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SUPPORTING INFORMATION

MESOIONIC COMPOUNDS: THE ROLE OF INTERMOLECULAR INTERACTIONS IN THEIR CRYSTALLINE DESIGN

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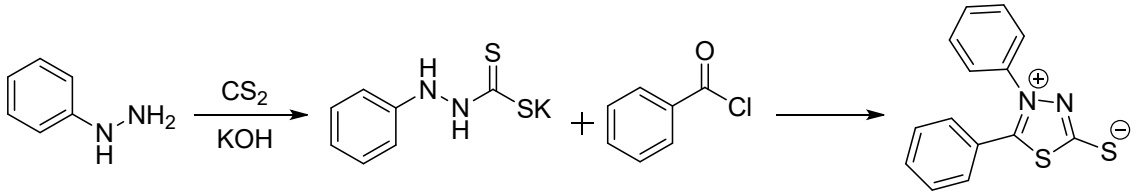
1. Synthesis of the mesoionic 1,3,4-thiadiazolium-5-thiolate (18)

The synthesis of mesoionic 1,3,4-thiadiazolium-5-thiolate (**18**) was initiated by the reaction of phenylhydrazine with CS_2 and KOH to form potassium β-phenyl-carbazoate. Potassium β-phenyl-carbazoate was reacted with benzoyl chloride giving the mesoionic system (**18**). Yield = 60% (Scheme 1).[1]



Scheme 1 Synthesis of the mesoionic 1,3,4-thiadiazolium-5-thiolate (**18**).

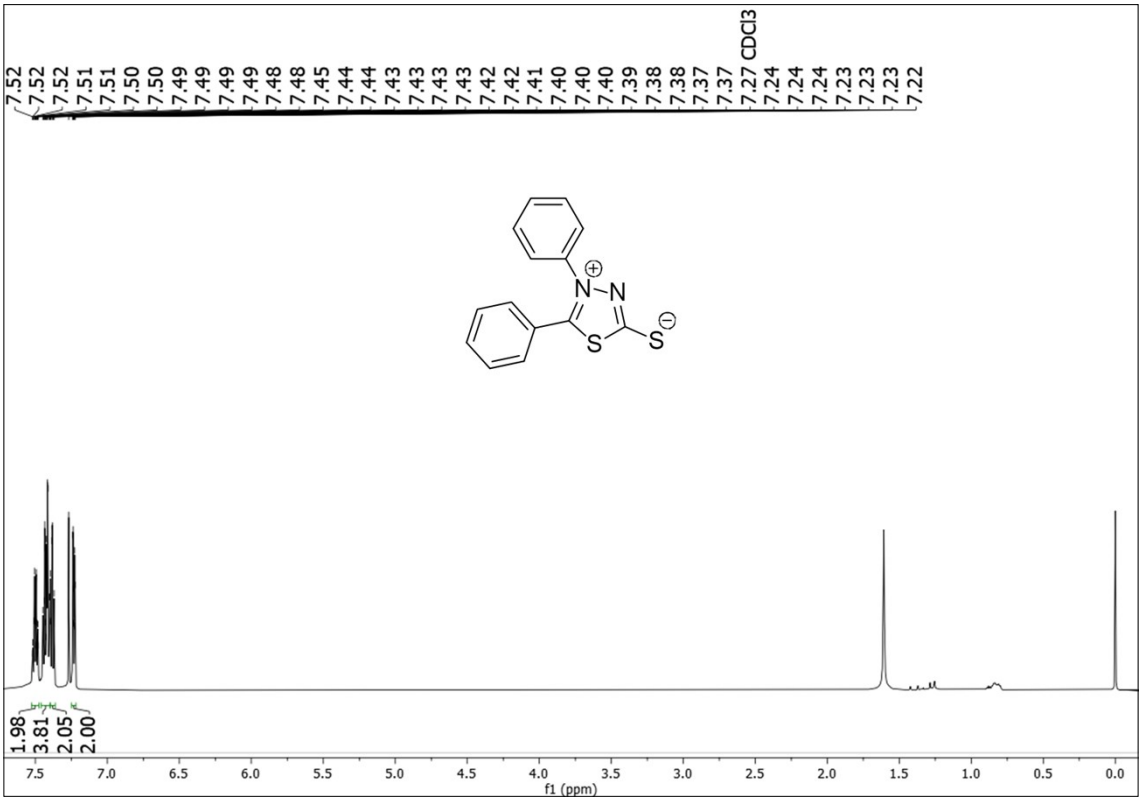


Figure S1 ^1H NMR spectra ($CDCl_3$, 600.13 MHz) for compound 1,3,4-thiadiazolium-5-thiolate (**18**)

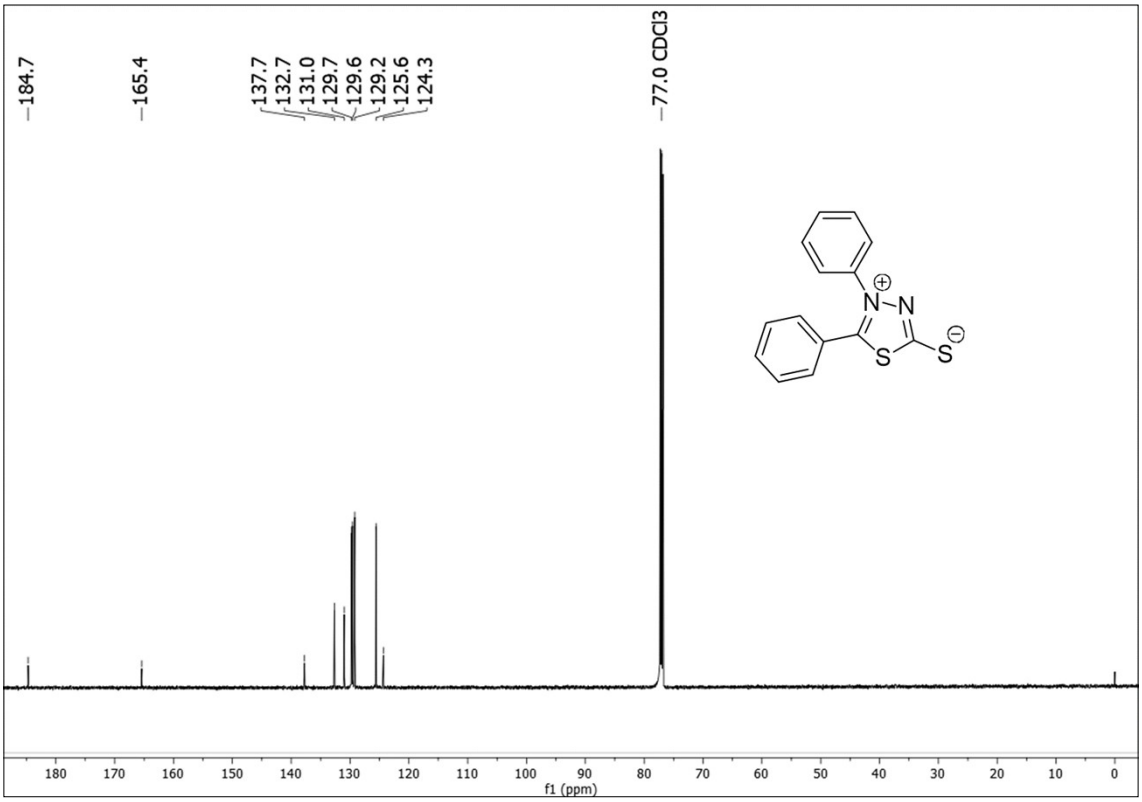


Figure S2 ^{13}C NMR spectra ($CDCl_3$, 150.90 MHz) for compound 1,3,4-thiadiazolium-5-thiolate (**18**)

2. Crystallographic data

Table S1 Crystal data for compound **18**

Compound	**18**
CCDC Number	1835915
Empirical formula	$C_{14}H_{10}N_2S_2$
Formula weight	270.36
Crystal system	monoclinic
Space group	$P2_1/n$
A (Å)	8.7734(3)
b (Å)	10.4120(3)
c (Å)	14.0300(5)
α (degree)	90
β (degree)	97.5020(10)
γ (degree)	90
Volume ($Å^3$)	1270.65(7)
Z	4
T (K)	296.15
ρ_{calc} (g/cm^3)	1.413
μ (mm^{-1})	3.636
Reflections collected	16780

Independent reflections	2255 [R_{int} = 0.0375, R_{sigma} = 0.0186]
Goodness-of-fit	1.054
R_1 [I>=2σ (I)]	0.0339
wR_2 [I>=2σ (I)]	0.0893
$Dr_{max.}$,$Dr_{min.}$ (e Å^{-3})	0.20/-0.22

3. Symmetry Codes, Contact Area, Stabilization Energy and Normalized Data

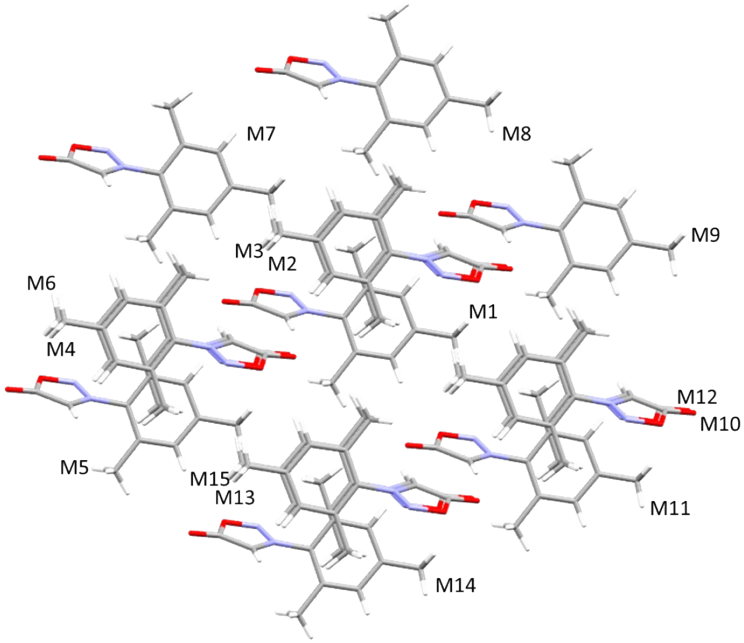


Figure S3 Supramolecular cluster of compound **1**

Table S2 Contact area and energetic data of each dimer from the supramolecular cluster of dimers of compound **1**

Dimer	Symmetry Code	$C_{M1\cdots MN}$ (Å^2)	$G_{M1\cdots MN}$ (kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	1-x,1-y,1-z	50.92	-11.08	2.62	2.47
M1···M3	-x,1-y,1-z	42.1	-10.44	2.16	2.33
M1···M4	x,-1+y,z	21.84	-4.94	1.12	1.10
M1···M5	x,y,1+z	9.04	0.21	0.46	-0.05
M1···M6	x,1+y,1+z	17.11	-3.80	0.88	0.85
M1···M7	1-x,2-y,1-z	13.37	-1.33	0.69	0.30
M1···M8	x,1+y,z	21.84	-4.94	1.12	1.10
M1···M9	-x,2-y,1-z	7.43	-0.76	0.38	0.17
M1···M10	1-x,1-y,-z	7.37	-1.31	0.38	0.29
M1···M11	x,y,-1+z	9.04	0.21	0.46	-0.05
M1···M12	-x,1-y,-z	15.67	-3.36	0.80	0.75

M1···M13	1-x,-y,-z	15.81	-10.85	0.81	2.42
M1···M14	x,-1+y,-1+z	17.11	-3.80	0.88	0.85
M1···M15	-x,-y,-z	23.95	-6.60	1.23	1.47
Total		272.60	-51.71	14.00	14.00

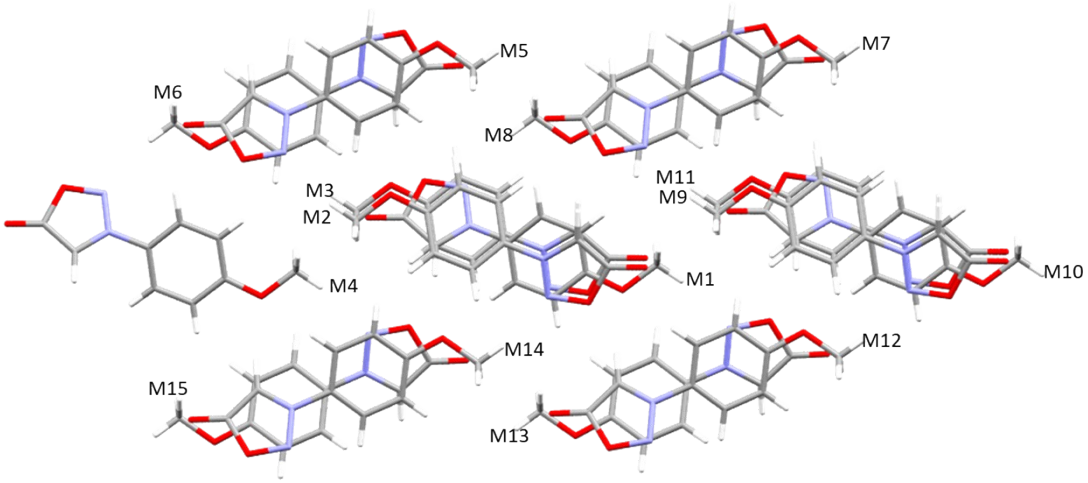


Figure S4 Supramolecular cluster of compound **2**

Table S3 Contact area and energetic data of each dimer from the supramolecular cluster of dimers of compound **2**

Dimer	Symmetry Code	$C_{M1\cdots MN}$ (Å^2)	$G_{M1\cdots MN}$ (kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	1/2+x,1.5-y,1-z	40.44	-13.79	2.40	2.97
M1···M3	-1/2+x,1.5-y,1-z	40.44	-13.79	2.40	2.97
M1···M4	x,y,1+z	8.28	-4.27	0.49	0.92
M1···M5	1/2-x,2-y,1/2+z	13.59	-3.11	0.81	0.67
M1···M6	-x,1/2+y,1.5-z	9.66	-4.85	0.57	1.04
M1···M7	1/2-x,2-y,-1/2+z	13.59	-3.11	0.81	0.67
M1···M8	-x,1/2+y,1/2-z	22.04	-3.19	1.31	0.69
M1···M9	1/2+x,1.5-y,-z	4.17	0.57	0.25	-0.12
M1···M10	x,y,-1+z	8.28	-4.27	0.49	0.92
M1···M11	-1/2+x,1.5-y,-z	4.17	0.57	0.25	-0.12
M1···M12	1/2-x,1-y,-1/2+z	19.58	-3.83	1.16	0.83
M1···M13	-x,-1/2+y,1/2-z	22.04	-3.19	1.31	0.69
M1···M14	1/2-x,1-y,1/2+z	19.58	-3.83	1.16	0.83
M1···M15	-x,-1/2+y,1.5-z	9.66	-4.85	0.57	1.04
Total		235.52	-51.16	14.00	14.00

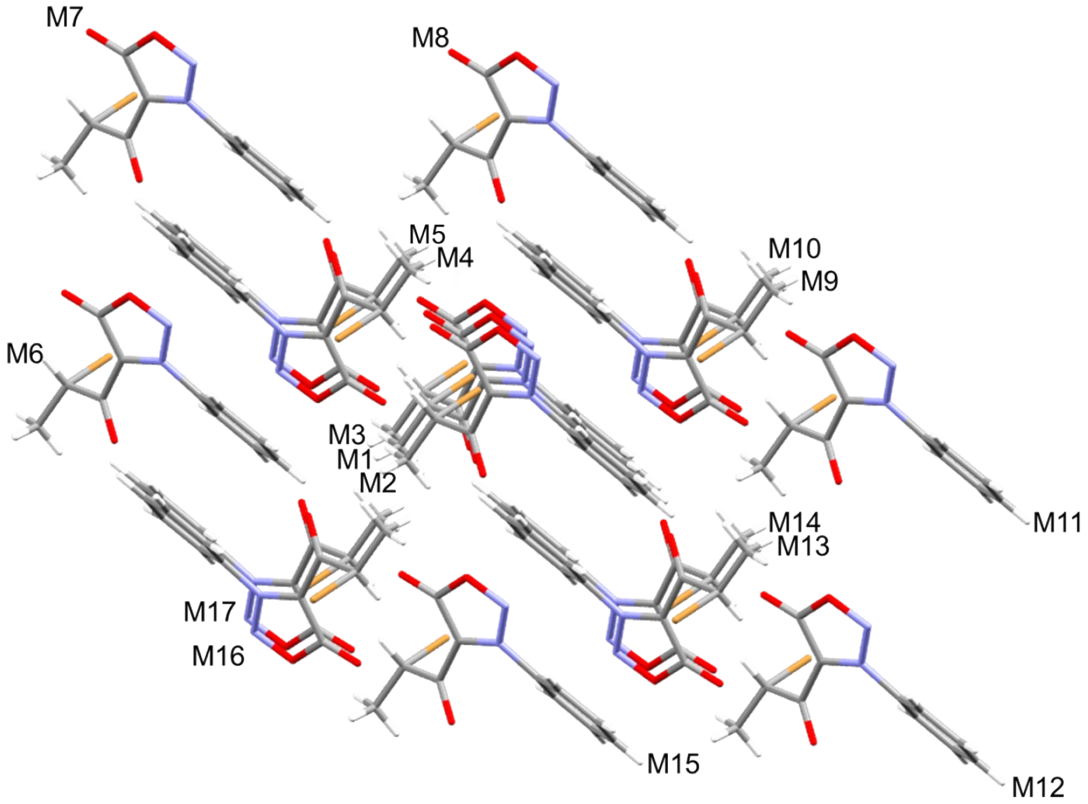


Figure S5 Supramolecular cluster of compound **3**

Table S4 Contact area and energetic data of each dimer from the supramolecular cluster of dimers of compound **3**

Dimer	Symmetry Code	$C_{M1\cdots MN}$ (Å^2)	$G_{M1\cdots MN}$ (kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	1+x,y,z	13.41	-1.79	0.73	0.49
M1···M3	-1+x,y,z	13.41	-1.79	0.73	0.49
M1···M4	1-x,1-y,2-z	32.22	-8.92	1.76	2.43
M1···M5	-x,1-y,2-z	28.09	-4.24	1.54	1.15
M1···M6	x,y,1+z	10.44	-0.09	0.57	0.02
M1···M7	-1+x,y,1+z	1.70	-1.22	0.09	0.33
M1···M8	x,1+y,z	7.13	-0.74	0.39	0.20
M1···M9	2-x,1-y,1-z	22.61	-5.19	1.24	1.41
M1···M10	1-x,1-y,1-z	43.97	-11.57	2.41	3.15
M1···M11	1+x,y,-1+z	10.44	-0.82	0.57	0.22
M1···M12	1+x,-1+y,-1+z	1.70	-1.22	0.09	0.33
M1···M13	1+x,y,-1+z	38.47	-8.56	2.11	2.33
M1···M14	1-x,-y,1-z	44.84	-7.80	2.46	2.12
M1···M15	x,-1+y,z	7.13	-0.74	0.39	0.20
M1···M16	1-x,-y,2-z	13.37	-3.31	0.73	0.90
M1···M17	-x,-y,2-z	3.22	-0.82	0.18	0.22
Total		292.15	-58.83	16.00	16.00

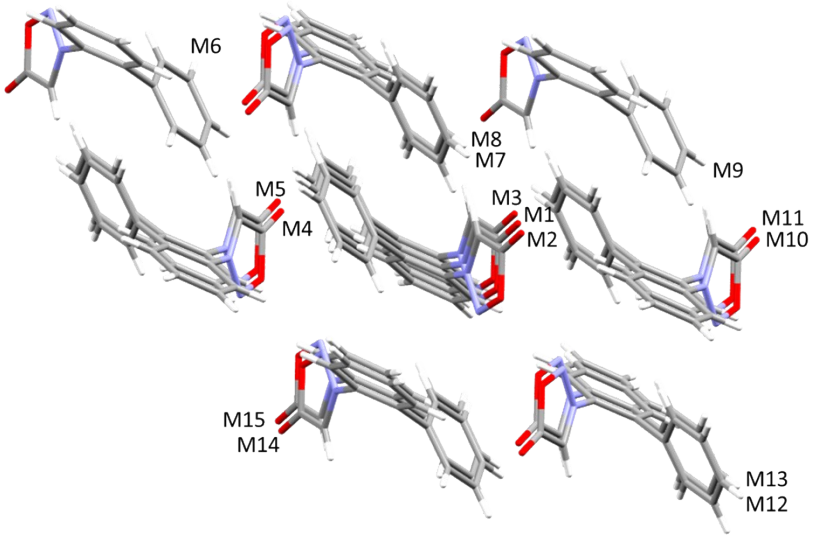


Figure S6 Supramolecular cluster of compound **4**

Table S5 Contact area and energetic data of each dimer from the supramolecular cluster of dimers of compound **4**

Dimer	Symmetry Code	$C_{M1\cdots MN}$ (Å^2)	$G_{M1\cdots MN}$ (kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	x,1+y,z	21.74	-3.40	1.04	0.71
M1···M3	x,-1+y,z	21.74	-3.40	1.04	0.71
M1···M4	-1/2+x,2.5-y,-1/2+z	6.94	-2.91	0.33	0.60
M1···M5	-1/2+x,1.5-y,-1/2+z	29.29	-8.27	1.41	1.72
M1···M6	-x,2-y,1-z	11.07	-1.29	0.53	0.27
M1···M7	1/2-x,1/2+y,1.5-z	37.55	-6.27	1.80	1.30
M1···M8	1/2-x,-1/2+y,1.5-z	37.55	-6.27	1.80	1.30
M1···M9	1-x,2-y,2-z	12.33	-8.25	0.59	1.72
M1···M10	1/2+x,2.5-y,1/2+z	6.94	-2.91	0.33	0.60
M1···M11	1/2+x,1.5-y,1/2+z	29.29	-8.27	1.41	1.72
M1···M12	1/2-x,1/2+y,2.5-z	11.63	-1.35	0.56	0.28
M1···M13	1/2-x,-1/2+y,2.5-z	11.63	-1.35	0.56	0.28
M1···M14	-x,2-y,2-z	14.93	-4.71	0.72	0.98
M1···M15	-x,1-y,2-z	39.10	-8.69	1.88	1.81
Total		291.73	-63.93	14.00	14.00

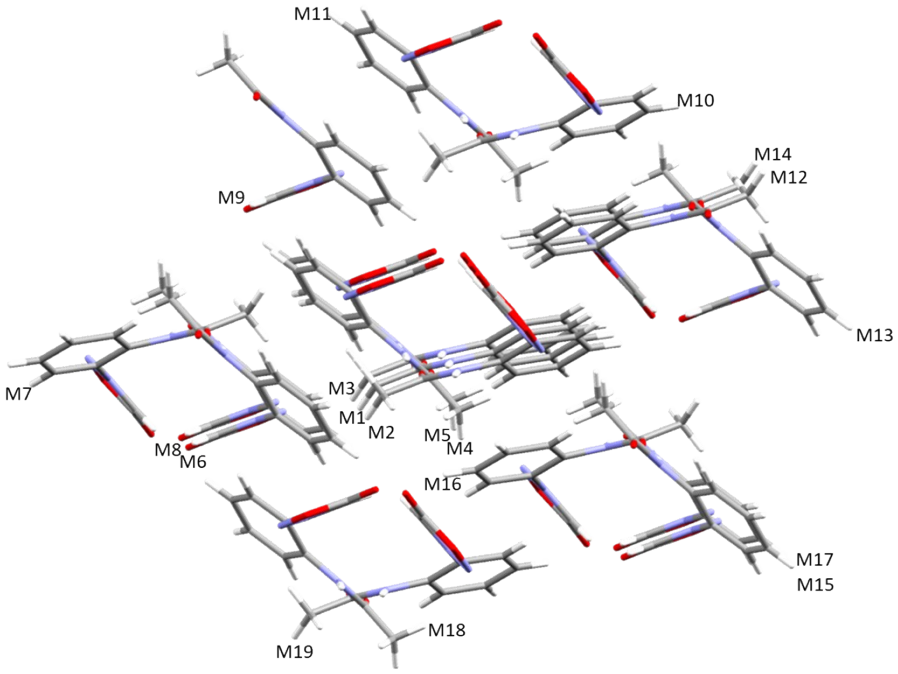


Figure S7 Supramolecular cluster of compound **5**

Table S6 Contact area and energetic data of each dimer from the supramolecular cluster of dimers of compound **5**

Dimer	Symmetry Code	$C_{M1\cdots MN}$ (Å^2)	$G_{M1\cdots MN}$ (kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	x,y,1+z	1.96	-0.89	0.13	0.21
M1···M3	x,y,-1+z	1.96	-0.89	0.13	0.21
M1···M4	x,1/2-y,1/2+z	42.92	-15.56	2.82	3.75
M1···M5	x,1/2-y,-1/2+z	42.92	-15.56	2.82	3.75
M1···M6	1-x,1/2+y,1/2-z	8.53	-1.86	0.56	0.45
M1···M7	1-x,1-y,-z	3.51	-0.29	0.23	0.07
M1···M8	1-x,1/2+y,-1/2-z	8.78	-1.17	0.58	0.28
M1···M9	2-x,1/2+y,1/2-z	11.96	-2.93	0.79	0.71
M1···M10	1+x,y,1+z	0.36	-0.64	0.02	0.15
M1···M11	1+x,1/2-y,1/2+z	11.59	-2.85	0.76	0.69
M1···M12	2-x,-y,1-z	25.89	-9.52	1.70	2.29
M1···M13	2-x,-1/2+y,1/2-z	11.96	-2.93	0.79	0.71
M1···M14	2-x,-y,-z	29.22	-4.88	1.92	1.17
M1···M15	1-x,-1/2+y,1/2-z	8.53	-1.86	0.56	0.45
M1···M16	1-x,-y,-z	43.14	-8.26	2.83	1.99
M1···M17	1-x,-1/2+y,-1/2-z	8.78	-1.17	0.58	0.28
M1···M18	-1+x,1/2-y,-1/2+z	11.59	-2.85	0.76	0.69
M1···M19	-1+x,y,-1+z	0.36	-0.64	0.02	0.15
Total		273.96	-73.86	18.00	18.00

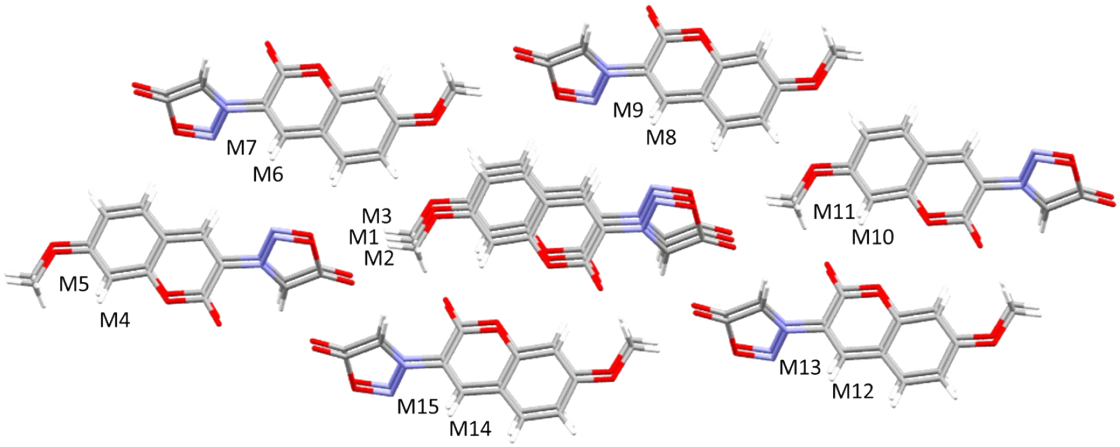


Figure S8 Supramolecular cluster of compound **6**

Table S7 Contact area and energetic data of each dimer from the supramolecular cluster of dimers of compound **6**

Dimer	Symmetry Code	$C_{M1\cdots MN}$ (Å^2)	$G_{M1\cdots MN}$ (kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	1+x,y,z	57.7	-10.82	2.81	1.86
M1···M3	-1+x,y,z	57.7	-10.82	2.81	1.86
M1···M4	x,-1+y,-1+z	5.86	-4.29	0.28	0.74
M1···M5	-1+x,-1+y,-1+z	7.22	-4.14	0.35	0.71
M1···M6	1-x,-y,1-z	21.65	-0.91	1.05	0.16
M1···M7	-x,-y,1-z	14.78	-1.49	0.72	0.26
M1···M8	2-x,1-y,2-z	15.13	-7.93	0.74	1.36
M1···M9	1-x,1-y,2-z	23.37	-8.56	1.14	1.47
M1···M10	1+x,1+y,1+z	7.22	-4.14	0.35	0.71
M1···M11	x,1+y,1+z	5.86	-4.29	0.28	0.74
M1···M12	2-x,2-y,2-z	11.48	-0.29	0.56	0.05
M1···M13	1-x,2-y,2-z	11.56	-6.15	0.56	1.05
M1···M14	2-x,1-y,1-z	19.88	-11.20	0.97	1.92
M1···M15	1-x,1-y,1-z	28.47	-6.62	1.38	1.14
Total		287.88	-70.81	14.00	14.00

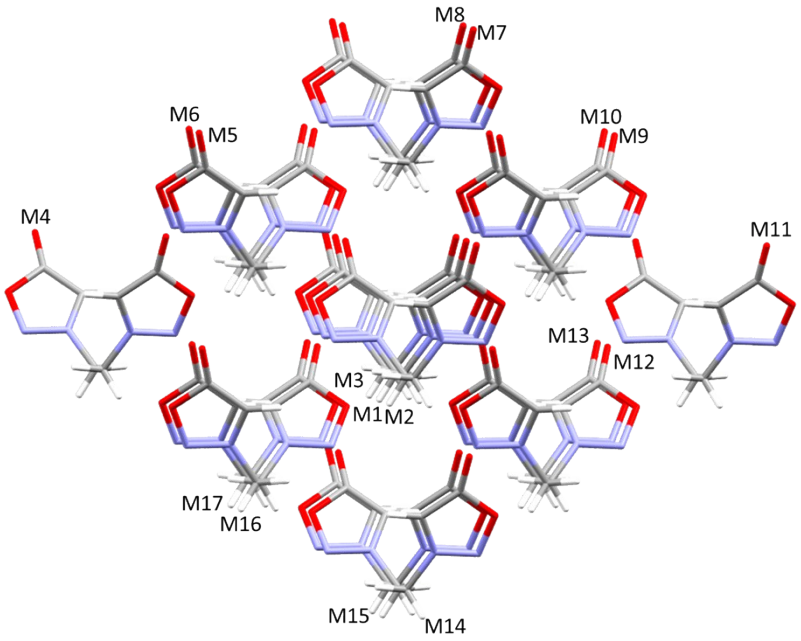


Figure S9 Supramolecular cluster of compound ***7***

Table S8 Contact area and energetic data of each dimer from the supramolecular cluster of dimers of compound ***7***

Dimer	Symmetry Code	$C_{M1\cdots MN}$ (Å^2)	$G_{M1\cdots MN}$ (kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	x,1+y,z	10.29	-0.32	0.72	0.08
M1···M3	x,-1+y,z	10.29	-0.29	0.72	0.08
M1···M4	-1/2+x,-1/2+y,z	4.75	1.23	0.33	-0.32
M1···M5	-1/4+x,1/4-y,-1/4+z	24.91	-3.38	1.75	0.88
M1···M6	-1/4+x,-3/4-y,-1/4+z	12.8	-6.32	0.90	1.65
M1···M7	x,1/2+y,-1/2+z	11.55	-6.05	0.81	1.58
M1···M8	x,-1/2+y,-1/2+z	11.55	-6.03	0.81	1.58
M1···M9	1/4+x,3/4-y,-1/4+z	12.8	-6.32	0.90	1.65
M1···M10	1/4+x,-1/4-y,-1/4+z	24.91	-3.41	1.75	0.89
M1···M11	1/2+x,1/2+y,z	4.75	1.23	0.33	-0.32
M1···M12	1/4+x,1/4-y,1/4+z	24.91	-3.38	1.75	0.88
M1···M13	1/4+x,-3/4-y,1/4+z	12.8	-6.32	0.90	1.65
M1···M14	x,1/2+y,1/2+z	11.55	-6.05	0.81	1.58
M1···M15	x,-1/2+y,1/2+z	11.55	-6.05	0.81	1.58
M1···M16	-1/4+x,3/4-y,1/4+z	12.8	-6.32	0.90	1.65
M1···M17	-1/4+x,-1/4-y,1/4+z	24.91	-3.38	1.75	0.88
Total		227.12	-60.86	16.00	16.00

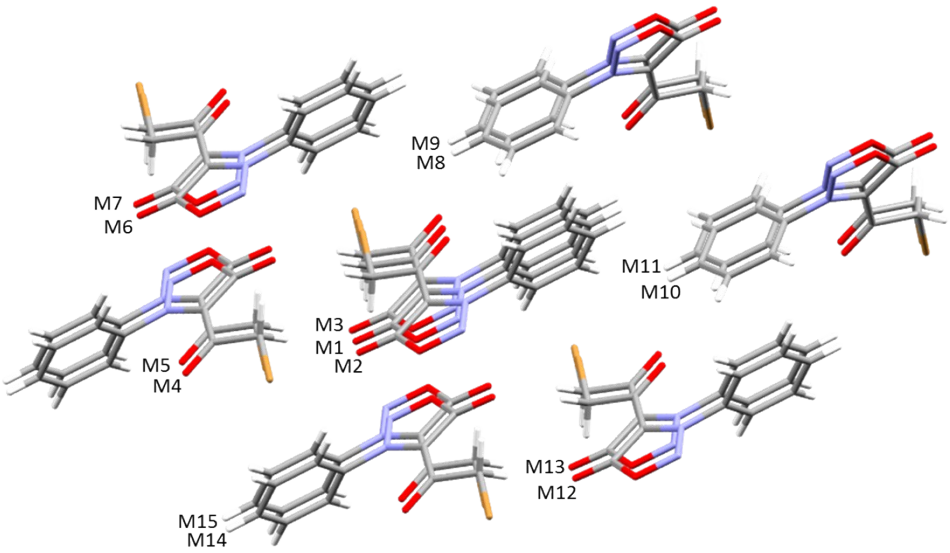


Figure S10 Supramolecular cluster of compound **8**

Table S9 Contact area and energetic data of each dimer from the supramolecular cluster of dimers of compound **8**

Dimer	Symmetry Code	$C_{M1\cdots MN}$ (Å^2)	$G_{M1\cdots MN}$ (kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	x,1+y,z	39.4	-8.22	1.95	2.07
M1···M3	x,-1+y,z	39.4	-8.22	1.95	2.07
M1···M4	2-x,2-y,-z	15.39	-4.16	0.76	1.05
M1···M5	2-x,1-y,-z	14.47	-0.93	0.72	0.23
M1···M6	1+x,y,z	15.09	-3.63	0.75	0.91
M1···M7	1+x,-1+y,z	10.37	-2.02	0.51	0.51
M1···M8	1-x,1/2+y,1/2-z	28.57	-5.95	1.42	1.50
M1···M9	1-x,-1/2+y,1/2-z	28.57	-5.95	1.42	1.50
M1···M10	-x,1/2+y,1/2-z	12.23	-0.38	0.61	0.09
M1···M11	-x,-1/2+y,1/2-z	12.23	-0.38	0.61	0.09
M1···M12	-1+x,1+y,z	10.37	-2.02	0.51	0.51
M1···M13	-1+x,y,z	15.09	-3.63	0.75	0.91
M1···M14	1-x,3-y,-z	6.95	-0.13	0.34	0.03
M1···M15	1-x,2-y,-z	34.04	-10.00	1.69	2.52
Total		282.17	-47.39	14.00	14.00

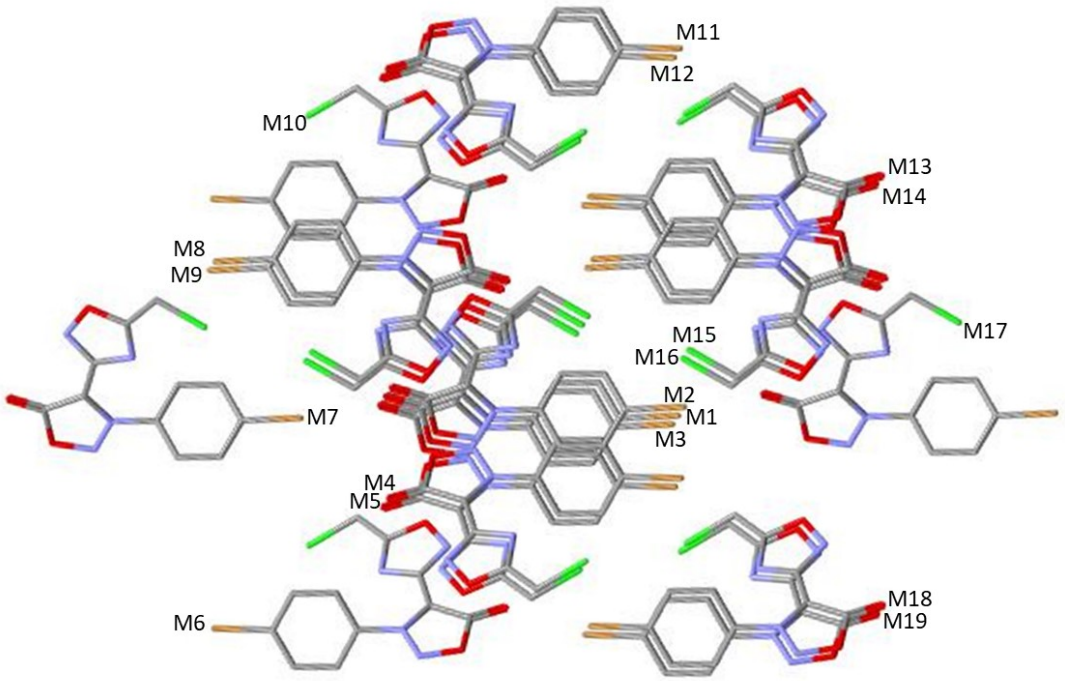


Figure S11 Supramolecular cluster of compound **9**

Table S10 Contact area and energetic data of each dimer from the supramolecular cluster of dimers of compound **9**

Dimer	Symmetry Code	$C_{M1\cdots MN}$ (Å^2)	$G_{M1\cdots MN}$ (kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	x,y,-1+z	8.58	-0.92	0.47	0.22
M1···M3	x,y,1+z	8.58	-0.92	0.47	0.22
M1···M4	x,1.5-y,-1/2+z	50.12	-7.64	2.73	1.81
M1···M5	x,1.5-y,1/2+z	50.12	-7.64	2.73	1.81
M1···M6	1-x,1/2+y,1.5-z	17.1	-6.08	0.93	1.44
M1···M7	-1+x,y,z	5.51	-1.76	0.30	0.42
M1···M8	1-x,1-y,1-z	32.57	-12.93	1.78	3.06
M1···M9	1-x,1-y,2-z	46.36	-19.08	2.53	4.52
M1···M10	1-x,-1/2+y,1.5-z	17.1	-6.08	0.93	1.44
M1···M11	x,1/2-y,-1/2+z	0.51	0.83	0.03	-0.20
M1···M12	x,1/2-y,1/2+z	0.51	0.83	0.03	-0.20
M1···M13	2-x,-1/2+y,1.5-z	14.35	-2.02	0.78	0.48
M1···M14	2-x,-1/2+y,2.5-z	1.22	-0.17	0.07	0.04
M1···M15	2-x,1-y,1-z	4.79	-1.00	0.26	0.24
M1···M16	2-x,1-y,2-z	51.64	-7.52	2.82	1.78
M1···M17	1+x,y,z	5.51	-1.76	0.30	0.42
M1···M18	2-x,1/2+y,1.5-z	14.35	-2.02	0.78	0.48
M1···M19	2-x,1/2+y,2.5-z	1.22	-0.17	0.07	0.04
Total		330.14	-76.05	18.00	18.00

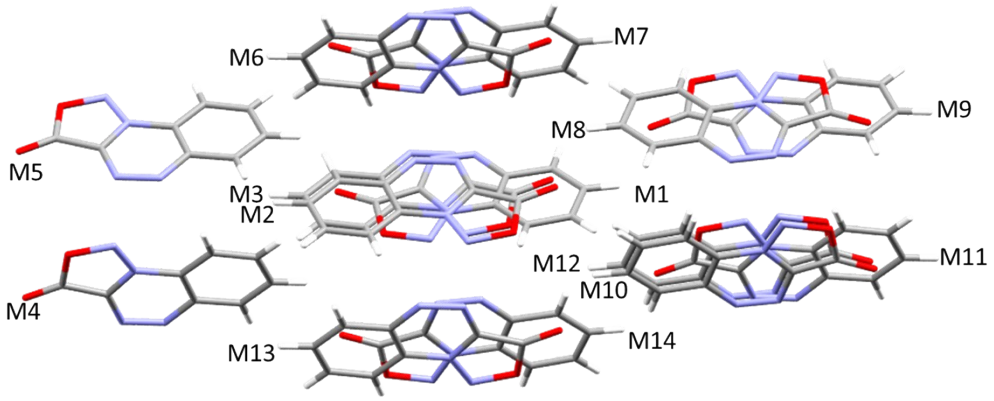


Figure S12 Supramolecular cluster of compound **10**

Table S11 Contact area and energetic data of each dimer from the supramolecular cluster of dimers of compound **10**

Dimer	Symmetry Code	$C_{M1\cdots MN}$ (Å^2)	$G_{M1\cdots MN}$ (kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	1.5-x,1/2+y,z	24.85	-9.12	1.49	2.00
M1···M3	1.5-x,-1/2+y,z	24.85	-9.12	1.49	2.00
M1···M4	1/2+x,y,1/2-z	13.23	-3.43	0.79	0.75
M1···M5	1/2+x,1.5-y,1-z	9.22	-4.04	0.55	0.89
M1···M6	1.5-x,2-y,1/2+z	23.56	-8.01	1.41	1.76
M1···M7	x,1.5-y,1/2+z	21.25	-4.35	1.27	0.96
M1···M8	1-x,2-y,1-z	17.75	-1.32	1.06	0.29
M1···M9	-1/2+x,1.5-y,1-z	9.22	-4.04	0.55	0.89
M1···M10	1-x,1/2+y,1/2-z	7.71	0.03	0.46	-0.01
M1···M11	-1/2+x,y,1/2-z	13.23	-3.43	0.79	0.75
M1···M12	1-x,-1/2+y,1/2-z	7.71	0.03	0.46	-0.01
M1···M13	1.5-x,2-y,-1/2+z	23.56	-8.01	1.41	1.76
M1···M14	x,1.5-y,-1/2+z	21.25	-4.35	1.27	0.96
Total		217.39	-50.04	13.00	13.00

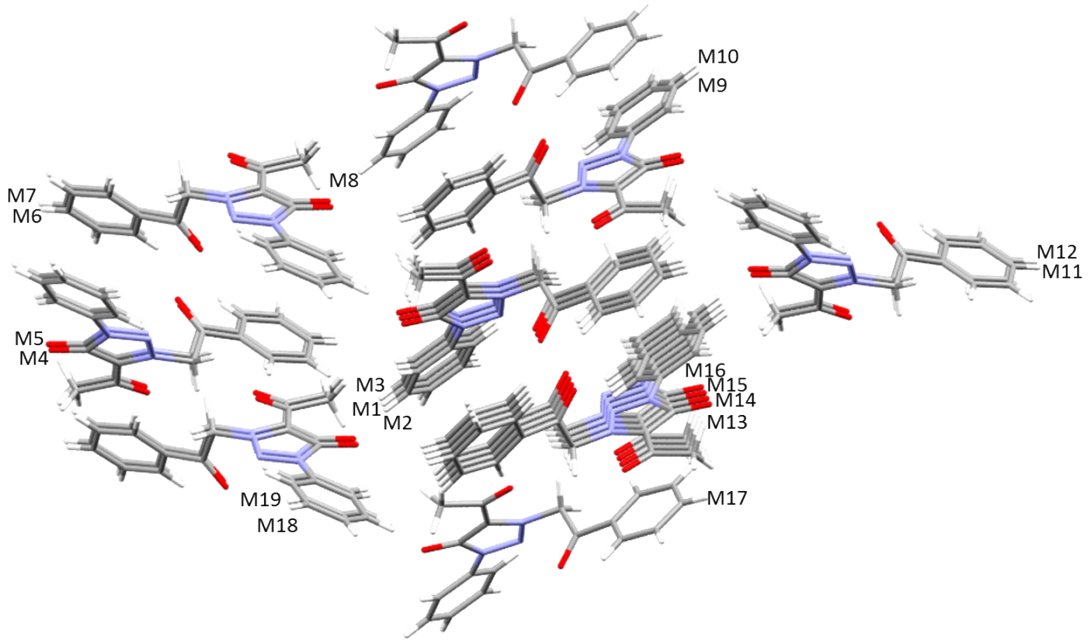


Figure S13 Supramolecular cluster of compound **11**

Table S12 Contact area and energetic data of each dimer from the supramolecular cluster of dimers of compound **11**

Dimer	Symmetry Code	$C_{M1\cdots MN}$ (Å^2)	$G_{M1\cdots MN}$ (kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	x,1+y,z	33.88	-6.08	1.53	1.40
M1···M3	x,-1+y,z	33.88	-6.08	1.53	1.40
M1···M4	1.5-x,2-y,-1/2+z	8.45	-2.29	0.38	0.53
M1···M5	1.5-x,1-y,-1/2+z	9.44	-1.47	0.43	0.34
M1···M6	1/2+x,1.5-y,-z	14.82	-1.60	0.67	0.37
M1···M7	1/2+x,1/2-y,-z	12.75	-3.47	0.58	0.80
M1···M8	1+x,1+y,z	5.16	-0.60	0.23	0.14
M1···M9	2-x,1/2+y,1/2-z	57.22	-13.06	2.59	3.01
M1···M10	2-x,-1/2+y,1/2-z	57.22	-13.06	2.59	3.01
M1···M11	1.5-x,2-y,1/2+z	8.45	-2.29	0.38	0.53
M1···M12	1.5-x,1-y,1/2+z	9.44	-1.47	0.43	0.34
M1···M13	1-x,1.5+y,1/2-z	12.73	-0.70	0.58	0.16
M1···M14	1-x,1/2+y,1/2-z	44.31	-9.72	2.01	2.24
M1···M15	1-x,-1/2+y,1/2-z	44.31	-9.72	2.01	2.24
M1···M16	1-x,-1.5+y,1/2-z	12.73	-0.70	0.58	0.16
M1···M17	-1+x,-1+y,z	5.16	-0.60	0.23	0.14
M1···M18	-1/2+x,1.5-y,-z	14.82	-1.60	0.67	0.37
M1···M19	-1/2+x,1/2-y,-z	12.75	-3.47	0.58	0.80
Total		397.52	-68.42	18.00	18.00

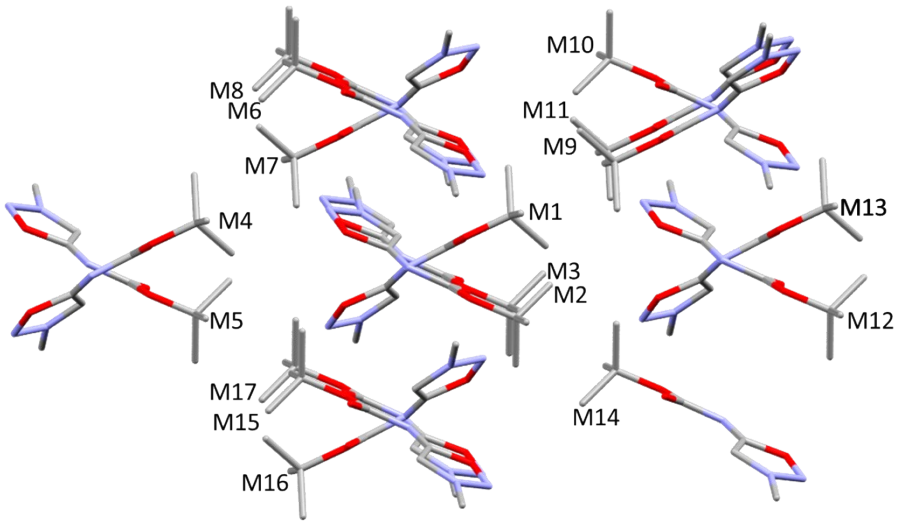


Figure S14 Supramolecular cluster of compound **12**

Table S13 Contact area and energetic data of each dimer from the supramolecular cluster of dimers of compound **12**

Dimer	Symmetry Code	$C_{M1\cdots MN}$ (Å^2)	$G_{M1\cdots MN}$ (kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	x,1/2-y,1/2+z	33.12	-9.75	1.91	2.54
M1···M3	x,1/2-y,-1/2+z	33.12	-9.75	1.91	2.54
M1···M4	-1+x,y,z	3.4	-0.17	0.20	0.05
M1···M5	-1+x,1/2-y,-1/2+z	14.71	-1.31	0.85	0.34
M1···M6	1-x,1/2+y,1.5-z	9.27	-0.29	0.53	0.08
M1···M7	1-x,1-y,1-z	28.24	-3.56	1.62	0.93
M1···M8	1-x,1/2+y,1/2-z	16.32	-5.29	0.94	1.38
M1···M9	2-x,1-y,2-z	1.39	-0.23	0.08	0.06
M1···M10	2-x,1/2+y,1.5-z	16	-1.54	0.92	0.40
M1···M11	2-x,1-y,1-z	16.99	-2.35	0.98	0.61
M1···M12	1+x,1/2-y,1/2+z	14.71	-1.31	0.85	0.34
M1···M13	1+x,y,z	3.4	-0.17	0.20	0.05
M1···M14	2-x,-1/2+y,1.5-z	16	-1.54	0.92	0.40
M1···M15	1-x,-1/2+y,1.5-z	9.27	-0.29	0.53	0.08
M1···M16	1-x,-y,1-z	45.82	-18.55	2.64	4.84
M1···M17	1-x,-1/2+y,1/2-z	16.32	-5.29	0.94	1.38
Total		278.08	-51.64	16.00	16.00

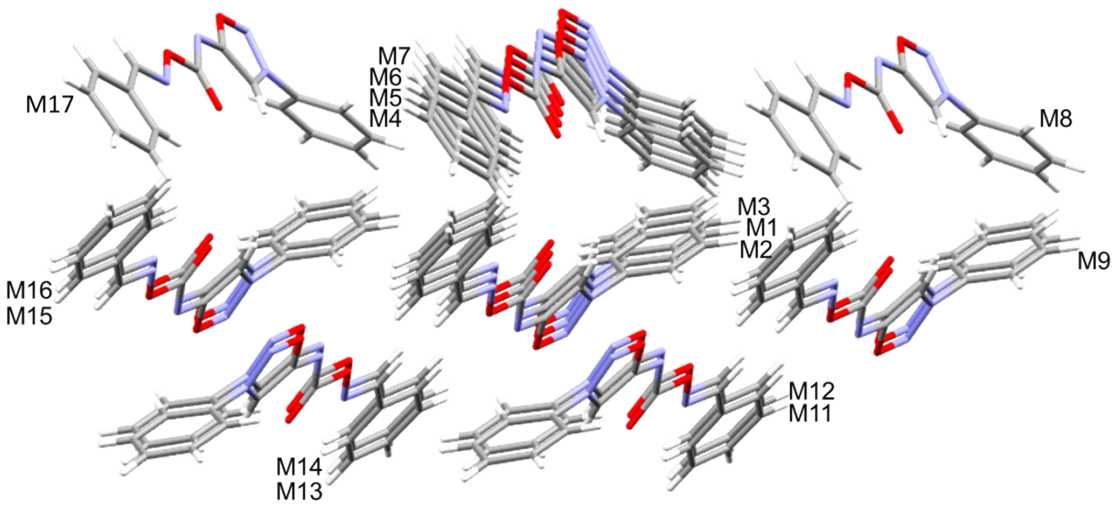


Figure S15 Supramolecular cluster of compound **13**

Table S14 Contact area and energetic data of each dimer from the supramolecular cluster of dimers of compound **13**

Dimer	Symmetry Code	$C_{M1\cdots MN}$ (Å^2)	$G_{M1\cdots MN}$ (kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	x,y,1+z	47.54	-12.21	1.91	2.14
M1···M3	x,y,-1+z	47.54	-12.21	1.91	2.14
M1···M4	x,1/2-y,-1.5+z	3.06	-1.04	0.12	0.18
M1···M5	x,1/2-y,-1/2+z	43.61	-6.98	1.75	1.22
M1···M6	x,1/2-y,1/2+z	43.61	-6.98	1.75	1.22
M1···M7	x,1/2-y,1.5+z	3.06	-1.04	0.12	0.18
M1···M8	1+x,1/2-y,1.5+z	11.94	-3.65	0.48	0.64
M1···M9	1+x,y,1+z	15.1	-4.43	0.61	0.78
M1···M10	1+x,y,2+z	15.16	-1.58	0.61	0.28
M1···M11	1-x,1-y,1-z	46.84	-15.82	1.88	2.77
M1···M12	1-x,1-y,2-z	20.1	-4.58	0.81	0.80
M1···M13	-x,1-y,-1-z	19.95	-3.01	0.80	0.53
M1···M14	-x,1-y,-z	37.94	-8.26	1.53	1.44
M1···M15	-1+x,y,-2+z	15.16	-1.58	0.61	0.28
M1···M16	-1+x,y,-1+z	15.10	-4.43	0.61	0.78
M1···M17	-1+x,1/2-y,-1.5+z	11.94	-3.65	0.48	0.64
Total		370.61	-83.37	16.00	16.00

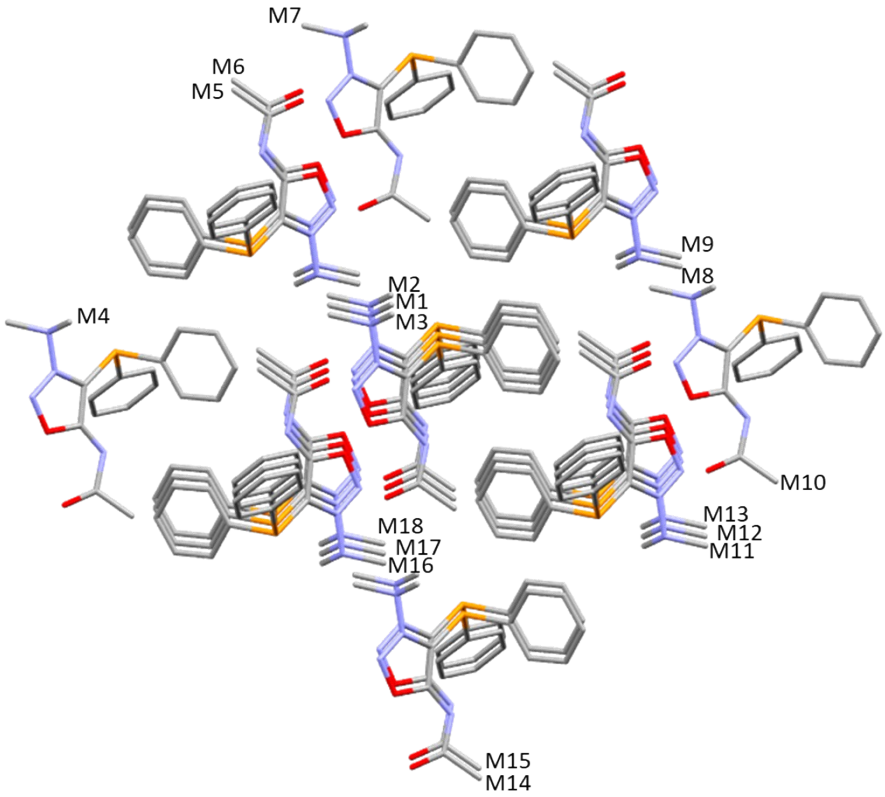


Figure S16 Supramolecular cluster of compound **14**

Table S15 Contact area and energetic data of each dimer from the supramolecular cluster of dimers of compound **14**

Dimer	Symmetry Code	$C_{M1\cdots MN}$ (Å^2)	$G_{M1\cdots MN}$ (kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	1+x,y,z	46.97	-9.61	1.76	1.79
M1···M3	-1+x,y,z	46.97	-9.61	1.76	1.79
M1···M4	x,y,1+z	11.27	-1.38	0.42	0.26
M1···M5	2-x,2-y,2-z	21.92	-1.06	0.82	0.20
M1···M6	1-x,2-y,2-z	27.08	-7.51	1.02	1.40
M1···M7	x,1+y,z	23.9	-5.73	0.90	1.07
M1···M8	2-x,2-y,1-z	25.45	-1.66	0.96	0.31
M1···M9	1-x,2-y,1-z	33.33	-6.29	1.25	1.17
M1···M10	x,y,-1+z	11.27	-1.38	0.42	0.26
M1···M11	2-x,1-y,1-z	10.66	-2.89	0.40	0.54
M1···M12	1-x,1-y,1-z	93.95	-14.99	3.53	2.80
M1···M13	-x,1-y,1-z	5.74	-1.41	0.22	0.26
M1···M14	x,-1+y,z	23.9	-5.73	0.90	1.07
M1···M15	-1+x,-1+y,z	0.08	-0.78	0.00	0.15
M1···M16	2-x,1-y,2-z	0.15	-2.83	0.01	0.53
M1···M17	1-x,1-y,2-z	64.4	-17.22	2.42	3.22
M1···M17	-x,1-y,2-z	5.53	-0.94	0.21	0.18
Total		452.57	-81.41	17.00	17.00

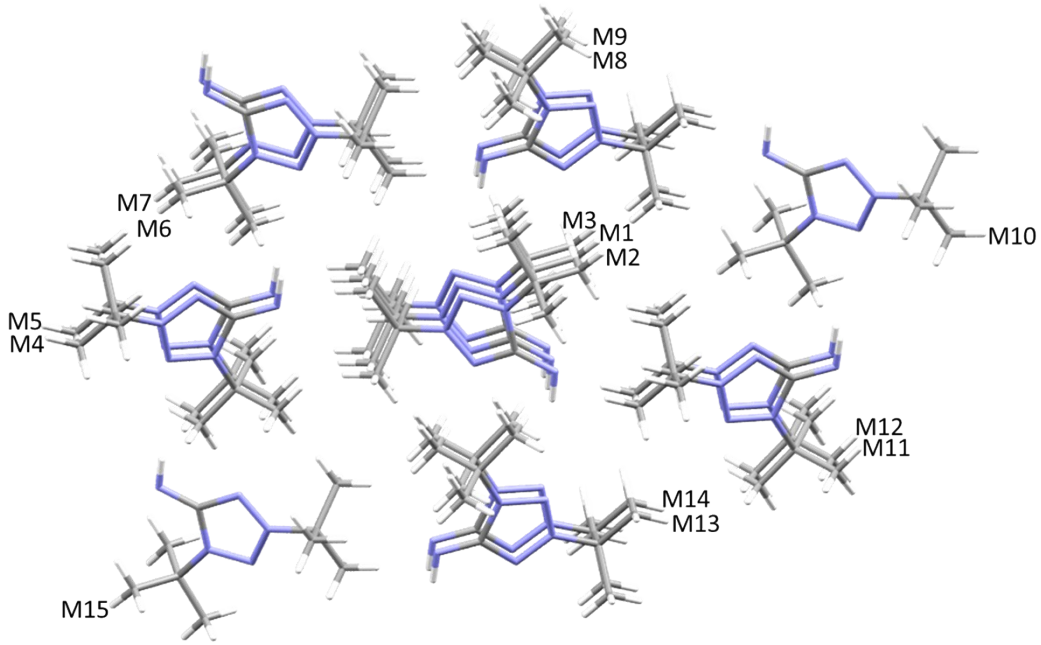


Figure S17 Supramolecular cluster of compound **15**

Table S16 Contact area and energetic data of each dimer from the supramolecular cluster of dimers of compound **15**

Dimer	Symmetry Code	$C_{M1\cdots MN}$ (Å^2)	$G_{M1\cdots MN}$ (kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	1+x,y,z	36.78	-4.62	1.75	1.31
M1···M3	-1+x,y,z	36.78	-4.62	1.75	1.31
M1···M4	1-x,-1/2+y,1/2-z	16.44	-2.79	0.78	0.79
M1···M5	-x,-1/2+y,1/2-z	17.66	-4.94	0.84	1.40
M1···M6	1-x,-y,1-z	22.22	-2.52	1.06	0.71
M1···M7	-x,-y,1-z	11.67	-1.71	0.56	0.49
M1···M8	1+x,1/2-y,1/2+z	23.36	-3.74	1.11	1.06
M1···M9	x,1/2-y,1/2+z	30.33	-5.17	1.44	1.47
M1···M10	1-x,1-y,1-z	3.46	-0.94	0.16	0.27
M1···M11	1-x,1/2+y,1/2-z	16.44	-2.79	0.78	0.79
M1···M12	-x,1/2+y,1/2-z	17.66	-4.94	0.84	1.40
M1···M13	x,1/2-y,-1/2+z	30.33	-5.17	1.44	1.47
M1···M14	-1+x,1/2-y,-1/2+z	23.36	-3.74	1.11	1.06
M1···M15	-x,-y,-z	7.72	-1.67	0.37	0.47
Total		294.21	-49.37	14.00	14.00

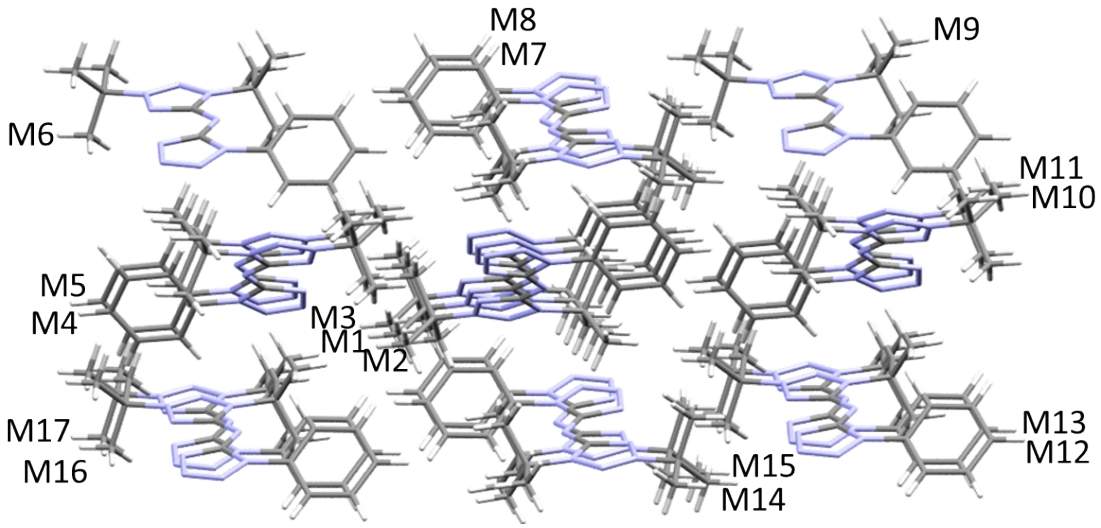


Figure S18 Supramolecular cluster of compound **16**

Table S17 Contact area and energetic data of each dimer from the supramolecular cluster of dimers of compound **16**

Dimer	Symmetry Code	$C_{M1\cdots MN}$ (Å^2)	$G_{M1\cdots MN}$ (kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	1+x,y,z	35.04	-9.13	1.29	1.37
M1···M3	-1+x,y,z	35.04	-9.13	1.29	1.37
M1···M4	1-x,1-y,1-z	38.10	-17.97	1.40	2.70
M1···M5	-x,1-y,1-z	17.38	-17.97	0.64	2.70
M1···M6	-1/2+x,1.5-y,1/2+z	7.32	-0.61	0.27	0.09
M1···M7	1.5-x,1/2+y,1/2-z	35.43	-9.86	1.30	1.48
M1···M8	1/2-x,1/2+y,1/2-z	70.45	-12.40	2.59	1.86
M1···M9	1/2+x,1.5-y,-1/2+z	7.32	-0.61	0.27	0.09
M1···M10	1-x,1-y,-z	32.18	-3.79	1.18	0.57
M1···M11	-x,1-y,-z	0.01	-0.04	0.00	0.01
M1···M12	1/2+x,1/2-y,-1/2+z	15.22	-0.97	0.56	0.15
M1···M13	-1/2+x,1/2-y,-1/2+z	10.08	-0.35	0.37	0.05
M1···M14	1.5-x,-1/2+y,1/2-z	35.43	-9.86	1.30	1.48
M1···M15	1/2-x,-1/2+y,1/2-z	70.45	-12.40	2.59	1.86
M1···M16	1/2+x,1/2-y,1/2+z	10.08	-0.35	0.37	0.05
M1···M17	-1/2+x,1/2-y,1/2+z	15.22	-0.97	0.56	0.15
Total		434.75	-106.41	16.00	16.00

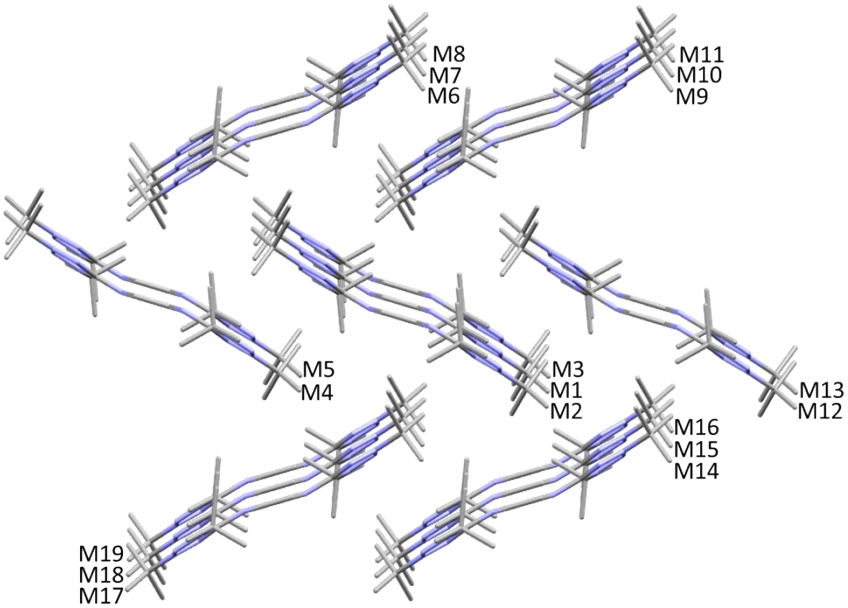


Figure S19 Supramolecular cluster of compound **17**

Table S18 Contact area and energetic data of each dimer from the supramolecular cluster of dimers of compound **17**

Dimer	Symmetry Code	$C_{M1\cdots MN}$ (Å^2)	$G_{M1\cdots MN}$ (kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	1+x,y,z	76.33	-12.25	2.24	2.30
M1···M3	-1+x,y,z	76.33	-12.25	2.24	2.30
M1···M4	x,-1+y,z	44.24	-9.38	1.30	1.76
M1···M5	-1+x,-1+y,z	45.52	-5.81	1.34	1.09
M1···M6	1-x,-1/2+y,1/2-z	3.40	-0.65	0.10	0.12
M1···M7	-x,-1/2+y,1/2-z	53.42	-7.95	1.57	1.49
M1···M8	-1-x,-1/2+y,1/2-z	13.24	-1.69	0.39	0.32
M1···M9	1-x,1/2+y,1/2-z	3.40	-0.65	0.10	0.12
M1···M10	-x,1/2+y,1/2-z	53.42	-7.95	1.57	1.49
M1···M11	-1-x,1/2+y,1/2-z	13.24	-1.69	0.39	0.32
M1···M12	1+x,1+y,z	45.52	-5.81	1.34	1.09
M1···M13	x,1+y,z	44.24	-9.38	1.30	1.76
M1···M14	1-x,1/2+y,-1/2-z	13.24	-1.69	0.39	0.32
M1···M15	-x,1/2+y,-1/2-z	53.42	-7.95	1.57	1.49
M1···M16	-1-x,1/2+y,-1/2-z	3.40	-0.65	0.10	0.12
M1···M17	1-x,-1/2+y,-1/2-z	13.24	-1.69	0.39	0.32
M1···M18	-x,-1/2+y,-1/2-z	53.42	-7.95	1.57	1.49
M1···M19	-1-x,-1/2+y,-1/2-z	3.4	-0.65	0.10	0.12
Total		612.42	-95.99	18.00	18.00

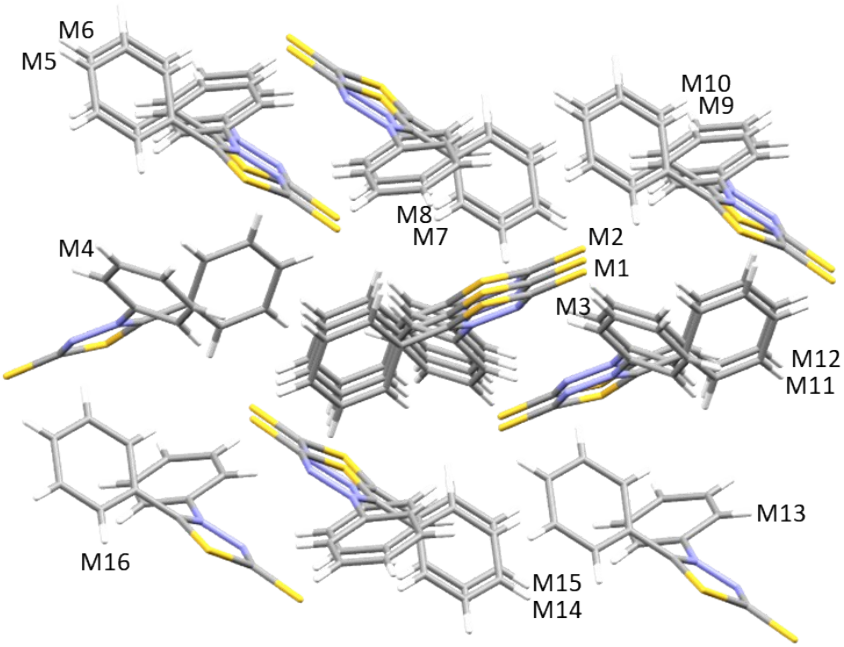


Figure S20 Supramolecular cluster of compound **18**

Table S19 Contact area and energetic data of each dimer from the supramolecular cluster of dimers of compound **18**

Dimer	Symmetry Code	$C_{M1\cdots MN}$ (Å^2)	$G_{M1\cdots MN}$ (kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	1+x,y,z	23.32	-1,67	1.09	0.31
M1···M3	-1+x,y,z	23.32	-1,67	1.09	0.31
M1···M4	1-x,1-y,2-z	45.59	-3,61	2.12	0.66
M1···M5	1/2+x,1.5-y,1/2+z	8.91	-4,67	0.42	0.85
M1···M6	-1/2+x,1.5-y,1/2+z	5.56	-3,24	0.26	0.59
M1···M7	1.5-x,1/2+y,1.5-z	11.74	-5,25	0.55	0.96
M1···M8	1/2-x,1/2+y,1.5-z	43.77	-8,83	2.04	1.61
M1···M9	1/2+x,1.5-y,-1/2+z	5.56	-3,24	0.26	0.59
M1···M10	-1/2+x,1.5-y,-1/2+z	8.91	-4,67	0.42	0.85
M1···M11	1-x,1-y,1-z	35.49	-16,90	1.65	3.09
M1···M12	-x,1-y,1-z	25.34	-12,53	1.18	2.29
M1···M13	-1/2+x,1/2-y,-1/2+z	14.45	-0,84	0.67	0.15
M1···M14	1.5-x,-1/2+y,1.5-z	11.74	-5,25	0.55	0.96
M1···M15	1/2-x,-1/2+y,1.5-z	43.77	-8,83	2.04	1.61
M1···M16	1/2+x,1/2-y,1/2+z	14.45	-0,84	0.67	0.15
Total		321.92	-82.02	15.00	15.00

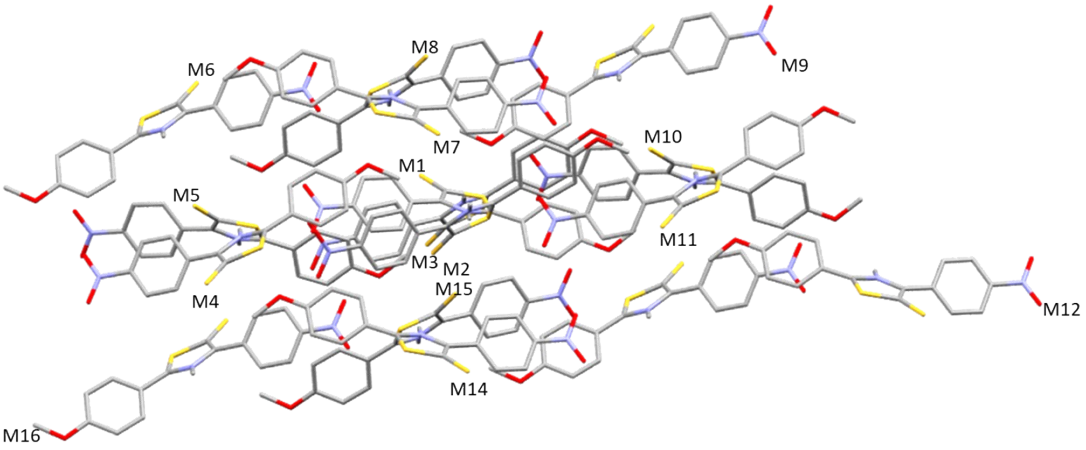


Figure S21 Supramolecular cluster of compound **19**

Table S20 Contact area and energetic data of each dimer from the supramolecular cluster of dimers of compound **19**

Dimer	Symmetry Code	$C_{M1\cdots MN}$ (Å^2)	$G_{M1\cdots MN}$ (kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	1.5-x,1/2+y,z	12.61	-5.32	0.46	0.78
M1···M3	1.5-x,-1/2+y,z	12.61	-5.32	0.46	0.78
M1···M4	1.5-x,1-y,-1/2+z	38.01	-7.88	1.39	1.15
M1···M5	x,1/2-y,-1/2+z	41.88	-8.50	1.54	1.24
M1···M6	1/2+x,y,1/2-z	12.84	-2.34	0.47	0.34
M1···M7	2-x,1-y,1-z	4.95	-4.22	0.18	0.62
M1···M8	1/2+x,1/2-y,1-z	36.07	-16.33	1.32	2.38
M1···M9	1/2+x,y,1.5-z	42.87	-7.26	1.57	1.06
M1···M10	1.5-x,1-y,1/2+z	38.01	-7.88	1.39	1.15
M1···M11	x,1/2-y,1/2+z	41.88	-8.50	1.54	1.24
M1···M12	1-x,1-y,2-z	3.59	0.60	0.13	-0.09
M1···M13	-1/2+x,y,1.5-z	42.87	-7.26	1.57	1.06
M1···M14	1-x,1-y,1-z	31.98	-3.87	1.17	0.56
M1···M15	-1/2+x,1/2-y,1-z	36.07	-16.33	1.32	2.38
M1···M16	-1/2+x,1/2-y,1-z	12.84	-2.34	0.47	0.34
Total		409.08	-97.42	15.00	15.00

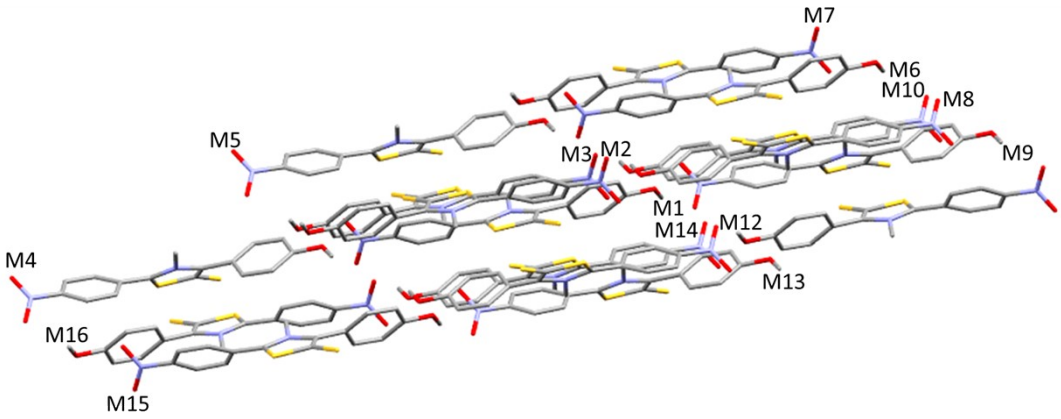


Figure S22 Supramolecular cluster of compound **20**

Table S21 Contact area and energetic data of each dimer from the supramolecular cluster of dimers of compound **20**

Dimer	Symmetry Code	$C_{M1\cdots MN}$ (Å^2)	$G_{M1\cdots MN}$ (kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	1-x,1-y,1-z	16.79	-12.39	0.64	1.78
M1···M3	1-x,-y,1-z	54.3	-5.56	2.07	0.80
M1···M4	1.5+x,1/2-y,1/2+z	15.55	-1.02	0.59	0.15
M1···M5	1/2+x,1/2-y,1/2+z	70.78	-23.72	2.70	3.41
M1···M6	-1+x,y,z	30.86	-5.27	1.18	0.76
M1···M7	-x,-y,1-z	4.05	-0.63	0.15	0.09
M1···M8	-1/2-x,1/2+y,1/2-z	11.94	-2.09	0.46	0.30
M1···M9	-1.5+x,1/2-y,-1/2+z	15.55	-1.02	0.59	0.15
M1···M10	-1/2-x,-1/2+y,1/2-z	11.94	-2.09	0.46	0.30
M1···M11	-1-x,-y,-z	7.84	-0.56	0.30	0.08
M1···M12	1/2-x,1/2+y,1/2-z	20.44	-9.55	0.78	1.37
M1···M13	-1/2+x,1/2-y,-1/2+z	70.78	-23.72	2.70	3.41
M1···M14	1/2-x,-1/2+y,1/2-z	20.44	-9.55	0.78	1.37
M1···M15	1+x,y,z	30.86	-5.27	1.18	0.76
M1···M16	2-x,-y,1-z	10.98	-2.03	0.42	0.29
Total		393.10	-92.09	15.00	15.00

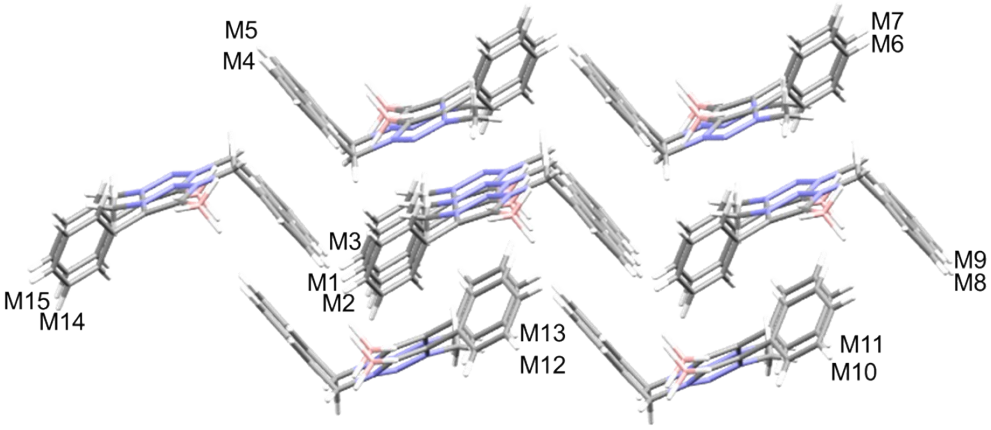


Figure S23 Supramolecular cluster of compound **21**

Table S22 Contact area and energetic data of each dimer from the supramolecular cluster of dimers of compound **21**

Dimer	Symmetry Code	$C_{M1\cdots MN}$ (Å^2)	$G_{M1\cdots MN}$ (kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	x,1+y,z	29.59	-4.25	1.10	0.73
M1···M3	x,-1+y,z	29.59	-4.25	1.10	0.73
M1···M4	x,-1+y,z	15.25	-5.18	0.56	0.88
M1···M5	1-x,-y,-z	64.95	-17.70	2.40	3.02
M1···M6	2-x,-y,-z	35.99	-8.37	1.33	1.43
M1···M7	2-x,-1-y,-z	6.20	-1.18	0.23	0.20
M1···M8	1+x,y,z	17.07	-3.06	0.63	0.52
M1···M9	1+x,-1+y,z	15.86	-1.30	0.59	0.22
M1···M10	2-x,1/2+y,1/2-z	16.26	-3.16	0.60	0.54
M1···M11	2-x,-1/2+y,1/2-z	16.26	-3.16	0.60	0.54
M1···M12	1-x,1/2+y,1/2-z	49.12	-13.03	1.82	2.22
M1···M13	1-x,-1/2+y,1/2-z	49.12	-13.03	1.82	2.22
M1···M14	-1+x,1+y,z	15.86	-1.30	0.59	0.22
M1···M15	-1+x,y,z	17.07	-3.06	0.63	0.52
M1···M16	x,1+y,z	29.59	-4.25	1.10	0.73
Total		378.19	-82.03	14.00	14.00

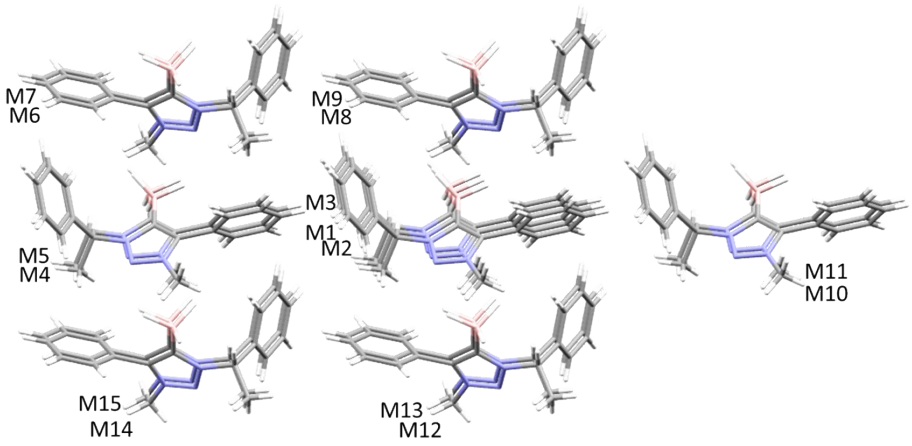


Figure S24 Supramolecular cluster of compound **22**

Table S23 Contact area and energetic data of each dimer from the supramolecular cluster of dimers of compound **22**

Dimer	Symmetry Code	$C_{M1\cdots MN}$ (Å^2)	$G_{M1\cdots MN}$ (kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	1+x,y,z	59.09	-9.92	2.06	1.74
M1···M3	-1+x,y,z	59.09	-9.92	2.06	1.74
M1···M4	1+x,y,1+z	10.86	-1.05	0.38	0.18
M1···M5	x,y,1+z	17.24	-3.37	0.60	0.59
M1···M6	1-x,1/2+y,2-z	12.42	-1.87	0.43	0.33
M1···M7	-x,1/2+y,2-z	0.49	-0.52	0.02	0.09
M1···M8	1-x,1/2+y,1-z	51.73	-12.03	1.80	2.11
M1···M9	-x,1/2+y,1-z	49.11	-11.14	1.71	1.96
M1···M10	x,y,-1+z	17.24	-3.37	0.60	0.59
M1···M11	-1+x,y,-1+z	10.86	-1.05	0.38	0.18
M1···M12	1-x,-1/2+y,1-z	51.73	-12.03	1.80	2.11
M1···M13	-x,-1/2+y,1-z	49.11	-11.14	1.71	1.96
M1···M14	1-x,-1/2+y,2-z	12.42	-1.87	0.43	0.33
M1···M15	-x,-1/2+y,2-z	0.49	-0.52	0.02	0.09
Total		401.88	-69.88	14.00	14.00

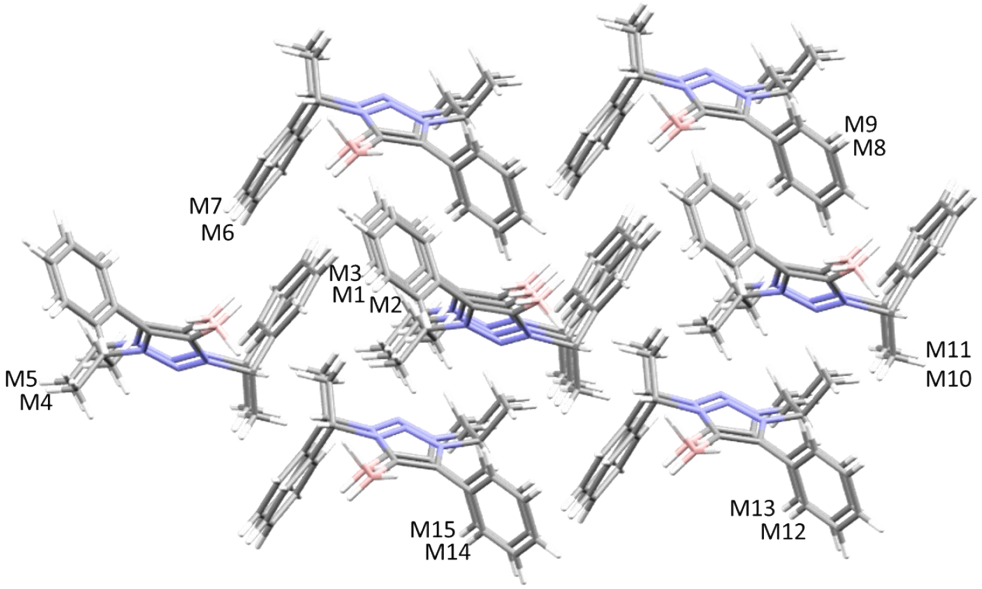


Figure S25 Supramolecular cluster of compound **23**

Table S24 Contact area and energetic data of each dimer from the supramolecular cluster of dimers of compound **23**

Dimer	Symmetry Code	$C_{M1\cdots MN}$ (Å^2)	$G_{M1\cdots MN}$ (kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	x,1+y,z	24.73	-4.81	0.80	0.83
M1···M3	x,-1+y,z	24.73	-4.81	0.80	0.83
M1···M4	1+x,1+y,z	13.68	-1.31	0.44	0.22
M1···M5	1+x,y,z	32.81	-6.13	1.06	1.05
M1···M6	1-x,1/2+y,1-z	50.7	-12.59	1.65	2.16
M1···M7	1-x,-1/2+y,1-z	50.7	-12.59	1.65	2.16
M1···M8	-x,1/2+y,1-z	19.11	-3.66	0.62	0.63
M1···M9	-x,-1/2+y,1-z	19.11	-3.66	0.62	0.63
M1···M10	-1+x,y,z	32.81	-6.13	1.06	1.05
M1···M11	-1+x,-1+y,z	13.68	-1.31	0.44	0.22
M1···M12	-x,1/2+y,-z	23.21	-4.25	0.75	0.73
M1···M13	-x,-1/2+y,-z	23.21	-4.25	0.75	0.73
M1···M14	1-x,1/2+y,-z	51.42	-8.06	1.67	1.38
M1···M15	1-x,-1/2+y,-z	51.42	-8.06	1.67	1.38
Total		431.32	-76.82	14.00	14.00

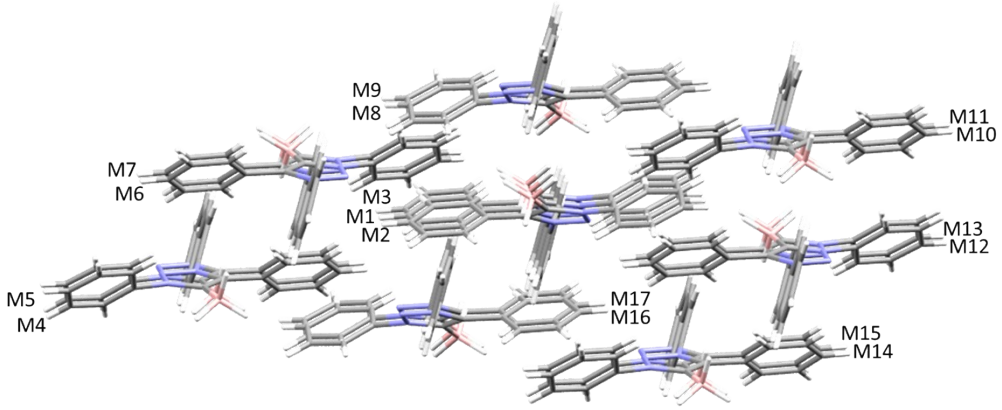


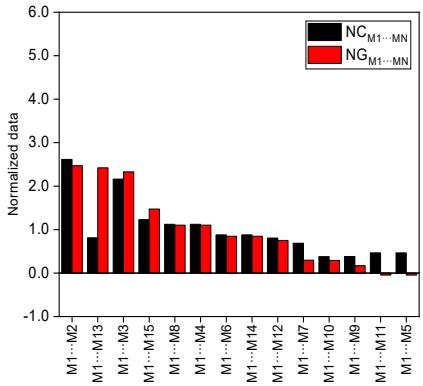
Figure S26 Supramolecular cluster of compound **24**

Table S25 Contact area and energetic data of each dimer from the supramolecular cluster of dimers of compound **24**

Dimer	Symmetry Code	$C_{M1\cdots MN}$ (Å^2)	$G_{M1\cdots MN}$ (kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	x,1+y,z	18.91	-4.91	0.71	0.86
M1···M3	x,-1+y,z	18.91	-4.91	0.71	0.86
M1···M4	-1/2-x,1/2+y,-1/2-z	2.77	-0.06	0.10	0.01
M1···M5	-1/2-x,-1/2+y,-1/2-z	2.77	-0.06	0.10	0.01
M1···M6	-1/2+x,1.5-y,-1/2+z	14.53	-3.71	0.55	0.65
M1···M7	-1/2+x,1/2-y,-1/2+z	29.97	-5.51	1.13	0.96
M1···M8	1-x,1-y,-z	77.12	-27.95	2.90	4.88
M1···M9	1-x,-y,-z	15.47	-1.41	0.58	0.25
M1···M10	1.5-x,1/2+y,1/2-z	25.72	-2.59	0.97	0.45
M1···M11	1.5-x,-1/2+y,1/2-z	25.72	-2.59	0.97	0.45
M1···M12	1/2+x,1.5-y,1/2+z	14.53	-3.71	0.55	0.65
M1···M13	1/2+x,1/2-y,1/2+z	29.97	-5.51	1.13	0.96
M1···M14	1/2-x,1/2+y,1/2-z	15.01	-2.95	0.56	0.52
M1···M15	1/2-x,-1/2+y,1/2-z	15.01	-2.95	0.56	0.52
M1···M16	-x,1-y,-z	72.77	-16.63	2.73	2.91
M1···M17	-x,-y,-z	46.59	-6.10	1.75	1.07
Total		425.77	-86.64	16.00	16.00

4. Normalized Data

Table S26 Contact area (NC) and energetic (NG) data normalized of all 24 compounds.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NG$_{M1\cdots MN}$
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2.0
1.0
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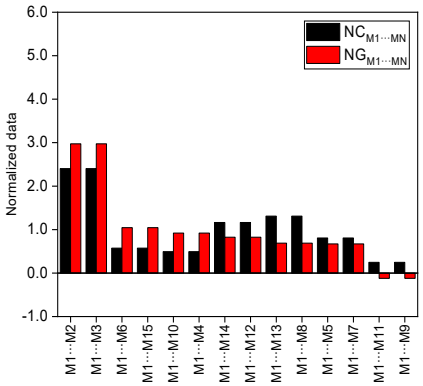
-1.0
M1···M2
M1···M13
M1···M3
M1···M15
M1···M8
M1···M4
M1···M6
M1···M14
M1···M12
M1···M7
M1···M10
M1···M9
M1···M11
M1···M5

1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NG$_{M1\cdots MN}$
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2.0
1.0
0.0
-1.0
M1···M2
M1···M3
M1···M6
M1···M15
M1···M10
M1···M4
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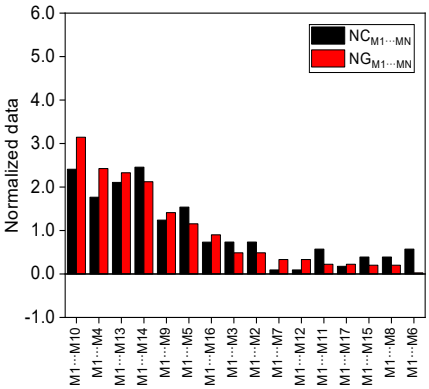
M1···M8
M1···M5
M1···M7
M1···M11
M1···M9

2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NG$_{M1\cdots MN}$
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3.0
2.0
1.0
0.0
-1.0
M1···M10
M1···M4
M1···M13
M1···M14
M1···M9
M1···M5
M1···M16
M1···M3
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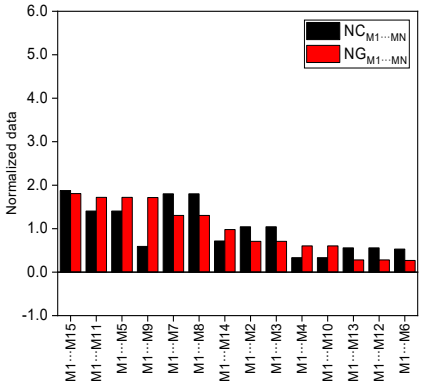
M1···M6

3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NG$_{M1\cdots MN}$
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2.0
1.0
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M1···M11
M1···M5
M1···M9
M1···M7
M1···M8
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M1···M4
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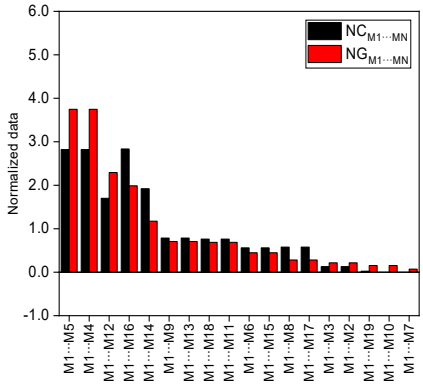
M1···M13
M1···M12
M1···M6

4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NG$_{M1\cdots MN}$
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1.0
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M1···M5
M1···M4
M1···M12
M1···M16
M1···M14
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M1···M13
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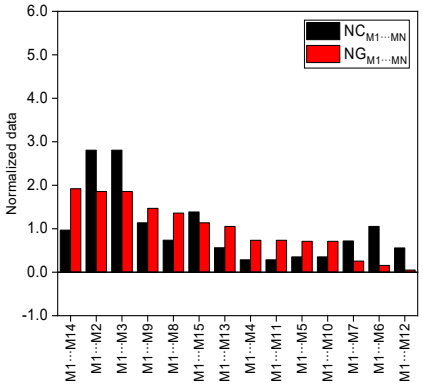
5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NG$_{M1\cdots MN}$
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M1···M3
M1···M9
M1···M8
M1···M15
M1···M13
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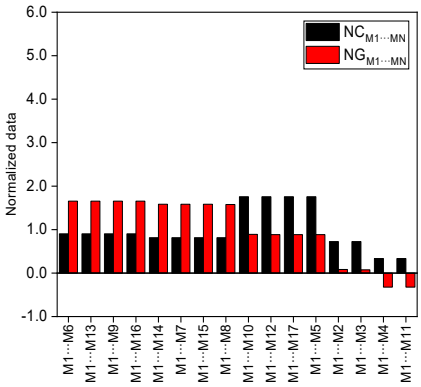
M1···M11
M1···M5
M1···M10
M1···M7
M1···M6
M1···M12

6


Normalized data
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NG M1···MN
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M1···M13
M1···M9
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M1···M7
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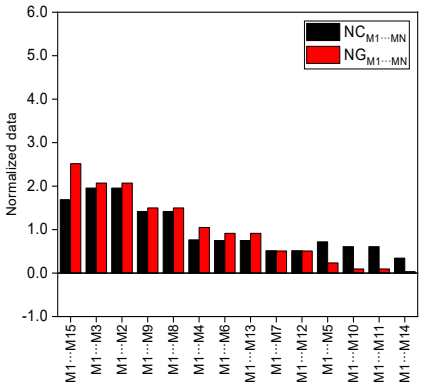
M1···M11

7


Normalized data
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NG M1···MN
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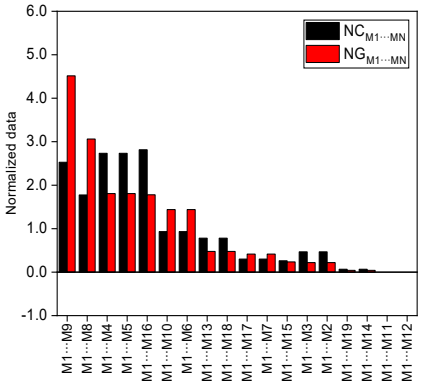
M1···M10
M1···M11
M1···M14

8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M1···M6
M1···M13
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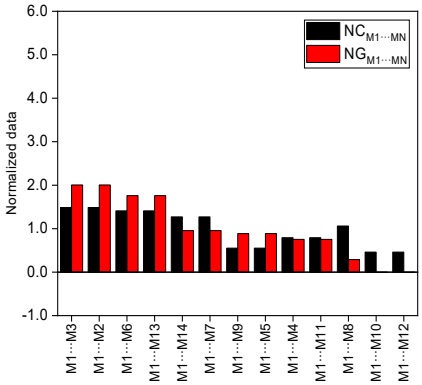
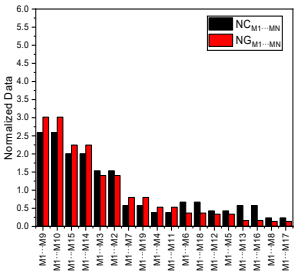
M1···M17
M1···M7
M1···M15
M1···M3
M1···M2
M1···M19
M1···M14
M1···M11
M1···M12

9


Normalized data
NC M1···MN
NG M1···MN
M1···M3
M1···M2
M1···M6
M1···M13
M1···M14
M1···M7
M1···M9
M1···M5
M1···M4
M1···M11
M1···M8
M1···M10
M1···M12

10


Normalized Data
NC M1···MN
NG M1···MN

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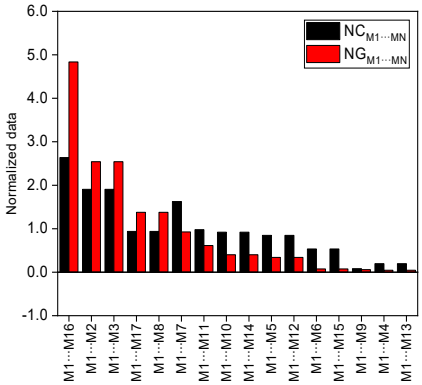
Normalized data
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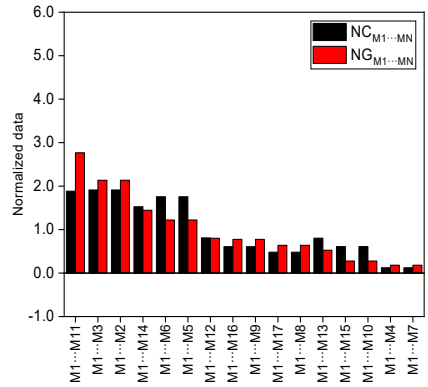
NG M1···MN
M1···M16
M1···M2
M1···M3
M1···M17
M1···M8
M1···M7
M1···M11
M1···M10
M1···M14
M1···M5
M1···M12
M1···M6
M1···M15
M1···M9
M1···M4
M1···M13

12



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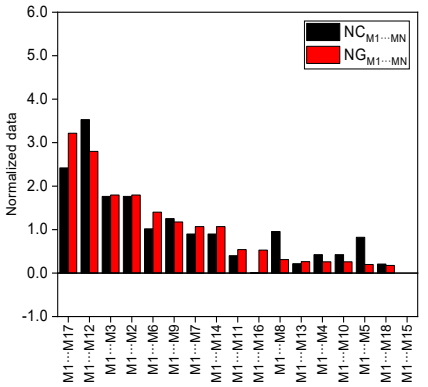

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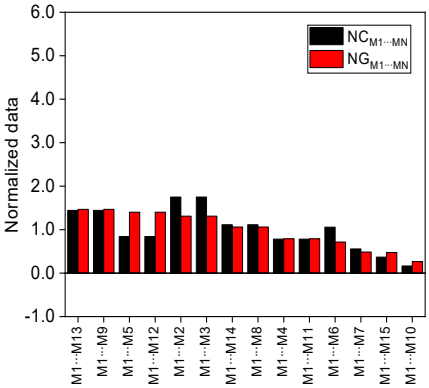

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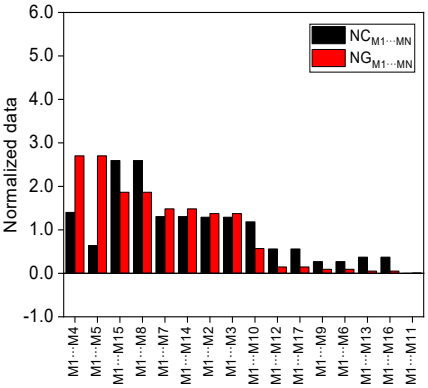

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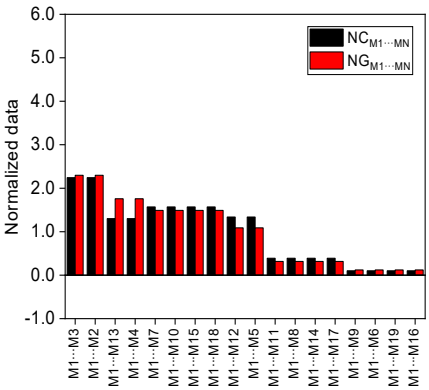

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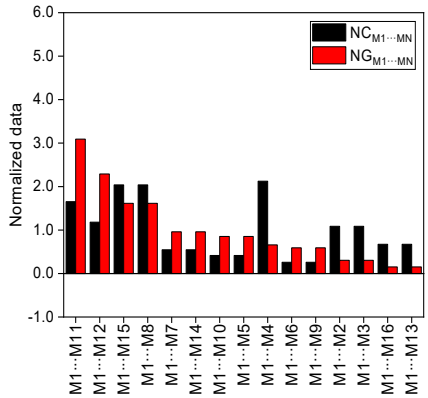

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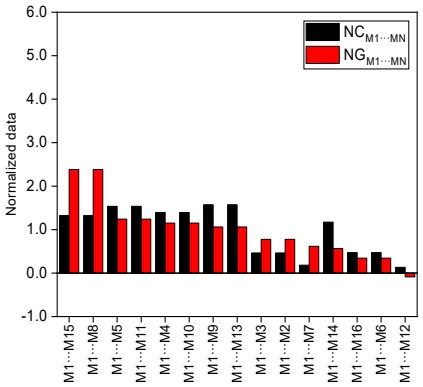

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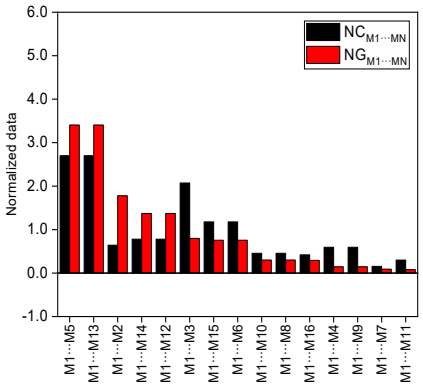

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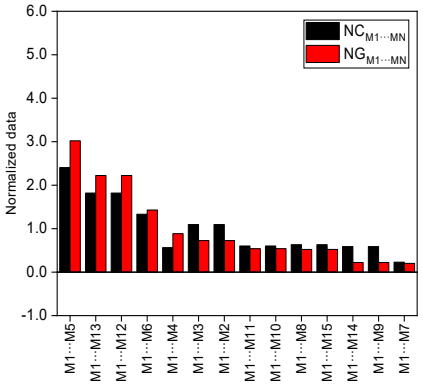

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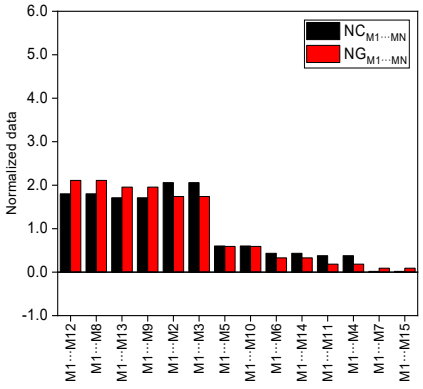

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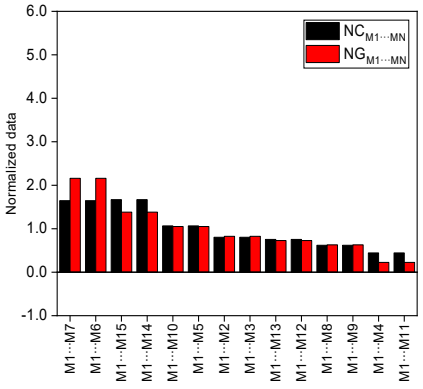

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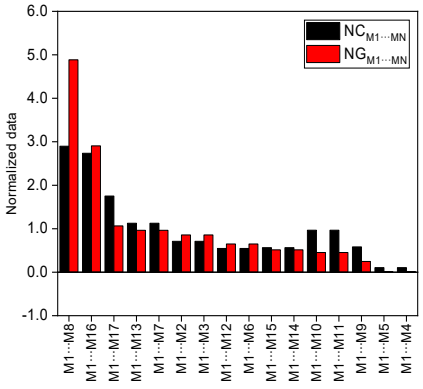


24

5. Supramolecular cluster data, CEE and CPE data

Table S27 Supramolecular cluster data, CEE and CPE data for structures **1-24**

Cpd	N	$C_{cluster}$[a]	$G_{cluster}$[b]	$SG_{M1\cdots MN}<0$	$SG_{M1\cdots MN}<0$	CEE[c]	CPE[d]
1	14	272.60	-62.79	-63.20	0.41	0.994	0.899
2	14	235.52	-64.95	-66.08	1.13	0.983	0.948
3	16	292.15	-58.83	-58.83	0.00	1.000	0.876
4	14	291.73	-67.34	-67.34	0.00	1.000	0.919
5	18	273.96	-74.75	-74.75	0.00	1.000	0.902
6	14	287.88	-81.64	-81.64	0.00	1.000	0.943
7	16	227.12	-61.18	-63.65	2.47	0.961	0.912
8	14	282.17	-55.62	-55.62	0.00	1.000	0.890
9	18	330.14	-76.05	-77.71	1.66	0.979	0.909
10	13	217.39	-59.16	-59.21	0.05	0.999	0.924
11	18	397.52	-77.97	-77.97	0.00	1.000	0.876
12	16	278.08	-61.39	-61.39	0.00	1.000	0.876
13	16	397.65	-91.46	-91.46	0.00	1.000	0.886
14	17	452.57	-91.03	-91.03	0.00	1.000	0.880
15	14	294.21	-49.37	-49.37	0.00	1.000	0.896
16	16	434.75	-106.41	-106.41	0.00	1.000	0.898
17	18	612.42	-95.99	-95.99	0.00	1.000	0.838
18	15	321.92	-82.02	-82.02	0.00	1.000	0.876
19	15	409.08	-102.74	-103.34	0.60	0.994	0.905
20	15	393.10	-104.47	-104.47	0.00	1.000	0.935
21	14	378.19	-82.03	-82.03	0.00	1.000	0.885
22	14	401.88	-79.80	-79.80	0.00	1.000	0.892
23	14	431.32	-81.63	-81.63	0.00	1.000	0.882
24	16	425.77	-91.55	-91.55	0.00	1.000	0.896

[a]In $Å^2$. [b]In kcal mol^{-1}. [c]Calculated with eq 1. [d]CPE = $(V_c-V_v)/V_c$; where CPE is the crystal packing efficiency; V_v, void volume (obtained using the CrystalExplorer software, with isovalue of 0.002e au^{-3}); and V_c, cell volume.

6. Crystallization Mechanisms

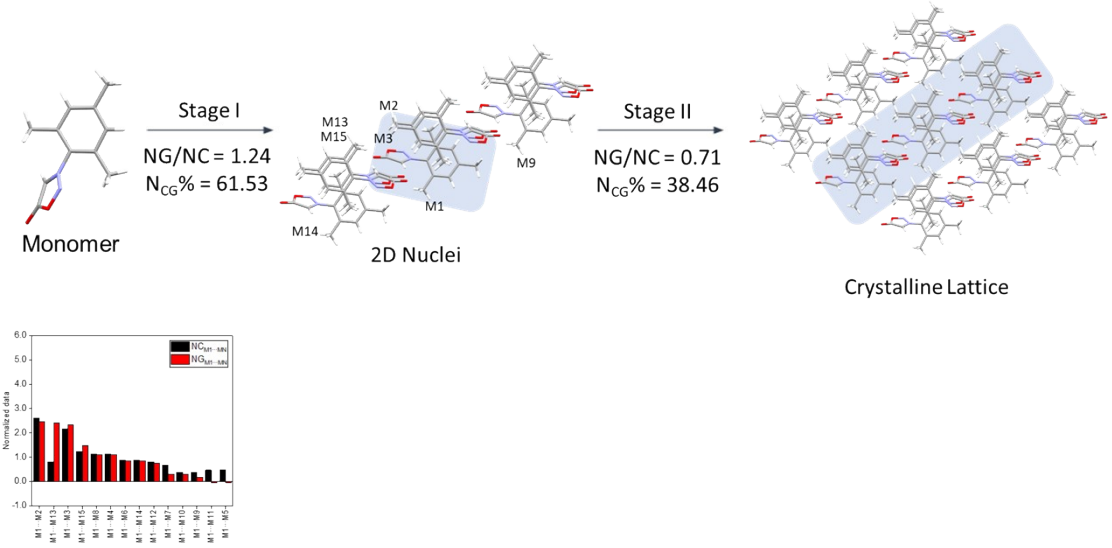


Figure S27 Crystallization mechanism of compound **1**

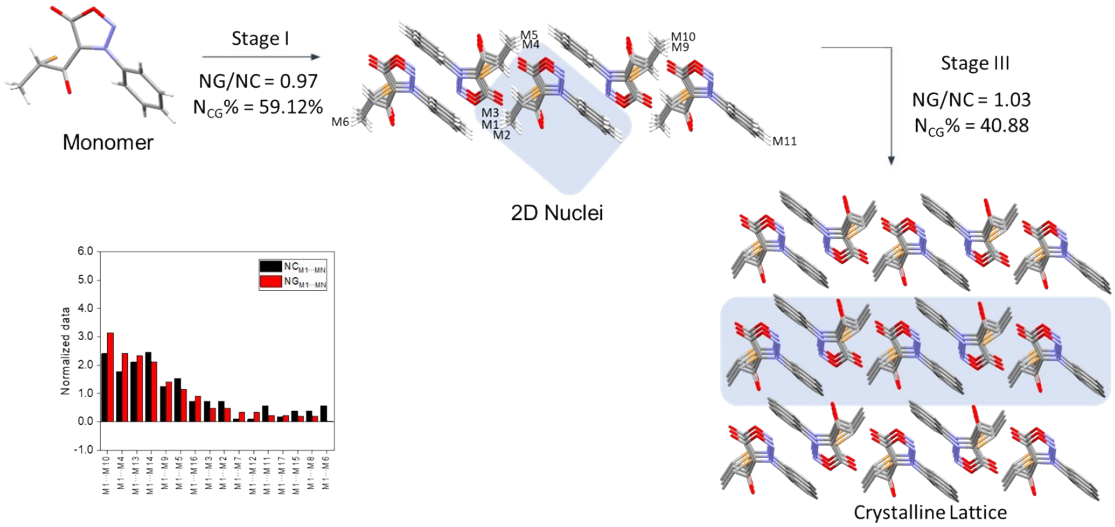


Figure S28 Crystallization mechanism of compound **3**

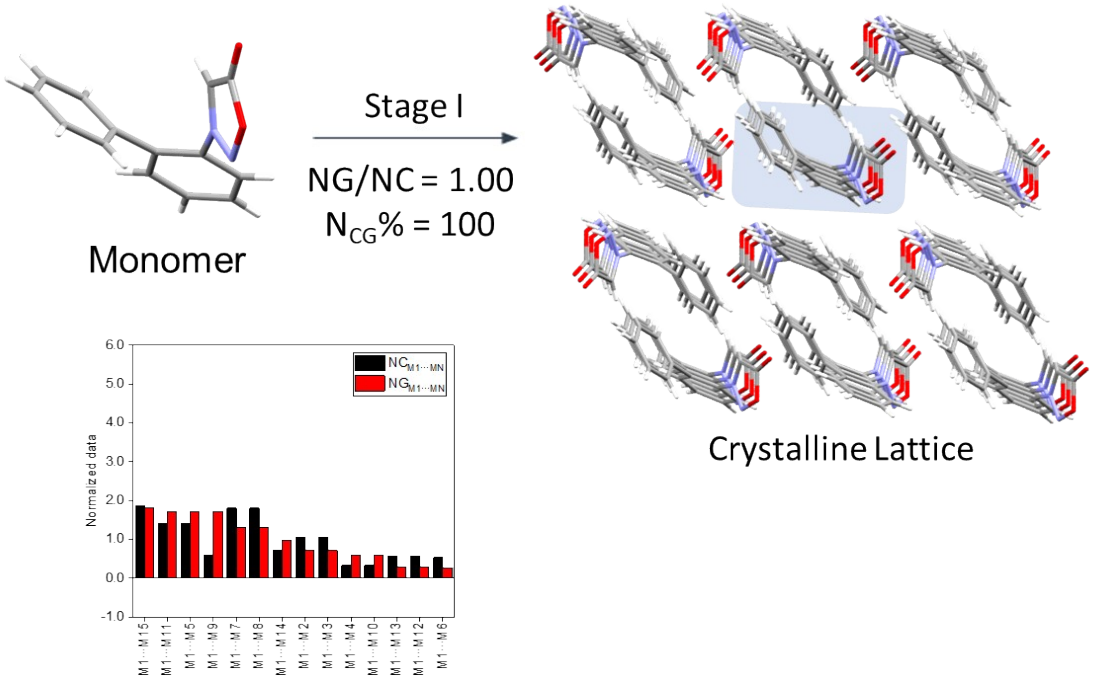


Figure S29 Crystallization mechanism of compound **4**

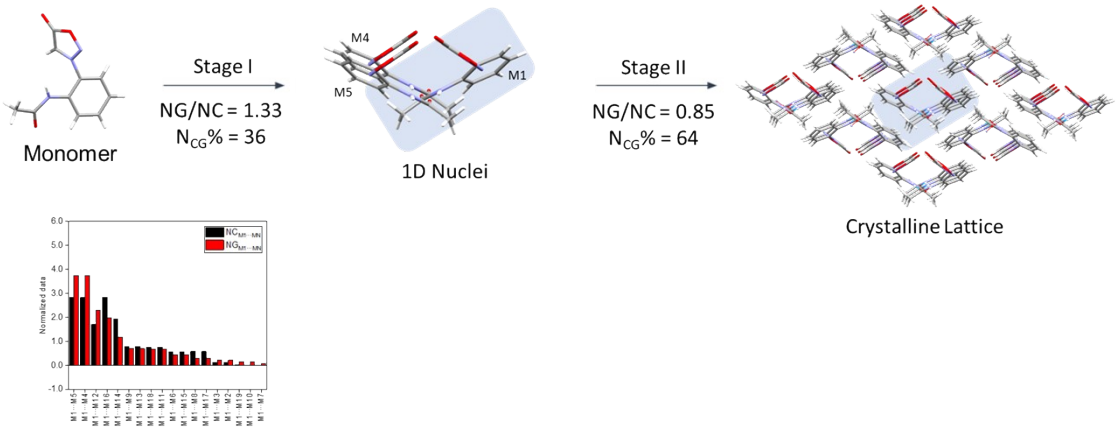


Figure S30 Crystallization mechanism of compound **5**

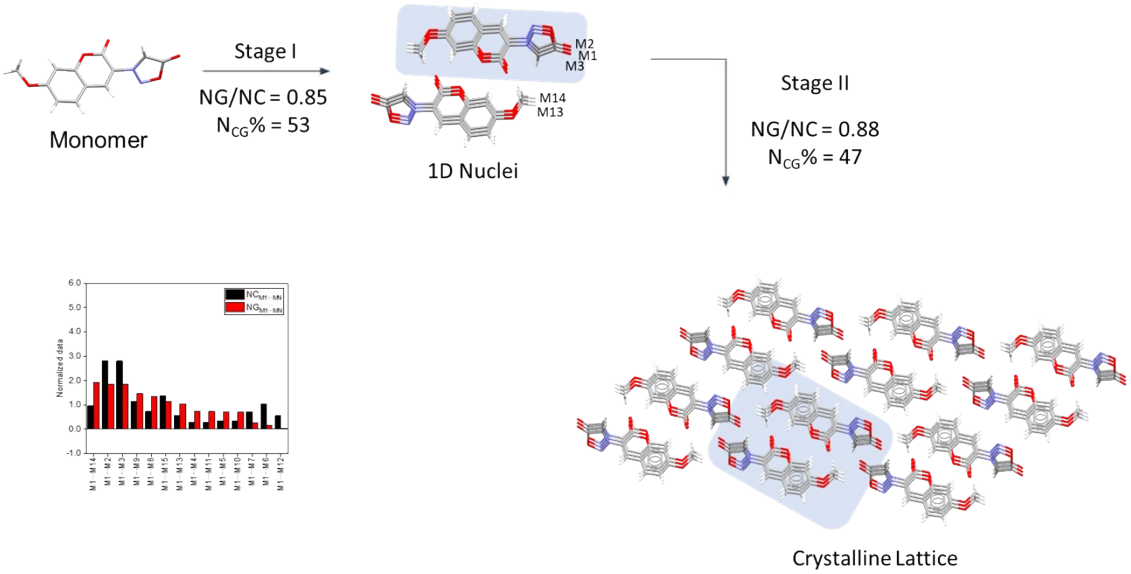


Figure S31 Crystallization mechanism of compound **6**

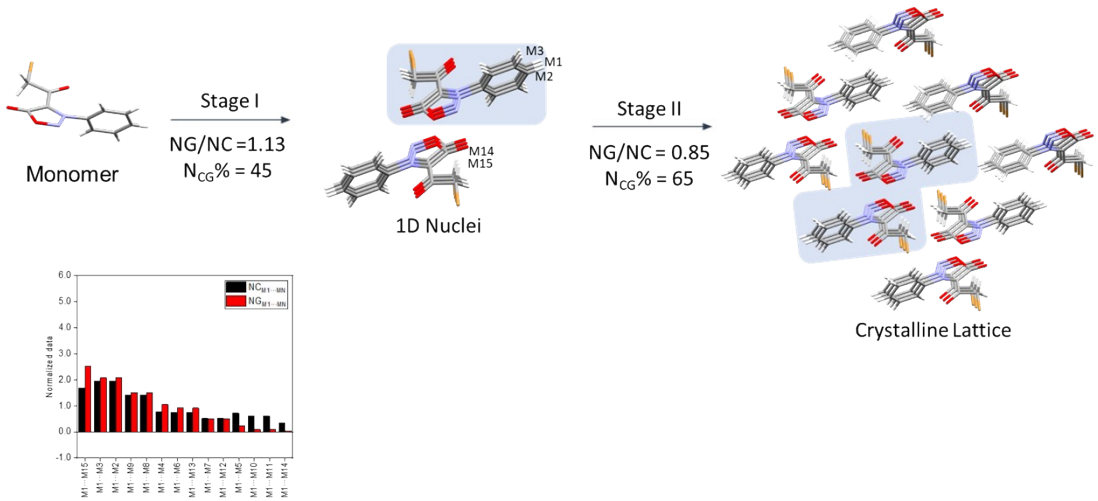


Figure S32 Crystallization mechanism of compound **8**

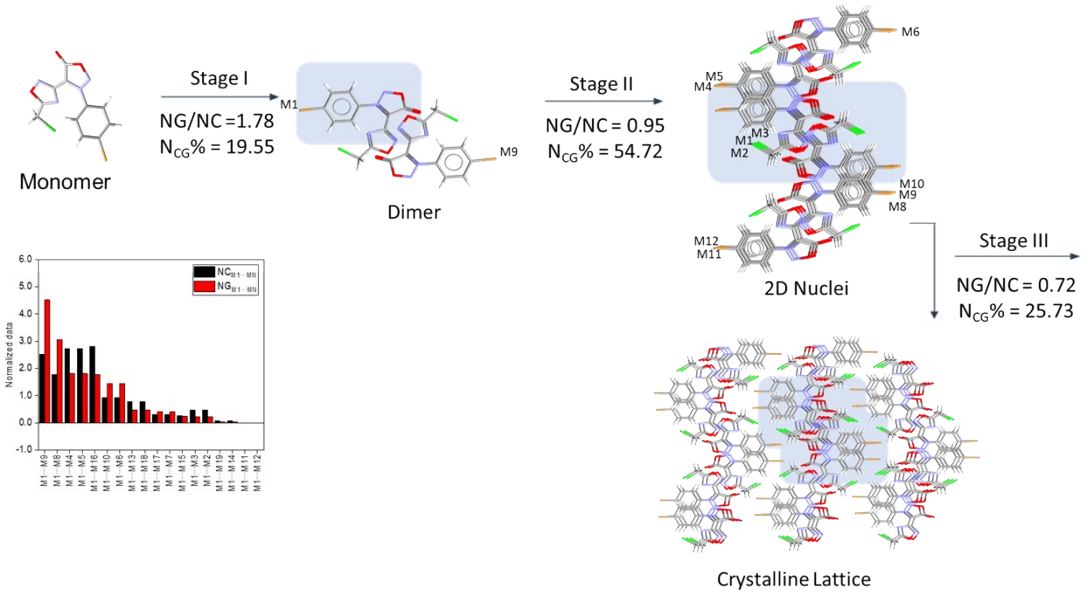


Figure S33 Crystallization mechanism of compound **9**

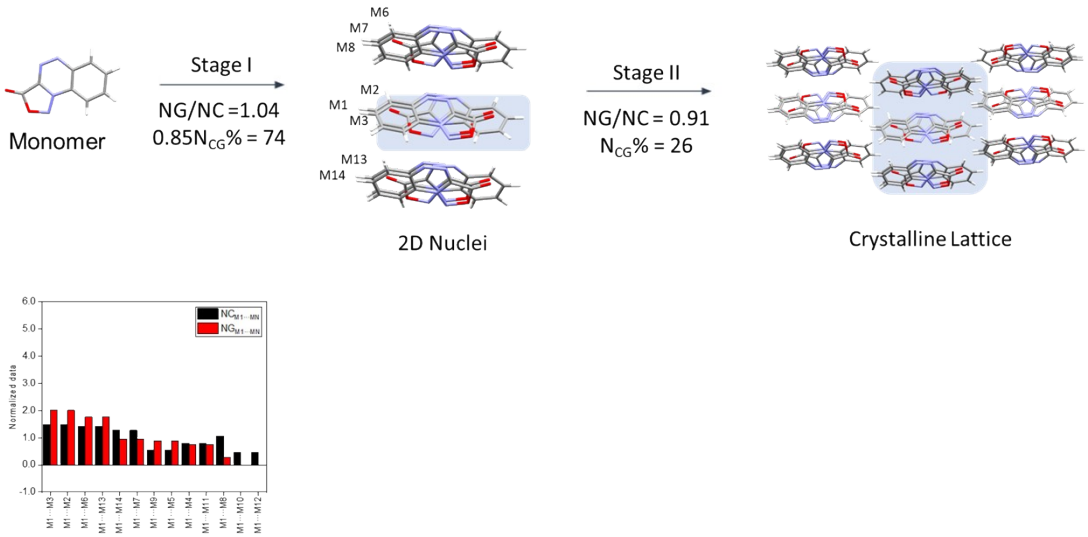


Figure S34 Crystallization mechanism of compound **10**

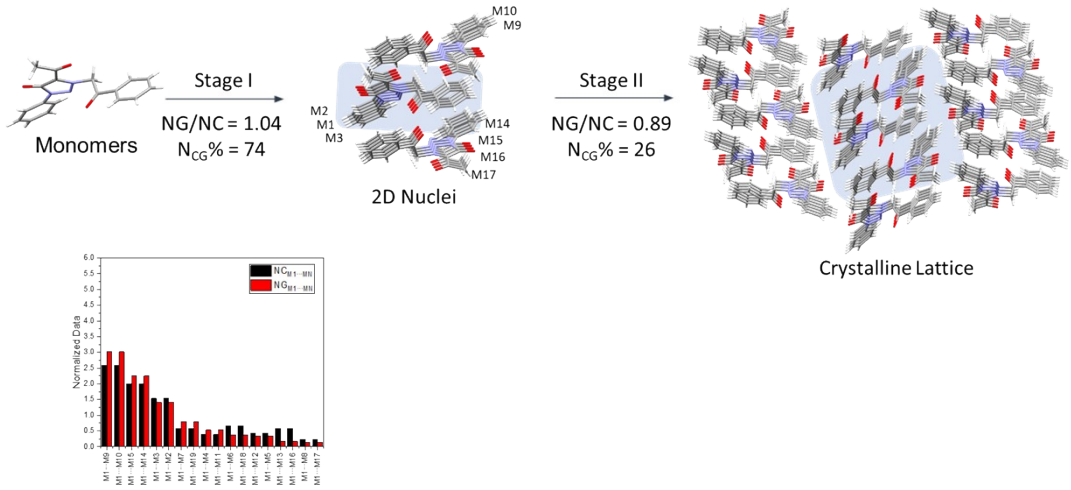


Figure S35 Crystallization mechanism of compound **11**

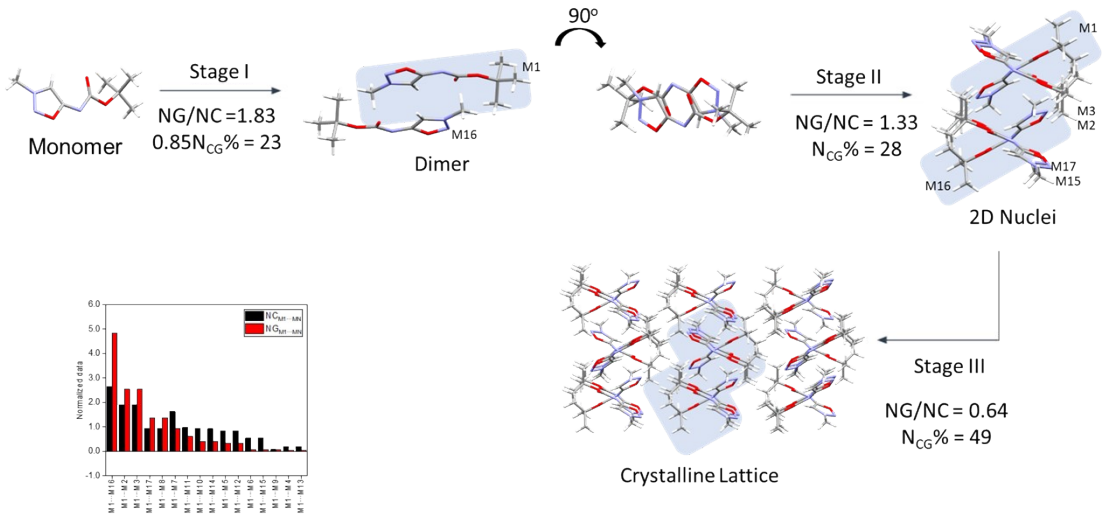


Figure S36 Crystallization mechanism of compound **12**

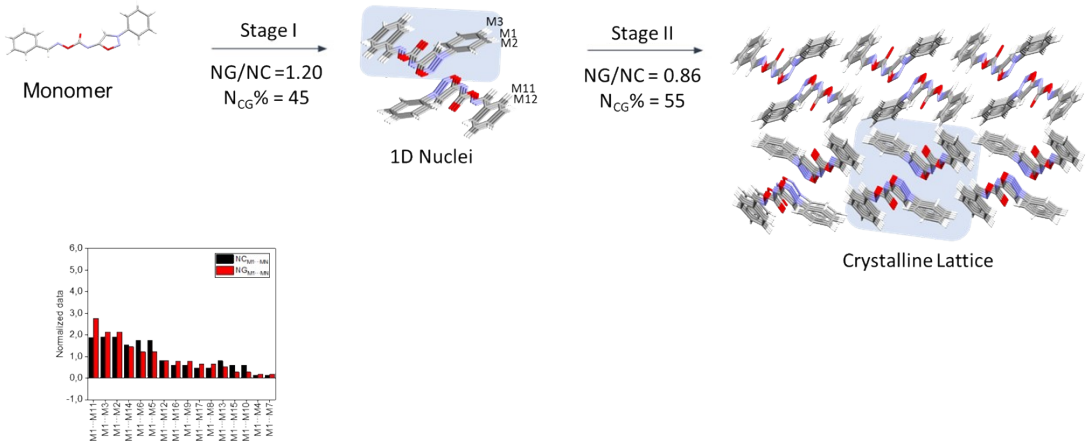


Figure S37 Crystallization mechanism of compound **13**

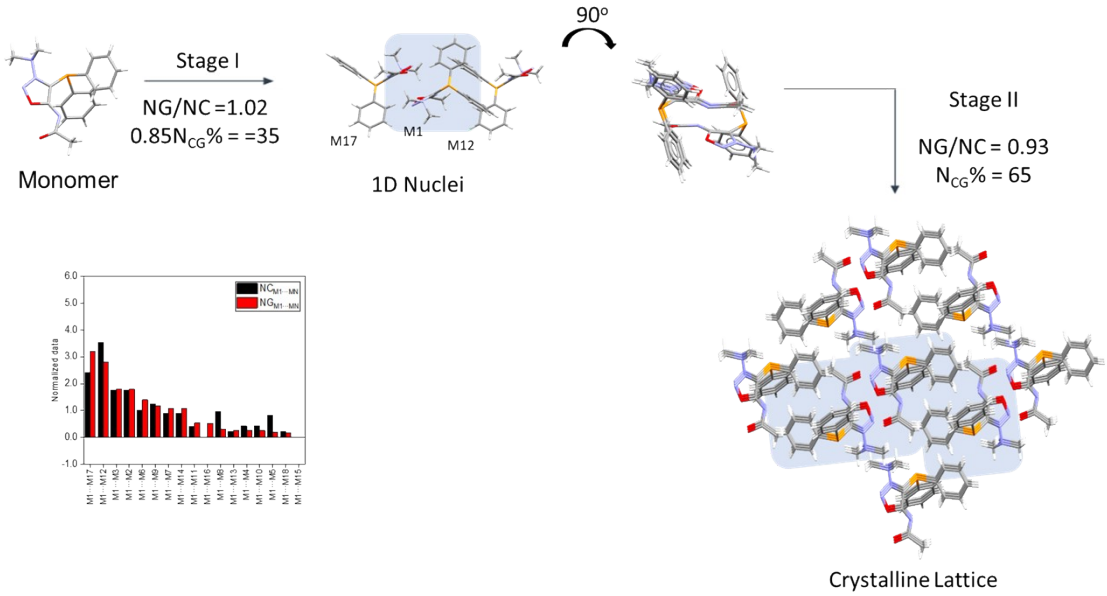


Figure S38 Crystallization mechanism of compound **14**

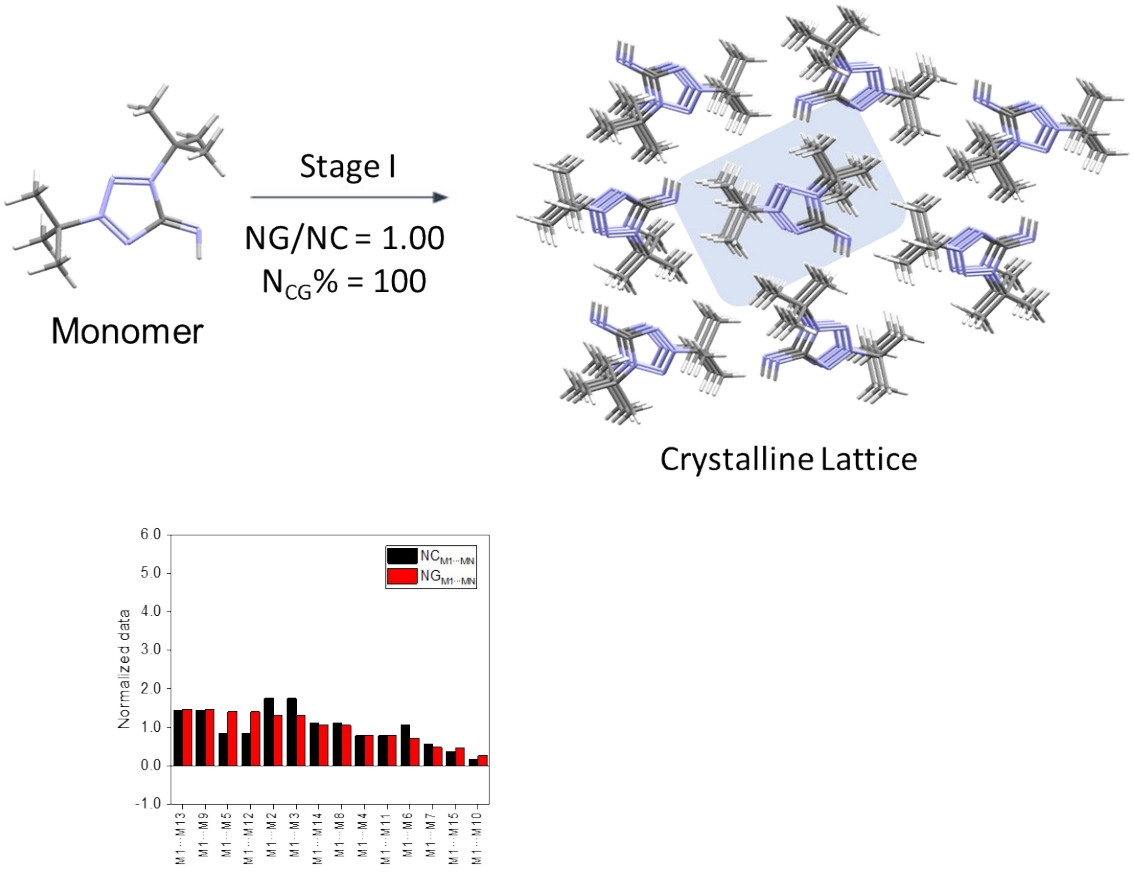


Figure S39 Crystallization mechanism of compound **15**

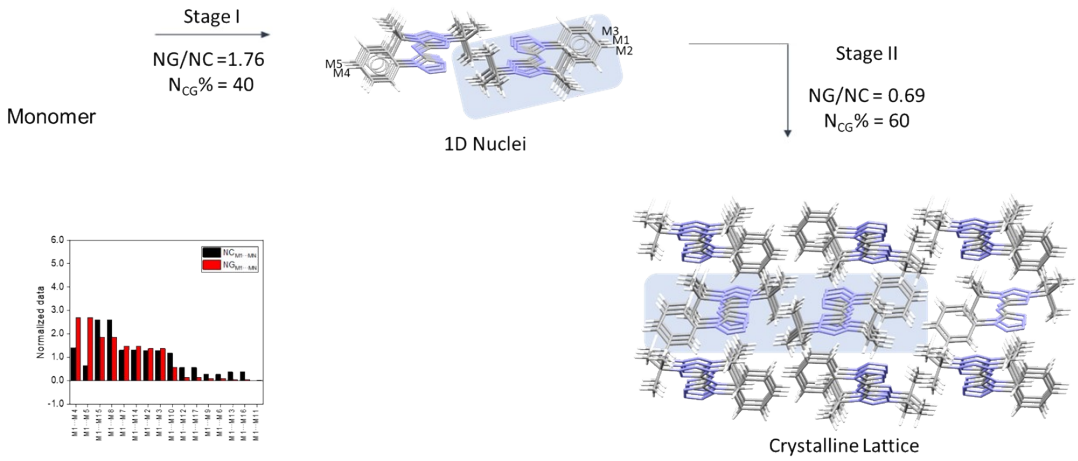


Figure S40 Crystallization mechanism of compound **16**

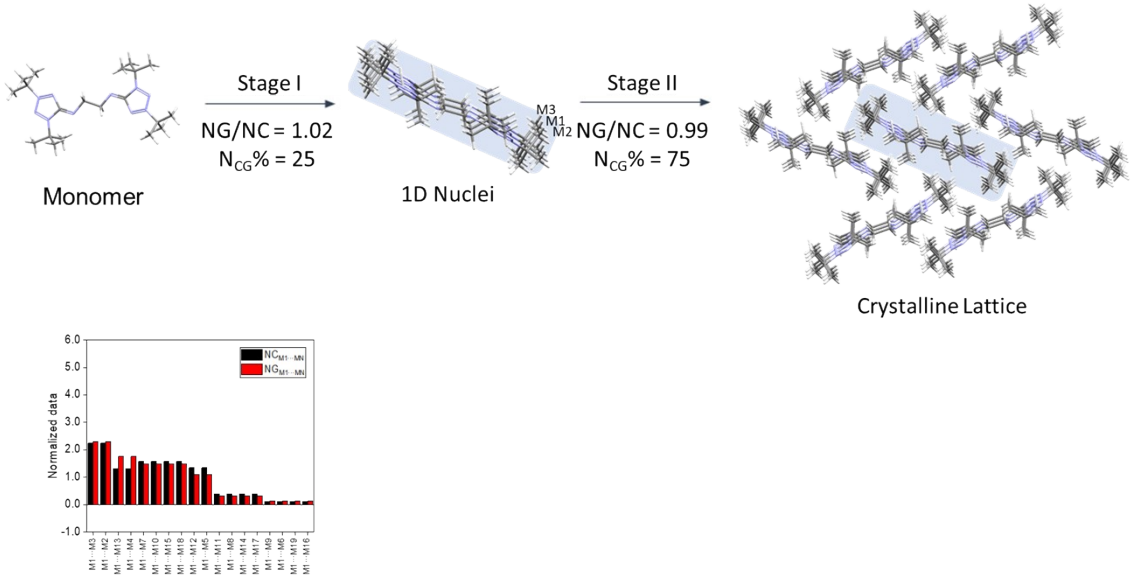


Figure S41 Crystallization mechanism of compound **17**

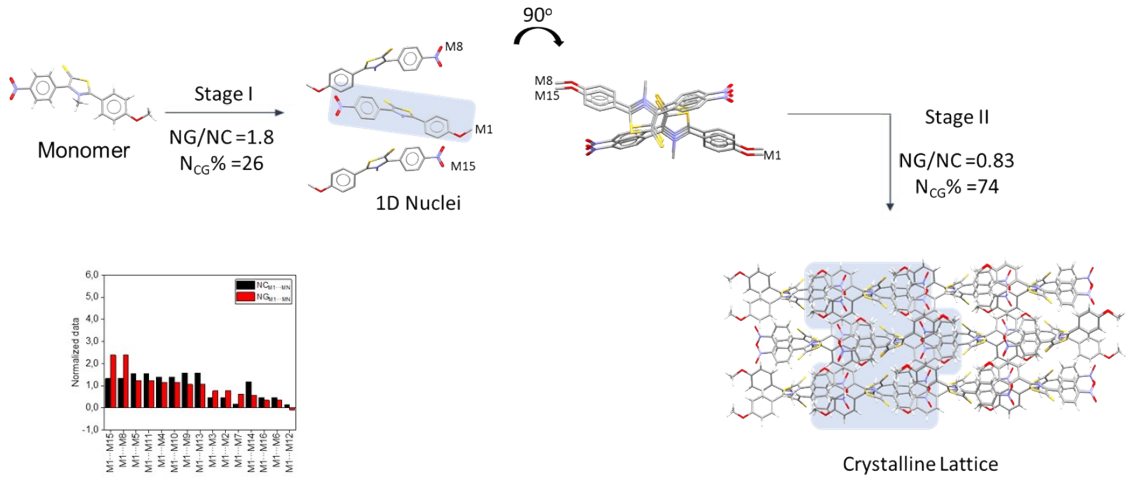


Figure S42 Crystallization mechanism of compound **19**

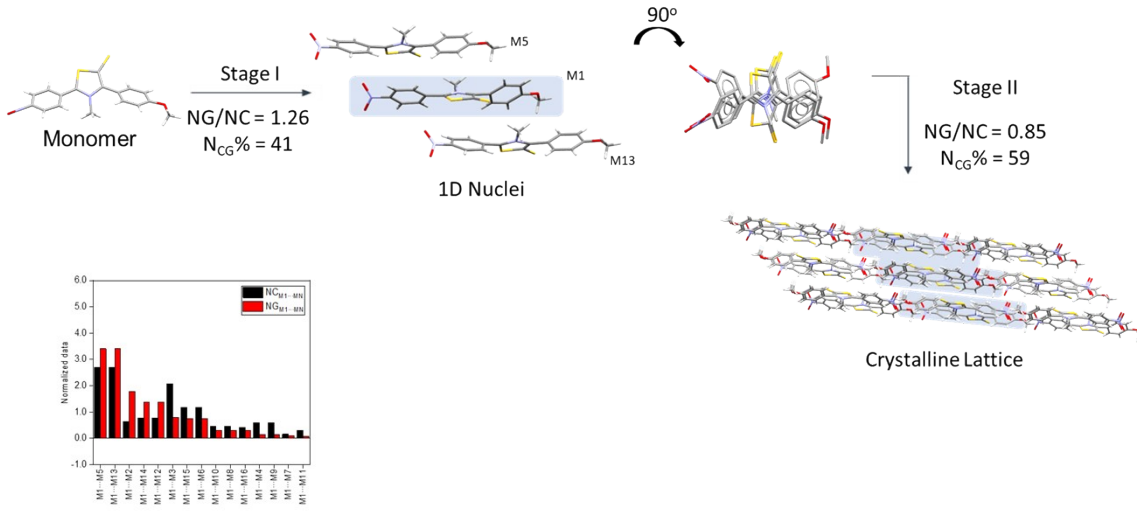


Figure S43 Crystallization mechanism of compound **20**

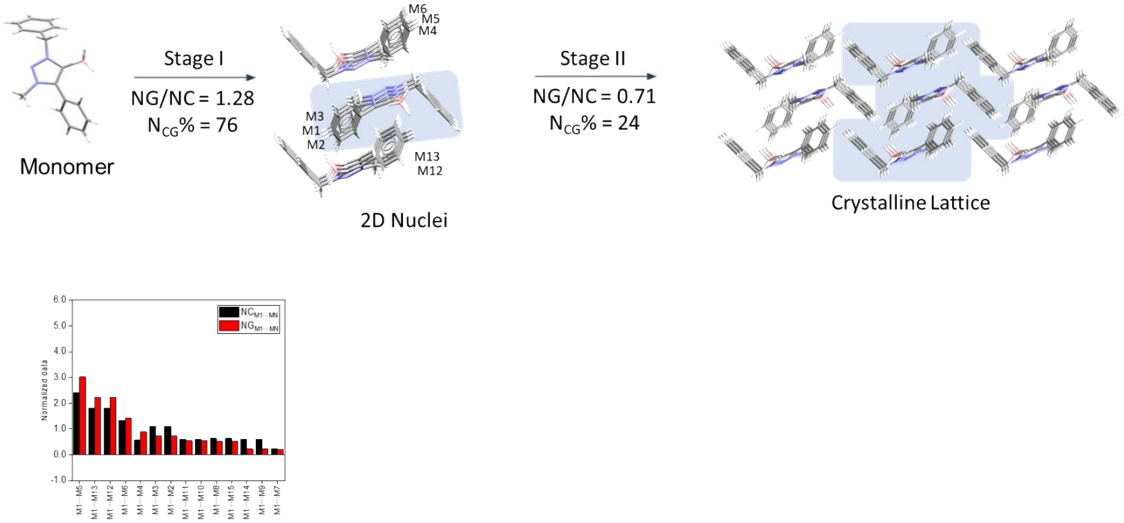


Figure S44 Crystallization mechanism of compound **21**

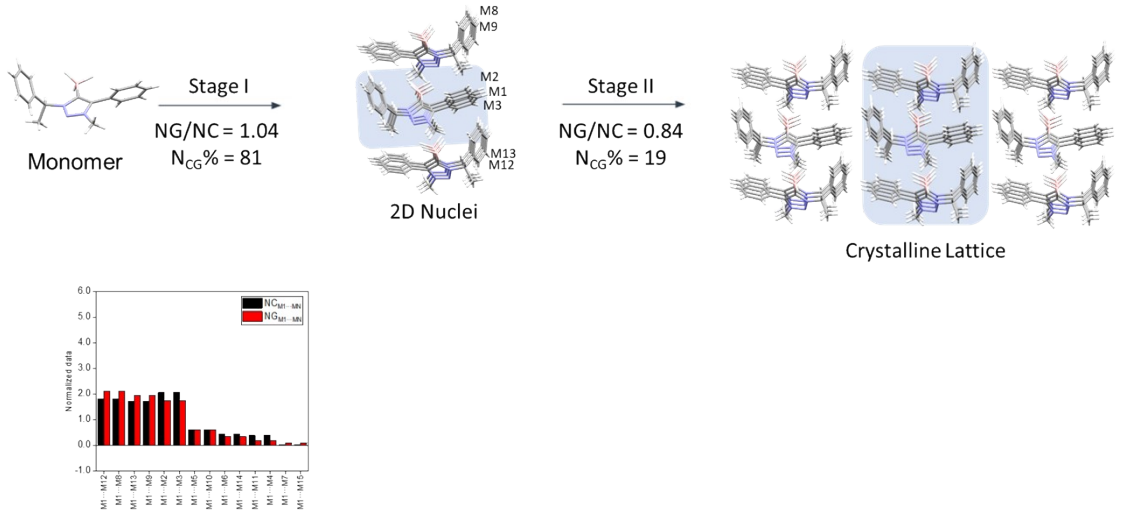


Figure S45 Crystallization mechanism of compound **22**

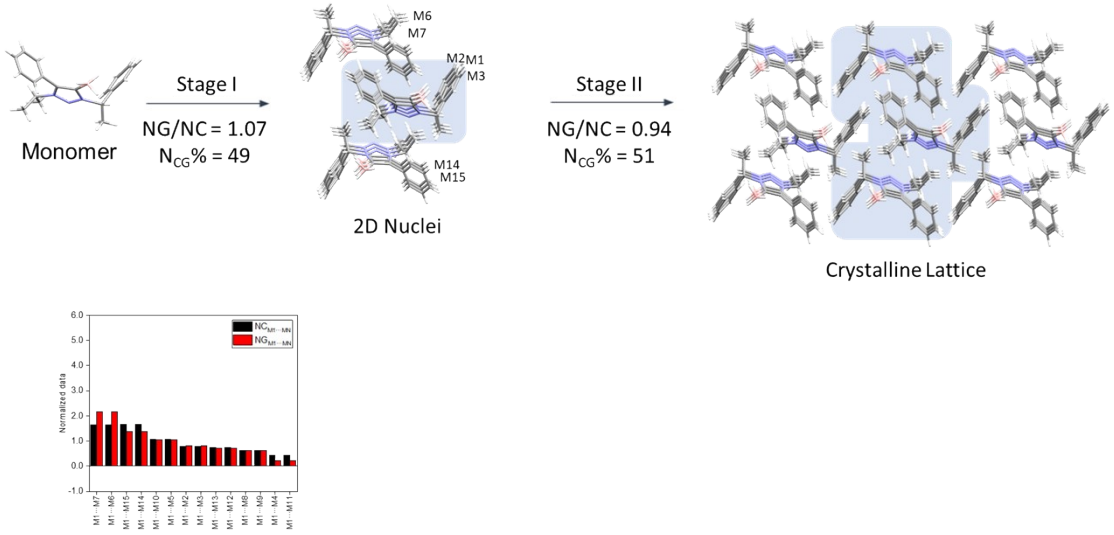


Figure S46 Crystallization mechanism of compound **23**

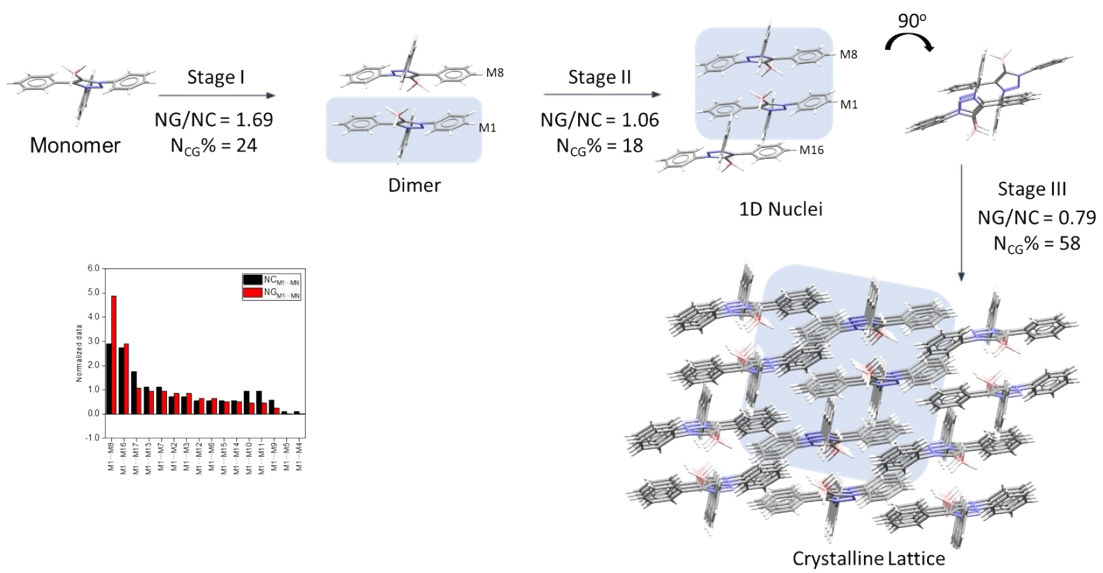


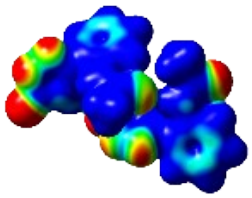
Figure S47 Crystallization mechanism of compound **24**

7. Molecular Electrostatic Potential (MEP)

Table S28 Molecular Eletrostatic Potencial of the most energetic dimers of structures **3-6**, **8-18**, **20-23.**

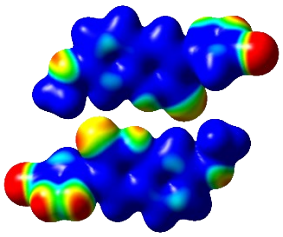
M1···M4 M1···M11

3



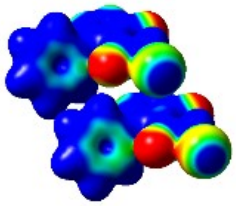
M1⋯M5

4



M1⋯M14

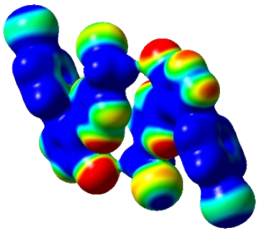
5



M1⋯M3

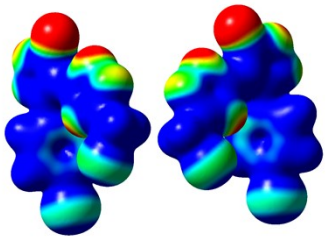
6

8



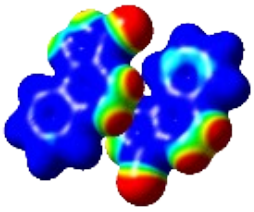
M1⋯M8
Most Stabilizing Dimer

9



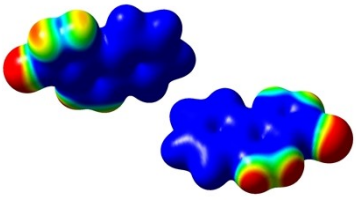
M1⋯M11
Most Destabilizing Dimer

9



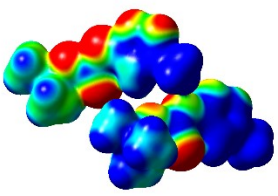
M1⋯M3
Most Stabilizing Dimer

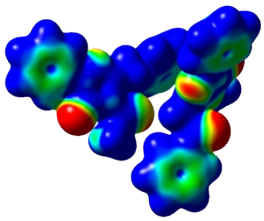
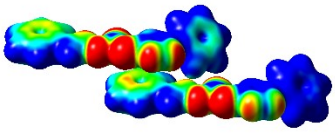
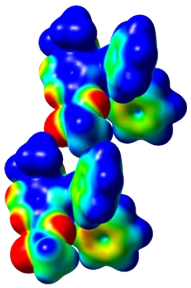
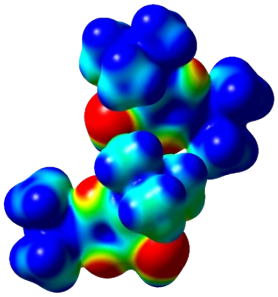
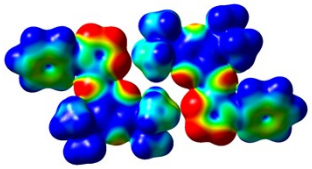
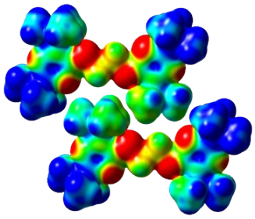
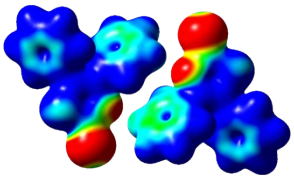
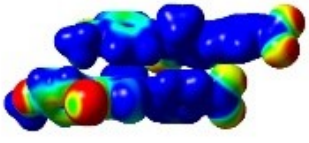
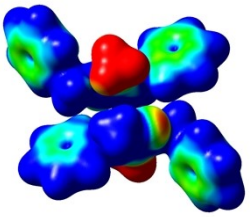
10

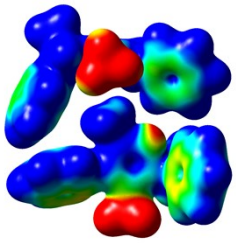


M1⋯M10
Most Destabilizing Dimer

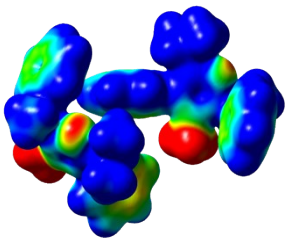
10



 M1⋯M9 **11**	M1⋯M2 **12**
 M1⋯M3 **13**	 M1⋯M7 **14**
 M1⋯M9 **15**	 M1⋯M5 **16**
 M1⋯M2 **17**	 M1⋯M12 **18**
 M1⋯M13 **20**	 M1⋯M5 **21**



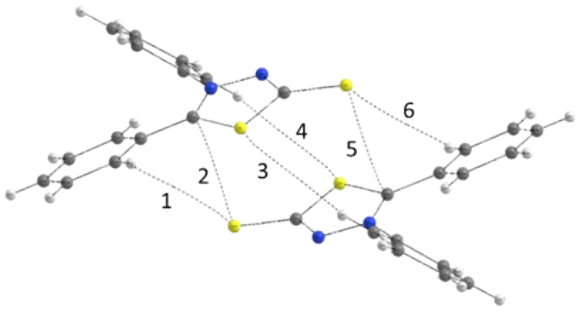
M1···M12
22



M1···M7
23

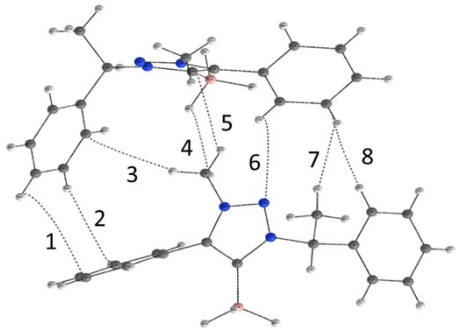
8. Quantum Theory of Atoms in Molecules (QTAIM)

Table S29 Quantum Theory of Atoms (QTAIM) of the most energetic dimer of structure **18.**



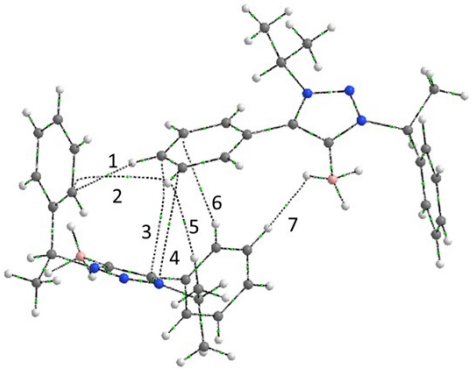
		Atoms	Interaction	ρ	Ellipticity	K	V	G	BPL	G_{AI}
M1···M11	1	H18··· S6	CH···S	0.005136	0.89153	-0.0011	-0.0024	0.00347	6.21514	-3.11
	2	C5··· S6	C···S	0.007227	0.69599	-0.0006	-0.0033	0.00395	6.66576	-4.38
	3	S4··· H12	CH···S	0.001572	0.31537	-0.0004	-0.0006	0.00101	6.88682	-0.95
	4	H8··· S4	CH···S	0.001572	0.31537	-0.0004	-0.0006	0.00101	6.88682	-0.95
	5	C5··· S6	C···S	0.007227	0.69599	-0.0006	-0.0033	0.00395	6.66576	-4.38
	6	H18··· S6	CH···S	0.005136	0.89153	-0.0011	-0.0024	0.00347	6.21514	-3.11
		Total		0.027870						-16.90

Table S30 Quantum Theory of Atoms (QTAIM) of the most energetic dimer to structure **22.**



		Atoms	Interaction	ρ	Ellipticity	K	V	G	BPL	G_{AI}
M1⋯M12	1	C15-H3A	CH-π	0.002352	0.79819	-0.0004	-0.001	0.0014	7.542755	-1.016
	2	C16-H4A	CH-π	0.004167	0.485994	-0.0006	-0.0019	0.0025	5.951807	-1.800
	3	H11C-C5	CH-π	0.002814	0.492582	-0.0005	-0.0012	0.00171	6.168536	-1.216
	4	H11B-H14	CH-H	0.004473	0.694646	-0.0013	-0.0018	0.00311	5.370844	-1.933
	5	H11A-C9	CH-C	0.005098	1.495309	-0.0009	-0.0025	0.00339	5.793293	-2.203
	6	N2-H17A	CH-N	0.002569	0.655024	-0.0007	-0.0012	0.00185	6.509034	-1.110
	7	H8C--H16A	CH-H	0.004586	0.100247	-0.001	-0.0026	0.00358	4.603646	-1.981
	8	H1A-C16	CH-π	0.001778	0.632409	-0.0004	-0.0007	0.00106	6.927292	-0.768
		Total		0.027837						-12.03

Table S31 Quantum Theory of Atoms (QTAIM) of the most energetic dimer to structure **23.**



		Atoms	Interaction	ρ	Ellipticity	K	V	G	BPL	G_{AI}
M1⋯M7	1		CH-π	0.004721	0.110745	-0.0008	0.0034	-0.0026	5.82972	-2.37
	2		CH-π	0.004468	0.783662	-0.0008	0.00281	-0.002	6.31358	-2.24
	3		π-π	0.002202	0.369983	-0.0002	0.00122	-0.001	7.59289	-1.10
	4		π-N	0.002233	0.302362	-0.0003	0.00147	-0.0011	7.40652	-1.12
	5		CH-H	0.00329	0.378914	-0.0009	0.00252	-0.0016	5.07527	-1.65
	6		CH-π	0.003826	0.109518	-0.0005	0.00234	-0.0018	6.00987	-1.92

	7		CH-H	0.004354	0.096795	-0.001	0.00296	-0.002	4.87499	-2.18
	Total			0.027870						-12.59

9. References

1. P. F. de Athayde-Filho, J. M. and A. M. Simas, Synthesis, Characterization and Evaluation of the Activity of Ten Mesoionic Compounds Against Microorganisms, Acta. Farm. Bonaerense, **1999**, 18, 17-22.