# Supporting Information

## *XPac* dissimilarity parameters as quantitative descriptors of isostructurality: the case of fourteen 4,5'-substituted benzenesulfonamido-2-pyridines obtained by substituent interchange involving $CF_3$/I/Br/Cl/ F/Me/H

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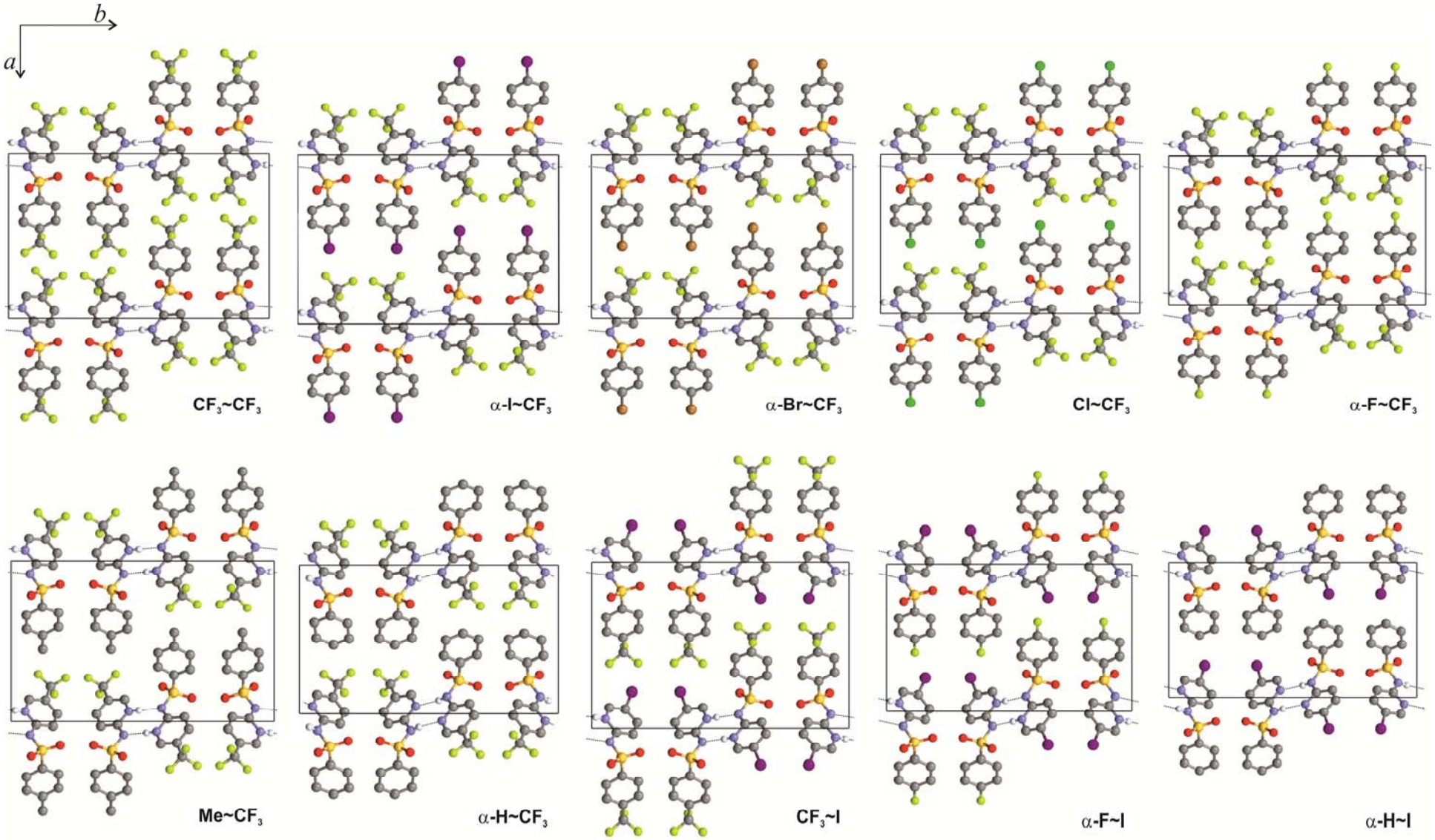
**Table S1** Parameters used to estimate the effective distance, defined as the distance between the centre of the C4 atom of the phenyl ring and the van der Waals surface of the substituent $R^1$ in direction of the C4-*X* bond (see Fig. 7). An approximation is used whereby the shape of all substituents is assumed to be spherical and $d_{eff} = d_{C4–X} + r$. Experimental $d_{C4–X}$ bond distances obtained in this study were used and the van der Waals radii *r* were taken from refs. 1 and 2).

| $R^1$ | *X* | $d_{C4–X}$ (Å) | *r* (Å) | $d_{eff}$ (Å) |
|---|---|---|---|---|
| $CF_3$ | C | 1.49 | 2.70 | 4.19 |
| I | I | 2.10 | 1.98 | 4.08 |
| Br | Br | 1.90 | 1.85 | 3.75 |
| Cl | Cl | 1.74 | 1.75 | 3.49 |
| Me | C | 1.50 | 2.00 | 3.50 |
| F | F | 1.38 | 1.47 | 2.85 |
| H | H | 0.95 | 1.20 | 2.15 |

**Table S2** Crystallographic data and calculated densities for polymorphic forms of the four $R^1$~$R^2$ compounds with $R^1$ = H or F and $R^2$ = I or $CF_3$. Details of the structures not belonging to structure type **A1** will be described in further publications.

| Form | Space group | *Z* | Type | *a* (Å) | *b* (Å) | *c* (Å) | *α* (°) | *β* (°) | *γ* (°) | $d_{calc}$ (g cm$^{-3}$) | *T* (K) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **α -H~CF$_3$** | $P2_1/c$ | 4 | **A1** | 10.88 | 18.80 | 6.15 | 90 | 95.2 | 90 | **1.604** | 120 |
| **β-H~CF$_3$** | $C2/c$ | 8 | | 20.64 | 8.43 | 15.70 | 90 | 115.5 | 90 | 1.628 | 120 |
| **γ-H~CF$_3$** | $P\bar{1}$ | 4 | | 10.31 | 10.69 | 12.13 | 77.4 | 83.7 | 72.1 | 1.618 | 120 |
| **α-H~I** | $P2_1/c$ | 4 | **A1** | 10.52 | 19.24 | 6.20 | 90 | 94.4 | 90 | **1.911** | 248 |
| **β-H~I** | $P\bar{1}$ | 4 | | 10.07 | 10.96 | 11.37 | 93.6 | 101.2 | 97.2 | 1.968 | 120 |
| **γ-H~I** | $C2/c$ | 8 | | 20.22 | 8.34 | 16.04 | 90 | 115.6 | 90 | 1.963 | 120 |
| **δ-H~I** | $P2_1/c$ | 4 | | 8.31 | 10.69 | 15.09 | 95.2 | 105.3 | 104.9 | 1.943 | 120 |
| **ε-H~I** | $P\bar{1}$ | 4 | | 7.99 | 12.95 | 11.80 | 90 | 98.9 | 90 | 1.982 | 120 |
| **α -F~CF$_3$** | $P2_1/c$ | 4 | **A1** | 11.19 | 19.09 | 5.96 | 90 | 97.4 | 90 | **1.686** | 120 |
| **β-F~CF$_3$** | $P\bar{1}$ | 2 | **A3a** | 6.52 | 9.44 | 10.57 | 94.3 | 99.4 | 93.1 | 1.667 | 120 |
| **γ-F~CF$_3$** | $P\bar{1}$ | 4 | | 5.12 | 15.65 | 16.20 | 89.6 | 84.7 | 84.0 | 1.656 | 120 |
| **α-F~I** | $P2_1/c$ | 4 | **A1** | 11.21 | 18.48 | 6.01 | 90 | 97.1 | 90 | **2.032** | 120 |
| **β-F~I** | $P2_1/n$ | 8 | | 10.62 | 15.71 | 15.00 | 90 | 94.0 | 90 | 2.013 | 120 |

Next page:
**Fig. S1** Crystal packing of ten 4,5'-substituted benzenesulfonamido-2-pyridines $R^1$~$R^2$. Each structure is viewed parallel to the crystallographic *c*-axis.

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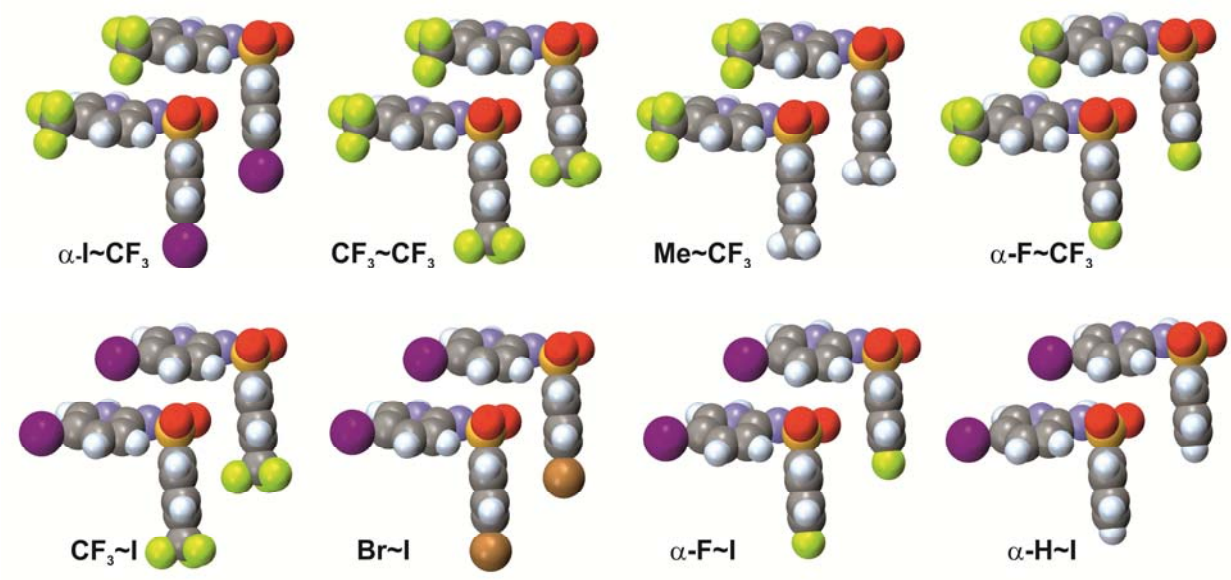


**Fig. S2.** Intermolecular contacts between two molecules within an **A**-type slipped stack of dimers propagating along [001].

## References

1. A. Bondi, *J. Phys. Chem.*, 1964, **68**, 441-451.
2. D. Seebach, *Angew. Chem. Int. Ed.*, 1990, **29**, 1320-1367.