Oral presentation

Aromatics Analyser 2 and a unified approach to aromatic interactions

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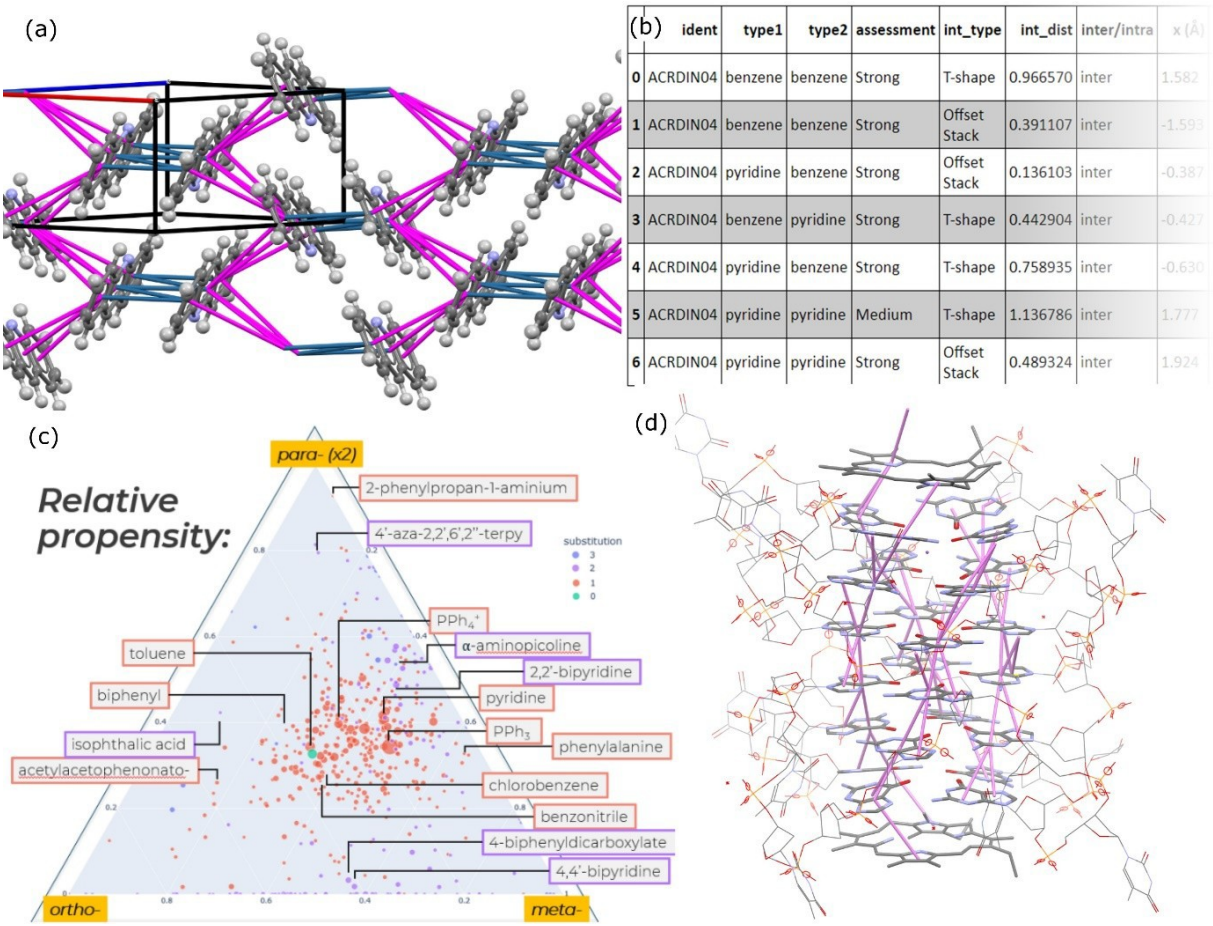
The interactions of aromatic systems are important in crystal form analysis and design, directing and informing properties of the crystalline solid state [1]. In presenting a new Aromatics Analyser (AA2) [2-3], we'll show how one can quantify these interactions across many heterocycle rings and interaction types, with a simple visualiser in Mercury and a notebook interface with the CSD Python API. This talk will cover the evolution of Aromatics Analyser, and report some of the insights to polymorphism, structure direction and stability, bio-macromolecules and semiconductor design from analysis of millions of unique interactions in the CSD.



	ident	type1	type2	assessment	int_type	int_dist	inter/intra	x (Å)
0	ACRDIN04	benzene	benzene	Strong	T-shape	0.966570	inter	1.582
1	ACRDIN04	benzene	benzene	Strong	Offset Stack	0.391107	inter	-1.593
2	ACRDIN04	pyridine	benzene	Strong	Offset Stack	0.136103	inter	-0.387
3	ACRDIN04	benzene	pyridine	Strong	T-shape	0.442904	inter	-0.427
4	ACRDIN04	pyridine	benzene	Strong	T-shape	0.758935	inter	-0.630
5	ACRDIN04	pyridine	pyridine	Medium	T-shape	1.136786	inter	1.777
6	ACRDIN04	pyridine	pyridine	Strong	Offset Stack	0.489324	inter	1.924

Figure 1. **(a)** Visualised aromatic interactions between acridine molecules in ACRDIN04, and **(b)** tabulated results. **(c)** Aromatic substitution can direct aromatic interactions in the solid state, as differently substituted rings will have different ortho- meta- and para- directed aromatic interactions **(d)** This program can also analyse bio-macromolecules such as this G-quadruplex – N-methylporphyrinium complex (PDB: 6p45)

[1] Pidcock, E., Sadiq, G., Stevens, J.S., Willacy, R.D. *Cryst. Growth Des.* (**2022)** *22* (1), 788-802.

[2] The CCDC open-source repository, https://github.com/CCDC-OpenSource.

[3] Publication forthcoming.