ESI Table. Some additional literature on miscellaneous topics related to CH/π hydrogen bonds in biological macromolecules. Titles and references are given.

(a) Carbohydrate/aromatic interactions in proteins
Carbohydrate Recognition through Noncovalent Interactions: A Challenge for Biomimetic and Supramolecular Chemistry.[1]
IR-Spectral Signatures of Aromatic–Sugar Complexes: Probing Carbohydrate–Protein Interactions[2]
Carbohydrate molecular recognition: a spectroscopic investigation of carbohydrate-aromatic interactions[3]
On the role of aromatic-sugar interactions in the molecular recognition of carbohydrates: A 3D view by using NMR[4]
Sugars stack up[5]
Solvent Effects in Carbohydrate Binding by Synthetic Receptors: Implications for the Role of Water in Natural Carbohydrate Recognition[6]
Carbohydrate-protein recognition probed by density functional theory and ab initio calculations including dispersive interactions[7]
Calorimetric measurement of the CH/π interaction involved in the molecular recognition of saccharides by aromatic compounds[8]
Carbohydrate-aromatic interactions: A computational and IR spectroscopic investigation of the complex, methyl α-l-fucopyranosidetoluene, isolated in the gas phase[9]
Progress in biomimetic carbohydrate recognition[10]
Enthalpic nature of the CH/π interaction involved in the recognition of carbohydrates by aromatic compounds, confirmed by a novel interplay of NMR, calorimetry, and theoretical calculations[11]
Carbohydrate binding sites in *Candida albicans* exo- β -1,3-glucanase and the role of the Phe-Phe 'clamp' at the active site entrance[12]
Three-Dimensional Potential Energy Surface of Selected Carbohydrates' CH/π Dispersion Interactions Calculated by High-Level Quantum Mechanical Methods[13]
Conformational mapping and energetics of saccharide–aromatic residue interactions: implications for the discrimination of anomers and epimers and in protein engineering[14]
Self-Assembled Multi-Component Catenanes: Structural Insights into an Adaptable Class of Molecular Receptors and [2]-Catenanes[15]
Self-Assembled Multi-Component Catenanes: The Effect of Multivalency and Cooperativity on Structure and Stability[16]

(b) CH/π hydrogen bonds in protein chemistry

The x-ray crystallographic study of covalently modified carboxypeptidase A by 2-benzyl-3,4-epoxybutanoic acid, a pseudomechanism-based inactivator[17]

Effect of side-chain structure on inhibition of yeast fatty-acid synthase by cerulenin analogues[18]

Crystal structure of neocarzinostatin, an antitumor protein-chromophore complex[19]

Solution structure of the antitumour antibiotic neocarzinostatin, a chromophore–protein complex[20]

Synthesis and Binding of Simple Neocarzinostatin Chromophore Analogues to the Apoprotein[21]

Induced Assembly of Aromatic Rings Caused by a CH/π Interaction[22]

Lipase-catalyzed esterification of 2-(4-substituted phenoxy)propionic acids in organic solvents: substituent effect controlling enantioselectivity toward racemic acids[23]

Enzymatic Properties of Phenylalanine101 Mutant Enzyme of Ribonuclease Rh from Rhizopus niveus[24] Three-dimensional structure of cyanobacterial photosystem I at 2.5 Å resolution[25]

How Does Lipase Flexibility Affect Its Enantioselectivity in Organic Solvents? Role of CH$\cdots\pi$ Association in Stabilization of Enzyme-Substrate Complex[26]

CH/π interactions involving aromatic amino acids: refinement of the CHARMM tryptophan force field[27]

Carbohydrate molecular recognition: a spectroscopic investigation of carbohydrate-aromatic interactions[28]

Design of artificial metalloenzymes using non-covalent insertion of a metal complex into a protein scaffold[29]

A circular loop of the 16-residue repeating units in ice nucleation protein[30]

Crystal structures of *Lymnaea stagnalis* AChBP in complex with neonicotinoid insecticides imidacloprid and clothianidin[31]

Critical contribution of aromatic rings to specific recognition of polyether rings[32]

N-domain of human adhesion/growth-regulatory galectin-9: preference for distinct conformers and non-sialylated N-glycans and detection of ligand-induced structural changes in crystal and solution[33]

Characterization of molecular recognition of STAT3 SH2 domain inhibitors through molecular simulation[34]

Insight into mechanism of small molecule inhibitors of the MDM2–p53 interaction: Molecular dynamics simulation and free energy analysis[35]

Strengthening π–π interactions while suppressing Csp^2–H$\cdots$π (T-shaped) interactions via perfluoroalkylation: A crystallographic and computational study that supports the beneficial formation of 1-D π–π stacked aromatic materials[36]

Aromatic-proline interactions: electronically tunable CH/π interactions[37]
(c) CH/π hydrogen bonds in nucleic acids
Most compact hairpin-turn structure exerted by a short DNA fragment, d(GCGAAGC) in solution: an extraordinarily stable structure resistant to nucleases and heat[38]
The structural basis of specific base-excision repair by uracil-DNA glycosylase[39]
Crystal structure and mutational analysis of human uracil-DNA glycosylase: Structural basis for specificity and catalysis[40]
An extended DNA structure through deoxyribose-base stacking induced by RecA protein[41]
Cross-strand purine-pyrimidine stack and sheared purine/pyrimidine pairing in the human HIV-1 reverse transcriptase inhibitors[42]
Solution structure of the ActD–5′ -CCGTT3GTGG-3′ complex: drug interaction with tandem G·T mismatches and hairpin loop backbone[43]
Common and selective molecular determinants involved in metabotropic glutamate receptor agonist activity[44]
Measurement of Nucleobase pKa Values in Model Mononucleotides Shows RNA−RNA Duplexes to be More Stable than DNA−DNA Duplexes[45]
An analysis of the different behavior of DNA and RNA through the study of the mutual relationship between stacking and hydrogen bonding[46]
Effect of the bases flanking an abasic site on the recognition of nucleobase by amiloride[47]
(d) CH/π hydrogen bonds in SBDD
Chymotrypsin Inhibition Induced by Side Chain-Side Chain Intramolecular CH/π Interaction in D-Thr-L-Phe Benzylamide[48]
Design of serine protease inhibitors with conformation restricted by amino acid side-chain-side-chain CH/π interaction[49]
A novel type of structurally simple nonpeptide inhibitors for alpha-chymotrypsin. Induced-fit binding of methyl 2-allyl-3-benzenepropanoate to the S2 subsite pocket[50]
Highly potent inhibitors of the Grb2-SH2 domain[51]
Structure-based Design of Compounds Inhibiting Grb2-SH2 Mediated Protein-protein Interactions in Signal Transduction Pathways[52]
Comparative molecular field analysis (CoMFA) and docking studies of non-nucleoside HIV-1 RT inhibitors (NNIs)[53]
Structure–Activity Relationship and Rational Design of 3,4-Dephostatin Derivatives as Protein

Tyrosine Phosphatase Inhibitors[54]

Structure of porcine pancreatic elastase complexed with FR901277, a novel macrocyclic inhibitor of elastases, at 1.6 Å resolution[55]

Molecular design and biological activities of protein-tyrosine phosphatase inhibitors[56]

Focused Library Approach for Identification of New N-Acylphenylalanines as VCAM/VLA-4 Antagonists[57]

The structure of human recombinant aldose reductase complexed with the potent inhibitor zenarestat[58]

Synthesis, dopamine D2 receptor binding studies and docking analysis of 5-[3-(4-arylpiperazin-1-yl)propyl]-1H-benzimidazole, 5-[2-(4-arylpiperazin-1-yl)ethoxy]-1H-benzimidazole and their analogs[59]

Structure-based design of derivatives of tyropeptin A as the potent and selective inhibitors of mammalian 20S proteasome[60]

Synthesis and c-Src inhibitory activity of imidazo[1,5-a]pyrazine derivatives as an agent for treatment of acute ischemic stroke[61]

Crystallographic investigation of the inhibition mode of a VIM-2 metallo-β-lactamase from *Pseudomonas aeruginosa* by a mercaptocarboxylate inhibitor[62]

Fatty acid amide hydrolase inhibitors. Surprising selectivity of chiral azetidine ureas[63]

Novel estrogen receptor (ER) modulators: carbamate and thiocarbamate derivatives with m-carborane bisphenol structure[64]

Inhibitors of human 2,3-oxidosqualene cyclase[65]

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