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Supporting information for article:

Polymorphism in some new bis-hydrazone compounds

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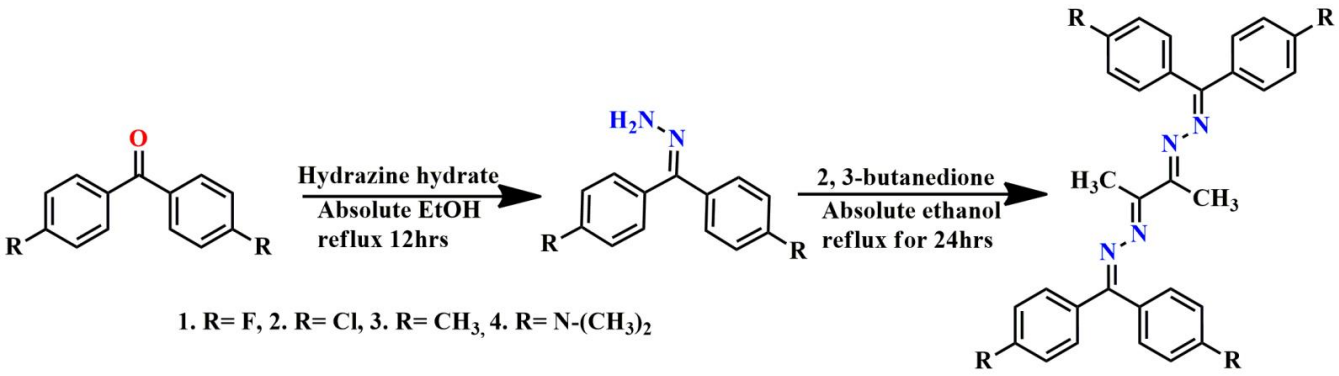
EXPERIMENTAL SECTION:

Synthesis of Compounds 1, 2, 3 and 4:

Synthetic scheme for compounds are shown in Scheme S1.



Scheme S1

Molecular structures of **1**, **2**, **3** and **4** were confirmed by ^{1}H NMR spectroscopy.

Compound **1:**

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.20 -7.67 (d, 4H), 7.18-7.19 (d, 4H), 7.05-7.10 (m, 8H), 2.18 (s, 6H).

Melting point: 160-163° C

Compound **2**:

^{1}H NMR (500 MHz, $CDCl_3$): δ7.60-7.61 (d, 4H), 7.35-7.38 (d, 4H), 7.12–7.26 (m, 8H), 2.18 (s, 6H).

Melting point: 190-192° C

Compound **3**:

^{1}H NMR (500 MHz, $CDCl_3$): δ7.05-7.08 (d, 4H), δ7.11-7.18 (m, 8H), δ7.53-7.68 (m, 4H), δ2.41-2.43 (d, 12H), δ2.01(s, 6H).

Melting point: 170-175° C

Compound **4**:

^{1}H NMR (500 MHz, $CDCl_3$): δ7.49-7.65 (m, 4H), δ7.07-7.19 (m, 4H), δ6.62-6.71 (m, 8H), δ3.07-3.08 (d, 24H), δ2.12(s, 6H).

Melting point: 235-240° C

Crystallization:

The compounds were crystallized by slow evaporation method in different solvents at room temperature. Solvents used for crystallization are shown in Table S1, S2, S3 and S4 for compound **1, 2, 3 and 4** respectively.

Table S1 Solvents used for crystallization of compound **1** and composition of crystals produced

Solvent used for crystallization of 1	**Crystalline form obtained**
CH_3CN	**1a**
DCM	**1b**
1,4-Dioxane	**1c**
Acetone	**1a** and **1c** concomitantly
$CHCl_3$	**1b**
Tertiary butanol	**1a**
Isopropyl alcohol	**1a**
Ethanol	**1a**
Sublimed crystal	**1c**

Table S2 Solvents used for crystallization of compound **2** and composition of crystals produced

Solvent used for crystallization of 2	**Crystalline form obtained**
CH_3CN	**2a**
DMSO	**2a** and **2b** concomitantly
DCM	**2a**
$CHCl_3$	**2a**
1,4-Dioxane	**2a**
Tertiary butanol	**2a**
Isopropyl alcohol	**2a**
Ethanol	**2a**
Acetone	**2a**

Table S3 List of solvents used for the synthesis of polymorphs of compound **3**.

Solvent used for crystallization of 3	**Polymorph obtained**
Carbontetrachloride	**3a**
Ethylacetate	**3a**
Acetone	**3a**
Diethyl ether	**3a**
Dimethyl Sulfoxide	**3a & 3b**concomitantly
Dimethylformamide	**3a**
Water	**3a**
Nitromethane	**3a**
n-Hexane	**3a**
Methanol	**3a**
Ethanol	**3a**
Isopropanol	**3a**
n-Propanol	**3a**
t-Butanol	**3a**
Acetonitrile	**3a**
n-Butanol	**3a**
Dimethylacetamide	**3a**
Tetrahydrofuran	**3a**
Furan	**3a**
1, 4-Dioxane	**3a & 3b** concomitantly
Cyclohexanone	**3a**
Cyclohexane	**3a**

Benzene	**3a**
Pyridine	**3a**
Toluene	**3a**
Fluorobenzene	**3a**
Anisole	**3a**
Nitrobenzene	**3a & 3b** concomitantly
m-Xylene	**3a**
Aniline	**3a**
Morpholine	**3a**
Piperidine	**3a**
Pyrrolidine	**3a**
m-Nitrotoluene	**3a**
Hexafluorobenzene	**3a**
Mesitylene	**3a**

Table S4 List of solvents used for the synthesis of polymorphs of compound **4**.

Solvent used for crystallization of 2	**Polymorph obtained**
CH_3CN	**4a**
EtOAc	**4a**
Mesitylene	**4b**

Thermal ellipsoid plots

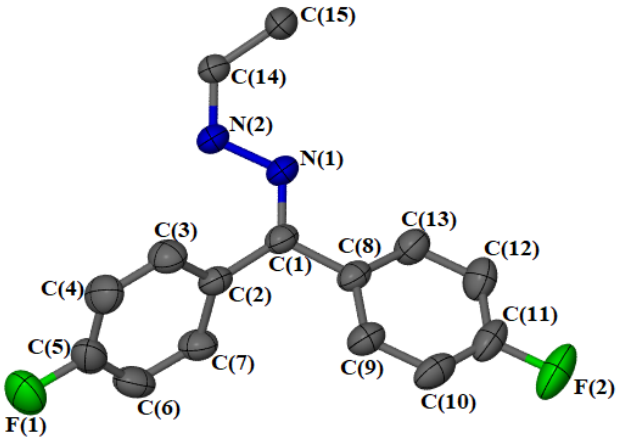


Figure S3 Thermal ellipsoid plot of the asymmetric unit of **1a**. Atoms are shown with 50% probability of thermal ellipsoids.

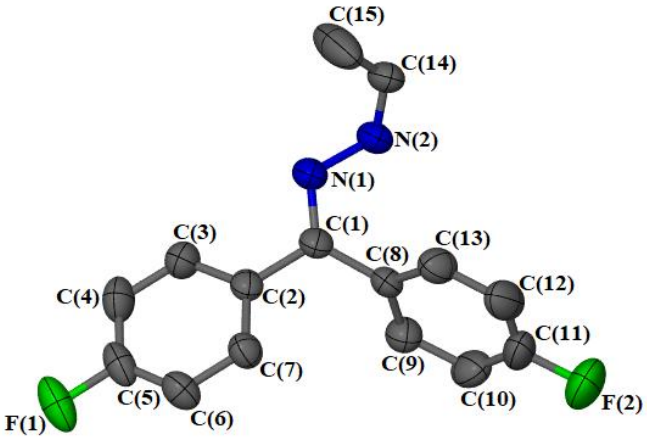


Figure S4 Thermal ellipsoid plot of the asymmetric unit of **1b**. Atoms are shown with 50% probability of thermal ellipsoids.

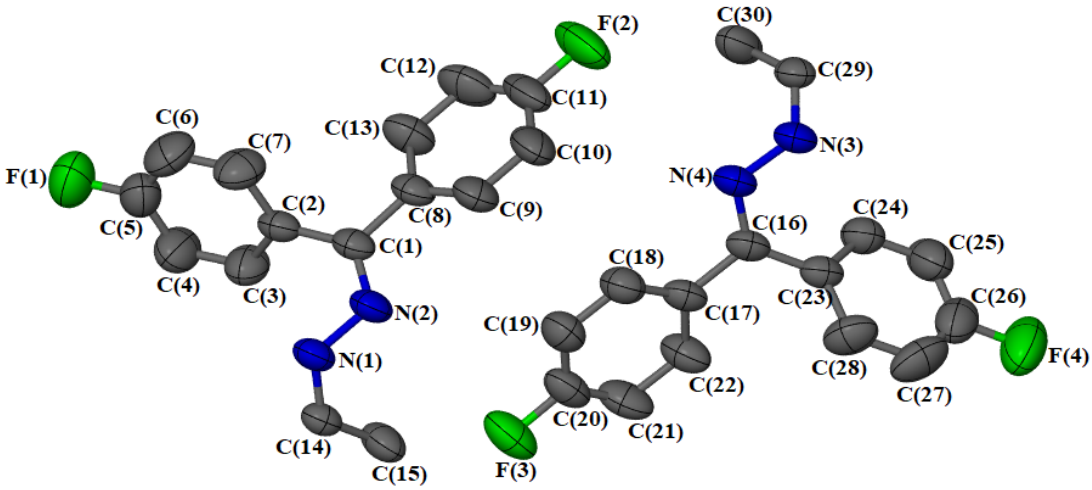


Figure S5 Thermal ellipsoid plot of the asymmetric unit of **1c**. Atoms are shown with 50% probability of thermal ellipsoids.

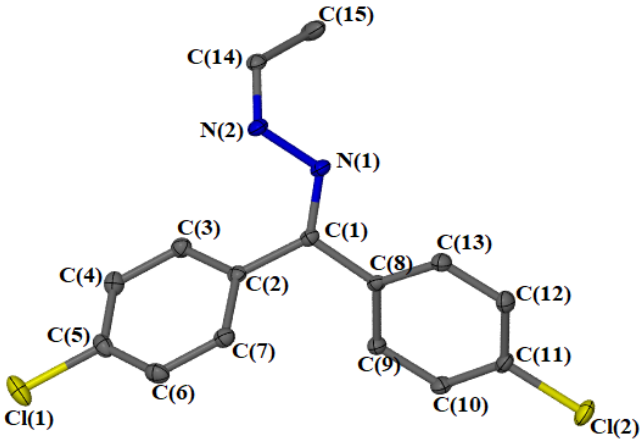


Figure S6 Thermal ellipsoid plot of the asymmetric unit of **2a**. Atoms are shown with 50% probability of thermal ellipsoids.

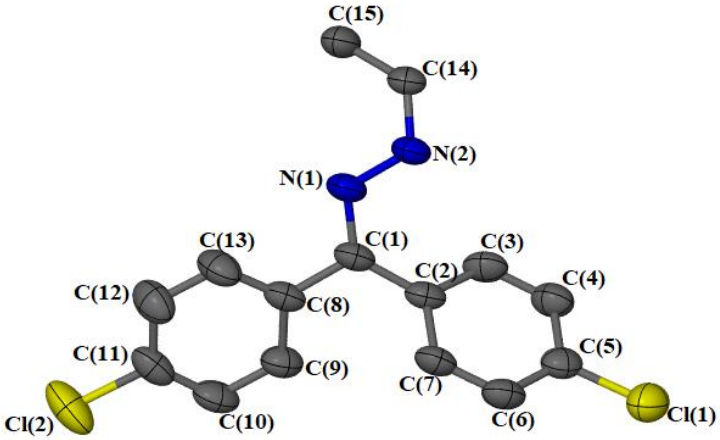


Figure S7 Thermal ellipsoid plot of the asymmetric unit of **2b**. Atoms are shown with 50% probability of thermal ellipsoids.

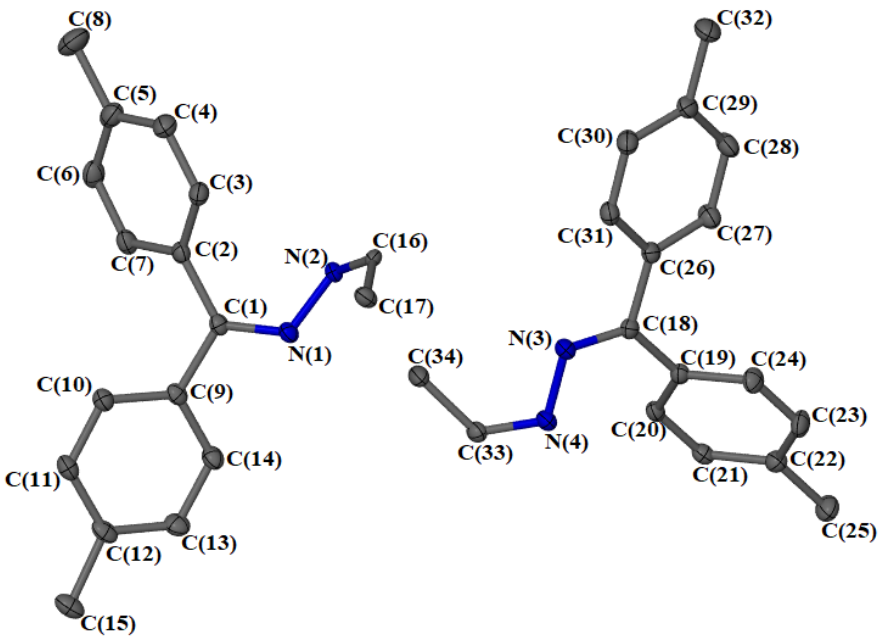


Figure S8 Thermal ellipsoid plot of the asymmetric unit of **3a**. Atoms are shown with 50% probability of thermal ellipsoids.

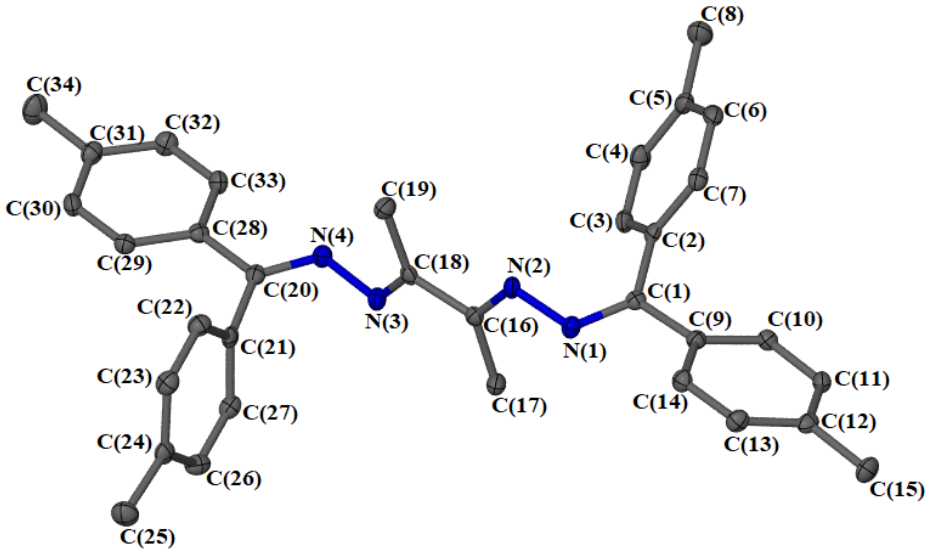


Figure S9 Thermal ellipsoid plot of the asymmetric unit of **3b**. Atoms are shown with 50% probability of thermal ellipsoids.

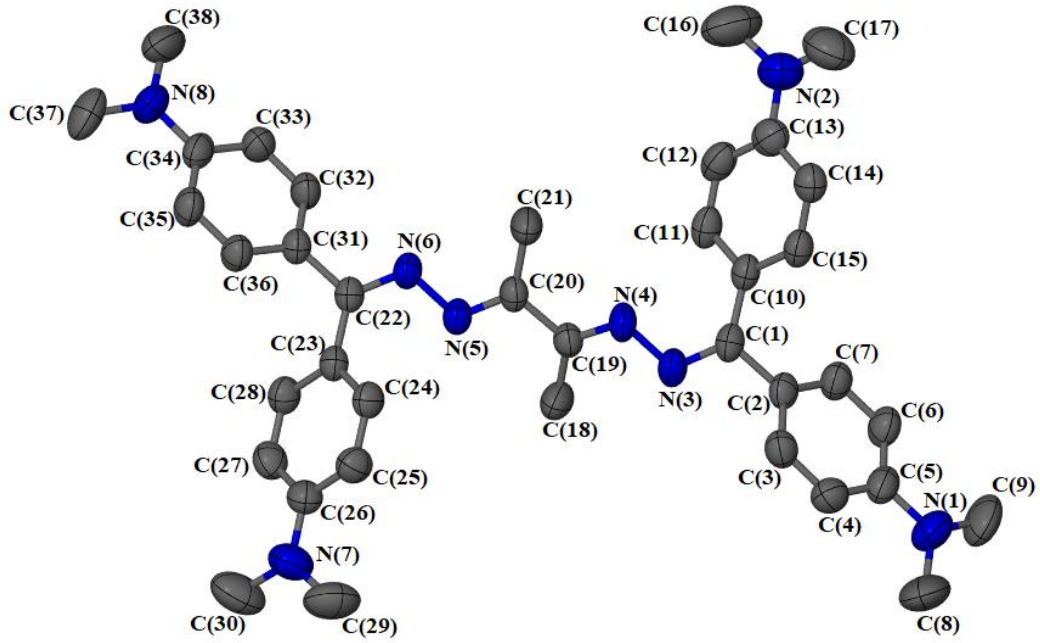


Figure S10 Thermal ellipsoid plot of the asymmetric unit of **4a**. Atoms are shown with 50% probability of thermal ellipsoids.

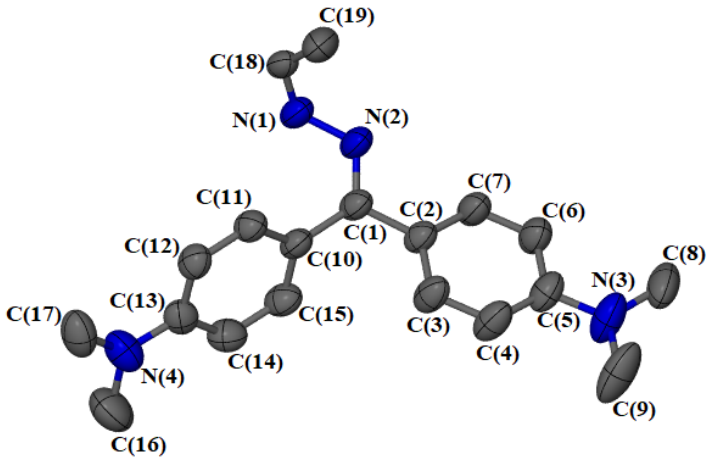


Figure S11 Thermal ellipsoid plot of the asymmetric unit of **4b**. Atoms are shown with 50% probability of thermal ellipsoids.

Hirshfeld surface analysis

Quantitative analysis of intermolecular interactions has been carried out using Crystal Explorer 3.1 program (Wolff *et al.*, 2012). Crystallographic information file (CIF) was used as input for the analysis. Details of Hirshfeld surface analysis and Finger print plots are shown in Fig. S15-S16.

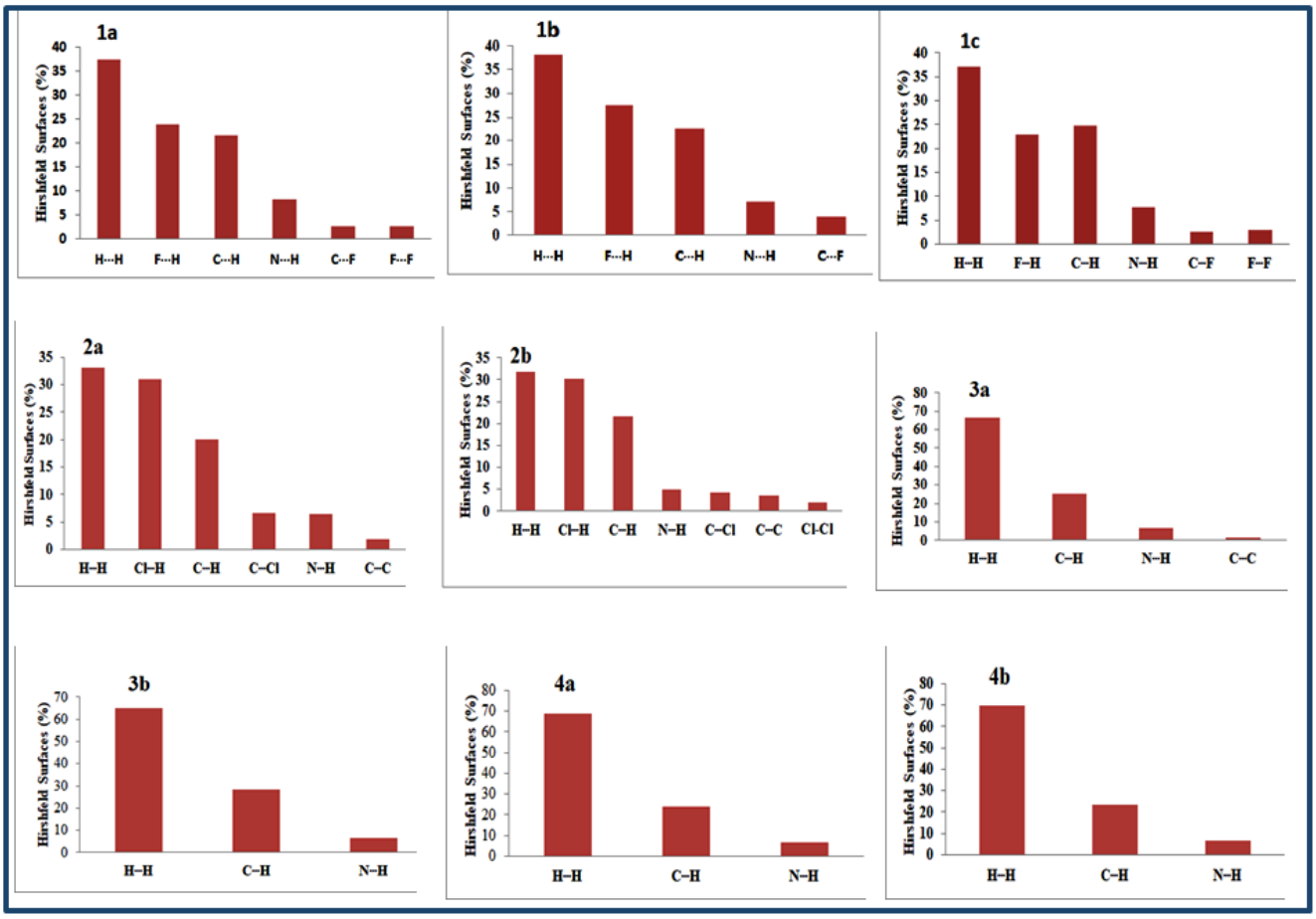


Figure S16 Graphical representation of relative contribution various inter-molecular interactions.

Finger print plot

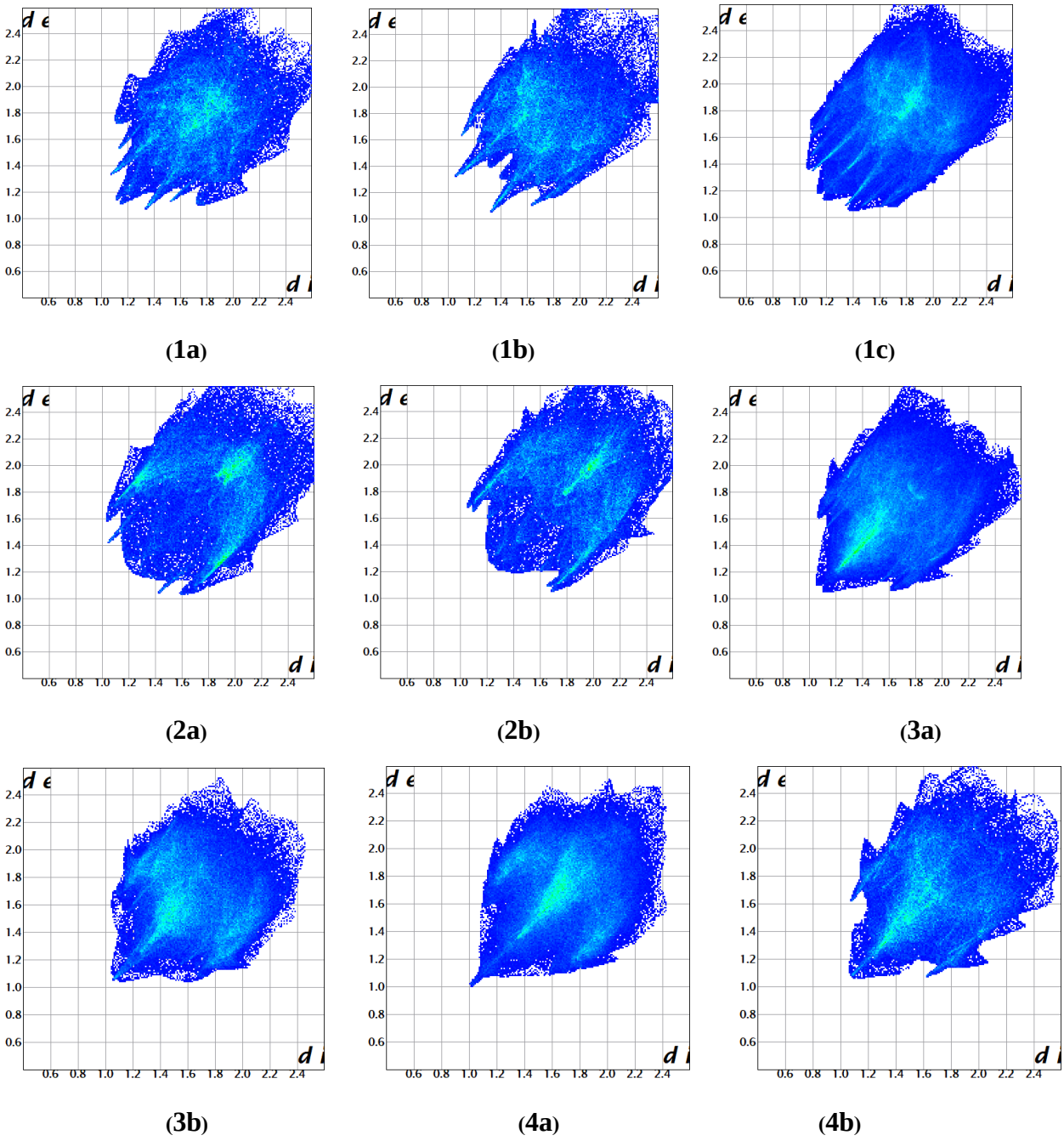


Figure S17 finger print plot of all the polymorphs.