

Supplementary Information

Molecular dynamics simulations of the adsorption of BMP-2 on surfaces with medical relevance

*Tillmann Utesch, Grazia Daminelli, Maria Andrea Mroginski**

Technische Universität Berlin, Institut für Chemie, Sekr. PC 14, 10623 Berlin, Germany

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- 1) Total energy curves for BMP2 thermal equilibration (Fig S1)
- 2) rmsd curves for SMD step (Fig S2)
- 3) Final structures of BMP2 adsorbed on surfaces (Fig S3,S4)
- 4) Desorption curves (Fig S5-FigS7)

Figure S1: Total energy curves for BMP2/graphite and BMP2/TiO₂ during the 200 ps thermal equilibration step

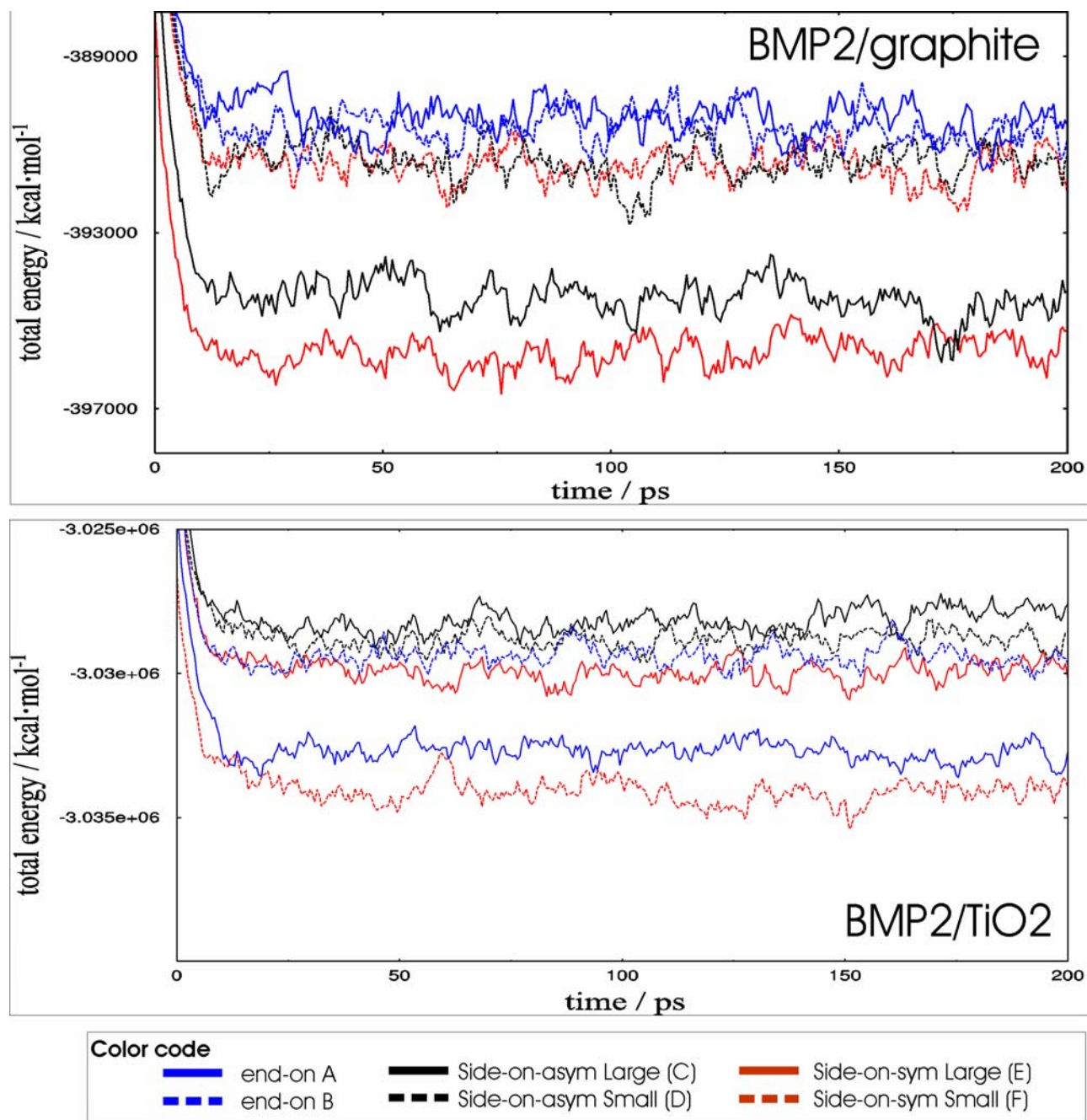


Figure S2: Root mean square deviation (rmsd) curves for heavy atoms on the BMP2 backbone during the SMD simulations of BMP2/graphite and BMP2/TiO₂ systems

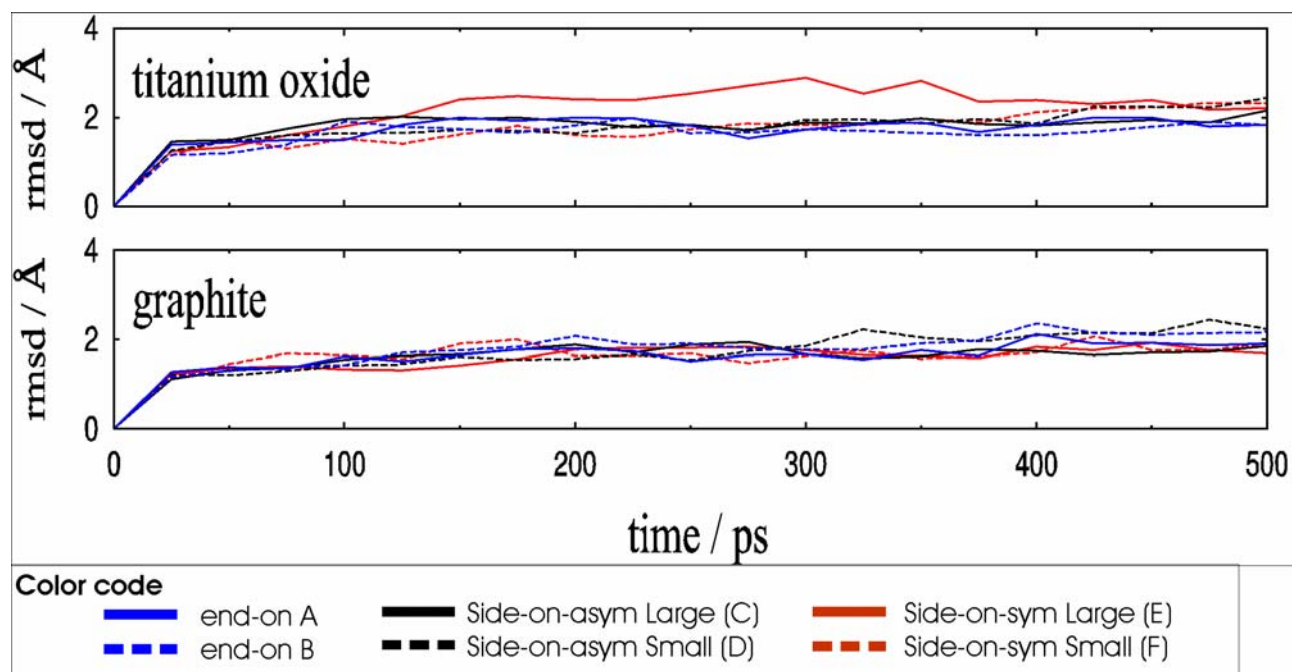
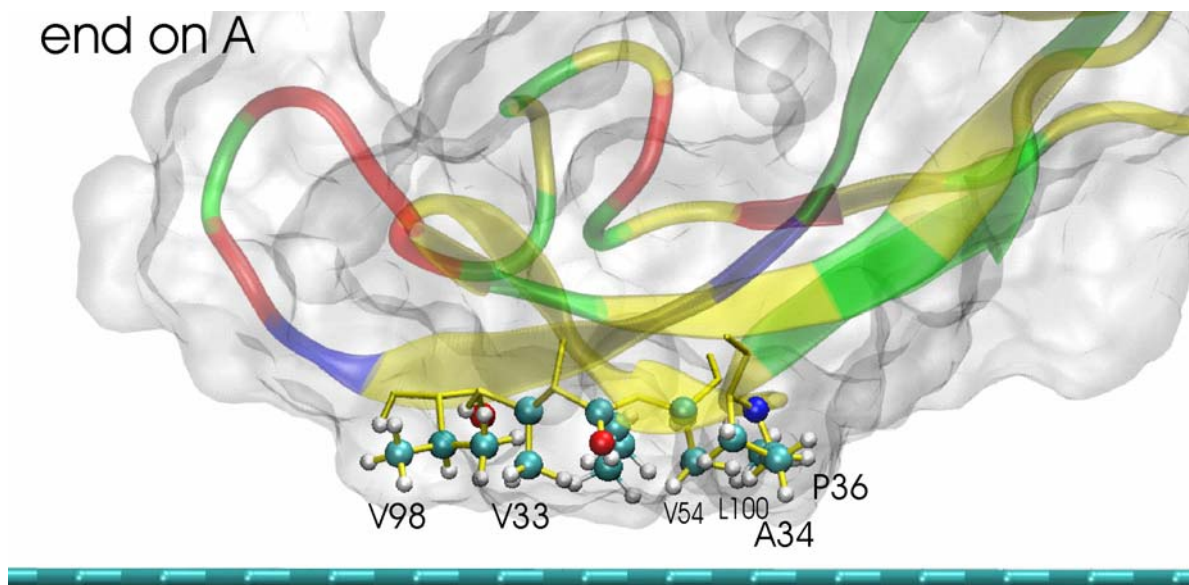


Figure S3: Final structures of BMP2 adsorbed on graphite surfaces

end on A



end on B

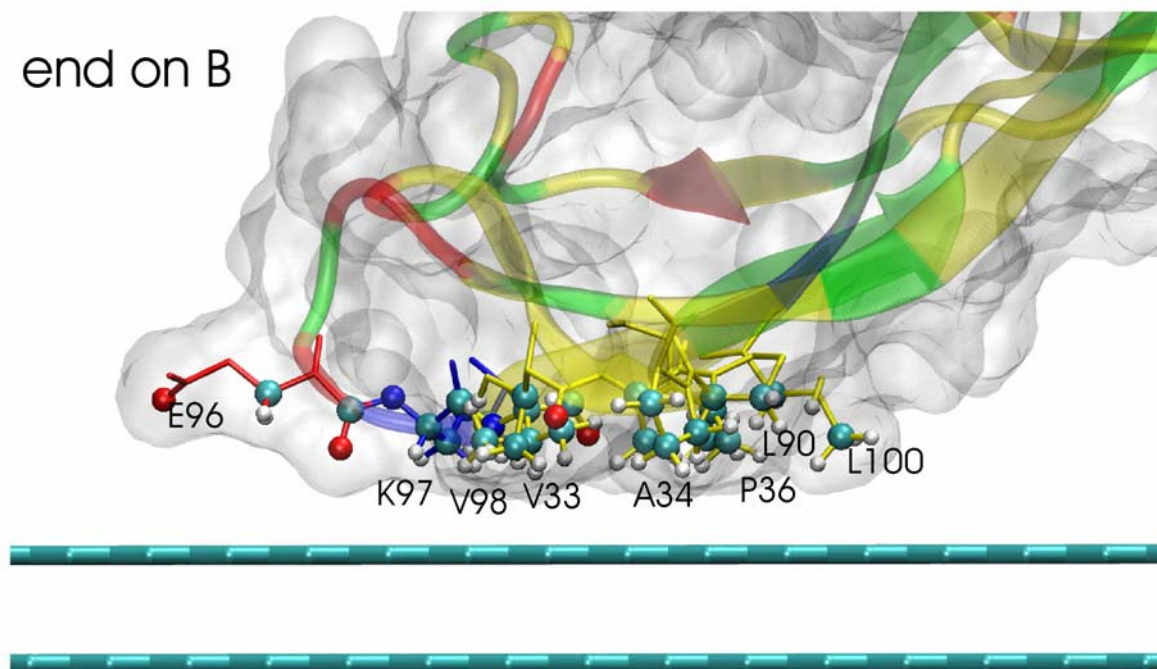
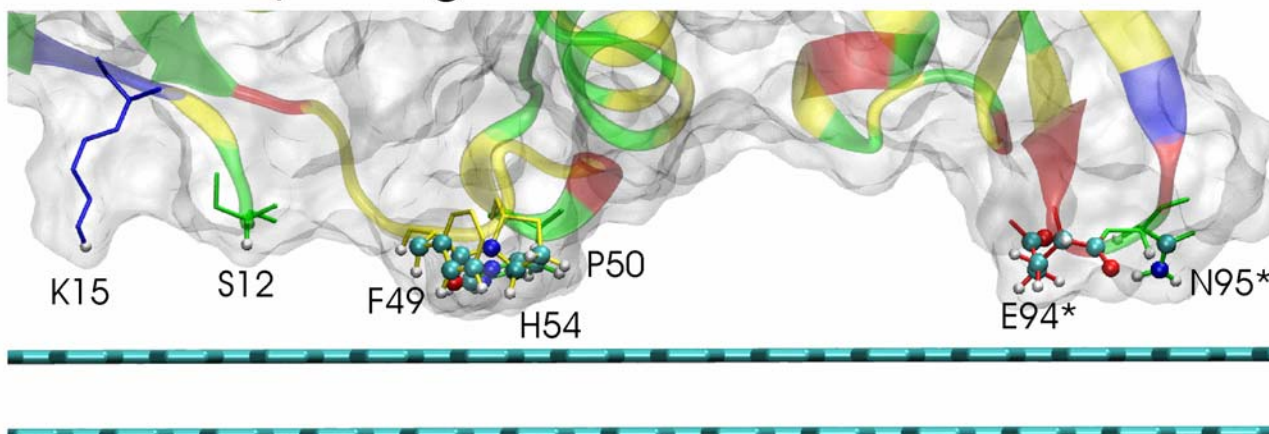
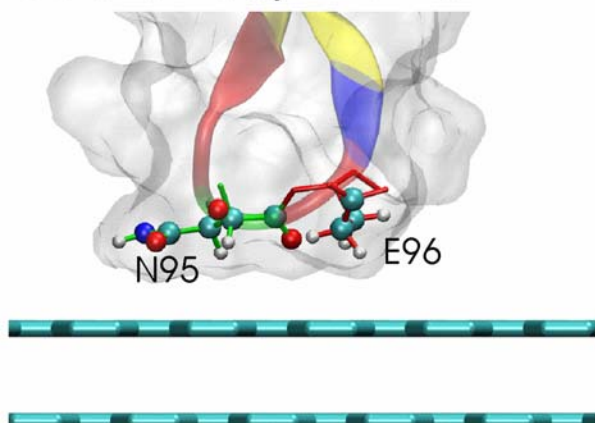


Figure S4: Final structures of BMP2 adsorbed on graphite surfaces

side-on-asym Large



side-on-asym Small



side-on-sym Small

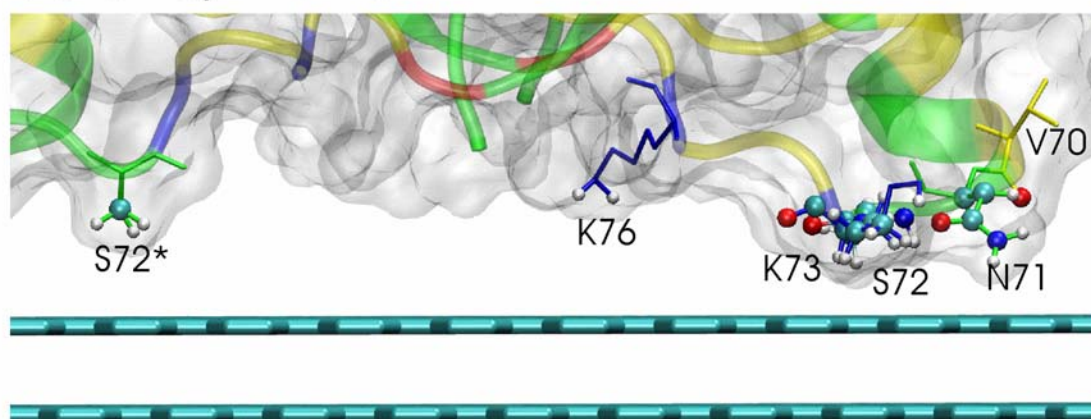


Figure S5: Desorption of BMP2 from the graphite forced by artificial forces pulling the dummy atom with a velocity $v=0.25 \text{ \AA/ps}$ and a force constant $k=50 \text{ kcal}/(\text{mol \AA})$. For the End-on A and B orientations, pulling forces, interaction energy between graphite and BMP2 and the surface separation distance of selected residues are plotted during SMD desorption.

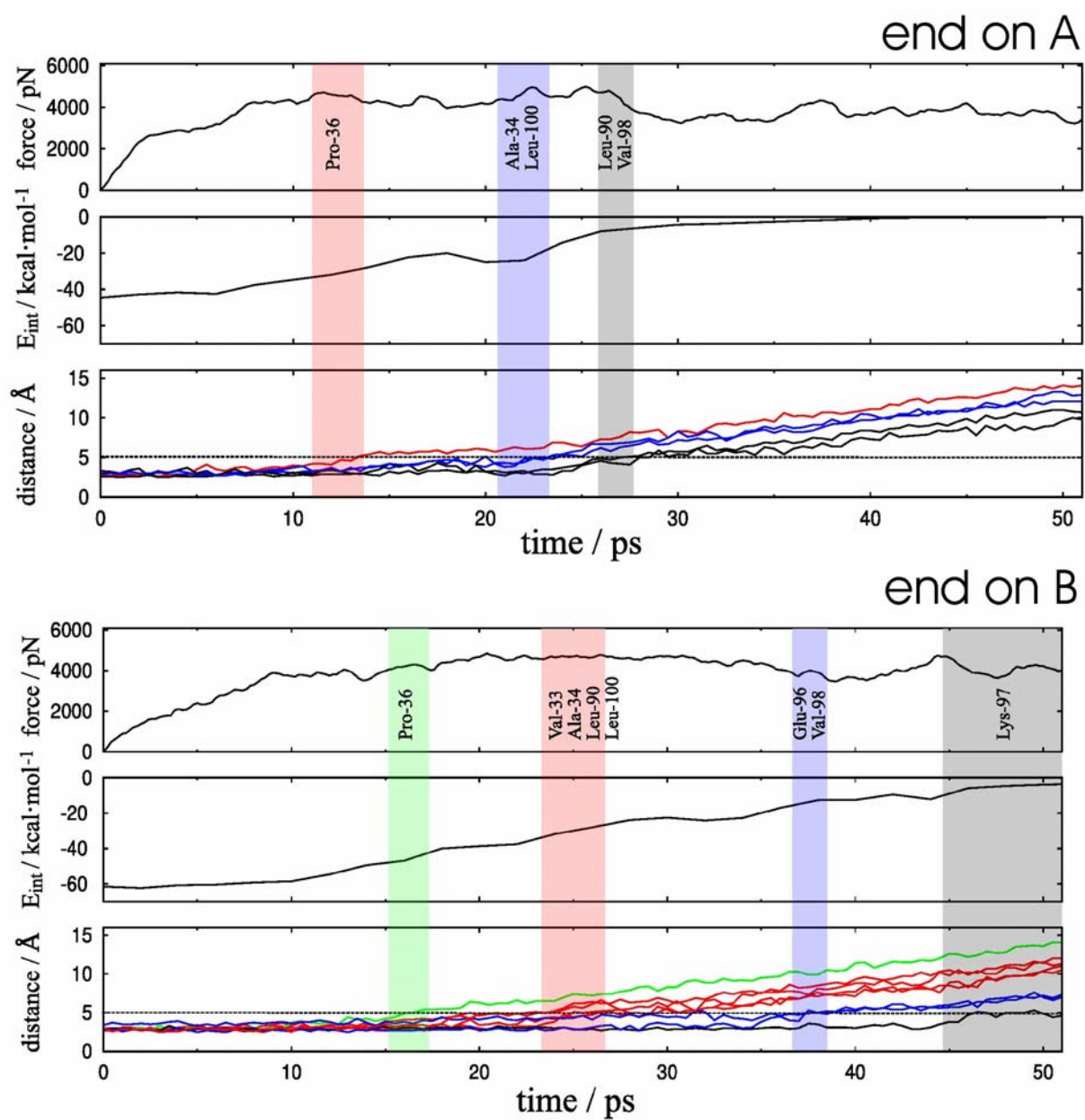


Figure S6: Desorption of BMP2 from the graphite forced by artificial forces pulling the dummy atom with a velocity $v=0.25 \text{ \AA/ps}$ and a force constant $k=50 \text{ kcal/(mol \AA)}$. For the side-on asymmetric orientations, pulling forces, interaction energy between graphite and BMP2 and the surface separation distance of selected residues are plotted during SMD desorption.

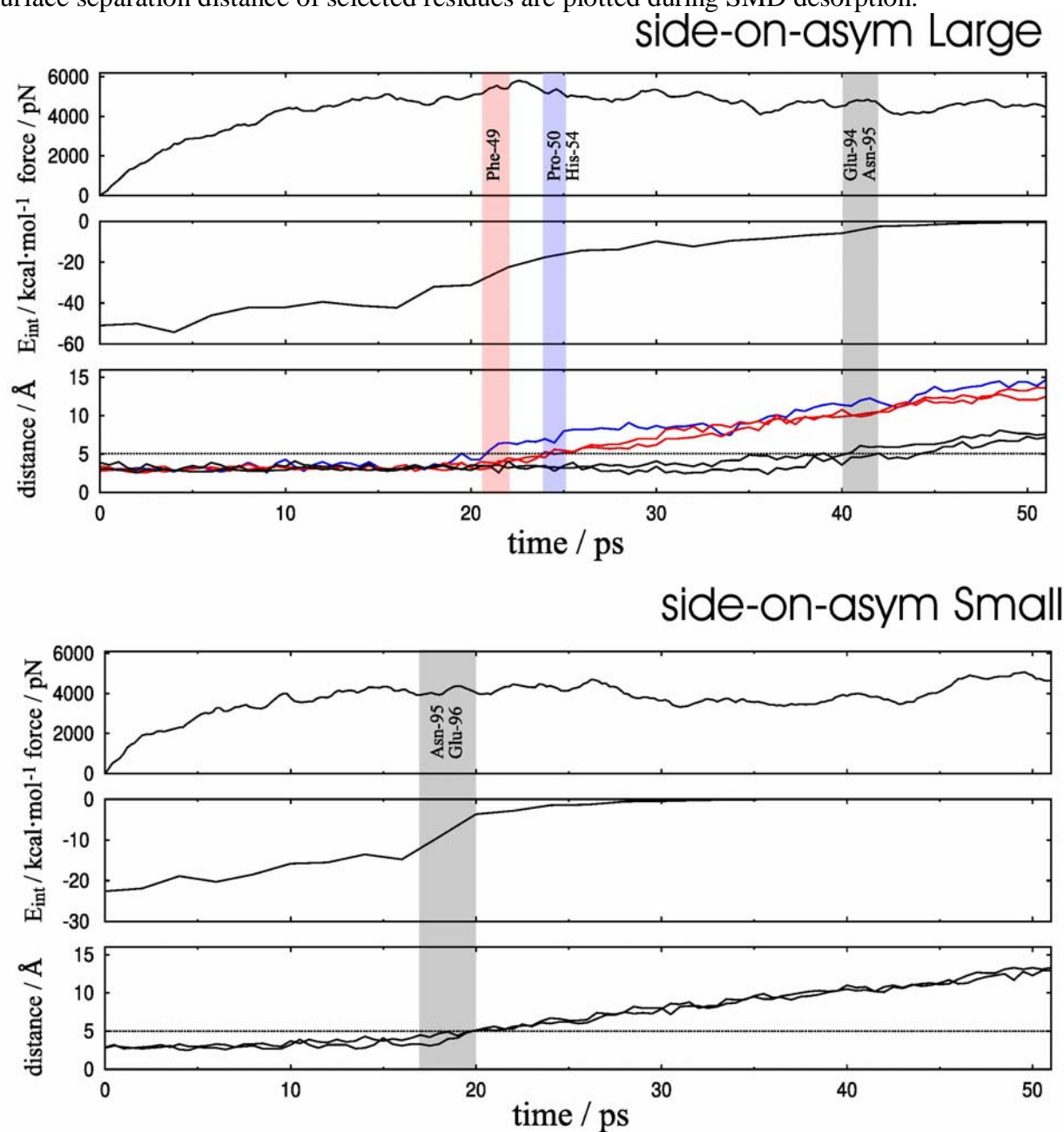
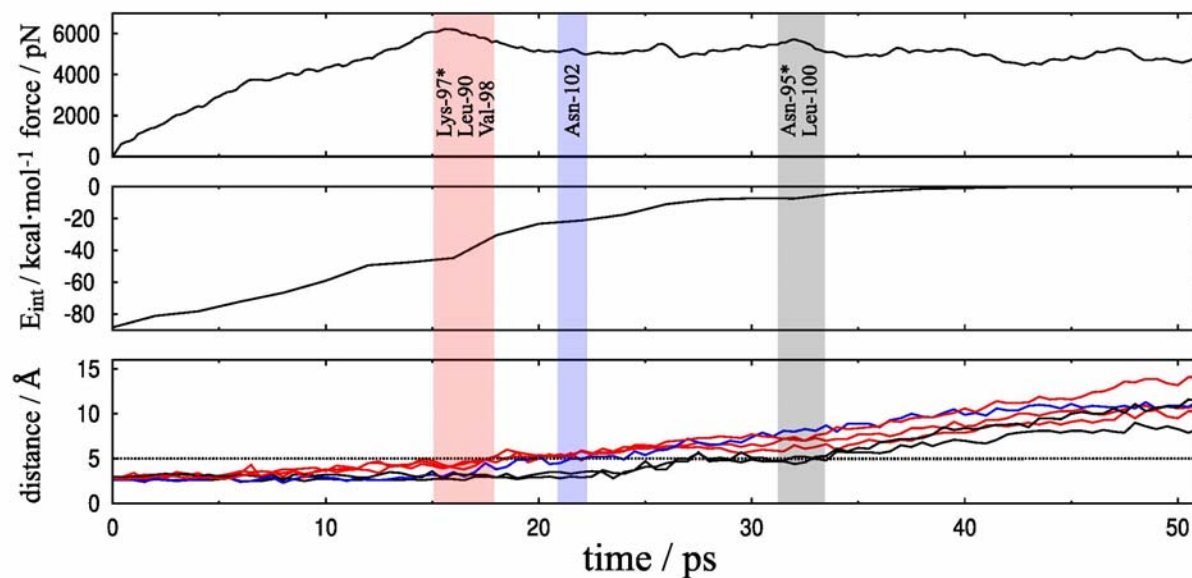


Figure S7: Desorption of BMP2 from the graphite forced by artificial forces pulling the dummy atom with a velocity $v=0.25 \text{ \AA/ps}$ and a force constant $k=50 \text{ kcal}/(\text{mol \AA})$. For the side-on symmetric orientations, pulling forces, interaction energy between graphite and BMP2 and the surface separation distance of selected residues are plotted during SMD desorption.

side-on-sym Large



side-on-sym Small

