Succinate Esters: Odd even effect in presence of alkyl side chain

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Supporting Information

ORTEP diagrams

Figure S1 ORTEP diagram of dimethyl succinate (DMS) with ellipsoids drawn at 50% probability

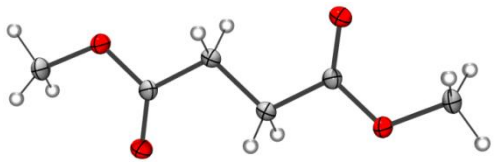


Figure S2 ORTEP diagram of diethyl succinate (DES) with ellipsoids drawn at 50% probability

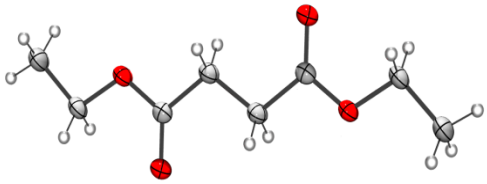


Figure S3 ORTEP diagram of di–*n*–propyl succinate (D*n*PS) with ellipsoids drawn at 50% probability

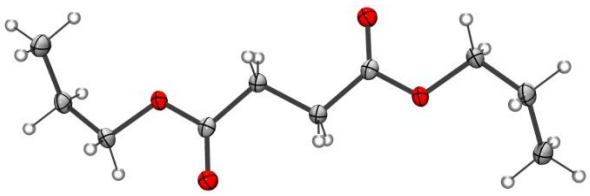
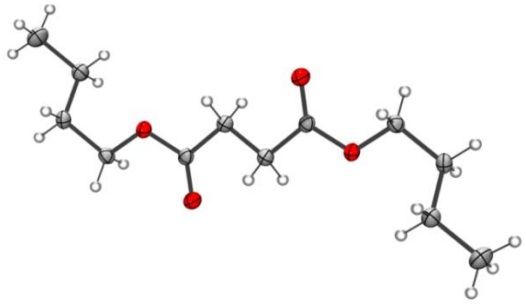


Figure S4 ORTEP diagram of di–*n*–butyl succinate (D*n*BS) with ellipsoids drawn at 50% probability



Hirshfeld surface analysis

A Hirshfeld surface of a particular molecule is generated based on the distribution of molecular electron density with respect to proximity of its nearest neighbors. The atoms in the molecule are defined by stockholder partitioning and is used to represent the molecule in the crystal. The Hirshfeld surface is drawn at $w(\boldsymbol{r}) = 0.5$ where $w(\boldsymbol{r})$ is the weight function of a molecule in the crystal given by $w(\boldsymbol{r}) = \frac{\sum_{i \in molecule\ A} \rho_i^{\mathrm{at}}(\boldsymbol{r})}{\sum_{i \in crystal} \rho_i^{\mathrm{at}}(\boldsymbol{r})}$ and $\rho_i(r)$ is the spherical atomic electron distribution located at the i^{th} nucleus. It is the ratio between the summation of spherical atom electron densities for any particular molecule and for entire crystal. At $w(\boldsymbol{r}) = 0.5$ it envelops a particular molecule and its shape is similar to the van der Waals surface. A plot of d_i verses d_e gives finger–print plot which can be considered as a map of different close interactions present.

In Figure S7 is shown the Hirshfeld surfaces, fingerprint plots and the percentage of corresponding close interactions of the dialkyl succinates in this study. The surfaces for the odd substituted succinates are of more symmetrical in shape compared to that of even numbered one.

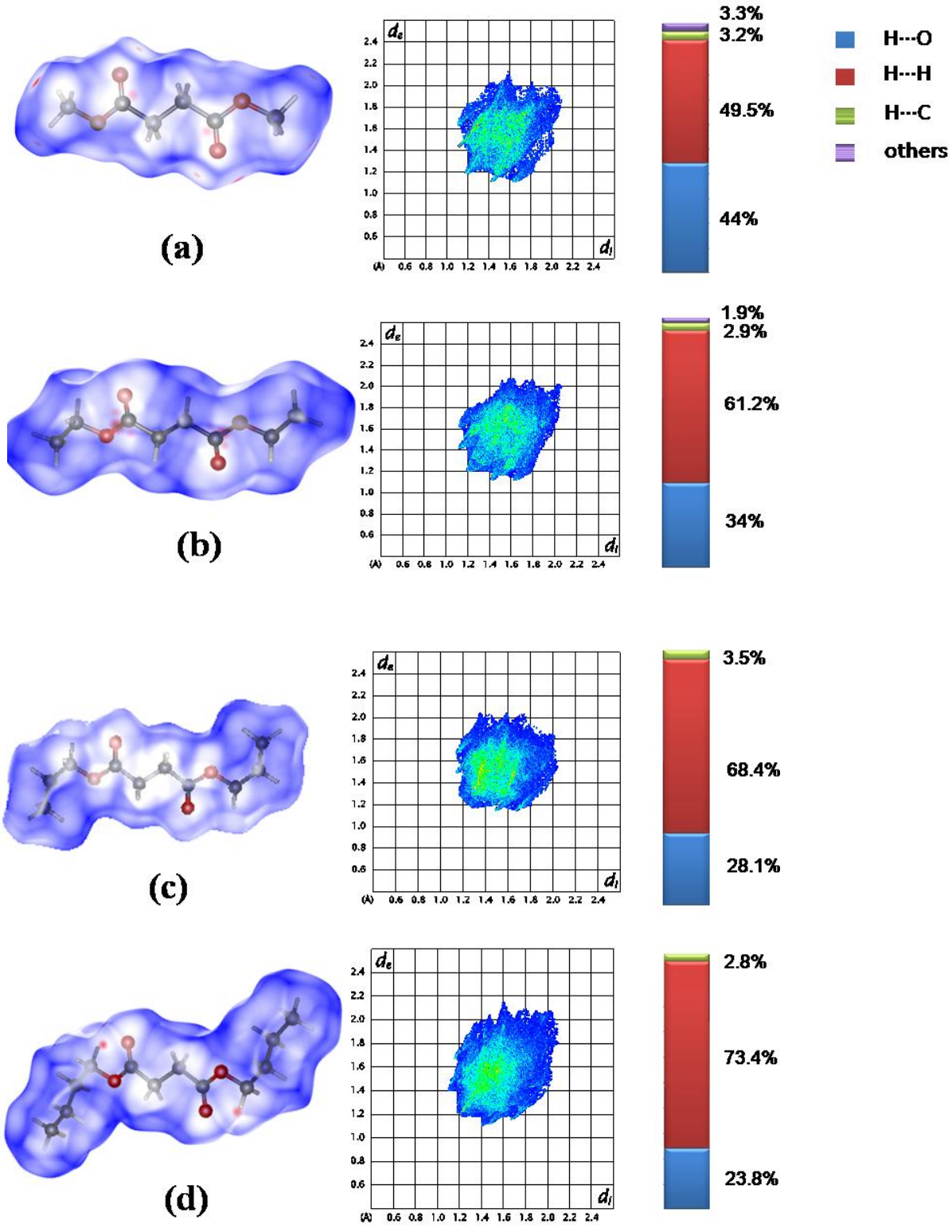


Figure S5 Hirshfeld surfaces, corresponding fingerprint plots and % of close interactions. (a) DMS, (b) DES, (c) D*n*PS and (d) D*n*BS

As the number of carbon atom in the alkyl side chain increases there is an increase in close H···H contacts due to increase in the dispersive interaction. H···O interactions decreases in percentage compared to H···H contacts can be explained since the proximity of H···H on surface increases with chain length while oxygen content remains constant.