S1. Similarity Indexes — Step by Step

The following general steps show how to obtain the proposed indexes. Additionally, the main steps of the process are demonstrated in Figure S2. The contact area index ($I^C$), in the supramolecular comparison between compound 3 (Cl) and 4 (Br), was used as an example. First, the two supramolecular clusters to be compared are constructed and numbered as observed in Figure S1. For further information, please check reference 1.

**Figure S1.** Supramolecular cluster of compound 1 (hydrogen atoms have been omitted for clarity).

From the supramolecular cluster — grown from the neighboring molecules around the reference molecule M1 — are obtained the dimers which will give us the geometric,
topological, and energetic information regarding the crystal structure. The neighboring
molecules represent the molecular coordination number (MCN). The dimers are
represented by the interaction between the M1 and MN molecules (e.g., M1⋯M10).
The geometrical data from the distances between all non-hydrogen atoms common to all
structures (Mercury), the contact area data from the contact surface area (ToposPro),
and the stabilization energy using computational calculation are obtained using all the
dimers. The equivalent dimers are chosen based on the geometric parameter, after the
overlay of the considered supramolecular clusters (see Figures S25-S39). The overlay
of the clusters were realized considering the M1 molecule as the reference point. An
overlay of the M1 molecule was carried choosing common atoms between the structures
using the Mercury software. After the overlay of the reference molecule, all the other
equivalent molecules can be found. The process of dimers selection can be difficult in
systems with lower similarity, but is necessary to always use the geometric parameter as
standard to define the molecules more close to the equivalence. Secondly, all data are
normalized with the number of molecules (N) from the MCN, and the geometric
parameter normalized with the product of N and the number of distances considered in
each comparison (m), following Eq. 1, Eq. 3 and Eq. 4 of the manuscript.
Example of the normalization of the raw data using compound 3 and 4 as example:

**Table S1.** Data for the normalization of the atom-atom distance (NDi):

| N | Number of atom-atom distances (m) | i (m X N) |
|---|-------------------------------|----------|
| 14 | 12 | 168 |

\[ NDi = i \times \left( \frac{\text{atom} - \text{atom distance}}{\sum \text{atom} - \text{atom distance}} \right) \]  
*(Eq. 1)*

**Table S2.** Normalization of the geometric data for structures 3 and 4.

| Dimer | 3 | 4 | 3 | 4 |
|-------|---|---|---|---|
| atom-atom distance (Å) | NDi | atom-atom distance (Å) | NDi | atom-atom distance (Å) | NDi |
| M1⋯M2 | 7.479 | 0.856 | 7.569 | 0.858 |
| | 7.426 | 0.850 | 7.525 | 0.853 |
| | 7.978 | 0.913 | 8.088 | 0.917 |
| | 8.105 | 0.928 | 8.210 | 0.930 |
| | 7.452 | 0.853 | 7.549 | 0.856 |
| | 8.419 | 0.963 | 8.487 | 0.962 |
| | 7.416 | 0.849 | 7.513 | 0.851 |
|       |       |       |       |
|-------|-------|-------|-------|
| M1···M3 | M1···M3 | M1···M3 | M1···M3 |
| 9.110 | 1.043 | 9.188 | 1.041 |
| 9.119 | 1.044 | 9.204 | 1.043 |
| 7.445 | 0.852 | 7.537 | 0.854 |
| 6.223 | 0.712 | 6.328 | 0.717 |
| 6.204 | 0.710 | 6.312 | 0.715 |
| M1···M4 | M1···M4 | M1···M4 | M1···M4 |
| 7.479 | 0.856 | 7.569 | 0.858 |
| 7.426 | 0.850 | 7.525 | 0.853 |
| 7.978 | 0.913 | 8.088 | 0.917 |
| 8.105 | 0.928 | 8.210 | 0.930 |
| 7.452 | 0.853 | 7.549 | 0.856 |
| 8.419 | 0.963 | 8.487 | 0.962 |
| 7.416 | 0.849 | 7.513 | 0.851 |
| 11.546 | 1.321 | 11.752 | 1.332 |
| 11.546 | 1.321 | 11.752 | 1.332 |
| 11.546 | 1.321 | 11.752 | 1.332 |
| 11.546 | 1.321 | 11.752 | 1.332 |
| 11.546 | 1.321 | 11.752 | 1.332 |
| M1···M5 | M1···M5 | M1···M5 | M1···M5 |
| 8.519 | 0.975 | 8.570 | 0.971 |
| 6.863 | 0.785 | 6.926 | 0.785 |
| 6.690 | 0.766 | 6.765 | 0.767 |
| 8.270 | 0.946 | 8.346 | 0.946 |
| 12.101 | 1.385 | 12.128 | 1.375 |
| 8.806 | 1.008 | 8.863 | 1.004 |
| 9.242 | 1.058 | 9.303 | 1.054 |
| 9.493 | 1.086 | 9.561 | 1.084 |
| 9.311 | 1.066 | 9.348 | 1.059 |
| 9.493 | 1.086 | 9.561 | 1.084 |
| M1···M6 | M1···M6 | M1···M6 | M1···M6 |
| 8.118 | 0.929 | 8.143 | 0.923 |
| 8.118 | 0.929 | 8.143 | 0.923 |
| 8.118 | 0.929 | 8.143 | 0.923 |
| 8.118 | 0.929 | 8.143 | 0.923 |
| M1···M7       |         |         |         |         |
|--------------|---------|---------|---------|---------|
|              | 8.118   | 0.929   | 8.143   | 0.923   |
|              | 8.118   | 0.929   | 8.143   | 0.923   |
|              | 8.118   | 0.929   | 8.143   | 0.923   |
|              | 8.118   | 0.929   | 8.143   | 0.923   |
|              | 8.118   | 0.929   | 8.143   | 0.923   |
|              | 8.118   | 0.929   | 8.143   | 0.923   |
|              | 8.118   | 0.929   | 8.143   | 0.923   |
|              | 8.118   | 0.929   | 8.143   | 0.923   |
|              |         |         |         |         |
| M1···M8      |         |         |         |         |
|              | 9.559   | 1.094   | 9.590   | 1.087   |
|              | 8.519   | 0.975   | 8.570   | 0.971   |
|              | 6.863   | 0.785   | 6.926   | 0.785   |
|              | 6.690   | 0.766   | 6.765   | 0.767   |
|              | 8.270   | 0.946   | 8.346   | 0.946   |
|              | 12.101  | 1.385   | 12.128  | 1.375   |
|              | 8.806   | 1.008   | 8.863   | 1.004   |
|              | 9.242   | 1.058   | 9.303   | 1.054   |
|              | 9.493   | 1.086   | 9.561   | 1.084   |
|              | 9.311   | 1.066   | 9.348   | 1.059   |
|              | 9.493   | 1.086   | 9.561   | 1.084   |
|              | 9.242   | 1.058   | 9.303   | 1.054   |
|              |         |         |         |         |
| M1···M9      |         |         |         |         |
|              | 11.546  | 1.321   | 11.752  | 1.332   |
|              | 11.546  | 1.321   | 11.752  | 1.332   |
|              | 11.546  | 1.321   | 11.752  | 1.332   |
|              | 11.546  | 1.321   | 11.752  | 1.332   |
|              | 11.546  | 1.321   | 11.752  | 1.332   |
|              | 11.546  | 1.321   | 11.752  | 1.332   |
|              | 11.546  | 1.321   | 11.752  | 1.332   |
|              | 11.546  | 1.321   | 11.752  | 1.332   |
|              | 11.546  | 1.321   | 11.752  | 1.332   |
|              |         |         |         |         |
| M1···M10     |         |         |         |         |
|              | 7.479   | 0.856   | 7.569   | 0.858   |

S4
|     |     |     |     |
|-----|-----|-----|-----|
| M1···M11 |     |     |     |
|     |     |     |     |
| M1···M12 |     |     |     |
|     |     |     |     |
| M1···M13 |     |     |     |
|     |     |     |     |
Normalization of the contact area (NC) (The normalization of the stabilization energy must be performed in an analogue way):

**Table S3.** Data for the normalization of the contact area (NC) and stabilization energy (NG).

| N   | NC \(g+897/g+869\) | G3G6 | NC \(g+897/g+898\) |
|-----|---------------------|------|---------------------|
| 14  |                     |      |                     |

\[
NC_{M1\cdots M14} = N \times \left( \frac{C_{M1\cdots M14}}{\sum C_{M1\cdots M14}} \right) \quad (\text{Eq. 3})
\]

**Table S4.** Normalization of the contact area data for structures 3 and 4.

| Dimer | 3   | 4   |
|-------|-----|-----|
| \(\Sigma\) | 1468.014 | 1482.358 |
| 168   | 168  |      |
|          | $C_{M1-MN}$ (Å²) | NC$_{M1-MN}$ | $C_{M1-MN}$ (Å²) | NC$_{M1-MN}$ |
|----------|------------------|-------------|------------------|-------------|
| M1···M2  | 39.34            | 1.55        | 39.10            | 1.51        |
| M1···M3  | 39.34            | 1.55        | 39.10            | 1.51        |
| M1···M4  | 11.24            | 0.44        | 11.22            | 0.43        |
| M1···M5  | 21.09            | 0.83        | 21.93            | 0.85        |
| M1···M6  | 16.07            | 0.63        | 16.89            | 0.65        |
| M1···M7  | 16.07            | 0.63        | 16.89            | 0.65        |
| M1···M8  | 21.09            | 0.83        | 21.93            | 0.85        |
| M1···M9  | 11.24            | 0.44        | 11.22            | 0.43        |
| M1···M10 | 39.34            | 1.55        | 39.10            | 1.51        |
| M1···M11 | 39.34            | 1.55        | 39.10            | 1.51        |
| M1···M12 | 34.91            | 1.37        | 35.96            | 1.39        |
| M1···M13 | 16.07            | 0.63        | 16.89            | 0.65        |
| M1···M14 | 16.07            | 0.63        | 16.89            | 0.65        |
| M1···M15 | 34.91            | 1.37        | 35.96            | 1.39        |
| Σ        | 356.12           | 14.00       | 362.18           | 14.00       |

With the dimers properly numbered and having all normalized data necessary to the calculation the similarity indexes can be obtained through the calculations steps. The main steps are mentioned below and a scheme is illustrated in Figure S2.

**Step 1.** A cluster overlay between the considered clusters for comparison have to be carried (see Figures S25-S39) using the reference molecule M1 as starting point.

**Step 2.** Then, it is necessary to find the geometric equivalent dimers between the clusters.

**Step 3.** With the equivalents tracked, it is time to correlate the considered normalized data (e.g., NC$_{M1-MN}$) in order to obtain the linear equation for the comparison parameter considered.
Figure S2. Representation of the three first steps for the similarity index approach.

Step 4. Using the data from the X axis in the linear equation generated by the correlation (step 3) the predicted value (NC\text{predict}) can be obtained. Obtaining the NC\text{predict} and the NC_{M1-MN} − NC\text{predict}:
Table S5. Calculation to obtain the NC\textsubscript{predict} and the NC\textsubscript{M1--MN} - NC\textsubscript{predict}.

| Dimer       | \(3\)     | \(4\)     | NC\textsubscript{predict} (\(Y'\)) | NC\textsubscript{M1--MN} - NC\textsubscript{predict} (\(Y' - Y\)) |
|-------------|------------|------------|-----------------------------------|---------------------------------------------------------------|
| M1···M2     | 1.55       | 1.51       | 1.53                              | -0.02                                                         |
| M1···M3     | 1.55       | 1.51       | 1.53                              | -0.02                                                         |
| M1···M4     | 0.44       | 0.43       | 1.53                              | -0.02                                                         |
| M1···M5     | 0.83       | 0.85       | 1.53                              | -0.02                                                         |
| M1···M6     | 0.63       | 0.65       | 1.36                              | 0.03                                                          |
| M1···M7     | 0.63       | 0.65       | 1.36                              | 0.03                                                          |
| M1···M8     | 0.83       | 0.85       | 1.36                              | 0.03                                                          |
| M1···M9     | 0.44       | 0.43       | 1.36                              | 0.03                                                          |
| M1···M10    | 1.55       | 1.51       | 0.64                              | 0.01                                                          |
| M1···M11    | 1.55       | 1.51       | 0.64                              | 0.01                                                          |
| M1···M12    | 1.37       | 1.39       | 0.64                              | 0.01                                                          |
| M1···M13    | 0.63       | 0.65       | 0.64                              | 0.01                                                          |
| M1···M14    | 0.63       | 0.65       | 0.46                              | -0.03                                                         |
| M1···M15    | 1.37       | 1.39       | 0.46                              | -0.03                                                         |
| \(\Sigma\)  | 14.00      | 14.00      | 14.00                             |                                                              |

Step 5. Now, the values can be applied to the proposed similarity equation. In this case, following Eq. 5 of the manuscript, the topological index was obtained for the supramolecular comparison considered. The same procedure must be carried for the geometric and energetic indexes, using the normalized atom-atom distances and stabilization energies, respectively. Applying the indexes equation:

Table S6. Calculation to obtain \(I^C\) index.

\[
NC_{M1--MN} - NC_{predict} (Y' - Y) \quad I^C = 1 - \sqrt{\frac{\sum (NC_{M1--MN} - NC_{predict})^2}{N}}
\]

\[-0.02\]
\[-0.02\]
\[-0.02\]
\[-0.02\]
\[0.03\]
\[0.03\]
\[0.01\]
\[0.01\]
\[0.01\]
\[0.01\]
\[-0.03\]
\[-0.03\]
\[0.981\]
After the calculation of the similarity indexes, using the geometric ($I^D$), contact area ($I^C$) and energetic ($I^E$) parameters, the multicomponent index of similarity ($I^X$) can be calculated.

The Eq. 7 of the manuscript was simplified form to facilitate the explanation of the method. It was used the values from the other equations (Eq. 2, Eq. 5 and Eq. 6) to achieve the $I^{DCG}$ index. It was applied the Root Mean Square Error (RMSE) in the considered values, following the same general idea from the first three indexes. The whole equation, using the three different parameters ($I^D$, $I^C$ and $I^E$), where $n = 3$ (geometric, topological and energetic parameters) should be write as follows:

$$I^{DCG} = 1 - \sqrt{\frac{\sum (ND_i - ND_{\text{predict}})^2}{\text{max}N}} + \sqrt{\frac{\sum (NC_N - NC_{\text{predict}})^2}{N}} + \sqrt{\frac{\sum (NG_N - NG_{\text{predict}})^2}{N}}$$

Changing all the ‘RMSE portions’ of each index for “$1-I^X$” we furnish a clear final equation, as demonstrated in Eq. 7 of the manuscript.

$$I^{mp} = 1 - \sqrt{\frac{\sum (1 - I^X)^2}{n}}$$  

(Eq. 7)
S2. Multi-parameter index ($I^{mp}$)

**Table S7.** Data of the multi-parameter index ($I^{DCG}$) of the supramolecular comparison for compounds 1-9.

| Parameter | Cl vs. Br | F vs. Cl | F vs. Br | H vs. Br | H vs. Cl | H vs. F | Me vs. OMe |
|-----------|-----------|-----------|-----------|-----------|-----------|---------|------------|
| N         | 14        | 14        | 14        | 14        | 14        | 14      | 16         |
| $I^{DCG}$ | 0.964     | 0.963     | 0.934     | 0.917     | 0.895     | 0.874   | 0.837      |
| Parameter | OMe vs. NO$_2$ | Me vs. NO$_2$ | Me vs. I | OMe vs. I | NO$_2$ vs. I | Pz vs. Me | Pz vs. OMe | Pz vs. NO$_2$ |
| N         | 16        | 16        | 16        | 16        | 16        | 16      | 16         | 16         |
| $I^{DCG}$ | 0.744     | 0.743     | 0.681     | 0.630     | 0.515     | 0.410   | 0.354      | 0.301      |

**Figure S3.** Overview of the similarity index ($I^{DCG}$), for compounds 1-9.

S3. XPac Analysis

The following data were provided by the XPac Software. All measures were carried out with default values, with filter settings of 10, 14 and 1.50, for the angular deviation (a), interplanar angular deviation (p) and corresponding molecular centroid distance deviation (d), respectively.
Figure S4. XPac data for the supramolecular comparison Cl vs. Br.

Figure S5. XPac data for the supramolecular comparison F vs. Cl.
Figure S6. XPac data for the supramolecular comparison F vs. Br.

Figure S7. XPac data for the supramolecular comparison H vs. F.
Figure S8. XPac data for the supramolecular comparison H vs. Cl.

Figure S9. XPac data for the supramolecular comparison H vs. Br.
Figure S10. XPac data for the supramolecular comparison Me vs. OMe.

Figure S11. XPac data for the supramolecular comparison Me vs. NO$_2$. 
Figure S12. XPac data for the supramolecular comparison OMe vs. NO$_2$.

Figure S13. XPac data for the supramolecular comparison Me vs. Pz.
Figure S14. XPac data for the supramolecular comparison I vs. OMe.

Figure S15. XPac data for the supramolecular comparison OMe vs. Pz.
Figure S16. X Pac data for the supramolecular comparison NO₂ vs. Pz.

Figure S17. X Pac data for the supramolecular comparison I vs. NO₂.
Figure S18. XPac data for the supramolecular comparison I vs. Me.

Figure S19. XPac data for the supramolecular comparison I vs. Pz.
S4. Effective distance

For compounds 1-4, the correlation between the absolute difference of the effective distance ($\Delta d_{\text{eff}}$) and the parameter ID was $\Delta d_{\text{eff}} = -26.808 \, I^D + 26.8821$, with $r = 0.971$. Gelbrich et al. (2012)\(^2\) showed that this parameter can be used to assess how different substituents can affect the overall molecular shape. The effective distance (along the C9–X bond) was considered to be between the center of the phenyl C9 atom and the boundary of the van der Waals surface of the substituent, as per **Eq. S1**:

$$d_{\text{eff}} = D_{\text{CPh-X}} + r \quad \text{(Eq. S1)}$$

The change to the molecules van der Waals surface, which resulted from the different substituents, is substantial in relation to its overall size. The data used to obtain the $\Delta d_{\text{eff}}$ are shown in **Table S8** and **Table S9**.

| Table S8. Data regarding the effective distance ($d_{\text{eff}}$) calculation. |
|---|---|---|---|
| R | X | $d_{\text{CPh-X}}$ (Å) | $r$ (Å) | $d_{\text{eff}}$ (Å) |
| H | H | 0.93 | 1.20 | 2.13 |
| F | F | 1.347 | 1.47 | 2.82 |
| Cl | Cl | 1.741 | 1.75 | 3.49 |
| Br | Br | 1.883 | 1.85 | 3.73 |

| Table S9. Data for the geometric parameter $I^D$ and the absolute difference of the effective distance ($\Delta d_{\text{eff}}$). |
|---|---|---|---|---|---|---|
| Parameter | Cl vs. Br | F vs. Cl | F vs. Br | H vs. F | H vs. Cl | H vs. Br |
| $I^D$ | 0.993 | 0.979 | 0.974 | 0.971 | 0.950 | 0.945 |
| $\Delta d_{\text{eff}}$ | 0.242 | 0.674 | 0.916 | 0.687 | 1.361 | 1.603 |

The correlation observed between $I^D$ and the $\Delta d_{\text{eff}}$ cannot be reproduced when compared with the topological ($I^C$) and energetic ($I^G$) indexes, which are based on more complex information - influence from the crystal packing and the types of interactions involved, respectively. The correlations mentioned show that it is not possible to attribute only one geometric parameter in order to compare the entire similarity of a system.
Figure S20. (a) Correlation between $\Delta d_{\text{eff}}$ and the contact area parameter $I_C$, for compounds 1–4 ($\Delta d_{\text{eff}} = -1.46144 I_D - 0.46045, r = 0.780$); and (b) Correlation between $\Delta d_{\text{eff}}$ and the energetic parameter $I_C$, for compounds 1–4 ($\Delta d_{\text{eff}} = 1.42708 I_D - 0.49866, r = 0.084$).

S5. Asphericity and CPE Parameters

The correlations between the $\Delta_{\text{CPE}}$ and $\Delta_{\Omega\text{cluster}}$ indexes are shown in Figure S21 and Figure S22, respectively.
**Figure S21.** Correlation between the Indexes ($I_{\text{index}}$) and $\Delta_{\text{CPE}}$. (a) Geometric index ($I^D$) ($y = -1.69x + 0.93; r = 0.668$); (b) Contact area index ($I^C$) ($y = -4.76x + 0.92; r = 0.772$); (c) Energetic index ($I^E$) ($y = -4.77x + 0.86; r = 0.739$); (d) Multi-component index ($I^{DCG}$) ($y = -3.98x + 0.90; r = 0.761$); (e) All index curves.
Figure S22. Correlation between the Indexes ($I^{\text{index}}$) and $\Delta_{\text{Cluster}}$. (a) Geometric index ($I^D$) ($y = -2.223x + 0.976; r = 0.795$); (b) Contact area index ($I^C$) ($y = -5.681x + 1.00; r = 0.798$); (c) Energetic index ($I^G$) ($y = -5.378x + 0.924; r = 0.726$); (d) Multi-component index ($I^{\text{DCG}}$) ($y = -4.645x + 0.959; r = 0.768$); (e) All index curves.
S6. Correlation between the contact area index (I_D) and the energetic index (I^G).

As expected, and as can be seen in Figure S23, the contact area (I_D) and energetic (I^G) indexes had an excellent correlation (r = 0.973).

**Figure S23.** Correlation between the contact area index (I_D) and the energetic index (I^G). I^G = 1.015 \times I^C - 0.072; r = 0.973.
S7. Ortep representations

Figure S24. Molecular structure of compounds 1-4, 6 and 7, represented by ORTEP diagrams, with thermal ellipsoids drawn at 50% probability.
### S8. Supramolecular clusters for all structures

| Compound | View Axis |
|----------|-----------|
|          | a         | b         | c         |
| 1        | ![Image](image1.png) | ![Image](image2.png) | ![Image](image3.png) |
| 2        | ![Image](image4.png) | ![Image](image5.png) | ![Image](image6.png) |
| 3        | ![Image](image7.png) | ![Image](image8.png) | ![Image](image9.png) |
| 4        | ![Image](image10.png) | ![Image](image11.png) | ![Image](image12.png) |
| 5        | ![Image](image13.png) | ![Image](image14.png) | ![Image](image15.png) |
Figure S25. Supramolecular clusters for the studied compounds 1-9, viewed from different axis.
S9. Supramolecular cluster overlay

Observation: Hydrogen atoms have been omitted for clarity.

**Figure S26.** Supramolecular cluster overlay of Cl (green) vs. Br (brown).

**Figure S27.** Supramolecular cluster overlay of F (yellow) vs. Cl (green).

**Figure S28.** Supramolecular cluster overlay of F (yellow) vs. Br (brown).
Figure S29. Supramolecular cluster overlay of H (black) vs. F (yellow).

Figure S30. Supramolecular cluster overlay of H (black) vs. Cl (green).

Figure S31. Supramolecular cluster overlay of H (black) vs. Br (brown).
Figure S32. Supramolecular cluster overlay of Me (orange) vs. OMe (magenta).

Figure S33. Supramolecular cluster overlay of Me (orange) vs. NO$_2$ (red).

Figure S34. Supramolecular cluster overlay of OMe (magenta) vs. NO$_2$ (red).
Figure S35. Supramolecular cluster overlay of Me (orange) vs. I (blue).

Figure S36. Supramolecular cluster overlay of NO$_2$ (red) vs. I (blue).

Figure S37. Supramolecular cluster overlay of OMe (magenta) vs. I (blue).
Figure S38. Supramolecular cluster overlay of Pz (grey) vs. OMe (magenta).

Figure S39. Supramolecular cluster overlay of Pz (grey) vs. Me (orange).

Figure S40. Supramolecular cluster overlay of Pz (grey) vs. NO₂ (red).
Table S10. Contact area and stabilization energy data of each dimer from the supramolecular cluster of compound 1 (X = H).

| Dimer | Symmetry Code                  | $C_{M1-MN}$ ($\text{Å}^2$) | $G_{M1-MN}$ (kcal mol$^{-1}$) | $NC_{M1-MN}$ | $NG_{M1-MN}$ |
|-------|--------------------------------|-----------------------------|--------------------------------|---------------|--------------|
| M1···M2 | -1/2-x, 1.5-y, -1/2+z         | 38.43                       | -6.59                          | 1.57          | 1.84         |
| M1···M3 | 1/2-x, 1.5-y, -1/2+z          | 38.43                       | -6.59                          | 1.57          | 1.84         |
| M1···M4 | x, y, -1+z                    | 13.96                       | -2.46                          | 0.57          | 0.69         |
| M1···M5 | -x, 2-y, -1/2+z               | 18.52                       | -1.87                          | 0.75          | 0.52         |
| M1···M6 | -1/2-x, 1/2+y, z              | 13.45                       | -1.42                          | 0.55          | 0.40         |
| M1···M7 | 1/2+x, 1/2+y, z               | 13.45                       | -1.42                          | 0.55          | 0.40         |
| M1···M8 | -x, 2-y, 1/2+z                | 18.52                       | -1.87                          | 0.75          | 0.52         |
| M1···M9 | x, y, 1+z                     | 13.96                       | -2.46                          | 0.57          | 0.69         |
| M1···M10 | -1/2+x, 1.5-y, 1/2+z          | 38.43                       | -6.59                          | 1.57          | 1.84         |
| M1···M11 | 1/2+x, 1.5-y, 1/2+z           | 38.43                       | -6.59                          | 1.57          | 1.84         |
| M1···M12 | -x, 1-y, 1/2+z               | 35.62                       | -4.73                          | 1.45          | 1.32         |
| M1···M13 | -1/2+x, -1/2+y, z             | 13.45                       | -1.42                          | 0.55          | 0.40         |
| M1···M14 | 1/2+x, -1/2+y, z              | 13.45                       | -1.42                          | 0.55          | 0.40         |
| M1···M15 | -x, 1-y, -1/2+z               | 35.62                       | -4.73                          | 1.45          | 1.32         |
|        | Cluster                        | 343.72                      | -50.16                         | 14.00         | 14.00        |
Table S11. Contact area and stabilization energy data of each dimer from the supramolecular cluster of compound 2 (X=F).

| Dimer   | Symmetry Code                  | $C_{M1\cdots MN}$ (Å²) | $G_{M1\cdots MN}$ (kcal mol⁻¹) | NC$_{M1\cdots MN}$ | NG$_{M1\cdots MN}$ |
|---------|--------------------------------|------------------------|--------------------------------|-------------------|-------------------|
| M1···M2 | -1/2-x, 1/2-y, -1/2+z          | 39.27                  | -6.97                          | 1.58              | 1.94              |
| M1···M3 | 1/2-x, 1/2-y, -1/2+z           | 39.27                  | -6.97                          | 1.58              | 1.94              |
| M1···M4 | x, y, -1+z                    | 10.45                  | -0.65                          | 0.42              | 0.18              |
| M1···M5 | -x, 1-y, -1/2+z                | 20.19                  | -1.98                          | 0.81              | 0.55              |
| M1···M6 | 1/2+x, 1/2+y, z                | 14.90                  | -1.85                          | 0.60              | 0.52              |
| M1···M7 | -x, 1-y, 1/2+z                 | 20.19                  | -1.98                          | 0.81              | 0.55              |
| M1···M8 | x, y, 1+z                     | 10.45                  | -0.65                          | 0.42              | 0.18              |
| M1···M9 | -1/2-x, 1/2-y, 1/2+z           | 39.27                  | -6.97                          | 1.58              | 1.94              |
| M1···M10| 1/2-x, 1/2-y, 1/2+z            | 39.27                  | -6.97                          | 1.58              | 1.94              |
| M1···M11| -x, y, 1/2+z                  | 34.97                  | -4.83                          | 1.41              | 1.35              |
| M1···M12| 1/2+x, -1/2+y, z              | 14.90                  | -1.85                          | 0.60              | 0.52              |
| M1···M13| 1/2+x, -1/2+y, z              | 14.90                  | -1.85                          | 0.60              | 0.52              |
| M1···M14| -x, -y, -1/2+z                 | 34.97                  | -4.83                          | 1.41              | 1.35              |
| Cluster |                                | 347.90                 | -50.20                         | 14.00             | 14.00             |
Table S12. Contact area and stabilization energy data of each dimer from the supramolecular cluster of compound 3 (X=Cl).

| Dimer   | Symmetry Code          | $C_{M1\cdots MN}$ (Å$^2$) | $G_{M1\cdots MN}$ (kcal mol$^{-1}$) | $N_{CM1\cdots MN}$ | $N_{GM1\cdots MN}$ |
|---------|------------------------|-----------------------------|-------------------------------------|---------------------|---------------------|
| M1···M2 | 1.5-x, 1/2-y, -1/2+z   | 39.34                       | -7.43                               | 1.55                | 1.90                |
| M1···M3 | 1/2-x, 1/2-y, -1/2+z   | 39.34                       | -7.43                               | 1.55                | 1.90                |
| M1···M4 | x, y, -1+z            | 11.24                       | -1.30                               | 0.44                | 0.33                |
| M1···M5 | 1-x, -y, -1/2+z       | 21.09                       | -2.49                               | 0.83                | 0.64                |
| M1···M6 | 1/2+x, -1/2+y, z     | 16.07                       | -1.96                               | 0.63                | 0.50                |
| M1···M7 | 1/2+x, -1/2+y, z     | 16.07                       | -1.96                               | 0.63                | 0.50                |
| M1···M8 | 1-x, -y, 1/2+z       | 21.09                       | -2.49                               | 0.83                | 0.64                |
| M1···M9 | x, y, 1+z            | 11.24                       | -1.30                               | 0.44                | 0.33                |
| M1···M10| 1/2+x, 1/2-y, 1/2+z  | 39.34                       | -7.43                               | 1.55                | 1.90                |
| M1···M11| 1/2-x, 1/2-y, 1/2+z  | 39.34                       | -7.43                               | 1.55                | 1.90                |
| M1···M12| 1-x, 1-y, 1/2+z      | 34.91                       | -4.80                               | 1.37                | 1.23                |
| M1···M13| 1/2+x, 1/2+y, z     | 16.07                       | -1.96                               | 0.63                | 0.50                |
| M1···M14| 1/2+x, 1/2+y, z     | 16.07                       | -1.96                               | 0.63                | 0.50                |
| M1···M15| 1-x, 1-y, -1/2+z    | 34.91                       | -4.80                               | 1.37                | 1.23                |
| Cluster |                        | 356.12                      | -54.74                              | 14.00               | 14.00               |
Table S13. Contact area and stabilization energy data of each dimer from the supramolecular cluster of compound 4 (X=Br).

| Dimer   | Symmetry Code          | $C_{M1-MN}$ ($\text{Å}^2$) | $G_{M1-MN}$ (kcal mol$^{-1}$) | $NC_{M1-MN}$ | $NG_{M1-MN}$ |
|---------|------------------------|----------------------------|-------------------------------|--------------|--------------|
| M1···M2 | 1.5-x, 1/2-y, -1/2+z   | 39.10                      | -7.60                         | 1.51         | 1.86         |
| M1···M3 | 1/2-x, 1/2-y, -1/2+z   | 39.10                      | -7.60                         | 1.51         | 1.86         |
| M1···M4 | x, y, -1+z             | 11.22                      | -2.06                         | 0.43         | 0.50         |
| M1···M5 | 1-x, -y, -1/2+z        | 21.93                      | -2.58                         | 0.85         | 0.63         |
| M1···M6 | 1/2+x, -1/2+y, z       | 16.89                      | -1.98                         | 0.65         | 0.48         |
| M1···M7 | -1/2+x, -1/2+y, z      | 16.89                      | -1.98                         | 0.65         | 0.48         |
| M1···M8 | 1-x, -y, 1/2+z         | 21.93                      | -2.58                         | 0.85         | 0.63         |
| M1···M9 | x, y, 1+z              | 11.22                      | -2.06                         | 0.43         | 0.50         |
| M1···M10| 1/2+x, 1/2-y, 1/2+z    | 39.10                      | -7.60                         | 1.51         | 1.86         |
| M1···M11| 1/2-x, 1/2-y, 1/2+z    | 39.10                      | -7.60                         | 1.51         | 1.86         |
| M1···M12| 1-x, 1-y, 1/2+z        | 35.96                      | -4.80                         | 1.39         | 1.17         |
| M1···M13| 1/2+x, 1/2+y, z        | 16.89                      | -1.98                         | 0.65         | 0.48         |
| M1···M14| -1/2+x, 1/2+y, +z      | 16.89                      | -1.98                         | 0.65         | 0.48         |
| M1···M15| 1-x, 1-y, -1/2+z       | 35.96                      | -4.80                         | 1.39         | 1.17         |
| Cluster |                        | 362.18                     | -57.20                        | 14.00        | 14.00        |
Table S14. Contact area and stabilization energy data of each dimer from the supramolecular cluster of compound 5 (X=I).

| Dimer    | Symmetry Code       | $C_{M1-\cdot\cdot\cdot M_N}$ (Å²) | $G_{M1-\cdot\cdot\cdot M_N}$ (kcal mol⁻¹) | $N_{C_{M1-\cdot\cdot\cdot M_N}}$ | $N_{G_{M1-\cdot\cdot\cdot M_N}}$ |
|----------|---------------------|----------------------------------|------------------------------------------|-------------------------------|-------------------------------|
| M1…M2   | 2-x, -1/2+y, 1-z    | 73.69                            | -12.65                                   | 3.15                          | 3.57                          |
| M1…M3   | 2-x, 1/2+y, 1-z     | 73.69                            | -12.65                                   | 3.15                          | 3.57                          |
| M1…M4   | 3-x, -1/2+y, 1-z    | 9.18                             | -1.94                                    | 0.39                          | 0.55                          |
| M1…M5   | 1+x, y, z           | 34.56                            | -4.17                                    | 1.48                          | 1.18                          |
| M1…M6   | 3-x, 1/2+y, 1-z     | 9.18                             | -1.94                                    | 0.39                          | 0.55                          |
| M1…M7   | 2.5-x, -y, -1/2+z   | 13.22                            | -1.67                                    | 0.57                          | 0.47                          |
| M1…M8   | 1/2+x, 1/2-y, 1/2-z | 15.7                             | -4.10                                    | 0.67                          | 1.16                          |
| M1…M9   | 2.5-x, 1-y, -1/2+z  | 13.22                            | -1.67                                    | 0.57                          | 0.47                          |
| M1…M10  | -1/2+x, 1/2-y, 1/2-z| 15.7                             | -4.10                                    | 0.67                          | 1.16                          |
| M1…M11  | 1-x, -1/2+y, 1-z    | 5.74                             | -0.03                                    | 0.25                          | 0.01                          |
| M1…M12  | -1+x, y, z          | 34.56                            | -4.17                                    | 1.48                          | 1.18                          |
| M1…M13  | 1-x, 1/2+y, 1-z     | 5.74                             | -0.03                                    | 0.25                          | 0.01                          |
| M1…M14  | -1/2+x, 1/2-y, 1.5-z| 21.67                            | -2.09                                    | 0.93                          | 0.59                          |
| M1…M15  | 2.5-x, -y, 1/2+z    | 13.22                            | -1.67                                    | 0.57                          | 0.47                          |
| M1…M16  | 1/2+x, 1/2-y, 1.5-z | 21.67                            | -2.09                                    | 0.93                          | 0.59                          |
| M1…M17  | 2.5-x, 1-y, 1/2+z   | 13.22                            | -1.67                                    | 0.57                          | 0.47                          |
| Cluster  |                     | 373.96                           | -56.64                                   | 16.00                         | 16.00                         |
Table S15. Contact area and stabilization energy data of each dimer from the supramolecular cluster of compound 6 (X=Me).

| Dimer  | Symmetry Code | $C_{M1-MN}$ (Å²) | $G_{M1-MN}$ (kcal mol⁻¹) | NC$_{M1-MN}$ | NG$_{M1-MN}$ |
|--------|---------------|------------------|--------------------------|-------------|-------------|
| M1···M2 | 2.5-x, 1/2+y, 2-z | 64.49 | -11.86 | 2.84 | 3.65 |
| M1···M3 | 2.5-x, -1/2+y, 2-z | 64.49 | -11.86 | 2.84 | 3.65 |
| M1···M4 | 1/2+x, 1/2+y, 1+z | 12.58 | -0.92 | 0.55 | 0.28 |
| M1···M5 | -3-x, y, 3-z | 34.91 | -6.14 | 1.54 | 1.89 |
| M1···M6 | 1/2+x, -1/2+y, 1+z | 12.99 | -1.02 | 0.57 | 0.31 |
| M1···M7 | -1/2+x, 1/2+y, z | 7.68 | -1.64 | 0.34 | 0.50 |
| M1···M8 | 2-x, y, 2-z | 20.54 | -2.34 | 0.91 | 0.72 |
| M1···M9 | -1/2+x, -1/2+y, z | 7.60 | -0.90 | 0.34 | 0.28 |
| M1···M10 | -1+x, y, -1+z | 11.29 | -1.46 | 0.50 | 0.45 |
| M1···M11 | -1/2+x, 1/2+y, -1+z | 12.99 | -1.02 | 0.57 | 0.31 |
| M1···M12 | 2-x, y, 1-z | 21.79 | -2.07 | 0.96 | 0.64 |
| M1···M13 | -1/2+x, -1/2+y, -1+z | 12.58 | -0.92 | 0.55 | 0.28 |
| M1···M14 | 1/2+x, 1/2+y, z | 7.60 | -0.90 | 0.34 | 0.28 |
| M1···M15 | 3-x, y, 2-z | 52.44 | -5.83 | 2.31 | 1.79 |
| M1···M16 | 1/2+x, -1/2+y, z | 7.68 | -1.64 | 0.34 | 0.50 |
| M1···M17 | 1+x, y, 1+z | 11.29 | -1.46 | 0.50 | 0.45 |
| Cluster | | 362.94 | -51.98 | 16.00 | 16.00 |
Table S16. Contact area and stabilization energy data of each dimer from the supramolecular cluster of compound 7 (X=OMe).

| Dimer    | Symmetry Code | $C_{M1-MN}$ (Å$^2$) | $G_{M1-MN}$ (kcal mol$^{-1}$) | NC$_{M1-MN}$ | NG$_{M1-MN}$ |
|----------|---------------|----------------------|-------------------------------|--------------|--------------|
| M1···M2  | 1-x, 2-y, 1-z | 60.84                | -10.43                        | 2.63         | 2.93         |
| M1···M3  | -x, 1-y, 1-z  | 74.96                | -14.31                        | 3.25         | 4.01         |
| M1···M4  | x, y, -1+z    | 16.32                | -1.45                         | 0.71         | 0.41         |
| M1···M5  | -x, 1-y, -z   | 38.52                | -7.48                         | 1.67         | 2.10         |
| M1···M6  | -1+x, -1+y, -1+z | 8.70            | -0.78                         | 0.38         | 0.22         |
| M1···M7  | 1+x, y, z     | 7.31                 | -1.21                         | 0.32         | 0.34         |
| M1···M8  | 1-x, 1-y, 1-z | 18.21                | -2.78                         | 0.79         | 0.78         |
| M1···M9  | x, -1+y, z    | 7.26                 | -1.11                         | 0.31         | 0.31         |
| M1···M10 | 1+x, y, 1+z   | 9.95                 | -1.85                         | 0.43         | 0.52         |
| M1···M11 | 1+x, 1+y, 1+z | 8.70                 | -0.78                         | 0.38         | 0.22         |
| M1···M12 | 1-x, 2-y, 2-z | 20.69                | -1.86                         | 0.90         | 0.52         |
| M1···M13 | x, y, 1+z     | 16.32                | -1.45                         | 0.71         | 0.41         |
| M1···M14 | x, 1+y, z     | 7.26                 | -1.11                         | 0.31         | 0.31         |
| M1···M15 | -x, 2-y, 1-z  | 57.2                 | -7.37                         | 2.48         | 2.07         |
| M1···M16 | -1+x, y, z    | 7.31                 | -1.21                         | 0.32         | 0.34         |
| M1···M17 | -1-x, y, -1+z | 9.95                 | -1.85                         | 0.43         | 0.52         |

Cluster | 369.50 | -57.03 | 16.00  | 16.00  |
Table S17. Contact area and stabilization energy data of each dimer from the supramolecular cluster of compound 8 (X=NO₂).

| Dimer    | Symmetry Code   | \(C_{M1-MN}\) (Å²) | \(G_{M1-MN}\) (kcal mol⁻¹) | NC_{M1-MN} | NG_{M1-MN} |
|----------|-----------------|---------------------|-----------------------------|-------------|-------------|
| M1···M2  | -x, -y, 2-z     | 49.51               | -10.81                      | 2.47        | 3.11        |
| M1···M3  | 1-x, 1-y, 2-z   | 52.47               | -10.98                      | 2.62        | 3.16        |
| M1···M4  | -1+x, -1+y, -1+z| 14.23               | -1.96                       | 0.71        | 0.56        |
| M1···M5  | -x, -y, 1-z     | 31.34               | -7.15                       | 1.56        | 2.06        |
| M1···M6  | x, y, -1+z      | 14.2                | -1.81                       | 0.71        | 0.52        |
| M1···M7  | -1+x, y, z      | 8.97                | -1.18                       | 0.45        | 0.34        |
| M1···M8  | -x, 1-y, 2-z    | 11.13               | -1.05                       | 0.56        | 0.30        |
| M1···M9  | x, 1+y, 1+z     | 6.18                | -1.17                       | 0.31        | 0.34        |
| M1···M10 | x, y, 1+z       | 14.2                | -1.81                       | 0.71        | 0.52        |
| M1···M11 | 1-x, 1-y, 3-z   | 16.00               | -2.25                       | 0.80        | 0.65        |
| M1···M12 | 1+x, 1+y, 1+z   | 14.23               | -1.96                       | 0.71        | 0.56        |
| M1···M13 | 2-x, 1-y, 3-z   | 0.33                | -0.08                       | 0.02        | 0.02        |
| M1···M14 | 1-x, -y, 2-z    | 60.73               | -8.03                       | 3.03        | 2.31        |
| M1···M15 | 1+x, y, z       | 8.97                | -1.18                       | 0.45        | 0.34        |
| M1···M16 | x, -1+y, -1+z   | 6.18                | -1.17                       | 0.31        | 0.34        |
| M1···M17 | 1-x, -y, 1-z    | 12.05               | -2.95                       | 0.60        | 0.85        |
| Cluster  |                 | 320.72              | -55.54                      | 16.00       | 16.00       |
Table S18. Contact area and stabilization energy data of each dimer from the supramolecular cluster of compound 9 (X=Pz).

| Dimer | Symmetry Code | $C_{M1-MN}$ (Å²) | $G_{M1-MN}$ (kcal mol⁻¹) | NC₉₁-MN | NG₉₁-MN |
|-------|---------------|------------------|--------------------------|---------|---------|
| M1···M2 | $x,1+y,z$ | 57.70 | -7.20 | 2.11 | 1.60 |
| M1···M3 | $x^-,1+y,z$ | 57.70 | -7.28 | 2.11 | 1.62 |
| M1···M4 | $-1+x,y,1+z$ | 11.09 | -1.79 | 0.41 | 0.40 |
| M1···M5 | $-1+x,-1+y,1+z$ | 15.60 | -0.90 | 0.57 | 0.20 |
| M1···M6 | $-1+x,1+y,z$ | 23.55 | -3.47 | 0.86 | 0.77 |
| M1···M7 | $-1+x,y,z$ | 59.75 | -12.53 | 2.19 | 2.79 |
| M1···M8 | $-1+x,-1+y,z$ | 6.27 | -0.96 | 0.23 | 0.21 |
| M1···M9 | $x,2+y,-1+z$ | 4.95 | -0.81 | 0.18 | 0.18 |
| M1···M10 | $x,1+y,-1+z$ | 39.59 | -8.09 | 1.45 | 1.80 |
| M1···M11 | $1+x,1+y,-1+z$ | 15.60 | -1.05 | 0.57 | 0.23 |
| M1···M12 | $1+x,y,-1+z$ | 11.09 | -1.84 | 0.41 | 0.41 |
| M1···M13 | $1+x,1+y,z$ | 6.27 | -0.77 | 0.23 | 0.17 |
| M1···M14 | $1+x,y,z$ | 59.75 | -12.53 | 2.19 | 2.79 |
| M1···M15 | $1+x,-1+y,z$ | 23.83 | -3.65 | 0.87 | 0.81 |
| M1···M16 | $x,-1+y,1+z$ | 39.59 | -8.19 | 1.45 | 1.82 |
| M1···M17 | $x,2+y,1+z$ | 4.95 | -0.82 | 0.18 | 0.18 |
| Cluster | | 437.28 | -71.90 | 16.00 | 16.00 |

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