Supplementary Information for

Polymorphism of the β,γ-hydroxylactone derived from indomethacin

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1. Powder X-ray diffraction patterns of the two polymorphs and the in situ prepared form I in bulk.

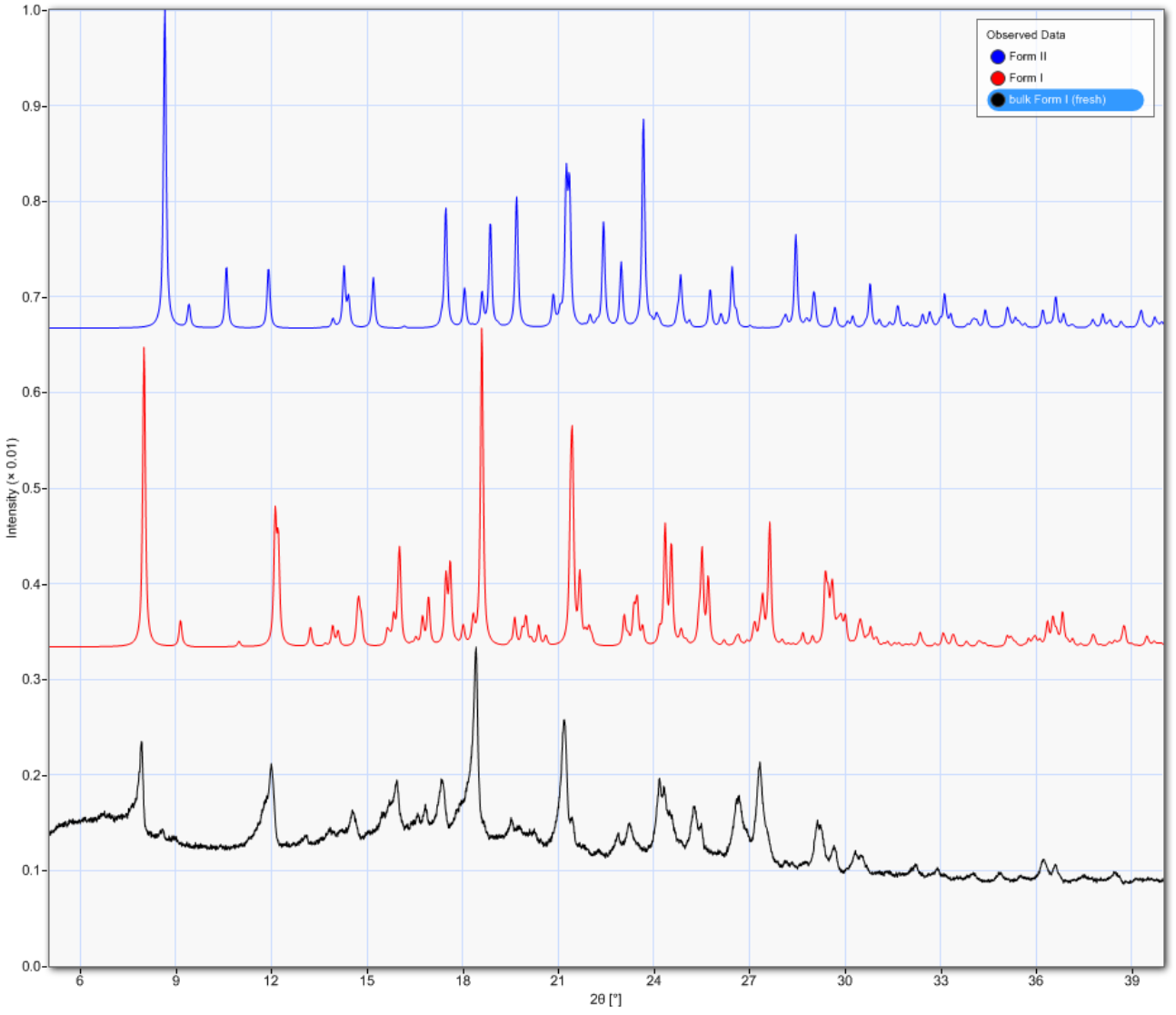

Figure 1S In situ preparation of Form I. Generated powder X-ray patterns of form II (blue), form I (red) and bulk material produced to obtain significant amount of the metastable form (black).

2. Differential Scanning Calorimetry

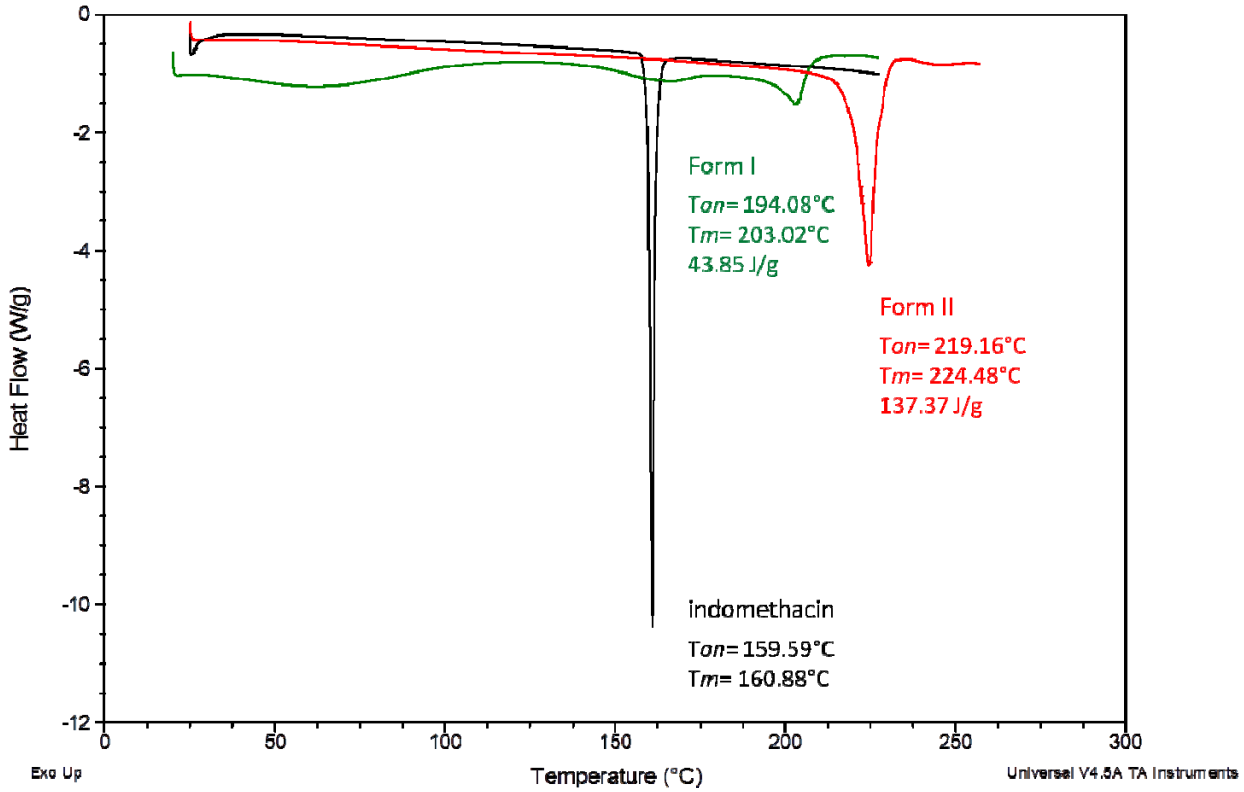

Figure 2S Melting points of γ-Indomethacin, and form I and II.

3. Computational chemistry details.

Applied basis set: B3LYP/6-31G**

Table 1S

	colour	molecule	Energy / kJ mol^{-1}
1	Red		0
2	Orange		0.73
3	Cyan		10.20
4	Green		9.63
5	Magenta		11.88
6	Dark gray		12.61
7	Light green		19.78
8	Pink		19.39
Crystal structure	Black		-

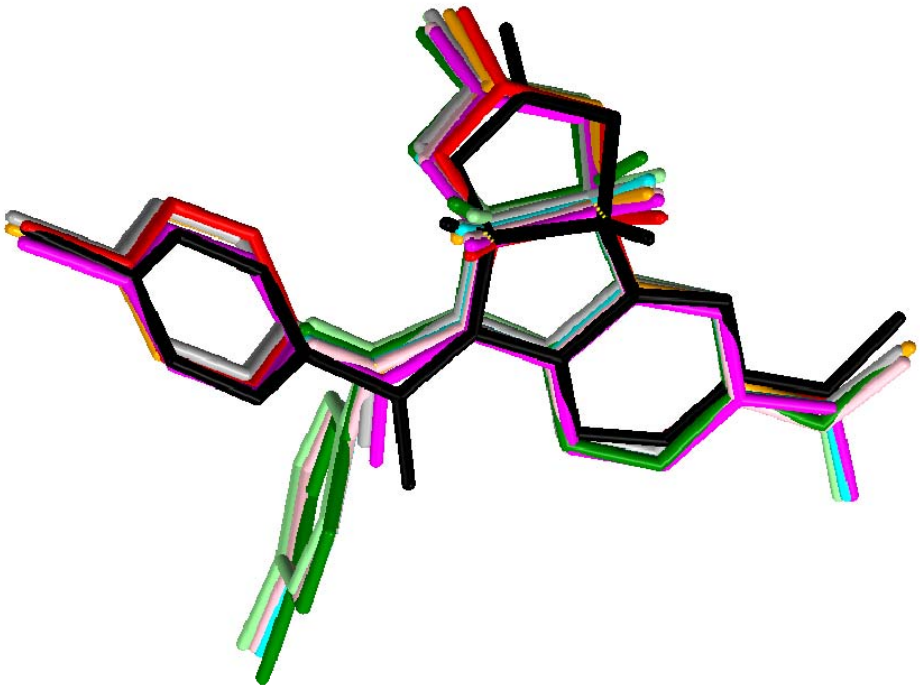

Figure 3S Overlay of the possible conformers.

4. Hydrogen bond pattern and intermolecular potentials in form I and II.

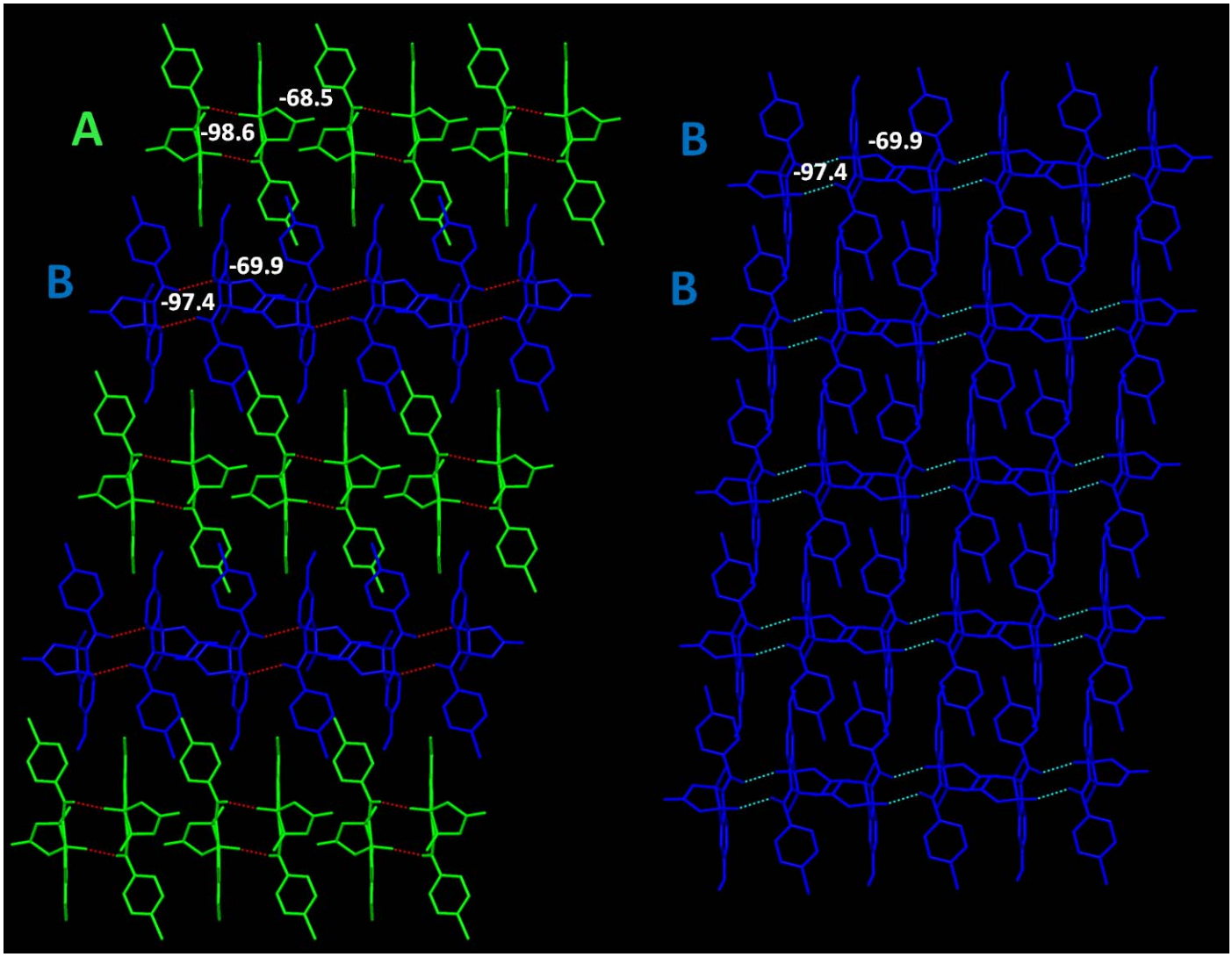

Figure 4S Packing diagrams are showing the hydrogen bond pattern in form I (left) and form II (right). Molecules are coloured by symmetry equivalence are showing the two types of centro-symmetrical dimers (A and B) and the calculated intermolecular potentials (kJ mol^{-1}) between the related molecules.

5. Hirshfeld surfaces and fingerprint plots for molecules

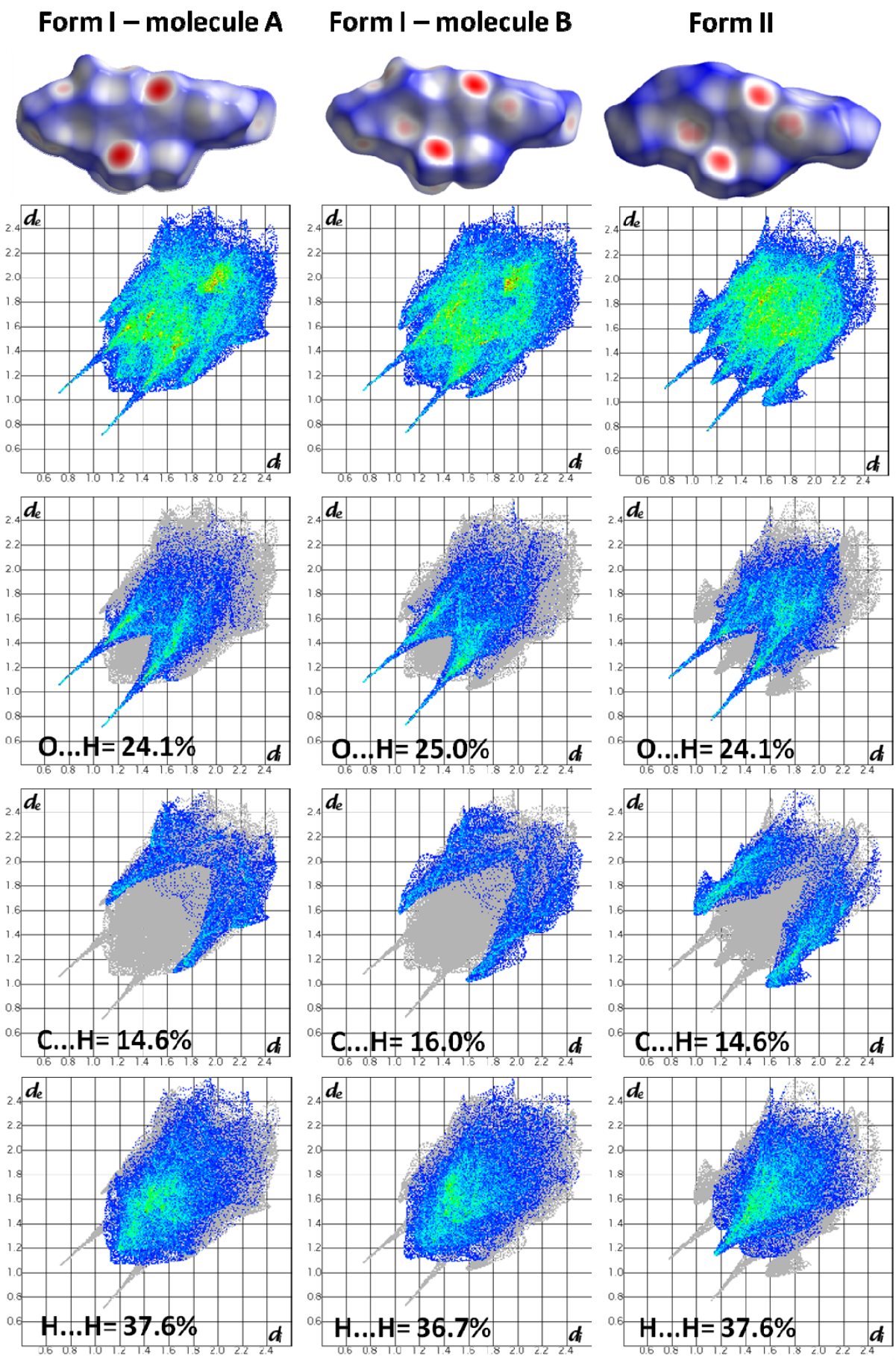

Figure 5S Hirshfeld surfaces and fingerprint plots of molecules in form I and II.

6. Hirshfeld surfaces and fingerprint plots for dimers

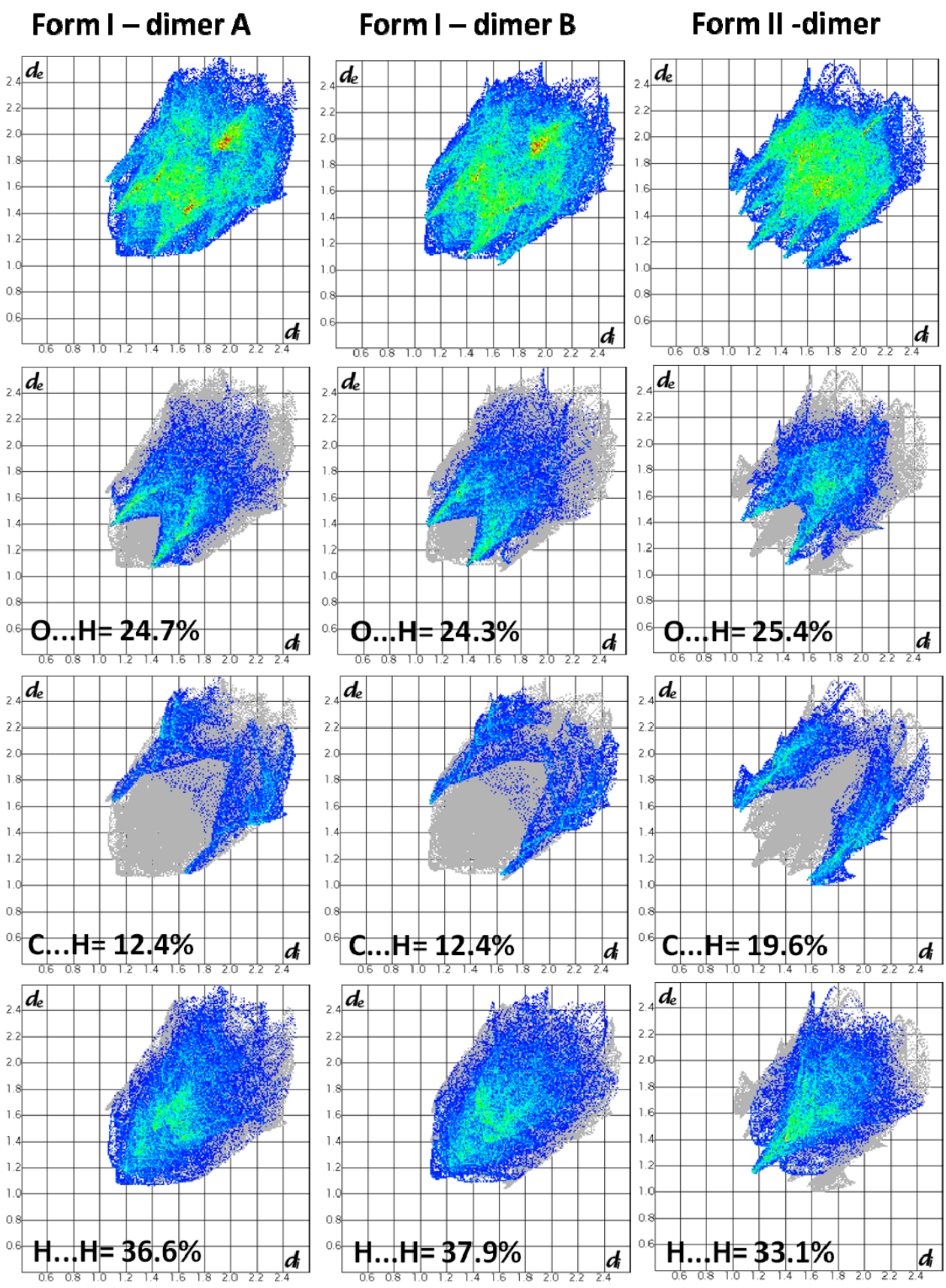

Figure 6S Hirshfeld surfaces and fingerprint plots of dimers in form I and II.