Supporting Information

Substituent Effects in the Crystallization Mechanisms of 7-chloro-4-substituted-Quinolines

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1. Synthesis of compounds 4, 5 and 8

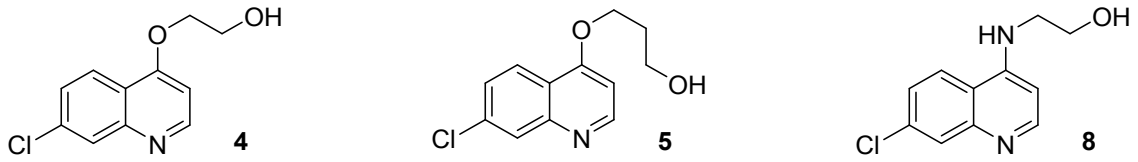


Figure S1. Compounds synthetized in this work.

Compound **4** and **5** were prepared following the described procedure reported Natarajan et al.[1] Spectroscopic data obtained are in accordance with those described by the authors.[1]

Compound **8** was prepared following conditions already reported by Oukoloff et al.[2] Spectroscopic data obtained are in accordance with those described by the authors.[2]

2. Crystallographic Data of new structures reported

Table S1. Crystallographic data of compounds **4, 5** and **8**.

Compound	**4**	**5**	**8**
CCDC number	1914635	1568275	1585679
Empirical formula	C_{11} H_{10} Cl N O_2	C_{12} H_{12} Cl N O_2	C_{11} H_{11} Cl N_2 O
Molecular weight	223,65	237,68	222.67
Temperature (K)	297(2)	293(2)	293(2)
Wavelength (Å)	0.71073	0.71073	0.56086
Crystal system	Monoclinic	Orthorhombic	Monoclinic
Space group	$P2_1$	P n a 2_1	$P2_1$/n
Cell parameters			
a (Å)	4.3139(2)	17.4385(6)	4.5838(2)
b (Å)	25.5732(14)	4.8748(2)	14.8986(7)
c (Å)	9.5710(5)	25.7168(9)	14.9416(7)
α (°)	90	90	90
β (°)	102.074(2)	90	93.4840(10)
γ (°)	90	90	90
V (Å^3)	1032.52(9)	2186.16(14)	1018.51(8)
Z	4	8	4
Calc. density (Mg m^{-3})	1.439	1.444	1.452
Abs. Coef. (mm^{-1})	0.347	0.332	0.185
F (000)	464	992	464
Crystal size (mm)	0.247 x 0.123 x 0.052	0.375 x 0.262 x 0.140	0.53 x 0.19 x 0.16
θ range for data collection (°)	2.317 to 27.128	2.336 to 30.939	2.41 to 21.086
Reflections collected/unique	17777 / 4540 [R(int) = 0.0379]	26505 / 5734 [R(int) = 0.0189]	14860 / 2235 [R(int) = 0.0377]
Completeness to theta (%)	99.6	98.9	99.7
Absorption correction	Multi-scan	Multi-scan	Multi-scan
Max. and min. transmission	0.7455 and 0.7057	0.7461 and 0.7127	0.7446 and 0.6687
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/restraints/parameters	4540 / 1 / 273	5734 / 1 / 289	2235 / 0 / 136
Goodness of fit on F^2	1.021	1.040	1.045
Final R indices	R1 = 0.0411, wR2 = 0.0786	R1 = 0.0266, wR2 = 0.0682	R1 = 0.0341, wR2 = 0.0953
R all data	R1 = 0.0624, wR2 = 0.0844	R1 = 0.0292, wR2 = 0.0696	R1 = 0.0434, wR2 = 0.1008
Extinction coefficient	None	None	None
$\Delta\rho_{máx.}$ and $\Delta\rho_{min}$ (e.A^{-3})	0.226 and -0.183	0.268 and -0.226	0.348 and -0.364

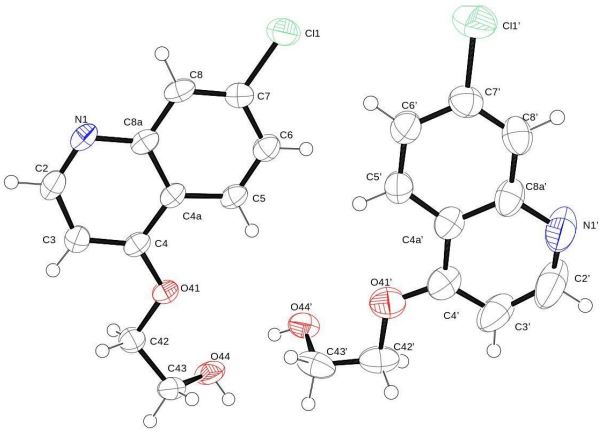


Figure S2. Asymmetric unit of compound **4**, represented by ORTEP diagrams with thermic ellipsoids drawn with 50% of probability.

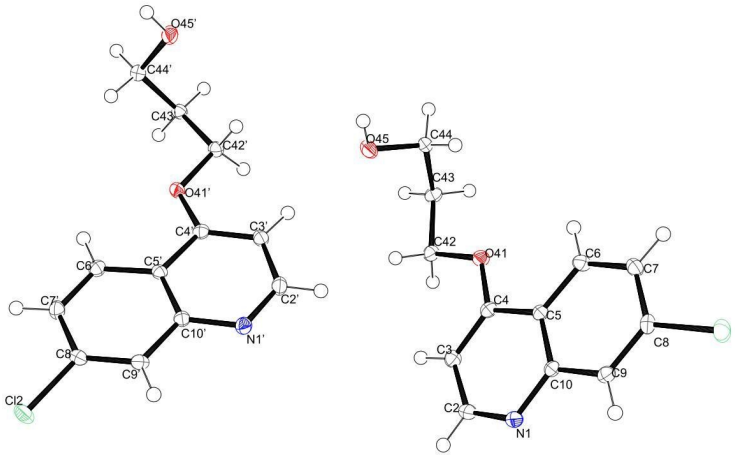


Figure S3. Asymmetric unit of compound **5**, represented by ORTEP diagrams with thermic ellipsoids drawn with 50% of probability.

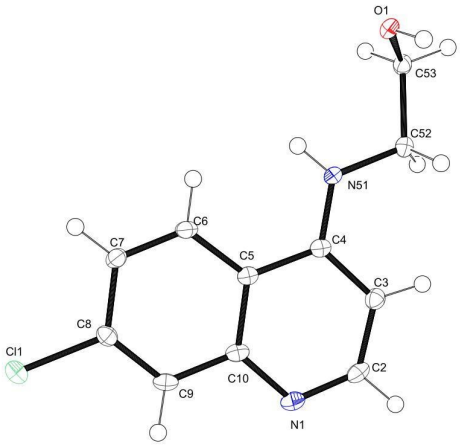


Figure S4. Asymmetric unit of compound **8**, represented by ORTEP diagrams with thermic ellipsoids drawn with 50% of probability.

3. Identification of the asymmetric unit molecules (*Z*')

Observation: Hydrogen atoms are omitted for clarity.

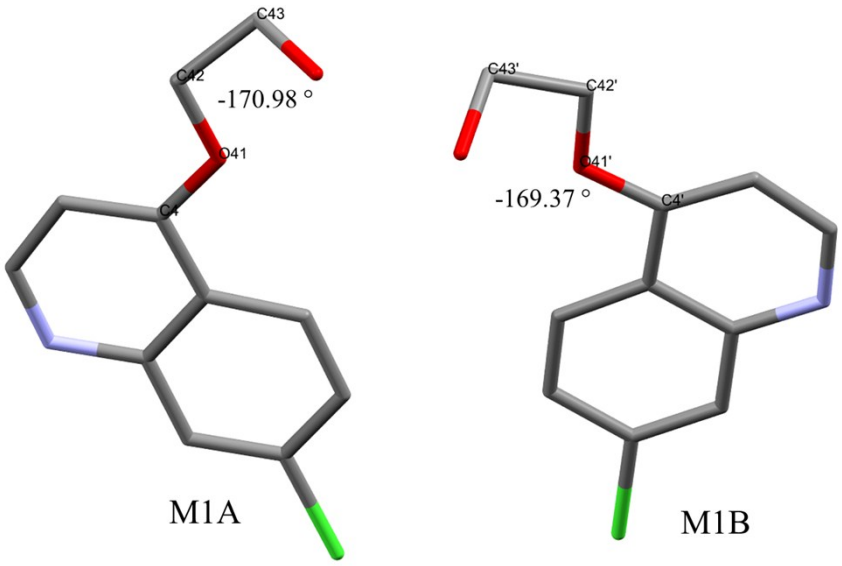


Figure S5. Asymmetric unit molecules for compound **4**. Torsion angles of -170.98 ° (M1A) e -169.37 ° (M1B) between the atoms C4-O41-C42-C43 and C4'-O41'-C42'-C43', respectively.

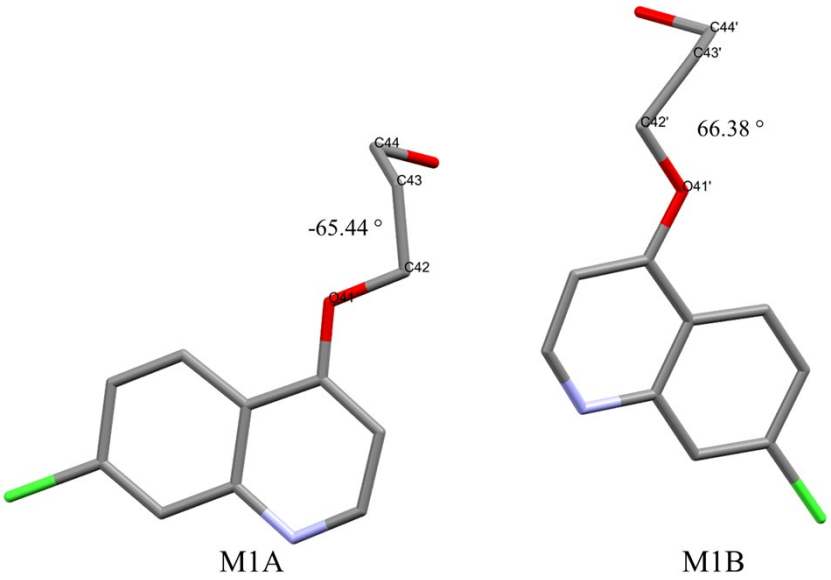


Figure S6. Asymmetric unit molecules for compound **5**. Torsion angles of -65.44 ° (M1A) and 66.38 ° (M1B) between atoms C44-C43-C42-O41 and C44'-C43'-C42'-O41', respectively.

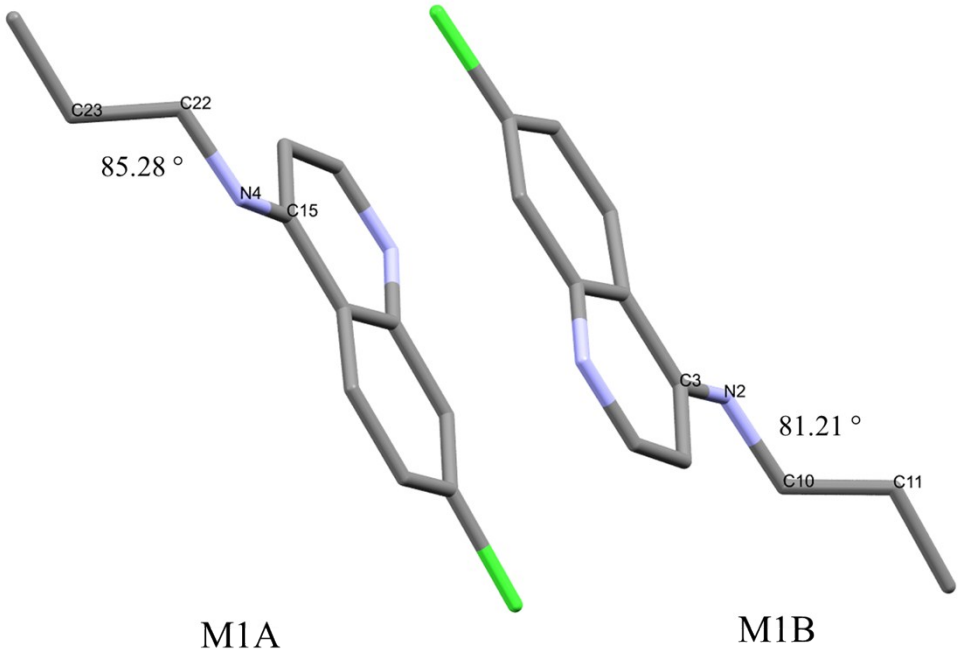


Figure S7. Asymmetric unit molecules for compound **6**. Torsions of 85.28 ° (M1A) e 81.21 ° (M1B) between the atoms C15-N4-C22-C23 and C3-N2-C10-C11, respectively.

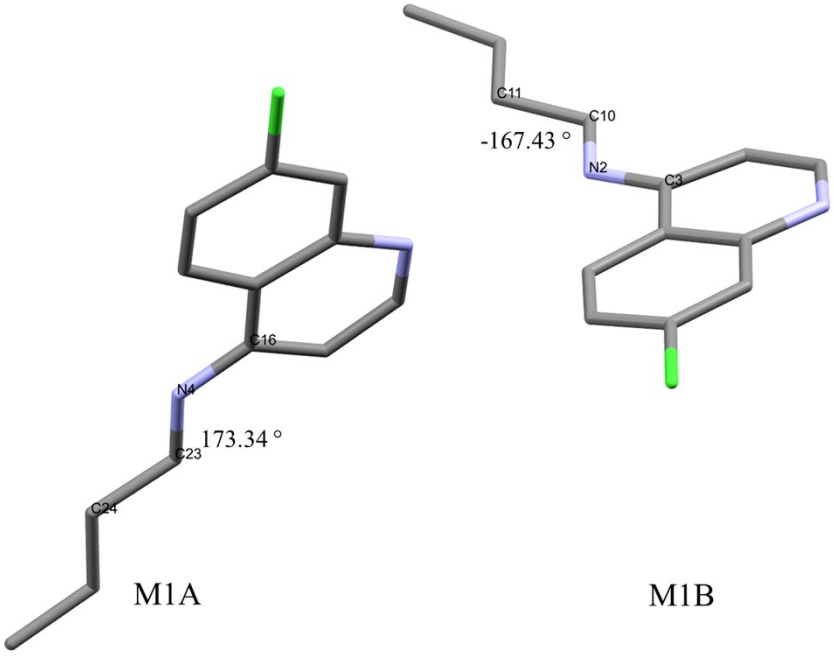


Figure S8. Asymmetric unit molecules for compound **7**. Torsions of 173.34 ° (M1A) and -167.43 ° (M1B) between the atoms C16-N4-C23-C24 and C3-N2-C10-C11 respectively.

4. Symmetry codes for the supramolecular clusters

Table S2. Symmetry codes of the molecules that compose the supramolecular cluster of compounds **1**, **2** and **3.**

Molecule	Symmetry Code		
	1	**2**	**3**
M1	x,y,z	x,y,z	x,y,z
M2	-1+x,y,z	-1+x,y,z	-1+x,y,z
M3	1+x,y,z	1+x,y,z	1+x,y,z
M4	1-x,-y,-z	2-x,-y,-z	-0.5+x,0.5-y,1-z
M5	2-x,-y,-z	1-x,1-y,-z	0.5+x,0.5-y,1-z
M6	1-x,1-y,-z	2-x,1-y,-z	-0.5+x,1.5-y,1-z
M7	2-x,1-y,-z	1-x,2-y,-z	0.5+x,1.5-y,1-z
M8	-1+x,1+y,z	-1+x,1+y,z	-1+x,1+y,z
M9	x,1+y,z	x,1+y,z	x,1+y,z
M10	0.5-x,0.5+y,0.5-z	0.5-x,0.5+y,0.5-z	-x,0.5+y,1.5-z
M11	1.5-x,0.5+y,0.5-z	1.5-x,0.5+y,0.5-z	1-x,0.5+y,1.5-z
M12	0.5-x,-0.5+y,0.5-z	0.5-x,-0.5+y,0.5-z	-x,-0.5+y,1.5-z
M13	1.5-x,-0.5+y,0.5-z	1.5-x,-0.5+y,0.5-z	1-x,-0.5+y,1.5-z
M14	x,-1+y,z	x,-1+y,z	x,-1+y,z
M15	1+x,-1+y,z	1+x,-1+y,z	1+x,-1+y,z

Table S3. Symmetry codes of the molecules that compose the supramolecular cluster of compounds **4 (M1A**,**M1B)** and **5 (M1A, M1B)**.

Molecule	Symmetry Code			
	4M1A	**4M1B**	**5M1A**	**5M1B**
M1	x,y,z	x,y,z	x,y,z	x,y,z
M2	-1+x,y,z	1+x,y,z	x,1+y,z	x,-1+y,z
M3	1+x,y,z	-1+x,y,z	x,-1+y,z	x,1+y,z
M4	-1+x,y,z	2+x,y,1+z	1.5-x,0.5+y,0.5+z	1.5-x,-0.5+y,-0.5+z
M5	x,y,z	1+x,y,1+z	1.5-x,-0.5+y,0.5+z	1.5-x,0.5+y,-0.5+z
M6	1+x,y,z	x,y,1+z	1-x,1-y,0.5+z	1-x,-y,-0.5+z
M7	-2+x,y,-1+z	1+x,y,z	1-x,-y,0.5+z	1-x,1-y,-0.5+z
M8	-1+x,y,-1+z	x,y,z	-0.5+x,1.5-y,z	-0.5+x,0.5-y,z
M9	x,y,-1+z	-1+x,y,z	-0.5+x,0.5-y,z	-0.5+x,1.5-y,z
M10	-x,0.5+y,1-z	-1+x,y,-1+z	x,1+y,z	-0.5+x,0.5-y,z
M11	1-x,0.5+y,1-z	-2+x,y,-1+z	x,y,z	-0.5+x,1.5-y,z
M12	1-x,0.5+y,2-z	x,y,-1+z	0.5+x,1.5-y,z	x,-1+y,z
M13	2-x,0.5+y,2-z	-1+x,y,-1+z	0.5+x,0.5-y,z	x,y,z
M14	x,y,1+z	-2+x,y,-1+z	0.5+x,1.5-y,z	0.5+x,0.5-y,z
M15	1+x,y,1+z	1-x,-0.5+y,1-z	0.5+x,0.5-y,z	0.5+x,1.5-y,z
M16	2+x,y,1+z	-x,-0.5+y,1-z	-	-
M17	1+x,y,1+z	2-x,-0.5+y,2-z	-	-
M18	2+x,y,1+z	1-x,-0.5+y,2-z	-	-

Table S4. Symmetry codes of the molecules that compose the supramolecular cluster of compound **6** dimeric nuclei.

Dimer	Symmetry Code	
	6	
D1	x,y,z	x,y,z
D2	-1+x,y,z	-1+x,y,z
D3	1+x,y,z	1+x,y,z
D4	1-x,0.5+y,1.5-z	1-x,0.5+y,1.5-z
D5	2-x,0.5+y,1.5-z	2-x,0.5+y,1.5-z
D6	-1+x,0.5-y,0.5+z	-1+x,0.5-y,0.5+z
D7	x,0.5-y,0.5+z	x,0.5-y,0.5+z
D8	1+x,0.5-y,0.5+z	1+x,0.5-y,0.5+z
D9	1-x,-0.5+y,1.5-z	1-x,-0.5+y,1.5-z
D10	2-x,-0.5+y,1.5-z	2-x,-0.5+y,1.5-z
D11	1-x,-y,1-z	1-x,-y,1-z
D12	2-x,-y,1-z	2-x,-y,1-z
D13	-1+x,0.5-y,-0.5+z	-1+x,0.5-y,-0.5+z
D14	x,0.5-y,-0.5+z	x,0.5-y,-0.5+z
D15	1+x,0.5-y,-0.5+z	1+x,0.5-y,-0.5+z
D16	2-x,1-y,1-z	2-x,1-y,1-z
D17	3-x,1-y,1-z	3-x,1-y,1-z

Table S5. Symmetry codes of the molecules that compose the supramolecular cluster of compounds **7 (7M1A, 7M1B)** and **8**.

Molecule	Symmetry Code		
	7M1A	**7M1B**	**8**
M1	x,y,z	x,y,z	x,y,z
M2	1-x,-y,1-z	-0.5+x,y,1.5-z	1+x,y,z
M3	2-x,-y,1-z	0.5+x,y,1.5-z	-1+x,y,z
M4	1.5-x,-0.5+y,z	1-x,-0.5+y,1.5-z	3-x,1-y,2-z
M5	1-x,-y,1-z	1.5-x,-0.5+y,z	2-x,1-y,2-z
M6	1.5-x,-y,-0.5+z	-1+x,y,z	1.5-x,0.5+y,1.5-z
M7	2-x,-y,1-z	1-x,-y,1-z	0.5-x,0.5+y,1.5-z
M8	2.5-x,-y,-0.5+z	x,y,z	1-x,1-y,1-z
M9	0.5+x,0.5-y,1-z	2-x,-y,1-z	-x,1-y,1-z
M10	1+x,0.5-y,-0.5+z	-1.5+x,0.5-y,1-z	-1-x,1-y,1-z
M11	1.5+x,0.5-y,1-z	0.5-x,0.5+y,z	-0.5+x,0.5-y,-0.5+z
M12	-0.5+x,0.5-y,1-z	-0.5+x,0.5-y,1-z	-1.5+x,0.5-y,-0.5+z
M13	1.5-x,0.5+y,z	1-x,0.5+y,1.5-z	1.5-x,-0.5+y,1.5-z
M14	0.5+x,0.5-y,1-z	1.5-x,0.5+y,z	0.5-x,-0.5+y,1.5-z
M15	-0.5+x,y,1.5-z	-1+x,0.5-y,0.5+z	1.5+x,0.5-y,0.5+z
M16	x,y,z	-0.5+x,y,1.5-z	0.5+x,0.5-y,0.5+z
M17	0.5+x,y,1.5-z	1.5-x,-y,0.5+z	-
M18	1+x,y,z	0.5+x,y,1.5-z	-
M19	0.5-x,-0.5+y,z	2.5-x,-y,0.5+z	-

Table S6. Symmetry codes of the molecules that compose the supramolecular cluster of compounds **9** and **10**.

Molecule	Symmetry Code	
	9	**10**
M1	x,y,z	x,y,z
M2	2-x,0.5+y,-z	-1+x,y,z
M3	x,1+y,z	1+x,y,z
M4	2-x,-0.5+y,-z	-1.5+x,-0.5+y,z
M5	x,-1+y,z	-0.5+x,-0.5+y,z
M6	2-x,0.5+y,1-z	-1+x,1-y,-0.5+z
M7	x,y,1+z	x,1-y,-0.5+z
M8	2-x,-0.5+y,1-z	1+x,1-y,-0.5+z
M9	1-x,0.5+y,-z	-0.5+x,1.5-y,-0.5+z
M10	-1+x,y,z	0.5+x,1.5-y,-0.5+z
M11	1-x,-0.5+y,-z	0.5+x,0.5+y,z
M12	1-x,0.5+y,-1-z	1.5+x,0.5+y,z
M13	-1+x,y,-1+z	-0.5+x,1.5-y,0.5+z
M14	1-x,-0.5+y,-1-z	0.5+x,1.5-y,0.5+z
M15	x,y,-1+z	-1+x,1-y,0.5+z
M16	1+x,y,z	x,1-y,0.5+z
M17	1+x,y,1+z	1+x,1-y,0.5+z

Table S7. Symmetry codes of the molecules that compose the supramolecular cluster of compounds **11** and **12** dimeric nuclei.

Dimer	Symmetry Code			
	11		**12**	
D1	x,y,z	0.5-x,0.5-y,0.5-z	x,y,z	0.5-x,0.5-y,0.5-z
D2	0.5-x,-0.5+y,z	x,-y,0.5-z	0.5-x,-0.5+y,z	x,-y,0.5-z
D3	x,1-y,0.5-z	0.5-x,0.5+y,z	x,1-y,0.5-z	0.5-x,0.5+y,z
D4	0.5+x,-y,z	1-x,-0.5+y,0.5-z	0.5+x,-y,z	1-x,-0.5+y,0.5-z
D5	1-x,0.5-y,z	0.5+x,y,0.5-z	1-x,0.5-y,z	0.5+x,y,0.5-z
D6	0.5+x,1-y,z	1-x,0.5+y,0.5-z	0.5+x,1-y,z	1-x,0.5+y,0.5-z
D7	1-x,1.5-y,z	0.5+x,1+y,0.5-z	1-x,1.5-y,z	0.5+x,1+y,0.5-z
D8	1.5-x,y,-z	1+x,0.5-y,-0.5+z	1.5-x,y,-z	1+x,0.5-y,-0.5+z
D9	1-x,1-y,-z	0.5+x,0.5+y,-0.5+z	0.5+x,0.5+y,-0.5+z	1-x,1-y,-z
D10	0.5-x,1-y,-0.5+z	x,0.5+y,-z	0.5-x,1-y,-0.5+z	x,0.5+y,-z
D11	0.5-x,y,-z	x,0.5-y,-0.5+z	x,0.5-y,-0.5+z	0.5-x,y,-z
D12	0.5-x,-y,-0.5+z	x,-0.5+y,-z	x,-0.5+y,-z	0.5-x,-y,-0.5+z
D13	-x,0.5+y,0.5-z	-0.5+x,1-y,z	-0.5+x,1-y,z	-x,0.5+y,0.5-z
D14	-0.5+x,y,0.5-z	-x,0.5-y,z	-0.5+x,y,0.5-z	-x,0.5-y,z
D15	-x,-0.5+y,0.5-z	-0.5+x,-y,z	-0.5+x,-y,z	-x,-0.5+y,0.5-z
D16	-0.5+x,-1+y,0.5-z	-x,-0.5-y,z	-x,-0.5-y,z	-0.5+x,-1+y,0.5-z
D17	0.5-x,-y,0.5+z	x,-0.5+y,1-z	0.5-x,-y,0.5+z	x,-0.5+y,1-z
D18	x,0.5-y,0.5+z	0.5-x,y,1-z	x,0.5-y,0.5+z	0.5-x,y,1-z
D19	x,0.5+y,1-z	0.5-x,1-y,0.5+z	0.5-x,1-y,0.5+z	x,0.5+y,1-z
D20	-0.5-x,y,1-z	-1+x,0.5-y,0.5+z	-0.5-x,y,1-z	-1+x,0.5-y,0.5+z
D21	-0.5+x,-0.5+y,0.5+z	-x,-y,1-z	-0.5+x,-0.5+y,0.5+z	-x,-y,1-z

Table S8. Symmetry codes of the molecules that compose the supramolecular cluster of compound **13** dimeric nuclei.

Dimer	Symmetry Code	
	13	
D1	x,y,z	1-x,1-y,1-z
D2	1-x,2-y,1-z	x,1+y,z
D3	1-x,-y,1-z	x,-1+y,z
D4	1+x,y,z	2-x,1-y,1-z
D5	2-x,-y,1-z	1+x,-1+y,z
D6	2-x,0.5+y,1.5-z	1+x,1.5-y,0.5+z
D7	2-x,-0.5+y,1.5-z	1+x,0.5-y,0.5+z
D8	1-x,0.5+y,1.5-z	x,1.5-y,0.5+z
D9	1-x,-0.5+y,1.5-z	x,0.5-y,0.5+z
D10	-x,0.5+y,1.5-z	-1+x,1.5-y,0.5+z
D11	-x,-0.5+y,1.5-z	-1+x,0.5-y,0.5+z
D12	-x,2-y,1-z	-1+x,1+y,z
D13	-x,1-y,1-z	-1+x,y,z
D14	-1+x,1.5-y,-0.5+z	-x,0.5+y,0.5-z
D15	-x,-0.5+y,0.5-z	-1+x,0.5-y,-0.5+z
D16	x,1.5-y,-0.5+z	1-x,0.5+y,0.5-z
D17	x,0.5-y,-0.5+z	1-x,-0.5+y,0.5-z
D18	2-x,0.5+y,0.5-z	1+x,1.5-y,-0.5+z
D19	2-x,-0.5+y,0.5-z	1+x,0.5-y,-0.5+z

Table S9. Symmetry codes of the molecules that compose the supramolecular cluster of compound **14**.

Molecule	Symmetry Code
	14
M1	x,y,z
M2	1+x,y,z
M3	-1+x,y,z
M4	2-x,-y,1-z
M5	1-x,-y,1-z
M6	1+x,0.5-y,0.5+z
M7	x,0.5-y,0.5+z
M8	2-x,0.5+y,0.5-z
M9	1-x,0.5+y,0.5-z
M10	x,0.5-y,-0.5+z
M11	-1+x,0.5-y,-0.5+z
M12	1-x,-y,-z
M13	-x,-y,-z
M14	2-x,-0.5+y,0.5-z
M15	1-x,-0.5+y,0.5-z
M16	1+x,y,z
M17	x,y,z
M18	x,0.5-y,-0.5+z
M19	1-x,-0.5+y,0.5-z

5. Contact area and stabilization energy data

Observation: Hydrogen atoms are omitted for clarity. Legend for all tables: [a]Å^2, contact area obtained by ToposPro. [b] kcal mol^{-1}, interaction energy using the equation $G_{M1\cdots MN} = G_{M1+MN} - (G_{M1} + G_{MN})$. [c] Determined using the equation $NC_{M1\cdots MN} = (MCN \times C_{M1\cdots MN})/ C_{Cluster.}$ [d] Determined using the equation $NG_{M1\cdots MN} = (MCN \times G_{M1\cdots MN})/ G_{Cluster.}$

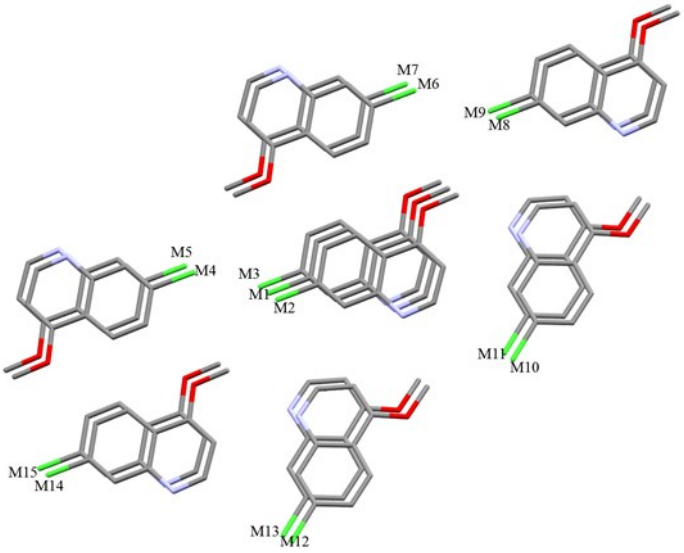


Figure S9. Supramolecular cluster of compound **1**.

Table S10. Contact area and energetic data of each dimer from the supramolecular cluster of compound **1**.

Dimer	$C_{M1\cdots MN}$[a] (Å^2)	$G_{M1\cdots MN}$[b] (kcal mol^{-1})	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]
M1···M2	39.34	-8.61	2.31	2.52
M1···M3	39.34	-8.61	2.31	2.52
M1···M4	0.52	-0.08	0.03	0.02
M1···M5	4.7	-0.04	0.28	0.01
M1···M6	31.3	-4.97	1.84	1.46
M1···M7	24.22	-3.53	1.42	1.03
M1···M8	4.04	-1.22	0.24	0.36
M1···M9	6.61	-1.37	0.39	0.40
M1···M10	21.11	-4.34	1.24	1.27
M1···M11	17.71	-4.04	1.04	1.18
M1···M12	21.11	-4.34	1.24	1.27
M1···M13	17.71	-4.04	1.04	1.18
M1···M14	6.61	-1.37	0.39	0.40
M1···M15	4.04	-1.22	0.24	0.36
Total	238.36	-47.80	14.00	14.00

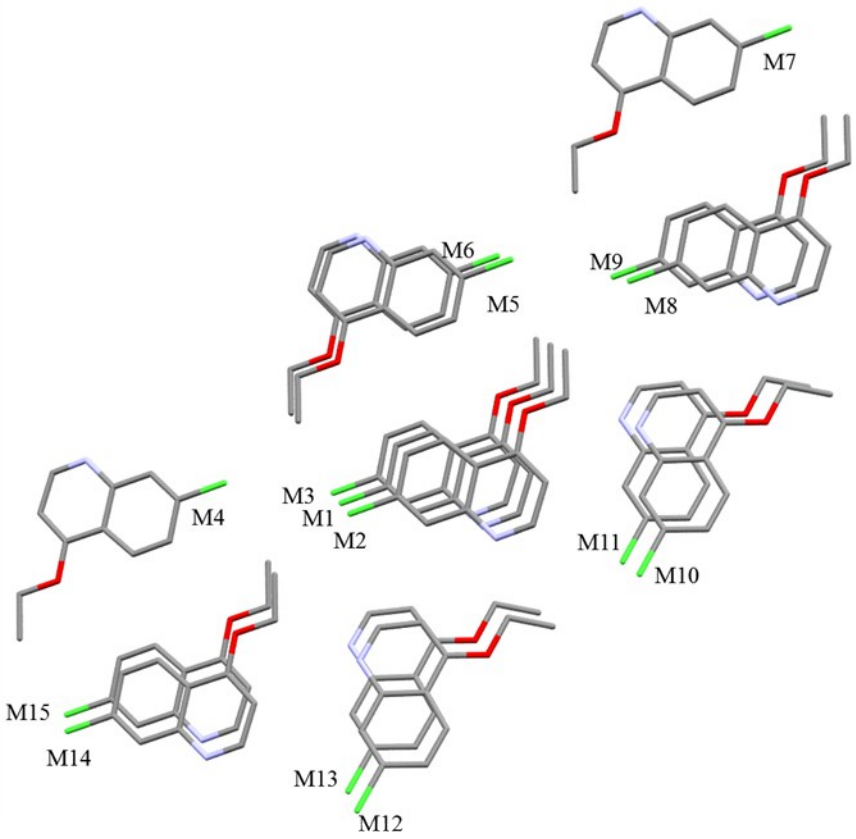


Figure S10. Supramolecular cluster of compound **2**.

Table S11. Contact area and energetic data of each dimer from the supramolecular cluster of compound **2**.

Dimer	$C_{M1\cdots MN}$[a] (Å^2)	$G_{M1\cdots MN}$[b] (kcal mol^{-1})	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]
M1···M2	46.36	-9.38	2.42	2.68
M1···M3	46.36	-9.38	2.42	2.68
M1···M4	2.04	-0.22	0.11	0.06
M1···M5	28.15	-4.44	1.47	1.27
M1···M6	36.98	-4.08	1.93	1.16
M1···M7	1.29	0.05	0.07	-0.01
M1···M8	5.07	-1.09	0.26	0.31
M1···M9	7.77	-1.10	0.41	0.31
M1···M10	22.06	-4.16	1.15	1.19
M1···M11	18.77	-4.44	0.98	1.27
M1···M12	22.06	-4.16	1.15	1.19
M1···M13	18.77	-4.44	0.98	1.27
M1···M14	7.77	-1.10	0.41	0.31
M1···M15	5.07	-1.09	0.26	0.31
Total	268.52	-49.05	14.00	14.00

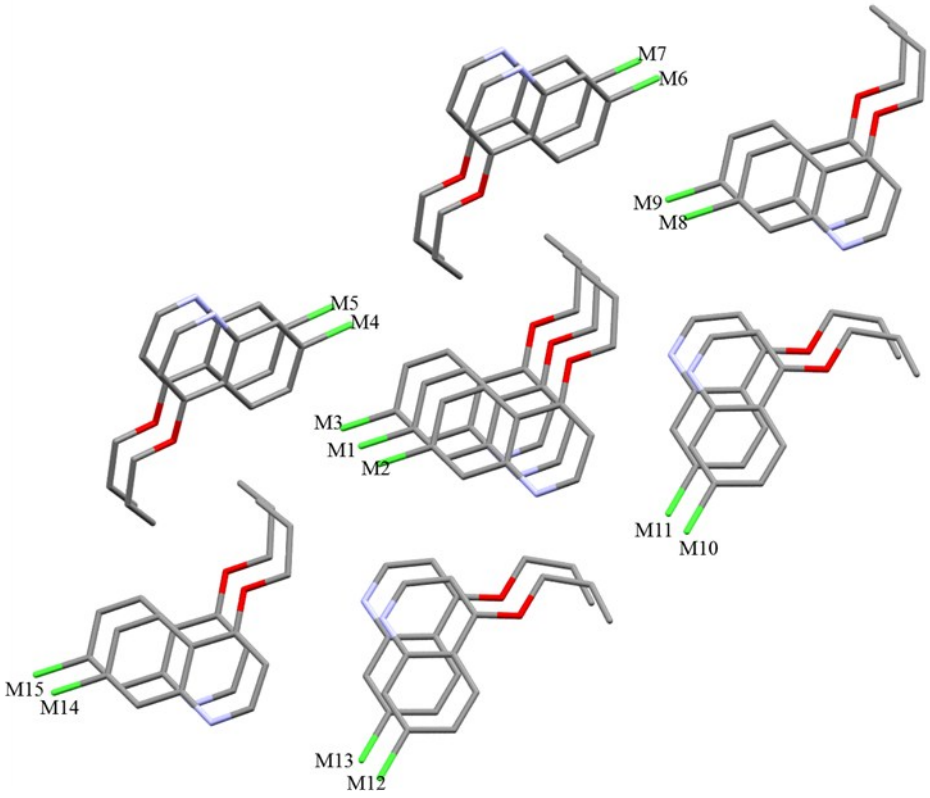


Figure S11. Supramolecular cluster of compound **3**.

Table S12. Contact area and energetic data of each dimer from the supramolecular cluster of compound **3**.

Dimer	$C_{M1\cdots MN}$[a] (Å^2)	$G_{M1\cdots MN}$[b] (kcal mol^{-1})	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]
M1···M2	48.01	-10.59	2.46	2.72
M1···M3	48.01	-10.59	2.46	2.72
M1···M4	11.01	-1.93	0.56	0.50
M1···M5	11.01	-1.93	0.56	0.50
M1···M6	25.24	-3.23	1.29	0.83
M1···M7	25.24	-3.23	1.29	0.83
M1···M8	3.52	-1.06	0.18	0.27
M1···M9	7.63	-1.16	0.39	0.30
M1···M10	22.12	-4.55	1.13	1.17
M1···M11	19.05	-4.75	0.98	1.22
M1···M12	22.12	-4.55	1.13	1.17
M1···M13	19.05	-4.75	0.98	1.22
M1···M14	7.63	-1.16	0.39	0.30
M1···M15	3.52	-1.06	0.18	0.27
Total	273.16	-54.57	14.00	14.00

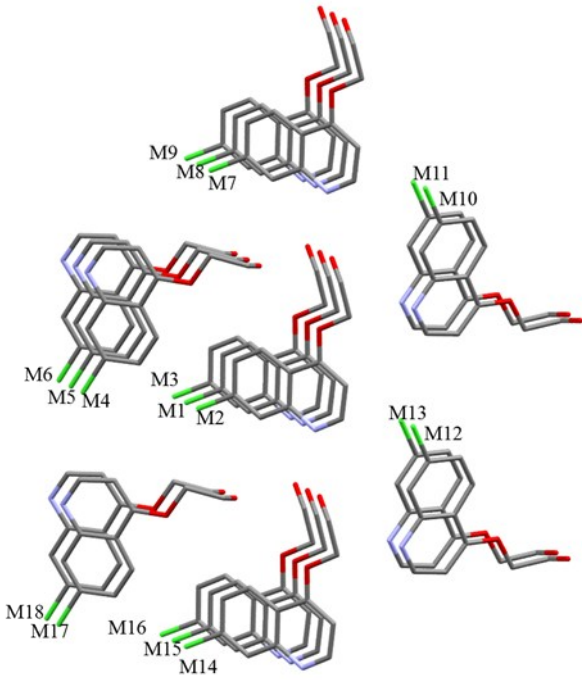


Figure S12. Supramolecular cluster of compound **4** considering **M1A**.

Table S13. Contact area and energetic data of each dimer from the supramolecular cluster of compound **4** considering **M1A**.

Dimer	$C_{M1\cdots MN}$[a] (Å^2)	$G_{M1\cdots MN}$[b] (kcal mol^{-1})	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]
M1···M2	47.64	-11.22	2.93	2.90
M1···M3	47.64	-11.22	2.93	2.90
M1···M4	3.29	0.24	0.20	-0.06
M1···M5	35.98	-7.03	2.21	1.82
M1···M6	22.61	-2.74	1.39	0.71
M1···M7	0.07	-1.18	0.00	0.30
M1···M8	14.03	-6.24	0.86	1.61
M1···M9	2.85	0.06	0.18	-0.02
M1···M10	19.68	-4.74	1.21	1.22
M1···M11	18.18	-4.63	1.12	1.20
M1···M12	10.85	-1.94	0.67	0.50
M1···M13	8.37	-0.71	0.51	0.18
M1···M14	2.85	0.06	0.18	-0.02
M1···M15	14.03	-6.24	0.86	1.61
M1···M16	0.07	-1.18	0.00	0.30
M1···M17	17.51	-4.78	1.08	1.24
M1···M18	10.66	-2.30	0.66	0.59
Total	276.31	-65.78	17.00	17.00

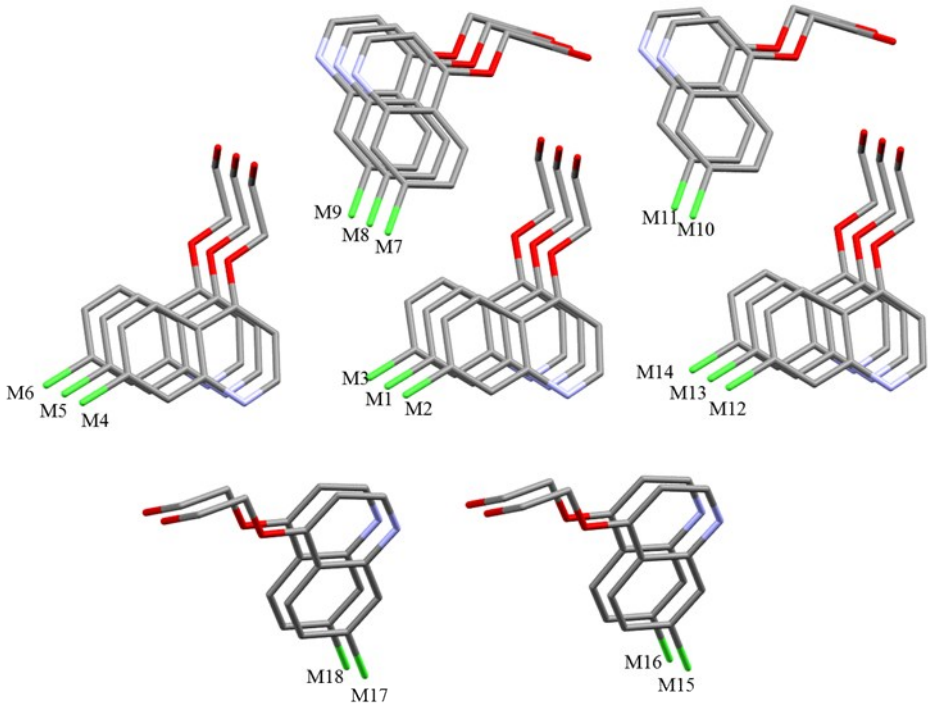


Figure S13. Supramolecular cluster of compound **4** considering **M1B**.

Table S14. Contact area and energetic data of each dimer from the supramolecular cluster of compound **4** considering **M1B**.

Dimer	$C_{M1\cdots MN}$[a] (Å^2)	$G_{M1\cdots MN}$[b] (kcal mol^{-1})	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]
M1···M2	49.64	-8.89	3.01	3.14
M1···M3	49.64	-8.89	3.01	3.14
M1···M4	0.6	-0.27	0.04	0.10
M1···M5	16.31	-0.68	0.99	0.24
M1···M6	0.03	0.07	0.00	-0.03
M1···M7	3.29	0.24	0.20	-0.08
M1···M8	35.98	-7.03	2.18	2.48
M1···M9	22.61	-2.74	1.37	0.97
M1···M10	17.51	-4.78	1.06	1.69
M1···M11	10.66	-2.30	0.65	0.81
M1···M12	0.03	0.07	0.00	-0.03
M1···M13	16.31	-0.68	0.99	0.24
M1···M14	0.6	-0.27	0.04	0.10
M1···M15	18.18	-4.63	1.10	1.64
M1···M16	19.68	-4.74	1.19	1.67
M1···M17	8.37	-0.71	0.51	0.25
M1···M18	10.85	-1.94	0.66	0.69
Total	280.29	-48.17	17.00	17.00

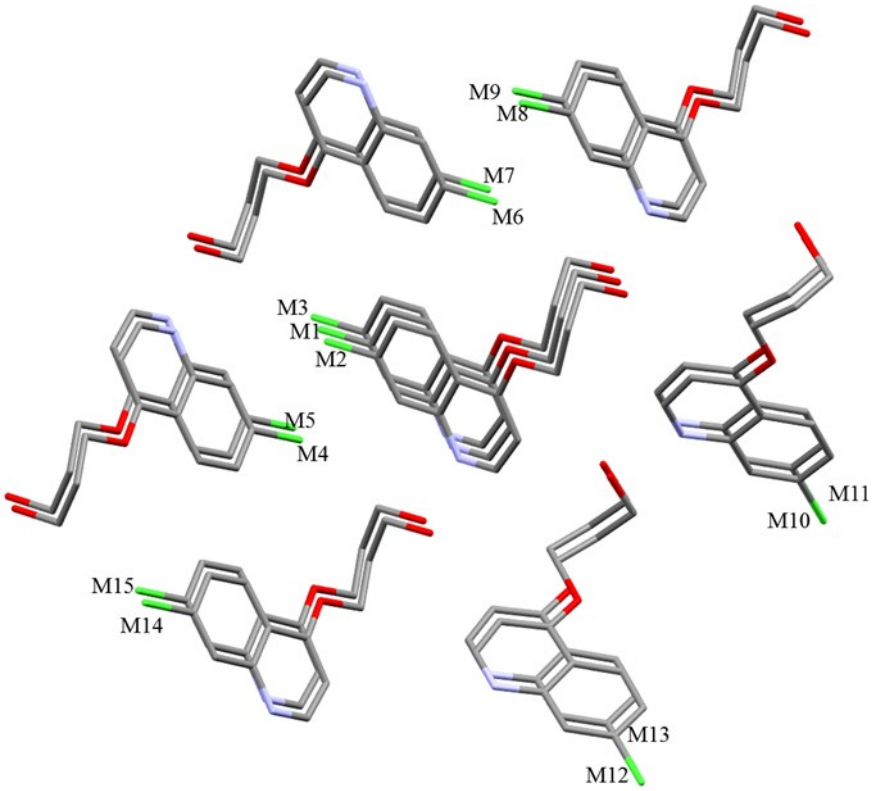


Figure S14. Supramolecular cluster of compound **5** considering **M1A**.

Table S15. Contact area and energetic data of each dimer from the supramolecular cluster of compound **5** considering **M1A**.

Dimer	$C_{M1\cdots MN}$[a] (Å^2)	$G_{M1\cdots MN}$[b] (kcal mol^{-1})	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]
M1···M2	47.84	-9.17	2.26	2.19
M1···M3	47.84	-9.17	2.26	2.19
M1···M4	11.97	-0.75	0.57	0.18
M1···M5	11.72	-0.83	0.55	0.20
M1···M6	40.64	-5.46	1.92	1.30
M1···M7	20.28	-4.37	0.96	1.04
M1···M8	11.84	-3.00	0.56	0.72
M1···M9	17.82	-6.22	0.84	1.49
M1···M10	9.63	-1.29	0.46	0.31
M1···M11	19.13	-3.49	0.90	0.83
M1···M12	22.66	-3.69	1.07	0.88
M1···M13	5.22	-1.96	0.25	0.47
M1···M14	11.84	-3.00	0.56	0.72
M1···M15	17.82	-6.22	0.84	1.49
Total	296.25	-58.63	14.00	14.00

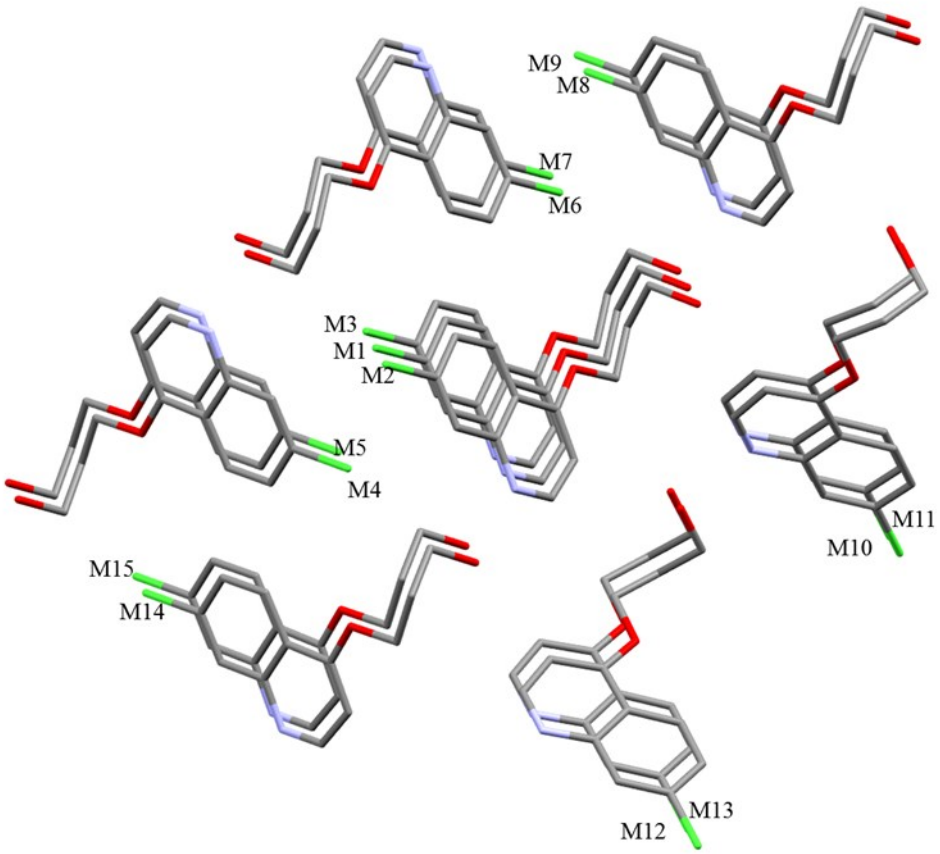


Figure S15. Supramolecular cluster of compound **5** considering **M1B**.

Table S16. Contact area and energetic data of each dimer from the supramolecular cluster of compound **5** considering **M1B**.

Dimer	$C_{M1\cdots MN}$[a] (Å^2)	$G_{M1\cdots MN}$[b] (kcal mol^{-1})	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]
M1···M2	48.47	-9.32	2.29	2.22
M1···M3	48.47	-9.32	2.29	2.22
M1···M4	11.97	-0.75	0.57	0.18
M1···M5	11.72	-0.83	0.55	0.20
M1···M6	20.28	-4.37	0.96	1.04
M1···M7	40.64	-5.46	1.92	1.30
M1···M8	18.08	-6.17	0.85	1.47
M1···M9	11.02	-3.01	0.52	0.72
M1···M10	5.22	-1.96	0.25	0.47
M1···M11	22.66	-3.69	1.07	0.88
M1···M12	9.63	-1.29	0.45	0.31
M1···M13	19.13	-3.49	0.90	0.83
M1···M14	18.08	-6.17	0.85	1.47
M1···M15	11.02	-3.01	0.52	0.72
Total	296.39	-58.84	14.00	14.00

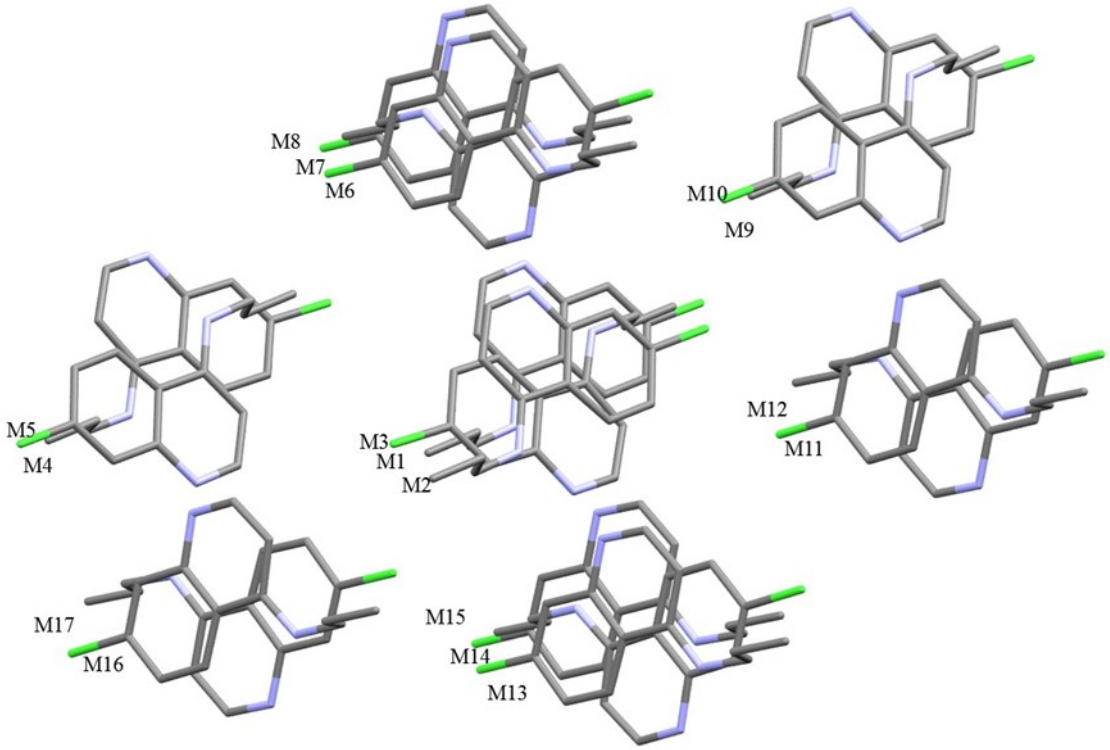


Figure S16. Supramolecular cluster of compound **6** considering **M1A**.

Table S17. Contact area and energetic data of each dimer from the supramolecular cluster of compound **6** considering **M1A**.

Dimer	$C_{M1\cdots MN}$[a] (Å^2)	$G_{M1\cdots MN}$[b] (kcal mol^{-1})	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]
M1···M2	56.79	-14.42	3.01	3.69
M1···M3	52.44	-11.00	2.78	2.82
M1···M4	17.48	-2.90	0.93	0.74
M1···M5	1.05	-1.59	0.06	0.41
M1···M6	12.67	-2.20	0.67	0.56
M1···M7	24.71	-9.82	1.31	2.52
M1···M8	13.26	-0.42	0.70	0.11
M1···M9	12.49	-1.99	0.66	0.51
M1···M10	8.67	-0.66	0.46	0.17
M1···M11	12.85	-1.90	0.68	0.49
M1···M12	13.63	-0.69	0.72	0.18
M1···M13	7.03	-0.11	0.37	0.03
M1···M14	24.71	-9.82	1.31	2.52
M1···M15	23.39	-2.58	1.24	0.66
M1···M16	12.85	-1.90	0.68	0.49
M1···M17	8.09	-0.47	0.43	0.12
Total	302.11	-62.47	16.00	16.00

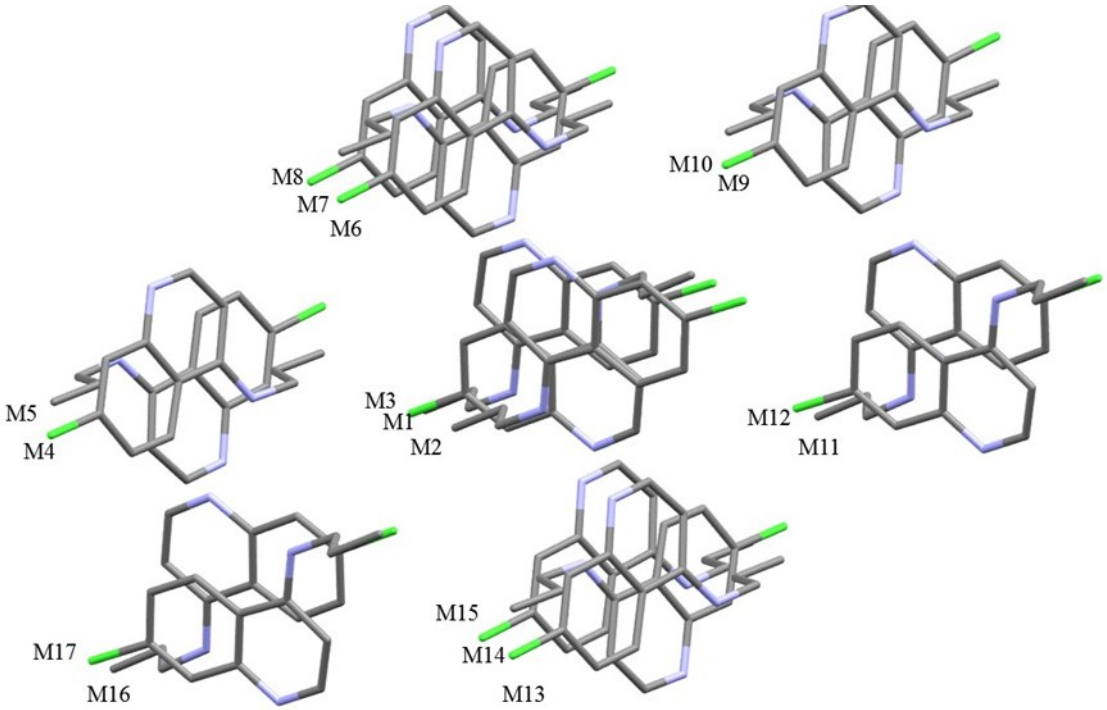


Figure S17. Supramolecular cluster of compound **6** considering **M1B**.

Table S18. Contact area and energetic data of each dimer from the supramolecular cluster of compound **6** considering **M1B**.

Dimer	$C_{M1\cdots MN}$[a] (Å^2)	$G_{M1\cdots MN}$[b] (kcal mol^{-1})	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]
M1···M2	52.44	-11.00	2.78	2.91
M1···M3	56.79	-14.42	3.01	3.82
M1···M4	12.67	-1.76	0.67	0.47
M1···M5	8.09	-0.47	0.43	0.12
M1···M6	13.26	-0.42	0.70	0.11
M1···M7	23.68	-10.09	1.25	2.67
M1···M8	12.67	-2.20	0.67	0.58
M1···M9	12.67	-1.76	0.67	0.47
M1···M10	13.63	-0.69	0.72	0.18
M1···M11	17.48	-1.51	0.93	0.40
M1···M12	10.38	-1.29	0.55	0.34
M1···M13	23.39	-2.58	1.24	0.68
M1···M14	23.68	-10.09	1.25	2.67
M1···M15	7.03	-0.11	0.37	0.03
M1···M16	12.49	-1.99	0.66	0.53
M1···M17	1.75	-0.04	0.09	0.01
Total	302.10	-60.42	16.00	16.00

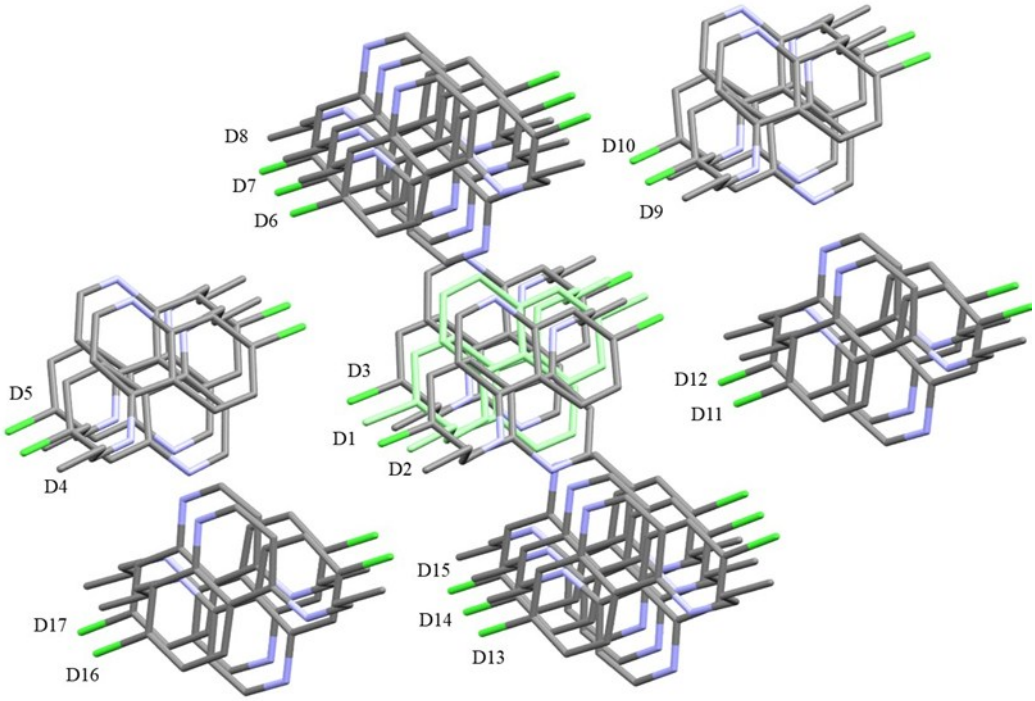


Figure S18. Supramolecular cluster of compound **6** considering M1A and M1B as D1. D1 dimeric nuclei was highlighted.

Table S19. Contact area and energetic data of each dimer from the supramolecular cluster of compound **6**.

Dimer	$C_{M1\cdots MN}$[a] (Å^2)	$G_{M1\cdots MN}$[b] (kcal mol^{-1})	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]
D1···D2	52.44	-11.23	1.71	1.83
D1···D3	52.44	-11.23	1.71	1.83
D1···D4	12.67	-2.22	0.41	0.36
D1···D5	34.57	-3.09	1.13	0.50
D1···D6	13.26	-2.60	0.43	0.42
D1···D7	68.1	-22.81	2.22	3.71
D1···D8	23.39	-2.60	0.76	0.42
D1···D9	12.67	-2.22	0.41	0.36
D1···D10	34.57	-3.09	1.13	0.50
D1···D11	45.34	-4.24	1.48	0.69
D1···D12	1.05	-1.13	0.03	0.18
D1···D13	23.39	-2.60	0.76	0.42
D1···D14	68.1	-22.81	2.22	3.71
D1···D15	13.26	-1.06	0.43	0.17
D1···D16	26.74	-4.49	0.87	0.73
D1···D17	8.67	-0.83	0.28	0.14
Total	490.66	-98.28	16.00	16.00

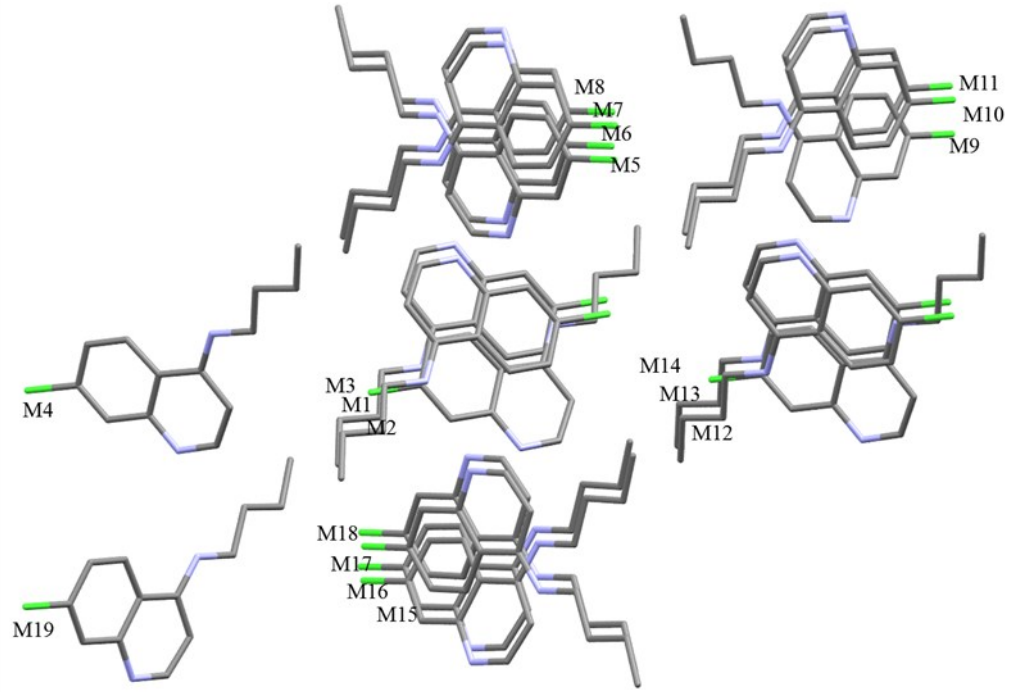


Figure S19. Supramolecular cluster of compound **7** considering **M1A**.

Table S20. Contact area and energetic data of each dimer from the supramolecular cluster of compound **7** considering **M1A**.

Dimer	$C_{M1\cdots MN}$[a] (Å^2)	$G_{M1\cdots MN}$[b] (kcal mol^{-1})	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]
M1···M2	41.61	-11.17	2.32	3.15
M1···M3	52.74	-11.81	2.94	3.33
M1···M4	10.92	-1.90	0.61	0.54
M1···M5	14	-1.85	0.78	0.52
M1···M6	26.04	-9.69	1.45	2.73
M1···M7	18.06	-2.22	1.01	0.62
M1···M8	7.47	-0.89	0.42	0.25
M1···M9	21.25	-1.84	1.19	0.52
M1···M10	5.82	-0.23	0.32	0.06
M1···M11	4.47	-0.28	0.25	0.08
M1···M12	19.34	-2.19	1.08	0.62
M1···M13	10.92	-1.90	0.61	0.54
M1···M14	19.34	-2.19	1.08	0.62
M1···M15	11.7	-1.09	0.65	0.31
M1···M16	24.45	-9.47	1.36	2.67
M1···M17	19.31	-3.41	1.08	0.96
M1···M18	9.37	-1.07	0.52	0.30
M1···M19	5.78	-0.67	0.32	0.19
Total	322.59	-63.87	18.00	18.00

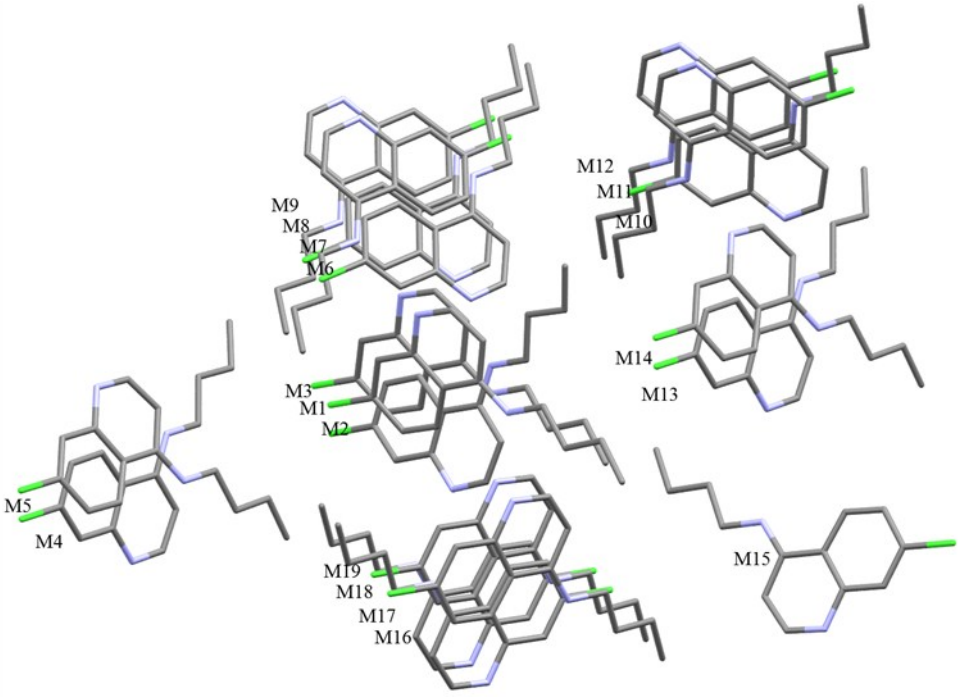


Figure S20. Supramolecular cluster of compound **7** considering **M1B**.

Table S21. Contact area and energetic data of each dimer from the supramolecular cluster of compound **7** considering **M1B**.

Dimer	$C_{M1\cdots MN}$[a] (Å^2)	$G_{M1\cdots MN}$[b] (kcal mol^{-1})	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]
M1···M2	52.51	-12.29	2.97	3.42
M1···M3	52.51	-12.29	2.97	3.42
M1···M4	14.79	-2.43	0.84	0.68
M1···M5	7.83	-1.27	0.44	0.35
M1···M6	9.37	-1.07	0.53	0.30
M1···M7	14	-1.85	0.79	0.51
M1···M8	24.45	-9.47	1.38	2.64
M1···M9	18.06	-2.22	1.02	0.62
M1···M10	4.47	-0.28	0.25	0.08
M1···M11	5.78	-0.67	0.33	0.19
M1···M12	21.25	-1.84	1.20	0.51
M1···M13	14.79	-2.43	0.84	0.68
M1···M14	7.83	-1.27	0.44	0.35
M1···M15	5.82	-0.23	0.33	0.06
M1···M16	19.31	-3.41	1.09	0.95
M1···M17	26.04	-9.69	1.47	2.70
M1···M18	11.7	-1.09	0.66	0.30
M1···M19	7.47	-0.89	0.42	0.25
Total	317.98	-64.69	18.00	18.00

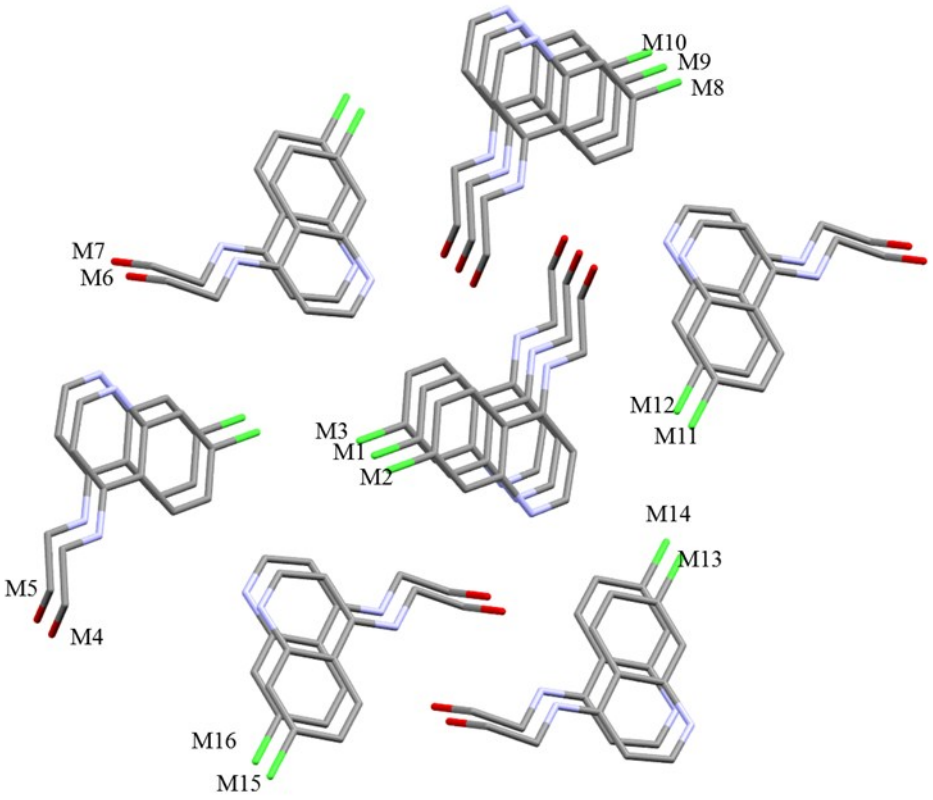


Figure S21. Supramolecular cluster of compound **8**.

Table S22. Contact area and energetic data of each dimer from the supramolecular cluster of compound **8**.

Dimer	$C_{M1\cdots MN}$[a] (Å^2)	$G_{M1\cdots MN}$[b] (kcal mol^{-1})	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]
M1···M2	44.75	-9.19	2.43	2.13
M1···M3	44.75	-9.19	2.43	2.13
M1···M4	0.99	0.01	0.05	0.00
M1···M5	8.03	-0.11	0.44	0.03
M1···M6	13.27	-3.12	0.72	0.72
M1···M7	11.36	-3.10	0.62	0.72
M1···M8	9.41	-1.10	0.51	0.25
M1···M9	28.99	-9.41	1.57	2.18
M1···M10	5.08	-0.20	0.28	0.05
M1···M11	23.32	-8.15	1.26	1.88
M1···M12	19.44	-3.45	1.05	0.80
M1···M13	13.27	-3.12	0.72	0.72
M1···M14	11.36	-3.10	0.62	0.72
M1···M15	19.44	-3.45	1.05	0.80
M1···M16	23.32	-8.15	1.26	1.88
Total	276.78	-64.82	15.00	15.00

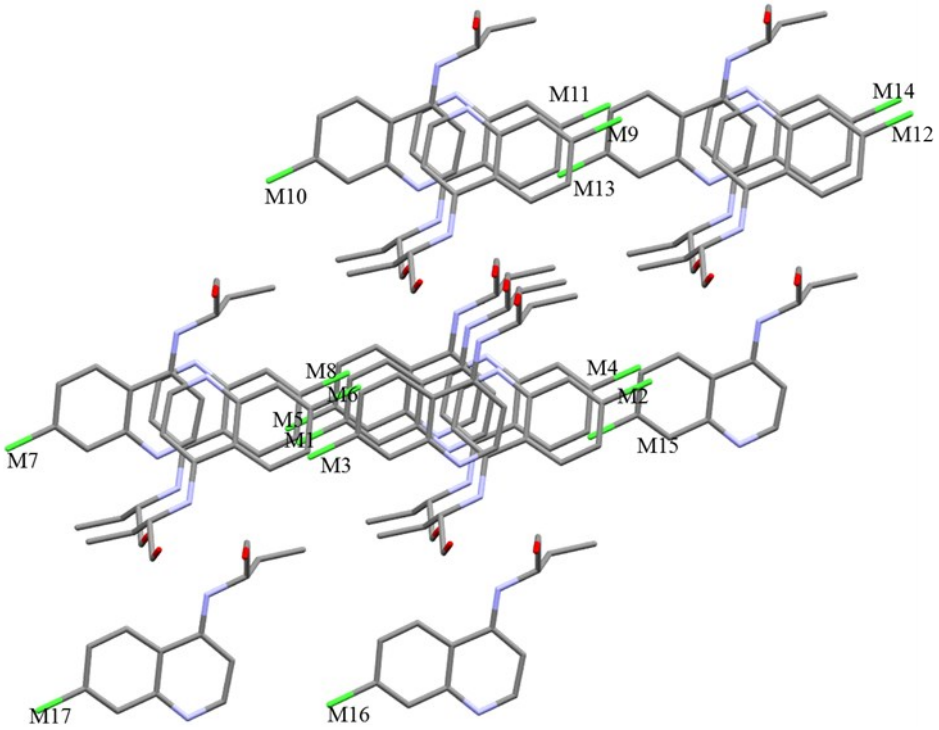


Figure S22. Supramolecular cluster of compound **9**.

Table S23. Contact area and energetic data of each dimer from the supramolecular cluster of compound **9**.

Dimer	$C_{M1\cdots MN}$[a] (Å^2)	$G_{M1\cdots MN}$[b] (kcal mol^{-1})	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]
M1···M2	49.51	-16.54	2.54	3.52
M1···M3	4.85	-1.46	0.25	0.31
M1···M4	49.51	-16.54	2.54	3.52
M1···M5	4.85	-1.46	0.25	0.31
M1···M6	16.81	-3.29	0.86	0.70
M1···M7	20.05	-1.60	1.03	0.34
M1···M8	16.81	-3.29	0.86	0.70
M1···M9	34.38	-9.40	1.76	2.00
M1···M10	8.47	-2.64	0.43	0.56
M1···M11	34.38	-9.40	1.76	2.00
M1···M12	10.25	-0.82	0.53	0.17
M1···M13	11.53	-1.85	0.59	0.39
M1···M14	10.25	-0.82	0.53	0.17
M1···M15	20.05	-1.60	1.03	0.34
M1···M16	8.47	-2.64	0.43	0.56
M1···M17	11.53	-1.85	0.59	0.39
Total	311.7	-75.19	16.00	16.00

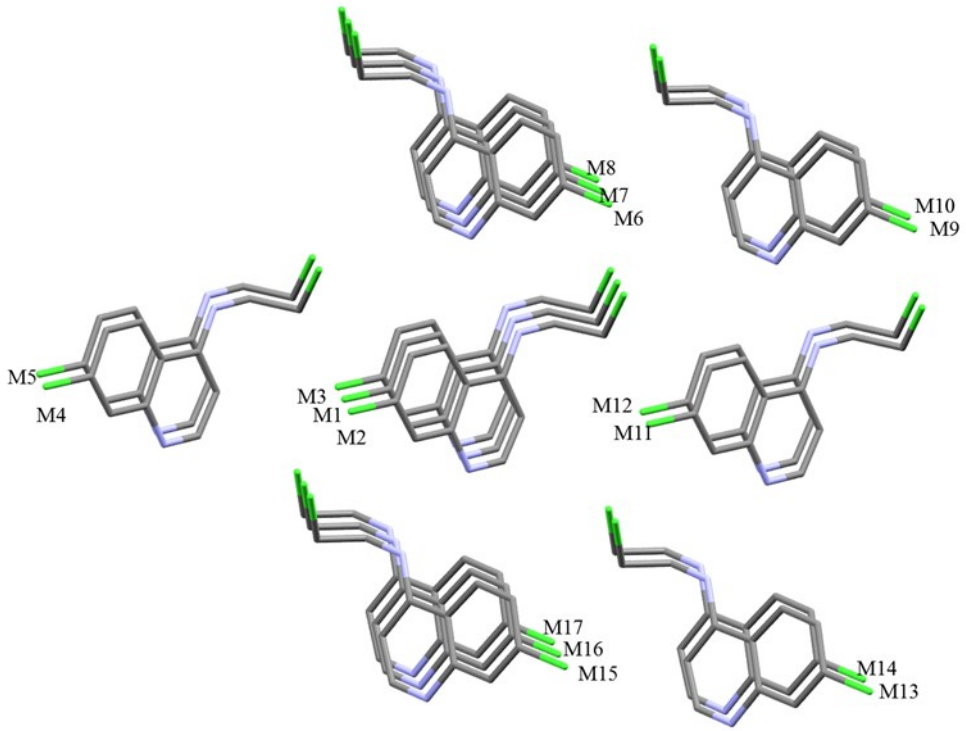


Figure S23. Supramolecular cluster of compound **10**.

Table S24. Contact area and energetic data of each dimer from the supramolecular cluster of compound **10**.

Dimer	$C_{M1\cdots MN}$[a] (Å^2)	$G_{M1\cdots MN}$[b] (kcal mol^{-1})	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]
M1···M2	49.93	-10.82	2.80	2.95
M1···M3	49.93	-10.82	2.80	2.95
M1···M4	13.08	-1.66	0.73	0.45
M1···M5	18.68	-3.15	1.05	0.86
M1···M6	10.91	-0.78	0.61	0.21
M1···M7	25.61	-9.79	1.43	2.67
M1···M8	13.82	-2.10	0.77	0.57
M1···M9	9.06	-0.95	0.51	0.26
M1···M10	1.73	-0.10	0.10	0.03
M1···M11	18.68	-3.15	1.05	0.86
M1···M12	13.08	-1.66	0.73	0.45
M1···M13	1.73	-0.10	0.10	0.03
M1···M14	9.06	-0.95	0.51	0.26
M1···M15	13.82	-2.10	0.77	0.57
M1···M16	25.61	-9.79	1.43	2.67
M1···M17	10.91	-0.78	0.61	0.21
Total	285.64	-58.67	16.00	16.00

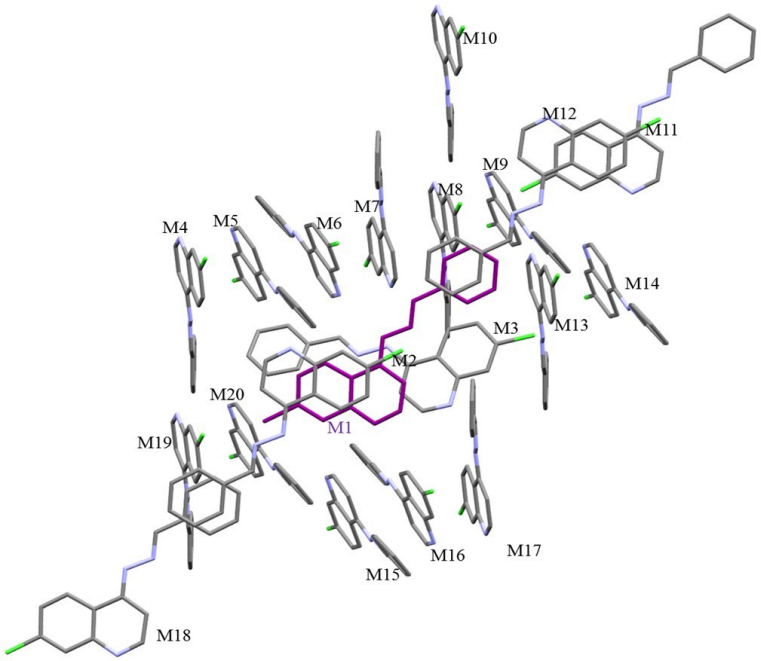


Figure S24. Supramolecular cluster of compound **11**.

Table S25. Contact area and energetic data of each dimer from the supramolecular cluster of compound **11**.

Dimer	$C_{M1\cdots MN}$[a] (Å^2)	$G_{M1\cdots MN}$[b] (kcal mol^{-1})	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]
M1···M2	50.94	-14.77	2.71	3.82
M1···M3	60.67	-12.22	3.23	3.16
M1···M4	9.45	-1.68	0.50	0.44
M1···M5	12.95	-1.26	0.69	0.33
M1···M6	24.8	-10.98	1.32	2.84
M1···M7	26.29	-3.12	1.40	0.81
M1···M8	9.45	-1.68	0.50	0.44
M1···M9	12.67	-0.92	0.68	0.24
M1···M10	9.58	-0.34	0.51	0.09
M1···M11	38.41	-5.80	2.05	1.50
M1···M12	9.76	-0.97	0.52	0.25
M1···M13	7.8	-1.23	0.42	0.32
M1···M14	8.09	-1.41	0.43	0.36
M1···M15	6	-0.38	0.32	0.10
M1···M16	24.80	-10.98	1.32	2.84
M1···M17	26.29	-3.12	1.40	0.81
M1···M18	9.76	-0.97	0.52	0.25
M1···M19	0.82	-0.21	0.04	0.06
M1···M20	8.09	-1.41	0.43	0.36
Total	356.62	-73.44	19.00	19.00

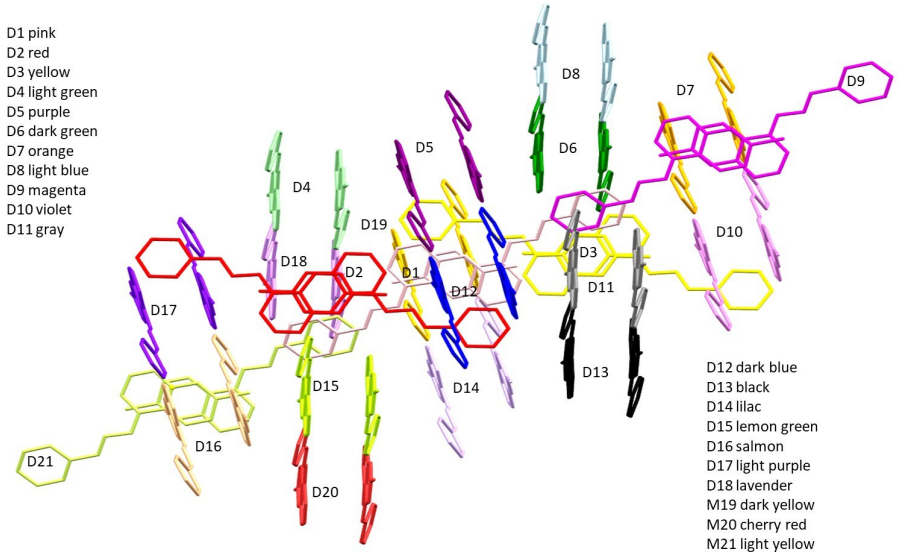


Figure S25. Supramolecular cluster of compound **11**. Dimer considered as the initial nucleus. Color were used for clarity.

Table S26. Contact area and energetic data of each dimer from the supramolecular cluster of compound **11**.

Dimer	$C_{M1\cdots MN}$[a] (Å^2)	$G_{M1\cdots MN}$[b] (kcal mol^{-1})	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]
D1···D2	60.67	-12.93	1.98	2.19
D1···D3	60.67	-12.93	1.98	2.19
D1···D4	35.74	-4.61	1.17	0.78
D1···D5	68.55	-24.75	2.24	4.20
D1···D6	35.74	-4.61	1.17	0.78
D1···D7	12.67	-0.88	0.41	0.15
D1···D8	9.58	-0.04	0.31	0.01
D1···D9	57.94	-7.54	1.90	1.28
D1···D10	8.09	-1.17	0.26	0.20
D1···D11	8.62	-1.28	0.28	0.22
D1···D12	8.09	-1.17	0.26	0.20
D1···D13	35.74	-4.61	1.17	0.78
D1···D14	68.55	-24.75	2.24	4.20
D1···D15	35.74	-4.61	1.17	0.78
D1···D16	12.67	-0.88	0.41	0.15
D1···D17	8.09	-1.17	0.26	0.20
D1···D18	8.62	-1.28	0.28	0.22
D1···D19	8.09	-1.17	0.26	0.20
D1···D20	9.58	-0.04	0.31	0.01
D1···D21	57.94	-7.54	1.90	1.28
Total	611.38	-117.93	20.00	20.00

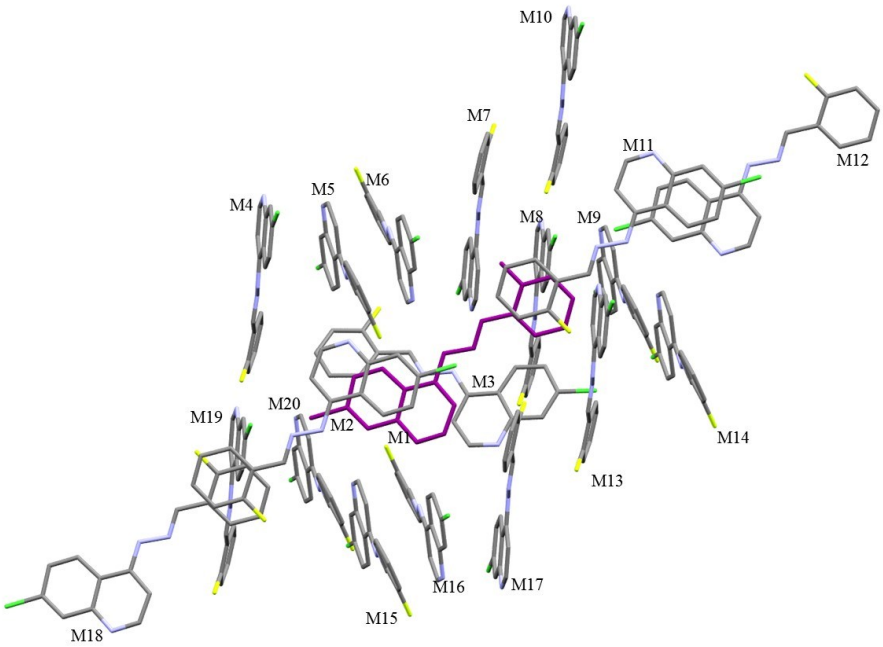


Figure S26. Supramolecular cluster of compound **12**.

Table S27. Contact area and energetic data of each dimer from the supramolecular cluster of compound **12**.

Dimer	$C_{M1\cdots MN}$[a] (Å^2)	$G_{M1\cdots MN}$[b] (kcal mol^{-1})	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]
M1···M2	51.55	-14.71	2.73	3.76
M1···M3	59.95	-12.69	3.17	3.24
M1···M4	9.67	-1.55	0.51	0.40
M1···M5	12.92	-1.16	0.68	0.30
M1···M6	24.99	-11.17	1.32	2.85
M1···M7	27.19	-3.11	1.44	0.80
M1···M8	9.67	-1.55	0.51	0.40
M1···M9	13.14	-0.82	0.70	0.21
M1···M10	10.42	-0.63	0.55	0.16
M1···M11	39.19	-5.90	2.07	1.51
M1···M12	9.85	-1.15	0.52	0.29
M1···M13	6.21	-0.87	0.33	0.22
M1···M14	7.74	-1.50	0.41	0.38
M1···M15	5.96	-0.46	0.32	0.12
M1···M16	24.99	-11.17	1.32	2.85
M1···M17	27.19	-3.11	1.44	0.80
M1···M18	9.85	-1.15	0.52	0.29
M1···M19	0.68	-0.15	0.04	0.04
M1···M20	7.74	-1.50	0.41	0.38
Total	358.9	-74.34	19.00	19.00

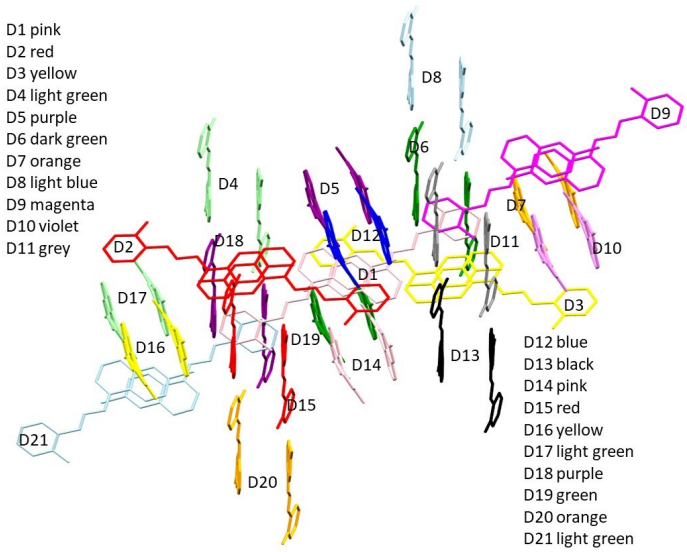


Figure S27. Supramolecular cluster of compound **12**. Dimer considered as the initial nucleus. Color were used for clarity.

Table S28. Contact area and energetic data of each dimer from the supramolecular cluster of compound **12**.

Dimer	$C_{M1\cdots MN}$[a] (Å^2)	$G_{M1\cdots MN}$[b] (kcal mol^{-1})	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]
D1···D2	59.95	-13.69	1.95	2.22
D1···D3	59.95	-13.69	1.95	2.22
D1···D4	36.86	-4.87	1.20	0.79
D1···D5	68.85	-24.83	2.24	4.03
D1···D6	36.86	-4.87	1.20	0.79
D1···D7	13.14	-0.87	0.43	0.14
D1···D8	10.42	-0.28	0.34	0.05
D1···D9	58.88	-8.09	1.92	1.31
D1···D10	7.74	-1.46	0.25	0.24
D1···D11	6.89	-1.17	0.22	0.19
D1···D12	7.74	-1.46	0.25	0.24
D1···D13	36.86	-4.87	1.20	0.79
D1···D14	68.85	-24.83	2.24	4.03
D1···D15	36.86	-4.87	1.20	0.79
D1···D16	13.14	-0.87	0.43	0.14
D1···D17	7.74	-1.46	0.25	0.24
D1···D18	6.89	-1.17	0.22	0.19
D1···D19	7.74	-1.46	0.25	0.24
D1···D20	10.42	-0.28	0.34	0.05
D1···D21	58.88	-8.09	1.92	1.31
Total	614.66	-123.20	20.00	20.00

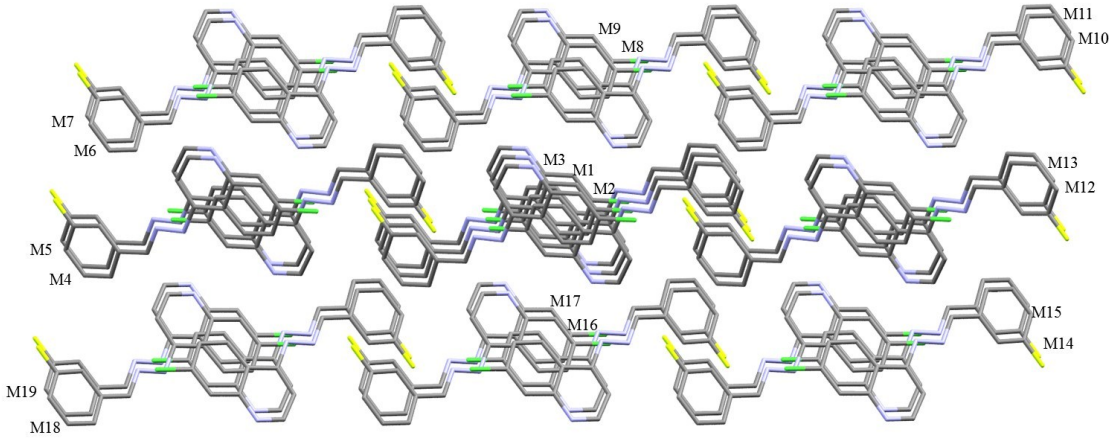


Figure S28. Supramolecular cluster of compound **13**. Dimer considered as the initial nucleus.

Table S29. Contact area and energetic data of each dimer from the supramolecular cluster of compound **13**.

Dimer	$C_{M1\cdots MN}$[a] (Å^2)	$G_{M1\cdots MN}$[b] (kcal mol^{-1})	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]
D1···D2	34.83	-10.04	1.03	1.40
D1···D3	34.83	-10.04	1.03	1.40
D1···D4	35.12	-6.95	1.04	0.97
D1···D5	39.18	-3.58	1.16	0.50
D1···D6	7.12	-1.31	0.21	0.18
D1···D7	7.12	-1.31	0.21	0.18
D1···D8	74.25	-17.14	2.20	2.40
D1···D9	74.25	-17.14	2.20	2.40
D1···D10	16.26	-3.44	0.48	0.48
D1···D11	16.26	-3.44	0.48	0.48
D1···D12	39.18	-3.58	1.16	0.50
D1···D13	35.12	-6.95	1.04	0.97
D1···D14	7.12	-1.31	0.21	0.18
D1···D15	7.12	-1.31	0.21	0.18
D1···D16	74.25	-17.14	2.20	2.40
D1···D17	74.25	-17.14	2.20	2.40
D1···D18	16.26	-3.44	0.48	0.48
D1···D19	16.26	-3.44	0.48	0.48
Total	608.78	-128.69	18.00	18.00

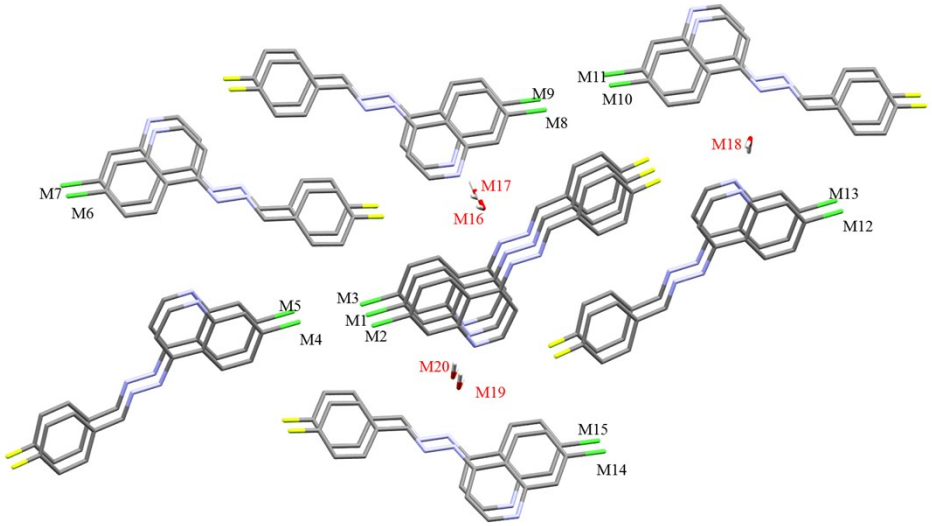
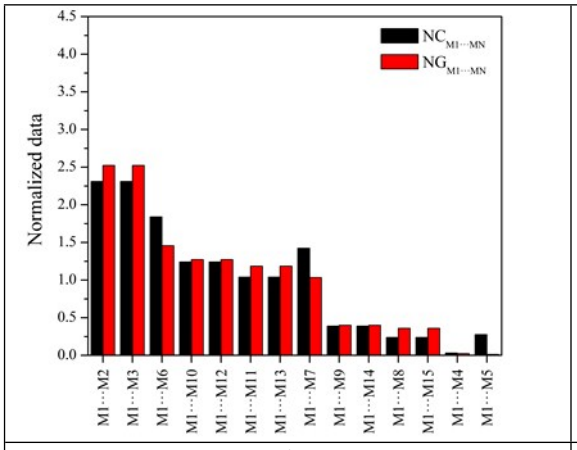


Figure S29. Supramolecular cluster of compound **14**. Dimer considered as the initial nucleus.

Table S30. Contact area and energetic data of each dimer from the supramolecular cluster of compound **14**.

Dimer	$C_{M1\cdots MN}$[a] (Å^2)	$G_{M1\cdots MN}$[b] (kcal mol^{-1})	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]
M1···M2	67.54	-15.22	3.58	3.83
M1···M3	67.54	-15.22	3.58	3.83
M1···M4	6.24	-0.03	0.33	0.01
M1···M5	2.02	-0.22	0.11	0.06
M1···M6	12.51	-1.99	0.66	0.50
M1···M7	11.89	-2.22	0.63	0.56
M1···M8	7.28	-2.92	0.39	0.74
M1···M9	17.9	-4.54	0.95	1.14
M1···M10	11.89	-2.22	0.63	0.56
M1···M11	12.51	-1.99	0.66	0.50
M1···M12	37.83	-4.91	2.00	1.24
M1···M13	34.48	-3.04	1.83	0.77
M1···M14	7.28	-2.92	0.39	0.74
M1···M15	17.9	-4.54	0.95	1.14
M1···M16	14.30	-6.19	0.76	1.56
M1···M17	7.76	0.38	0.41	-0.10
M1···M18	0.15	-0.14	0.01	0.03
M1···M19	11.4	-3.75	0.60	0.95
M1···M20	10.3	-3.77	0.55	0.95
Total	358.72	-75.44	19.00	19.00

6. Normalized data



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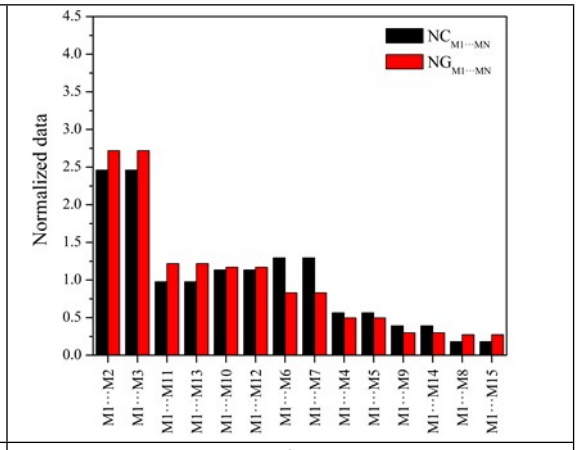

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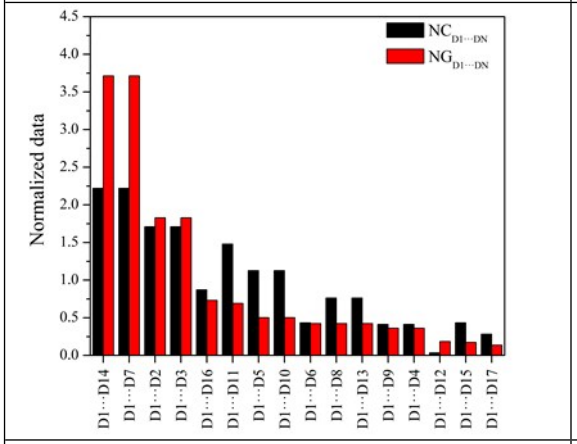

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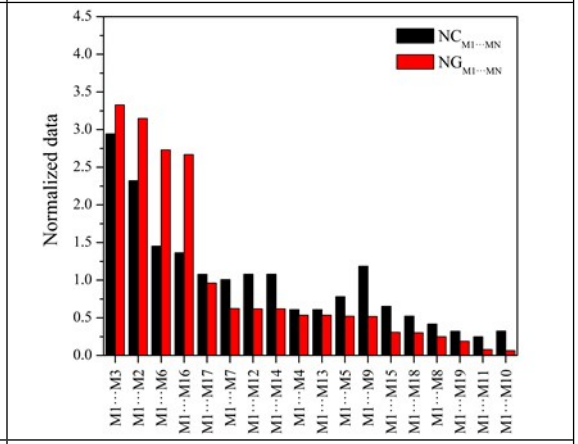

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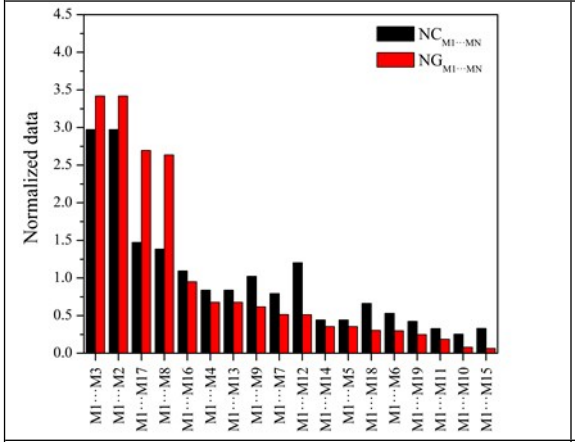

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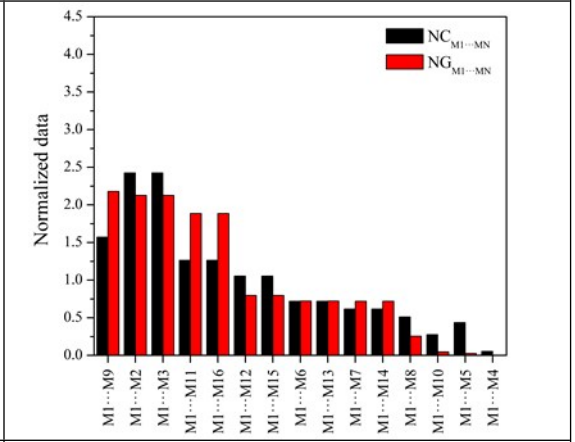

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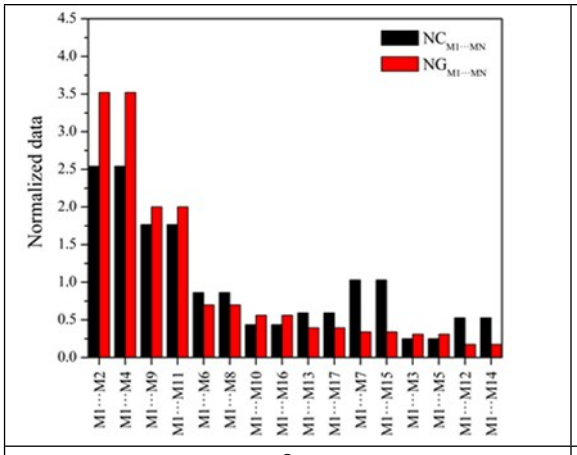

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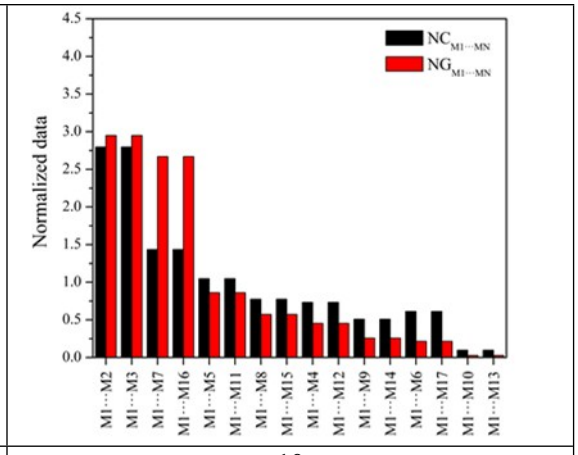

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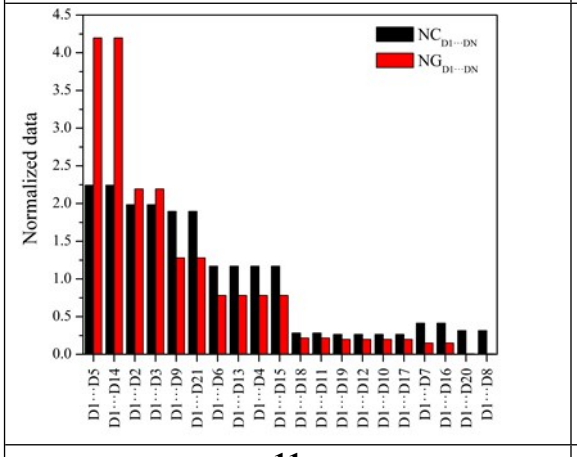

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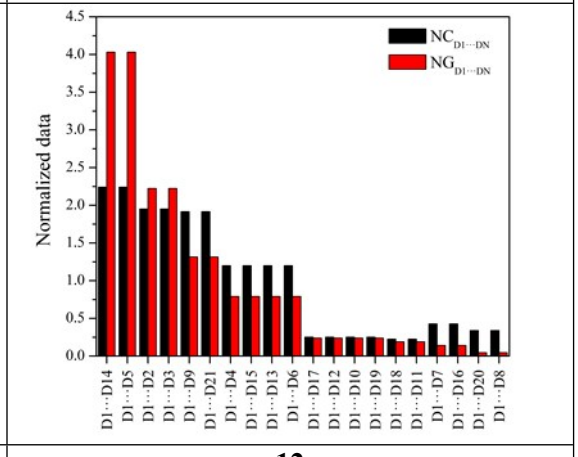

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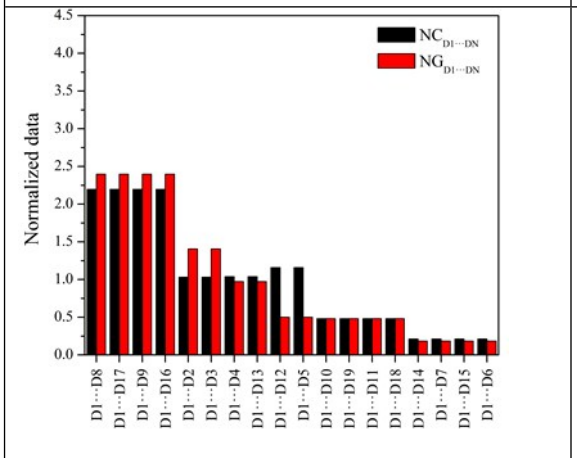

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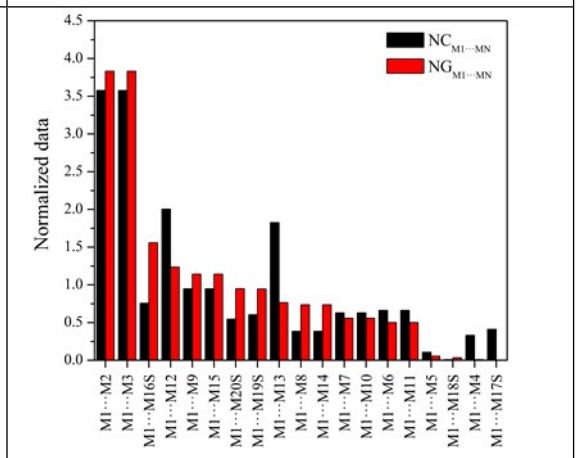


14

7. Concentration dependent ^{1}H-NMR experiments

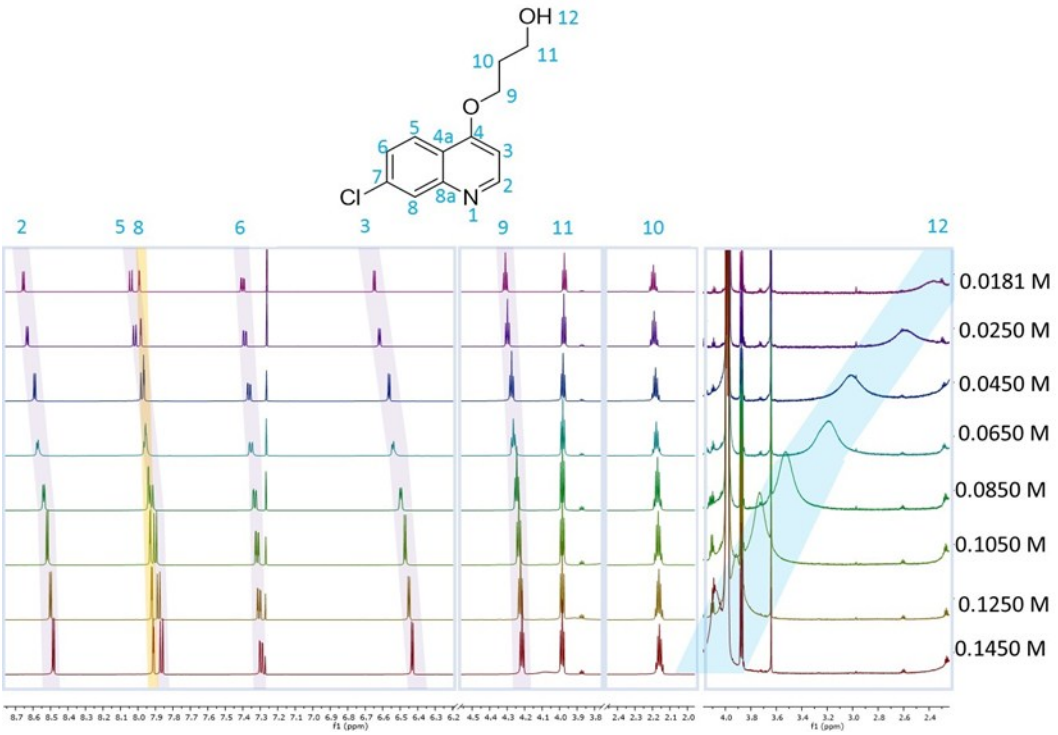
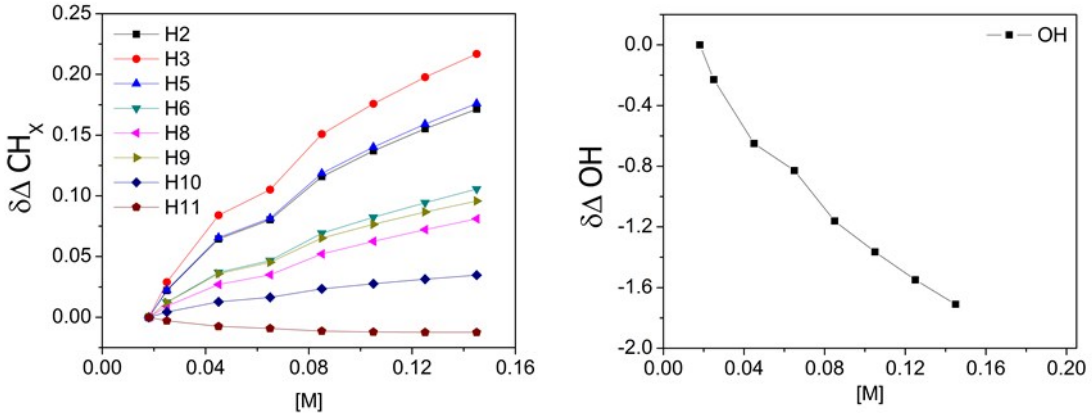


Figure S30. Concentration-dependent ^{1}H-NMR experiments of compound **5** using $CDCl_3$.



(a) (b)

Figure S31. Concentration-dependent ^{1}H-NMR chemical shift changes of signals of (a) CH_X and (b) OH for compound **5,** in $CDCl_3$.

8. Crystallization Mechanisms

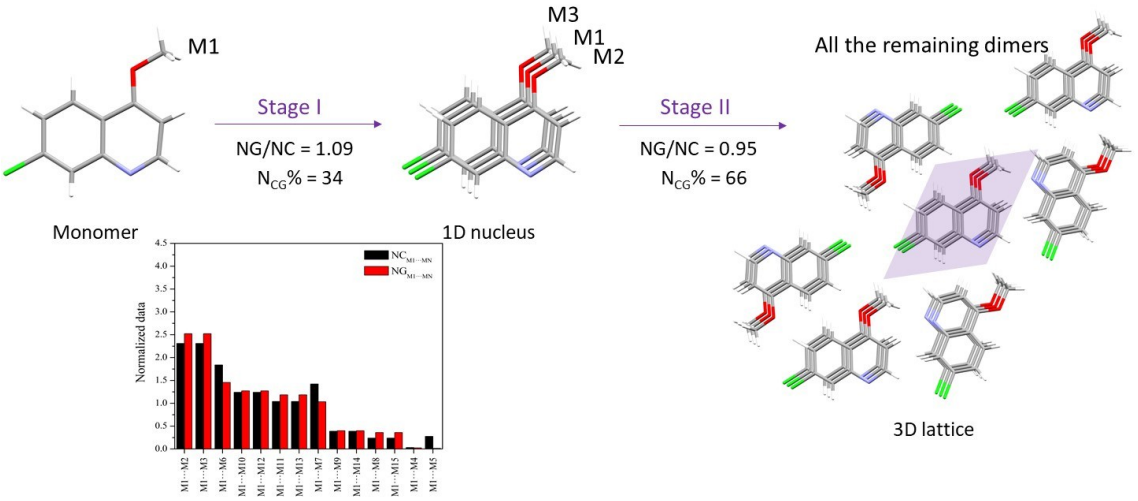


Figure S32. Crystallization mechanism for compound **1**. The shaded area represents the portion of the previous stage.

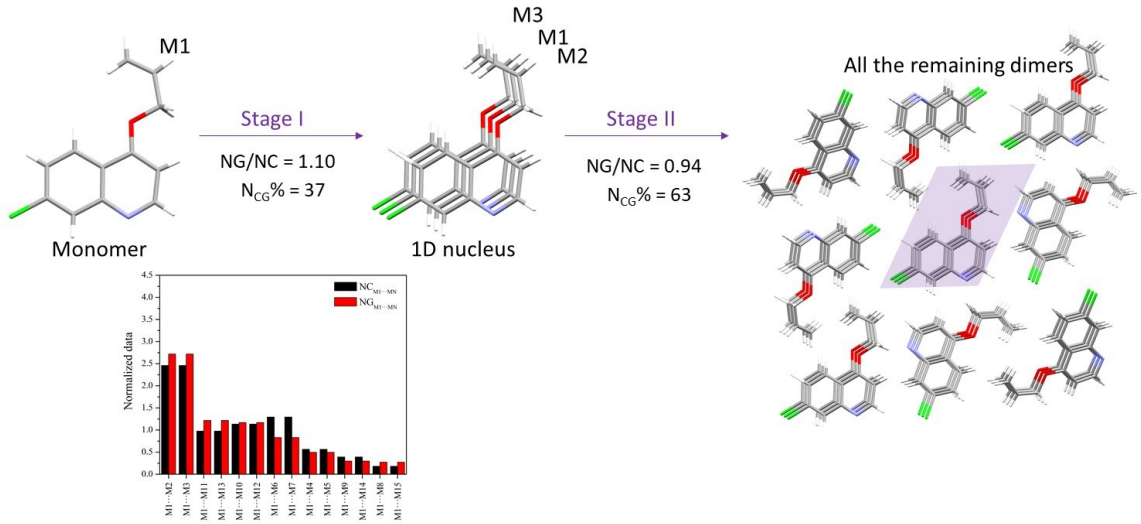


Figure S33. Crystallization mechanism for compound **3**. The shaded area represents the portion of the previous stage.

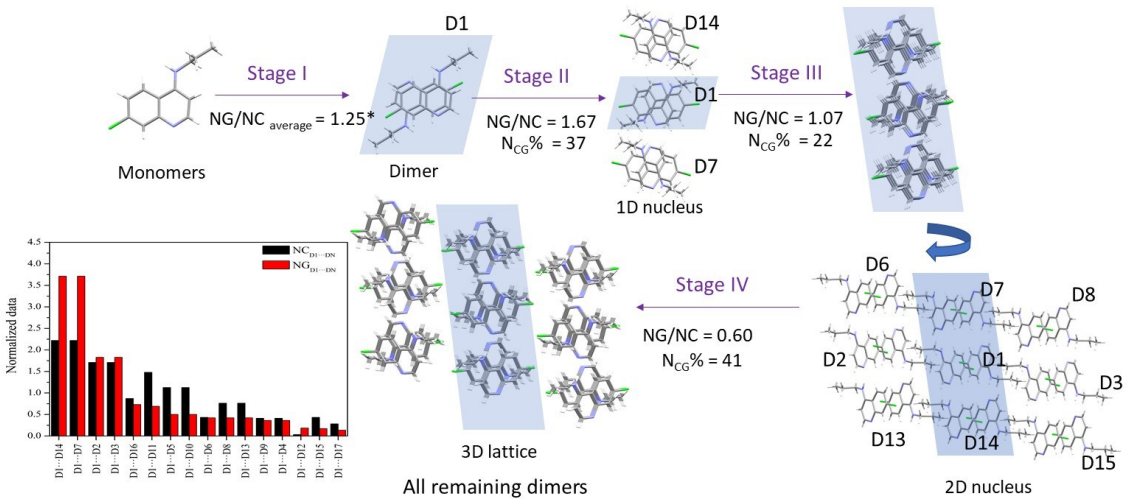


Figure S34. Crystallization mechanism of compound **6**. Dimer formed between M1A and M1B molecules considered as new reference D1 (dimer 1). The shaded area represents the portion of the previous stage. *NG/NC calculated from the supramolecular cluster considering the central molecule as the monomer M1

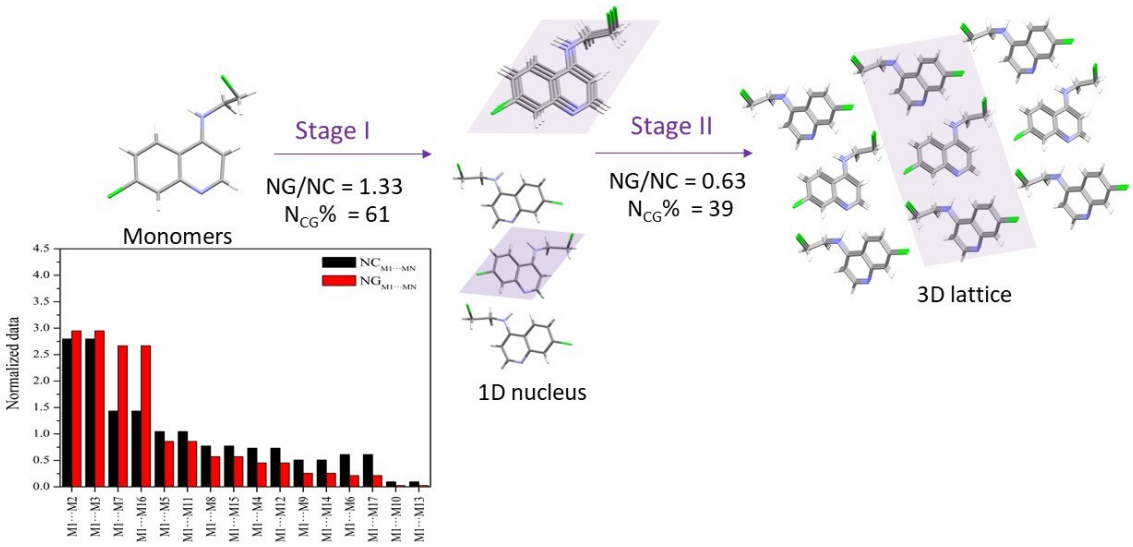


Figure S35. Crystallization mechanism for compound **10**. The shaded area represents the portion of the previous stage.

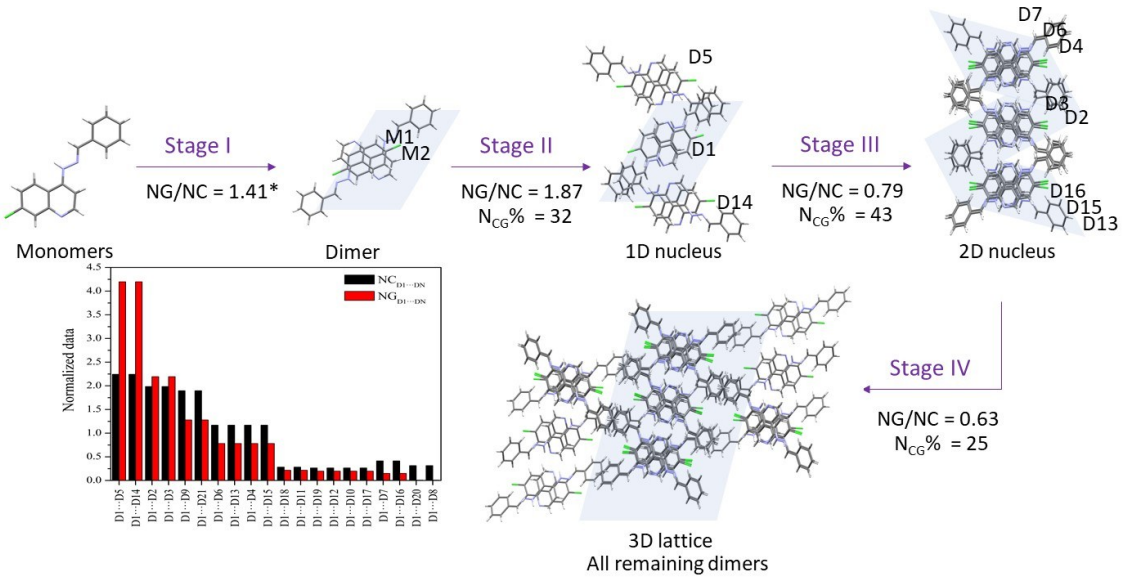


Figure S36. Crystallization mechanism for compound **11**. Dimer formed between M1A and M1B molecules considered as new reference D1 (dimer 1). The shaded area represents the portion of the previous stage. *NG/NC calculated from the supramolecular cluster considering the central molecule as the monomer M1.

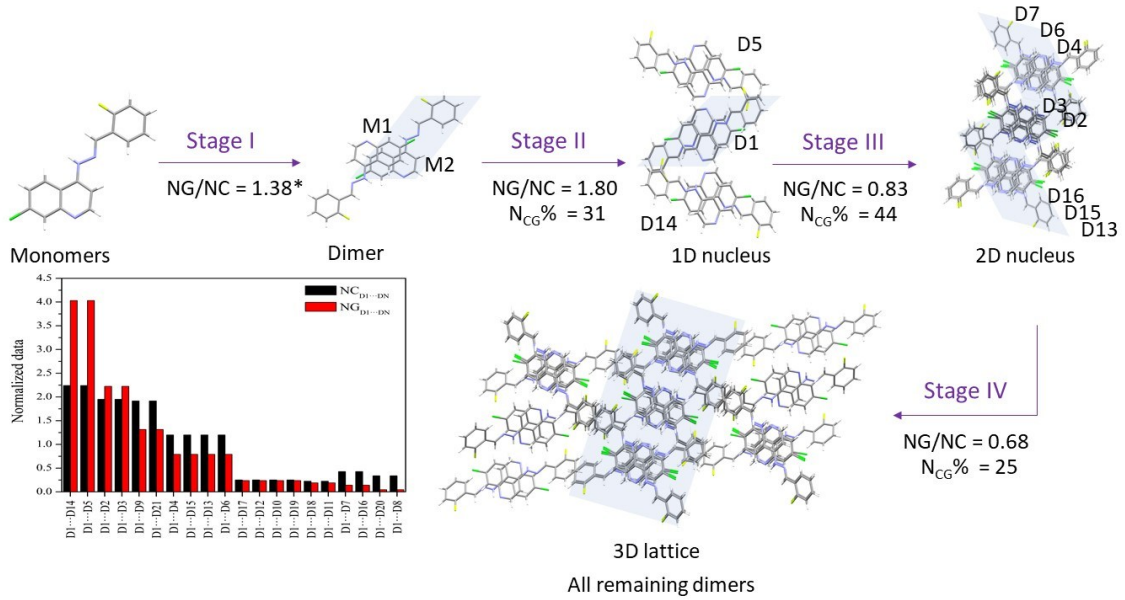


Figure S37. Crystallization mechanism for compound **12**. Dimer formed between M1A and M1B molecules considered as new reference D1 (dimer 1). The shaded area represents the portion of the previous stage. *NG/NC calculated from the supramolecular cluster considering the central molecule as the monomer M1.

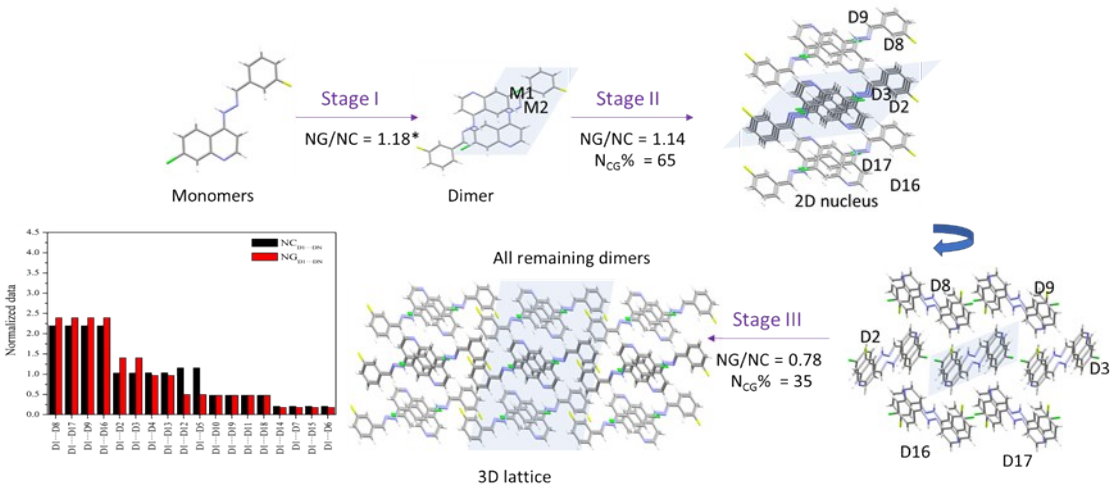
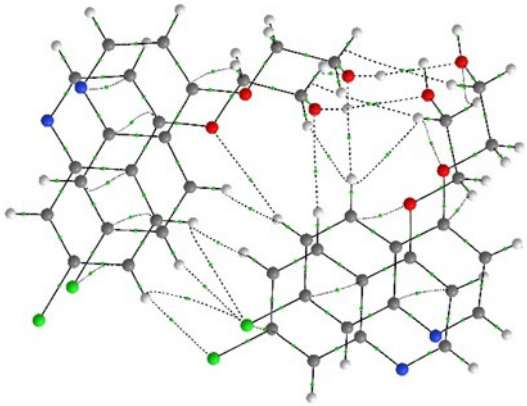


Figure S38. Crystallization mechanism for compound **13**. Dimer formed between M1A and M1B molecules considered as new reference D1 (dimer 1). The shaded area represents the portion of the previous stage. *NG/NC calculated from the supramolecular cluster considering the central molecule as the monomer M1.

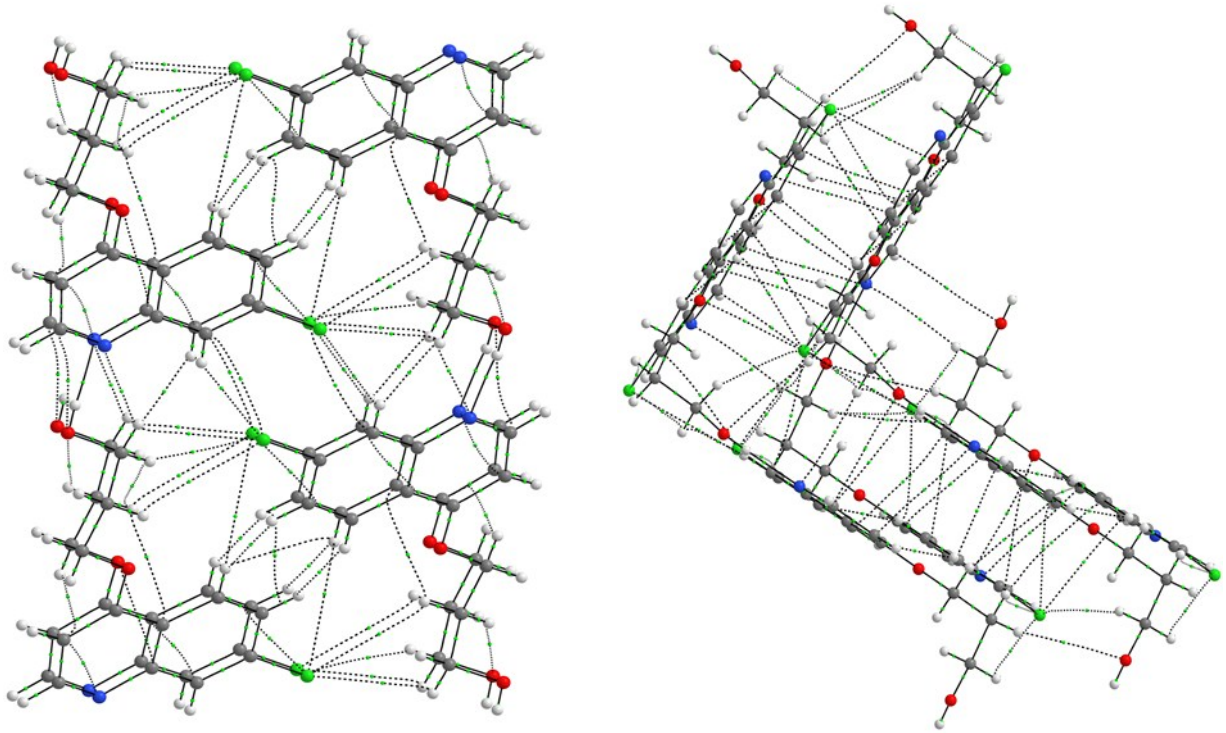
9. QTAIM Data

Table S31. Intermolecular interactions paths data for compound **4**.



Atoms	Interaction	ρ_{int} (a.u.)	$\nabla^2\rho$	$\mathcal{E}$	$G_{AI(X\cdots Y)}$ (kcal mol^{-1})	%
N1' - C3'	arylN···π	0.002761	0.007936	2.231469	-0.67	1.81
H5 - H43D	arylCH···HC	0.004122	0.017248	0.661928	-1.00	2.70
H5 - H43A	CH···HC	0.001765	0.006996	0.604329	-0.43	1.15
H5' - H6	arylCH···HCaryl	0.003806	0.016616	1.925313	-0.92	2.49
H6 - H5'	arylCH···HCaryl	0.003791	0.016673	1.924715	-0.92	2.48
H5 - O44'	arylCH···OH	0.007171	0.021572	0.042175	-1.74	4.69
H5 - 044'	arylCH···OH	0.007068	0.021410	0.028068	-1.71	4.62
H6 - O41'	arylCH···O	0.001664	0.007394	0.603007	-0.40	1.09
C5 - O41	O···π	0.004145	0.013768	0.312594	-1.00	2.71
C7 - C4A	π···π	0.005563	0.014465	0.992107	-1.35	3.64
C8A - C3	π···π	0.005367	0.013303	0.691998	-1.30	3.51
C8A - C4'	π···π	0.002910	0.007451	0.777228	-0.70	1.90
C8' - C4A'	π···π	0.003263	0.007830	1.286325	-0.79	2.13
C7'- C5'	π···π	0.003117	0.007939	3.998503	-0.75	2.04
Cl1 - C6	Cl···π	0.005669	0.015954	2.210964	-1.37	3.71
Cl1' - C6'	Cl···π	0.003788	0.010024	2.473938	-0.92	2.48
Cl1 - H6'	Cl···HCaryl	0.004032	0.013941	0.200826	-0.98	2.64
Cl1 - H6'	Cl···HCaryl	0.003030	0.011796	1.340255	-0.73	1.98
Cl1 - H5'	Cl···HCaryl	0.003667	0.012886	0.324778	-0.89	2.40
H66' - Cl1	Cl···HCaryl	0.004063	0.013916	0.203529	-0.98	2.66
C4' - H42C	CH···π	0.003121	0.010422	0.482405	-0.76	2.04
C4 - H42B	CH···π	0.004034	0.013766	0.288573	-0.98	2.64
O41 - H43A	O···HC	0.002461	0.012116	0.240344	-0.60	1.61
O44 - H43B	HO···HC	0.004719	0.022610	1.292587	-1.14	3.09
O44' - H43C	OH···HC	0.007854	0.032983	0.543375	-1.90	5.14
O44 - O44'	HO···OH	0.021760	0.073320	0.011993	-5.27	14.23
044 - O44'	O···O	0.021818	0.073505	0.013371	-5.28	14.27
H43A - C43'	CH···CH	0.003208	0.015211	0.216802	-0.78	2.10
H43A - C43'	CH···CH	0.003201	0.015196	0.190886	-0.77	2.09
Total		0.152938			-37.03	100.00

Table S32. Intermolecular interactions paths data for compound **5**.



Atoms	Interaction	ρ_{int} (a.u.)	$\nabla^2\rho$	$\mathcal{E}$	$G_{AI(X\cdots Y)}$ (kcal mol^{-1})	%
H44A - H43B	CH···HC	0.001059	0.004422	0.801276	-0.34	0.34
H43B - H44A	CH···HC	0.001063	0.004416	0.898742	-0.35	0.35
H9 - Cl2	Cl···HCaryl	0.001407	0.004899	5.811998	-0.46	0.46
Cl1 - H9'	Cl···HCaryl	0.001554	0.005407	4.518278	-0.51	0.51
Cl1 - H9'	Cl···HCaryl	0.001565	0.005444	4.453615	-0.51	0.51
H6 - Cl2	Cl···HCaryl	0.002236	0.00784	0.632562	-0.73	0.73
H6 - Cl2	Cl···HCaryl	0.002237	0.007835	0.637547	-0.73	0.73
Cl1 - H6'	Cl···HCaryl	0.002358	0.008237	0.539232	-0.77	0.77
Cl1 - H6'	Cl···HCaryl	0.002363	0.008257	0.539567	-0.77	0.77
H44A - Cl2	Cl···HC	0.001861	0.00682	0.0380360	-0.61	0.61
Cl2 - H44A	Cl···HC	0.001902	0.006892	0.071179	-0.62	0.62
Cl1 - H44D	Cl···HC	0.001928	0.00704	0.041334	-0.63	0.63
Cl1 - H44D	Cl···HC	0.001954	0.007088	0.084398	-0.64	0.64
H43B - Cl2	Cl···HC	0.003247	0.011384	0.846664	-1.06	1.06
H43B - Cl2	Cl···HC	0.003258	0.011418	0.792283	-1.06	1.06
H43B - Cl2	Cl···HC	0.003273	0.011413	0.806699	-1.07	1.06
H43B - Cl2	Cl···HC	0.003298	0.011463	0.800107	-1.07	1.07
Cl1 - H43C	Cl···HC	0.003754	0.012957	0.487177	-1.22	1.22
Cl1 - H43C	Cl···HC	0.003764	0.01292	0.45936	-1.23	1.22
Cl1 - H43C	Cl···HC	0.003764	0.01293	0.474687	-1.23	1.22
Cl1 - H43C	Cl···HC	0.003789	0.012984	0.473028	-1.23	1.23
Cl1 - H44C	Cl···HC	0.004733	0.017085	0.201395	-1.54	1.54
Cl1 - H44C	Cl···HC	0.004745	0.017166	0.211003	-1.54	1.54
Cl1 - H44C	Cl···HC	0.004752	0.017274	0.214815	-1.55	1.55
Cl1 - H44C	Cl···HC	0.004761	0.017091	0.198763	-1.55	1.55
H44B - Cl2	Cl···HC	0.004911	0.017697	0.174534	-1.60	1.60
H44A - Cl2	Cl···HC	0.004913	0.017513	0.161336	-1.60	1.60
H44B - Cl2	Cl···HC	0.004939	0.017601	0.162323	-1.61	1.61

H44A - Cl2	Cl···HC	0.004969	0.01761	0.16038	-1.62	1.62
H6 - H6'	arylCH···Hcaryl	0.002501	0.011704	69.430646	-0.81	0.81
H6 - H7'	arylCH···HCaryl	0.003928	0.016854	0.156653	-1.28	1.28
H6 - H7'	arylCH···HCaryl	0.00394	0.016849	0.156249	-1.28	1.28
H6 - H7'	arylCH···HCaryl	0.003947	0.016891	0.158187	-1.28	1.28
H6 - H7'	arylCH···HCaryl	0.003964	0.016909	0.158354	-1.29	1.29
H7 - H6'	arylCH···HCaryl	0.004038	0.017269	0.140688	-1.31	1.31
H7 - H6'	arylCH···HCaryl	0.00404	0.017252	0.138652	-1.32	1.31
H7 - H6'	arylCH···HCaryl	0.004046	0.017238	0.137874	-1.32	1.32
H7 - H6'	arylCH···HCaryl	0.004061	0.017282	0.140223	-1.32	1.32
H9 - H44B	arylCH···HC	0.003875	0.016306	0.400794	-1.26	1.26
H9' - H44C	arylCH···HC	0.004434	0.018576	0.353743	-1.44	1.44
H9' - H44C	arylCH···HC	0.004458	0.018485	0.355366	-1.45	1.45
O45' - C2'	HO···π	0.002621	0.009935	0.663379	-0.85	0.85
O45 - C2	HO···π	0.002623	0.009735	0.442152	-0.85	0.85
C2 - O45	HO···π	0.002656	0.009776	0.424895	-0.86	0.86
O45 - H43A	HO···HC	0.002756	0.011478	0.028915	-0.90	0.90
O45 - H43A	HO···HC	0.002795	0.011459	0.017962	-0.91	0.91
H43D - O45'	HO···HC	0.00305	0.012315	0.02529	-0.99	0.99
O45' - H43D	HO···HC	0.003082	0.012289	0.016856	-1.00	1.00
N1' - C3'	N···π	0.003892	0.010242	0.802639	-1.27	1.27
C3' - N1'	N···π	0.003916	0.01038	0.753245	-1.27	1.27
N1 - C3	N···π	0.004011	0.010485	0.665917	-1.31	1.30
N1 - C3	N···π	0.004048	0.010661	0.620782	-1.32	1.32
C10 - O41	O···π	0.004058	0.01452	3.748196	-1.32	1.32
C10 - O41	O···π	0.004065	0.014524	4.360813	-1.32	1.32
N1 - H44B	N···HC	0.00426	0.014282	0.230274	-1.39	1.39
N1 - H44B	N···HC	0.004283	0.014087	0.236344	-1.39	1.39
H44C - N1'	N···HC	0.004644	0.015041	0.262329	-1.51	1.51
H43C - C5'	CH···π	0.00428	0.013818	2.011099	-1.39	1.39
C51 - H43C	CH···π	0.004297	0.013851	2.028717	-1.40	1.40
C5 - H43B	CH···π	0.004521	0.014797	1.574246	-1.47	1.47
C5 - H43B	CH···π	0.004525	0.014802	1.57094	-1.47	1.47
H42C - C4'	CH···π	0.005244	0.016274	2.5673	-1.71	1.71
H42C - C4'	CH···π	0.005245	0.016295	2.537219	-1.71	1.71
H42B - C3	CH···π	0.005463	0.016537	1.725602	-1.78	1.78
H42B - C3	CH···π	0.005464	0.016546	1.730371	-1.78	1.78
C9 - C5	π···π	0.004384	0.011142	3.190047	-1.43	1.43
C9' - C5'	π···π	0.004384	0.011167	4.488396	-1.43	1.43
C5' - C9'	π···π	0.004414	0.011211	4.850084	-1.44	1.44
C9 - C5	π···π	0.004424	0.011211	3.415023	-1.44	1.44
C7 - H7'	arylCH···π	0.005783	0.024475	7.676948	-1.88	1.88
C7 - H7'	arylCH···π	0.005802	0.024368	6.558891	-1.89	1.89
Cl1 - C7	Cl···π	0.005804	0.014905	0.746527	-1.89	1.89
Cl2 - C7'	Cl···π	0.005821	0.014937	0.768373	-1.89	1.89
Cl1 - C7	Cl···π	0.005831	0.01496	0.724379	-1.90	1.90
Cl2 - C7'	Cl···π	0.00586	0.015009	0.745716	-1.91	1.91
Cl1 - C9'	Cl···π	0.007153	0.021304	0.396326	-2.33	2.33
Cl2 - C9	Cl···π	0.007244	0.021629	0.465732	-2.36	2.36
Cl2 - C9	Cl···π	0.007245	0.021642	0.4719	-2.36	2.36
Total					-100.11	100.00

10. References

1 J. K. Natarajan, J. N. Alumasa, K. Yearick, K. A. Ekoue-Kovi, L. B. Casabianca, A. C. de Dios, C. Wolf and P. D. Roepe, *J. Med. Chem.*, 2008, **51**, 3466–3479.

2 K. Oukoloff, N. Coquelle, M. Bartolini, M. Naldi, R. Le Guevel, S. Bach, B. Josselin, S. Ruchaud, M. Catto, L. Pisani, N. Denora, R. M. Iacobazzi, I. Silman, J. L. Sussman, F. Buron, J. P. Colletier, L. Jean, S. Routier and P. Y. Renard, *Eur. J. Med. Chem.*, 2019, **168**, 58–77.