Targeting the Protein Backbone with Aryl Halides: Systematic Comparison of Halogen Bonding and $\pi\cdots\pi$ Interactions using $N$-methylacetamide

M. O. Zimmermann$^{a,b}$ and F. M. Boeckler$^{a,b}$

$^a$ Department of Pharmaceutical and Medicinal Chemistry, Institute of Pharmaceutical Sciences, Eberhard Karls Universität Tübingen, Auf der Morgenstelle 8, 72076 Tübingen, Germany.

$^b$ Center for Bioinformatics Tuebingen (ZBIT), Eberhard Karls University Tuebingen, Sand 1, 72076 Tuebingen, Germany.

**Figure S1.** Planescans for chlorobenzene and bromobenzene with $N$-methylacetamide in distances of 3.0, 3.5, and 4.0 Å calculated using TPSS(D3)/TZVPP. Positive energy values (> 0 kJ/mol) are omitted. The setup of the scan is similar to that shown in Figure 2. The most favourable interaction energies for chlorobenzene and bromobenzene are -8.7 kJ/mol and -10.1 kJ/mol, respectively (at a distance of 3.5 Å).
Figure S2. Tilted plane scans of chlorobenzene, bromobenzene, and iodobenzene with N-methylacetamide for tilt angles 0° (regular plane scan), 45°, and 90° in a distance of 3.5 Å. Positive energy values (> 0 kJ/mol) are omitted. Energy values < -10 kJ/mol are highlighted with a black border. Calculations were performed using TPSS(D3)/TZVPP.