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Targeting the Protein Backbone with Aryl Halides: Systematic Comparison of Halogen Bonding and π···π Interactions using *N*-methylacetamide

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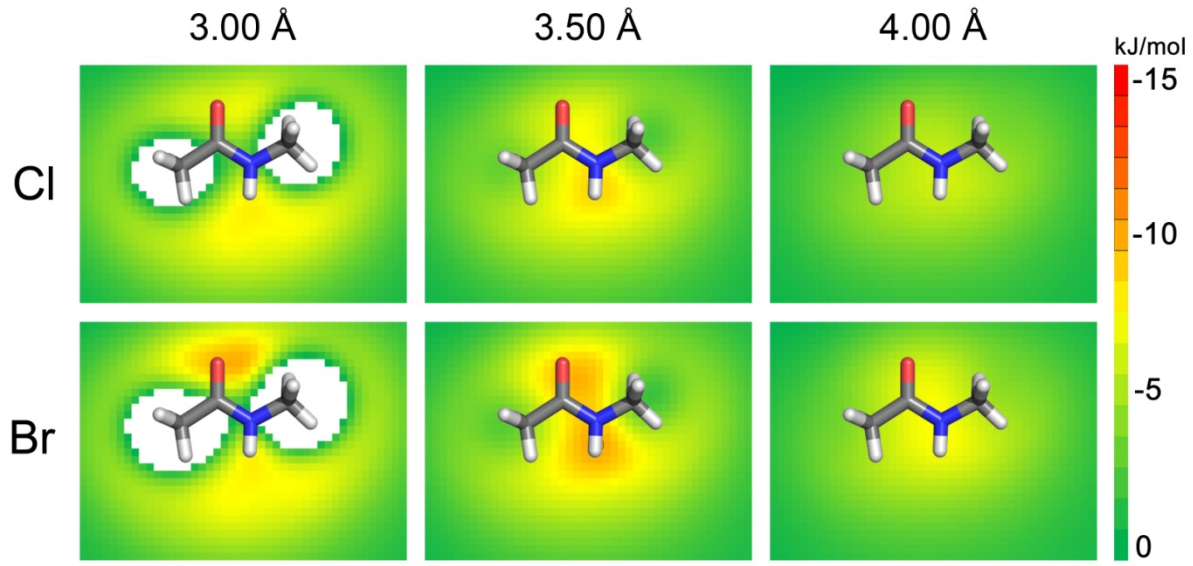

Figure S1. Planescans for chlorobenzene and bromobenzene with *N*-methylacetamide in distances of 3.0, 3.5, and 4.0 Å calculated using TPSS(D3)/TZVPP. Positive energy values (> 0 kJ/mol) are omitted. The setup of the scan is similar to that shown in Figure 2. The most favourable interaction energies for chlorobenzene and bromobenzene are -8.7 kJ/mol and -10.1 kJ/mol, respectively (at a distance of 3.5 Å).

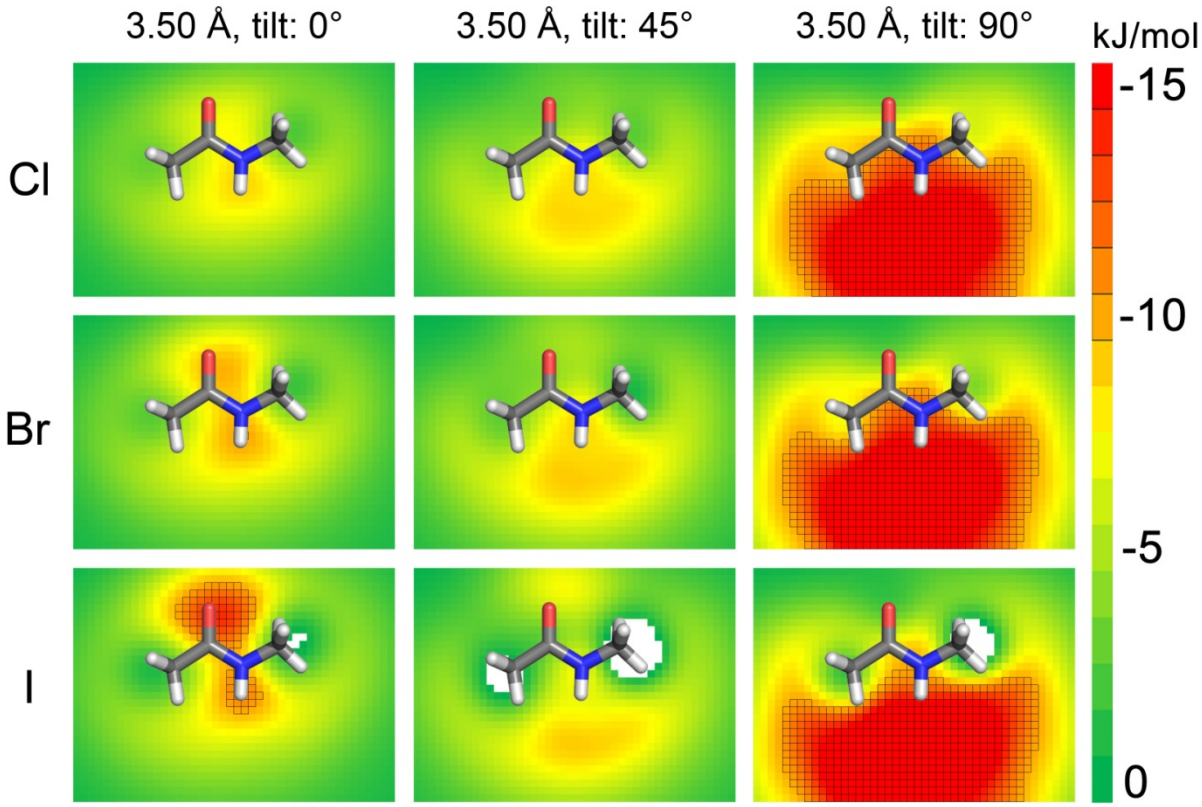

Figure S2. Tilted plane scans of chlorobenzene, bromobenzene, and iodobenzene with *N*-methylacetamide for tilt angles 0° (regular plane scan), 45°, and 90° in a distance of 3.5 Å. Positive energy values (> 0 kJ/mol) are omitted. Energy values < -10 kJ/mol are highlighted with a black border. Calculations were performed using TPSS(D3)/TZVPP.