SUPPORTING INFORMATION

Insights on Conformation in the Solid State: A Case Study ─ *s-cis* and/or *s-trans* Crystallization of 5(3)-Aryl-3(5)-Carboxyethyl-1-*tert*-butylpyrazoles

Geórgia C. Zimmer,[a] Anderson B. Pagliari,[a] Caroline R. Bender,[a] Paulo R. S. Salbego,[a] Tainára Orlando,[a] Manfredo Horner,[a] Nilo Zanatta, Helio G. Bonacorso[a] and Marcos A. P. Martins*[a]

[a]Núcleo de Química de Heterociclos (NUQUIMHE) Department of Chemistry, Federal University of Santa Maria (UFSM), CEP 97105-900 Santa Maria, Rio Grande do Sul, Brazil

*E-mail of corresponding author: marcos.nuquimhe@gmail.com

1. ORTEP of compounds 1d and 2b-d.

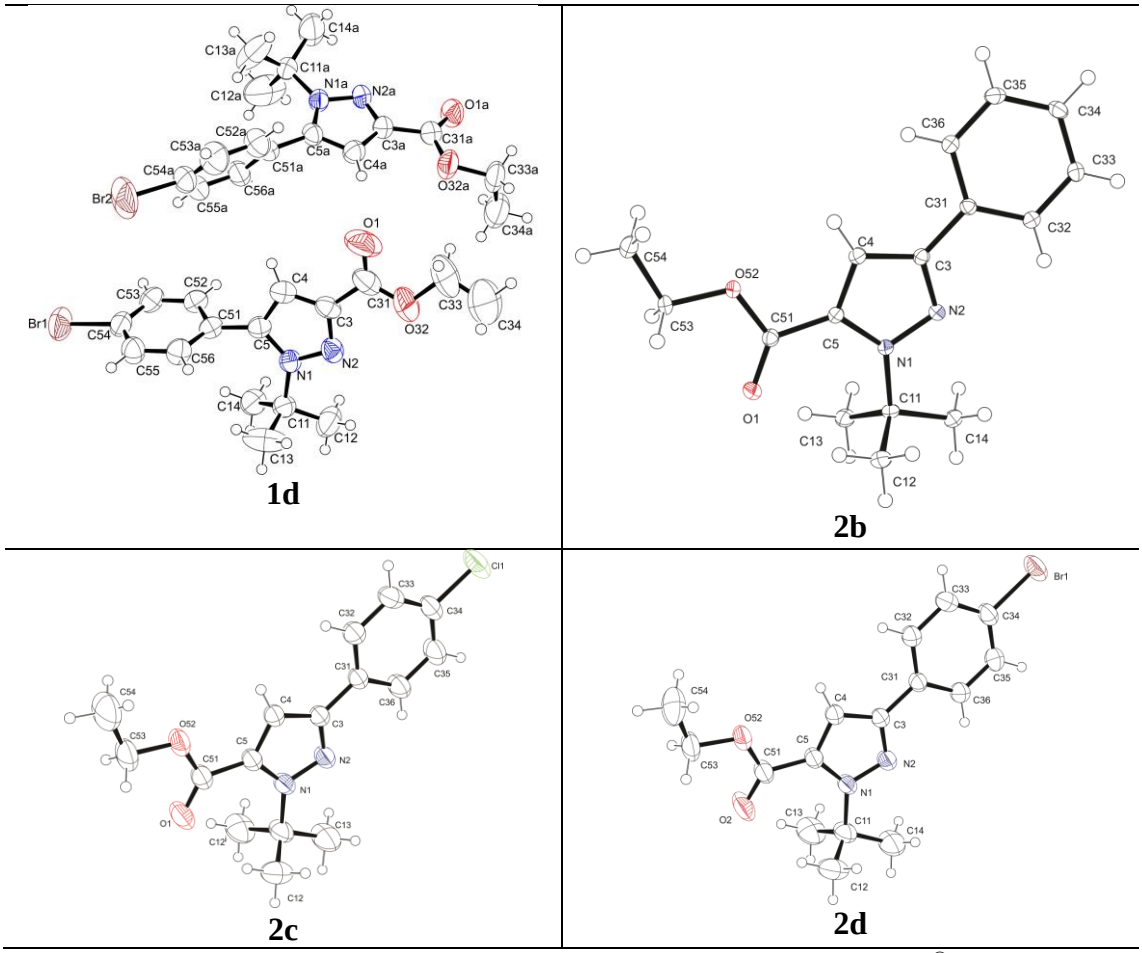


Figure S1. Molecular structure of **1d** and **2b-d** represented by ORTEP® diagram, with thermal ellipsoids drawn at 50% probability level.

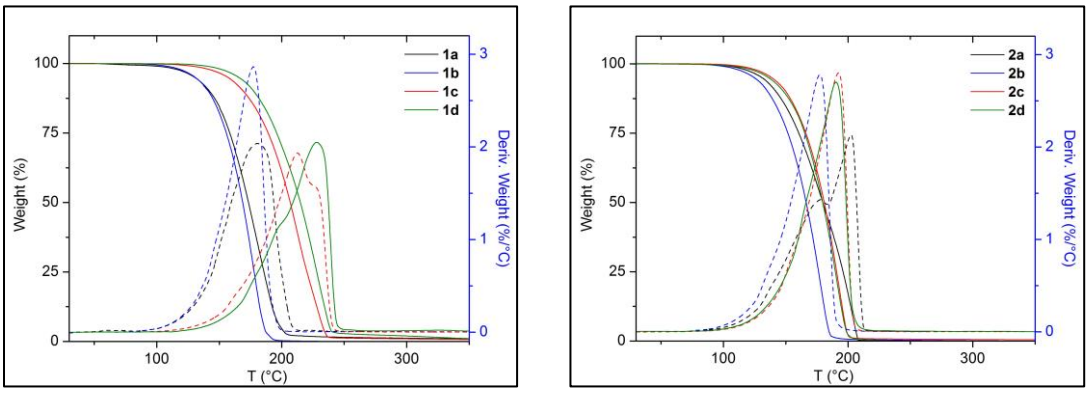
Table S1. X-ray data for compounds **1a-d**.

Compound	**1a**	**1b**	**1c**	**1d**
Empirical formula	$C_{16}H_{20}N_2O_2$	$C_{16}H_{19}FN_2O_2$	$C_{16}H_{19}ClN_2O_2$	$C_{32}H_{38}Cl_2N_4O_4$
Mw	272.34	290.33	306.78	702,48
T [K]	293(2)	293(2)	293(2)	293(2)
Crystal system	Monoclinic	Monoclinic	Triclinic	Triclinic
Space group	$P2_1/n$	$P2_1/c$	P-1	P-1
a [Å]	8.0704(9)	6.9381(7)	10.9637(5)	10.8799(6)
b [Å]	10.6122(13)	18.463(3)	13.2546(6)	13.3677(7)
c [Å]	17.698(4)	12.600(2)	13.9344(6)	13.9345(8)
α [°]	90	90	62.661(2)	62.953(3)
β [°]	93.130(11)	103.702(10)	67.366(2)	68.018(3)
γ [°]	90	90	81.873(3)	82.371(3)
V [Å^3]	1513.5(4)	1568.1(4)	1658.68(13)	1672.04(16)
Z	4	4	4	2
$D_{calcd.}$ [g cm^{-3}]	1.195	1.230	1.228	1.395
μ [mm^{-1}]	0.636	0.740	0.236	2.464
F(000)	584	616	648	720
Crystal size (mm)	0.29 x 0.22 x 0.16	0.29 x 0.25 x 0.15	0.58 x 0.16 x 0.10	0.42 x 0.33 x 0.10
θ range for data Collection (deg) h, k, l range	5.01 to 68.33 -9≤h≤9 -12≤k≤12 -21≤l≤20	4.33 to 72.13 -8≤h≤8 -22≤k≤22 -15≤l≤15	1.73 to 27.30 -14≤h≤14 -17≤k≤16 -17≤l≤17	1.71 to 27.22 -13≤h≤13 -17≤k≤17 -17≤l≤17
Reflections collected/unique	13793 / 2685 [R_{int} = 0.019]	29117 / 3058 [R_{int} = 0.0276]	50297 / 7388 [R_{int} = 0.0742]	45369 / 7398 [R_{int} = 0.0520]
Data/restraints/parameters	2685 / 0 / 181	3058 / 0 / 190	7388 / 1 / 380	7390 / 1 / 379
Absoption correction	Multi-scan	Multi-scan	Gaussian	Gaussian
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Final R indices	R1 = 0.0725, wR2 = 0.1928	R1 = 0.0438, wR2 = 0.1194	R1 = 0.0707, wR2 = 0.1897	R1 = 0.0553, wR2 = 0.1291
R all data	R1 = 0.0770, wR2 = 0.1967	R1 = 0.0516, wR2 = 0.1264	R1 = 0.1641, wR2 = 0.2439	R1 = 0.1240, wR2 = 0.1531
Goodness of fit on F^2	1.052	1.030	1.030	1.034
Largest diff. peak and hole (e Å^3)	0.633 and -0.430	0.172 and -0.176	0.610 and -0.293	0.654 and -0.896

Table S2. Data of X-ray for compounds **2a-d**.

Compound	**2a**	**2b**	**2c**	**2d**
Empirical formula	$C_{16}H_{20}N_2O_2$	$C_{16}H_{19}FN_2O_2$	$C_{16}H_{19}ClN_2O_2$	$C_{16}H_{19}BrN_2O_2$
Mw	272.34	290.33	306.78	351.24
T [K]	293(2)	293(2)	293(2)	293(2)
Crystal system	Monoclinic	Triclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	P-1	$P2_1/m$	C2/c
a [Å]	8.900(5)	8.5662(3)	9.077(2)	26.040(3)
b [Å]	8.307(4)	8.9965(3)	6.9098(15)	9.0972(11)
c [Å]	19.352(11)	10.0893(4)	13.708(2)	13.8867(19)
α [°]	90	92.860(2)	90	90
β [°]	91.44(2)	100.776(2)	107.735(7)	91.957
γ [°]	90	91.266(2)	90	90
V [Å^3]	1430.2(13)	762.49(5)	819.0(3)	3287.7(7)
Z	4	2	2	8
$D_{calcd.}$ [g cm^{-3}]	1.265	1.265	1.244	1.419
μ [mm^{-1}]	0.084	0.092	0.239	3.456
F(000)	584	308	324	1440
Crystal size (mm)	0.29 x 0.22 x 0.16	0.75 x 0.49 x 0.39	0.26 x 0.19 x 0.13	0.75 x 0.49 x 0.39
θ range for data	2.29 to 30.12	2.06 to 27.12	2.40 to 27.12	3.40 to 70.24
Collection (deg) *h, k, l* range	$-12 \le h \le 12$ $-11 \le k \le 11$ $-22 \le l \le 27$	$-10 \le h \le 10$ $-10 \le k \le 11$ $-12 \le l \le 12$	$-11 \le h \le 11$ $-8 \le k \le 8$ $-17 \le l \le 17$	$-31 \le h \le 31$ $-11 \le k \le 11$ $-16 \le l \le 16$
Reflections collected/unique	23991 / 4174 [R_{int} = 0.0311]	21320 / 3352 [R_{int} = 0.0186]	10540 / 1940 [R_{int} = 0.0289]	23652 / 3043 [R(int)=0.023]
Data/restraints/parameters	4174 / 0 / 181	3352 / 0 / 190	1940 / 0 / 131	3043 / 0 / 190
Absoption correction	Multi-scan	Gaussian	Multi-scan	Multi-scan
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Final *R* indices	R1 = 0.0417, wR2 = 0.0993	R1 = 0.0392 wR2 = 0.1187	R1 = 0.0443 wR2 = 0.1127	R1 = 0.0319 wR2 = 0.0843
R all data	R1 = 0.0557, wR2 = 0.1061	R1 = 0.0474 wR2 = 0.1285	R1 = 0.0681, wR2 = 0.1257	R1 = 0.0335 wR2 = 0.0855
Goodness of fit on F^2	1.040	0.947	1.035	1.035
Largest diff. peak and hole (*e* Å^3)	0.352 and -0.229	0.206 and -0.167	0.166 and -0.176	0.261 and -0.493

2. Thermal Analysis



(a) (b)

Figure S2**.** TGA curves of (a) **1a-d** and (b) **2a-d**.

Table S3**.** Thermogravimetric data obtained by TGA in a heating rate of 10 °C min^{-1}.

Compounds	T_i[a](°C)	T_f[b](°C)	T_d[c](°C)
1a	92.11	230.12	180.02
1b	96.83	211.21	177.18
1c	109.12	268.88	212.16
1d	120.47	267.93	229.17
2a	87.38	235.79	201.71
2b	83.60	214.99	176.24
2c	96.83	232.01	191.36
2d	82.65	232.96	189.47

[a]Initial decomposition temperature. [b]Final decomposition temperature. [c]Temperature of maximum decomposition.

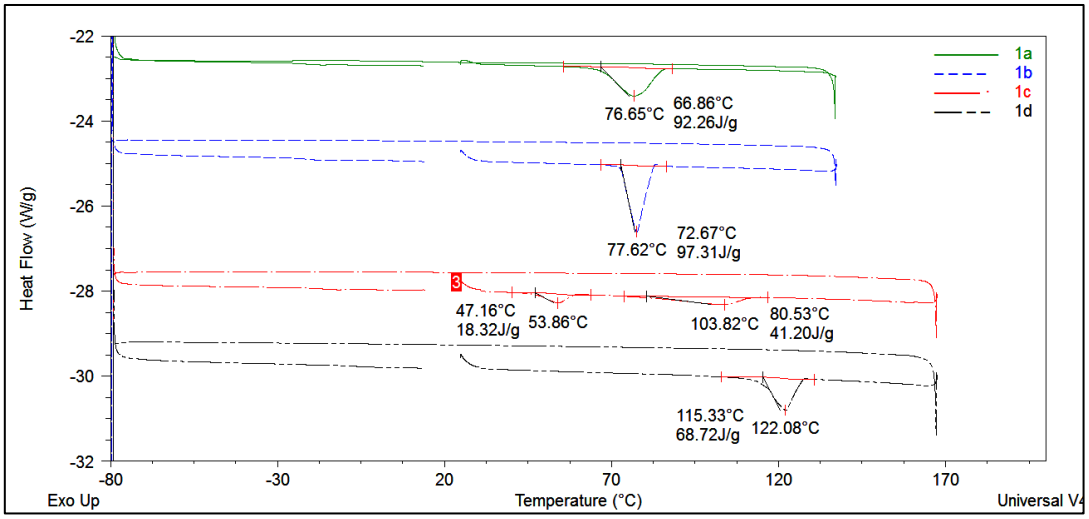


Figure S3**.** DSC curves for **1a-d** at heating rate of 5 °C min^{-1}.

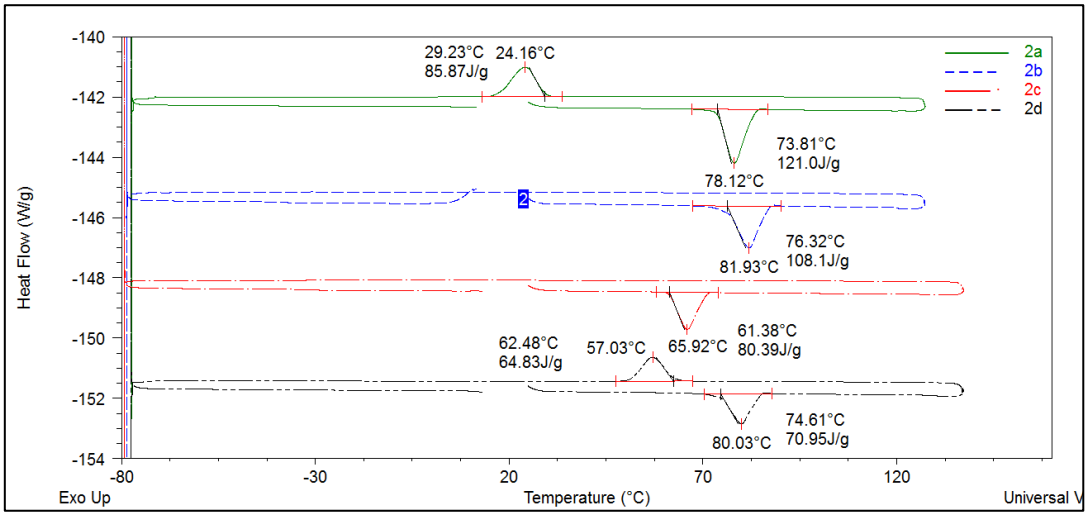


Figure S4**.** DSC curves for **2a-d** at heating rate of 5 °C min^{-1}.

3. PXRD pattern of compounds 1,3-pyrazole and 1,5-pyrazole regioisomers.

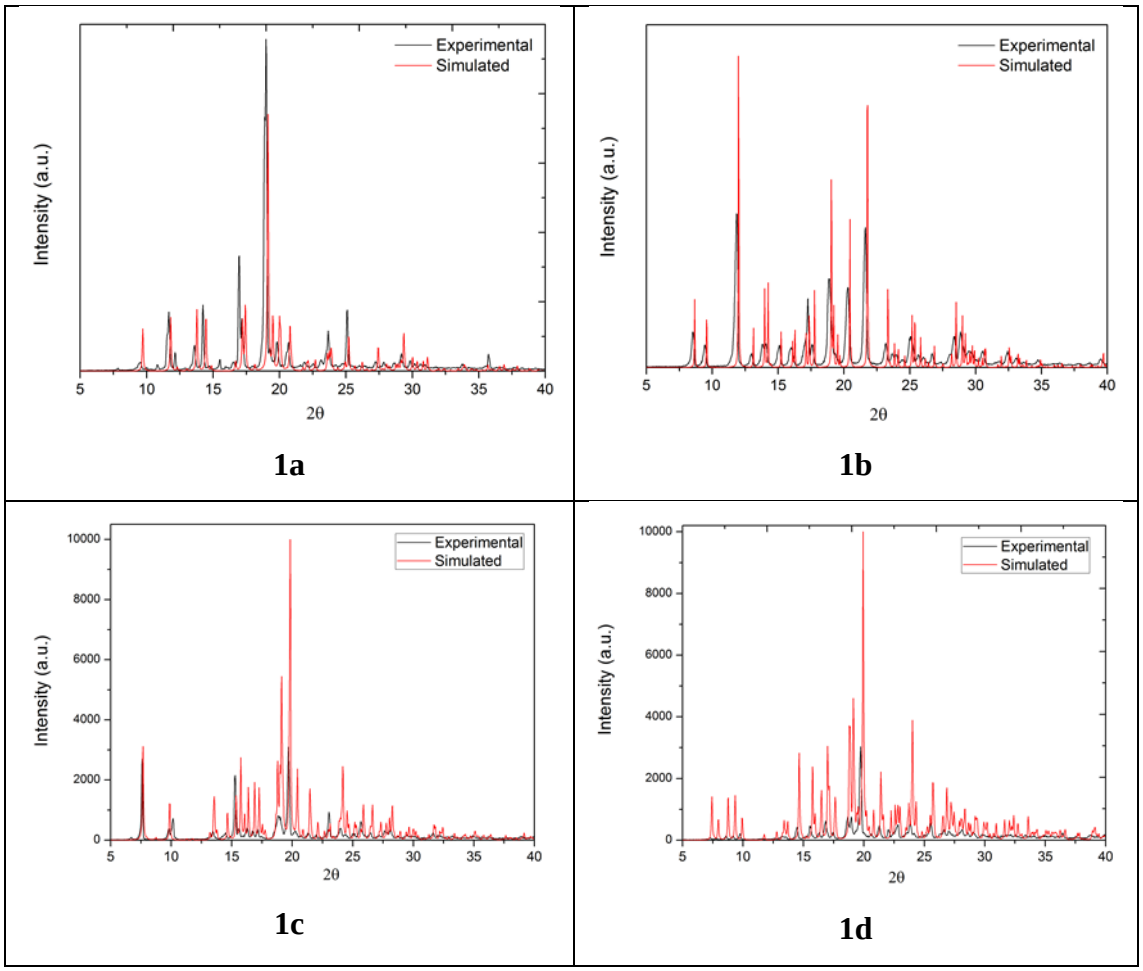


Figure S5**.** PXRD pattern of **1a-d**.

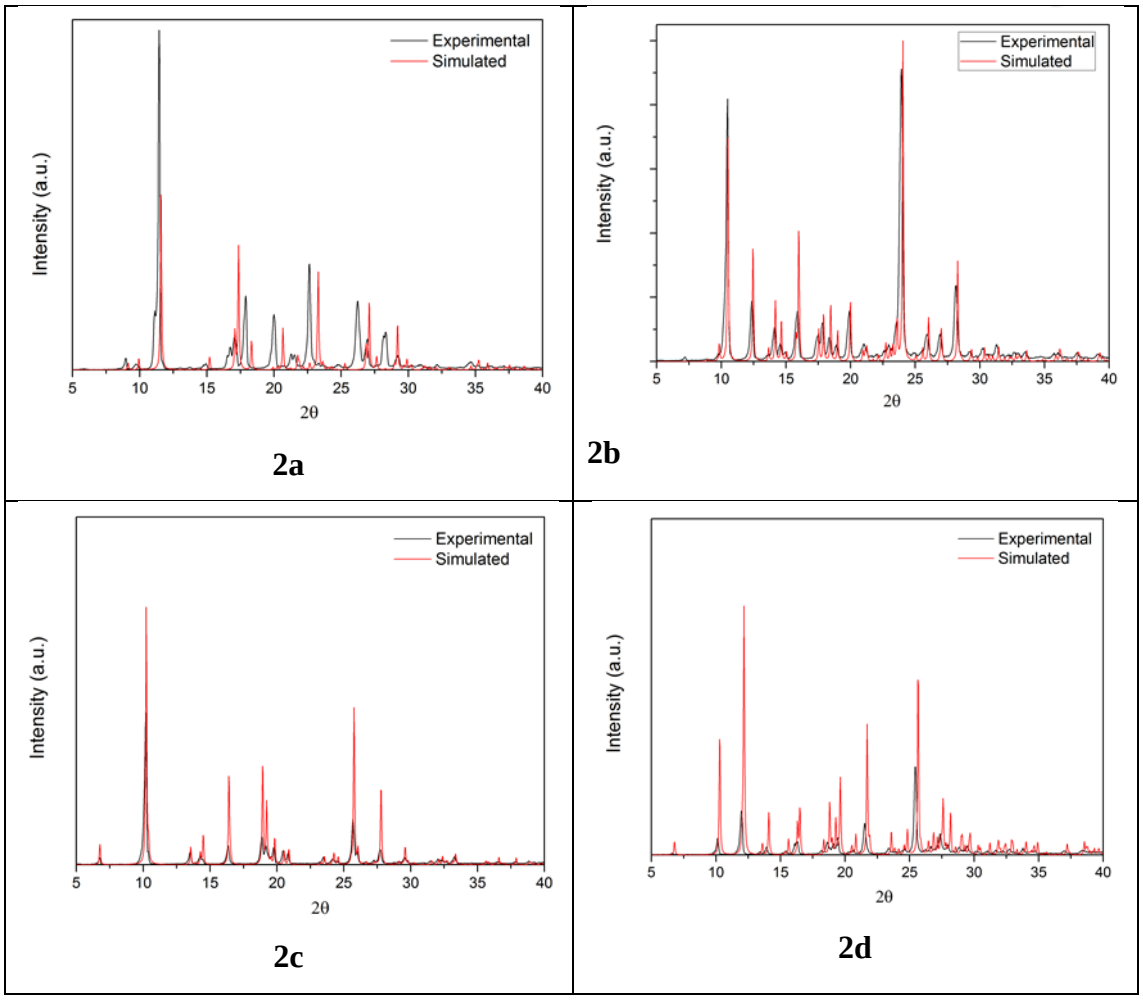


Figure S6. PXRD pattern of **2a-d**.

4. NMR in liquid and solid State.

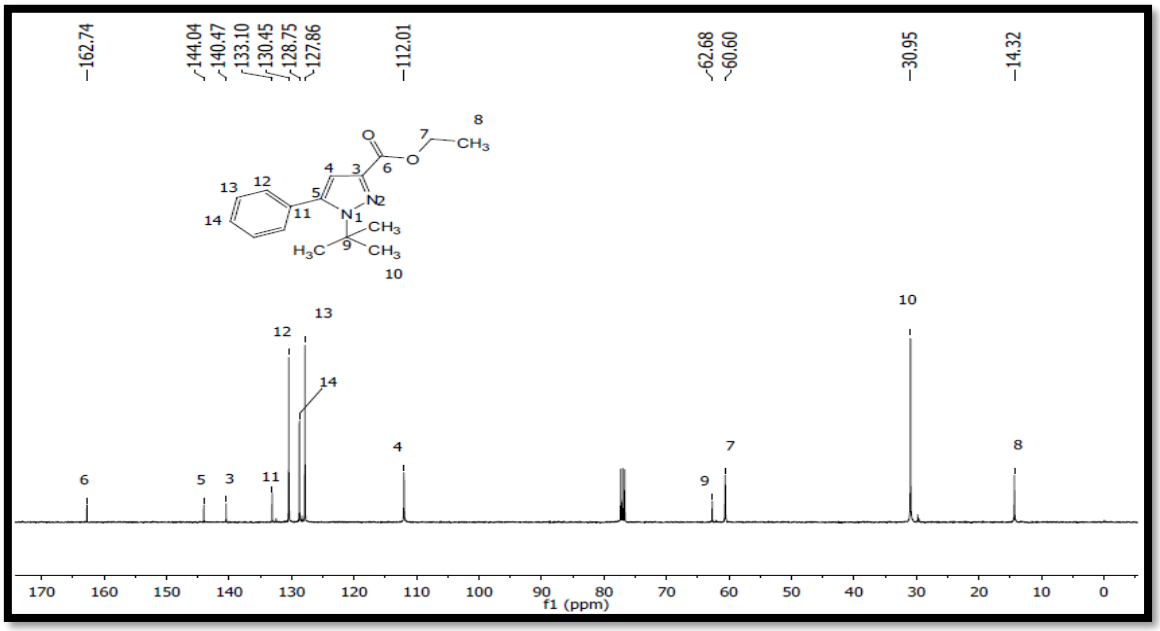


Figure S7. ^{13}C NMR (150.903 MHz, $CDCl_3$) spectrum of **1a**.

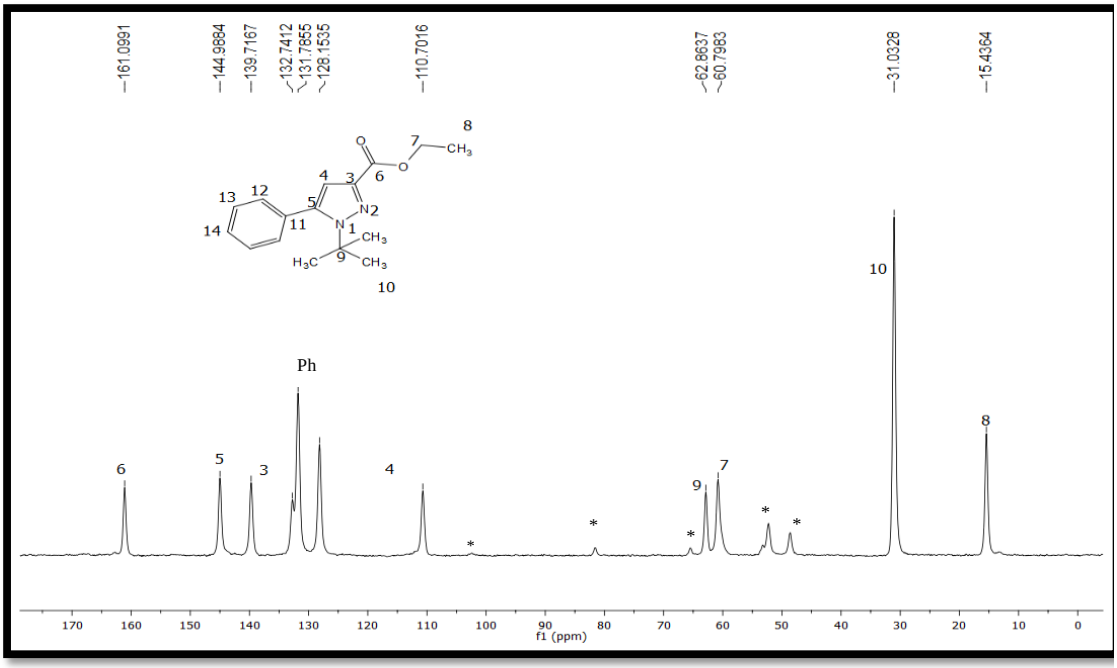


Figure S8. ^{13}C NMR (150.903 MHz) spectrum of **1a** in solid state.

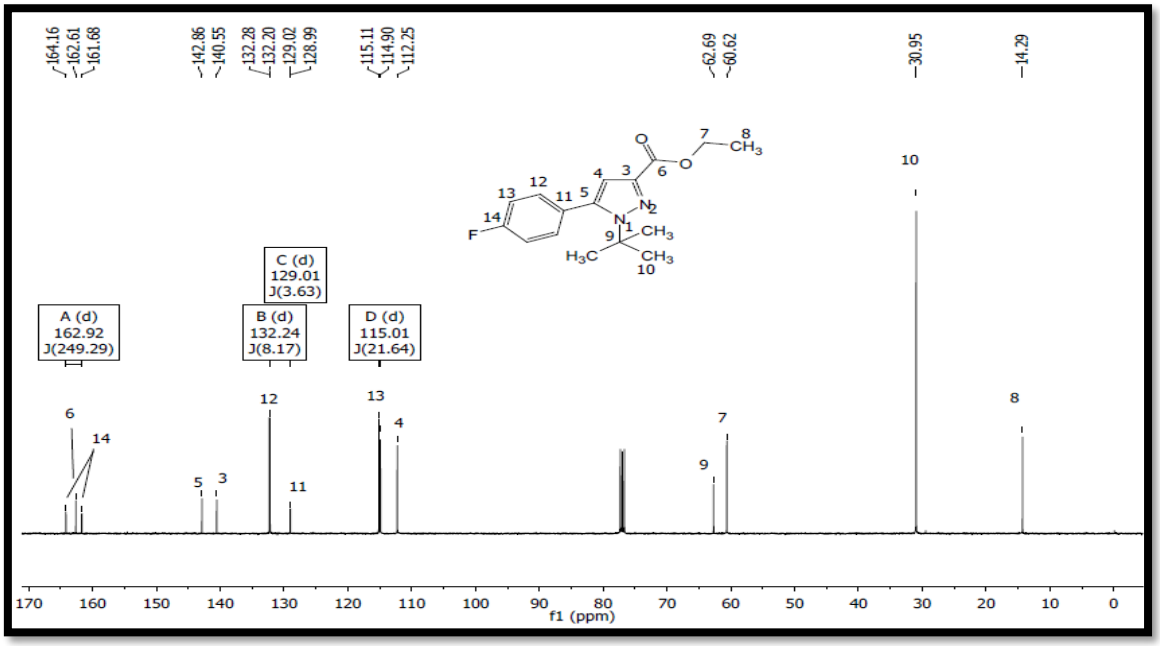


Figure S9: ^{13}C NMR (150.903 MHz, $CDCl_3$) spectrum of **1b**.

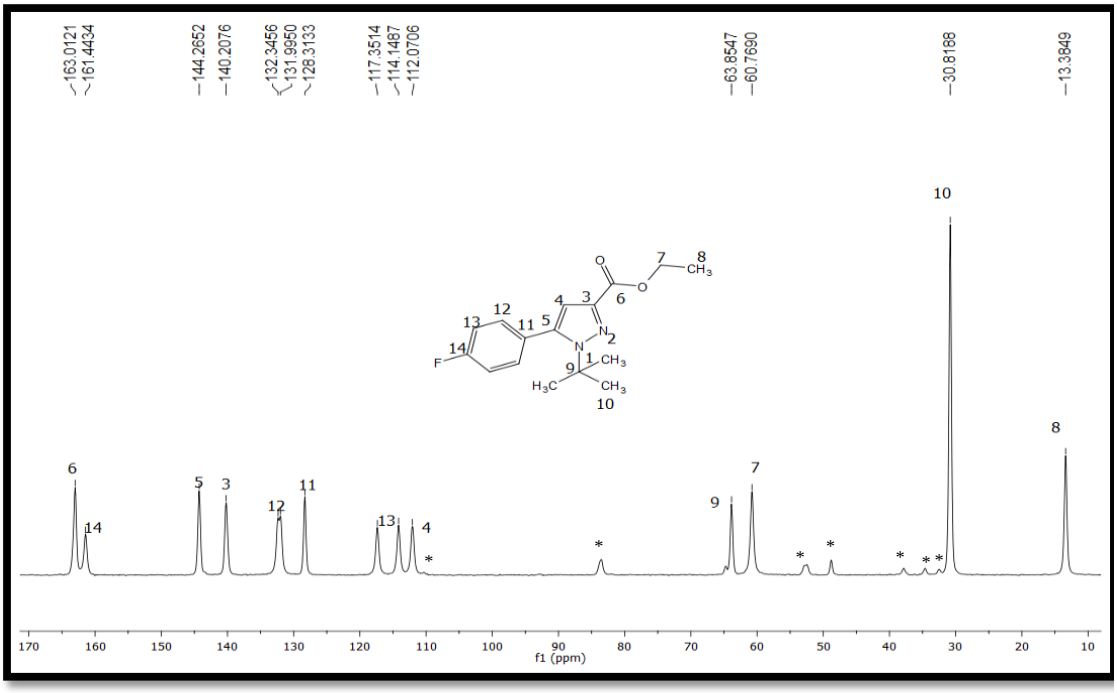


Figure S10. ^{13}C NMR (150.903 MHz) spectrum of **1b** in solid state.

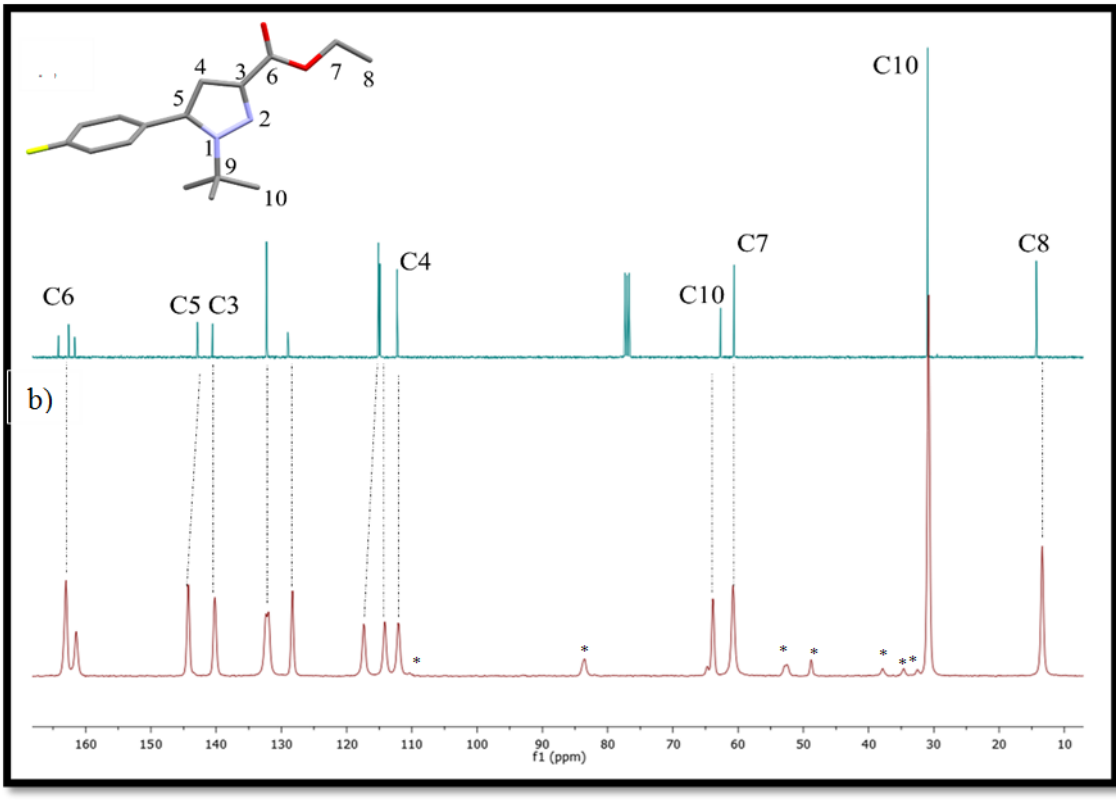


Figure S11. ^{13}C NMR (150.903 MHz) spectrum: a) liquid state in $CDCl_3$; b) solid state of compound **1b**.

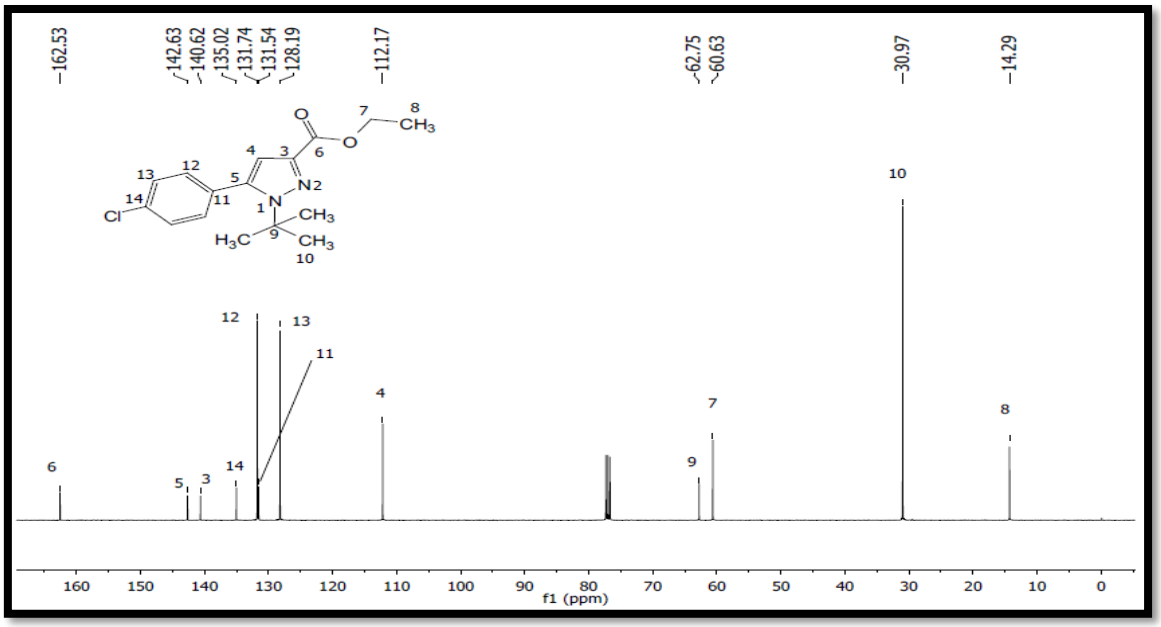


Figure S12. ^{13}C NMR (150.903 MHz. $CDCl_3$) spectrum of **1c.**

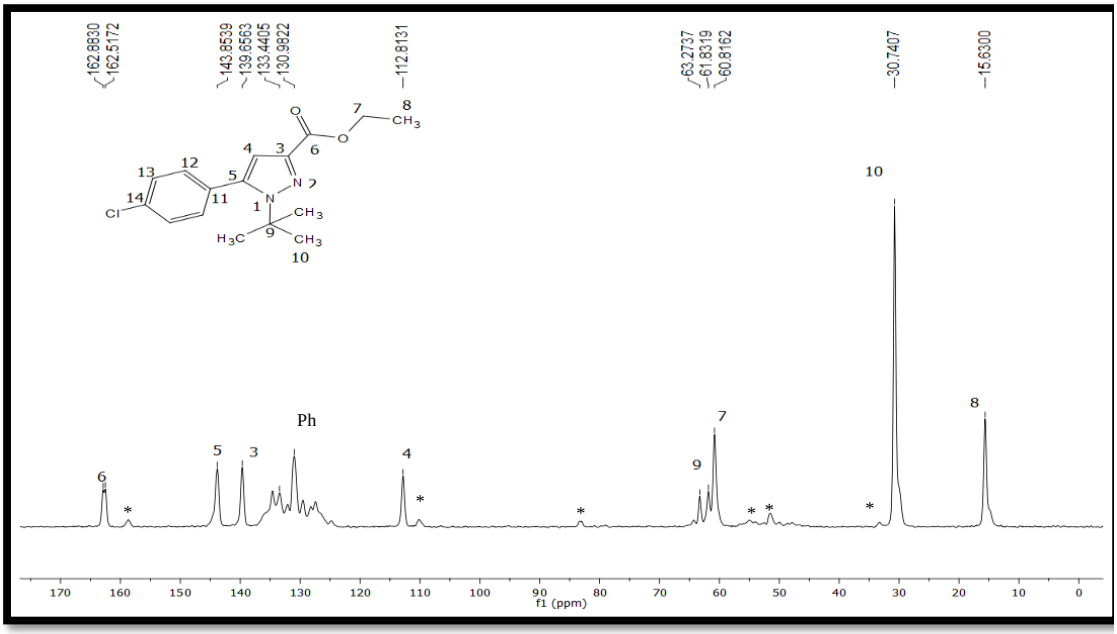


Figure S13. ^{13}C NMR (150.903 MHz) spectrum of **1c** in solid state.

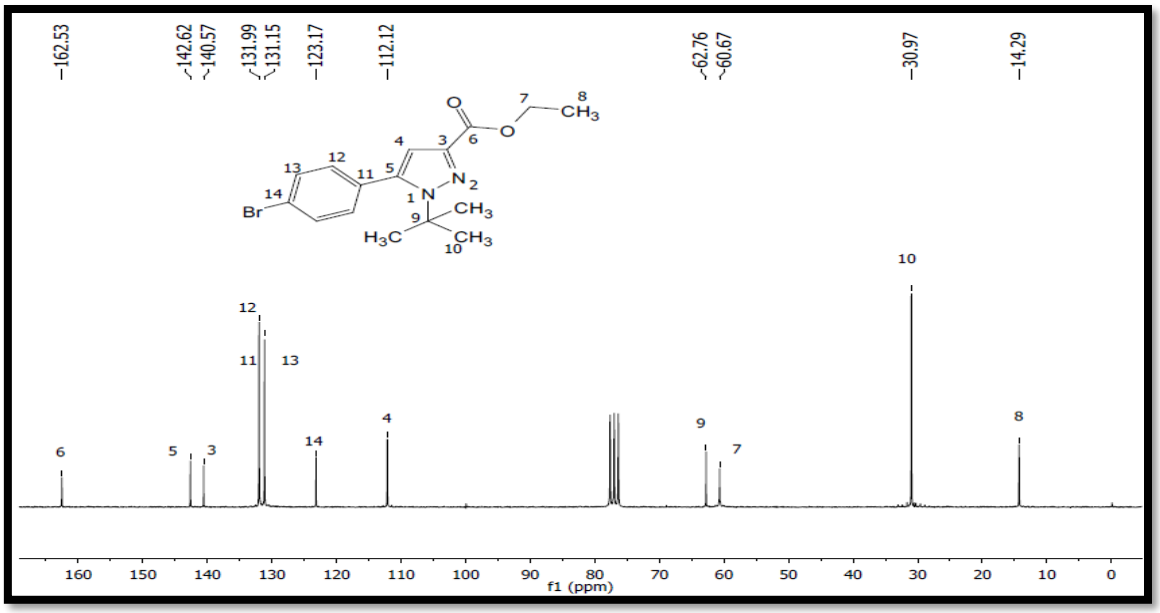


Figure S14: ^{13}C NMR (150.903 MHz. $CDCl_3$) spectrum of **1d.**

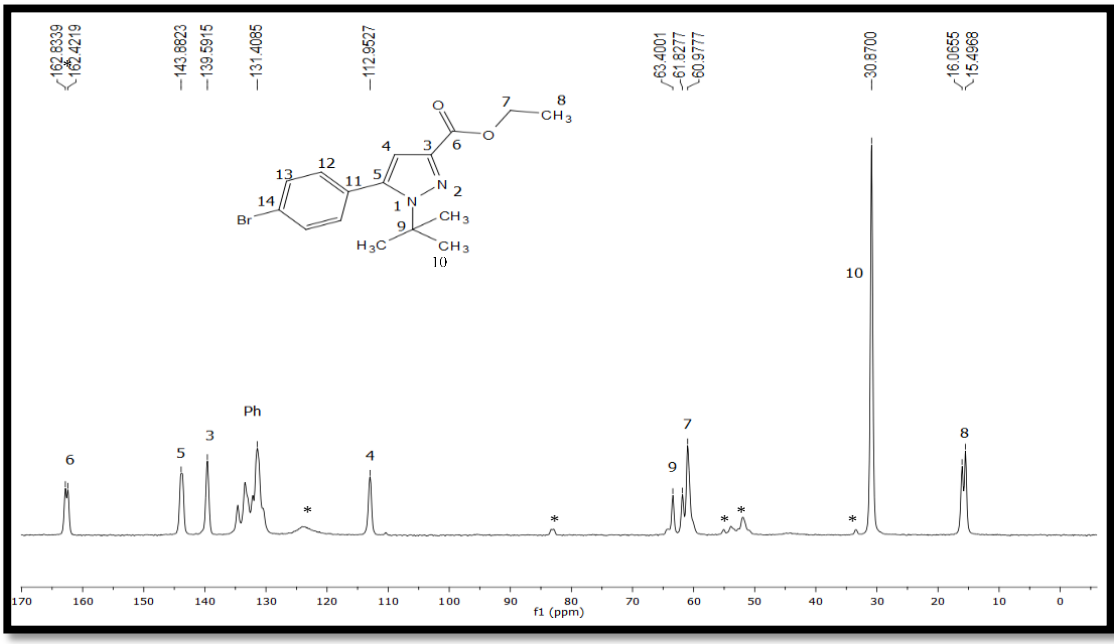


Figure S15. ^{13}C NMR (150.903 MHz) spectrum of **1d** in solid state.

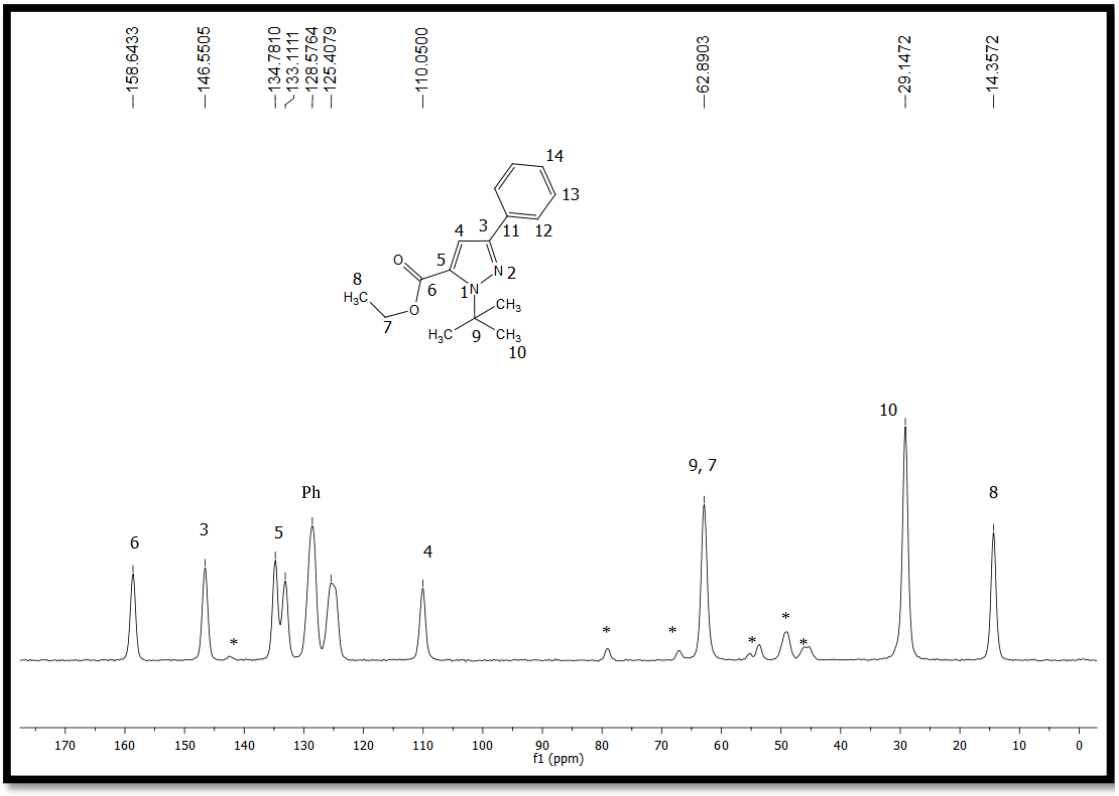


Figure S16. ^{13}C NMR (150.903 MHz) spectrum of **2a** in solid state.

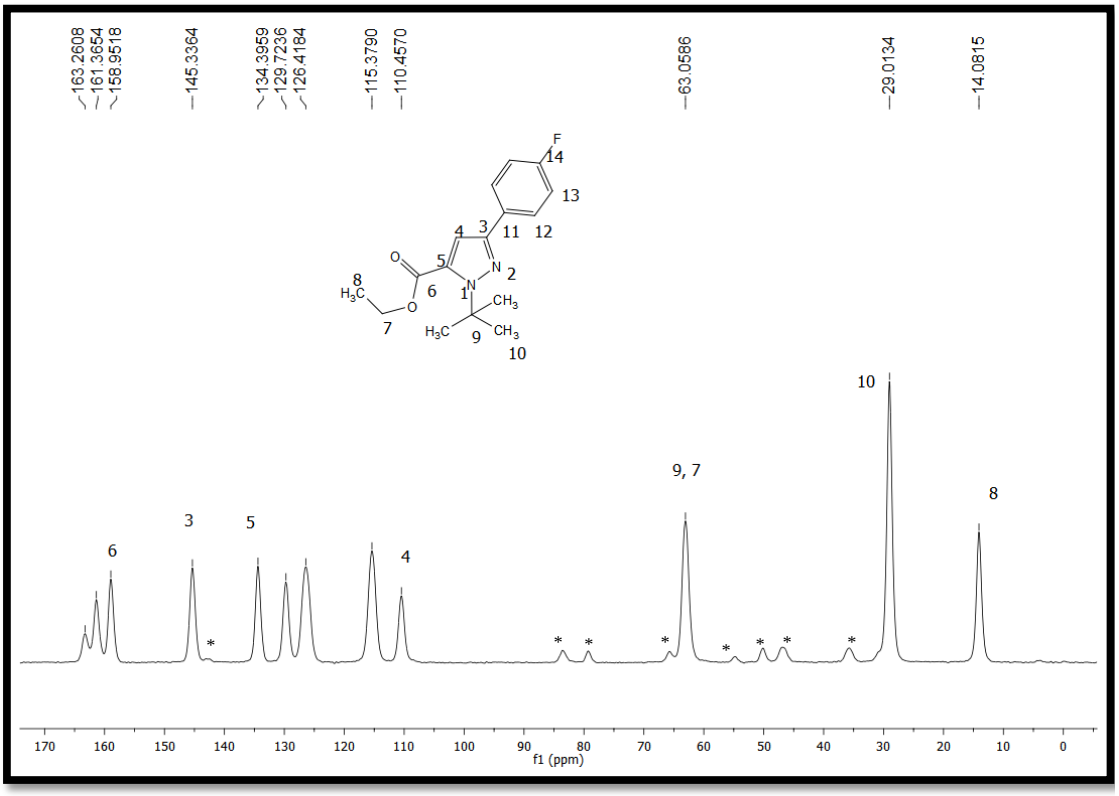


Figure S17. ^{13}C NMR (150.903 MHz) spectrum of **2b** in solid state.

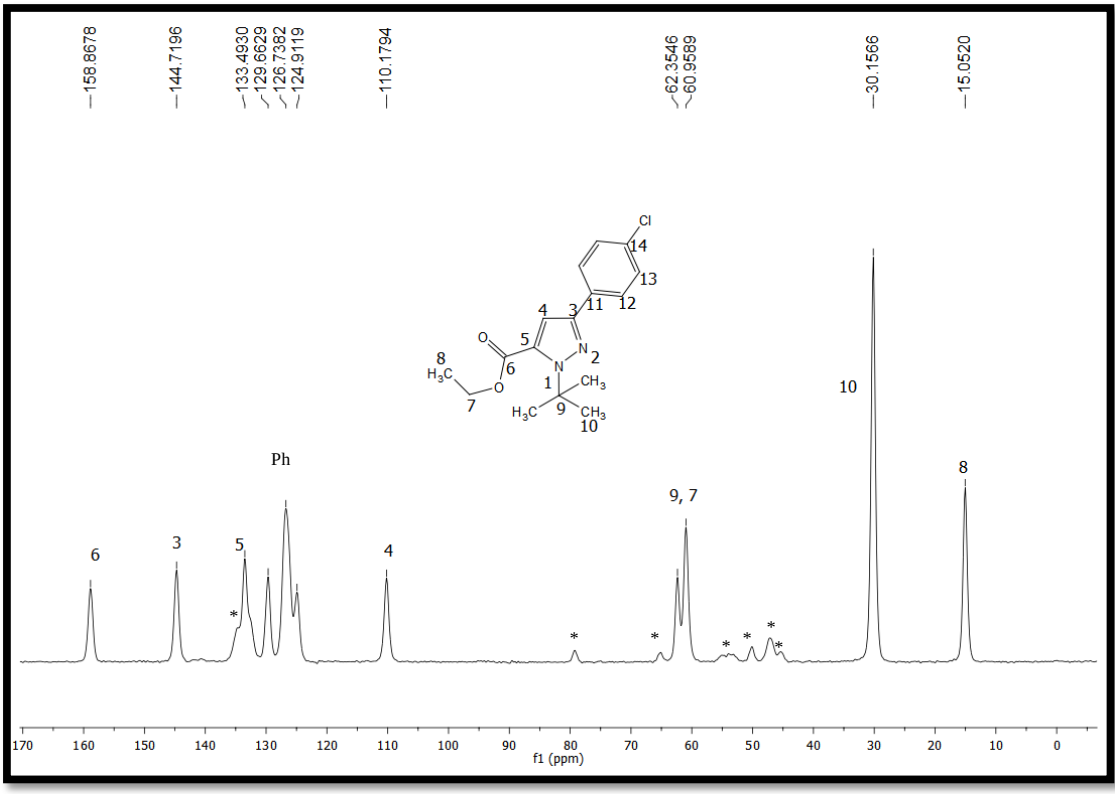


Figure S18. ^{13}C NMR (150.903 MHz) spectrum of **2c** in solid state.

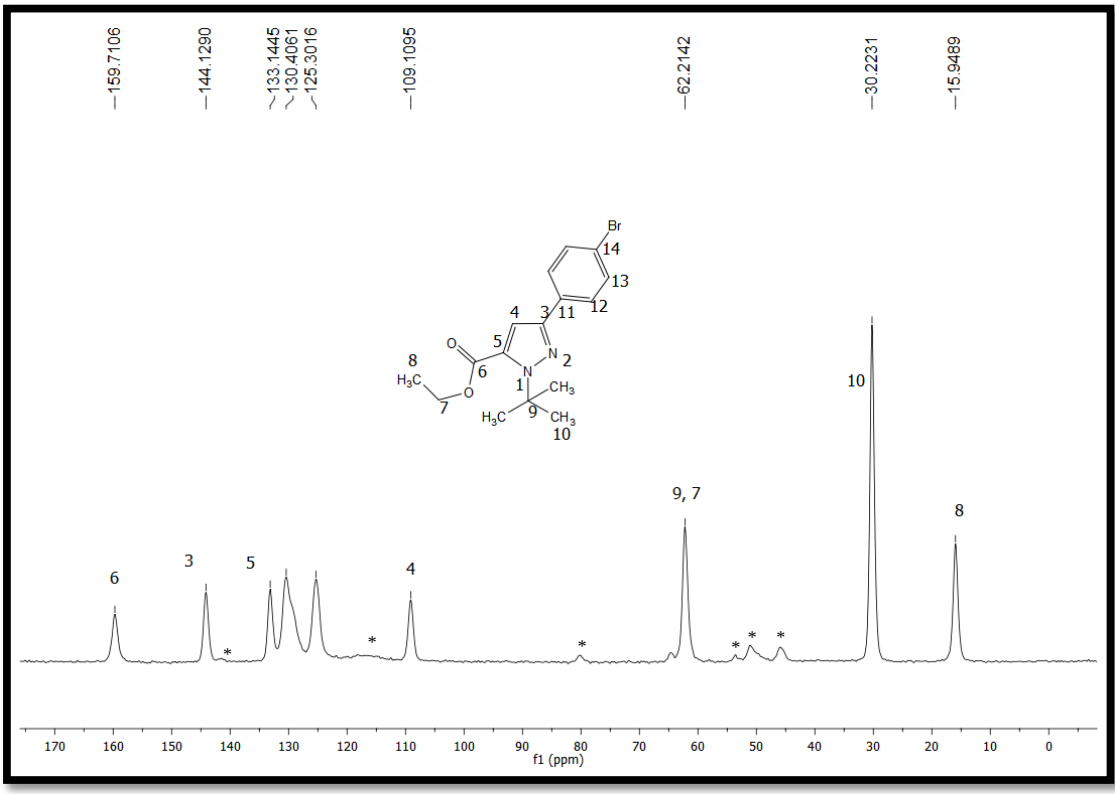


Figure S19. ^{13}C NMR (150.903 MHz) spectrum of **2d** in solid state.

5. Infrared Graph

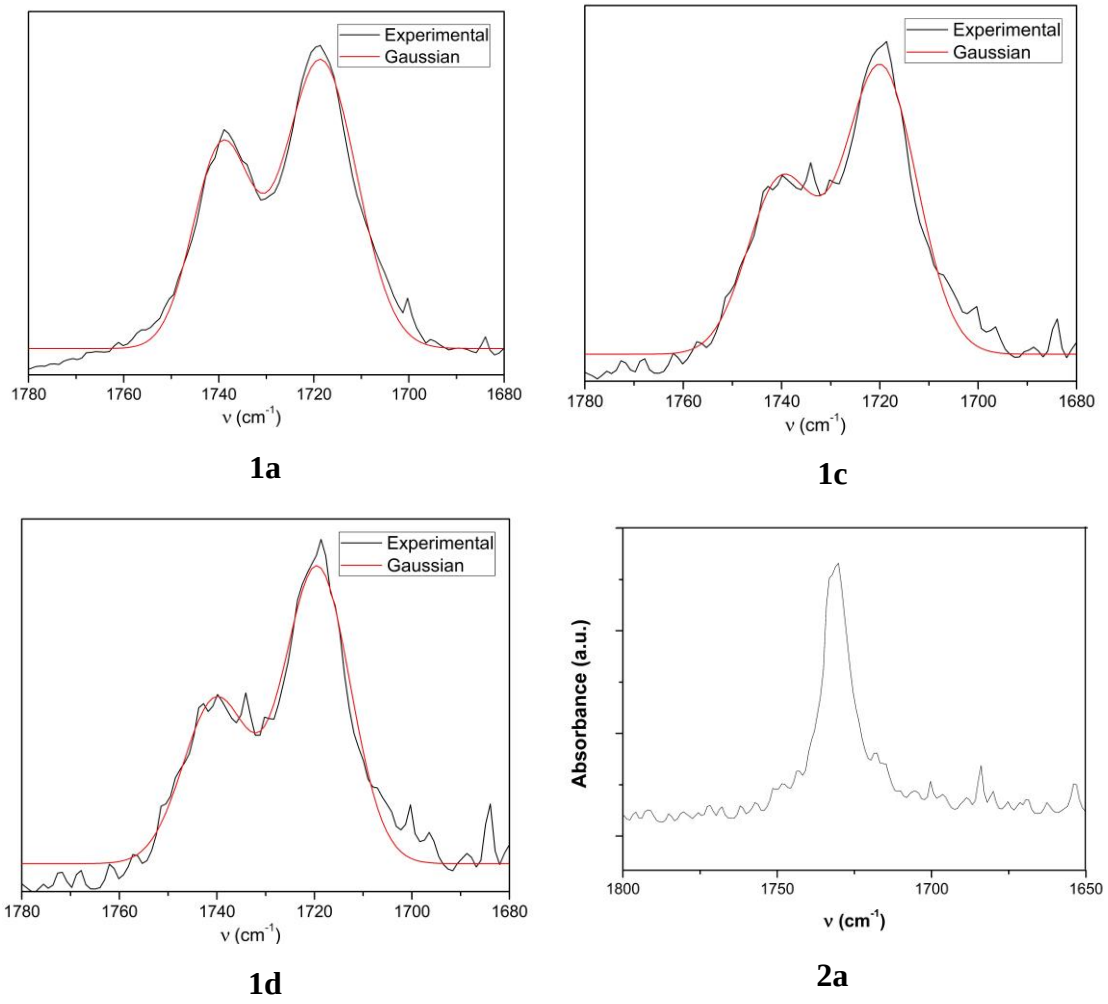
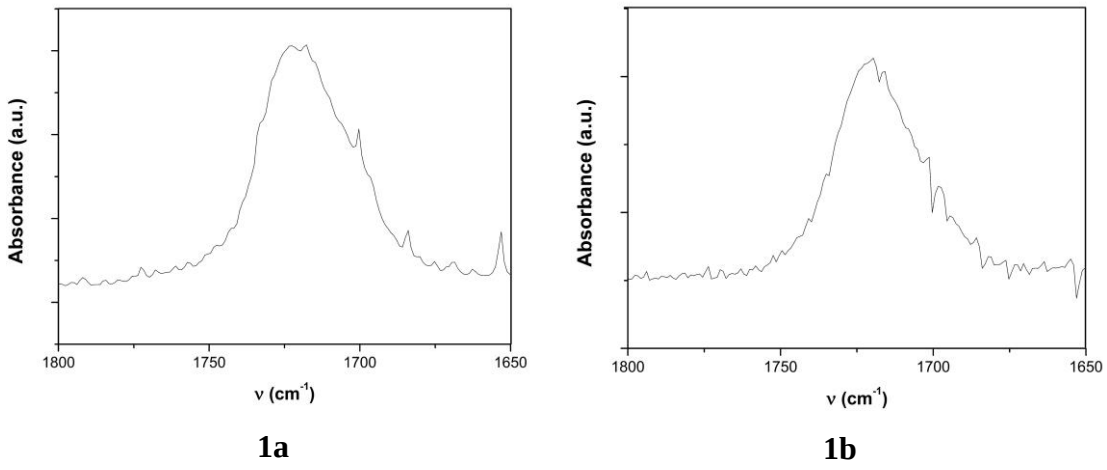


Figure S20. Infrared graph for compound **1a**, **1c-d** and **2a** in CCl_4.



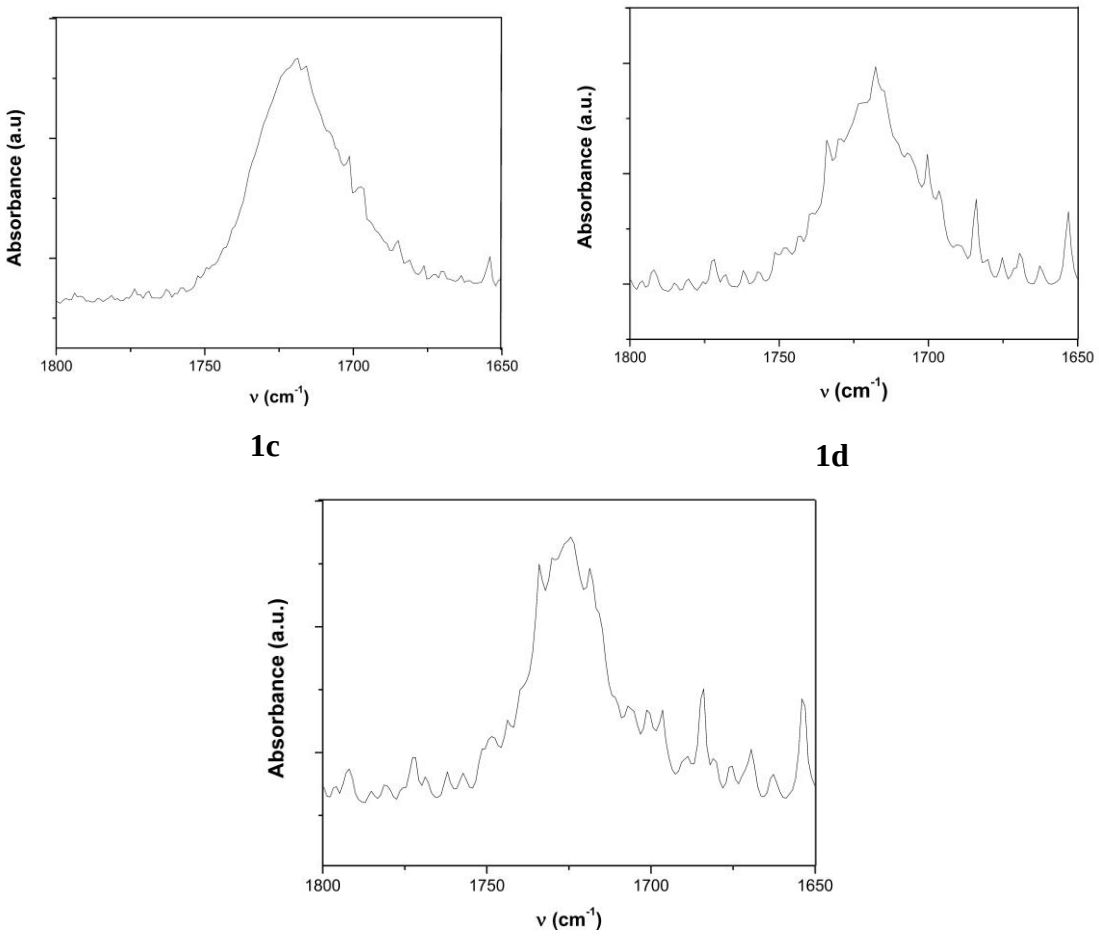
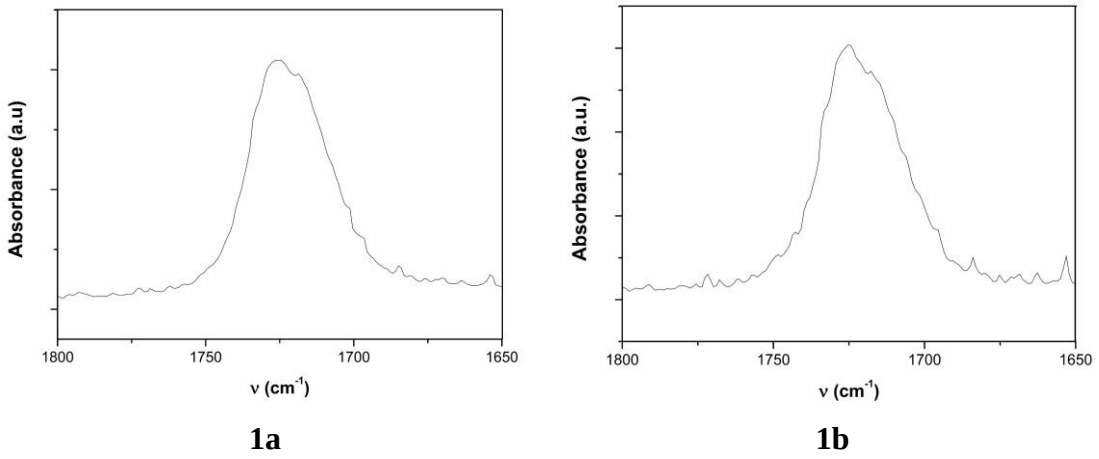


Figure S21. Infrared graph for compound **1a-d** and **2a** in $CHCl_3$.



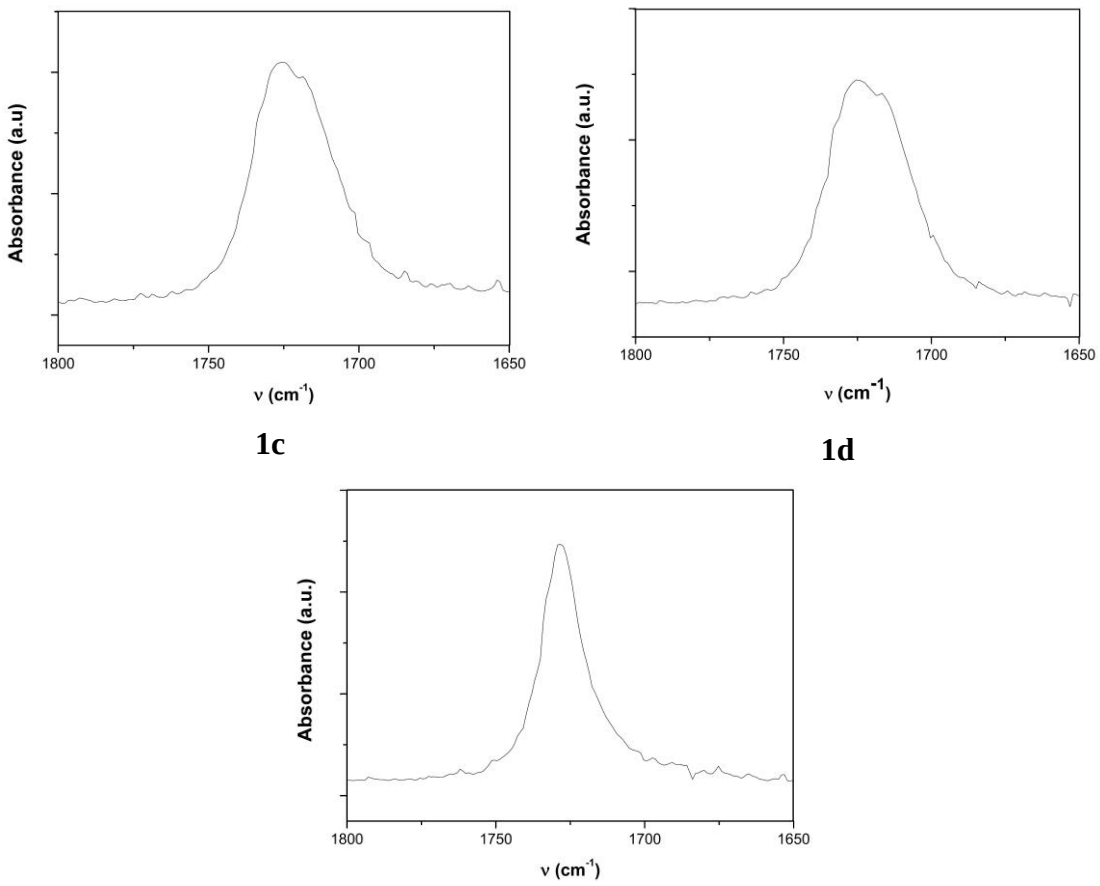
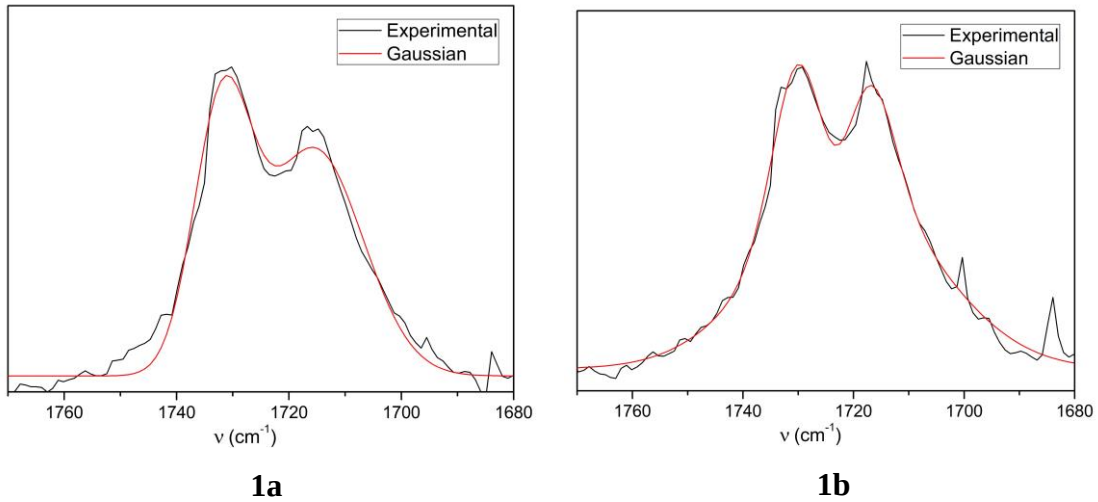


Figure S22. Infrared graph for compound **1a-d** and **2a** in CH_2Cl_2.



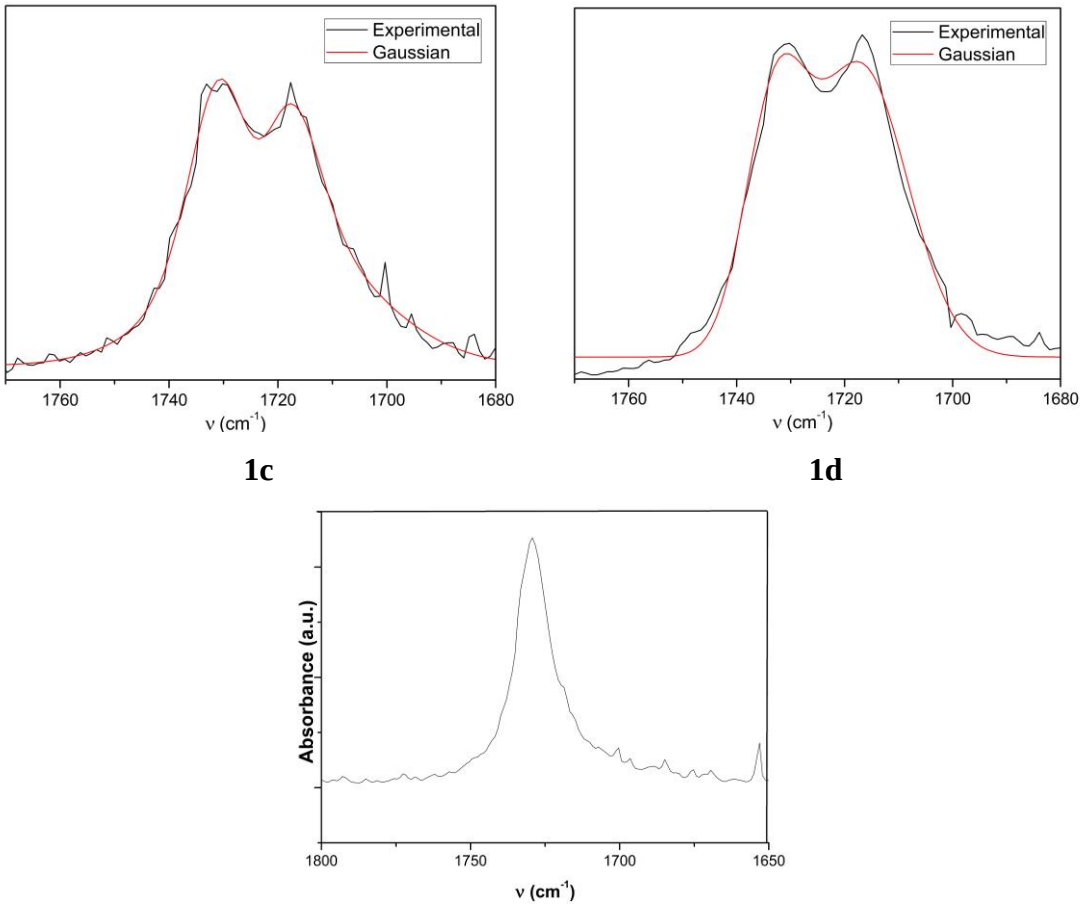


Figure S23. Infrared graph for compound **1a-d** and **2a** in CH_3CN.

Table S4. The IR spectra datas, region υ(C=O) for the compounds **1a-d** and **2a**.

Compound	solvent	Peak 1 (ν cm^{-1})	Pike 2 (ν cm^{-1})	**Deconvolution %**	
		experimental		Peak 1	Peak 2
1a	CCl_4	1719	1739	63	37
	$CHCl_3$	1722	-	-	-
	CH_2Cl_2	1727	-	-	-
	CH_3CN	1716	1731	46	54
1b	CCl_4	1720	1739	67	33
	$CHCl_3$	1721	-	-	-
	CH_2Cl_2	1725	-	-	-
	CH_3CN	1718	1730	51	49
1c	CCl_4	1719	1739	66	34
	$CHCl_3$	1720	-	-	-
	CH_2Cl_2	1725	-	-	-
	CH_3CN	1718	1731	48	52
1d	CCl_4	1719	1740	67	33
	$CHCl_3$	1718	-	-	-
	CH_2Cl_2	1725	-	-	-
	CH_3CN	1717	1731	55	45
2a	CCl_4	1730	-	-	-
	$CHCl_3$	1725	-	-	-
	CH_2Cl_2	1729	-	-	-

	CH_3CN	1729	-	-	-

Table S5. The calculated IR spectra data[a] for compound **1c** and **2a**, region υ(C=O).

Compound	Solvent	*s-cis* (ν cm^{-1})	*s-trans* (ν cm^{-1})
1c	CCl_4	1749	1724
	CH_3CN	1721	1705
	Vacuo	1769	1741
2a	CCl_4	1715	1725
	CH_3CN	1700	1711
	Vacuo	1726	1734

[a] scaled by 0.9876 for B3LYP/cc-pVTZ level of theory from optimized structures.

6. Calculation of Gibbs free energy (G)

Through the Gibbs free energy (G) of each isomer, one can determine the equilibrium constant K. For a given interconversion between conformations s-*cis* and s-*trans*, represented by M_1 and M_2, can be written the equation (1).

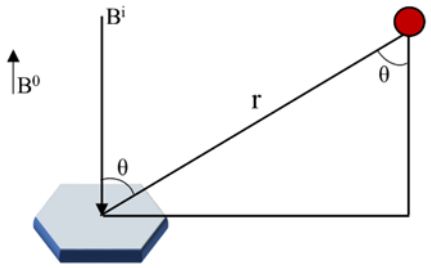
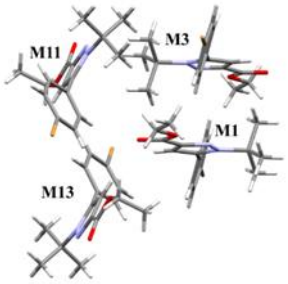
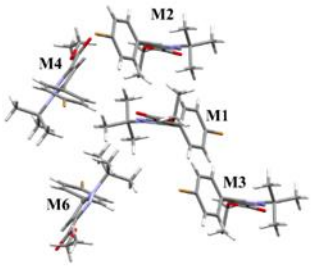
$$K = \frac{[M_1]}{[M_2]} - e^{-(\Delta G/RT)} \qquad (1)$$

Where ΔG represents the Gibbs free energy difference between two conformations M_1 and M_2, R is denoted by the ideal gases and T is the temperature. The Gibbs free energy for the conformers was obtained from the theoretical calculations at 298.15 K. Geometry optimization and calculated frequencies of all the studied species was carried out at the B3LYP/cc-pVTZ level of theory. Table S6 shows the Gibbs free energy values for *1,3*-pyrazole and *1,5*-pyrazole used in equation (1).

Table S6. Gibbs free energy values for conformers of *1,3*-pyrazole compound **1c** and *1,5*-pyrazole compound **2a**.

1,3-Pyrazole	Gibbs free energy (u.a.)	1,5-Pyrazole	Gibbs free energy (u.a.)
s-trans	-1341.377924	*s-trans*	-1341.384307
s-cis	-1341.376682	*s-cis*	-1341.379481

Table S7. Calculation of the chemical shift for compound **1d**.

		$\Delta\delta = K\frac{(3cos^2\theta)-1}{r^3}$			
	Conformer	Dimers	r	θ	Δδ
	s-trans C=O	M1···M13Ph	5.342	25	0.0096
		M1···M13Pi	5.286	79	-0.0060
		M1···M11Ph	5.549	67	-0.0032
		M1···M11Pi	5.780	26	0.0074
		M1···M3Ph	5.113	82	-0.0070
		M1···M3Pi	7.007	48	0.0010
	Total				0.0017
	*s-cis* C=O	M1···M4Ph	5.6780	84	-0.0053
		M1···M4Pi	7.684	48	0.0008
		M1···M2Ph	5.156	83	-0.0070
		M1···M2Pi	6.017	39	0.0037
		M1···M3Ph	5.850	76	-0.0041
		M1···M3Pi	8.388	60	-0.0004
		M1···M6Ph	7.259	27	0.0036
		M1···M6Pi	7.045	88	-0.0028
	Total				-0.0115
	s-trans -CH_2	M1···M8Ph	7.976	20	0.0032
		M1···M8Pi	8.248	90	-0.0018
		M1···M3Ph	5.959	81	-0.0045
		M1···M3Pi	8.78	58	-0.0002
		M1···M13Ph	7.194	37	0.0025
		M1···M13Pi	6.068	88	-0.0045
		M1···M11Ph	4.774	50	0.0022
		M1···M11Pi	6.304	46	0.0018
		M1···M10Ph	7.299	66	-0.0013

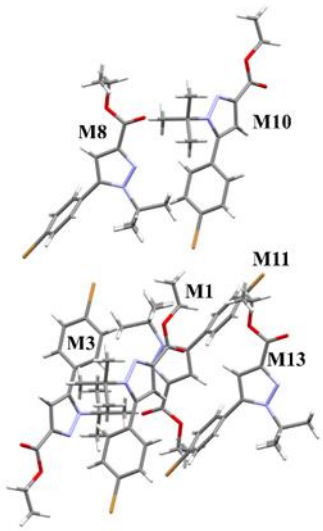
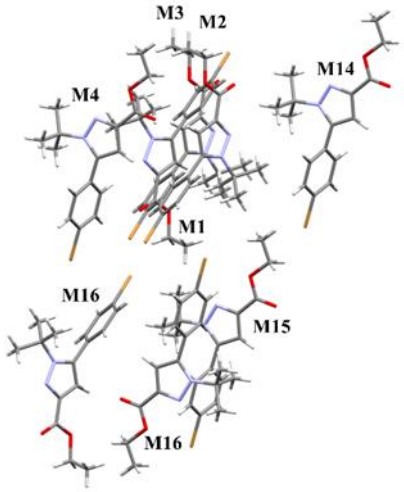
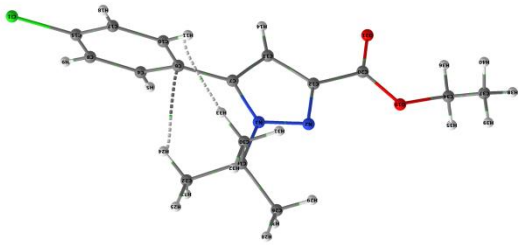
	Total	M1···M10Pi	11.074	79	-0.0007 -0.0032
	s-trans -CH_3	M1···M8Ph	7.062	26	0.0040
		M1···M8Pi	6.986	89	-0.0029
		M1···M3Ph	6.303	87	-0.0040
		M1···M3Pi	9.501	61	-0.0003
		M1···M13Ph	8.505	36	0.0016
		M1···M13Pi	7.206	87	-0.0027
		M1···M11Ph	5.536	41	0.0042
		M1···M11Pi	7.286	51	0.0005
		M1···M10Ph	6.571	57	-0.0004
		M1···M10Pi	10.221	79	-0.0008
	Total				-0.0008
	*s-cis* -CH_2	M1···M3Ph	5.998	84	-0.0045
		M1···M3Pi	8.701	60	-0.0004
		M1···M15Ph	9.119	67	-0.0008
		M1···M15Pi	5.86	83	-0.0047
		M1···M18Ph	6.879	84	-0.0030
		M1···M18Pi	10.898	89	-0.0008
		M1···M4Ph	7.044	78	-0.0025
		M1···M4Pi	8.955	49	0.0004
		M1···M2Ph	6.290	64	-0.0017
		M1···M2Pi	7.526	52	0.0003
		M1···M14Ph	10.847	39	0.0006
		M1···M14Pi	13.794	84	-0.0004
		M1···M16Ph	5.951	41	0.0034
		M1···M16Pi	8.587	63	-0.0006
	Total				-0.0146
	s-cis -CH_3	M1···M3Ph	6.906	79	-0.0027
		M1···M3Pi	9.633	54	0.0000
		M1···M15Ph	8.731	75	-0.0012
		M1···M15Pi	5.201	74	-0.0055
		M1···M18Ph	6.784	78	-0.0028
		M1···M18Pi	10.767	83	-0.0008
		M1···M4Ph	7.242	66	-0.0013
		M1···M4Pi	9.092	51	0.0003
		M1···M2Ph	5.620	52	0.0008
		M1···M2Pi	7.084	63	-0.0011
		M1···M14Ph	9.794	46	0.0005
		M1···M14Pi	12.908	86	-0.0005
		M1···M16Ph	4.828	50	0.0021
		M1···M16Pi	7.873	65	-0.0010
	Total				-0.0131

Table S8. Data of QTAIM analysis for intramolecular interactions of compounds **1a-d** and **2a-d.**

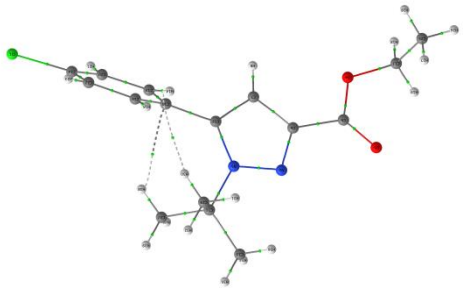
Comp.		ρ	$\nabla^2\rho$	ε	k	V	G	H_c
1a	CH···π	0.00919	+0.03008	1.30858	-0.00138	-0.00475	+0.00614	0.00139
		0.00923	+0.02992	1.40425	-0.00135	-0.00479	+0.00614	0.00135
1b	CH···π	0.00744	+0.03010	0.90748	-0.00172	-0.00408	+0.00580	0.00172
		0.01139	+0.03796	0.22007	-0.00145	-0.00658	+0.00803	0.00145

1c	CH···HC	0.00588	+0.02467	0.52900	-0.00148	-0.00321	+0.00469	0.00148
	CH···π (*s-trans*)	0.01290	+0.04339	0.02831	-0.00150	-0.00786	+0.00935	0.00149
	CH···HC	0.00660	+0.02703	0.75629	-0.00161	-0.00354	+0.00515	0.00161
	CH···π (*s-cis*)	0.01236	+0.04193	0.07143	-0.00151	-0.00747	+0.00897	0.00150
1d	CH···HC	0.00607	+0.02536	0.45027	-0.00148	-0.00339	+0.00486	0.00147
	CH···π (*s-trans*)	0.01296	+0.04381	0.05260	-0.00152	-0.00791	+0.00943	0.00152
	CH···HC	0.00669	+0.02767	0.59600	-0.00162	-0.00368	+0.00530	0.00162
	CH···π (*s-cis*)	0.01258	+0.04281	0.01530	-0.00152	-0.00765	+0.00918	0.00153
2a	CH···O	0.0137	+0.04511	0.101645	-0.00050	-0.01027	+0.01077	0.000503
		0.0158	+0.05284	0.058971	-0.00061	-0.01199	+0.01260	0.000611
2b	CH···O	0.0138	+0.04534	0.105465	-0.00051	-0.01032	+0.01083	0.000511
		0.0159	+0.05338	0.052123	-0.00064	-0.01206	+0.01270	0.000642
2c	CH···O	0.01561	+0.05168	0.080369	-0.00056	-0.01180	+0.01236	0.000563
		0.01561	+0.05169	0.080351	-0.00056	-0.01181	+0.01236	0.000554
2d	CH···O	0.01486	+0.04974	0.06835	-0.00062	-0.01120	+0.01182	0.00062
		0.01553	+0.05101	0.08994	-0.00051	-0.01174	+0.01225	0.00051

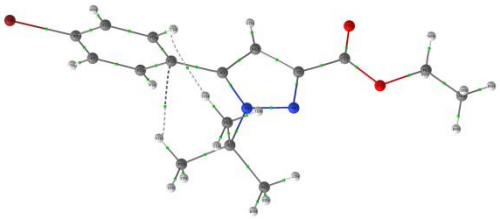
Hc= Vc + Gc



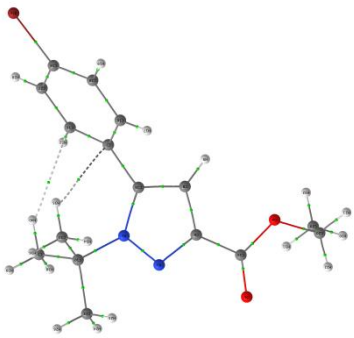
1c (*s-trans*)



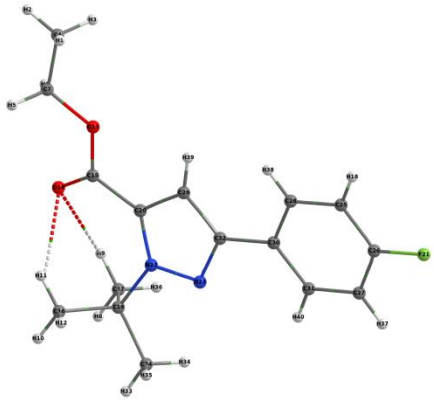
1c (*s-cis*)



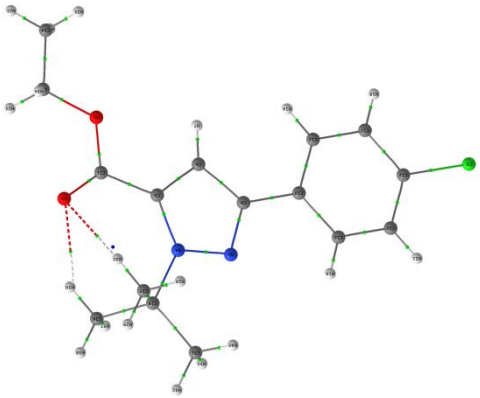
1d (*s-trans*)



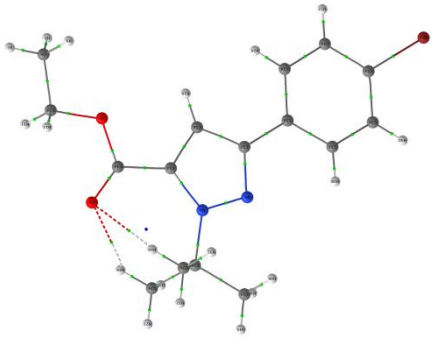
1d (*s-cis*)



2b (*s-trans*)

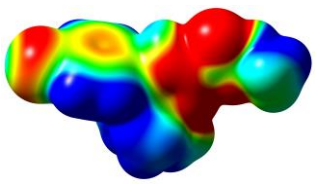


2c (*s-trans*)

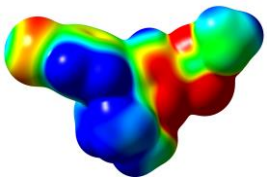


2d (*s-trans*)

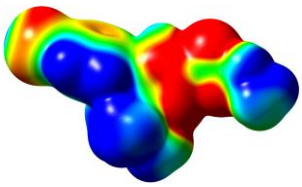
Figure S24. View of the intramolecular interactions of compounds **1c-d** and **2b-d**.



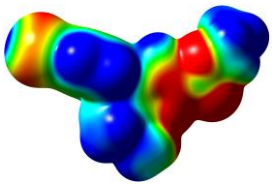
1c *s-trans*



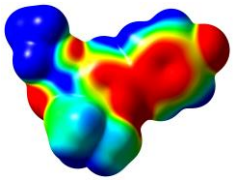
1c *s-cis*



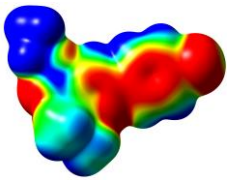
1d *s-trans*



1d *s-cis*



2b



2c

Compound	V_{min} (C=O)

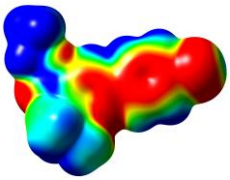
 **2d**	**1c** *s-trans*	-0.065
	1c *s-cis*	-0.079
	1d *s-trans*	-0.062
	1d *s-cis*	-0.079
	2b	-0.043
	2c	-0.042
	2d	-0.042

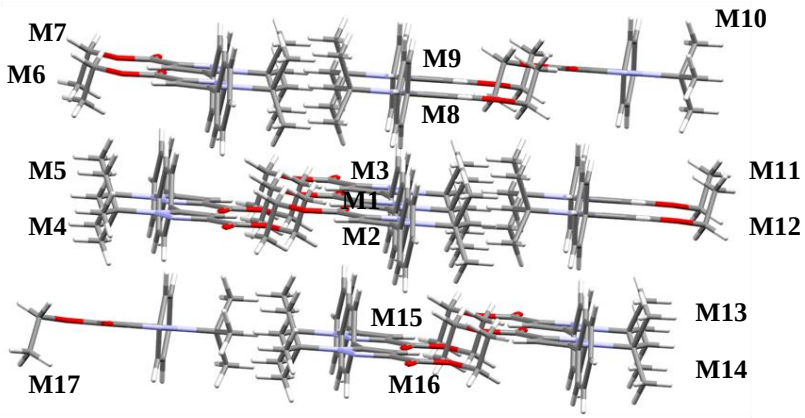
Figure S25. The Molecular Electrostatic Potential of compounds **1c-d** and **2b-d**.

7. Cluster Supramolecular

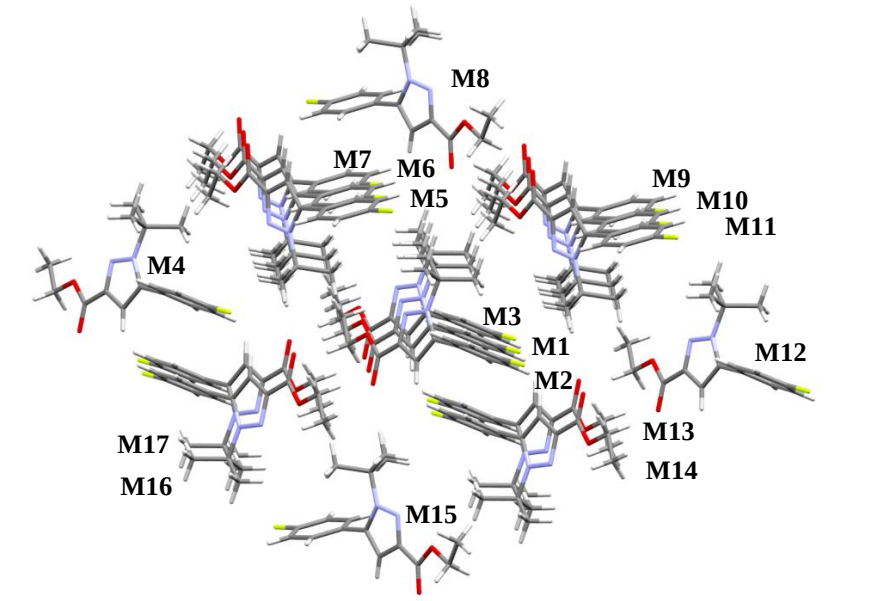
Table S9. Molecular Coordination Number[a] (MCN) for compounds **1a-d** and **2a-d**

Compound	NCM
1a	16
1b	16
1c	15:17[b]
1d	15:17[b]
2a	15
2b	15
2c	16
2d	17

[a] NCM obtained by TOPOS® program. [b] Cluster A: Cluster B

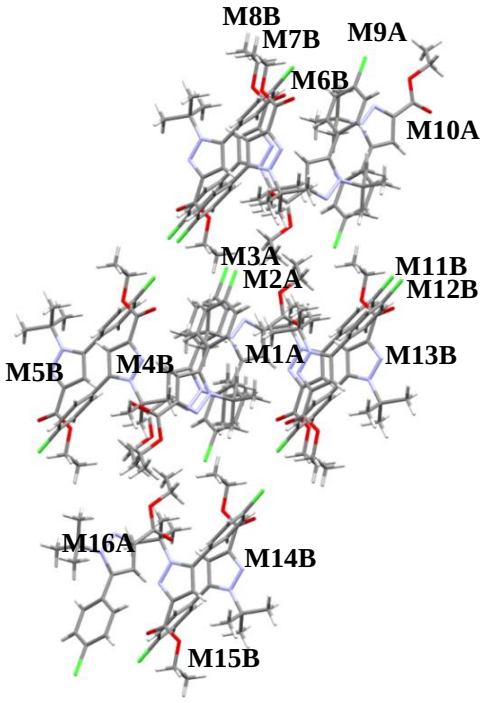


1a

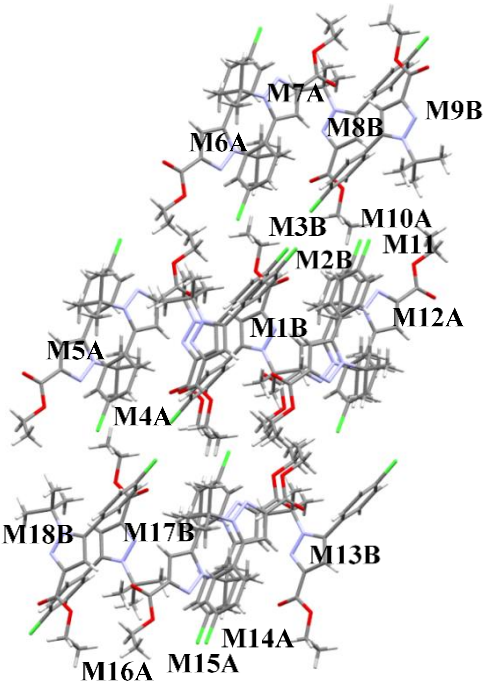


1b

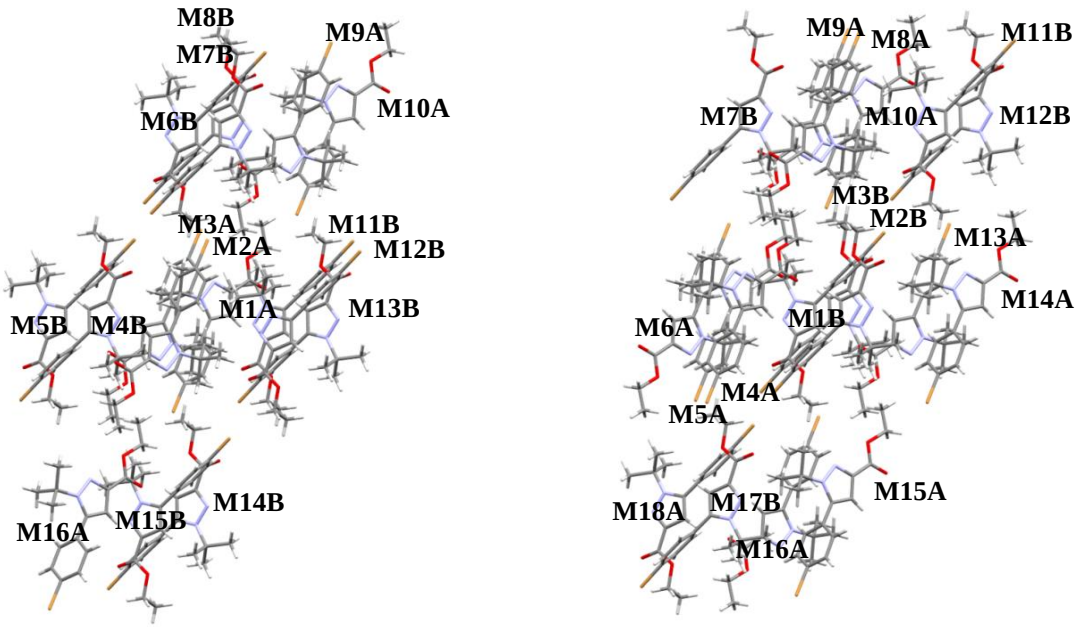
Figure S26. Supramolecular cluster of *1,3*-isomers.



1c Cluster A *(s-trans)*



1c Cluaster B (*s-cis*)



1d Cluster A (*s-trans*) **1d** Cluaster B (*s-cis*)

Figure S27. Supramolecular cluster of *1,3*-isomers.

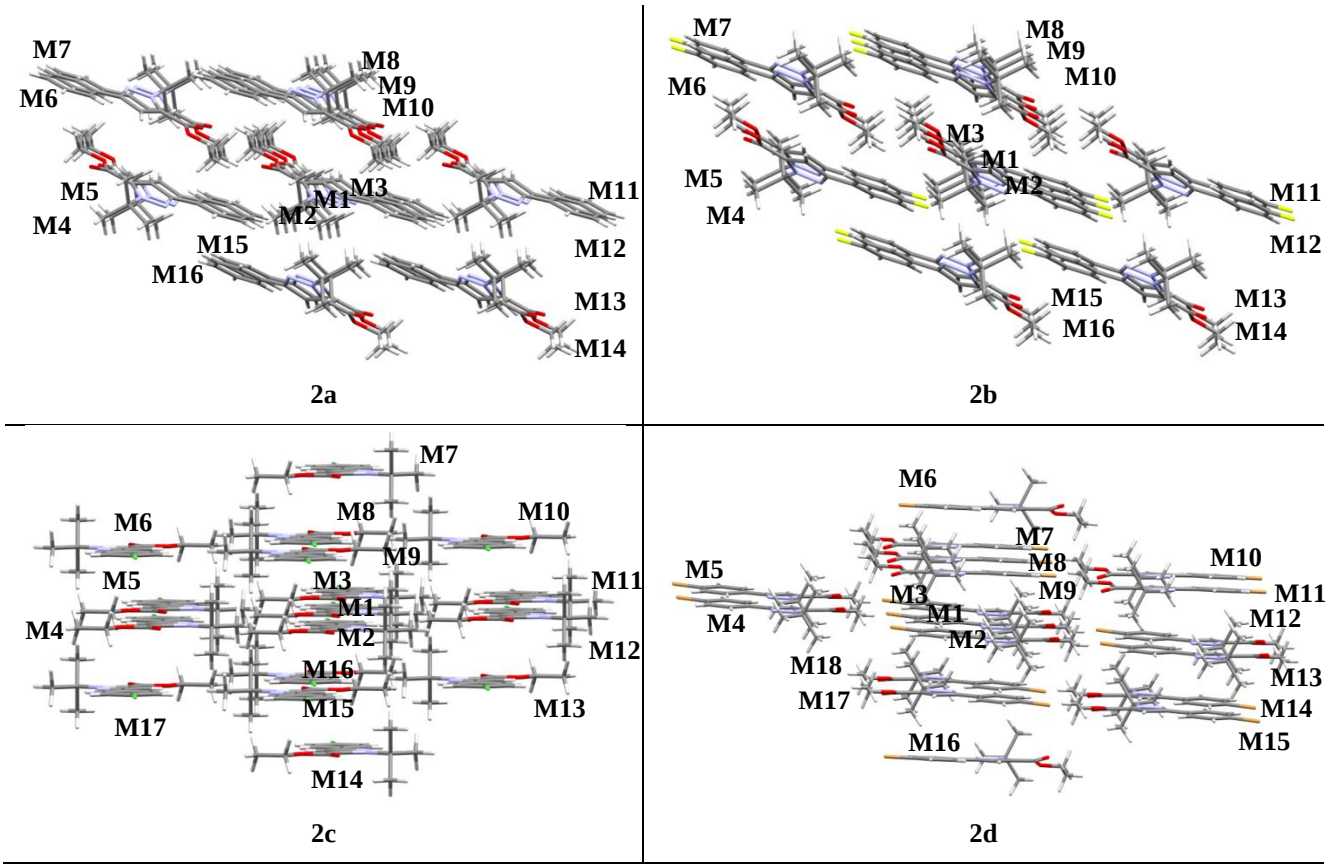


Figure S28. Supramolecular cluster of *1,5*-isomers.

Table S10. Topological[a] and energetic[b] data of each dimer from the supramolecular cluster of compound **1b**.

Dimer	Symmetry code	$C_{M1\cdots MN}$ (Å)	$G_{M1\cdots MN}$ (Kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	1+x,y,z	58.71	-10.67	2.35	2.72
M1···M3	-1+x,y,z	58.71	-10.67	2.35	2.72
M1···M4	-1+x,y,1+z	0.82	-0.24	0.03	0.06
M1···M5	1+x,1,5-y,1/2+z	1.46	-0.35	0.06	0.09
M1···M6	x1,5-y,1/2+z	52.02	-6.09	2.08	1.55
M1···M7	-1+x,1,5-y,1/2+z	21.04	-2.17	0.84	0.55
M1···M8	1-x,1/2+y,1,5-z	9.06	-2.74	0.36	0.70
M1···M9	-1+x,1,5-y,- 1/2+z	1.46	-0.35	0.06	0.09
M1···M10	x,1,5-y,-1,2+z	52.02	-6.09	2.08	1.55
M1···M11	1+x,1,5-y,-1/2+z	21.04	-2.17	0.84	0.55
M1···M12	1+x,y,-1+z	0.82	-0.24	0.03	0.06
M1···M13	1-x,1-y,1-z	33.82	-7.15	1.35	1.82
M1···M14	2-x,1-y,1-z	36.51	-5.60	1.46	1.43
M1···M15	1-x,-1/2+y,1,5-z	9.06	-2.74	0.36	0.70
M1···M16	1-x,1-y,2-z	20.17	-2.89	0.81	0.74
M1···M17	-x,1-y,2-z	23.00	-2.60	0.92	0.66
Total		399.72	-62.76		

[a] Contact surface obtained by TOPOS®.[b] Interaction energy obtained by Gaussian 09® (theory level ωB97X-D/cc-pVDZ).

Table S11. Topological[a] and energetic[b] data of each dimer from the supramolecular cluster of compound **1cA**.

Dimer	Symmetry code	$C_{M1\cdots MN}$ (Å)	$G_{M1\cdots MN}$ (Kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1A	x,y,z				
M1···M2A	-x,2-y,-z	36.16	-4.60	1.36	1.06
M1···M3A	1-x,2-y,-z	75.83	-14.81	2.85	3.41
M1···M4B	x,y,z	46.36	-7.90	1.74	1.82
M1···M5B	1-x,1-y,-z	13.60	-1.74	0.51	0.40
M1···M6B	1-x,2-y,-1-z	24.03	-2.68	0.90	0.62
M1···M7B	x,1+y,-1+z	2.07	-0.77	0.08	0.18
M1···M8B	1+x,1+y,- 1+z	16.43	-1.54	0.62	0.35
M1···M9A	1-x,3-y,-1-z	25.51	-4.44	0.96	1.02
M1···M10A	1+x,1+y,- 1+z	5.92	-0.85	0.22	0.20
M1···M11B	1-x,2-y,-z	27.59	-4.97	1.04	1.14
M1···M12B	-x,2-y,-z	39.17	-9.62	1.47	2.22
M1···M13B	x,1+y,z	46.20	-6.53	1.74	1.50
M1···M14B	x,y,1+z	14.90	-1.32	0.56	0.30
M1···M15B	-x,1-y,1-z	19.55	-2.49	0.73	0.57
M1···M16A	-1+x,- 1+y,1+z	5.92	-0.85	0.22	0.20
Total		399.24	-65.10		

[a] Contact surface obtained by TOPOS®.[b] Interaction energy obtained by Gaussian 09® (theory level ωB97X-D/cc-pVDZ).

Table S12. Topological[a] and energetic[a] data of each dimer from the supramolecular cluster of compound **1cB**.

Dimer	Symmetry code	$C_{M1\cdots MN}$ (Å)	$G_{M1\cdots MN}$ (Kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1B	x,y,z				
M1···M2B	-x,1-y,-z	77.33	-13.95	3.29	3.78
M1···M3B	1-x,1-y,-z	38.92	-5.76	1.66	1.56
M1···M4A	x,-1+y,z	46.20	-6.53	1.97	1.77
M1···M5A	1-x,1-y,-z	13.60	-1.74	0.58	0.47
M1···M6A	1-x,2-y,-1-z	24.03	-2.68	1.02	0.73
M1···M7A	x,y,-1+z	14.90	-1.32	0.63	0.36
M1···M8B	1-x,2-y,-1-z	3.30	-0.71	0.14	0.19
M1···M9B	x,1+y,-1+z	12.43	-0.74	0.53	0.20
M1···M10A	1-x,2-y,-z	27.59	-4.97	1.17	1.35
M1···M11A	-x,2-y,-z	39.17	-9.62	1.67	2.61
M1···M12A	x,y,z	46.36	-7.90	1.97	2.14
M1···M13B	-x,1-y,1-z	1.01	-0.48	0.04	0.13
M1···M14A	-1+x,-1+y,1+z	16.43	-1.54	0.70	0.42
M1···M15A	x,-1+y,1+z	2.07	-0.77	0.09	0.21
M1···M16A	-x,1-y,1-z	19.55	-2.49	0.83	0.68
M1···M17B	x,-1+y,1+z	12.43	-0.74	0.53	0.20
M1···M18B	-x,-y,1-z	3.98	-0.75	0.17	0.20
Total		399.3	-62.68		

[a] Contact surface obtained by TOPOS®.[b] Interaction energy obtained by Gaussian 09® (theory level ωB97X-D/cc-pVDZ).

Table S13. Topological[a] and energetic[b] data of each dimer from the supramolecular cluster of compound **1dA**.

Dimer	Symmetry code	$C_{M1\cdots MN}$ (Å)	$G_{M1\cdots MN}$ (Kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1A	x,y,z				
M1···M2A	1-x,1-y,-z	37.40	-5.10	1.38	1.11
M1···M3A	2-x,1-y,-z	78.12	-15.60	2.88	3.40
M1···M4B	x,-1+y,z	46.90	-8.21	1.73	1.79
M1···M5B	2-x,1-y,-z	13.13	-1.83	0.48	0.40
M1···M6B	2-x,2-y,-1-z	26.14	-2.82	0.96	0.62
M1···M7B	x,y,-1+z	1.98	-0.93	0.07	0.20
M1···M8B	1+x,y,-1+z	16.96	-1.57	0.63	0.34
M1···M9A	2-x,2-y,-1-z	27.80	-3.87	1.02	0.84
M1···M10A	1+x,1+y,-1+z	6.12	-1.32	0.23	0.29
M1···M11B	2-x,2-y,-z	48.09	-7.33	1.77	1.60
M1···M12B	1-x,2-y,-z	26.84	-4.71	0.99	1.03
M1···M13B	x,y,z	37.30	-9.41	1.37	2.05
M1···M14B	x,-1+y,2+z	13.62	-1.45	0.50	0.32
M1···M15B	1-x,1-y,1-z	20.45	-3.28	0.75	0.72
M1···M16A	-1+x,-1+y,1+z	6.12	-1.32	0.23	0.29
Total		406.97	-68.75		

[a] Contact surface obtained by TOPOS®.[b] Interaction energy obtained by Gaussian 09® (theory level ωB97X-D/cc-pVDZ).

Table S14. Topological[a] and energetic[b] data of each dimer from the supramolecular cluster of compound **1dB**.

Dimer	Symmetry code	$C_{M1\cdots MN}$ (Å)	$G_{M1\cdots MN}$ (Kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1B	x,y,z				
M1···M2B	1-x,2-y,-z	38.52	-5.91	1.62	1.53
M1···M3B	2-x,2-y,-z	78.08	-14.22	3.29	3.68
M1···M4A	1-x,2-y,-z	26.84	-4.71	1.13	1.22
M1···M5A	2-x,2-y,-z	37.30	-9.41	1.57	2.44
M1···M6A	x,1+y,z	46.90	-8.21	1.97	2.13
M1···M7B	1-x,2-y,-z	2.04	-0.31	0.09	0.08
M1···M8A	-1+x,y,1+z	1.98	-0.93	0.08	0.24
M1···M9A	x,y,1+z	16.96	-1.57	0.71	0.41
M1···M10A	1-x,1-y,1-z	20.45	-3.28	0.86	0.85
M1···M11B	x,-1+y,1+z	12.45	-1.00	0.52	0.26
M1···M12B	1-x,1-y,1-z	5.06	-0.86	0.21	0.22
M1···M13A	x,y,z	48.09	-7.33	2.02	1.90
M1···M14A	1-x,1-y,-z	13.13	-1.83	0.55	0.47
M1···M15A	2-x,2-y,-1-z	26.14	-2.83	1.10	0.73
M1···M16A	x,1+y,-1+z	13.62	-1.45	0.57	0.38
M1···M17B	2-x,3-y,-1-z	3.87	-0.78	0.16	0.20
M1···M18B	x,1+y,-1+z	12.45	-1.00	0.52	0.26
Total		403.88	-65.63		

[a] Contact surface obtained by TOPOS®.[b] Interaction energy obtained by Gaussian 09® (theory level ωB97X-D/cc-pVDZ).

Table S15. Topological[a] and energetic[b] data of each dimer from the supramolecular cluster of compound **2a**.

Dimer	Symmetry code	$C_{M1\cdots MN}$ (Å)	$G_{M1\cdots MN}$ (Kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	x,1+y,z	23.30	-3.55	0.99	0.80
M1···M3	x,-1+y,z	23.30	-3.55	0.99	0.80
M1···M4	-1+x,1+y,z	13.30	-1.56	0.56	0.35
M1···M5	-1+x,y,z	29.65	-6.32	1.26	1.43
M1···M6	-x,1-y,1-z	27.33	-5.68	1.16	1.29
M1···M7	-x,-y,1-z	8.78	-0.43	0.37	0.10
M1···M8	1-x,-y,1-z	14.22	-2.11	0.60	0.48
M1···M9	1-x,1-y,1-z	73.76	-14.77	3.13	3.34
M1···M10	1-x,2-y,1-z	7.54	-1.36	0.32	0.31
M1···M11	1+x,-1+y,z	13.30	-1.56	0.56	0.35
M1···M12	1+x,y,z	29.65	-6.32	1.26	1.43
M1···M13	2-x,-1/2+y,1.5-z	11.03	-3.75	0.47	0.85
M1···M14	2-x,1/2+y,1.5-z	24.12	-3.75	1.02	0.85
M1···M15	1-x,1/2+y,1.5-z	27.00	-5.79	1.15	1.31
M1···M16	1-x,-1/2+y,1.5-z	27.00	-5.79	1.15	1.31
Total		353.28	-66.31		

[a] Contact surface obtained by TOPOS®.[b] Interaction energy obtained by Gaussian 09® (theory level ωB97X-D/cc-pVDZ).

Table S16. Topological[a] and energetic[b] data of each dimer from the supramolecular cluster of compound **2b**.

Dimer	Symmetry code	$C_{M1\cdots MN}$ (Å)	$G_{M1\cdots MN}$ (Kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	-1+x, y, z	24.19	-3.07	1.00	0.80
M1···M3	1+x,y,z	24.19	-3.07	1.00	0.80
M1···M4	x,1+y,z	29.22	-5.55	1.21	1.44
M1···M5	1+x,1+y,z	16.41	-1.98	0.68	0.51
M1···M6	-x,1-y,2-z	8.74	-0.44	0.36	0.11
M1···M7	1-x,1-y,2-z	30.14	-5.83	1.25	1.51
M1···M8	2-x,-y,2-z	7.36	-1.10	0.30	0.29
M1···M9	1-x,-y,2-z	76.54	-14.39	3.16	3.73
M1···M10	-x,-y,2-z	20.98	-2.06	0.87	0.53
M1···M11	x,-1+y,z	29.22	-5.55	1.21	1.44
M1···M12	-1+x,-1+y,z	16.41	-1.98	0.68	0.51
M1···M13	1-x,-1-y,1-z	37.81	-4.69	1.56	1.21
M1···M14	-x,-1-y,1-z	17.15	-2.74	0.71	0.71
M1···M15	2-x,-y,1-z	5.70	-0.66	0.24	0.17
M1···M16	1-x,-y,1-z	43.10	-8.70	1.78	2.25
Total		387.16	-61.79		

[a] Contact surface obtained by TOPOS®.[b] Interaction energy obtained by Gaussian 09® (theory level ωB97X-D/cc-pVDZ).

Table S17. Topological[a] and energetic[b] data of each dimer from the supramolecular cluster of compound **2c**.

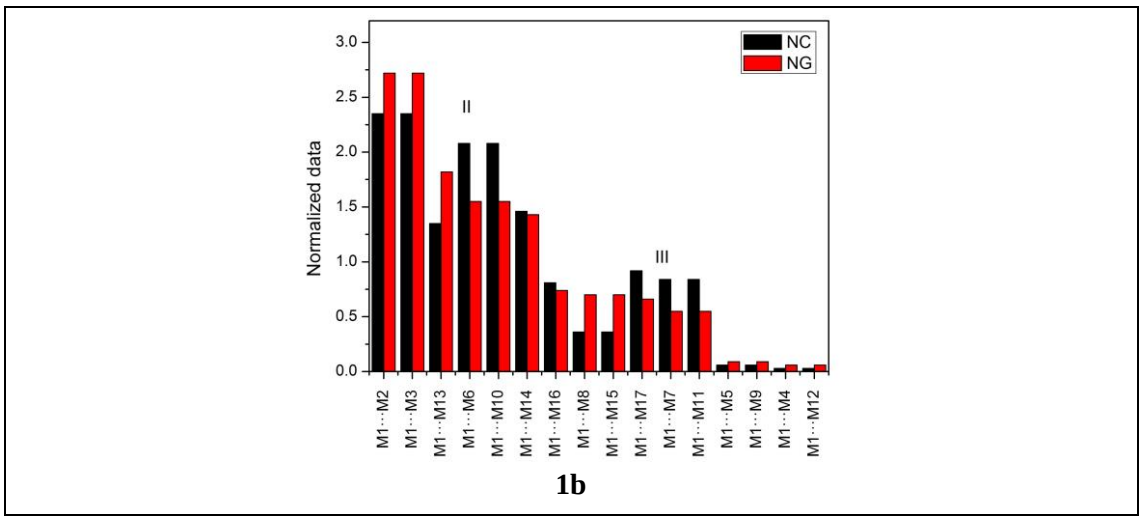
Dimer	Symmetry code	$C_{M1\cdots MN}$ (Å)	$G_{M1\cdots MN}$ (Kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	x, y, 1+z	9.34	-0.89	0.38	0.25
M1···M3	x, y, -1+z	9.34	-0.89	0.38	0.25
M1···M4	1+x, y, 1+z	31.15	-0.45	1.27	0.13
M1···M5	1+x, y, z	5.47	-2.67	0.22	0.76
M1···M6	2-x, -1/2 +y, 2-z	37.11	-0.64	1.51	0.18
M1···M7	x, -1+y, z	4.80	-0.96	0.20	0.27
M1···M8	1-x, -1/2+y,1-z	72.44	-13.68	2.96	3.87
M1···M9	1-x, -1/2+y, 2-z	26.78	-3.60	1.09	1.02
M1···M10	-x, -1/2+y, 1-z	8.91	-5.37	0.36	1.52
M1···M11	-1+x, y, -1+z	31.15	-0.45	1.27	0.13
M1···M12	-1+x, y, z	5.47	-2.67	0.22	0.76
M1···M13	-x, ½+y, 1-z	8.91	-5.37	0.36	1.52
M1···M14	x,1+y,z	4.80	-0.96	0.20	0.27
M1···M15	1-x,1/2+y,2-z	26.78	-3.60	1.09	1.02
M1···M16	1-x,1/2+y,1-z	72.44	-13.68	2.96	3.87
M1···M17	2-x,1/2+y,2-z	37.11	-0.64	1.51	0.18
Total		392.00	-56.48		

[a] Contact surface obtained by TOPOS®.[b] Interaction energy obtained by Gaussian 09® (theory level ωB97X-D/cc-pVDZ).

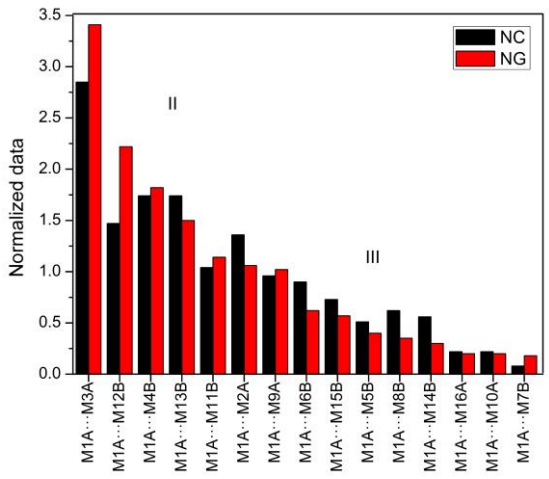
Table S18. Topological[a] and energetic[b] data of each dimer from the supramolecular cluster of compound **2d**.

Dimer	Symmetry code	$C_{M1\cdots MN}$ (Å)	$G_{M1\cdots MN}$ (Kcal mol^{-1})	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z				
M1···M2	x,-1+y,z	29.57	-2.50	1.28	0.70
M1···M3	x,1+y,z	29.57	-2.50	1.28	0.70
M1···M4	-1/2+x,-1/2+y,z	6.52	-0.88	0.28	0.25
M1···M5	-1/2+x,1/2+y,z	9.60	-1.72	0.41	0.48
M1···M6	x,-y,1/2+z	4.90	-0.92	0.21	0.26
M1···M7	1-x,1+y,1.5-z	12.46	-2.02	0.54	0.57
M1···M8	1-x,y,1.5-z	83.89	-16.08	3.62	4.52
M1···M9	1-x,-1+y,1.5-z	12.46	-2.02	0.54	0.57
M1···M10	1.5-x,1/2+y,1.5-z	20.28	-2.70	0.88	0.76
M1···M11	1.5-x,-1/2+y,1.5-z	20.28	-2.70	0.88	0.76
M1···M12	1/2+x,1/2+y,z	6.52	-0.88	0.28	0.25
M1···M13	1/2+x,-1/2+y,z	9.60	-1.72	0.41	0.48
M1···M14	1.5-x,1.5-y,1-z	9.32	-0.33	0.40	0.09
M1···M15	1.5-x,1/2-y,1-z	20.36	-2.11	0.88	0.59
M1···M16	x,-y,-1/2+z	4.90	-0.92	0.21	0.26
M1···M17	1-x,-y,1-z	36.63	-5.23	1.58	1.47
M1···M18	1-x,1-y,1-z	77.02	-15.28	3.32	4.29
Total		393.88	-60.48		

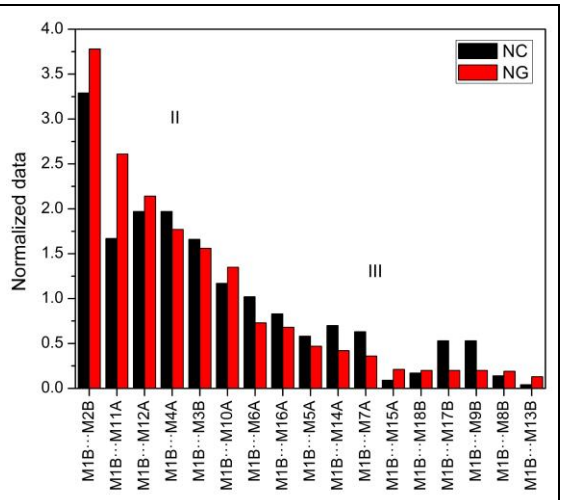
[a] Contact surface obtained by TOPOS®.[b] Interaction energy obtained by Gaussian 09® (theory level ωB97X-D/cc-pVDZ).



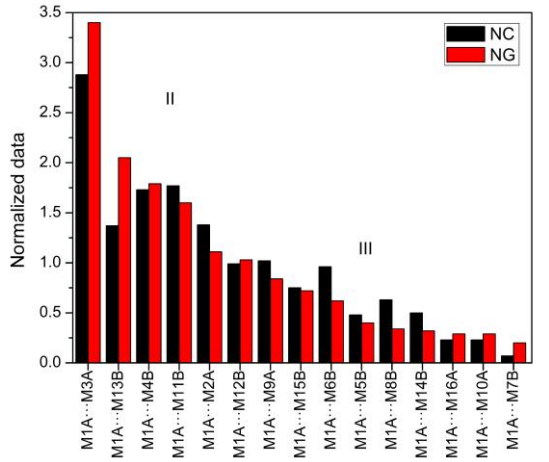
1b



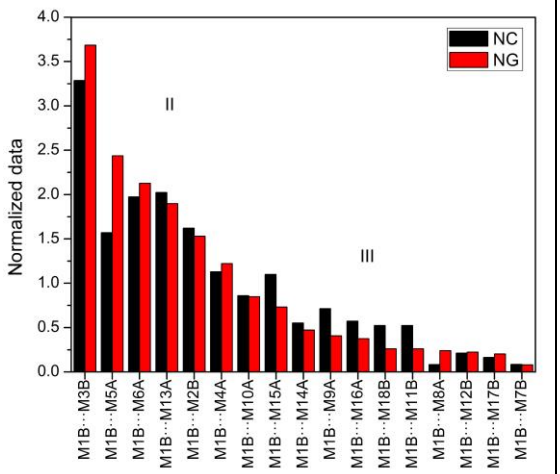
1c cluster A



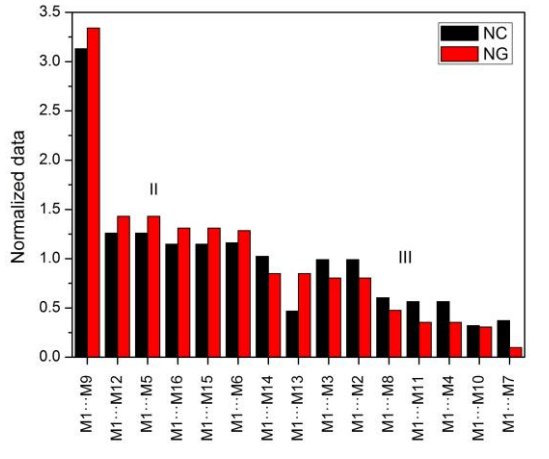
1c Cluster B



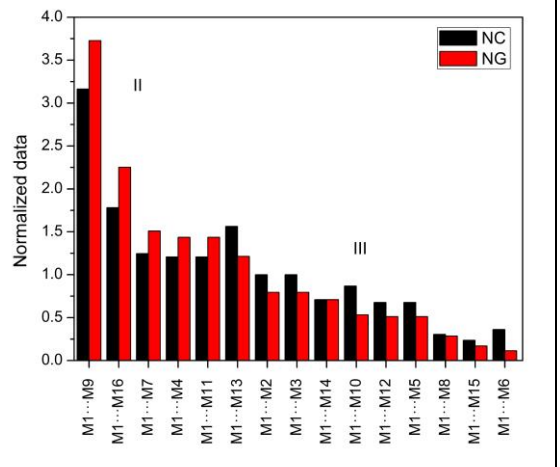
1d Cluster A



1d Cluster B



2a



2b

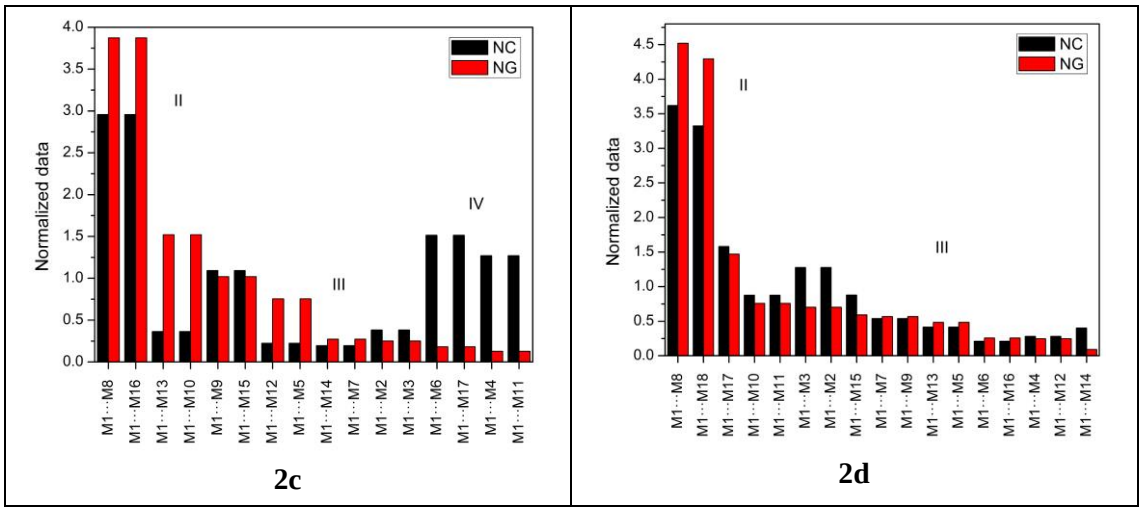
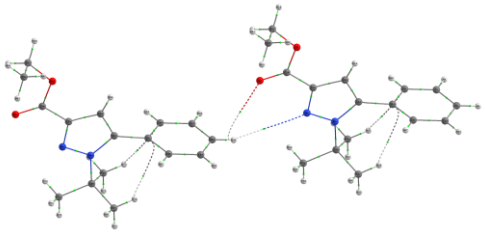
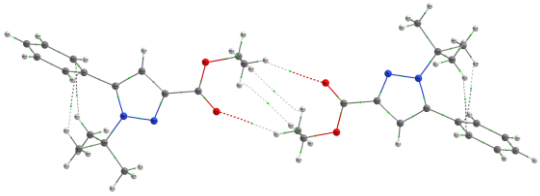
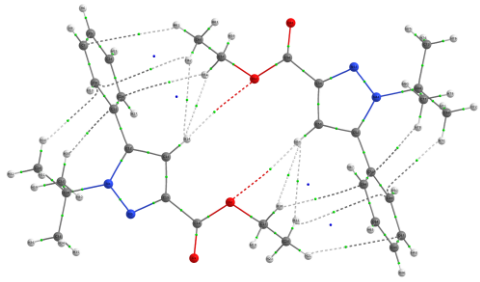


Figure S29. Topological and energetic normalized data of each dimer from the supramolecular cluster of compounds **1b-d** and **2a-d**.

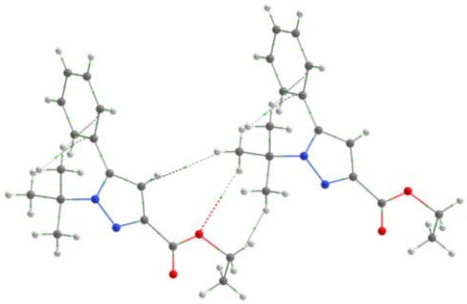
8. QTAIM Supramolecular

Table S19. View of the dimer interactions from QTAIM analysis of compound **1a.**

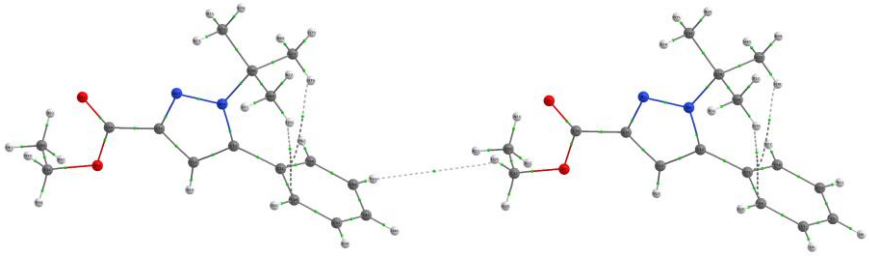
	
M1···M2/M1···M3	M1···M4



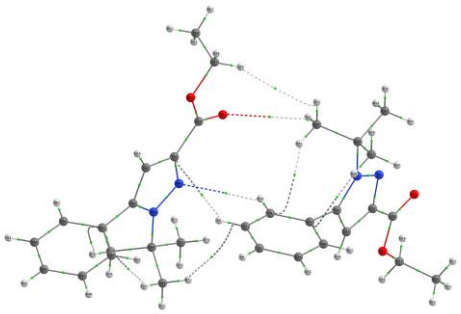
M1···M5



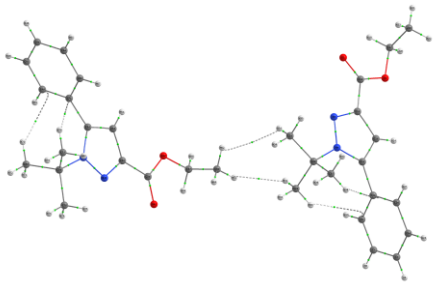
M1···M6/ M1···M13



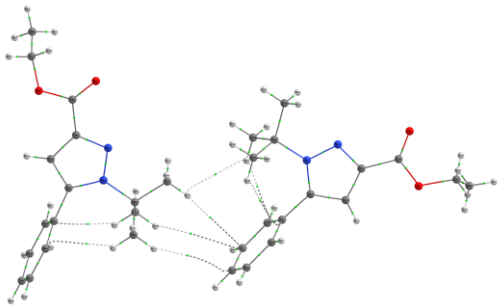
M1···M7/ M1···M14



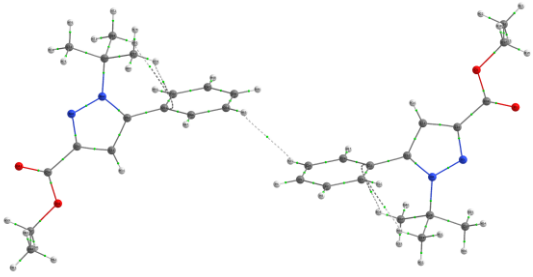
M1···M8/ M1···M9



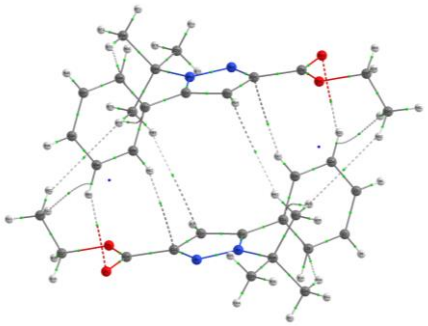
M1···M10/ M1···M17



M1···M11/M1···M12



M1···M15



M1···M16

Table S20. QTAIM data and G_{AI} of dimers of compound **1a**.

Dimer	Interaction	ρ_{INT}	$\nabla^2\rho$	ε	K	V	G	H	G_{AI}[a]
M1···M16	CH···HC	0.001312	0.005144	0.433189	-0.000405	-0.000476	0.000881	0.000405	-0.56
	CH···HC	0.001312	0.005144	0.433157	-0.000405	-0.000476	0.000881	0.000405	-0.56
	CH···πPi	0.001400	0.004891	0.451069	-0.00036	-0.000502	0.000862	0.00036	-0.60
	CH···πPi	0.001406	0.004891	0.451049	-0.00036	-0.000502	0.000862	0.00036	-0.60
	CH···HC	0.002578	0.009777	0.693528	-0.000706	-0.001032	0.001738	0.000706	-1.11
	CH···HC	0.002578	0.009777	0.693334	-0.000706	-0.001032	0.001738	0.000706	-1.11
	CH···O	0.003561	0.014946	0.110693	-0.000802	-0.002132	0.002934	0.000802	-1.53
	CH···O	0.003562	0.014947	0.110661	-0.000802	-0.002133	0.002935	0.000802	-1.53
	CH···πPi	0.005013	0.015732	0.272544	-0.000704	-0.002524	0.003229	0.000705	-2.15
	CH···πPi	0.005013	0.015732	0.272611	-0.000704	-0.002524	0.003229	0.000705	-2.15
M1···M5	CH···HC	0.002120	0.010378	1.208164	-0.00081	-0.000974	0.001784	0.00081	-0.51
	CH···HC	0.002120	0.010378	1.207871	-0.00081	-0.000974	0.001784	0.00081	-0.51
	CH···Oet	0.002196	0.009967	0.474996	-0.000615	-0.001262	0.001877	0.000615	-0.52
	CH···Oet	0.002196	0.009967	0.475039	-0.000615	-0.001262	0.001877	0.000615	-0.52
	CH···HC	0.002429	0.011044	0.25093	-0.00079	-0.00118	0.001971	0.000791	-0.58
	CH···HC	0.002429	0.011045	0.250828	-0.00079	-0.00118	0.001971	0.000791	-0.58
	CH···πPh	0.003055	0.01028	0.903743	-0.000627	-0.001316	0.001943	0.000627	-0.73
	CH···πPh	0.003055	0.010281	0.903601	-0.000627	-0.001316	0.001943	0.000627	-0.73
	CH···πPh	0.003386	0.010896	2.34694	-0.000537	-0.00165	0.002187	0.000537	-0.81
	CH···πPh	0.003386	0.010897	2.34838	-0.000537	-0.00165	0.002187	0.000537	-0.81
	CH···πPh	0.004146	0.012531	0.295072	-0.000625	-0.001883	0.002508	0.000625	-0.99
	CH···πPh	0.004146	0.012532	0.295202	-0.000625	-0.001883	0.002508	0.000625	-0.99

Dimer	Interaction	ρ_{INT}	$\nabla^2\rho$	ε	K	V	G	H	G_{AI}[a]
M1···M9	CH···HC	0.001818	0.007303	0.590521	-0.000558	-0.000709	0.001268	0.000559	-0.77
M1···M8	CH···πPh	0.002431	0.008385	0.466078	-0.000581	-0.000933	0.001515	0.000582	-1.03
	CH···O	0.003537	0.016032	0.27864	-0.000986	-0.002037	0.003022	0.000985	-1.50
	CH···πPi	0.004325	0.01626	2.616438	-0.000769	-0.002526	0.003296	0.00077	-1.83
	CH···N	0.004361	0.01591	0.211154	0.000766	-0.002447	0.003213	0.000766	-1.84
M1···M12	CH···πPh	0.00147	0.004785	1.269363	-0.000324	-0.000548	0.000872	0.000324	-0.62
M1···M11	CH···πPh	0.002504	0.007851	0.056325	-0.000489	-0.000985	0.001474	0.000489	-1.06
	CH···HC	0.003129	0.013092	0.458476	-0.000926	-0.001421	0.002347	0.000926	-1.32
	CH···πPh	0.003279	0.009775	0.940838	-0.000478	-0.001488	0.001966	0.000478	-1.38
M1···M4	CH···HC	0.001777	0.007891	0.406792	-0.000618	-0.000736	0.001354	0.000618	-0.54
	CH···HC	0.001777	0.007891	0.406546	-0.000618	-0.000736	0.001355	0.000619	-0.54
	CH···O	0.004269	0.017495	0.058397	-0.000814	-0.002746	0.00356	0.000814	-1.29
	CH···O	0.004269	0.017495	0.058393	-0.000814	-0.002746	0.00356	0.000814	-1.29
M1···M6	CH···πPi	0.001898	0.006507	0.516377	-0.00046	-0.000707	0.001167	0.00046	-0.87
M1···M13	CH···HC	0.002092	0.009023	0.54485	-0.000699	-0.000857	0.001556	0.000699	-0.96
	CH···Oet	0.003919	0.016672	0.044144	0.000855	-0.002457	0.003313	0.000856	-1.80
M1···M3	CH···N	0.0017	0.006758	0.696011	-0.000481	-0.000728	0.001209	0.000481	-0.67
M1···M2	CH···O	0.004343	0.020255	0.856742	-0.001282	-0.002499	0.003782	0.001283	-1.71
M1···M10	CH···HC	0.001239	0.005066	0.502009	-0.00041	-0.000446	0.000856	0.00041	-0.40
M1···M17	CH···HC	0.003748	0.01548	0.182344	0.001016	-0.001838	0.002854	0.001016	-1.21
M1···M15	CH···HC	0.003014	0.013287	1.605336	0.001011	-0.001299	0.00231	0.001011	-1.5
M1···M7	CH···HC	0.000405	0.001587	0.92108	-0.00013	-0.000137	0.000267	0.00013	-0.55
M1···M14									

a Atom···atom interaction. G_{AI} = Atom···atom interaction energy (kcal mol^{-1}).

Table S21. View of the dimer interactions from QTAIM analysis of compound **1b.**

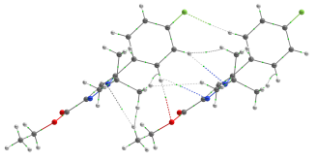
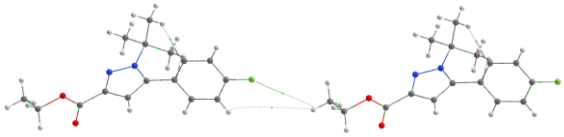
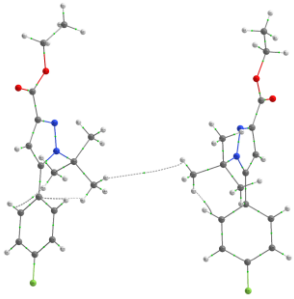
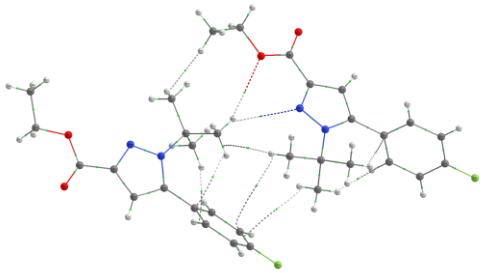
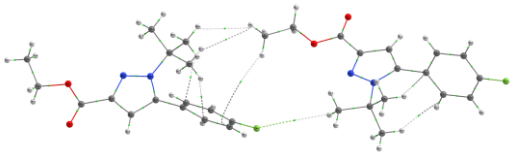
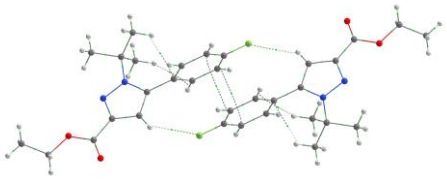
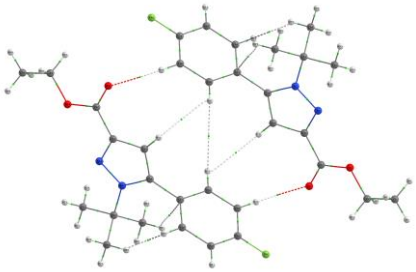
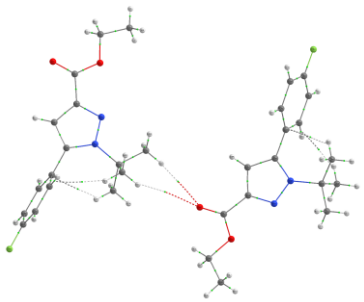
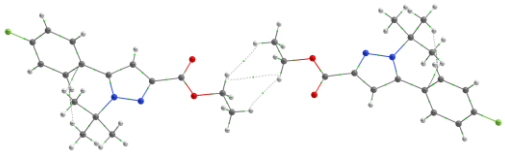
 M1···M2/M1···M3	 M1···M4/ M1···M12
 M1···M5/M1···M9	 M1···M6/ M1···M10
 M1···M7/M1···M11	 M1···M14/M1···M16
 M1···M13	 M1···M8/M1···M15
 M1···M17	

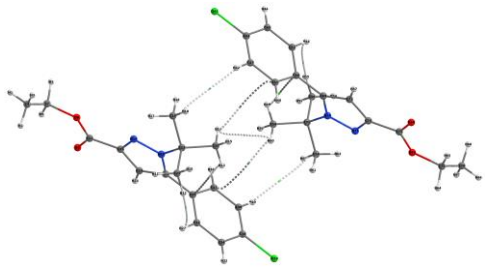
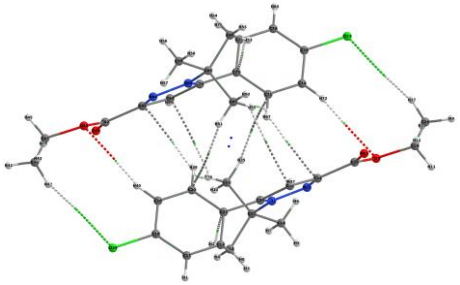
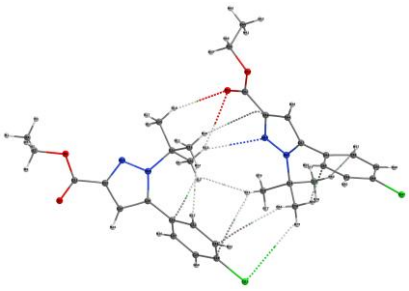
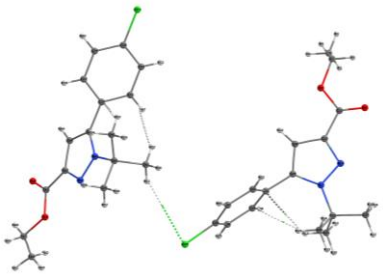
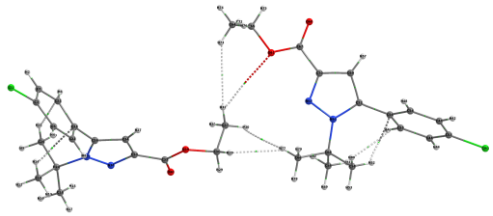
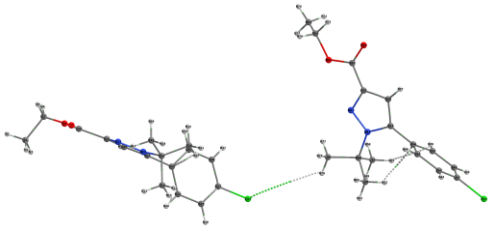
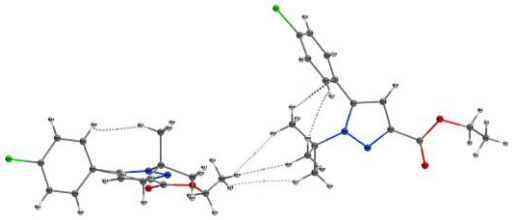
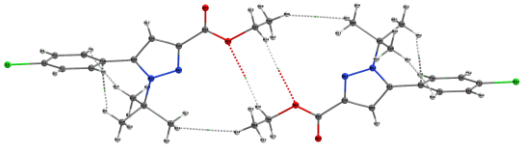
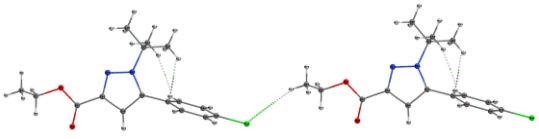
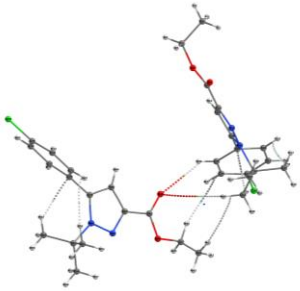
Table S22. QTAIM data and G_{AI} of dimers of compound **1b**

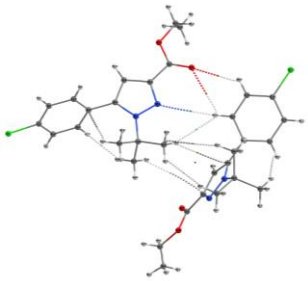
Dimer	Interaction	ρ_{INT}	$\nabla^2\rho$	ε	K	V	G	H	G_{AI}[a]
	CH···HC	0.00121	0.004973	0.231473	-0.000401	-0.000441	0.000842	0.000401	-0.49
	CH···F	0.001706	0.009021	0.060406	-0.000705	-0.000845	0.00155	0.000705	-0.69
	CH···HC	0.00211	0.009048	0.235129	-0.000678	-0.000906	0.001584	0.000678	-0.85
M1···M2	CH···HC	0.002685	0.011573	1.721625	-0.000809	-0.001275	0.002084	0.000809	-1.08
M1···M3	CH···πPi	0.003287	0.011634	3.476110	-0.000563	-0.001782	0.002345	0.000563	-1.32
	CH···N	0.004835	0.017744	0.385902	-0.000843	-0.00275	0.003593	0.000843	-1.94
	CH···Oet	0.004924	0.018718	0.105100	-0.000755	-0.003169	0.003924	0.000755	-1.98
	CH···N	0.005781	0.020488	0.827096	-0.000534	-0.004054	0.004588	0.000534	-2.32
TOTAL		0.026538							-10.67
M1···M13	CH···HC	0.001255	0.004974	0.478271	-0.000413	-0.000417	0.00083	0.000413	-0.51
	CH···HC	0.001997	0.007967	0.671334	-0.000609	-0.000774	0.001383	0.000609	-0.81
	CH···HC	0.001997	0.007968	0.671243	-0.000609	-0.000774	0.001383	0.000609	-0.81
	CH···O	0.0062	0.020615	0.026797	-0.000514	-0.004125	0.00464	0.000515	-2.51
	CH···O	0.0062	0.020615	0.026795	-0.000514	-0.004125	0.00464	0.000515	-2.51
TOTAL		0.017649							-7.15
M1···M6	CH···HC	0.001784	0.007263	0.953345	-0.000562	-0.000691	0.001253	0.000562	-0.65
M1···M10	CH···πPh	0.001969	0.006251	1.018032	-0.000398	-0.000766	0.001164	0.000398	-0.72
	CH···N	0.002974	0.011243	0.385620	-0.000679	-0.001453	0.002132	0.000679	-1.08
	CH···Oet	0.003021	0.013755	0.057839	-0.000845	-0.001749	0.002594	0.000845	-1.10
	CH···HC	0.003237	0.013301	0.071816	-0.000859	-0.001606	0.002466	0.00086	-1.18
	CH···πPh	0.003746	0.012388	0.390985	-0.00078	-0.001538	0.002317	0.000779	-1.36
TOTAL		0.016731							-6.09
M1···M14	CH···F	0.004865	0.023616	0.030969	-0.001116	-0.003672	0.004788	0.001116	-1.38
	CH···F	0.004865	0.023616	0.030968	-0.001116	-0.003672	0.004788	0.001116	-1.38
	Phπ···πPh	0.005008	0.011627	0.927182	-0.000417	-0.002073	0.00249	0.000417	-1.42
	Phπ···πPh	0.005008	0.011627	0.927169	-0.000417	-0.002073	0.00249	0.000417	-1.42
TOTAL		0.019746							-5.60
M1···M16	O···O	0.003034	0.013411	0.224325	-0.000741	-0.00187	0.002611	0.000741	-0.79
	CH···O	0.004044	0.016106	0.043254	-0.000755	-0.002517	0.003272	0.000755	-1.05
	CH···O	0.004044	0.016107	0.043248	-0.000755	-0.002518	0.003272	0.000754	-1.05
TOTAL		0.011122							-2.89
M1···M8	CH···O	0.001158	0.0059	5.627038	-0.000741	-0.00187	0.002611	0.000741	-0.69
M1···M15	CH···O	0.00343	0.014116	0.046920	-0.000755	-0.002517	0.003272	0.000755	-2.05
TOTAL		0.004588							-2.74

Dimer	Interaction	ρ_{INT}	$\nabla^2\rho$	ε	K	V	G	H	G_{AI}[a]
M1···M17	CH···HC	0.003716	0.016529	0.532422	-0.001115	-0.001903	0.003017	0.001114	-0.86
	CH···HC	0.003716	0.016529	0.532326	-0.001115	-0.001903	0.003017	0.001114	-0.86
	CH···HC	0.003776	0.020121	3.676149	-0.001561	-0.001908	0.003469	0.001561	-0.88
TOTAL		0.011208							-2.60
M1···M7	CH···πPh	0.000482	0.001807	4.626078	-0.000149	-0.000154	0.000303	0.000149	-0.20
M1···M11	CH···F	0.000523	0.003111	0.335394	-0.00027	-0.000238	0.000508	0.00027	-0.22
	CH···HC	0.00202	0.00856	0.137908	-0.000658	-0.000824	0.001482	0.000658	-0.85
	CH···HC	0.00213	0.008952	0.192381	0.000683	-0.000872	0.001555	0.000683	-0.90
TOTAL		0.005155							-2.17
M1···M5	CH···HC	0.000068	0.000266	0.269934	-0.000023	-0.000021	0.000044	0.000023	-0.35
M1···M9									
M1···M4	CH···HC	0.000057	0.000222	1.425203	-0.00002	-0.000016	0.000035	0.000019	-0.11
M1···M12	CH···F	0.000073	0.000594	0.403660	-0.000059	-0.000031	0.00009	0.000059	-0.14
		0.000130							-0.24

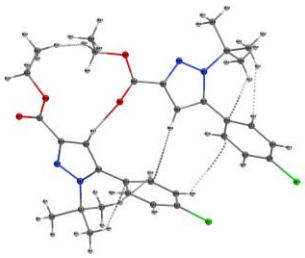
[a]Atom···atom interaction. G_{AI} = Atom···atom interaction energy (kcal mol^{-1}).

Table S23. View of the dimer interactions from QTAIM analysis of compound **1c** (Cluster A and B).

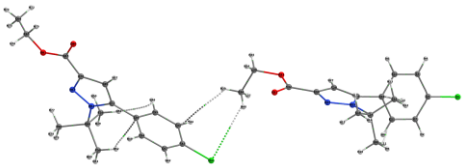
 M1A···M2A	 M1A···M3A
 M1A···M4B/ M1B···M12A	 M1A···M5B/ M1B···M5A
 M1A···M6B/ M1B···M6A	 M1A···M7B/ M1B···M15A
 M1A···M8B/ M1B···M14A	 M1A···M9A
 M1A···M10A/ M1A···M16A	 M1A···M11B/ M1B···M10A



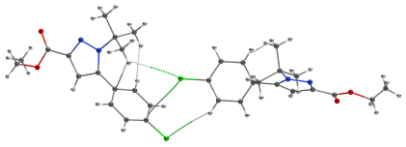
M1A···M12B/ M1B···M11A



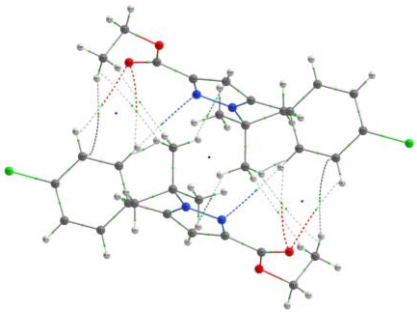
M1A···M13B/ M1B···M4A



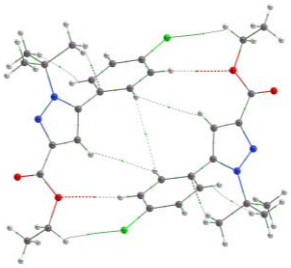
M1A···M14B/ M1B···M7A



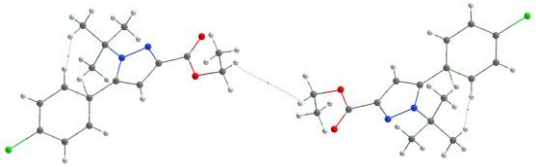
M1A···M15B/ M1B···M16A



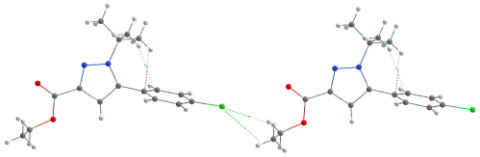
M1B···M2B



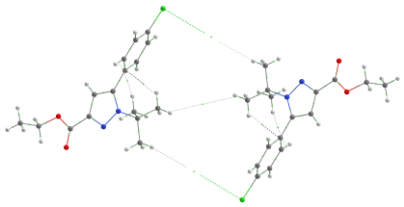
M1B···M3B



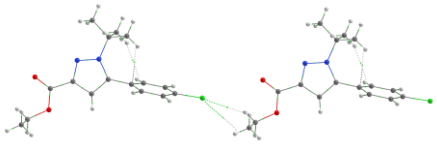
M1B···M8B



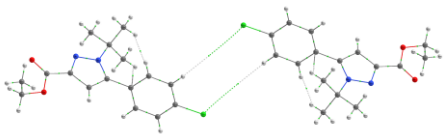
M1B···M9B



M1B···M13B



M1B···M17B



M1B···M18B

Table S24. QTAIM data and G_{AI} of dimers of compound **1c**

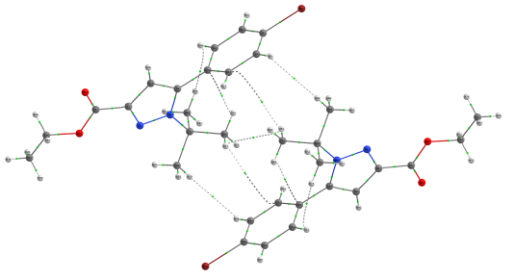
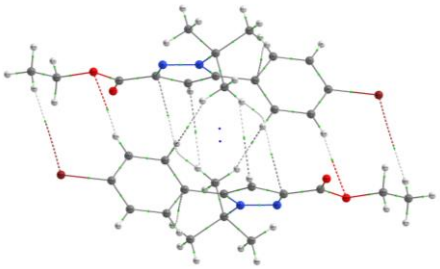
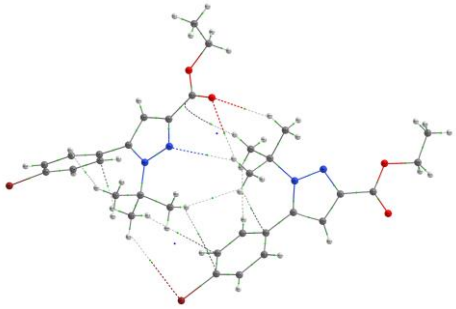
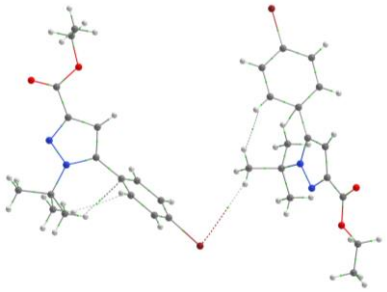
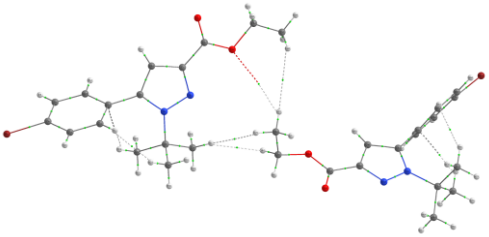
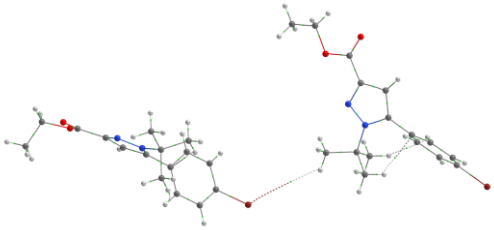
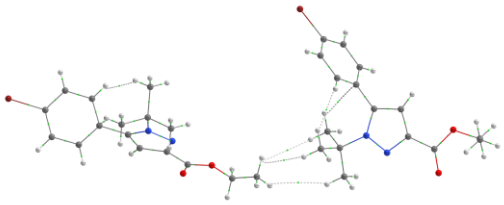
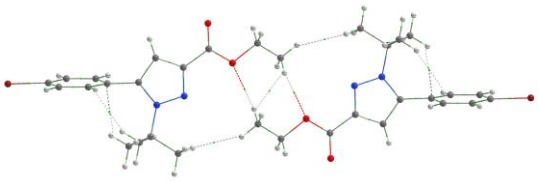
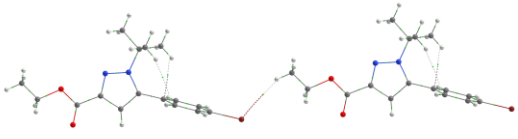
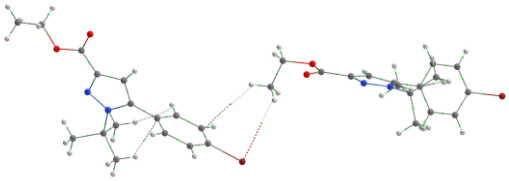
Dimer	Interaction	ρ_{INT}	$\nabla^2\rho$	ε	K	V	G	H	G_{AI}[a]
M1A···M3A	CH···Cl	0.00091	0.003333	0.012823	-0.000247	-0.000339	0.000586	0.000247	-0.44
	CH···Cl	0.00091	0.003334	0.012393	-0.000247	-0.000339	0.000586	0.000247	-0.44
	CH···πPh	0.002881	0.009417	0.091296	-0.000594	-0.001166	0.00176	0.000594	-1.38
	CH···πPh	0.002882	0.009423	0.091693	-0.000594	-0.001167	0.001762	0.000595	-1.38
	CH···πPi	0.003097	0.009246	0.063974	-0.000517	-0.001278	0.001795	0.000517	-1.48
	CH···πPi	0.003098	0.009249	0.064335	-0.000517	-0.001278	0.001795	0.000517	-1.48
	CH···Oet	0.003425	0.013446	0.293867	-0.000688	-0.001985	0.002673	0.000688	-1.64
	CH···Oet	0.003432	0.013465	0.292957	-0.000688	-0.00199	0.002678	0.000688	-1.64
	CH···πPi	0.005136	0.018288	2.12895	-0.000802	-0.002968	0.00377	0.000802	-2.46
	CH···πPi	0.005142	0.018308	2.12011	-0.000802	-0.002973	0.003775	0.000802	-2.46
TOTAL		0.030913							-14.81
M1A···M12B	CH···πPi	0.001608	0.005499	0.553282	-0.000357	-0.000661	0.0010180	0.000357	-0.65
M1B···M11A	CH···HC	0.001923	0.008508	2.127294	-0.000634	-0.000859	0.0014930	0.000634	-0.77
	CH···HC	0.00244	0.009878	0.666165	-0.000736	-0.000997	0.0017330	0.000736	-0.98
	CH···HC	0.002715	0.011317	0.048645	-0.000760	-0.001309	0.0020690	0.00076	-1.09
	CH···N	0.002758	0.009462	0.197331	-0.000503	-0.001359	0.0018620	0.000503	-1.11
	CH···πPi	0.003516	0.011592	1.179545	-0.000564	-0.001770	0.0023340	0.000564	-1.42
	CH···O	0.003706	0.01715	0.544693	-0.001024	-0.002239	0.0032630	0.001024	-1.49
	CH···O	0.005223	0.02351	0.204333	-0.001100	-0.003677	0.0047770	0.0011	-2.10
TOTAL		0.023889							-9.62
M1A···M4B	CH···πPh	0.001471	0.005125	0.980676	-0.000322	-0.000637	0.000959	0.000322	-0.47
M1B···M12A	CH···πPh	0.001482	0.004777	0.306362	-0.000311	-0.000573	0.000884	0.000311	-0.48
	CH···Cl	0.001719	0.006274	0.177386	-0.000414	-0.000741	0.001155	0.000414	-0.55
	CH···πPi	0.001926	0.006775	1.196006	-0.000430	-0.000833	0.001264	0.000431	-0.62
	CH···CH	0.003884	0.015435	0.169226	-0.000945	-0.001969	0.002914	0.000945	-1.25
	CH···O	0.00408	0.015931	0.171048	-0.000731	-0.002521	0.003252	0.000731	-1.31
	CH···O	0.004345	0.016722	0.091222	-0.000739	-0.002702	0.003441	0.000739	-1.40
	CH···N	0.005693	0.018127	0.090310	-0.000606	-0.003319	0.003926	0.000607	-1.83
TOTAL		0.0246							-7.90
M1A···M13B	CH···CH	0.002542	0.010653	0.1502	-0.0007	-0.0012	0.0019	0.000735	-0.91
M1B···M4A	CH···πPh	0.002783	0.009089	0.9483	-0.0005	-0.0013	0.0018	0.000489	-0.99
	CH···πPh	0.004098	0.013134	1.3270	-0.0008	-0.0017	0.0025	0.000794	-1.46
	CH···O	0.008893	0.02917	0.0370	-0.0005	-0.0064	0.0068	0.000464	-3.17
TOTAL		0.018316							-6.53

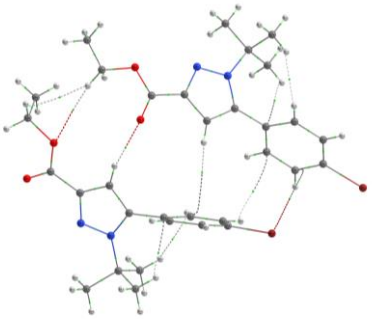
Dimer	Interaction	ρ_{INT}	$\nabla^2\rho$	ε	K	V	G	H	G_{AI}[a]
M1A···M11B	CH···O	0.000557	0.002833	2.083489	-0.000258	-0.000191	0.000450	0.000259	-0.22
M1B···M10A	CH···HC	0.001723	0.006463	0.495287	-0.000478	-0.000659	0.001138	0.000479	-0.68
	CH···πPh	0.002605	0.008897	0.932249	-0.000582	-0.001060	0.001642	0.000582	-1.02
	CH···O	0.007761	0.030582	0.144448	-0.000977	-0.005692	0.006669	0.000977	-3.05
TOTAL		0.012646							-4.97
M1A···M2A	CH···CH	0.001671	0.00706	2.77693	-0.00059	-0.00059	0.00118	0.000587	-0.64
	CH···HC	0.001671	0.00706	2.79728	-0.00059	-0.00059	0.00118	0.000586	-0.64
	CH···HC	0.00263	0.01100	0.72447	-0.00082	-0.00110	0.00193	0.000824	-1.01
	CH···πPh	0.003001	0.00948	0.46628	-0.00060	-0.00118	0.00177	0.000596	-1.15
	CH···πPh	0.003003	0.00948	0.46457	-0.00060	-0.00118	0.00177	0.000596	-1.15
TOTAL		0.011976							-4.60
M1A···M9A	CH···CH	0.000989	0.004184	0.06308	-0.000351	-0.000345	0.000695	0.00035	-1.05
	CH···CH	0.000989	0.004184	0.06308	-0.000351	-0.000345	0.000695	0.00035	-1.05
	CH···Oet	0.001093	0.005658	0.114082	-0.000456	-0.000502	0.000958	0.000456	-1.16
	CH···Oet	0.001093	0.005658	0.114082	-0.000456	-0.000502	0.000958	0.000456	-1.16
TOTAL		0.004164							-4.44
M1A···M6B	CH···Oet	0.001403	0.00702	0.292425	-0.000553	-0.000649	0.001202	0.000553	-0.32
M1B···M6A	CH···CH	0.001515	0.006113	0.102976	-0.000477	-0.000575	0.001052	0.000477	-0.35
	CH···CH	0.003472	0.014958	1.052449	-0.00098	-0.001779	0.002759	0.00098	-0.80
	CH···CH	0.005192	0.021524	0.165994	-0.001154	-0.003073	0.004227	0.001154	-1.20
TOTAL		0.011582							-2.68
M1A···M15B	CH···Cl	0.001556	0.005661	0.546236	-0.000385	-0.000646	0.001031	0.000385	-0.55
M1B···M16A	CH···Cl	0.001877	0.007211	0.285365	-0.000471	-0.000862	0.001332	0.00047	-0.66
	Cl···πPh	0.003652	0.009954	1.690851	-0.00038	-0.001729	0.002109	0.00038	-1.29
TOTAL		0.007085							-2.49
M1A···M5B M1B···M5A	CH···Cl	0.002712	0.009659	0.100079	-0.000559	-0.001298	0.001856	0.000558	-1.74
M1A···M8B	CH···CH	0.001337	0.005319	1.460156	-0.000424	-0.000482	0.000906	0.000424	-0.26
M1B···M14A	CH···CH	0.002038	0.008274	0.984211	-0.000612	-0.000845	0.001457	0.000612	-0.39
	CH···CH	0.004599	0.016517	0.038697	-0.000812	-0.002506	0.003318	0.000812	-0.89
TOTAL		0.007974							-1.54
M1A···M14B	CH···π	0.002878	0.010141	0.287793	-0.000685	-0.001165	0.00185	0.000685	-0.62
M1B···M7A	CH···Cl	0.003302	0.01139	0.147867	-0.00063	-0.001587	0.002217	0.00063	-0.71
TOTAL		0.00618							-1.32

Dimer	Interaction	ρ_{INT}	$\nabla^2\rho$	ε	K	V	G	H	G_{AI}[a]
M1A···M16A	CH···Cl	0.002016	0.007232	0.249761	-0.000463	-0.000881	0.001345	0.000464	-0.85
M1A···M10A									
M1A···M7B	CH···Cl	0.000811	0.003089	0.068665	-0.000232	-0.000307	0.00054	0.000233	-0.77
M1B···M2B	CH···πPh	0.000754	0.002628	0.527696	-0.000203	-0.000251	0.000454	0.000203	-0.31
	CH···πPh	0.000754	0.002629	0.527311	-0.000203	-0.000251	0.000454	0.000203	-0.31
	CH···HC	0.001397	0.005475	7.28310	-0.000442	-0.000484	0.000927	0.000443	-0.58
	CH···HC	0.001397	0.005475	7.28310	-0.000442	-0.000484	0.000927	0.000443	-0.58
	CH···HC	0.001565	0.006391	0.69469	-0.00051	-0.000578	0.001088	0.00051	-0.65
	CH···HC	0.001565	0.006391	0.69469	-0.00051	-0.000578	0.001088	0.00051	-0.65
	CH···O	0.002115	0.010615	0.589014	-0.000755	-0.001143	0.001899	0.000756	-0.87
	CH···O	0.002115	0.010615	0.589014	-0.000755	-0.001143	0.001899	0.000756	-0.87
	CH···O	0.003035	0.012974	1.053454	-0.000788	-0.001668	0.002456	0.000788	-1.25
	CH···O	0.003035	0.012974	1.053454	-0.000788	-0.001668	0.002456	0.000788	-1.25
	CH···N	0.003682	0.011688	0.841218	-0.000499	-0.001925	0.002423	0.000498	-1.52
	CH···N	0.003682	0.011688	0.841218	-0.000499	-0.001925	0.002423	0.000498	-1.52
	CH···πPi	0.004367	0.013447	0.243683	-0.000726	-0.00191	0.002636	0.000726	-1.80
	CH···πPi	0.004367	0.013447	0.243683	-0.000726	-0.00191	0.002636	0.000726	-1.80
TOTAL		0.033830							-13.95
M1B···M3B	CH···CH	0.000637	0.002278	0.507777	-0.000194	-0.000182	0.000376	0.000194	-0.28
	CH···CH	0.001069	0.004512	0.517692	-0.000374	-0.000381	0.000754	0.000373	-0.47
	CH···CH	0.001069	0.004512	0.517692	-0.000374	-0.000381	0.000754	0.000373	-0.47
	CH···Cl	0.001129	0.004208	0.043864	-0.000301	-0.000451	0.000751	0.0003	-0.50
	CH···Cl	0.001129	0.004208	0.043935	-0.000301	-0.000451	0.000751	0.0003	-0.50
	CH···O	0.004006	0.015161	0.023006	-0.000656	-0.002478	0.003134	0.000656	-1.77
	CH···O	0.004007	0.015161	0.022999	-0.000656	-0.002478	0.003134	0.000656	-1.77
TOTAL		0.013046							-5.76
M1B···M18B	CH···Cl	0.000167	0.000655	0.037089	-0.000059	-0.000045	0.000105	0.00006	-0.37
	CH···Cl	0.000167	0.000655	0.037104	-0.000059	-0.000045	0.000105	0.00006	-0.37
TOTAL		0.000334							-0.75
M1B···M17B	CH···Cl	0.003338	0.013212	0.968076	-0.000839	-0.001626	0.002465	0.000839	-0.27
M1B···M9B	CH···Cl	0.005928	0.022971	0.095338	-0.001105	-0.003532	0.004637	0.001105	-0.47
TOTAL		0.009266							-0.74
M1B···M8B	CH···CH	0.000187	0.000684	0.674369	-0.000055	-0.000061	0.000116	0.000055	-0.71
M1B···M13B	CH···CH	0.000113	0.000428	0.153263	-0.000037	-0.000034	0.00007	0.000036	-0.48

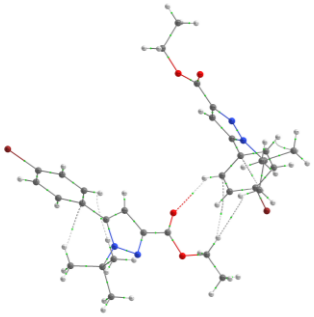
[a]Atom···atom interaction. G_{AI} = Atom···atom interaction energy (kcal mol^{-1}).

Table S25. View of the dimer interactions from QTAIM analysis of compound **1d** (Cluster A and B).

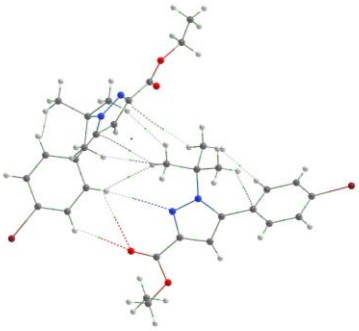
 M1A···M2A	 M1A···M3A
 M1A···M4B/ M1B···M6A	 M1A···M5B/ M1B···M14A
 M1A···M6B/ M1B···M15A	 M1A···M7B/ M1B···M8A
 M1A···M8B/ M1B···M9A	 M1A···M9A
 M1A···M10A/ M1A···M16A	 M1A···M14B/ M1B···M16A



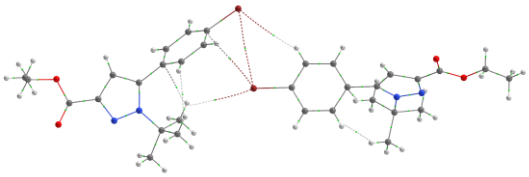
M1A···M11B/ M1B···M13A



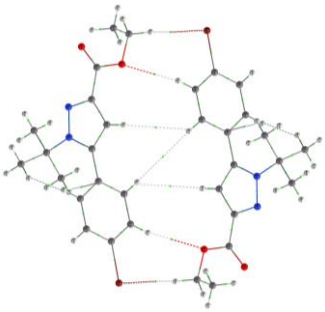
M1A···M12B/ M1B···M4A



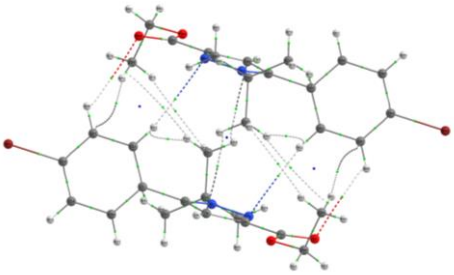
M1A···M13B// M1B···M5A



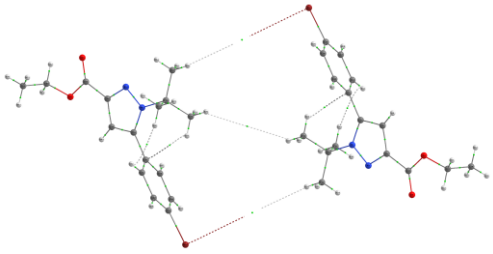
M1A···M15B/ M1B···M10A



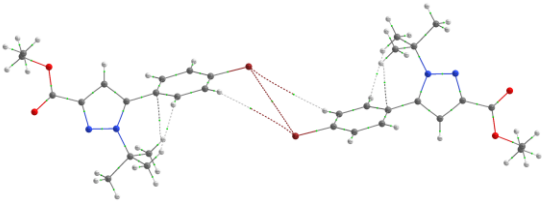
M1B···M2B



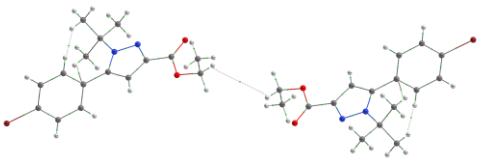
M1B···M3B



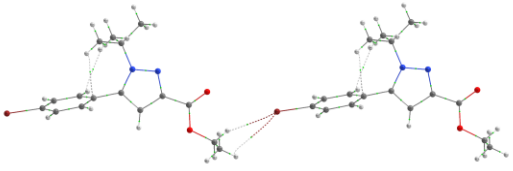
M1B···M7B



M1B···M12B



M1B···M12B



M1B···M11B/ M1B···M18B

Table S26. QTAIM data and G_{AI} of dimers of compound **1d**

Dimer	Interaction	ρ_{INT}	$\nabla^2\rho$	ε	K	V	G	H	G_{AI}[a]
M1A···M3A	CH···Br	0.001295	0.004388	0.009242	-0.00031	-0.00048	0.000789	0.000308	-0.61
	CH···Br	0.001295	0.004388	0.009242	-0.00031	-0.00048	0.000789	0.000308	-0.61
	CH···πPh	0.003113	0.010197	0.06762	-0.00064	-0.00128	0.001912	0.000637	-1.47
	CH···πPh	0.003114	0.010198	0.067682	-0.00064	-0.00128	0.001913	0.000637	-1.47
	CH···πPi	0.00336	0.009992	0.060445	-0.00055	-0.00141	0.001952	0.000545	-1.58
	CH···πPi	0.00336	0.009992	0.060469	-0.00055	-0.00141	0.001952	0.000545	-1.58
	CH···OEt	0.00366	0.014265	0.256618	-0.00069	-0.00219	0.00288	0.000687	-1.73
	CH···OEt	0.003661	0.014266	0.256374	-0.00069	-0.00219	0.00288	0.000686	-1.73
	CH···πPi	0.005114	0.018529	2.398319	-0.00081	-0.003	0.003818	0.000814	-2.41
	CH···πPi	0.005114	0.01853	2.397605	-0.00081	-0.003	0.003818	0.000814	-2.41
TOTAL		0.033086							-15.60
M1A···M13B	CH···Pi	0.001876	0.00628	0.645848	-0.00039	-0.00078	0.001176	0.000394	-0.79
M1B···M5A	CH···HC	0.002054	0.009063	1.11727	-0.00066	-0.00094	0.001602	0.000663	-0.86
	CH···HC	0.002482	0.010075	0.4357	-0.00075	-0.00102	0.001767	0.000752	-1.04
	CH···N	0.002562	0.008894	0.18513	-0.0005	-0.00123	0.001728	0.000495	-1.08
	CH···HC	0.002837	0.011735	0.056963	-0.00077	-0.00139	0.002164	0.00077	-1.19
	CH···O	0.002868	0.013681	0.754843	-0.0009	-0.00161	0.002516	0.000905	-1.21
	CH···πPi	0.003396	0.011266	1.106.618	-0.00056	-0.00169	0.002253	0.000563	-1.43
	CH···O	0.004302	0.019868	0.19621	-0.00102	-0.00292	0.003944	0.001024	-1.81
TOTAL		0.022377							-9.41
M1A···M4B	CH···πPh	0.001332	0.00442	0.329977	-0.0003	-0.00051	0.000809	0.000295	-0.43
M1B···M6A	CH···πPh	0.001678	0.005776	1.14711	-0.00035	-0.00074	0.001093	0.000351	-0.54
	CH···πCO	0.00208	0.007464	2.41941	-0.00048	-0.00091	0.001385	0.00048	-0.67
	CH···Br	0.00223	0.007429	0.151166	-0.00046	-0.00093	0.001396	0.000462	-0.72
	CH···HC	0.004128	0.016269	0.13815	-0.00096	-0.00214	0.003105	0.000963	-1.33
	CH···O	0.004209	0.016277	0.154703	-0.00073	-0.00262	0.003343	0.000726	-1.35
	CH···O	0.004463	0.017147	0.095595	-0.00074	-0.00281	0.00355	0.000736	-1.43
	CH···N	0.005455	0.017669	0.072712	-0.00063	-0.00316	0.00379	0.000628	-1.75
TOTAL		0.025575							-8.21
M1A···M11B	Br···πPh	0.001697	0.00487	2.937466	-0.00022	-0.00078	0.000997	0.00022	-0.57
M1B···M13A	CH···HC	0.002176	0.01043	1.197537	-0.0008	-0.00102	0.001812	0.000796	-0.74
	CH···Oet	0.002372	0.010767	0.410764	-0.00066	-0.00137	0.002029	0.000664	-0.80
	CH···πPh	0.002595	0.008745	1.324985	-0.00048	-0.00123	0.001709	0.000478	-0.88
	CH···πPh	0.004128	0.01371	1.201975	-0.00088	-0.00167	0.002548	0.000879	-1.39

	CH···O	0.008711	0.028795	0.038841	-0.00049	-0.00622	0.006711	0.000488	-2.94
TOTAL		0.021679							-7.33
M1A···M2A	CH···HC	0.001944	0.008383	0.682559	-0.00067	-0.00075	0.001421	0.000674	-0.76
	CH···HC	0.001944	0.008383	0.682242	-0.00067	-0.00075	0.001421	0.000674	-0.76
	CH···HC	0.002547	0.010607	0.76738	-0.0008	-0.00106	0.001853	0.000798	-1.00
	CH···πPh	0.003295	0.010439	0.446195	-0.00066	-0.0013	0.001955	0.000655	-1.29
	CH···πPh	0.003295	0.01044	0.446265	-0.00066	-0.0013	0.001955	0.000654	-1.29
TOTAL		0.013025							-5.10
M1A···M12B	CH···HC	0.001948	0.007969	0.337254	-0.0006	-0.00079	0.001393	0.000599	-0.75
M1B···M4A	CH···πPh	0.002247	0.007259	0.474555	-0.00045	-0.00091	0.00136	0.000454	-0.86
	CH···O	0.008062	0.030882	0.10387	-0.0009	-0.00592	0.006818	0.000902	-3.10
TOTAL		0.012257							-4.71
M1A···M9A	CH···HC	0.001364	0.005821	0.035685	-0.00047	-0.00052	0.000987	0.000469	-0.48
	CH···HC	0.001364	0.005821	0.03571	-0.00047	-0.00052	0.000987	0.000469	-0.48
	CH···HC	0.001963	0.008665	0.869375	-0.00066	-0.00085	0.00151	0.000657	-0.69
	CH···OEt	0.003158	0.012946	0.046644	-0.00071	-0.00182	0.002529	0.000707	-1.11
	CH···OEt	0.003158	0.012946	0.046636	-0.00071	-0.00182	0.002529	0.000707	-1.11
TOTAL		0.011007							-3.87
M1A···M15B	CH···Br	0.002174	0.007217	0.376322	-0.00044	-0.00092	0.00136	0.000444	-0.51
M1B···M10A	CH···Br	0.002715	0.009503	0.31516	-0.00058	-0.00122	0.0018	0.000576	-0.63
	Br···Br	0.004568	0.012005	0.876718	-0.00041	-0.00218	0.00259	0.000411	-1.06
	Br···πPh	0.004614	0.012211	1.456318	-0.00046	-0.00214	0.002594	0.000459	-1.07
TOTAL		0.014071							-3.28
M1A···M6B	CH···O	0.001078	0.005578	0.737185	-0.00046	-0.00048	0.000938	0.000457	-0.27
M1B···M15A	CH···HC	0.00146	0.006117	0.230443	-0.00049	-0.00055	0.001038	0.000491	-0.37
	CH···HC	0.003744	0.015833	0.636768	-0.00099	-0.00197	0.002965	0.000994	-0.94
	CH···HC	0.00497	0.020993	0.199476	-0.00118	-0.00289	0.004071	0.001177	-1.25
TOTAL		0.011252							-2.82
M1A···M5B M1B···M14A	CH···Br	0.003133	0.010109	0.089902	-0.00055	-0.00144	0.001981	0.000546	-1.83
M1A···M8B	CH···HC	0.001685	0.006994	0.23967	-0.00054	-0.00067	0.00121	0.000538	-0.34
M1B···M9A	CH···HC	0.00287	0.011753	0.044837	-0.00081	-0.00133	0.002133	0.000806	-0.57
	CH···HC	0.003297	0.013701	0.378695	-0.00094	-0.00155	0.002487	0.000939	-0.66
TOTAL		0.007852							-1.57
M1A···M14B	CH···πPh	0.002394	0.008394	0.271054	-0.00058	-0.00095	0.001522	0.000576	-0.58
M1B···M16A	CH···Br	0.003601	0.011425	0.142896	-0.00061	-0.00165	0.002251	0.000605	-0.87

TOTAL		0.005995							-1.45
M1A···M16A M1A···M10A	CH···Br	0.002511	0.008085	0.050056	-0.00047	-0.00109	0.001554	0.000468	-1.32
M1A···M7B M1B···M8A	CH···Br	0.000956	0.00335	0.035449	-0.00025	-0.00034	0.00059	0.000248	-0.93
M1B···M3B	CH···πPh	0.000773	0.002708	0.128991	-0.000212	-0.000254	0.000465	0.000211	-0.37
	CH···πPh	0.000773	0.002708	0.128872	-0.000212	-0.000254	0.000465	0.000211	-0.37
	CH···HC	0.001201	0.004567	1.232496	-0.000366	-0.000409	0.000776	0.000367	-0.57
	CH···HC	0.001201	0.004568	1.211303	-0.000366	-0.000409	0.000776	0.000367	-0.57
	CH···HC	0.001302	0.005195	0.919574	-0.000419	-0.000462	0.000880	0.000418	-0.62
	CH···HC	0.001302	0.005195	0.919308	-0.000419	-0.000462	0.000880	0.000418	-0.62
	CH···O	0.003044	0.014171	0.164152	-0.000860	-0.001822	0.002682	0.000860	-1.45
	CH···O	0.003045	0.014171	0.164196	-0.000860	-0.001822	0.002682	0.000860	-1.45
	CH···πPi	0.004294	0.013473	0.225723	-0.000763	-0.001842	0.002605	0.000763	-2.04
	CH···πPi	0.004294	0.013473	0.225764	-0.000763	-0.001842	0.002605	0.000763	-2.04
	CH···N	0.004366	0.013415	0.821582	-0.000501	-0.002351	0.002852	0.000501	-2.07
	CH···N	0.004366	0.013415	0.821662	-0.000501	-0.002351	0.002852	0.000501	-2.07
TOTAL		0.029961							-14.22
M1B···M2B	CH···HC	0.00058	0.00206	1.0990150	-0.0001760	-0.0001630	0.0003390	0.000176	-0.26
	CH···Br	0.001115	0.003909	0.0397290	-0.0002790	-0.0004190	0.0006980	0.000279	-0.50
	CH···Br	0.001115	0.003909	0.0396930	-0.0002790	-0.0004190	0.0006980	0.000279	-0.50
	CH···HC	0.001153	0.004914	0.3538940	-0.0004080	-0.0004120	0.0008200	0.000408	-0.51
	CH···HC	0.001153	0.004914	0.3539840	-0.0004080	-0.0004120	0.0008200	0.000408	-0.51
	CH···Oet	0.00408	0.015356	0.0208170	-0.0006520	-0.0025360	0.0031870	0.000651	-1.82
	CH···Oet	0.00408	0.015356	0.0208380	-0.0006520	-0.0025360	0.0031870	0.000651	-1.82
TOTAL		0.013276							-5.91
M1B···M18B	CH···Br	0.003641	0.013422	0.533216	-0.000833	-0.00169	0.002523	0.000833	-0.38
M1B···M11B	CH···Br	0.006058	0.021253	0.121913	-0.000995	-0.003323	0.004318	0.000995	-0.63
TOTAL		0.009699						0.000000	-1.01
M1B···M12B	CH···Br	0.000408	0.001442	0.130419	-0.000122	-0.000116	0.000239	0.000123	-0.28
	CH···Br	0.000408	0.001442	0.130418	-0.000122	-0.000116	0.000239	0.000123	-0.28
	Br···Br	0.000419	0.001781	0.578442	-0.000141	-0.000164	0.000305	0.000141	-0.29
TOTAL		0.001235							-0.85
M1B···M17B	CH···HC	0.000183	0.000664	0.41682	-0.000054	-0.000057	0.000112	0.000055	0.78
M1B···M7B	CH···HC	0.000088	0.00034	0.166222	-0.000029	-0.000027	0.000056	0.000029	-0.31

[a]Atom···atom interaction. G_{AI} = Atom···atom interaction energy (kcal mol^{-1}).

Table S27. View of the dimer interactions from QTAIM analysis of compound **2a**.

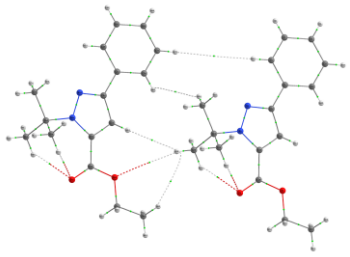
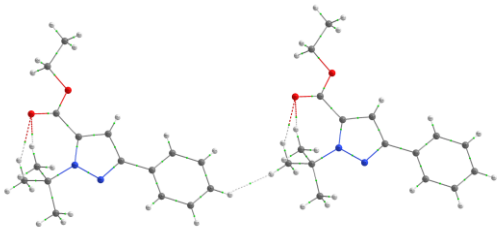
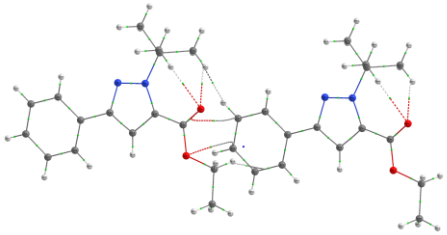
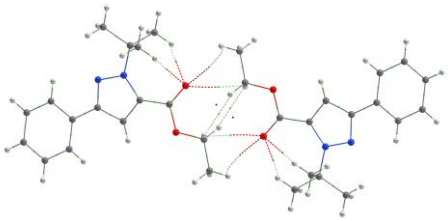
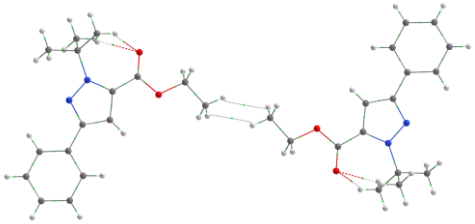
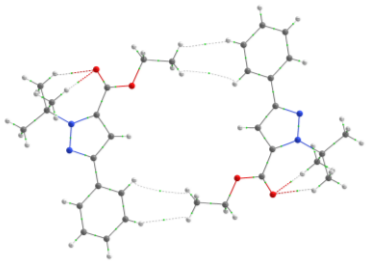
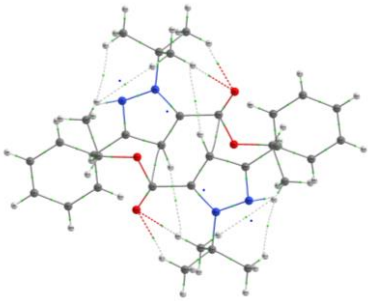
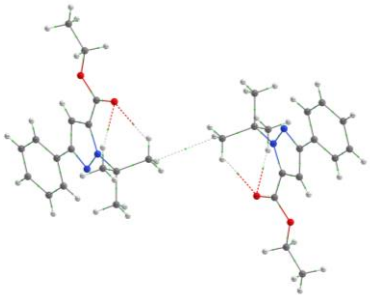
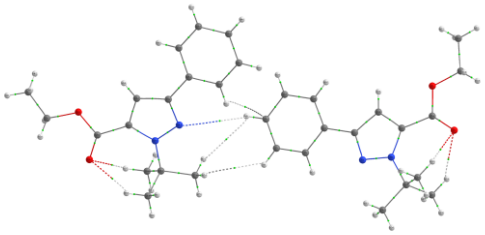
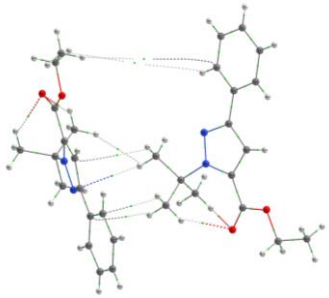
 M1···M2/ M1···M3	 M1···M4/ M1···M11
 M1···M5/ M1···M12	 M1···M6
 M1···M7	 M1···M8
 M1···M9	 M1···M10
 M1···M13	 M1···M15/ M1···M16

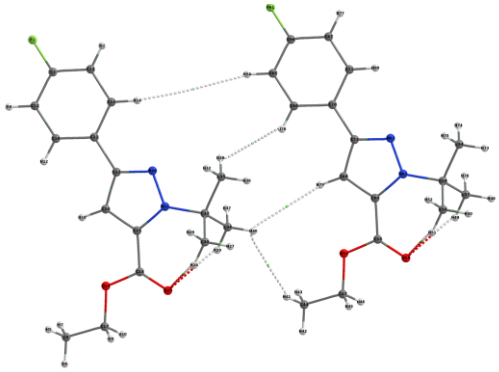
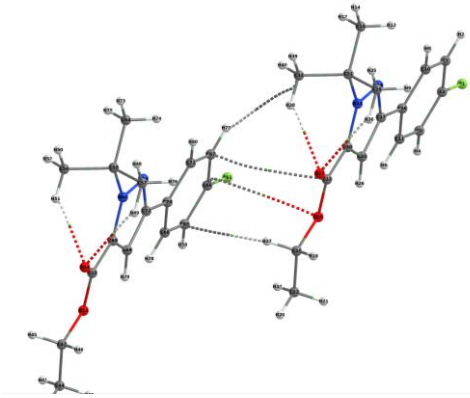
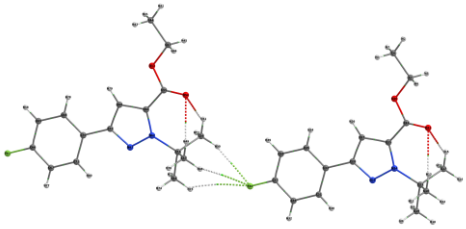
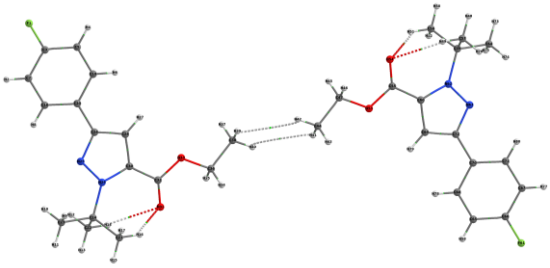
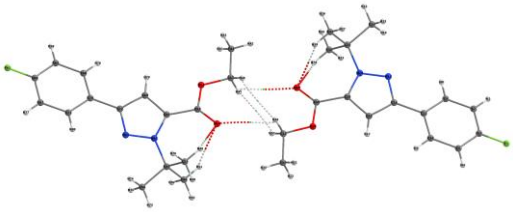
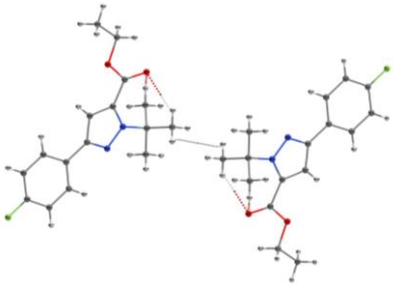
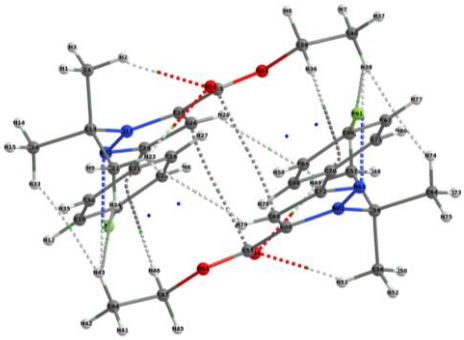
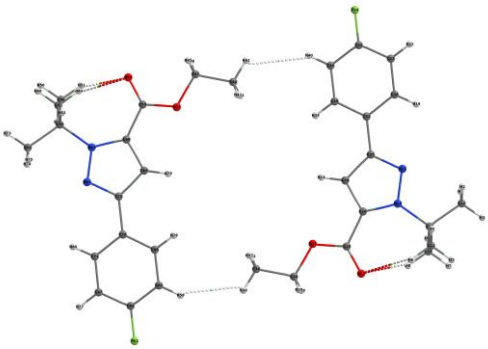
Table S28. QTAIM data and G_{AI} of dimers of compound **2a**

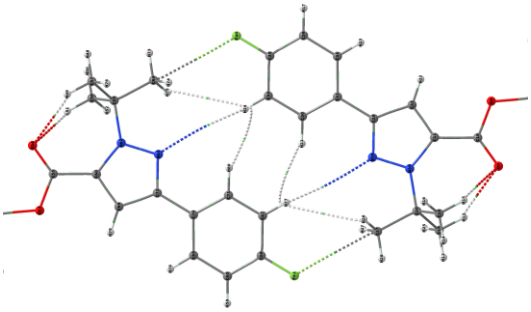
Dimer	Interaction	ρ_{INT}	$\nabla^2\rho$	ε	K	V	G	H	G_{AI}[a]
M1···M9	H···H	0.001659	0.007228	0.444255	-0.000568	-0.00067	0.001239	0.000569	-0.53
	H···H	0.001659	0.007228	0.444377	-0.000568	-0.00067	0.001239	0.000569	-0.53
	H···H	0.002576	0.011073	0.677213	-0.000765	-0.001239	0.002004	0.000765	-0.83
	H···H	0.002576	0.011074	0.67692	-0.000765	-0.001239	0.002004	0.000765	-0.83
	H···H	0.003684	0.014735	0.087367	-0.000863	-0.001957	0.00282	0.000863	-1.18
	H···H	0.003685	0.014736	0.087369	-0.000863	-0.001957	0.002821	0.000864	-1.18
	CH···N	0.004304	0.015392	0.180777	-0.000713	-0.002422	0.003135	0.000713	-1.38
	CH···N	0.004304	0.015391	0.180772	-0.000713	-0.002422	0.003135	0.000713	-1.38
	π···π	0.005009	0.016349	0.461762	-0.000942	-0.002204	0.003146	0.000942	-1.61
	π···π	0.005009	0.01635	0.461736	-0.000942	-0.002204	0.003146	0.000942	-1.61
	CH···π	0.005806	0.018204	1.535601	-0.000778	-0.002995	0.003773	0.000778	-1.86
	CH···π	*0.005807*	0.018206	1.535285	-0.000778	-0.002996	0.003774	0.000778	-1.86
TOTAL		0.046078	0.165966						-14.77
M1···M12	CH···CH	0.003548	0.01643	6.686639	-0.001251	-0.001605	0.002856	0.001251	-1.33
M1···M5	π···π	0.003781	0.012542	3.651281	-0.000754	-0.001628	0.002382	0.000754	-1.41
	LP···π	0.004029	0.01331	1.036099	-0.000559	-0.00221	0.002769	0.000559	-1.51
	CH···π	0.005552	0.01828	4.339799	-0.00077	-0.00303	0.0038	0.00077	-2.07
TOTAL		0.016910	0.060562						-6.32
M1···M16	CH···π	0.002127	0.00702	1.469952	-0.000395	-0.000965	0.00136	0.000395	-0.74
M1···M15	H···H	0.002426	0.0102	0.124581	-0.000727	-0.001095	0.001823	0.000728	-0.85
	CH···N	0.002752	0.010869	0.382676	-0.000624	-0.00147	0.002094	0.000624	-0.96
	CH···π	0.004392	0.01546	4.619899	-0.00094	-0.001986	0.002925	0.000939	-1.53
	CH···π	0.004921	0.015525	1.633245	-0.000811	-0.00226	0.003071	0.000811	-1.72
TOTAL		0.016618	0.059074						-5.79
M1···M6	CH···O	0.003732	0.017982	1.683657	-0.001087	-0.002322	0.003409	0.001087	-0.79
	CH···O	0.003733	0.017984	1.683314	-0.001087	-0.002323	0.003409	0.001086	-0.79
	H···H	0.004512	0.019805	0.172351	-0.001275	-0.002401	0.003676	0.001275	-0.96
	H···H	0.004513	0.019805	0.172269	-0.001275	-0.002401	0.003676	0.001275	-0.96
	CH···O	0.005147	0.025399	0.63529	-0.001508	-0.003333	0.004841	0.001508	-1.09
	CH···O	0.005148	0.025403	0.636077	-0.001509	-0.003333	0.004842	0.001509	-1.09
TOTAL		0.026785	0.126378						-5.68
M1···M14	H···H	0.002194	0.010127	0.287253	-0.000756	-0.00102	0.001776	0.000756	-0.69
M1···M13	CH···N	0.002195	0.008995	0.413069	-0.000608	-0.001033	0.001641	0.000608	-0.69

	H···H	0.002748	0.012243	1.156129	-0.000933	-0.001195	0.002128	0.000933	-0.86
	CH···π	0.004846	0.016725	0.479676	-0.00104	-0.002102	0.003142	0.00104	-1.52
TOTAL		0.011983	0.04809						-3.75
M1···M2	H···H	0.000181	0.000553	0.195731	-0.000042	-0.000053	0.000096	0.000043	-0.08
M1···M3	CH···OEt	0.001452	0.007103	0.527383	-0.000557	-0.000661	0.001218	0.000557	-0.61
	H···H	0.001931	0.008312	0.159638	-0.000629	-0.000819	0.001448	0.000629	-0.81
	H···H	0.002021	0.008676	1.468273	-0.000689	-0.000791	0.00148	0.000689	-0.84
	H···H	0.00291	0.012496	0.229789	-0.000897	-0.00133	0.002227	0.000897	-1.22
TOTAL		0.008495							-3.55
M1···M8	H···H	0.001937	0.008371	2.229425	-0.000629	-0.000835	0.001464	0.000629	-0.31
	H···H	0.001937	0.008371	2.22247	-0.000629	-0.000835	0.001464	0.000629	-0.31
	H···H	0.004551	0.019113	0.071352	-0.001155	-0.002469	0.003623	0.001154	-0.74
	H···H	0.004552	0.019114	0.071368	-0.001155	-0.002469	0.003624	0.001155	-0.74
TOTAL		0.012977							-2.11
M1···M4 M1···M11	H···H	0.00304	0.013174	0.117858	-0.000852	-0.001589	0.002441	0.000852	-1.56
M1···M10	H···H	0.002625	0.010942	0.559675	-0.000822	-0.001092	0.001913	0.000821	-1.36
M1···M7	H···H	0.002481	0.010819	0.732894	-0.000828	-0.001048	0.001877	0.000829	-0.215
	H···H	0.002481	0.010820	0.73265	-0.000828	-0.001048	0.001877	0.000829	-0.215
TOTAL		0.004962							-0.43

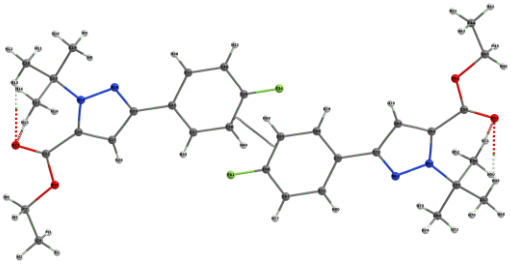
[a]Atom···atom interaction. G_{AI} = Atom···atom interaction energy (kcal mol^{-1}).

Table S29. View of the dimer interactions from QTAIM analysis of compound **2b**.

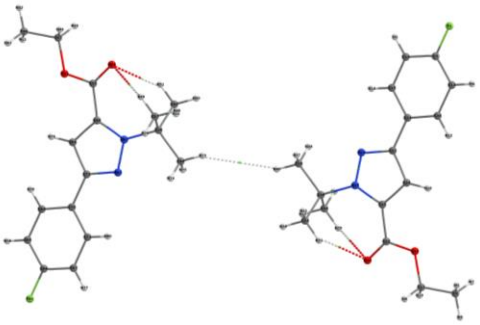
 M1···M2/ M1···M3	 M1···M4/ M1···M11
 M1···M5/ M1···M12	 M1···M6
 M1···M7	 M1···M8
 M1···M9	 M1···M10



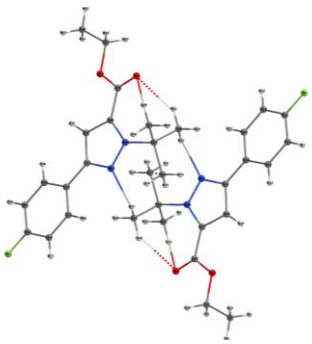
M1···M13



M1···M14



M1···M15



M1···M16

Table S30. QTAIM data and G_{AI} of dimers of compound **2b**

Dimer	Interaction	ρ_{INT}	$\nabla^2\rho$	ε	K	V	G	H	G_{AI}[a]
M1···M9	H···H	0.00174	0.007526	0.397941	-0.000593	-0.000695	0.001288	0.000593	-0.67
	H···H	0.001741	0.007525	0.395855	-0.000593	-0.000695	0.001288	0.000593	-0.67
	H···H	0.002178	0.009372	0.157761	-0.000679	-0.000986	0.001664	0.000678	-0.83
	H···H	0.002187	0.009401	0.154039	-0.00068	-0.00099	0.00167	0.00068	-0.84
	CH···N	0.00286	0.011391	0.354344	-0.000673	-0.001501	0.002175	0.000674	-1.10
	CH···N	0.002861	0.011389	0.354125	-0.000673	-0.001502	0.002174	0.000672	-1.10
	H···H	0.003172	0.012865	0.073701	-0.000799	-0.001618	0.002417	0.000799	-1.21
	H···H	0.003182	0.01289	0.073737	-0.000799	-0.001624	0.002423	0.000799	-1.22
	πhole··· π	0.004184	0.013097	1.511789	-0.000734	-0.001807	0.002541	0.000734	-1.60
	πhole··· π	0.004187	0.013104	1.508571	-0.000734	-0.001808	0.002542	0.000734	-1.60
	CH··· π	0.004647	0.014326	1.729213	-0.000634	-0.002314	0.002948	0.000634	-1.78
	CH··· π	0.00465	0.014336	1.73266	-0.000634	-0.002316	0.00295	0.000634	-1.78
TOTAL		0.037589							-14.39
M1···M16	CH···N	0.006593	0.019478	0.262167	-0.000481	-0.003907	0.004388	0.000481	-4.35
	CH···N	0.006597	0.019482	0.261716	-0.000481	-0.003909	0.00439	0.000481	-4.35
TOTAL		0.01319							-8.70
M1···M7	H···H	0.003438	0.015467	0.150338	-0.001096	-0.001675	0.002771	0.001096	-1.07
-5.83	H···H	0.003439	0.015463	0.149922	-0.001095	-0.001675	0.00277	0.001095	-1.07
	CH···O	0.005935	0.026872	0.194182	-0.001357	-0.004005	0.005361	0.001356	-1.84
	CH···O	0.005936	0.026875	0.194555	-0.001357	-0.004005	0.005362	0.001357	-1.84
TOTAL		0.018748							-5.83
M1···M4	πhole··· π	0.002742	0.008986	3.690961	-0.000541	-0.001164	0.001705	0.000541	-1.24
M1···M11	H···H	0.002849	0.012979	15.183146	-0.001023	-0.001199	0.002222	0.001023	-1.29
	EtO··· π	0.002888	0.010378	1.55392	-0.00052	-0.001555	0.002075	0.00052	-1.31
	CH··· π	0.003779	0.012872	2.398953	-0.000613	-0.001992	0.002605	0.000613	-1.71
TOTAL		0.012258							-5.55
M1···M13	CH···N	0.00136	0.005624	2.747515	-0.000426	-0.000553	0.00098	0.000427	-0.35
	CH···N	0.00136	0.005624	2.747514	-0.000426	-0.000553	0.00098	0.000427	-0.35
	H···H	0.002142	0.009472	0.215362	-0.00073	-0.000908	0.001638	0.00073	-0.55
	H···H	0.002142	0.009472	0.215362	-0.00073	-0.000908	0.001638	0.00073	-0.55
	H···H	0.002233	0.009336	1.524367	-0.000688	-0.000958	0.001646	0.000688	-0.58
	H···H	0.002233	0.009336	1.524367	-0.000688	-0.000958	0.001646	0.000688	-0.58
	CH···F	0.003313	0.017532	0.266466	-0.001322	-0.001739	0.003061	0.001322	-0.86

	CH···F	0.003313	0.017532	0.266466	-0.001322	-0.001739	0.003061	0.001322	-0.86
TOTAL		0.018096							-4.69
M1···M2	H···H	0.000098	0.000295	0.337728	-0.000022	-0.00003	0.000052	0.000022	-0.06
M1···M3	H···H	0.001094	0.004541	0.188208	-0.000375	-0.000386	0.00076	0.000374	-0.63
	H···H	0.001713	0.007266	0.113437	-0.000576	-0.000665	0.001241	0.000576	-0.99
	H···H	0.002389	0.010225	0.287291	-0.00076	-0.001036	0.001796	0.00076	-1.39
TOTAL		0.005294							-3.07
M1···M14	π··· π	0.00394	0.008926	8.124341	-0.000319	-0.001593	0.001913	0.00032	-2.74
M1···M10	H···H	0.003073	0.013341	0.086239	-0.000916	-0.001503	0.002419	0.000916	-1.03
	H···H	0.003075	0.013355	0.086031	-0.000917	-0.001505	0.002422	0.000917	-1.03
TOTAL		0.006148							-2.06
M1···M12	CH···F	0.001799	0.010303	0.834004	-0.000799	-0.000979	0.001777	0.000798	-0.36
M1···M5	CH···F	0.001954	0.011213	0.899995	-0.00082	-0.001158	0.001978	0.00082	-0.39
	CH···F	0.006128	0.025998	0.022479	-0.000955	-0.004583	0.005538	0.000955	-1.23
TOTAL		0.009881							-1.98
M1···M8	H···H	0.00206	0.008367	0.422244	-0.000636	-0.00082	0.001456	0.000636	-1.10
M1···M15	H···H	0.001087	0.004593	0.040418	-0.000383	-0.000381	0.000765	0.000384	-0.66
M1···M6	H···H	0.001792	0.007612	1.115513	-0.000609	-0.000684	0.001294	0.00061	-0.22
	H···H	0.001794	0.007621	1.103655	-0.00061	-0.000685	0.001295	0.00061	-0.22
TOTAL		0.003586							-0.44

[a]Atom···atom interaction. G_{AI} = Atom···atom interaction energy (kcal mol^{-1}).

Table S31. View of the dimer interactions from QTAIM analysis of compound **2c**.

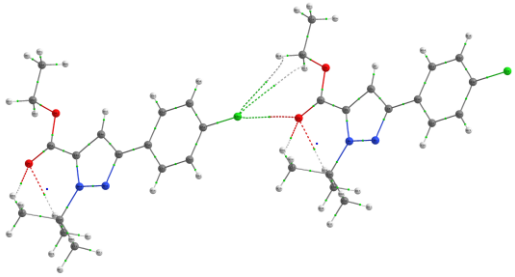
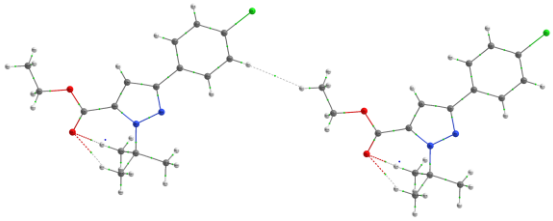
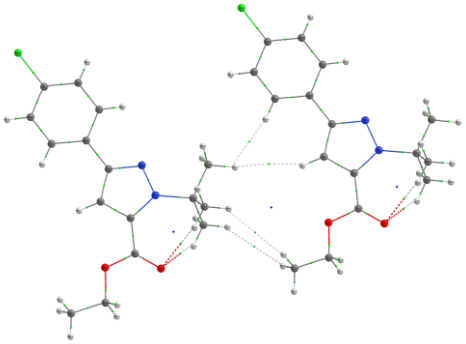
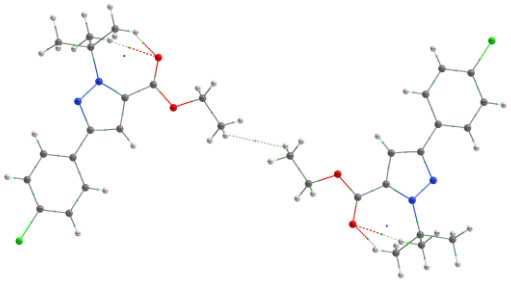
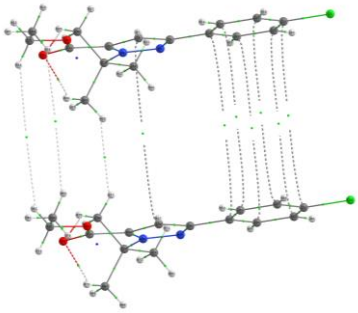
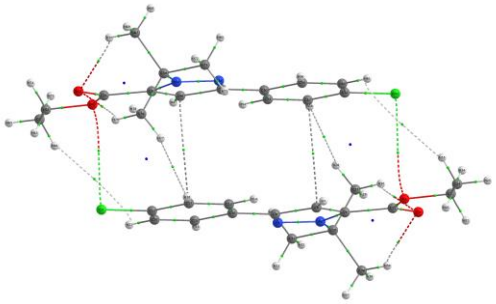
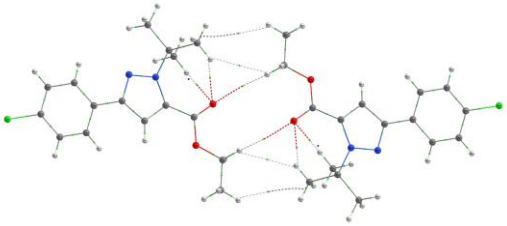
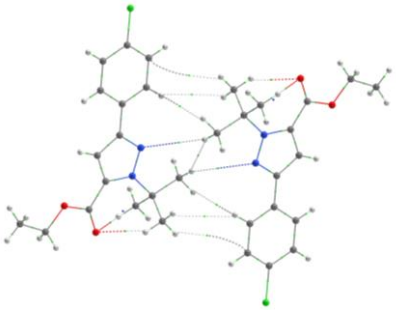
 M1···M2/ M1···M3	 M1···M4/ M1···M11
 M1···M5/ M1···M12	 M1···M6/ M1···M17
 M1···M7/ M1···M14	 M1···M8/ M1···M16
 M1···M9/ M1···M15	 M1···M10/ M1···M13

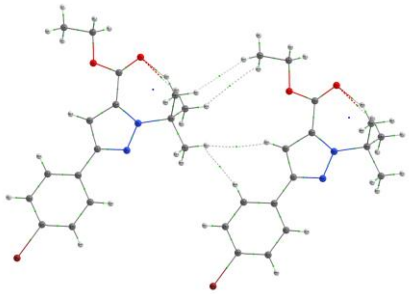
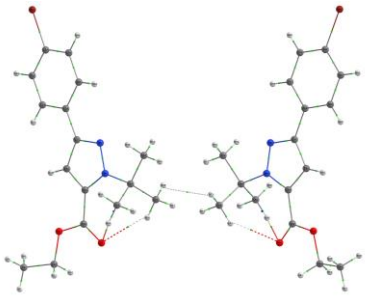
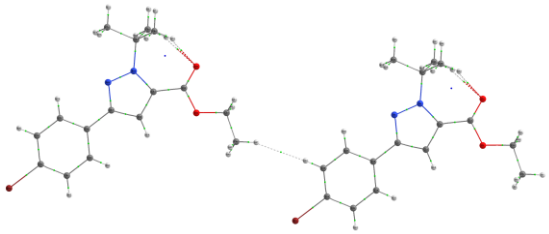
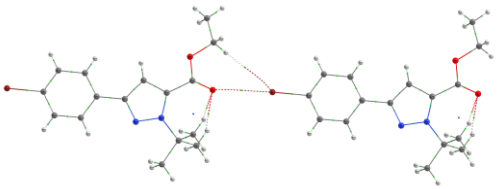
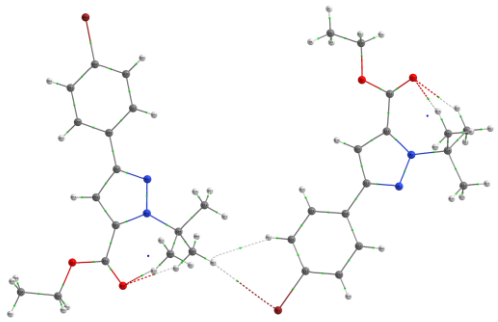
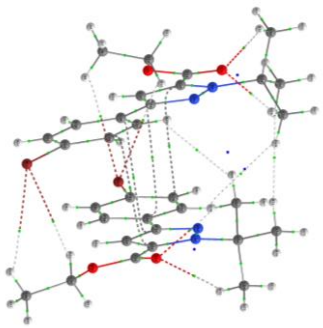
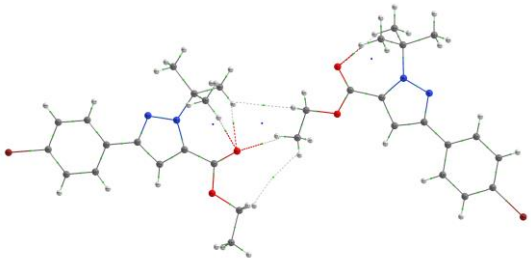
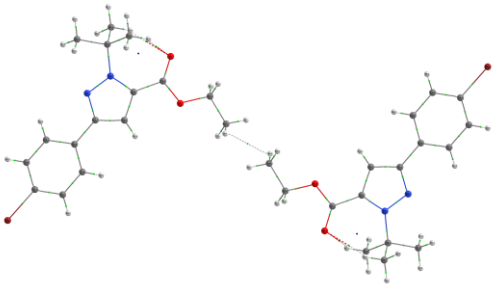
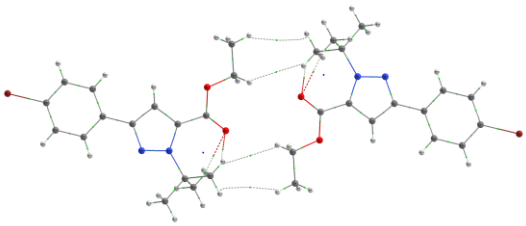
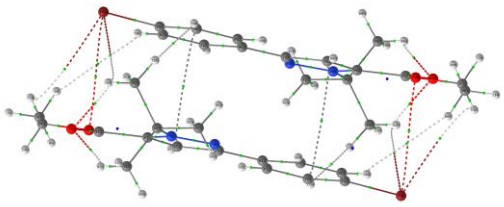
Table S32. QTAIM data and G_{AI} of dimers of compound **2c**

Dimer	Interaction	ρ_{INT}	$\nabla^2\rho$	ε	K	V	G	H	G_{AI}[a]
M1···M8	H···H	0.000526	0.002082	1.014266	-0.000178	-0.000164	0.000342	0.000178	-0.29
M1···M16	H···H	0.000526	0.002082	1.01453	-0.000178	-0.000164	0.000342	0.000178	-0.29
	H···H	0.001504	0.006409	0.115487	-0.00051	-0.000582	0.001092	0.00051	-0.83
	H···H	0.001504	0.006409	0.115482	-0.00051	-0.000582	0.001092	0.00051	-0.83
	O···Cl	0.004812	0.017803	3.817467	-0.000828	-0.002794	0.003623	0.000829	-2.67
	O···Cl	0.004812	0.017804	3.824962	-0.000828	-0.002794	0.003623	0.000829	-2.67
	Phπ···πPi	0.005496	0.013625	3.715107	-0.000473	-0.002459	0.002933	0.000474	-3.05
	PhCH···πPi	0.005496	0.013625	3.714339	-0.000473	-0.002459	0.002933	0.000474	-3.05
TOTAL		0.024676							-13.68
M1···M13	CH···πPh	0.00128	0.004107	0.869838	-0.000281	-0.000465	0.000746	0.000281	-0.44
M1···M10	CH···πPh	0.00128	0.004107	0.872282	-0.000281	-0.000465	0.000746	0.000281	-0.44
	CH···πPh	0.001796	0.006131	2.123699	-0.000416	-0.000702	0.001117	0.000415	-0.62
	CH···πPh	0.001797	0.006132	2.121516	-0.000416	-0.000702	0.001117	0.000415	-0.62
	CH···N	0.001838	0.007288	0.187855	-0.000502	-0.000819	0.00132	0.000501	-0.63
	CH···N	0.001839	0.007289	0.187786	-0.000502	-0.000819	0.001321	0.000502	-0.64
	H···H	0.001887	0.008158	0.613457	-0.000645	-0.000749	0.001394	0.000645	-0.65
	H···H	0.001887	0.008159	0.613343	-0.000645	-0.000749	0.001394	0.000645	-0.65
	H···H	0.001935	0.008299	0.28769	-0.000618	-0.00084	0.001457	0.000617	-0.67
TOTAL		0.015539							-5.37
M1···M9	H···H	0.001398	0.005525	1.730061	-0.000431	-0.00052	0.000951	0.000431	-0.50
M1···M15	H···H	0.001399	0.005526	1.731093	-0.000431	-0.00052	0.000951	0.000431	-0.50
	CH···O	0.001639	0.007733	0.586441	-0.000572	-0.000789	0.001361	0.000572	-0.59
	CH···O	0.001639	0.007735	0.585898	-0.000572	-0.000789	0.001361	0.000572	-0.59
	H···H	0.001982	0.008681	0.292517	-0.000637	-0.000897	0.001533	0.000636	-0.71
	H···H	0.001982	0.008682	0.292533	-0.000637	-0.000897	0.001533	0.000636	-0.71
TOTAL		0.010039							-3.60

M1···M12	H···H	0.001607	0.006829	0.06348	-0.000534	-0.000639	0.001173	0.000534	-0.39
M1···M5	H···H	0.001607	0.006829	0.063467	-0.000534	-0.000639	0.001173	0.000534	-0.39
	H···H	0.00218	0.009083	0.637007	-0.000641	-0.000988	0.00163	0.000642	-0.53
	H···H	0.005518	0.01976	0.101715	-0.000904	-0.003132	0.004036	0.000904	-1.35
TOTAL		0.010912							-2.67
M1···M14	H···H	0.001685	0.007048	0.061801	-0.000541	-0.000681	0.001221	0.00054	-0.96
M1···M7									
M1···M3	H···Cl	0.003245	0.013556	2.260538	-0.000923	-0.001543	0.002466	0.000923	-0.22
M1···M2	H···Cl	0.003245	0.013555	2.260047	-0.000923	-0.001543	0.002466	0.000923	-0.22
	Cl···O	0.006476	0.025422	0.035644	-0.001047	-0.004261	0.005308	0.001047	-0.44
TOTAL		0.012966							-0.88
M1···M6	H···H	0.002265	0.009562	0.277025	-0.000713	-0.000965	0.001678	0.000713	-0.64
M1···M17									
M1···M4	H···H	0.001536	0.006595	0.007476	-0.000498	-0.000652	0.001151	0.000499	-0.45
M1···M11									

[a]Atom···atom interaction. G_{AI} = Atom···atom interaction energy (kcal mol^{-1}).

Table S33. View of the dimer interactions from QTAIM analysis of compound **2d**.

 M1···M2/ M1···M3	 M1···M6/ M1···M16
 M1···M4/ M1···M12	 M1···M5/ M1···M13
 M1···M7/ M1···M9	 M1···M8
 M1···M10/ M1···M11	 M1···M14
 M1···M15	 M1···M18

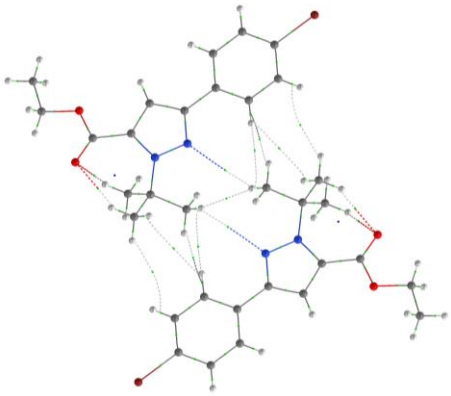
 M1···M17	

Table S34. QTAIM data and G_{AI} of dimers of compound **2d**

Dimer	Interaction	ρ_{INT}	$\nabla^2\rho$	ε	K	V	G	H	G_{AI}[a]
M1···M8	H···H	0.00153	0.006536	0.010486	-0.0005	-0.0006	0.00113	0.00051	-0.59
	H···H	0.0019	0.008401	0.234823	-0.0006	-0.0008	0.00145	0.00065	-0.74
	H···H	0.0019	0.008401	0.234871	-0.0006	-0.0008	0.00145	0.00065	-0.74
	CH···Br	0.0041	0.013361	0.364401	-0.0007	-0.002	0.00266	0.00068	-1.58
	CH···Br	0.0041	0.013361	0.3643610	-0.0007	-0.002	0.00266	0.00068	-1.58
	Phπ···πPi	0.00456	0.011043	3.6663660	-0.0003	-0.0021	0.00241	0.00035	-1.76
	Phπ···πPi	0.00456	0.011043	3.6618360	-0.0003	-0.0021	0.00241	0.00035	-1.76
	CH···Br	0.00467	0.015878	0.2681330	-0.0008	-0.0023	0.00313	0.00084	-1.80
	CH···Br	0.00467	0.015878	0.2681250	-0.0008	-0.0023	0.00313	0.00084	-1.80
	Phπ···πPi	0.00482	0.011093	1.2755590	-0.0003	-0.0021	0.00244	0.00033	-1.86
	Phπ···πPi	0.00482	0.011094	1.2742080	-0.0003	-0.0021	0.00244	0.00033	-1.86
TOTAL		0.04164							-16.08
M1···M18	H···H	0.00118	0.005034	0.4119110	-0.0004	-0.0004	0.00084	0.00042	-0.50
	H···H	0.00118	0.005034	0.4116680	-0.0004	-0.0004	0.00084	0.00042	-0.50
	H···H	0.00151	0.006455	0.0697290	-0.0005	-0.0006	0.0011	0.00052	-0.64
	H···H	0.00151	0.006455	0.0697590	-0.0005	-0.0006	0.0011	0.00052	-0.64
	CH···Br	0.00181	0.006353	0.6662400	-0.0004	-0.0007	0.00117	0.00042	-0.77
	CH···Br	0.00181	0.006353	0.6662710	-0.0004	-0.0007	0.00117	0.00042	-0.77
	CH···Br	0.00352	0.013658	8.3740780	-0.0008	-0.0018	0.00261	0.00081	-1.49
	CH···Br	0.00352	0.013659	8.3296220	-0.0008	-0.0018	0.00261	0.00081	-1.49
	Phπ···πPi	0.00489	0.011917	5.7727860	-0.0004	-0.0022	0.0026	0.00038	-2.07
	Phπ···πPi	0.00489	0.011917	5.7653410	-0.0004	-0.0022	0.0026	0.00038	-2.07
	Br-O	0.00512	0.017371	0.5900490	-0.0006	-0.0031	0.0037	0.00064	-2.17
	Br-O	0.00512	0.01737	0.5900540	-0.0006	-0.0031	0.0037	0.00064	-2.17
TOTAL		0.03605							-15.28
M1···M17	H···H	0.00145	0.006035	0.9873090	-0.0005	-0.0005	0.00102	0.00049	-0.40
	H···H	0.00145	0.006035	0.9859520	-0.0005	-0.0005	0.00102	0.00049	-0.40
	H···H	0.00151	0.005848	3.3595520	-0.0004	-0.0006	0.00102	0.00044	-0.42
	H···H	0.00151	0.005848	3.3641660	-0.0004	-0.0006	0.00102	0.00044	-0.42
	H···H	0.0016	0.006669	3.0558490	-0.0006	-0.0006	0.00112	0.00055	-0.44
	H···H	0.00161	0.006669	3.0536790	-0.0006	-0.0006	0.00112	0.00055	-0.44
	CH···πPh	0.00163	0.005806	1.6462290	-0.0004	-0.0006	0.00101	0.00044	-0.45
	CH···πPh	0.00163	0.005807	1.6476750	-0.0004	-0.0006	0.00101	0.00044	-0.45
	CH···N	0.00193	0.007733	0.4842930	-0.0005	-0.0009	0.0014	0.00053	-0.53

	CH···N	0.00193	0.007733	0.4840370	-0.0005	-0.0009	0.0014	0.00053	-0.53
	H···H	0.00273	0.01132	0.1480950	-0.0007	-0.0014	0.0021	0.00073	-0.75
TOTAL		0.01898							-5.23
M1···M10	H···H	0.00099	0.004186	3.651332	-0.0004	-0.0003	0.00068	0.00037	-0.45
M1···M11	H···H	0.0024	0.010649	0.126267	-0.0008	-0.0011	0.0019	0.00077	-1.08
	CH···O	0.00261	0.013036	0.615581	-0.0009	-0.0014	0.00232	0.00094	-1.17
TOTAL		0.006							-2.70
M1···M2	H···H	0.00159	0.006924	1.472801	-0.0005	-0.0007	0.0012	0.00053	-0.44
M1···M3	H···H	0.00161	0.006849	0.084965	-0.0005	-0.0006	0.00118	0.00054	-0.45
	H···H	0.00186	0.00782	0.907461	-0.0006	-0.0007	0.00134	0.00062	-0.52
	H···H	0.00394	0.015584	0.118646	-0.0009	-0.0021	0.00299	0.0009	-1.10
TOTAL		0.009							-2.50
M1···M15	H···H	0.0008	0.003035	0.474306	-0.0002	-0.0003	0.00052	0.00024	-0.46
	H···H	0.0008	0.003035	0.474157	-0.0002	-0.0003	0.00052	0.00024	-0.46
	H···H	0.00102	0.00422	0.224531	-0.0003	-0.0004	0.00071	0.00034	-0.59
	H···H	0.00102	0.004221	0.224486	-0.0003	-0.0004	0.00071	0.00034	-0.59
TOTAL		0.00363							-2.11
M1···M7	H···H	0.00208	0.00897	1.374227	-0.0007	-0.0008	0.00154	0.00071	-0.80
M1···M9	CH···Br	0.00316	0.009704	0.058278	-0.0005	-0.0014	0.00193	0.0005	-1.22
TOTAL		0.00525							-2.02
M1···M13	CH···Br	0.00371	0.012196	0.148385	-0.0006	-0.0018	0.0024	0.00065	-0.57
M1···M5	Br···O	0.00754	0.028375	0.083313	-0.0011	-0.0048	0.00595	0.00114	-1.15
TOTAL		0.01125							-1.72
M1···M4 M1···M12	H···H	0.00287	0.011598	0.005503	-0.0007	-0.0015	0.0022	0.0007	-0.9
M1···M6 M1···M16	H···H	0.0014	0.005794	0.073486	-0.0005	-0.0005	0.00099	0.00046	-0.9
M1···M14	H···H	0.00443	0.018726	0.329133	-0.0012	-0.0023	0.00349	0.00119	-0.3

[a]Atom···atom interaction. G_{AI} = Atom···atom interaction energy (kcal mol^{-1}).

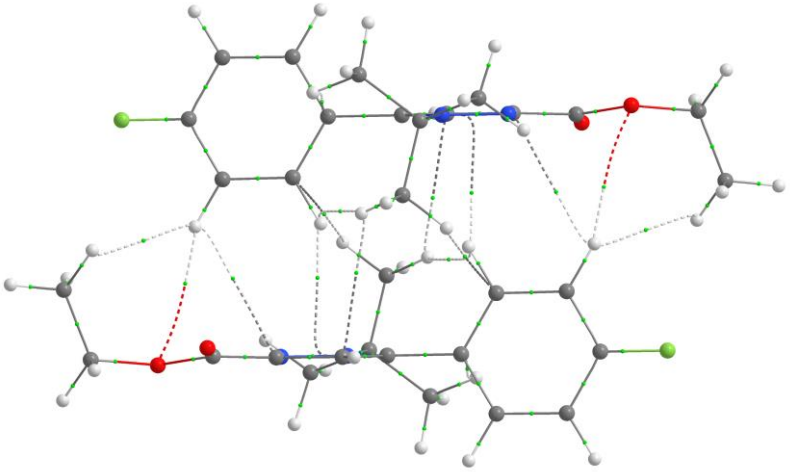


Figure S30. QTAIM analysis from optimization dimer structure for compound **1b**. The dimer structure was obtained from *s-trans* dimer **1cA**, with the change of the halogen by F.

9. Crystallization Mechanism

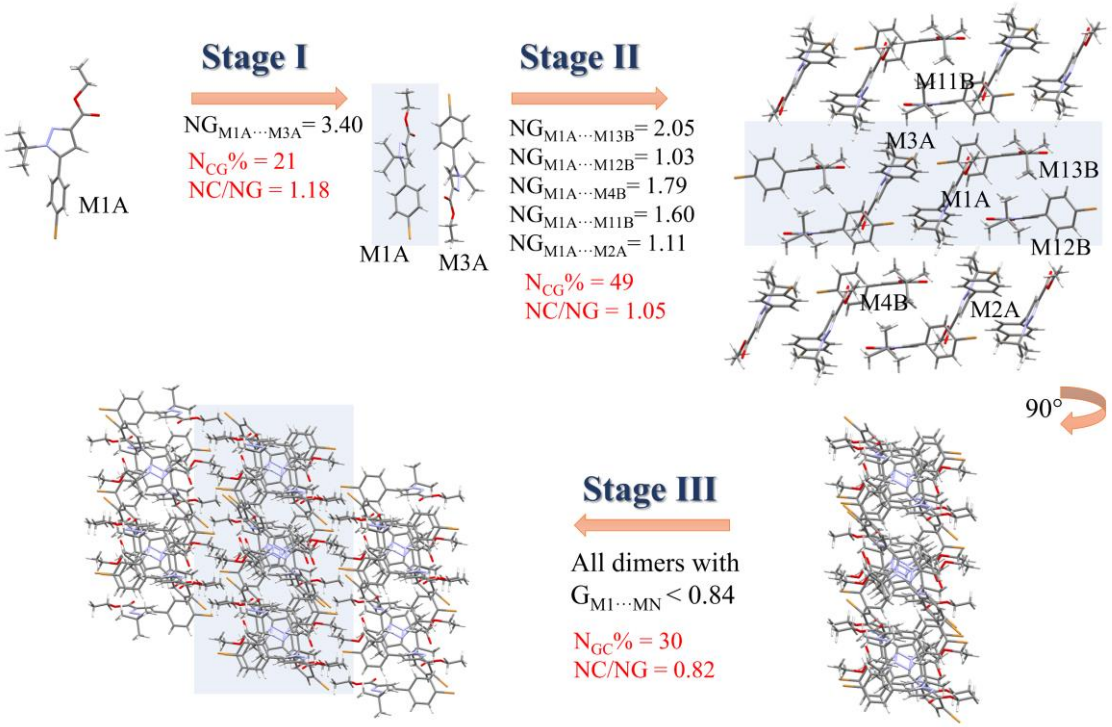


Figure S31. Proposal of crystallization mechanism of compound **1d** from data of cluster A.

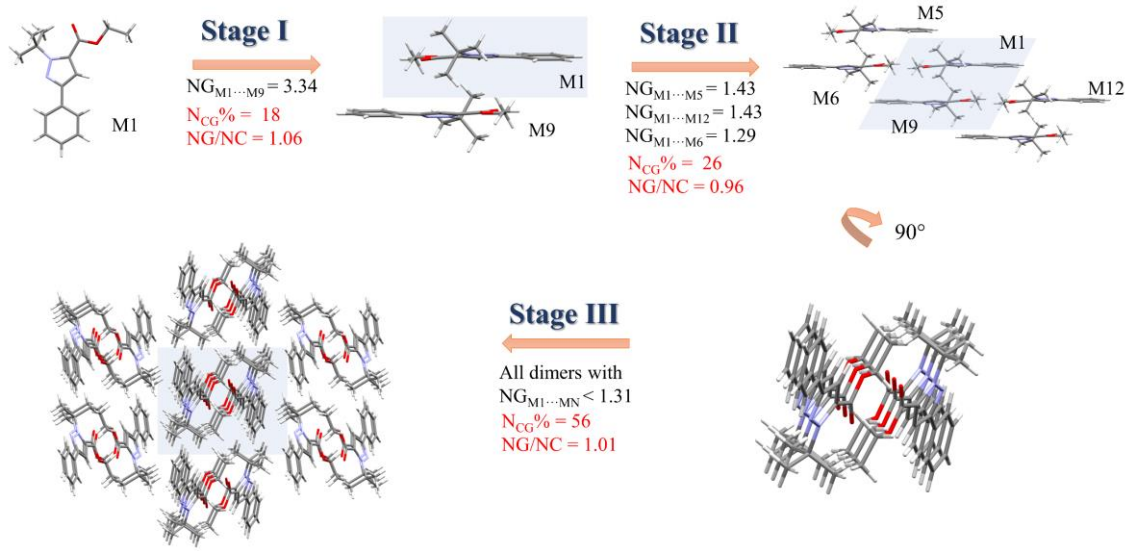


Figure S32. Proposal of crystallization mechanism of compound **2a**.

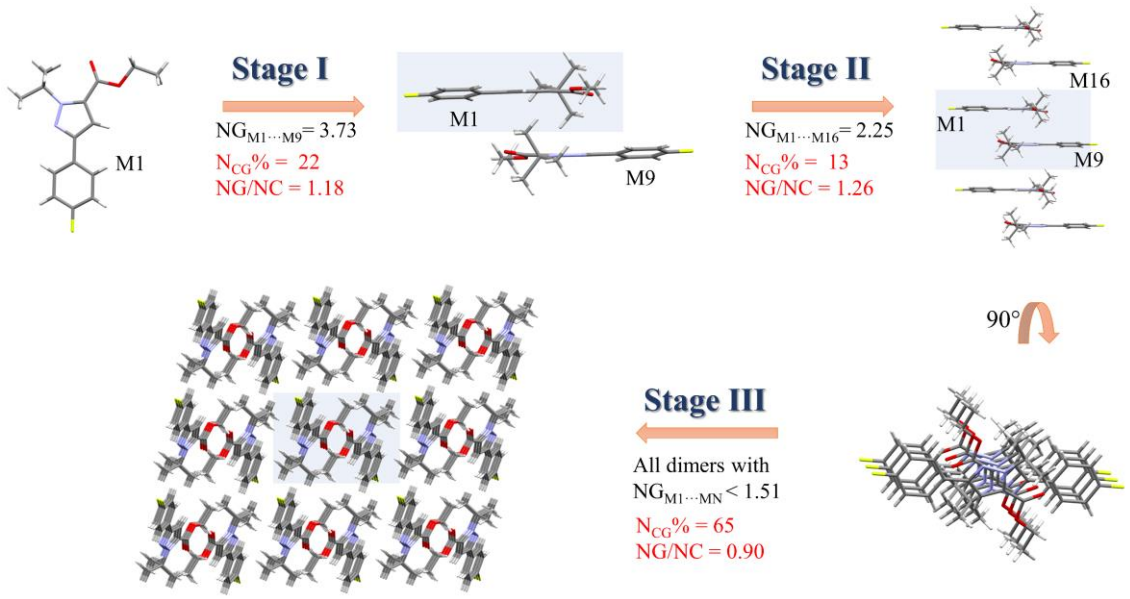


Figure S33. Proposal of crystallization mechanism of compound **2b**.

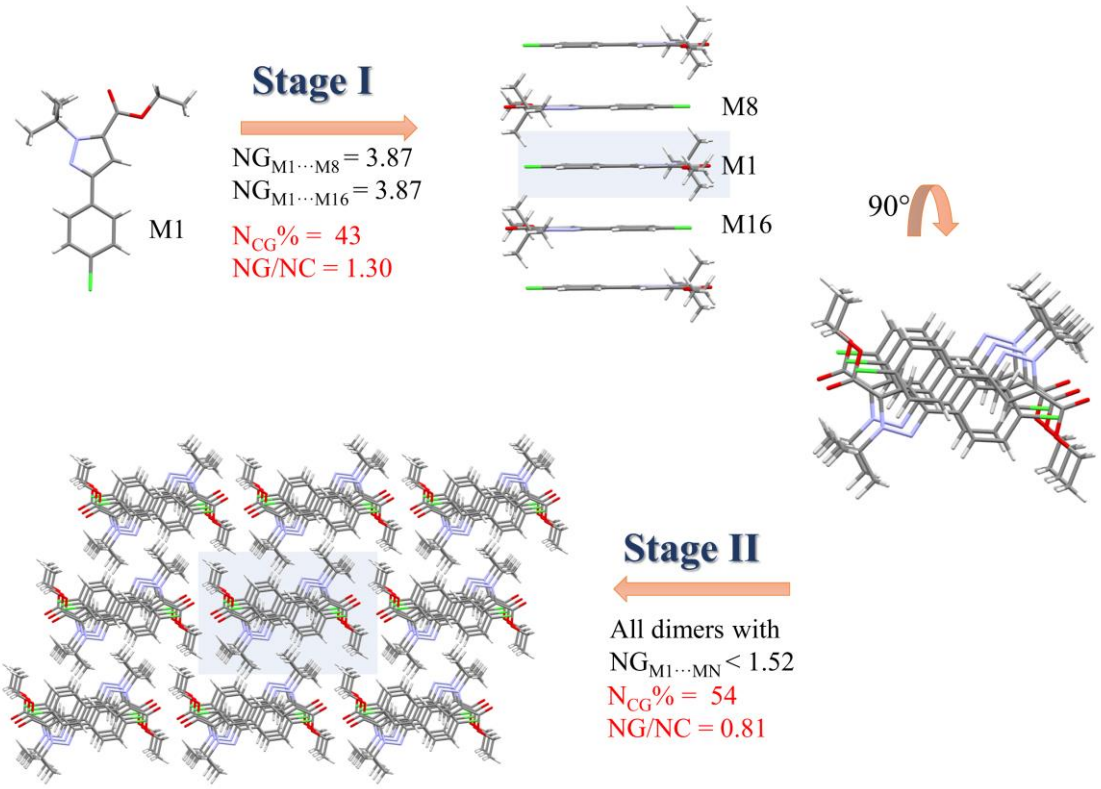


Figure S34. Proposal of crystallization mechanism of compound **2c**.

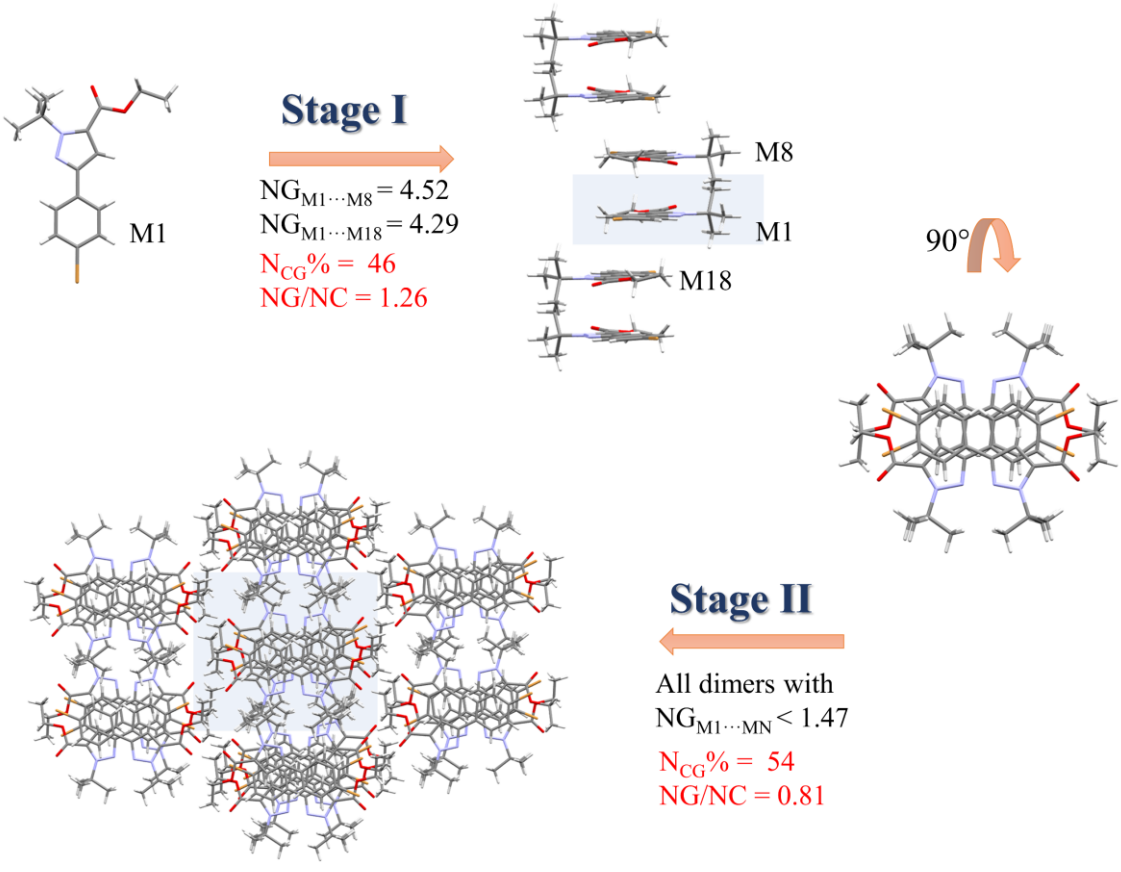


Figure S35. Proposal of crystallization mechanism of compound **2d**.