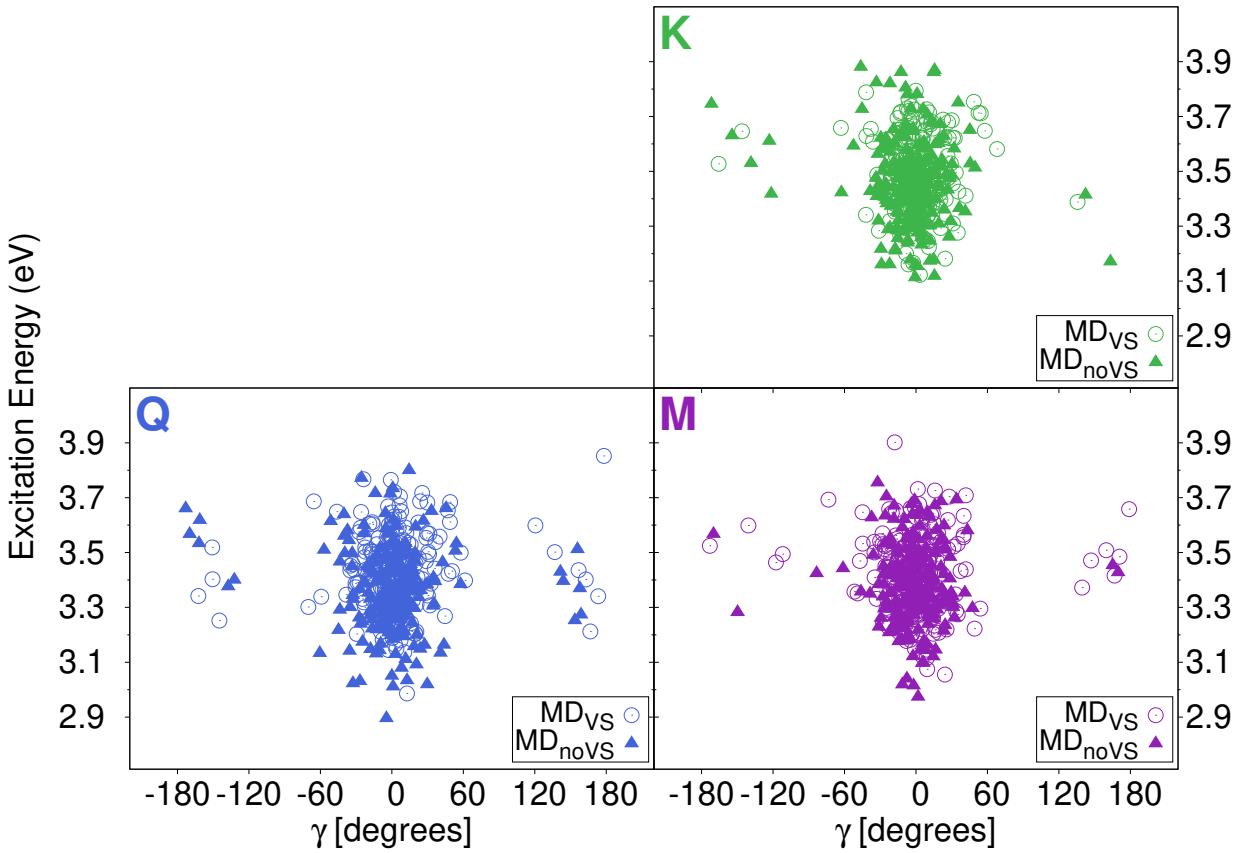

Figure S10: QM/FQ Excitation Energies of the first electronic transition as a function of γ dihedral angle.