

1. Calculation of the dimensions of the molecular clips and tweezers:

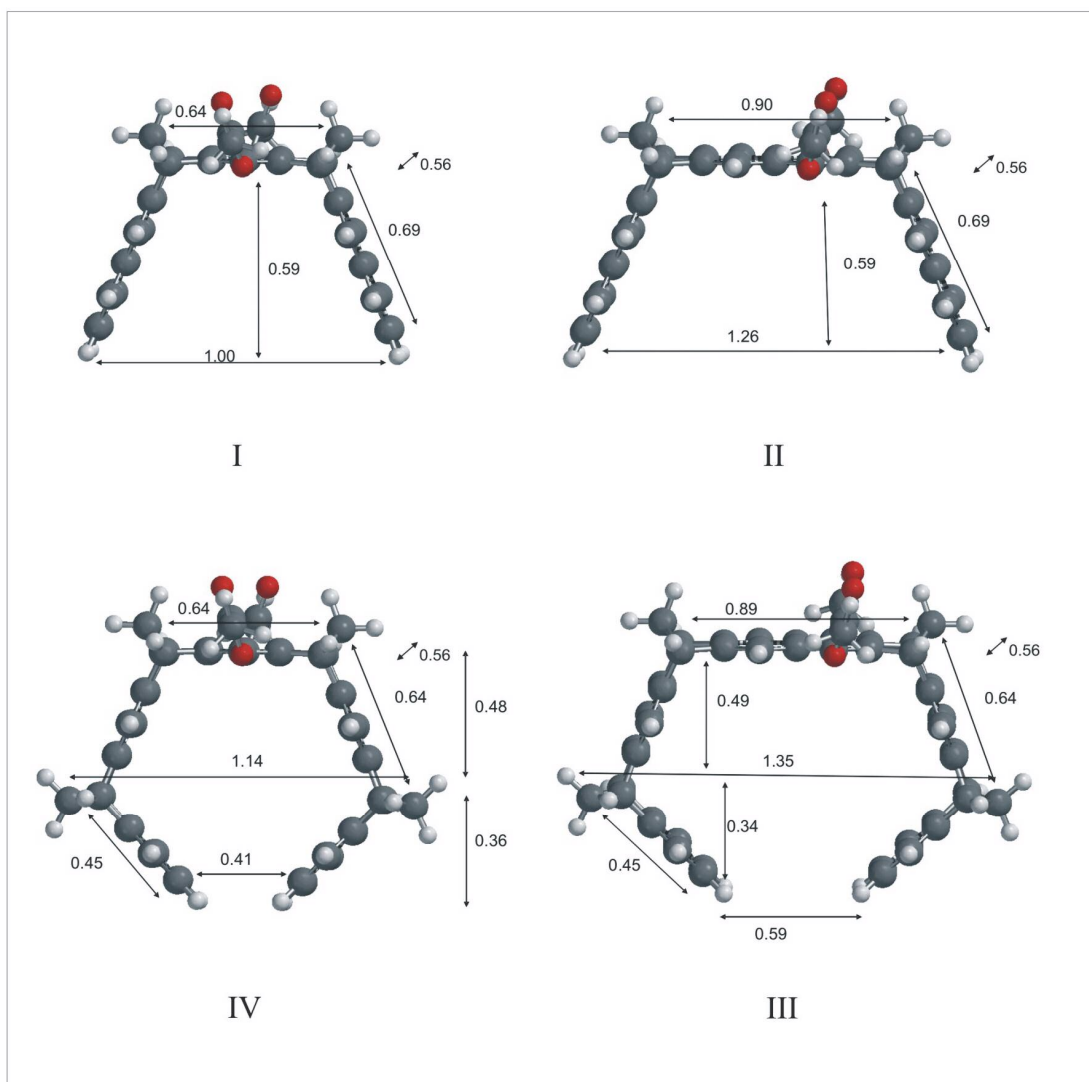


Figure 1: Dimensions of the four investigated receptor molecules calculated by means of force field methods (MMFF94, Monte-Carlo conformer search)

With the values of figure 1 we are able to calculate the area of different sides of the molecules. This is shown exemplary for the molecular clip I in figure 2.

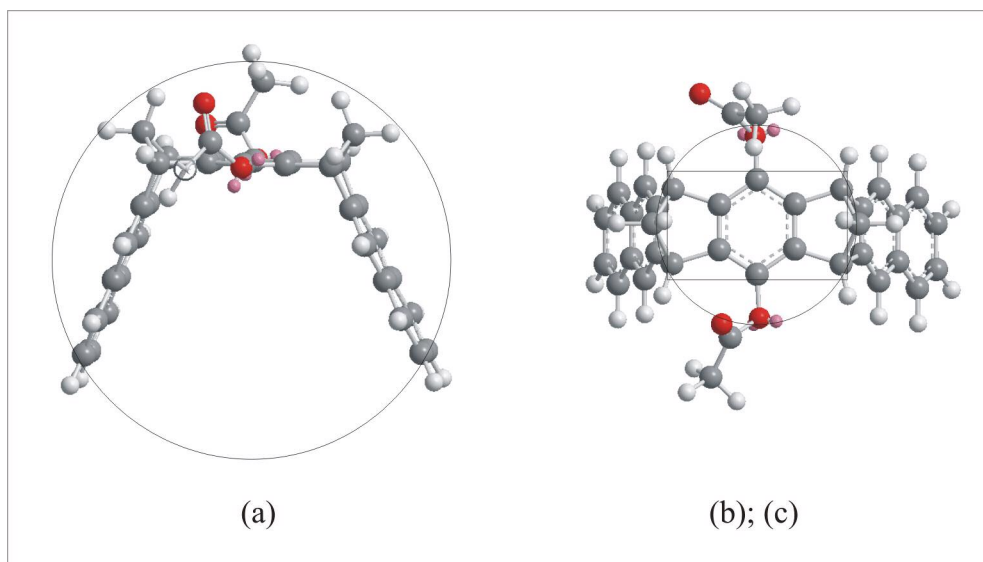


Figure 2: Two different sides of the molecule were chosen to calculate the required area the molecules: (a) The molecules lie flatly onto the water surface and (b) the molecules are oriented with the aromatic side arms perpendicular to the water surface. (c) The molecules are oriented with the aromatic side arms perpendicular to the water surface and can't rotate.

Table 1 shows the results of the calculation of the area.

Table 1: Theoretical areas calculated for the used tweezers and clips lying flat on the water surface (a), oriented perpendicular to the water surface (b) and oriented perpendicular to the water surface without a rotation. The characters correspond to figure 2.

Typ	Calculated area [nm ²]		
	(a)	(b)	(c)
I	0.79	0.34	0,33
II	1.25	0.62	0,46
III	1.43	0.62	0,46
IV	1.02	0.34	0,33