

# 1 PIPSA analysis

Various research areas have utilized PIPSA (Protein Interaction Property Similarity Analysis) Wade et al. (2001) for quantification of Molecular Interaction Field (MIF) differences. PIPSA allows the selection of different regions for comparison, such as a skin of adjustable thickness defined using surface probes of adjustable radius around the whole protein or in defined spherical or conical region. The definition of regions is useful to restrict comparison of the MIFs to the sites where the interaction occurs for a given system. For example, for comparing the interaction fields of binding sites for relating enzyme kinetic parameters Gabdoulline et al. (2007), a spherical restriction of the surface skin was used. surface skin was used.

Some geometries of interaction sites are not well covered using the restrictions methods already implemented in PIPSA (cone and sphere). Therefore, a cylindrical restriction was implemented in addition. To be able to better verify the selected region, a method to visualize the selected region was also added to PIPSA (see 1). The cylindrical region needs to overlap with the protein skin, as do the other geometric restriction methods in PIPSA. The cylinder is specified by the start and end coordinates of the central axis and the radius of the cylinder Mendes et al. (2022).

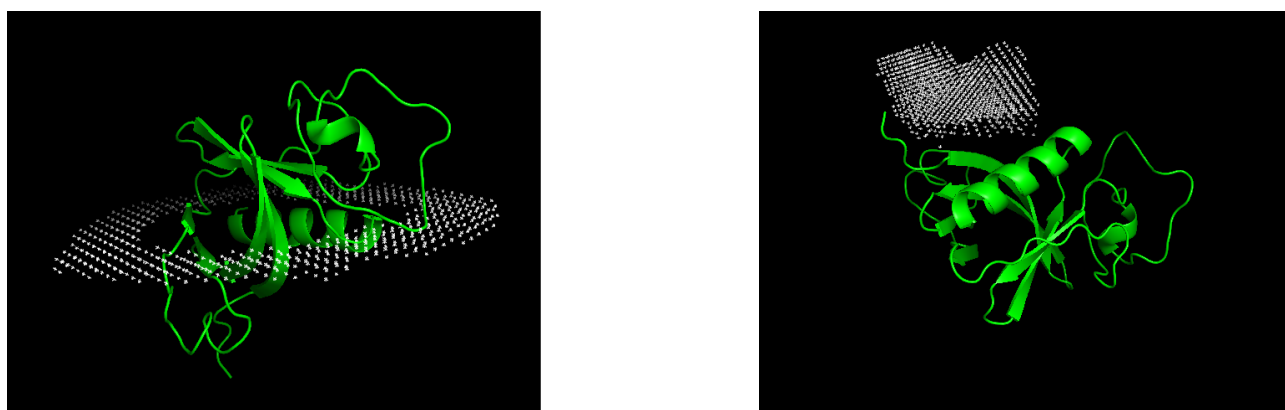


Figure 1: Pleckstrin Homology (PH) domain with two different cylinder definitions for PIPSA. PIPSA now allows visualization of the volume selected using a command line flag ‘-pv filename.pdb’. Left: The cylinder is defined by the axis  $x_0=21.771$ ,  $y_0=12.558$ ,  $z_0=11.517$  and  $x_1=20.771$ ,  $y_1=11.558$ ,  $z_1=10.517$ , radius=30 Å. Right: The cylinder is defined by the axis  $x_0=21.771$ ,  $y_0=12.558$ ,  $z_0=11.517$  and  $x_1=0.0$ ,  $y_1=0.0$ ,  $z_1=0.0$  and radius=10 Å. In both cases, the probe radius and skin thickness were set to 3.0 and 4.0 Å, respectively.

## References

- Gabdoulline, R. R., Stein, M. & Wade, R. C. (2007), ‘qpipsa: relating enzymatic kinetic parameters and interaction fields’, *BMC bioinformatics* **8**(1), 373.
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- Wade, R., Gabdoulline, R. & De Rienzo, F. (2001), ‘Protein interaction property similarity analysis’, *International Journal of Quantum Chemistry* **83**(3-4), 122–127.