Comparison of Solvent Accessible Surface Area (SASA) for Omega Basic No. of cheminfor-matics structures 7.0 7.5 8.0 8.5 No. of cheminfor-matics structures 7.5 8.0 8.5 7.5 8.0 8.5 7.5 8.0 8.5 No. of cheminfor-matics structures No. of cheminformatics structures 7.5 5.6 5.8 7.0 No. of cheminfor-matics structures SASA [nm²] No. of cheminformatics structures GaMD SASA [nm²] SASA [nm²] SASA [nm²] SASA [nm²] SASA [nm²] cMD