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Supporting information for article:

Influence of *ortho*-substituent on the molecular and crystal structures of 2-(N-arylimino)coumarin-3-carboxamide: isotypic and polymorphic structures

Svitlana V. Shishkina, Irina S. Konovalova, Sergiy M. Kovalenko, Pavlo V. Trostianko, Anna O. Geleverya, Lyudmila L. Nikolayeva and Natalya D. Bunyatyan

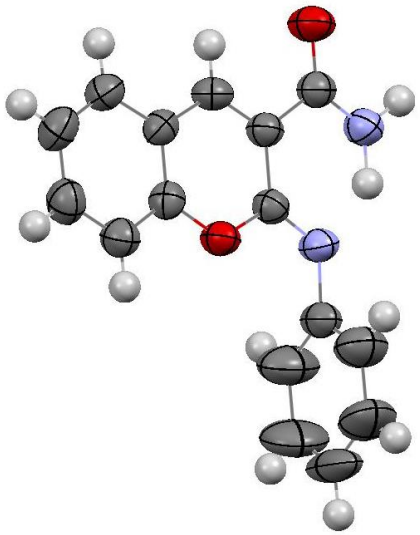

Fig. S1. Molecular structure of **1h**.

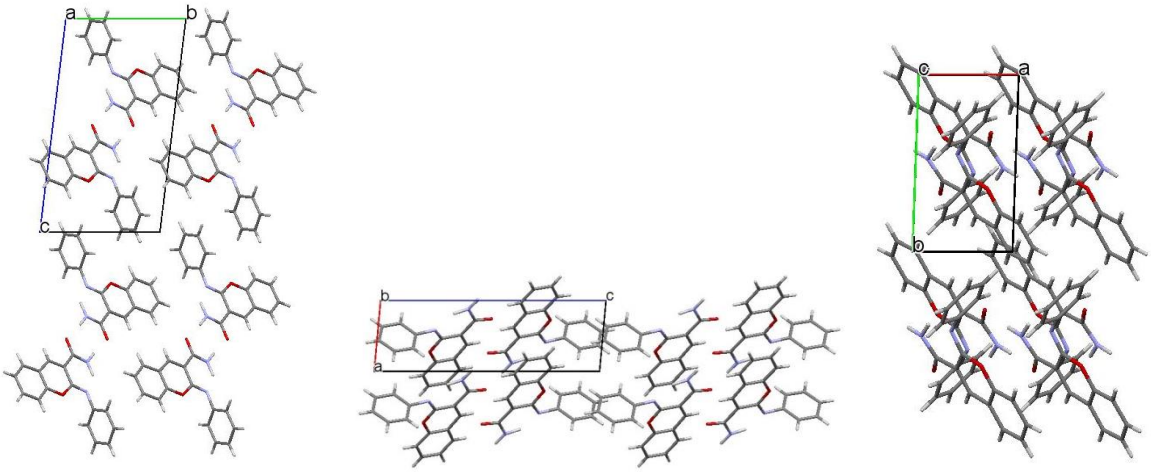

Fig. S2. Molecules packing in structure **1h**.

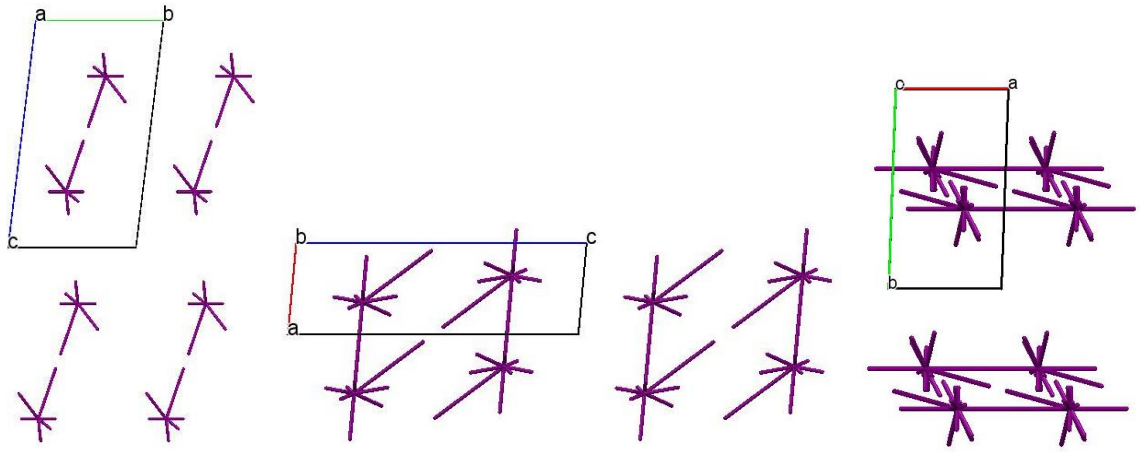

Fig. S3. Packing of energy-vector diagrams in structure **1h**.

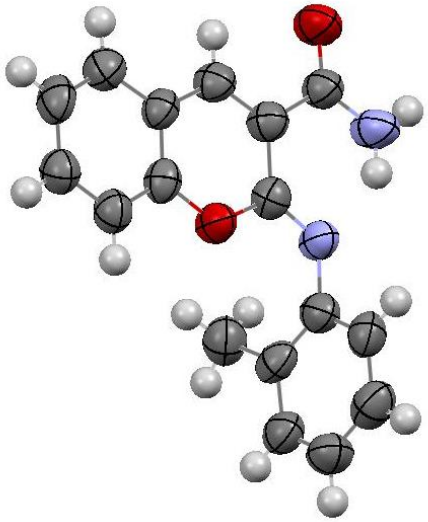

Fig. S4. Molecular structure of **1me**.

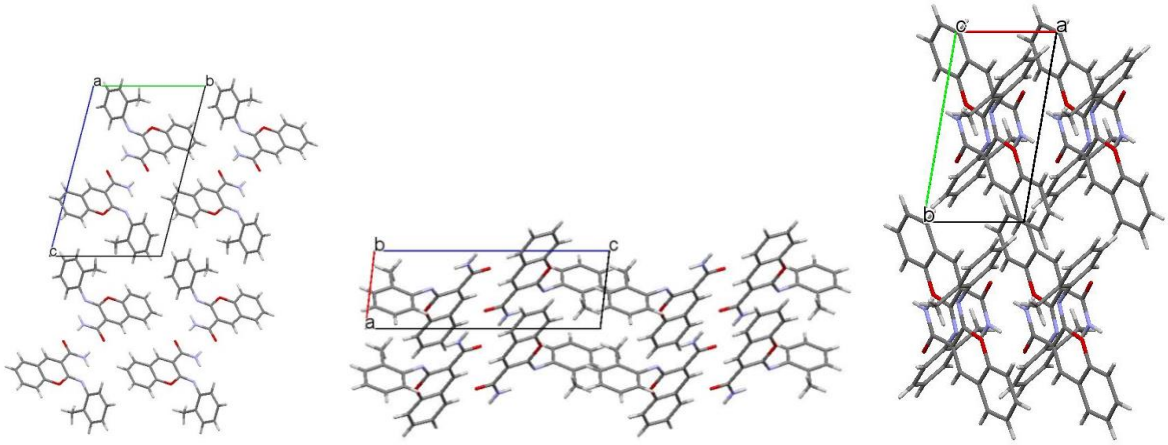

Fig. S5. Molecules packing in structure **1me**.

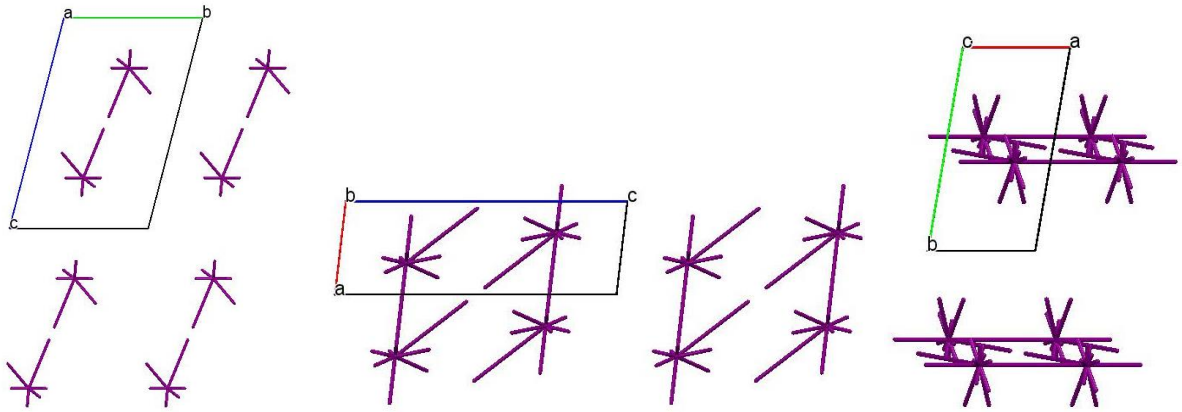

Fig. S6. Packing of energy-vector diagrams in structure **1me**.

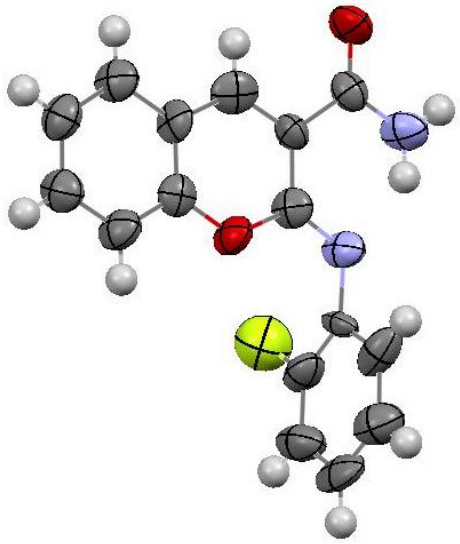

Fig. S7. Molecular structure of **1f_1**.

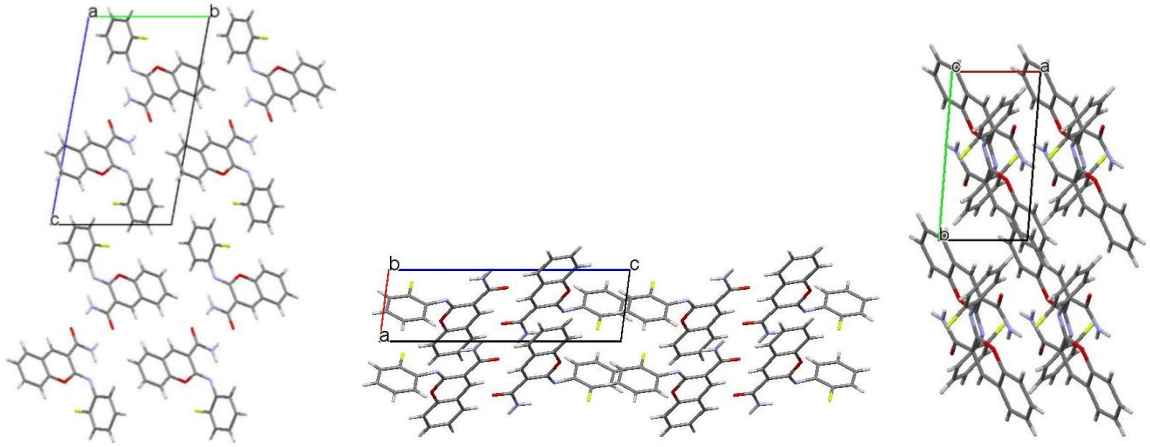

Fig. S8. Molecules packing in structure **1f_1**.

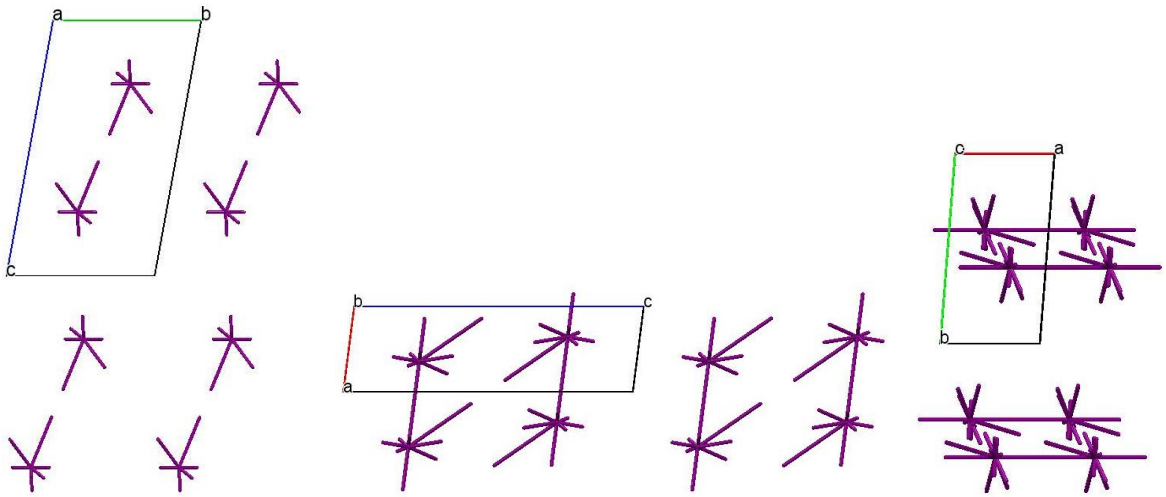

Fig. S9. Packing of energy-vector diagrams in structure **1f_1**

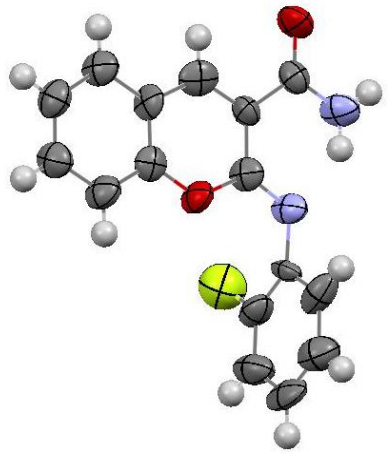

Fig. S10. Molecular structure of **1f_2**.

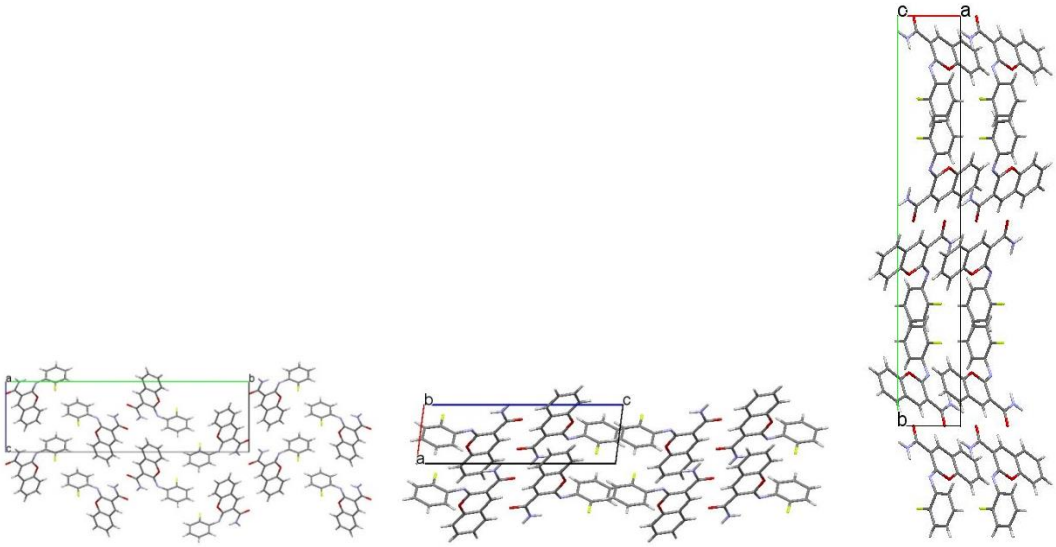

Fig. S11. Molecules packing in structure **1f_2**.

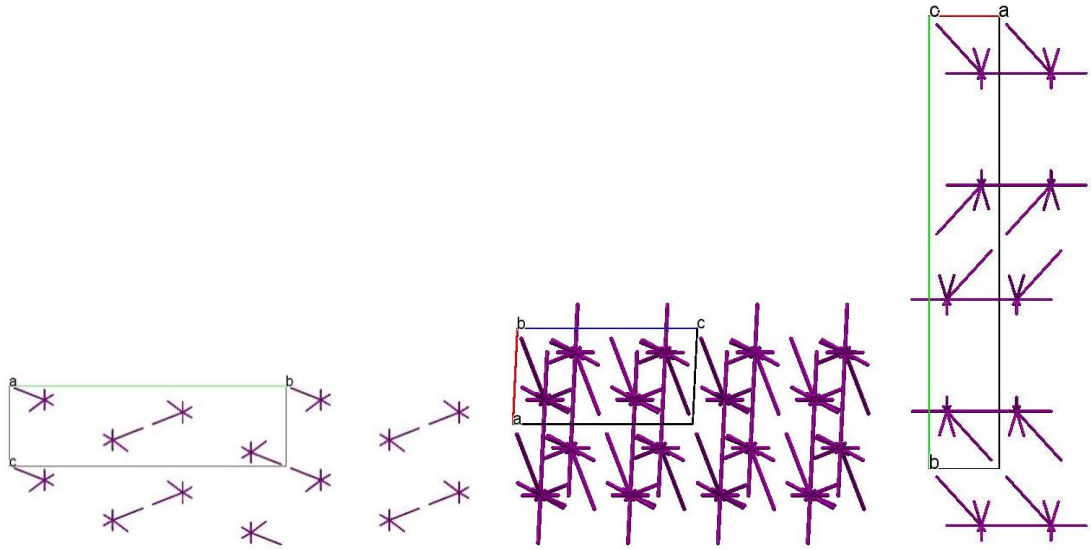

Fig. S12. Packing of energy-vector diagrams in structure **1f_2**.

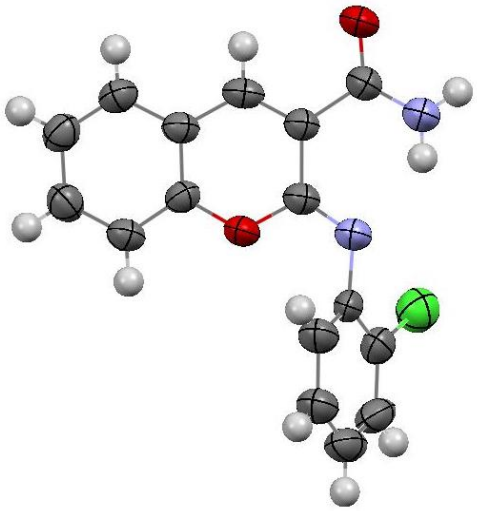

Fig. S13. Molecular structure of **1cl**.

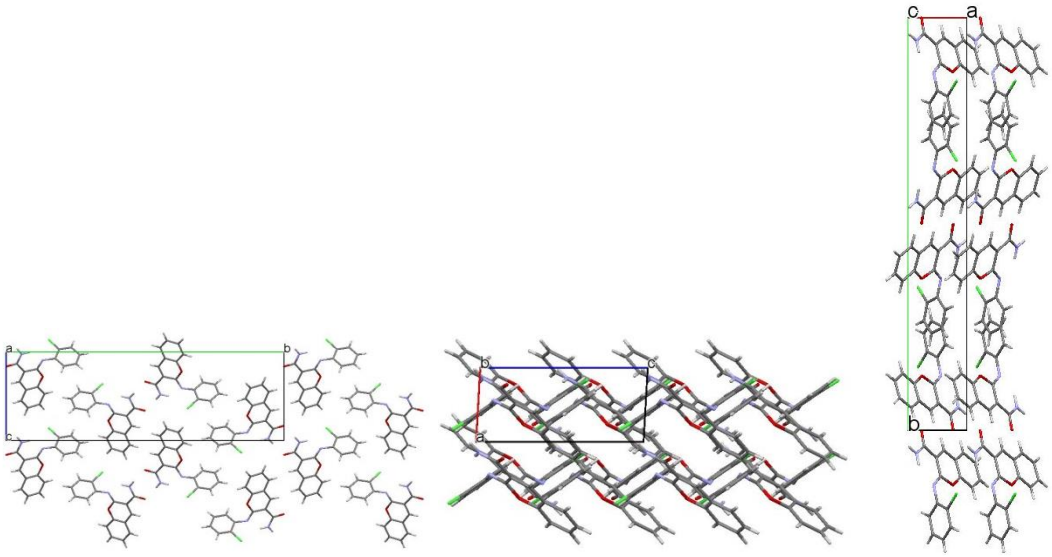

Fig. S14. Molecules packing in structure **1cl**.

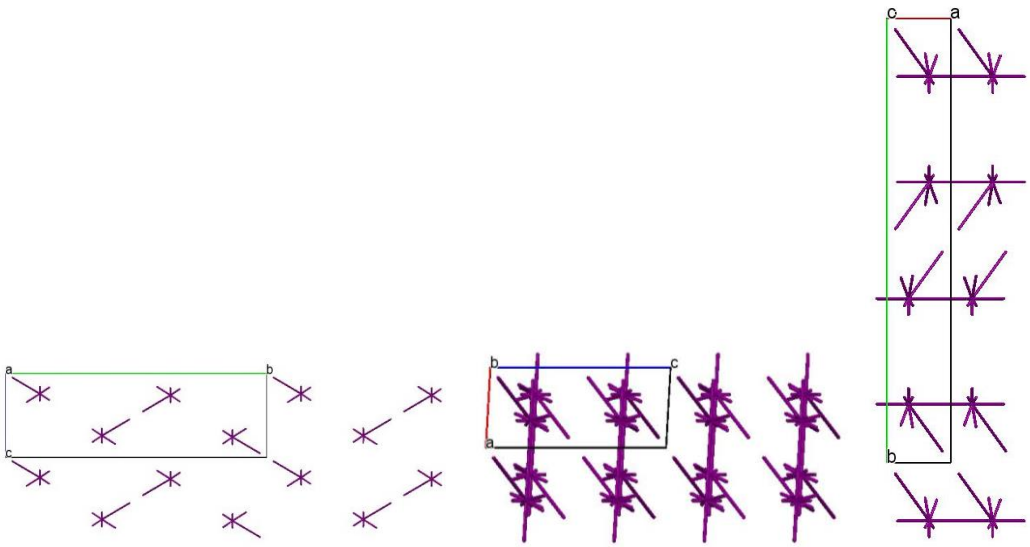

Fig. S15. Packing of energy-vector diagrams in structure **1cl**.

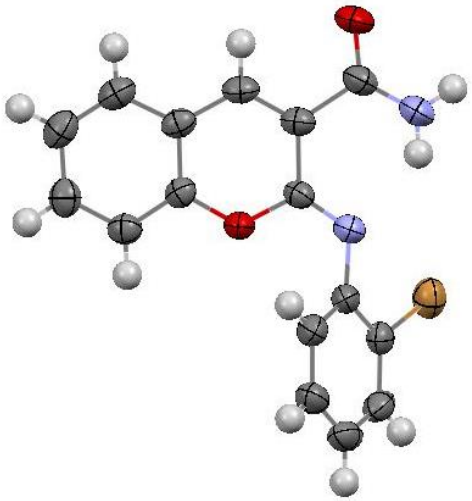

Fig. S16. Molecular structure of **1br**_**l**.

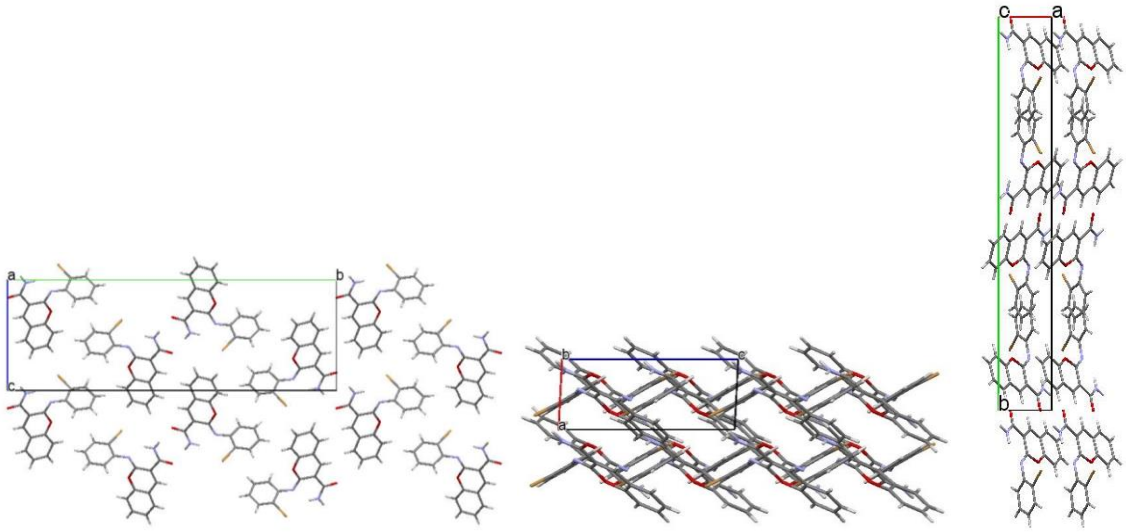

Fig. S17. Molecules packing in structure **1br**_**l**.

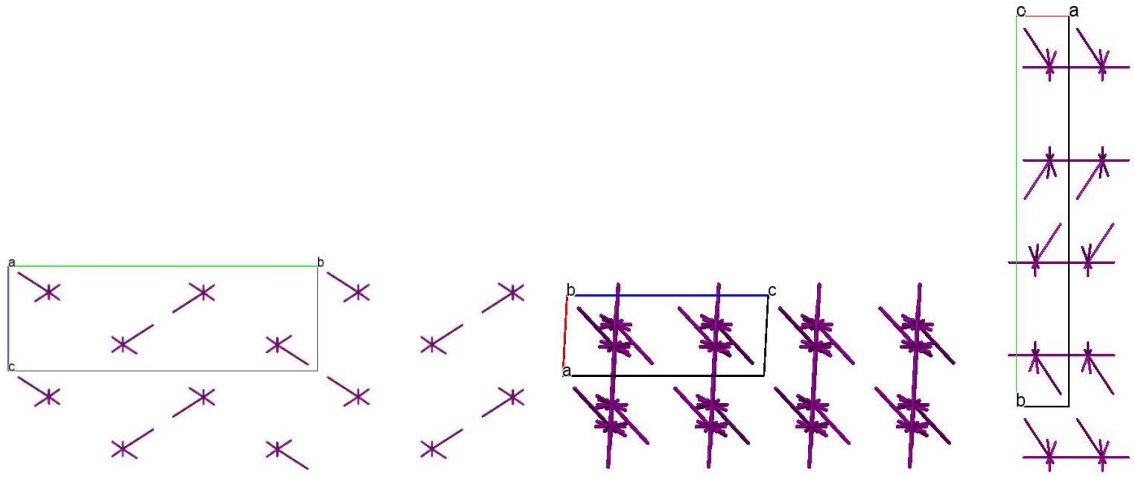

Fig. S18. Packing of energy-vector diagrams in structure **1br**_**1**.

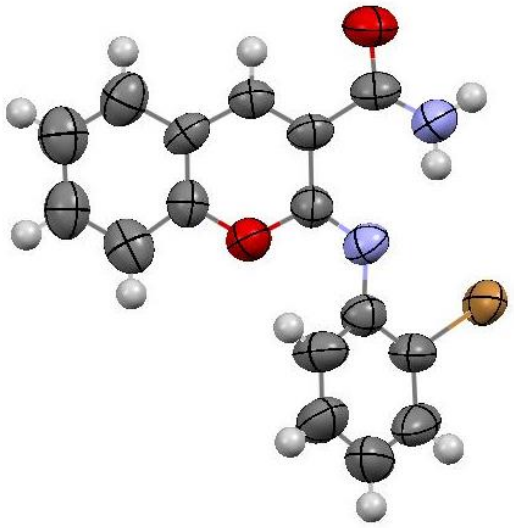

Fig. S19. Molecular structure of **1br_II**.

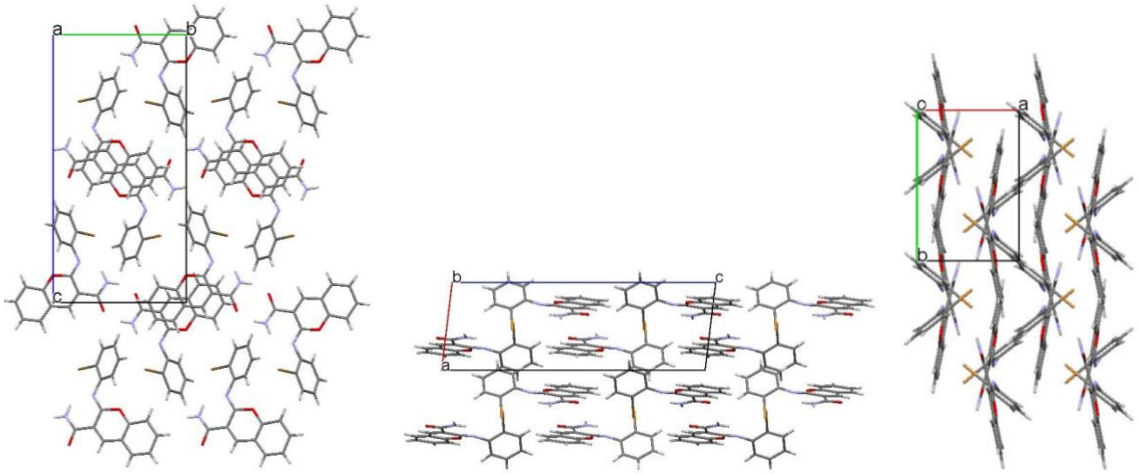

Fig. S20. Molecules packing in structure **1br_II**.

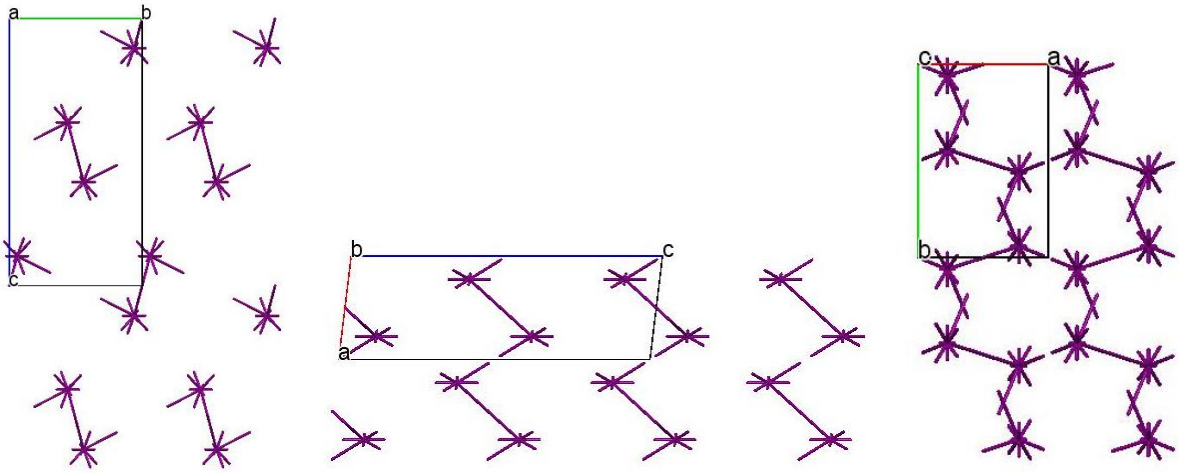

Fig. S21. Packing of energy-vector diagrams in structure **1br_2**.

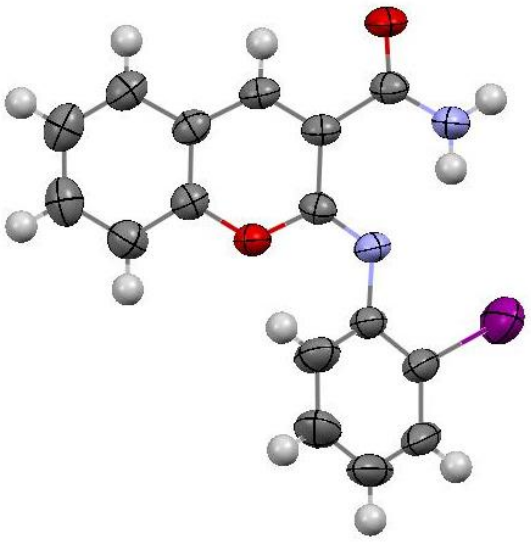

Fig. S22. Molecular structure of **1i**.

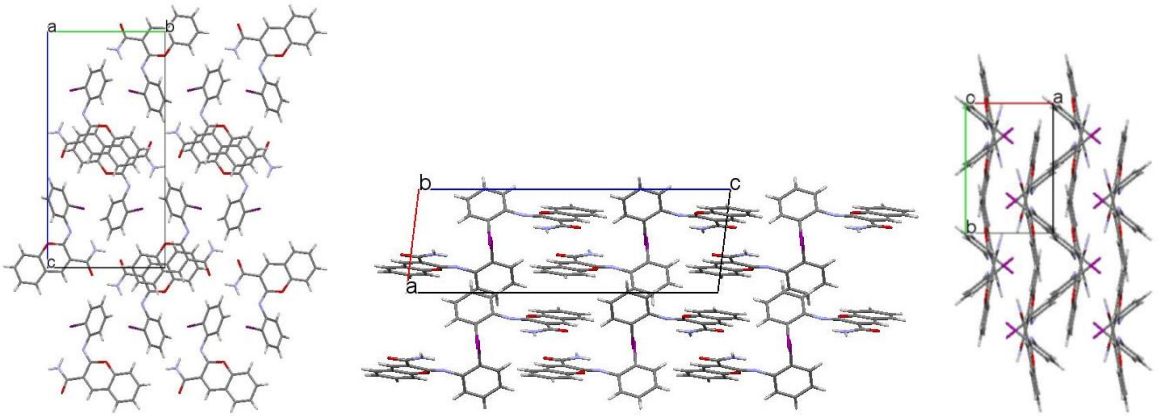

Fig. S23. Molecules packing in structure **1i**.

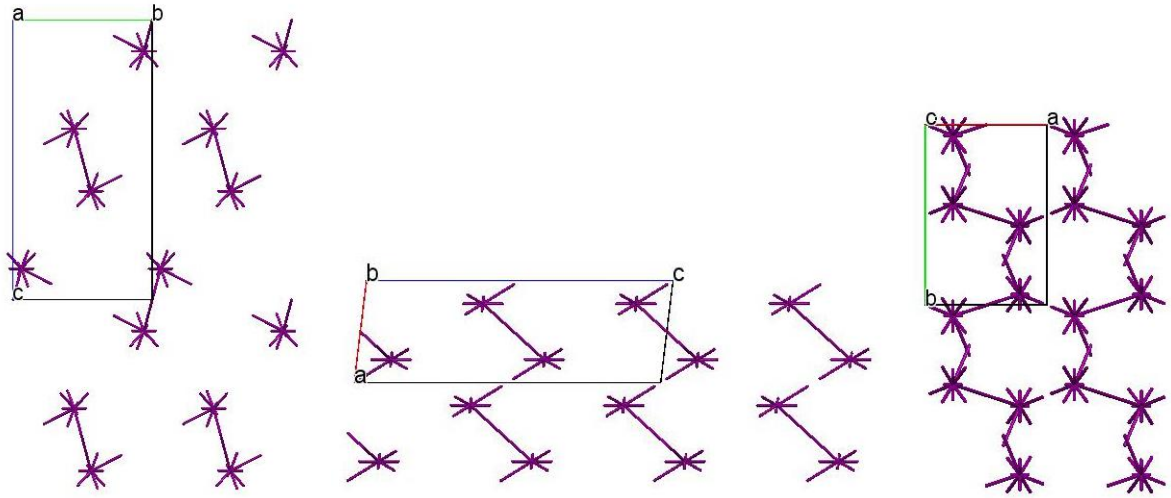

Fig. S24. Packing of energy-vector diagrams in structure **1i**.

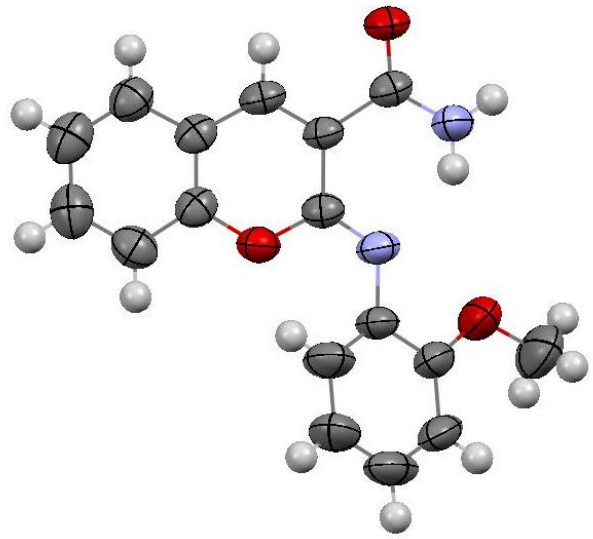

Fig. S25. Molecular structure of **1ome**.

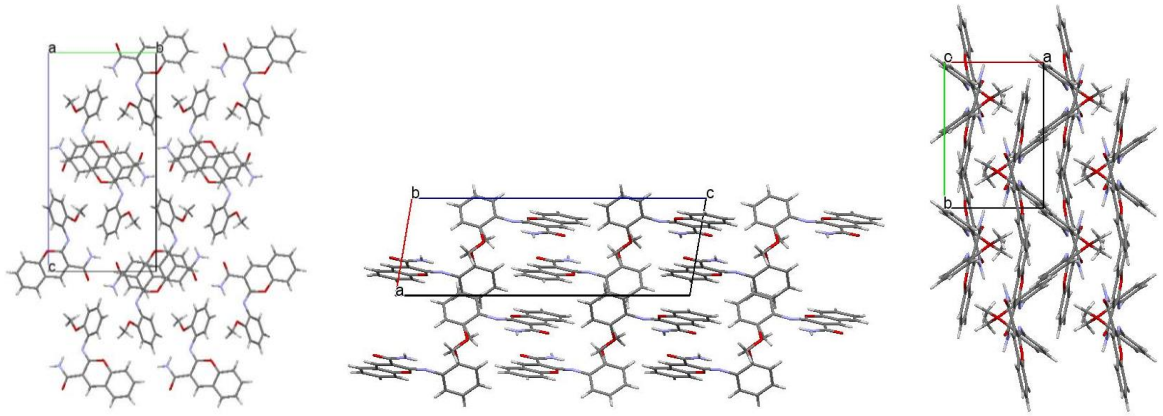

Fig. S26. Molecules packing in structure **1ome**.

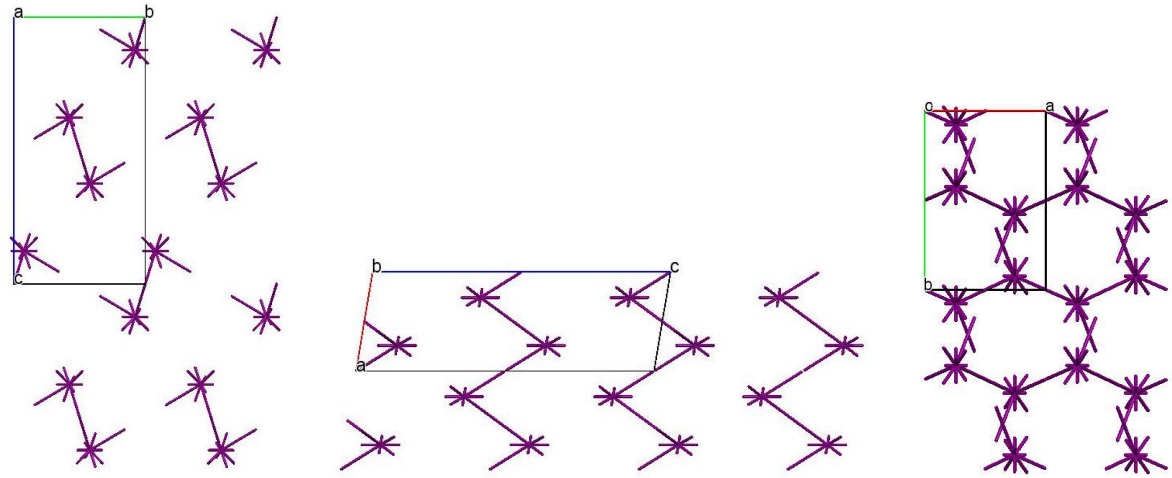

Fig. S27. Packing of energy-vector diagrams in structure **1ome**.

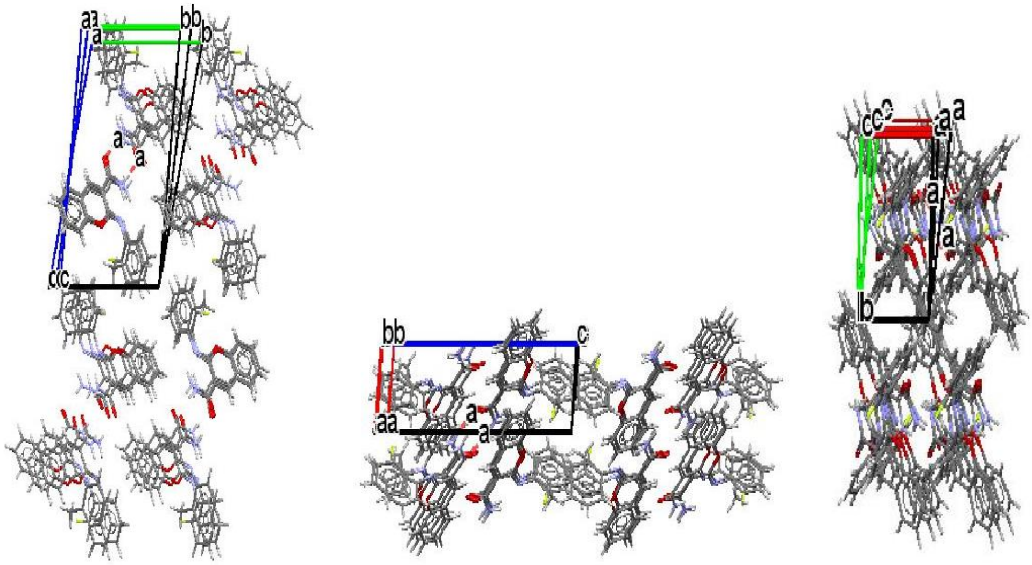

Fig. S28. Supramolecular cluster overlay of **1h**, **1me** and **1f_1**.

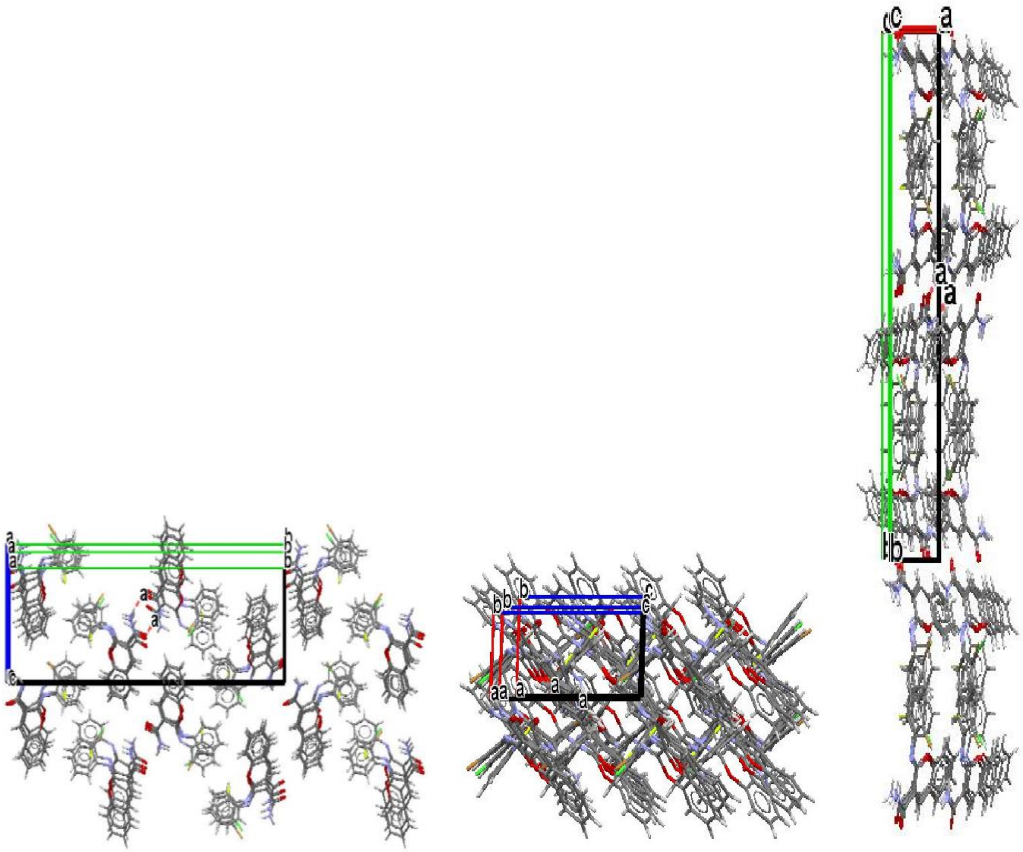

Fig. S29. Supramolecular cluster overlay of **1f_2**, **1cl** and **1br_1**.

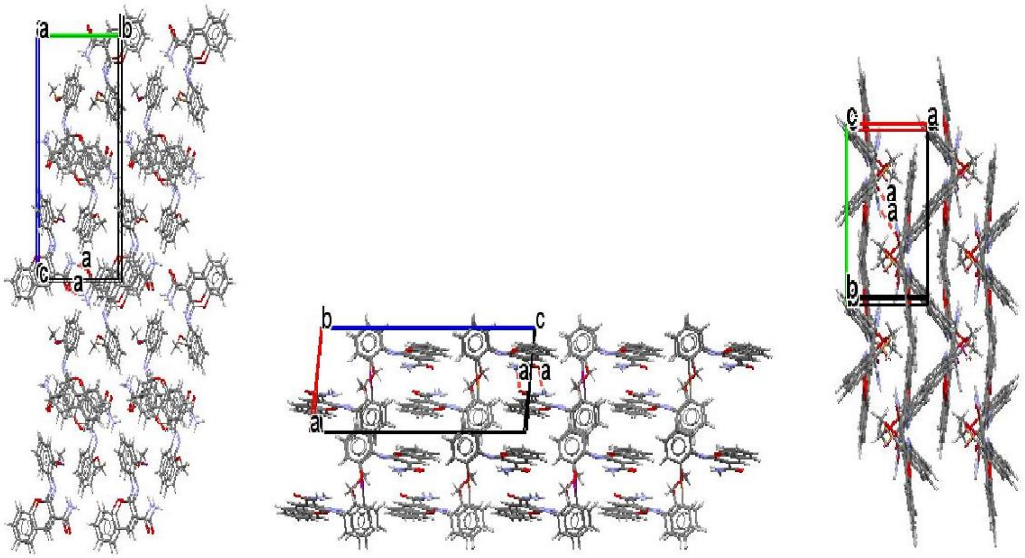

Fig. S30. Supramolecular cluster overlay of **1br_2**, **1i** and **1ome**.

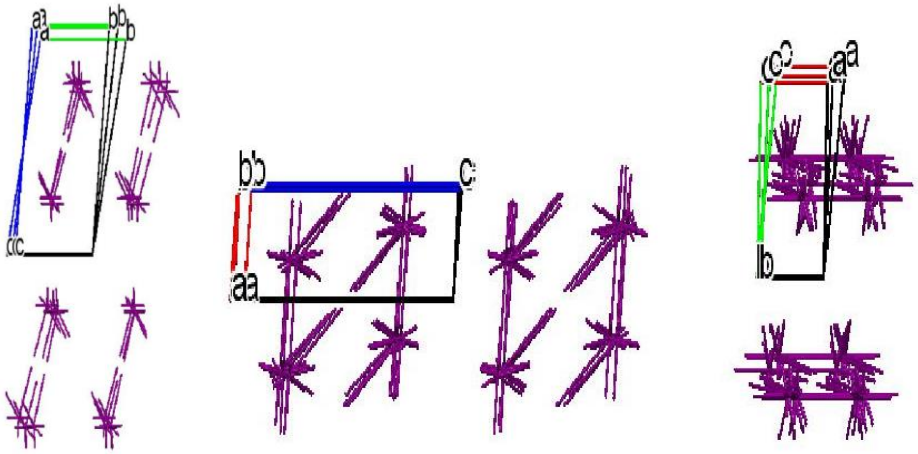

Fig. S31. Energy-vector diagrams overlay of **1h**, **1me** and **1f_1**.

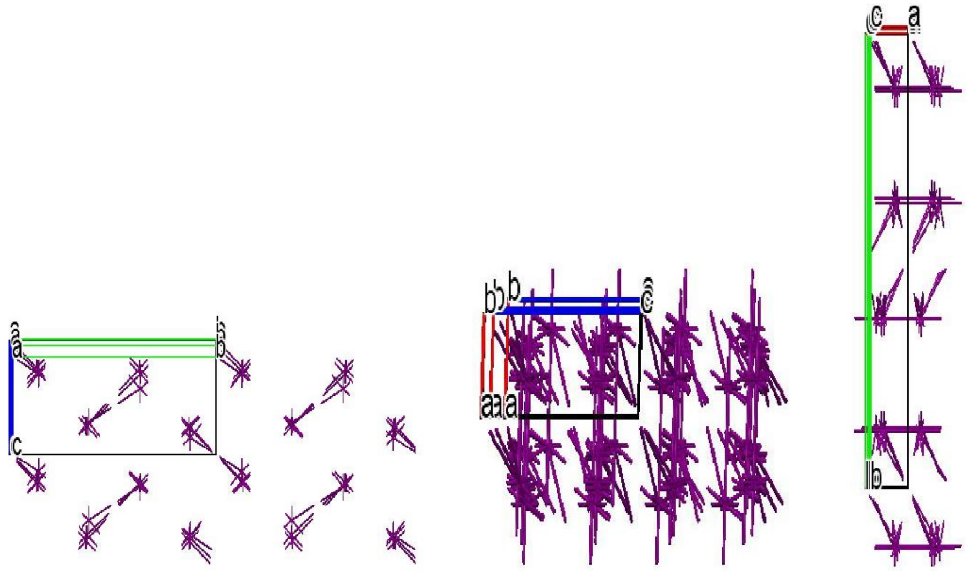

Fig. S32. Energy-vector diagrams overlay of **1f_2**, **1cl** and **1br_1**.

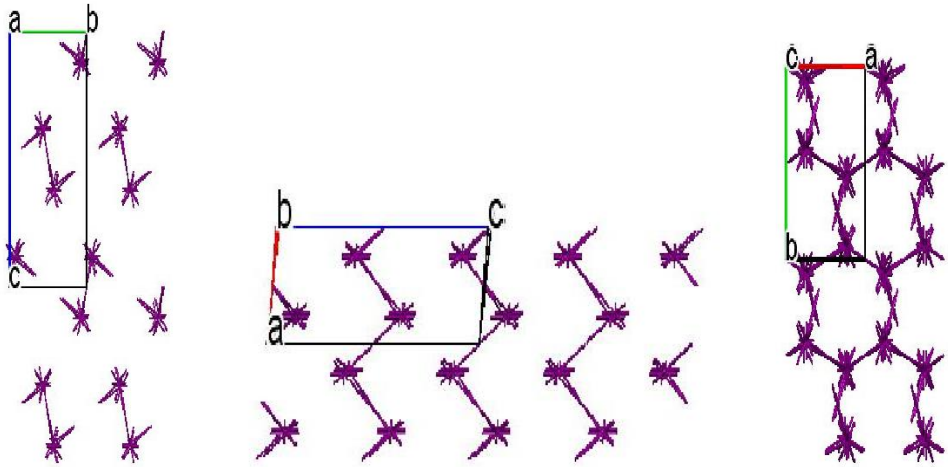

Fig. S33. Energy-vector diagrams overlay of **1br_2**, **1i** and **1ome**.

Table S1. Calculated pairwise interaction energies in structure **1h**.

Dimer	Symmetry operation	E_{int}, kJ/mol	Contribution to the total interaction energy, %	Interaction type
1h_d1	1+x,y,z	-59.50	17.1	Stacking 3.44
1h_d2	-1+x,y,z	-59.50	17.1	Stacking 3.44
1h_d3	2-x,1-y,1-z	-51.92	14.9	N-H…O
1h_d4	1-x,-y,1-z	-26.48	7.6	Non-specific
1h_d5	1-x,1-y,2-z	-23.47	6.7	Non-specific
1h_d6	-x,-y,1-z	-22.80	6.5	Non-specific
1h_d7	1-x,1-y,1-z	-17.99	5.2	Non-specific
1h_d8	1+x,1+y,z	-15.77	4.5	C-H…π
1h_d9	-1+x,-1+y,z	-15.77	4.5	C-H…π
1h_d10	x,1 +y,z	-12.47	3.6	C-H…π
1h_d11	x,-1+y,z	-12.47	3.6	C-H…π
1h_d12	-x,1-y,2-z	-10.63	3.1	Non-specific
1h_d13	1-x,2-y,2-z	-10.33	3.0	Non-specific
1h_d14	2-x,1-y,2-z	-6.19	1.8	Non-specific
1h_d15	-x,2-y,2-z	-3.14	0.9	Non-specific
		-348.44		

Table S2. Calculated pairwise interaction energies in structure **1me**.

Dimer	Symmetry operation	E_{int}, kJ/mol	Contribution to the total interaction energy, %	Interaction type
1me_d1	1+x,y,z	-60.12	16.8	Stacking 3.57
1me_d2	-1+x,y,z	-60.12	16.8	Stacking 3.50
1me_d3	2-x,1-y,1-z	-53.18	14.9	N-H…O
1me_d4	-x,-y,1-z	-27.24	7.6	Non-specific
1me_d5	1-x,-y,1-z	-26.94	7.5	C-H…O
1me_d6	1-x,1-y,2-z	-20.96	5.9	Non-specific
1me_d7	1-x,1-y,1-z	-19.00	5.3	Stacking carbamide 3.67
1me_d8	-x,1-y,2-z	-16.99	4.8	Non-specific
1me_d9	1+x,1+y,z	-15.10	4.2	C-H…π
1me_d10	-1+x,-1+y,z	-15.10	4.2	C-H…π
1me_d11	x,1+y,z	-10.79	3.0	C-H…π
1me_d12	x,-1+y,z	-10.79	3.0	C-H…π
1me_d13	1-x,2-y,2-z	-10.29	2.9	Non-specific
1me_d14	2-x,1-y,2-z	-5.31	1.5	Non-specific
1me_d15	-x,2-y,2-z	-5.02	1.4	Non-specific
		-357.06		

Table S3. Calculated pairwise interaction energies in structure **1f_1**.

Dimer	Symmetry operation	E_{int}, kJ/mol	Contribution to the total interaction energy, %	Interaction type
1f1_d1	1+x,y,z	-60.54	18.1	Stacking 3.44
1f1_d2	-1+x,y,z	-60.54	18.1	Stacking 3.44
1f1_d3	2-x,1-y,1-z	-47.45	14.2	N-H…O
1f1_d4	1-x,-y,1-z	-26.82	8.0	C-H…O
1f1_d5	-x,-y,1-z	-24.31	7.3	Non-specific
1f1_d6	1-x,1-y,2-z	-21.80	6.5	Non-specific
1f1_d7	1+x,1+y,z	-15.02	4.5	C-H..π
1f1_d8	-1+x,-1+y,z	-15.02	4.5	C-H…π
1f1_d9	1-x,1-y,1-z	-13.43	4.0	Stacking carbonyl 3.65
1f1_d10	x,1+y,z	-11.55	3.5	C-H…π
1f1_d11	x,-1+y,z	-11.55	3.5	C-H…π
1f1_d12	1-x,2-y,2-z	-10.08	3.0	Non-specific
1f1_d13	-x,1-y,2-z	-8.62	2.6	Non-specific
1f1_d14	2-x,1-y,2-z	-8.12	2.4	C-H…F
		-334.89		

Table S4. Calculated pairwise interaction energies in structure **1f_2**.

Dimer	Symmetry operation	E_{int}, kJ/mol	Contribution to the total interaction energy, %	Interaction type
1f2_d1	1+x,y,z	-59.50	17.4	Stacking 3.42
1f2_d2	-1+x,y,z	-59.50	17.4	Stacking 3.42
1f2_d3	-x,1-y,1-z	-50.92	14.9	N-H…O
1f2_d4	1-x,1-y,2-z	-25.36	7.4	C-H…O
1f2_d5	2-x,1-y,2-z	-24.85	7.3	Non-specific
1f2_d6	x,1/2-y,1/2+z	-15.61	4.6	Non-specific
1f2_d7	x,1/2-y,-1/2+z	-15.61	4.6	Non-specific
1f2_d8	1+x,y,1+z	-15.31	4.5	C-H…π
1f2_d9	-1+x,y,-1+z	-15.31	4.5	C-H…π
1f2_d10	1-x,1-y,1-z	-15.23	4.5	Stacking carbonyl 3.60
1f2_d11	x,y,1+z	-11.67	3.4	C-H…π
1f2_d12	x,y,-1+z	-11.67	3.4	C-H…π
1f2_d13	1+x,1/2-y,-1/2+z	-5.52	1.6	Non-specific
1f2_d14	-1+x,1/2-y,1/2+z	-5.52	1.6	Non-specific
1f2_d15	1+x,1/2-y,1/2+z	-5.23	1.5	Non-specific
1f2_d16	-1+x,1/2-y,-1/2+z	-5.23	1.5	Non-specific
		-342.04		

Table S5. Calculated pairwise interaction energies in structure **1cl**.

Dimer	Symmetry operation	E_{int}, kJ/mol	Contribution to the total interaction energy, %	Interaction type
1cl_d1	1+x,y,z	-66.86	18.8	Stacking 3.45
1cl_d2	-1+x,y,z	-66.86	18.8	Stacking 3.45
1cl_d3	2-x,1-y,1-z	-53.89	15.2	N-H…O
1cl_d4	1-x,1-y,-z	-26.07	7.3	Non-specific
1cl_d5	-x,1-y,-z	-24.02	6.8	Non-specific
1cl_d6	x,3/2-y,1/2+z	-20.17	5.7	Non-specific
1cl_d7	x,3/2-y,-1/2+z	-20.17	5.7	Non-specific
1cl_d8	1+x,y,1+z	-11.42	3.2	C-H…Cl 2.76
1cl_d9	-1+x,y,-1+z	-11.42	3.2	C-H…Cl
1cl_d10	1+x,3/2-y,1/2+z	-8.79	2.5	Non-specific
1cl_d11	-1+x,3/2-y,-1/2+z	-8.79	2.5	Non-specific
1cl_d12	x,y,1+z	-8.66	2.4	Cl…π 3.41
1cl_d13	x,y,-1+z	-8.66	2.4	Cl…π 3.41
1cl_d14	1+x,3/2-y,-1/2+z	-6.74	1.9	Non-specific
1cl_d15	-1+x,3/2-y,1/2+z	-6.74	1.9	Non-specific
1cl_d16	1-x,1-y,1-z	-6.23	1.8	Non-specific
		-355.56		

Table S6. Calculated pairwise interaction energies in structure **1br_I**.

Dimer	Symmetry operation	E_{int}, kJ/mol	Contribution to the total interaction energy, %	Interaction type
1br1_d1	1+x,y,z	-72.59	19.8	Stacking 3.48
1br1_d2	-1+x,y,z	-72.59	19.8	Stacking 3.48
1br1_d3	2-x,1-y,1-z	-55.02	15.0	N-H…O
1br1_d4	1-x,1-y,-z	-24.94	6.8	Non-specific
1br1_d5	-x,1-y,-z	-22.05	6.0	Non-specific
1br1_d6	x,3/2-y,1/2+z	-20.50	5.6	C-H…π
1br1_d7	x,3/2-y,-1/2+z	-20.50	5.6	C-H…π
1br1_d8	x,y,1+z	-9.83	2.7	Br…π 3.47
1br1_d9	x,y,-1+z	-9.83	2.7	Br…π 3.47
1br1_d10	1+x,y,1+z	-9.50	2.6	C-H…Br
1br1_d11	-1+x,y,-1+z	-9.50	2.6	C-H…Br
1br1_d12	1+x,3/2-y,1/2+z	-8.49	2.3	Non-specific
1br1_d13	-1+x,3/2-y,-1/2+z	-8.49	2.3	Non-specific
1br1_d14	1+x,3/2-y,-1/2+z	-7.53	2.1	Non-specific
1br1_d15	-1+x,3/2-y,1/2+z	-7.53	2.1	Non-specific
1br1_d16	1-x,1-y,1-z	-7.32	2.0	Non-specific
		-366.14		

Table S7. Calculated pairwise interaction energies in structure **1br_II**.

Dimer	Symmetry operation	E_{int}, kJ/mol	Contribution to the total interaction energy, %	Interaction type
1br2_d1	1-x,1-y,1-z	-71.00	20.1	Stacking 3.37
1br2_d2	-x,1-y,1-z	-59.79	17.0	Stacking 3.48
1br2_d3	1-x,-y,1-z	-40.04	11.3	N-H…O
1br2_d4	-x,1/2+y,1/2-z	-27.61	7.8	C-H…π
1br2_d5	-x,-1/2+y,1/2-z	-27.61	7.8	C-H…π
1br2_d6	1-x,1/2+y,1/2-z	-19.83	5.6	Br…π
1br2_d7	1-x,-1/2+y,1/2-z	-19.83	5.6	Br…π
1br2_d8	x,1/2-y,1/2+z	-18.58	5.3	C-H…O
1br2_d9	x,1/2-y,-1/2+z	-18.58	5.3	C-H…O
1br2_d10	x,1+y,z	-11.97	3.4	Non-specific
1br2_d11	x,-1+y,z	-11.97	3.4	Non-specific
1br2_d12	1+x,y,z	-7.61	2.2	Non-specific
1br2_d13	-1+x,y,z	-7.61	2.2	Non-specific
1br2_d14	x,3/2-y,1/2+z	-5.36	1.5	Non-specific
1br2_d15	x,3/2-y,-1/2+z	-5.36	1.5	Non-specific
		-352.79		

Table S8. Calculated pairwise interaction energies in structure **1i**.

Dimer	Symmetry operation	E_{int}, kJ/mol	Contribution to the total interaction energy, %	Interaction type
1i_d1	1-x,1-y,1-z	-72.34	19.6	Stacking 3.40 h-t
1i_d2	-x,1-y,1-z	-60.46	16.4	Stacking 3.46 h-t
1i_d3	1-x,-y,1-z	-35.73	9.7	N-H…O
1i_d4	-x,1/2+y,1/2-z	-27.74	7.5	C-H…I, C-H…N
1i_d5	-x,-1/2+y,1/2-z	-27.74	7.5	C-H…I, C-H…N
1i_d6	1-x,1/2+y,1/2-z	-26.82	7.2	I…π
1i_d7	1-x,-1/2+y,1/2-z	-26.82	7.2	I…π
1i_d8	x,1/2-y,1/2+z	-18.24	4.9	C-H…O
1i_d9	x,1/2-y,-1/2+z	-18.24	4.9	C-H…O
1i_d10	x,1+y,z	-12.01	3.3	Non-specific
1i_d11	x,-1+y,z	-12.01	3.3	Non-specific
1i_d12	1+x,y,z	-9.92	2.7	Non-specific
1i_d13	-1+x,y,z	-9.92	2.7	Non-specific
1i_d14	x,3/2-y,1/2+z	-5.69	1.5	Non-specific
1i_d15	x,3/2-y,-1/2+z	-5.69	1.5	Non-specific
1i_d16	-x,2-y,1-z	-0.29	0.1	Non-specific
		-369.70		

Table S9. Calculated pairwise interaction energies in structure **1ome.**

Dimer	Symmetry operation	E_{int}, kJ/mol	Contribution to the total interaction energy, %	Interaction type
1ome_d1	1-x,2-y,2-z	-64.18	18.3	Stacking 3.44
1ome_d2	2-x,2-y,2-z	-61.71	17.6	Stacking 3.48
1ome_d3	1-x,1-y,2-z	-40.12	11.4	N-H…O
1ome_d4	2-x,1/2+y,5/2-z	-25.02	7.1	C-H…π
1ome_d5	2-x,-1/2+y,5/2-z	-25.02	7.1	C-H…π
1ome_d6	1-x,1/2+y,5/2-z	-20.63	5.9	C-H…π
1ome_d7	1-x,-1/2+y,5/2-z	-20.63	5.9	C-H…π
1ome_d8	x,3/2-y,1/2+z	-15.94	4.5	C-H…O
1ome_d9	x,3/2-y,-1/2+z	-15.94	4.5	C-H…O
1ome_d10	x,1+y,z	-11.88	3.4	Non-specific
1ome_d11	x,-1+y,z	-11.88	3.4	Non-specific
1ome_d12	1+x,y,z	-10.88	3.1	Non-specific
1ome_d13	-1+x,y,z	-10.88	3.1	Non-specific
1ome_d14	x,5/2-y,1/2+z	-7.11	2.0	Non-specific
1ome_d15	x,5/2-y,-1/2+z	-7.11	2.0	Non-specific
1ome_d16	2-x,3-y,2-z	-1.88	0.5	Non-specific
		-350.91		