Synthesis and solid state structure for a series of poly(1-pyrrolylmethyl)benzene derivatives. Control of the interplaying $\pi$-$\pi$ and C–H···$\pi$ interactions?

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Supplementary Material (ESI)

A CSD search for intermolecular C–H···$\pi$(heterocycles) interactions.

A Cambridge Structural Database search for non-bonded contacts (Chart 1) was carried out using the program ConQuest (version 1.7). i The search criteria (CSD dated February 2005) were error and disorder free only structures (organic and organometallic) with $R$ factors less than 0.1 (H normalized). Normalised structures were retrieved from the Cambridge Structural Database and analysed using VISTA (version 2.1). ii Of the 104 hits, 89 corresponded to C–H···$\pi$(N containing heterocycles).
Chart 1. Parameters used for the search

\[ QA = \text{O, S, Se, N} \]
\[ \alpha = 90-180^\circ \]
\[ \theta = 0-90^\circ \]
\[ d = 0-3.2 \text{ Å} \]

\( M = \text{Centroid} \)

Figure 1. Scattergrams for the geometry of the retrieved intermolecular C–H···π(heterocycle) interactions (see Chart 1 for nomenclature).
Figure II. Histogram of $\theta$ (THETA) angles ($^\circ$).
