Electronic Supporting Information

For paper

Use of quantum chemical methods to study concomitant polymorphs of new benzimidazole-1,2,3-triazole hybrid compound

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(E_{int}, kcal/mol), the contribution of this energy to the total interaction energy (%) and bonding type in crystals of **1t**.

Table S4 Symmetry codes, interaction energy of the basic **dimer** with neighbouring ones (E_{int}, kcal/mol), the contribution of this energy to the total interaction energy (%) and bonding type in crystals of **1m**.

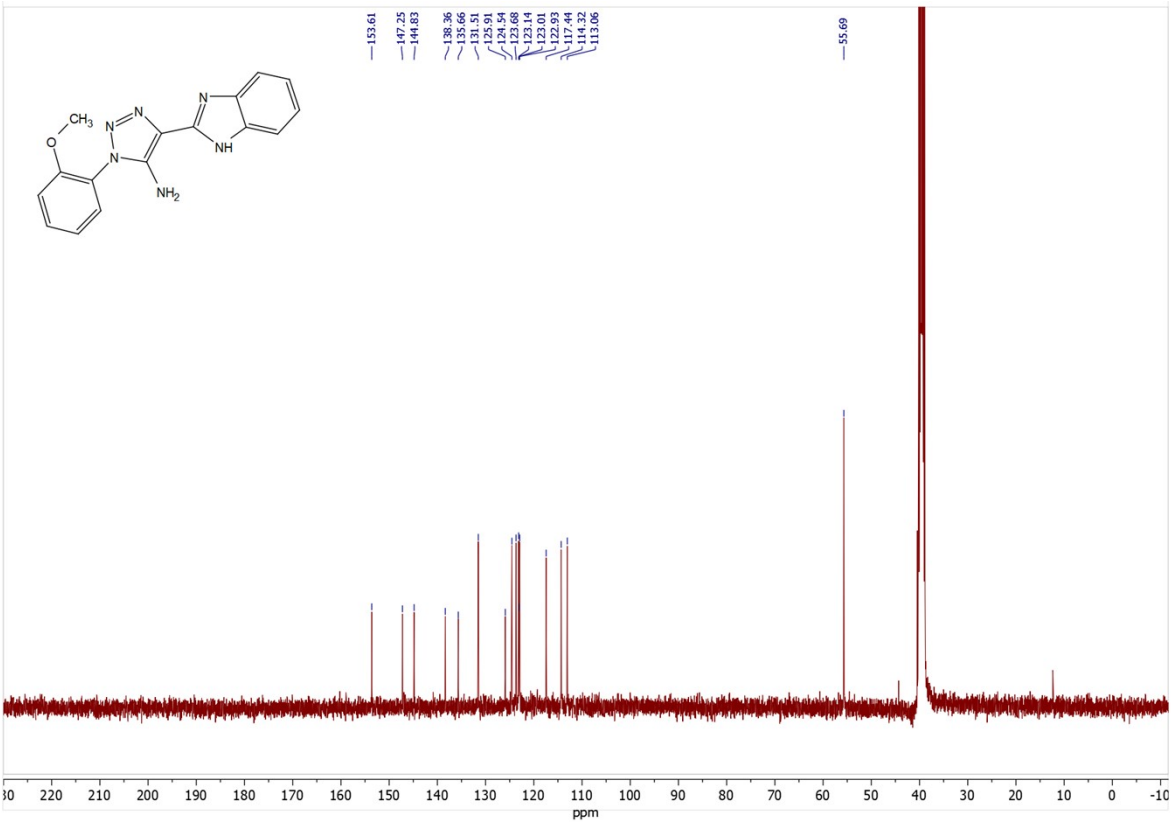


Figure S1. ^{13}C NMR spectrum (100 MHz, DMSO-d6) of the title compound.

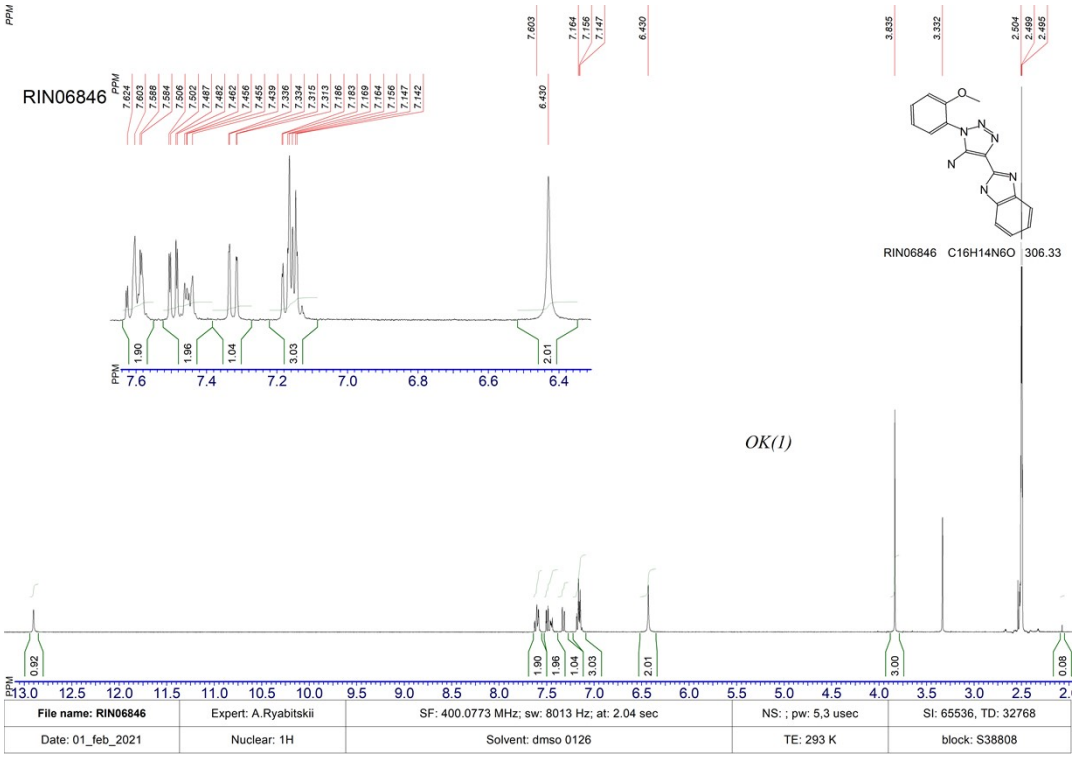
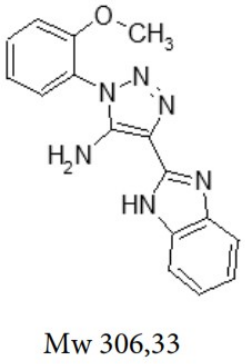


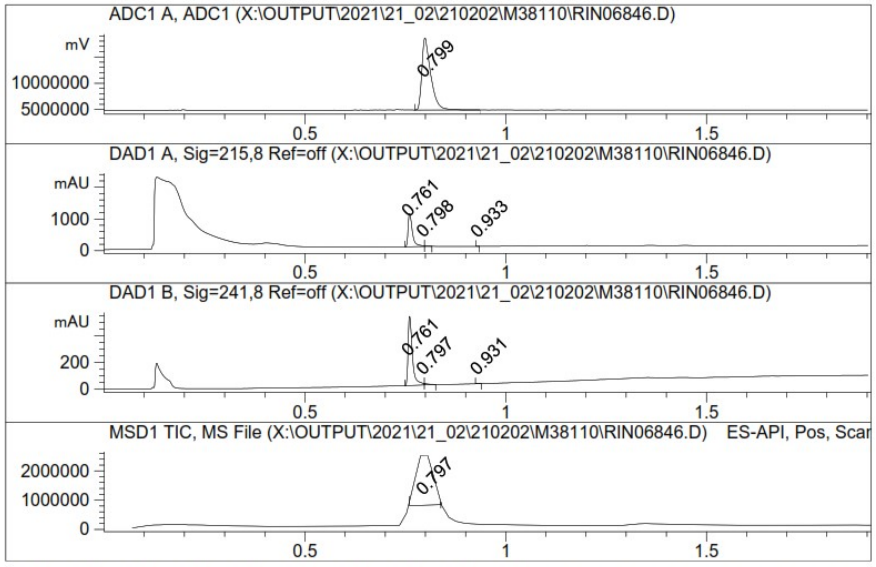
Figure S2. ^{1}H NMR spectrum (400 MHz, DMSO-d6) of the title compound.

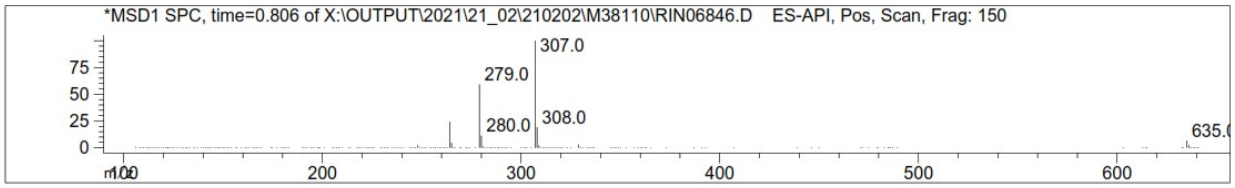
Agilent 1260 LC/MSD SL
Diodearrey G1315B (DAD1A-215nm; DAD1B-241nm)
Mass Quad G6140 (MSD1-Pos, MSD2-Neg)
ELSD Softa 1400 (ADC1 A, ELSD)

Mobile Phase:A-H2O+0.1%HCOOH;B-MeCN+0.1HCOOH
Separation column: **98%**
Rapid Resolutionn HT Cartige 4.6x30mm,
1.8-Micron, Zorbx SB-C18



Mw 306,33





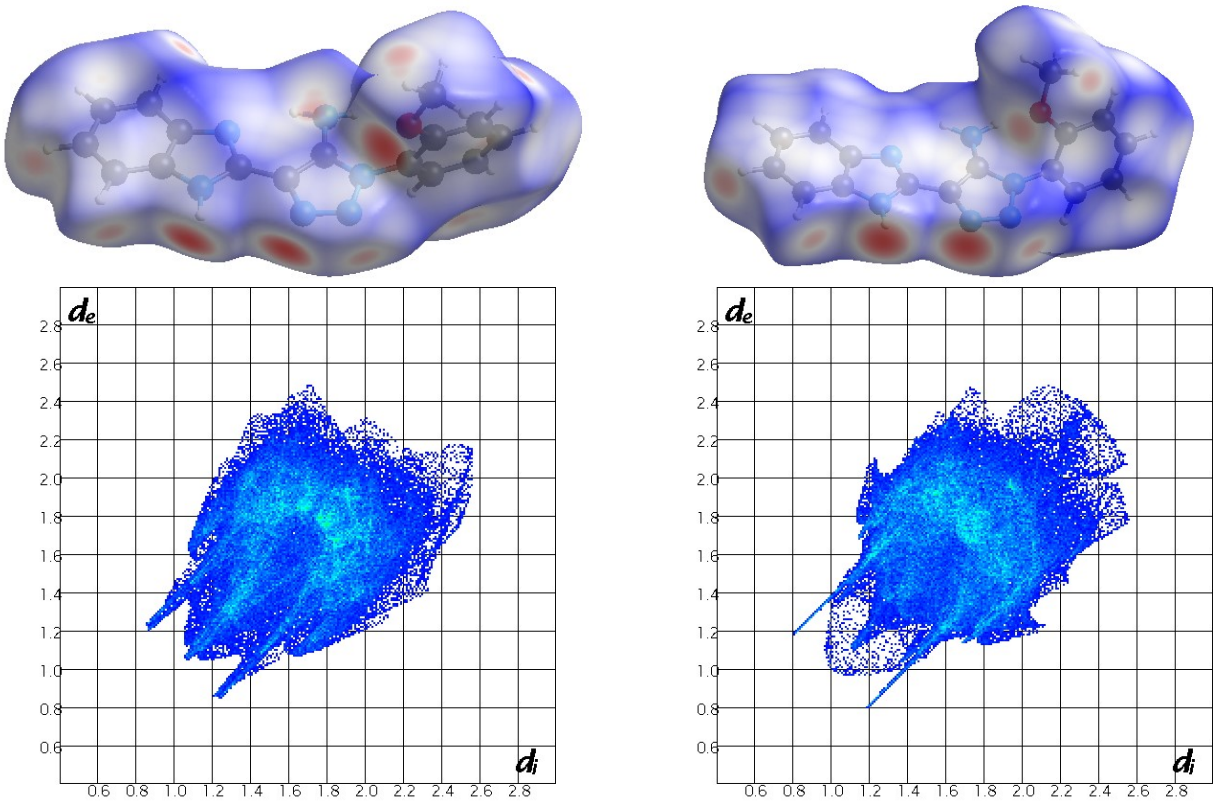
#	Signal	R.Time	Area %
1	ADC1 A, ADC1	0.799	100.000

#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	0.761	98.800
2		0.798	1.093
3		0.933	0.108

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,8 Ref=off	0.761	98.036
2		0.797	1.909
3		0.931	0.055

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.797	100.000

Figure S3. LC/MS data for the title compound.



1t **1m**

Figure S4 Hirshfeld surfaces mapped over d_{norm} (at the top) and two-dimensional fingerprint plots (at the bottom) of the molecule in structures **1t** and **1m**.

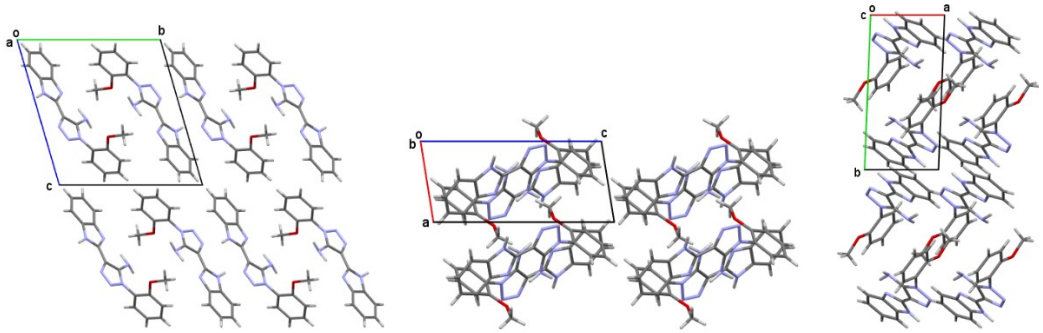


Figure S5 Molecules packing in structure **1t**.

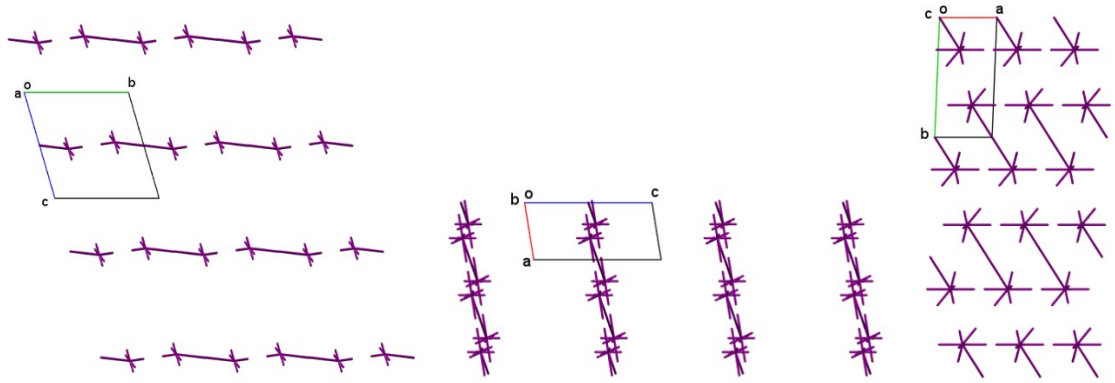


Figure S6 Packing of energy-vector diagrams in structure **1t**.

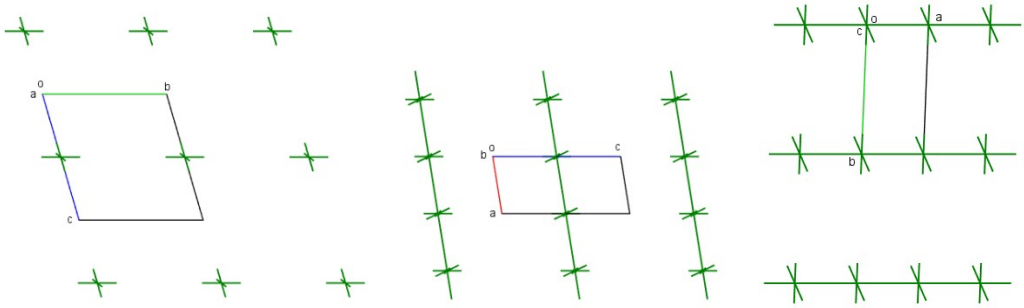


Figure S7 Packing of DBU in structure **1t**.

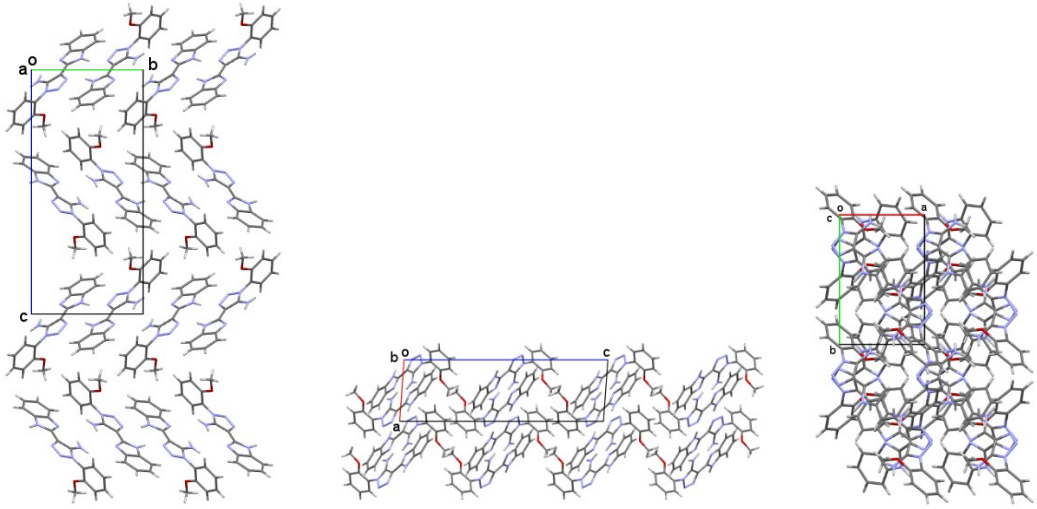


Figure S8 Molecules packing in structure **1m**.

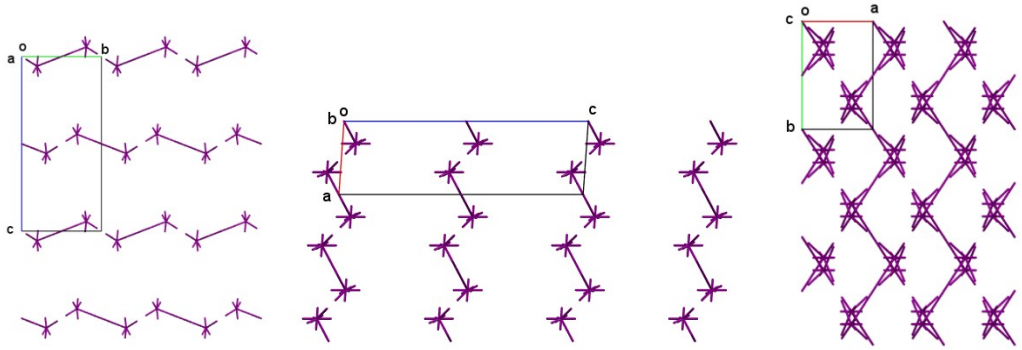


Figure S9 Packing of energy-vector diagrams in structure **1m**.

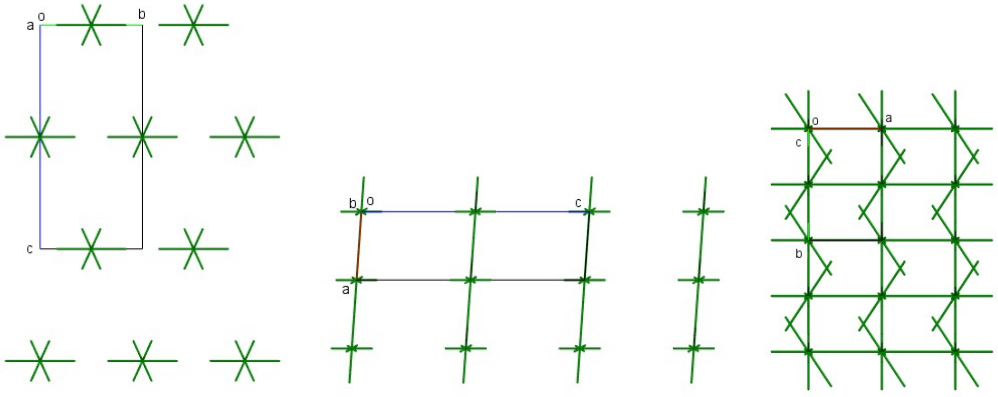


Figure S10 Packing of DBU in structure **1m**.

Table S1 Symmetry codes, interaction energy of the basic **molecule** with neighbouring ones (E_{int}, kcal/mol), the contribution of this energy to the total interaction energy (%) and bonding type in crystals of **1t**.

Dimer	Symmetry operation	E_{int}, kcal/mol	Contribution to the total interaction energy, %	Interaction type
t_1	-x,-y,1-z	-17.39	18.7	N2–H…N3
t_2	-1+x,y,z	-14.23	15.3	N6–H…O1
t_3	1+x,y,z	-14.23	15.3	N6–H…O1
t_4	-x,1-y,1-z	-10.07	10.8	C16–H…C9(π)
t_5	1-x,-y,1-z	-9.13	9.8	stacking
t_6	1-x,1-y,1-z	-8.56	9.2	non-specific
t_7	x,y,-1+z	-3.50	3.8	non-specific
t_8	x,y,1+z	-3.50	3.8	non-specific
t_9	1+x,y,-1+z	-3.17	3.4	non-specific
t_10	-1+x,y,1+z	-3.17	3.4	non-specific
t_11	-x,1-y,2-z	-2.18	2.3	non-specific
t_12	2-x,-y,-z	-1.74	1.9	non-specific
t_13	1-x,1-y,2-z	-1.17	1.3	non-specific
t_14	1-x,-y,-z	-1.16	1.2	non-specific
		E_{int}(total) -93.18 kcal/mol		

Table S2 Symmetry codes, interaction energy of the basic **molecule** with neighbouring ones (E_{int}, kcal/mol), the contribution of this energy to the total interaction energy (%) and bonding type in crystals of **1m**.

Dimer	Symmetry operation	E_{int}, kcal/mol	Contribution to the total interaction energy, %	Interaction type
m_1	2-x,2-y,1-z	-18.77	20.7	N2–H…N3
m_2	2-x,1-y,1-z	-13.25	14.6	C–H…π
m_3	1-x,2-y,1-z	-13.16	14.5	stacking
m_4	1-x,1-y,1-z	-12.84	14.2	non-specific
m_5	1+x,y,z	-5.49	6.1	non-specific
m_6	-1+x,y,z	-5.49	6.1	non-specific
m_7	x,3/2-y,-1/2+z	-4.30	4.7	non-specific
m_8	x,3/2-y,1/2+z	-4.30	4.7	non-specific
m_9	2-x,1/2+y,1/2-z	-3.53	3.9	non-specific
m_10	2-x,-1/2+y,1/2-z	-3.53	3.9	non-specific
m_11	1+x,3/2-y,-1/2+z	-1.66	1.8	non-specific
m_12	-1+x,3/2-y,1/2+z	-1.66	1.8	non-specific
m_13	1-x,1/2+y,1/2-z	-1.40	1.5	non-specific
m_14	1-x,-1/2+y,1/2-z	-1.40	1.5	non-specific
		E_{int}(total) -90.77 kcal/mol		

Table S3 Symmetry codes, interaction energy of the basic **dimer** with neighbouring ones (E_{int}, kcal/mol), the contribution of this energy to the total interaction energy (%) and bonding type in crystals of **1t**.

Dimer	Symmetry operation	E_{int}, kcal/mol	Contribution to the total interaction energy, %	Interaction type
dt_1	-1+x,y,z	-36.59	23.3	Stacking/N–H…O
dt_2	1+x,y,z	-36.59	23.3	Stacking/N–H…O
dt_3	x,-1+y,z	-11.43	7.3	C16–H…C9(π)
dt_4	x,1+y,z	-11.43	7.3	C16–H…C9(π)
dt_5	-1+x,-1+y,z	-9.90	6.3	non-specific
dt_6	1+x,1+y,z	-9.90	6.3	non-specific
dt_7	x,y,1+z	-8.25	5.2	non-specific
dt_8	x,y,-1+z	-8.25	5.2	non-specific
dt_9	1+x,y,-1+z	-7.17	4.6	non-specific
dt_10	-1+x,y,1+z	-7.17	4.6	non-specific
dt_11	x,-1+y,-1+z	-2.23	1.4	non-specific
dt_12	x,1+y,1+z	-2.23	1.4	non-specific
dt_13	-2+x,y,1+z	-1.95	1.2	non-specific
dt_14	2+x,y,-1+z	-1.95	1.2	non-specific
dt_15	1+x,1+y,1+z	-1.15	0.7	non-specific
dt_16	-1+x,-1+y,-1+z	-1.15	0.7	non-specific
		E_{int}(total) -157.34 kcal/mol		

Table S4 Symmetry codes, interaction energy of the basic **dimer** with neighbouring ones (E_{int}, kcal/mol), the contribution of this energy to the total interaction energy (%) and bonding type in crystals of **1m**.

Dimer	Symmetry operation	E_{int}, kcal/mol	Contribution to the total interaction energy, %	Interaction type
dm_1	1+x,y,z	-22.50	15.0	stacking
dm_2	-1+x,y,z	-22.50	15.0	stacking
dm_3	x,-1+y,z	-15.10	10.1	C–H…π
dm_4	x,1+y,z	-15.10	10.1	C–H…π
dm_5	-1+x,-1+y,z	-13.87	9.3	non-specific
dm_6	1+x,1+y,z	-13.87	9.3	non-specific
dm_7	2-x,-1/2+y,3/2-z	-7.94	5.3	non-specific
dm_8	2-x,-1/2+y,1/2-z	-7.94	5.3	non-specific
dm_9	2-x,1/2+y,3/2-z	-7.94	5.3	non-specific
dm_10	2-x,1/2+y,1/2-z	-7.94	5.3	non-specific
dm_11	1-x,1/2+y,3/2-z	-2.02	1.4	non-specific
dm_12	1-x,-1/2+y,3/2-z	-2.02	1.4	non-specific
dm_13	3-x,1/2+y,1/2-z	-2.02	1.4	non-specific
dm_14	3-x,-1/2+y,1/2-z	-2.02	1.4	non-specific
dm_15	3-x,-1/2+y,3/2-z	-1.69	1.1	non-specific
dm_16	3-x,1/2+y,3/2-z	-1.69	1.1	non-specific
dm_17	1-x,-1/2+y,1/2-z	1.69	1.1	non-specific
dm_18	1-x,1/2+y,1/2-z	-1.69	1.1	non-specific
		E_{int}(total) -149.58 kcal/mol		