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Supporting information for article:

Three polymorphs of 3-(3-phenyl-1*H*-1,2,4-triazol-5-yl)-2*H*-1-benzopyran-2-one formed from different solvents

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Supporting information

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

Dimer	Molecules	Symmetry operation	E_{int}, kcal/mol	The contribution to the total interaction energy, %
		Molecule **1t_A**		
1t_d1	**A-A**	2-x,1-y,-z	-17.6	23.6
1t_d2	**A-A**	1-x,2-y,-z	-15.9	21.3
1t_d3	**A-A**	2-x,2-y,-z	-7.4	9.9
1t_d4	**A-A**	1-x,1-y,-z	-7.3	9.9
1t_d5	**A-A**	1+x,y,z	-5.4	7.2
1t_d6	**A-A**	-1+x,y,z	-5.4	7.2
1t_d7	**A-B**	x,1+y,-1+z	-4.2	5.6
1t_d8	**A-B**	1-x,1-y,1-z	-3.3	4.5
1t_d9	**A-B**	x,y,z	-2.8	3.7
1t_d10	**A-B**	2-x,1-y,-z	-2.0	2.6
1t_d11	**A-B**	1+x,y,z	-1.3	1.7
1t_d12	**A-B**	2-x,1-y,1-z	-1.1	1.4
1t_d13	**A-B**	1-x,1-y,-z	-1.0	1.4
		Molecule **1t_B**		
1t_d14	**B-B**	1-x,1-y,1-z	-16.6	22.4
1t_d15	**B-B**	2-x,-y,1-z	-16.4	22.1
1t_d16	**B-B**	2-x,1-y,1-z	-7.8	10.5
1t_d17	**B-B**	1-x,-y,1-z	-7.1	9.6
1t_d18	**B-B**	1+x,y,z	-5.4	7.2
1t_d19	**B-B**	-1+x,y,z	-5.4	7.2
1t_d20	**B-A**	x,-1+y,1+z	-4.2	5.6
1t_d21	**B-A**	1-x,1-y,1-z	-3.3	4.5
1t_d22	**B-A**	x,y,z	-2.8	3.7
1t_d23	**B-A**	2-x,1-y,-z	-2.0	2.6
1t_d24	**B-A**	-1+x,y,	-1.3	1.7
1t_d25	**B-A**	2-x,1-y,1-z	-1.1	1.4
1t_d26	**B-A**	1-x,1-y,-z	-1.0	1.4

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

Dimer	Molecules	Symmetry operation	E_{int}, kcal/mol	The contribution to the total interaction energy, %
		Molecule **1m_A**		
1m_d1	**A-B**	1+x,y,z	-17.23	23.6
1m_d2	**A-B**	x,y,-1+z	-15.74	21.6
1m_d3	**A-B**	1+x,y,-1+z	-7.58	10.4
1m_d4	**A-B**	x,y,z	-7.24	9.9
1m_d5	**A-A**	1+x,y,z	-5.15	7.1
1m_d6	**A-A**	-1+x,y,z	-5.15	7.1
1m_d7	**A-B**	1-x,1/2+y,1-z	-3.23	4.4
1m_d8	**A-A**	2-x,1/2+y,1-z	-2.53	3.5
1m_d9	**A-A**	2-x,-1/2+y,1-z	-2.53	3.5
1m_d10	**A-B**	1-x,-1/2+y,1-z	-1.90	2.6
1m_d11	**A-A**	3-x,1/2+y,1-z	-1.29	1.8
1m_d12	**A-A**	3-x,-1/2+y,1-z	-1.29	1.8
1m_d13	**A-B**	2-x,1/2+y,1-z	-1.05	1.4
1m_d14	**A-B**	2-x,-1/2+y,1-z	-1.04	1.4
		Molecule **1m_B**		
1m_d15	**B-A**	-1+x,y,z	-17.23	23.2
1m_d16	**B-A**	x,y,1+z	-15.74	21.2
1m_d17	**B-A**	-1+x,y,1+z	-7.58	10.2
1m_d18	**B-A**	x,y,z	-7.24	9.8
1m_d19	**B-B**	1+x,y,z	-5.28	7.1
1m_d20	**B-B**	-1+x,y,z	-5.28	7.1
1m_d21	**B-B**	1-x,1/2+y,2-z	-4.31	5.8
1m_d22	**B-B**	1-x,-1/2+y,2-z	-4.31	5.8
1m_d23	**B-A**	1-x,-1/2+y,1-z	-3.23	4.4
1m_d24	**B-A**	1-x,1/2+y,1-z	-1.90	2.6
1m_d25	**B-A**	2-x,1/2+y,1-z	-1.04	1.4
1m_d26	**B-A**	2-x,-1/2+y,1-z	-1.05	1.4

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

Dimer	Symmetry operation	E_{int}, kcal/mol	The contribution to the total interaction energy, %
1r_d1	3/2-x,1/2+y,z	-14.02	18.3
1r_d2	3/2-x,-1/2+y,z	-14.02	18.3
1r_d3	1-x,1-y,1-z	-10.02	13.1
1r_d4	2-x,1-y,1-z	-5.21	6.8
1r_d5	x,3/2-y,1/2+z	-4.81	6.3
1r_d6	x,3/2-y,-1/2+z	-4.81	6.3
1r_d7	3/2-x,1-y,1/2+z	-4.56	6.0
1r_d8	3/2-x,1-y,-1/2+z	-4.56	6.0
1r_d9	1-x,1/2+y,1/2-z	-3.14	4.1
1r_d10	1-x,-1/2+y,1/2-z	-3.14	4.1
1r_d11	1/2+x,y,1/2-z	-2.32	3.0
1r_d12	-1/2+x,y,1/2-z	-2.32	3.0
1r_d13	1/2+x,1/2-y,1-z	-1.80	2.3
1r_d14	-1/2+x,1/2-y,1-z	-1.80	2.3