

Supporting Information to
A Medicinal Chemist's Guide to Molecular Interactions

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Additional Figures S-1 to S-8 cited in the main text

Figure S-1: Median hydrogen bond distances as well as upper and lower 90% quantiles (dotted lines) of for various donor-acceptor pairs derived from the CSD

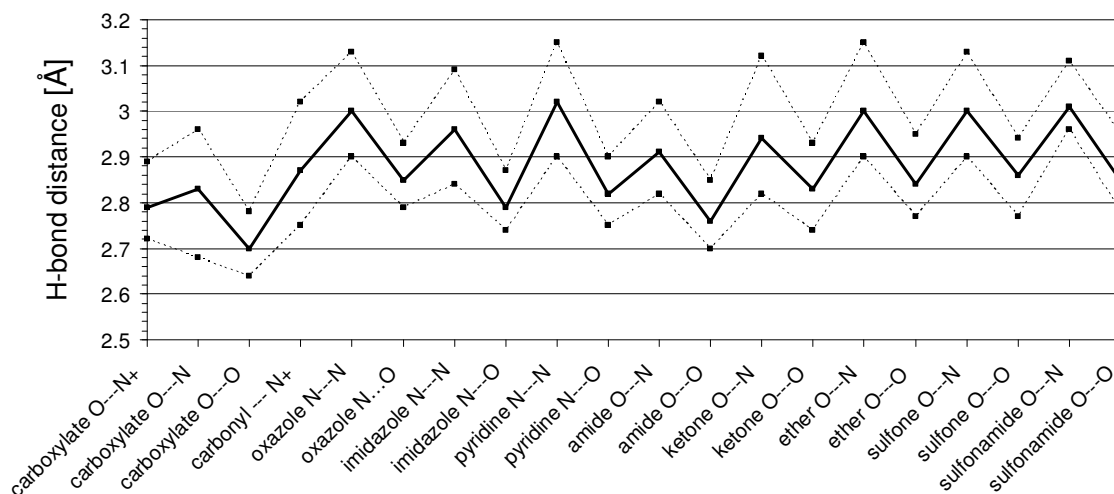


Figure S-2: Difference between the sum of the van der Waals radii and the median hydrogen bond distance found in the CSD for various donor-acceptor pairs

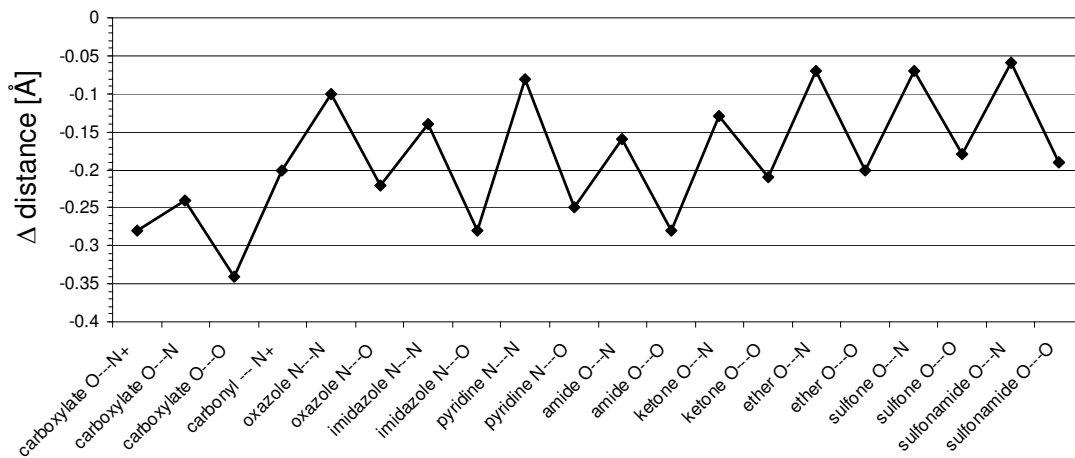


Figure S-3: Scatter plot of CH-F angle versus H-F distance for interactions between phenyl CH groups and F atoms bound to aromatic rings (CSD data). F atoms with a distance of no more than 1.5 Å to the phenyl plane were selected.

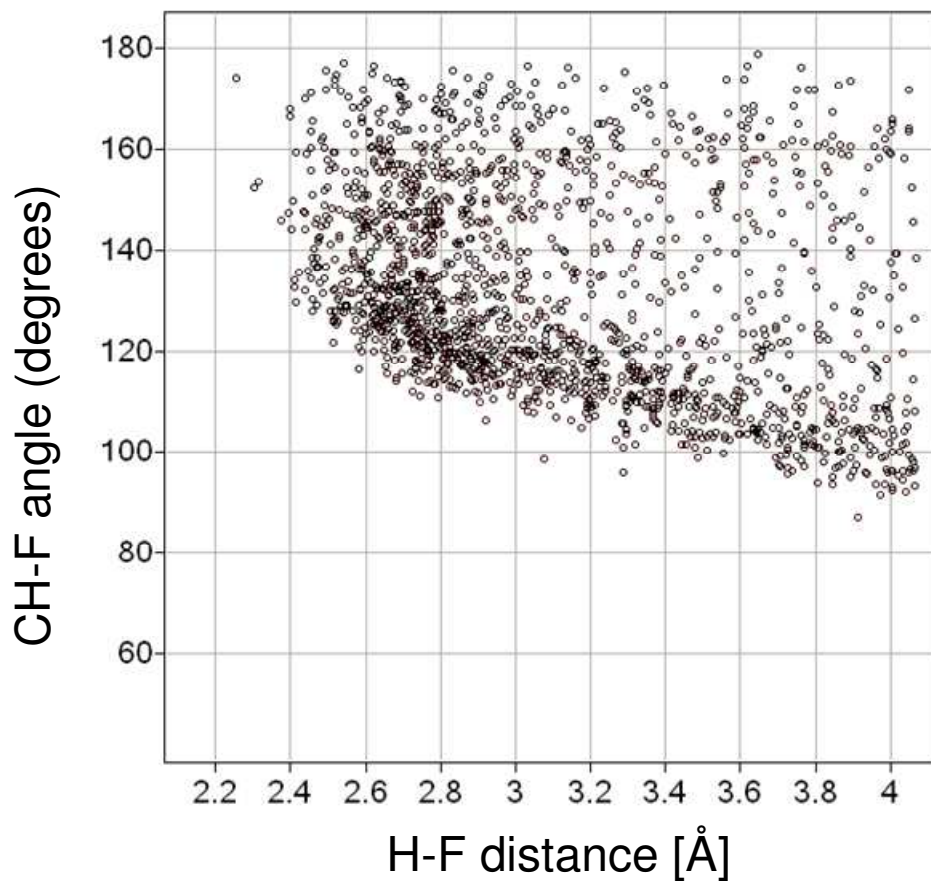


Figure S-4: Distribution of fluorine atoms around phenyl rings in the CSD. (a, b) F bound to sp^3 carbon, (c, d) F bound to aryl rings. (a, c) Radial distribution functions. Darker grey corresponds to higher density; peaks above a numerical value of 90 are colored red. (b, d) Scatter plots of all hits colored by the angle between the phenyl plane and the C-F vector from blue (0° , in plane) to green (90° , orthogonal).

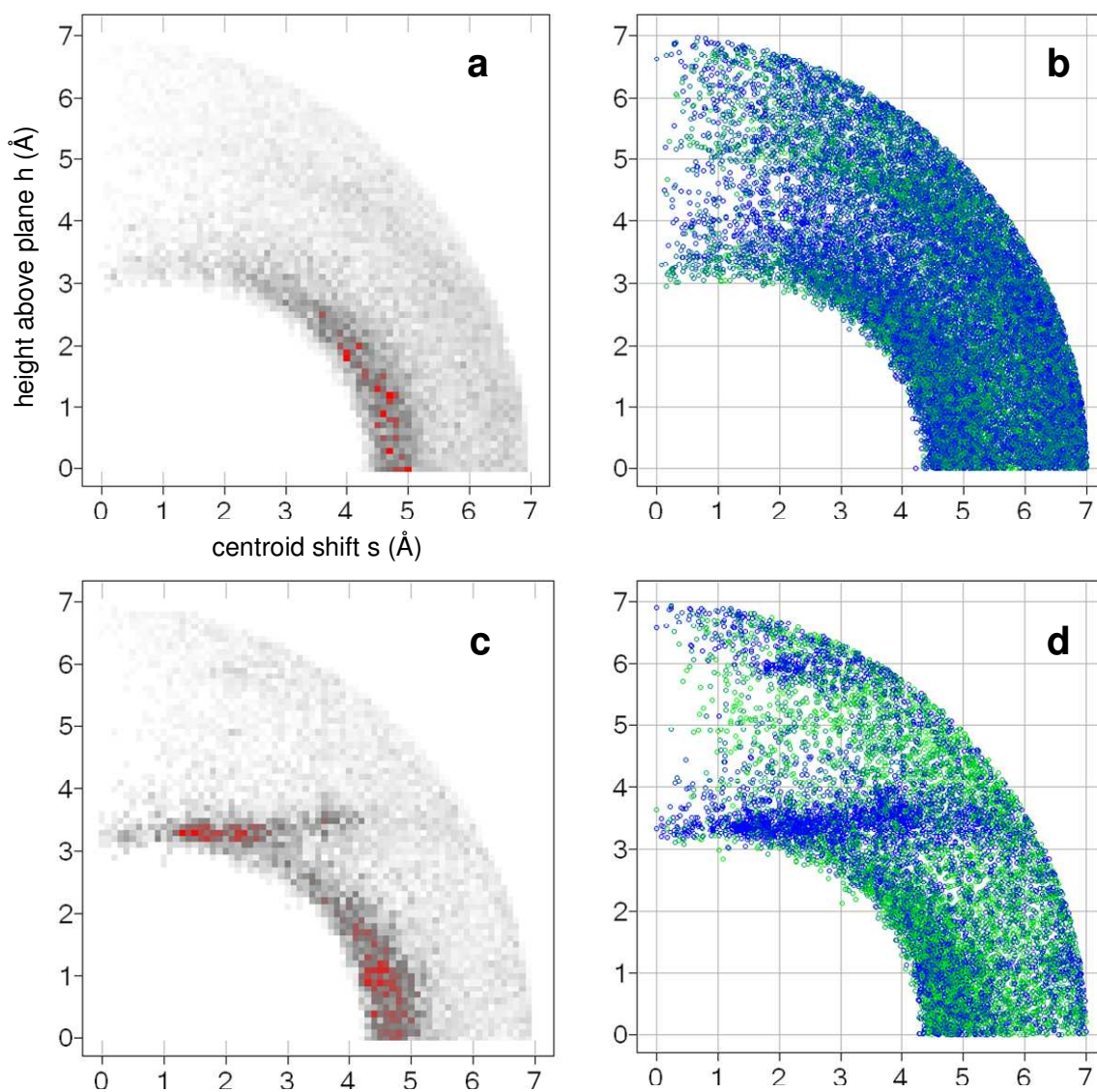


Figure S-5: Distribution of chlorine atoms around phenyl rings in the CSD. (a, b) Cl bound to sp^3 carbon, (c, d) Cl bound to aryl rings. (a, c) Radial distribution functions. Darker grey corresponds to higher density; peaks above a numerical value of 90 are colored red. (b, d) Scatter plots of all hits colored by the angle between the phenyl plane and the C-Cl vector from blue (0° , in plane) to green (90° , orthogonal).

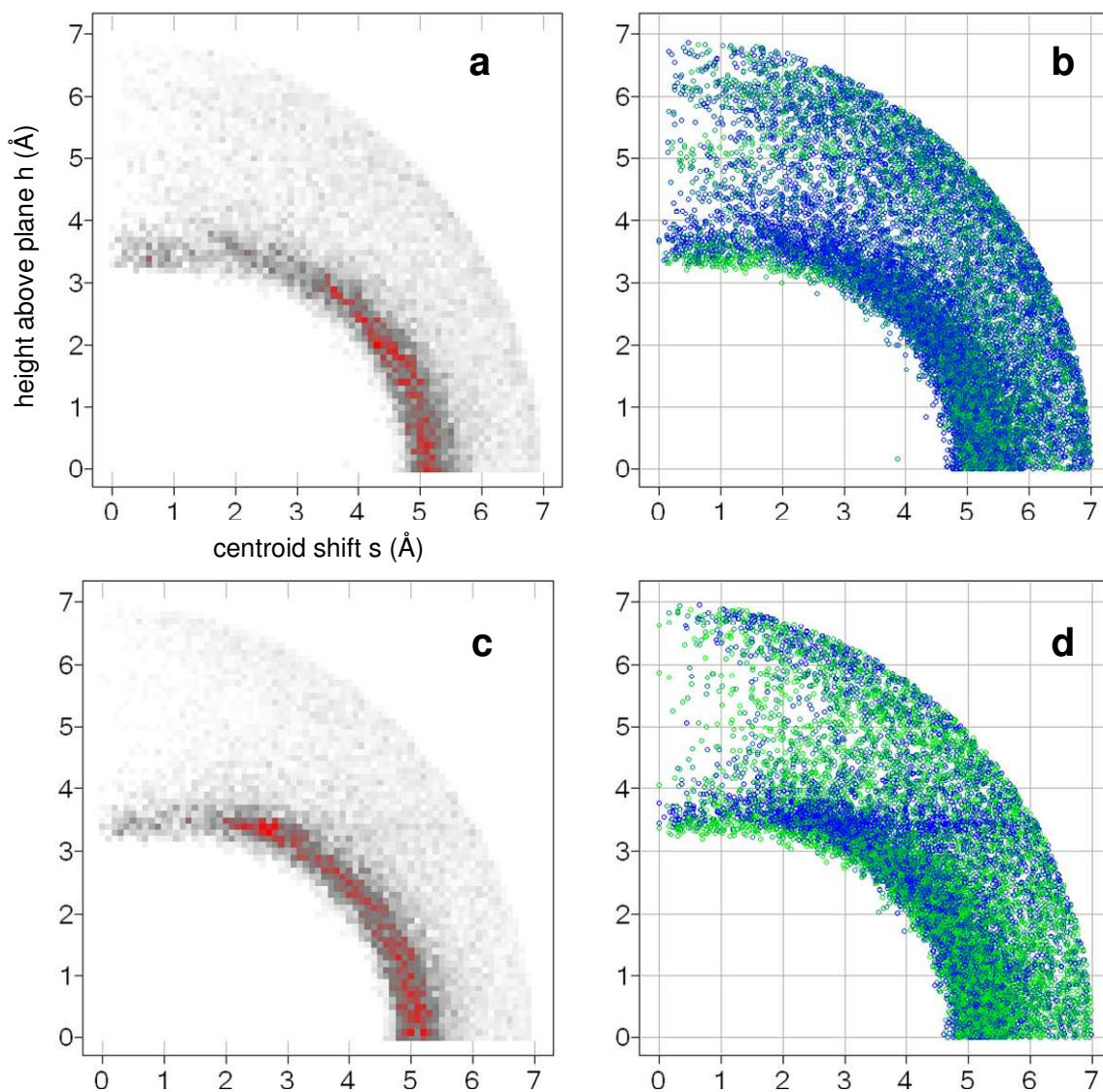


Figure S-6: Distribution of bromine atoms around phenyl rings in the CSD. (a, b) Br bound to sp^3 carbon, (c, d) Br bound to aryl rings. (a, c) Radial distribution functions. Darker grey corresponds to higher density; peaks above a numerical value of 90 are colored red. (b, d) Scatter plots of all hits colored by the angle between the phenyl plane and the C-Br vector from blue (0° , in plane) to green (90° , orthogonal).

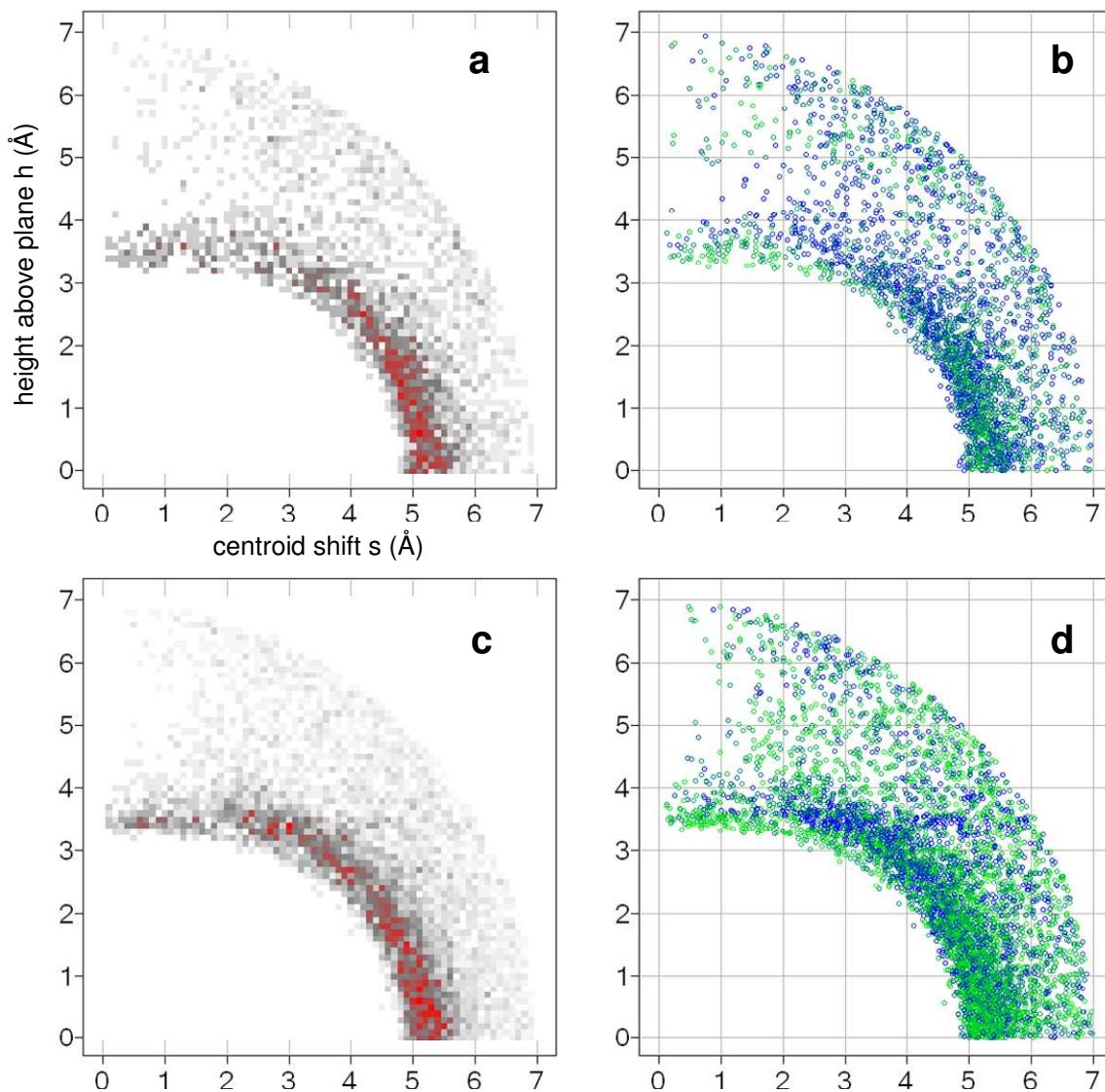


Figure S-7: Examples of Cation- π interactions a) Carbamoylcholine (orange, PDB code 1uw6) and Nicotine (green, PDB code 1iv6) bound to Acetylcholine binding protein b) Donepezil binding to Acetylcholine esterase (PPB code 1eve)

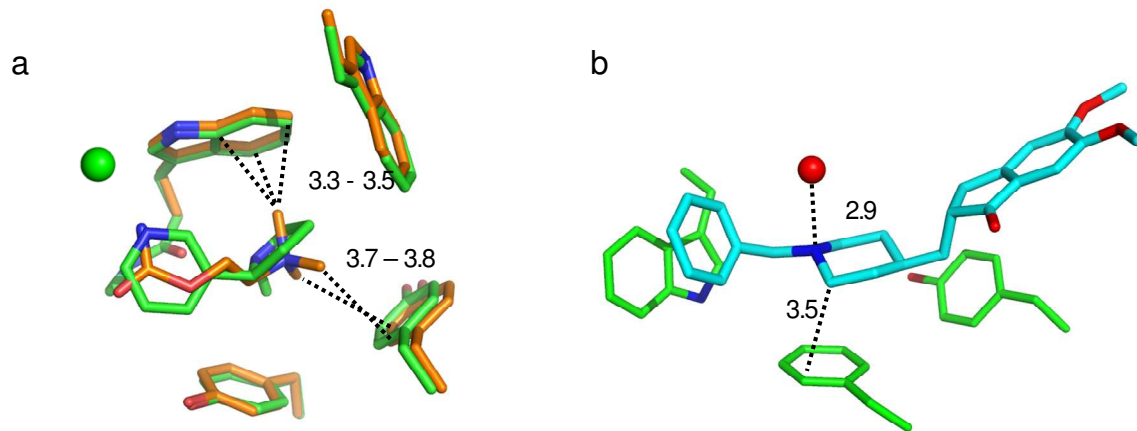


Figure S-8: Radial distribution functions of thioether sulfur atoms around phenyl rings
Darker grey corresponds to higher density; peaks above a numerical value of 90 are colored red. Left: CSD statistics, right: PDB statistics

