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Supporting information for article:

Interactions in flavanone and chalcone derivatives: Hirshfeld surface analysis and energy framework and global reactivity descriptors

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Fig S22. The energy frameworks for FL6, CH6A/B Fl7 and CH7 with interactions to Br atoms

Table S1. Geometrical parameters (Å, °) for hydrogen bonds

	d(D-H)	d(H...A)	d(D...A)	<D-H...A	symmetry
FL4 NUYRII01					
O3-H9…O2	0.84	1.87	2.7045(18)	175	-1+x,3/2-y,-1/2+z
C1-H2…O3	0.99	2.62	3.275(18)	124	x,3/2-y,1/2+z
FL7 YIVREA					
C16-H10…O2	1.09(3)	1.87(3)	2.84(2)	146(2)	intra
C5-H3…Br1	1.11(3)	2.99(3)	4.094(3)	170(2)	2-x,1/2+y,1-z
C8-H6…O2	1.06(2)	2.64(2)	3.545(2)	143(2)	-1+x,y,z
CH1 REPXIW					
O1-H1…O2	0.99(3)	1.62(3)	2.520(2)	150(2)	intra
CH3 URESOA					
O1-H16…O2	0.95(2)	1.65(2)	2.511(2)	149(2)	intra
C11-H6…O3	0.93	2.60	3.432(2)	149	x, 3/2-y, ½+z
C9-H5…O3	0.93	2.64	3.488(2)	149	x, 3/2-y, ½+z
C12-H7…O2	0.93	2.66	3.494(2)	150	x, ½-y, -½+z
CH5 QEXLAH					
O1-H1…O2	0.84(2)	1.76(2)	2.535(2)	152(2)	intra
C1-H2…O1	0.93	2.63	3.248(2)	125	x,-1+y,z
C14-H10…Cl1	0.93	2.93	3.700(2)	142	-x,-y,1-z
C11-H8…O2	0.93	2.66	3.409(2)	138	1-x,2-y,1-z
CH6A IKOFAR					
O1-Hl1…O2	0.87(7)	1.84(14)	2.513(11)	133(12)	intra
C1-H2…O1	0.93	2.61	3.418(11)	146	-1+x,y,z
C14-H9…O2	0.93	2.66	3.301(11)	127	-1+x,1+y,z
CH6B IKOFAR01					
O2-Hl1…O1	0.82	1.81	2.533(5)	147	intra
C3-H3…O2	0.93	2.67	3.320(5)	128	x,-1+y,z
CH7 YIVPUO					
O1-H15…O2	0.89(4)	2.08(5)	2.573(15)	114(3)	intra
O3-H30…O4	1.11(5)	1.52(5)	2.549(15)	151(3)	intra
C2-H1…O2	1.02(5)	2.60(4)	3.520(18)	150(4)	1-x,-1/2+y,-1/2-z
C5-H3…O4	1.11(5)	2.42(4)	3.323(19)	138(3)	1/2+x,3/2-y,1-z
C20-H17…Br2	1.24(4)	2.79(4)	3.847(16)	142(3)	1/2-x,2-y,1/2+z
C31 –H23…O2	1.11(4)	2.55(4)	3.652(17)	172(4)	-1/2+x,3/2-y,-z
C33-H26…O3	1.01(4)	2.55(4)	3.245(19)	126(3)	1/2-x,1-y,-1/2+z

Table S2. Geometrical parameters for C-H…π interactions for flavanones and chalcones

	d(C-H)	d(H...Cg)	d(C...Cg)	<C-H…Cg	symmetry
FL1					
C11-H11B…Cg2	0.98	2.69	3.605(2)	156	1-x, -y, 1-z
C14-H14…Cg1	0.95	2.83	3.658(2)	146	1+x, y, z
C16-H16…Cg2	0.95	2.69	3.544(2)	150	2-x, -½+y, ½-z
FL2					
C18-H18A…Cg2	0.98	2.89	3.786(3)	153	3/2-x, ½+y, z
C2B-H2B…Cg1	1.00	2.92	3.778(3)	145	½-x, -½+y, z
FL3					
C2A-H2A…Cg1	1.00	2.89	3.874(4)	168	2-x, 1-y, 1-z
C18-H18A…Cg5	0.98	2.99	3.863(3)	149	x, y, z
C53A-H53A…Cg4	0.99	2.97	3.731(2)	135	½-x, -½+y, ½-z
C53A-H53B…Cg1	0.99	2.84	3.683(2)	143	3/2-x,- ½+y, ½-z
C61-H61C…Cg5	0.98	2.94	3.769(2)	143	½-x, ½+y, ½-z
C52-H52B…Cg1	1.00	2.92	3.754(2)	142	3/2 -x,- ½+y, ½-z
C53B-H53C…Cg4	0.99	2.69	3.259(2)	117	½-x, -½+y, ½-z
FL4 NUYRII01					
C4-H6…Cg3	0.95	2.88	3.669(3)	142	2-x, 1-y, 1-z
C6-H8…Cg3	0.95	2.79	3.597(2)	143	x, y, z
FL5_FL5					
C7-H7…Cg2	0.95	2.80	3.610(2)	144	-1+x, 3/2-y, ½+z
C9-H9…Cg2	0.95	2.92	3.639(2)	134	1-x, 1-y, 1-z
C13-H13…Cg1	0.95	2.92	3.675(2)	137	1+x, y, z
FL6 BRFLAY					
C7-H4…Cg2	0.96	2.87	3.709(2)	147	-1+x,y,z
C12-H9…Cg3	0.85	2.98	3.738(2)	149	1+x,-3/2-y,-1/2+z
C14-H11…Cg3	1.08	2.91	3.724(2)	132	1-x,-1-y,-1-z
FL8_FL3					
C64-H64…Cg1	0.95	2.96	3.838(5)	155	½-x, - ½+y, ½-z
CH2					
C7-O2…Cg1		3.8677(14)	3.6750(18)	71.82(9)	x, -1+y, z
CH3 URESOA					
C16-H12…Cg1	0.96	2.81	3.580(2)	138	-x, -y, -z
C17-H15…Cg2	0.96	2.89	3.770(2)	152	1+x, 2-y, -z
CH7 YIVPUO					
C16-H11…Cg4	1.07(4)	2.89	3.933(17)	163	1/2+x,3/2-y,1-z

for FL1, FL2, FL3, Fl5, FL8: Cg1 – a center of gravity for ring C5/C6/C7/C8/C9/C10; Cg2 - a center of gravity for ring C12/C13/C14/C15/C16/C17; Cg4 – a center of gravity for ring C55/C56/C57/C58/C59/C60; Cg5 – a center of gravity for ring C62/C63/C64/C65/C66/C67;

for FL4: Cg3 – a center of gravity for ring C9/C11/C12/C13/C14/C15;

for FL6: Cg2 – a center of gravity for ring C1/C11/C12/C13/C14/C15, Cg3 – a center of gravity for ring C2/C3/C4/C5/C6/C7;

for CH2: Cg1 – a center of gravity for ring C1/C2/C3/C4/C5/C6

for CH3: Cg1 – a center of gravity for ring C1/C2/C3/C4/C5/C6; Cg2 –– a center of gravity for ring C10/C11/C12/C13/C14/C15;

for CH7: Cg4 –– a center of gravity for ring C27/C28/C29/C30/C31/C32

Table S3. Geometrical parameters for π…π interactions for flavanones and chalcones.

Interaction	Cg(I)···Cg(J)	α	Cg(I)perp	Cg(J)perp	Slippage	Symmetry
FL1						
Cg1···Cg1	3.8602(9)	0.02(7)	3.4867(6)	3.4866(6)	1.657	1-x, 1-y, 1-z
FL7 YIVREA						
Cg2…Cg2	4.194(4)	0.0(4)	3.845(3)	3.845(3)	1.675	-1+x,y,z
Cg2…Cg2	4.194(4)	0.0(4)	3.845(3)	3.845(3)	1.675	1+x,y,z
FL8						
Cg1···Cg3	3.6746(18)	2.69(15)	3.4862(13)	3.5368(13)		
Cg3···Cg3	3.7772(18	0.00	3.5126(13)	3.5126(13)	1.389	1-x, 1-y, -z
CH1						
Cg2···Cg2	4.5241(10)	0.00(8)	3.3078(7)	3.3079(7)	3.086	1-x, 2-y, 1-z
CH2						
Cg1···Cg1	4.0469(11)	0.00(8)	3.4895(7)	3.4895(7)	2.050	x, -1+y, z
Cg1···Cg1	4.0469(11)	0.00(8)	3.4895(7)	3.4895(7)	2.050	x, 1+y, z
Cg2···Cg2	4.0469(11)	0.03(8)	3.5542(7)	3.5542(7)	1.935	x, -1+y, z
Cg2···Cg2	4.0469(11)	0.03(8)	3.5542(7)	3.5541(7)	1.935	x, 1+y, z
CH3 URESOA						
Cg2···Cg2	3.9070(10)	0.00(6)	3.5835(6)	3.5836(6)	1.557	1-x, 1-y, -z
CH4						
Cg1…Cg1	3.9413(12)	0.00(10)	3.4744(8)	-3.4744(8)	1.861	-1+x, y, z
Cg2…Cg2	3.9412(12)	0.03(10)	3.5180(8)	-3.5180(8)	1.777	-1+x, y, z
Cg3…Cg3	3.9412(12)	0.03(10)	3.4959(9)	-3.4959(9)	1.820	1+x, y, z
Cg4…Cg4	3.9415(12)	0.02(10)	3. 4276(9)	-3. 4276 (9)	1.946	1+x, y, z
CH5 QEXLAH						
Cg2···Cg2	3.8150(7)	0.02(6)	3.5591(5)	3.5592(5)	1.373	-x, 1-y, 1-z
CH6A IKOFAR						
Cg1…Cg1	4.003(7)	0.0(6)	3.517(5)	3.516(5)	1.912	x, -1+y, z
Cg1…Cg1	4.002(7)	0.0(6)	3.516(5)	3.517(5)	1.912	x, 1+y, z
Cg2…Cg2	4.002(7)	0.0(4)	3.625(4)	3.625(4)	1.697	x, -1+y, z
Cg2…Cg2	4.003(7)	0.0(4)	3.625(4)	3.625(4)	1.697	x, 1+y, z
CH6B IKOFAR01						
Cg1…Cg1	3.996(3)	0.0(2)	3.6975(17)	3.6977(17)	1.514	-x, 2-y,1-z
CH7 YIVPUO						
Cg1…Cg4	4.016(9)	7.0(8)	3.357(6)	3.597(6)	1.786	1-x,1/2+y,1/2-z
Cg3…Cg2	3.993(9)	16.1(8)	3.375(7)	3.777(6)	1.297	1-x,-1/2+y,1/2-z

Cg···*Cg* – distance between ring centroids; α - dihedral angle between planes I and J; *Cg*(I)$_{perp}$ a nd *Cg*(J)$_{perp}$ - (interplanar spacing) perpendicular distance of *Cg*(I) on ring J and *Cg*(J) on ring I, respectively; slippage - distance between *Cg*(I) and perpendicular projection of *Cg*(J) on ring I.

for FL1, FL8: Cg1 – a center of gravity for ring C1/C2/C3/C4/C5/C6; Cg2 – a center of gravity for ring C10/C11/C12/C13/C14/C15; Cg3 – a center of gravity for ring C55/C56/C57/C58/C59/C60; Cg4 – a center of gravity for ring C60/C61/C62/C63/C64/C65

for FL7 YIVREA: Cg2 – a center of gravity for ring C1/C2/C3/C4/C5/C6

for CH1, CH2, CH3, CH4, CH5, CH6A, CH6B Cg1 – a center of gravity for ring C1/C2/C3/C4/C5/C6; Cg2 – a center of gravity for ring C10/C11/C12/C13/C14/C15; Cg3 – a center of gravity for ring C51/C52/C53/C54/C55/C56; Cg4 - a center of gravity for ring C60/C61/C62/C63/C64/C65

for CH7 YIVPUO: Cg3 – a center of gravity for ring C18/C19/C20/C21/C22/C23; Cg4 – a center of gravity for ring C27/C28/C29/C30/C31/C32

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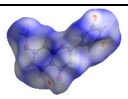
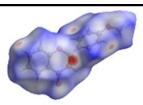
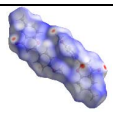
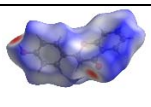
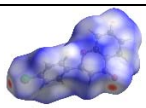
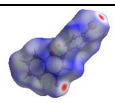
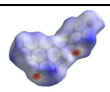
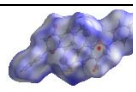
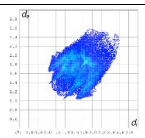
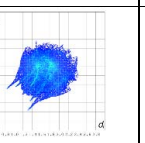
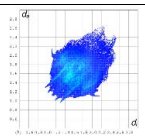
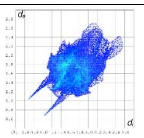
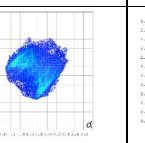
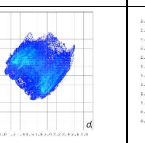
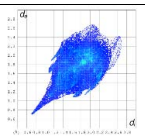
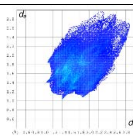
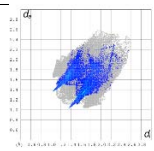
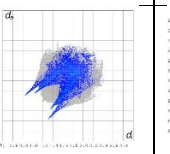
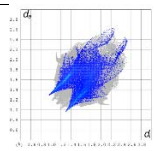
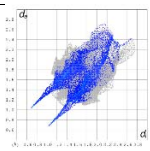
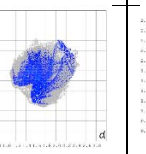
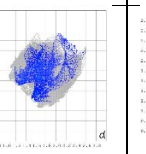
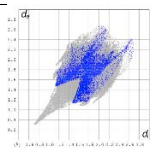
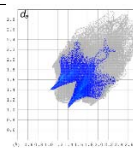
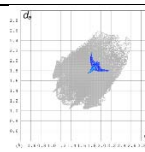
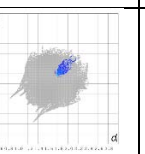
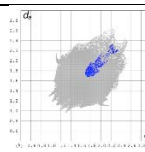
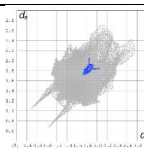
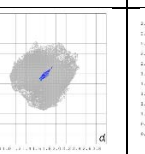
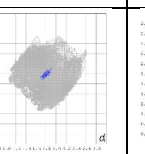
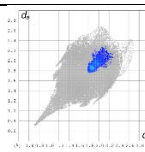
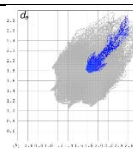
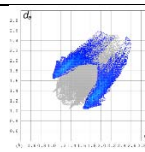
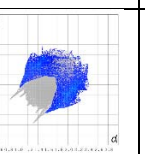
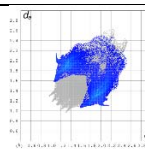
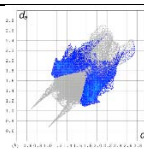
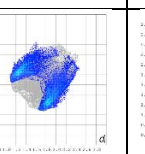
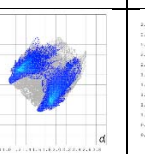
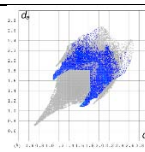
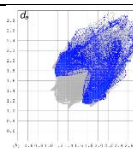
HS								
all								
O…H								
C…C								
C…H								
H…H								
	CH1	**CH2**	**CH3**	**CH4**	**CH5**	**CH6A**	**CH6B**	**CH7**
HS								
all								
O…H								
C…C								
C…H								

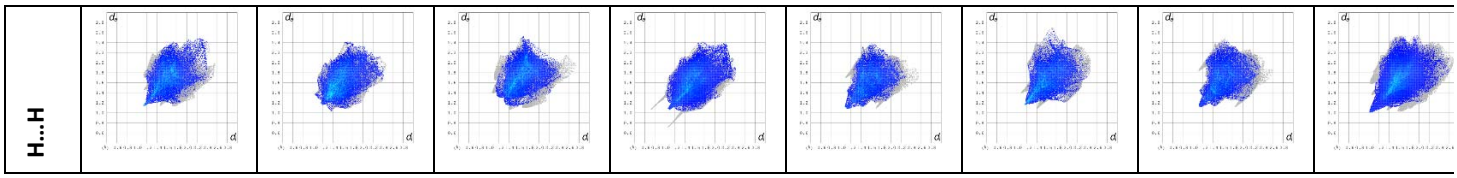


Figure S1. Hirshfeld surface analysis displaying the d_{norm} surfaces of examined compounds (first row) and corresponding 2D fingerprint plots with all, O…H, C…C, C…H and H…H interactions

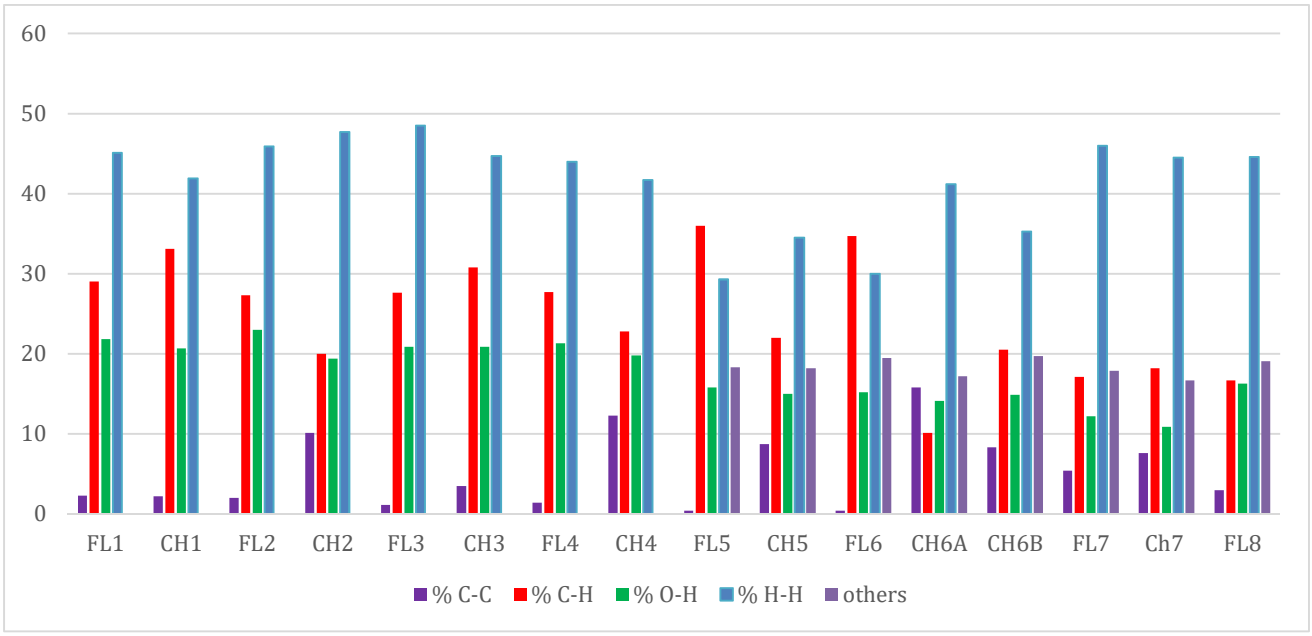
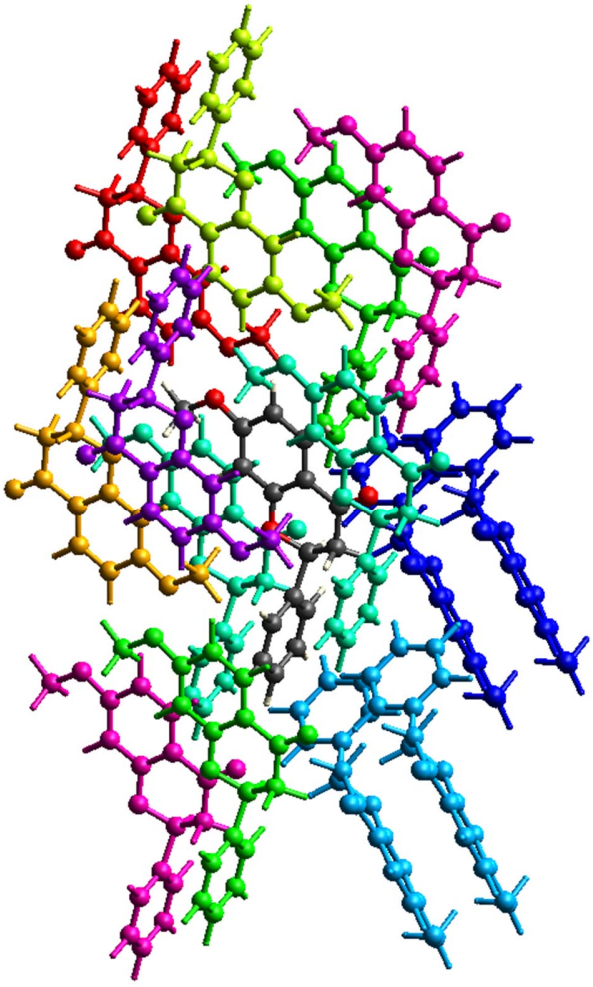
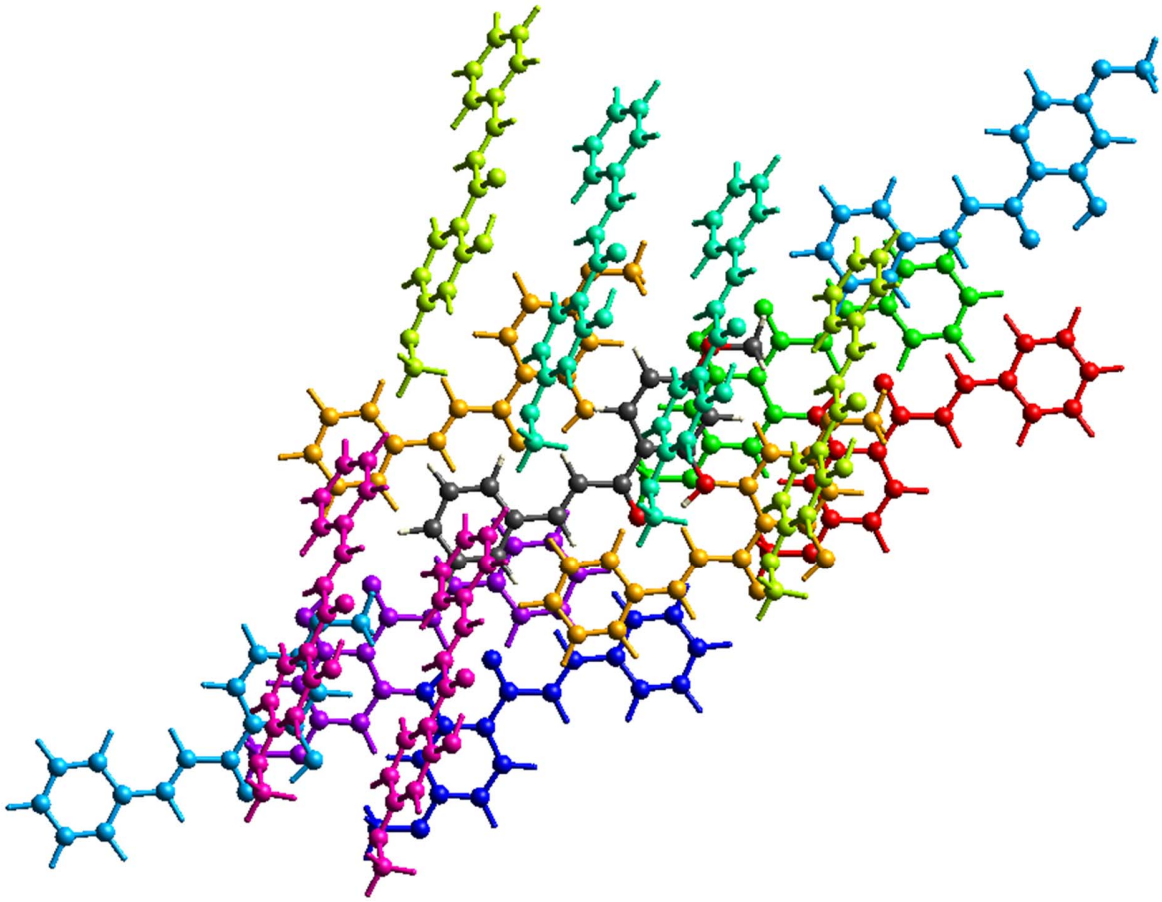


Figure S2. Relative contributions of various intermolecular contacts to the Hirshfeld surface area in series of flavanones and chalcones.



	N	**FL1**	R	E_ele	E_pol	E_dis	E_rep	E_tot	
	1	-x, -y, -z	11.99	-1.5	-0.2	-2.6	0.0	-4.0	
	1	-x, -y, -z	7.02	-16.8	-4.6	-40.1	29.7	-37.7	C-H…pi
	1	-x, -y, -z	11.27	-5.3	-0.9	-12.3	9.4	-11.1	
	2	x, y, z	8.52	-3.4	-0.7	-19.0	11.9	-13.4	C7-H7…O2
	2	x, y, z	6.60	-7.1	-2.5	-21.7	9.6	-22.4	C-H…π
	2	-x, y+1/2, -z+1/2	10.38	-4.9	-0.7	-20.8	16.3	-13.7	C-H… π
	2	-x, y+1/2, -z+1/2	7.39	-3.8	-3.1	-13.3	5.4	-14.5	
	1	-x, -y, -z	5.70	-10.2	-2.5	-53.3	23.6	-44.4	π…π
	2	x, y, z	10.78	-8.6	-2.0	-11.6	13.6	-12.3	C15-H15…O4
							Sum	-249.8	Elatt= -124.9

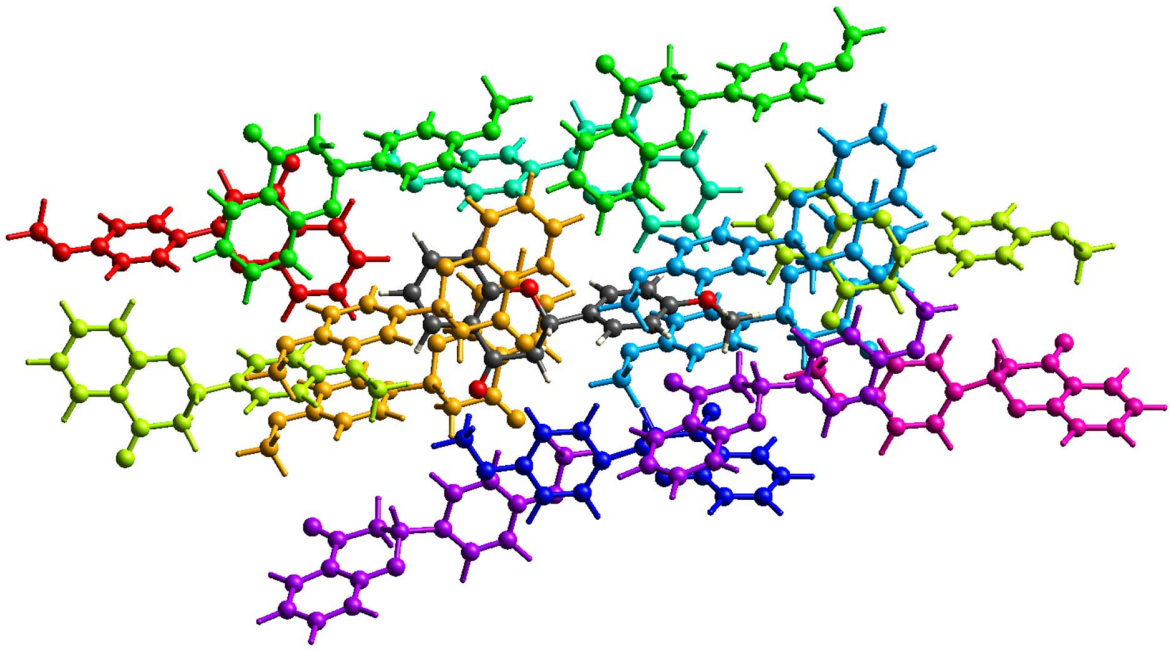
Fig. S3. Output of interaction energy calculations for flavanone **FL1** using CrystalExplorer. In table there is row with sum of the total energy and Elatt energy.



	N	**CH1**	R	E_ele	E_pol	E_dis	E_rep	E_tot	
	1	-x, -y, -z	10.68	-17.0	-4.0	-16.5	13.8	-26.8	C2-H2…O2
	2	x, y, z	5.48	-2.2	-2.0	-36.3	14.8	-26.3	C-H…O
	2	-x, y+1/2, -z+1/2	10.30	1.5	-0.3	-3.6	1.0	-1.2	
	1	-x, -y, -z	8.18	-2.1	-1.9	-32.7	12.6	-24.3	O…O stacked
	2	-x, y+1/2, -z+1/2	6.78	-9.1	-1.5	-30.8	16.6	-27.3	C-H…pi
	2	x, y, z	16.26	1.2	-0.5	-6.0	3.5	-2.2	
	1	-x, -y, -z	9.00	-8.1	-3.1	-17.7	11.6	-19.2	
	1	-x, -y, -z	9.69	-7.0	-0.9	-31.1	19.9	-23.0	C-H…π

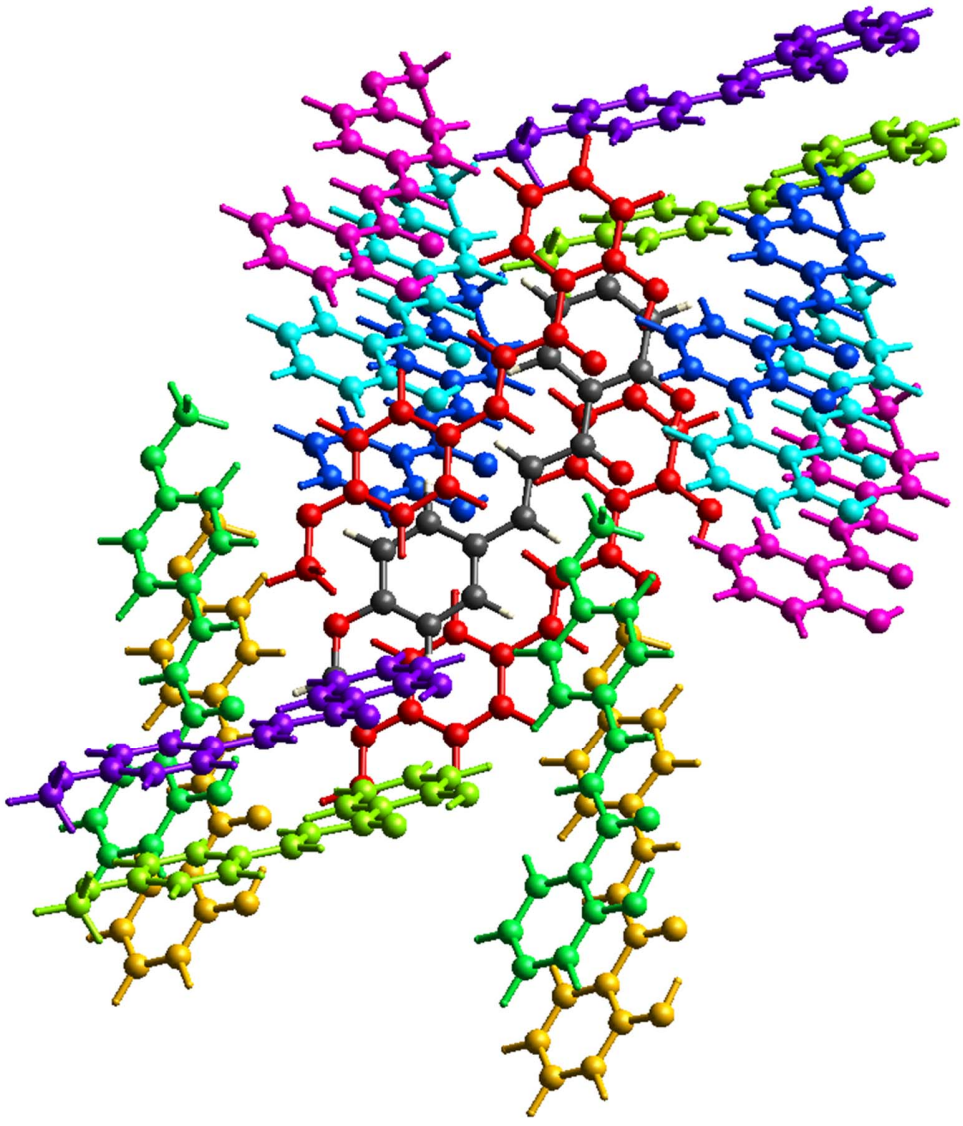
	2	-x, y+1/2, -z+1/2	11.94	-2.4	-0.5	-14.5	9.2	-9.8	
							Sum	-226.9	Elatt= -113.45

Fig. S4. Output of interaction energy calculations for flavanone **CH1** using CrystalExplorer. In table there is row with sum of the total energy and Elatt energy.



	N	**FL2**	R	E_ele	E_pol	E_dis	E_rep	E_tot	
	1	-x, -y, -z	12.56	-3.4	-0.3	-10.4	7.8	-8.0	
	2	-x+1/2, y+1/2, z	6.35	-20.7	-4.0	-44.2	39.2	-39.1	C2-H2A...O4 C16-H16..O4
	2	x, y, z	12.77	-5.2	-0.9	-11.5	7.1	-11.8	
	2	x+1/2, -y+1/2, -z	8.93	-5.9	-0.9	-17.7	13.5	-13.9	
	1	-x, -y, -z	6.15	-5.1	-0.6	-22.1	14.9	-15.9	
	2	-x+1/2, y+1/2, z	9.13	-3.6	-1.2	-28.0	16.5	-18.9	pi...π or C-H...π
	1	-x, y, -z+1/2	6.15	-6.4	-3.6	-31.6	17.2	-26.5	C18-H18B...O4
	2	x+1/2, y+1/2, -z+1/2	9.69	-7.4	-3.0	-10.3	9.5	-13.2	
	1	-x, y, -z+1/2	15.62	1.5	-0.6	-7.1	6.8	-0.8	
							Sum	-245.0	Elatt= -122.5

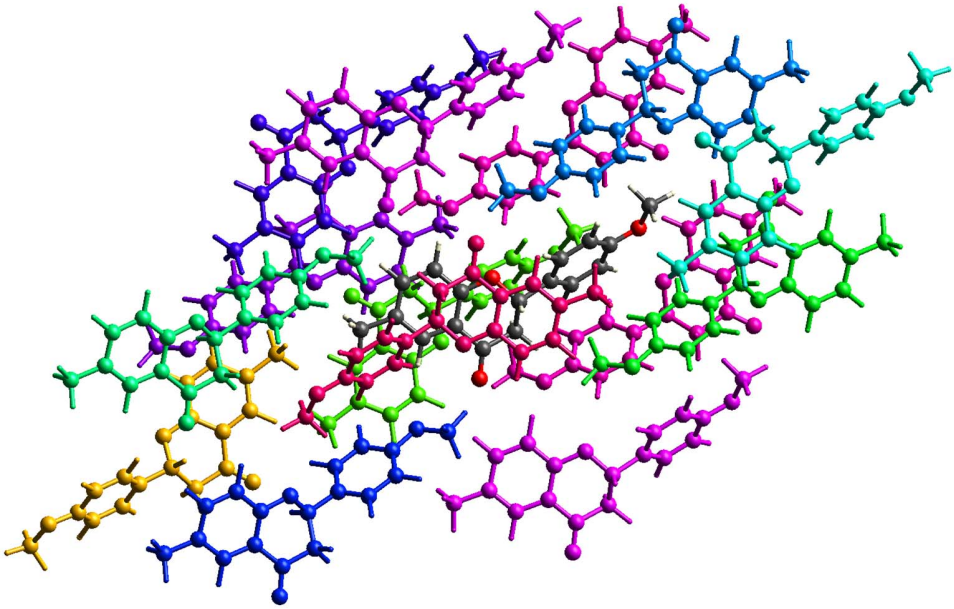
Fig. S5. Output of interaction energy calculations for flavanone **FL2** using CrystalExplorer. In table there is row with sum of the total energy and Elatt energy.



	N	**CH2**	R	E_ele	E_pol	E_dis	E_rep	E_tot	
	2	x, y, z	4.05	-0.7	-2.9	-69.4	38.5	-39.5	π …π
	2	-x, -y, z+1/2	11.32	-4.6	-1.1	-9.6	4.5	-11.3	

	2	x+1/2, -y, z	12.71	-1.8	-1.2	-13.1	9.5	-8.4	
	2	-x, -y, z+1/2	10.07	-7.7	-1.7	-16.7	11.1	-17.1	Csp3-H…O
	2	-x+1/2, y, z+1/2	8.00	-14.1	-3.5	-19.2	19.9	-21.9	C-H…O
	2	-x+1/2, y, z+1/2	8.97	-1.3	-0.6	-10.9	7.6	-6.7	
	2	x+1/2, -y, z	12.95	0.5	-0.6	-7.8	3.8	-4.3	
	2	-x+1/2, y, z+1/2	8.97	-4.0	-0.9	-6.1	2.9	-8.4	
							Sum	-258.2	Elatt= -129.1

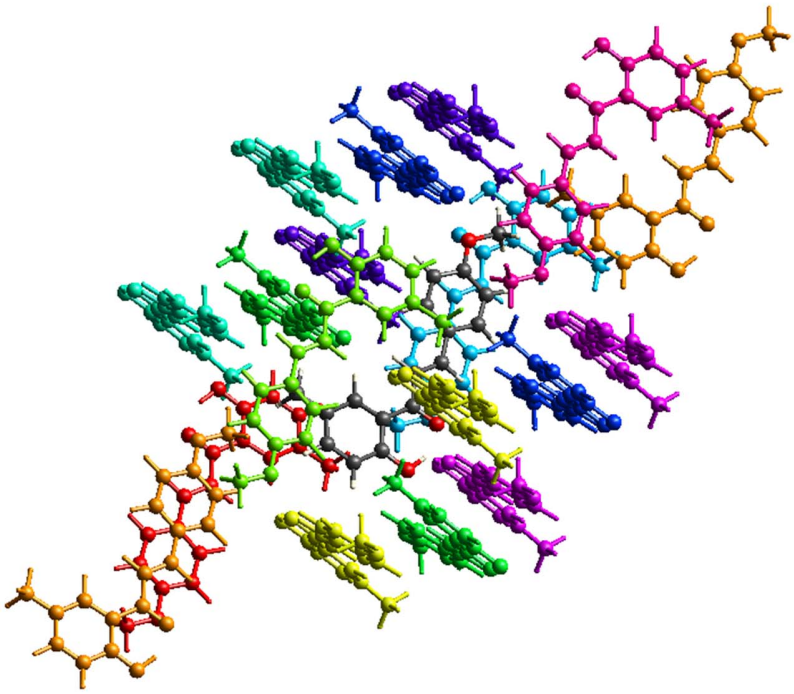
Fig. S6. Output of interaction energy calculations for flavanone **CH2** using CrystalExplorer. In table there is row with sum of the total energy and Elatt energy.



	N	**FL3**	R	E_ele	E_pol	E_dis	E_rep	E_tot	
	1	-x, -y, -z	13.45	-1.7	-0.5	-7.4	2.4	-7.1	
	2	-x+1/2, y+1/2, -z+1/2	6.08	-20.5	-5.2	-49.5	42.7	-42.3	C-H…O
	1	-	15.53	-0.2	-0.0	-6.4	4.4	-3.1	
	1	-x, -y, -z	14.97	0.3	-0.1	-4.2	1.3	-2.6	
	2	x+1/2, -y+1/2, z+1/2	11.39	-1.6	-0.4	-13.3	7.7	-8.7	
	1	-	4.88	-18.8	-3.7	-66.4	41.9	-54.6	π…π
	1	-	9.38	-9.6	-1.8	-32.3	21.2	-26.5	C-H…π

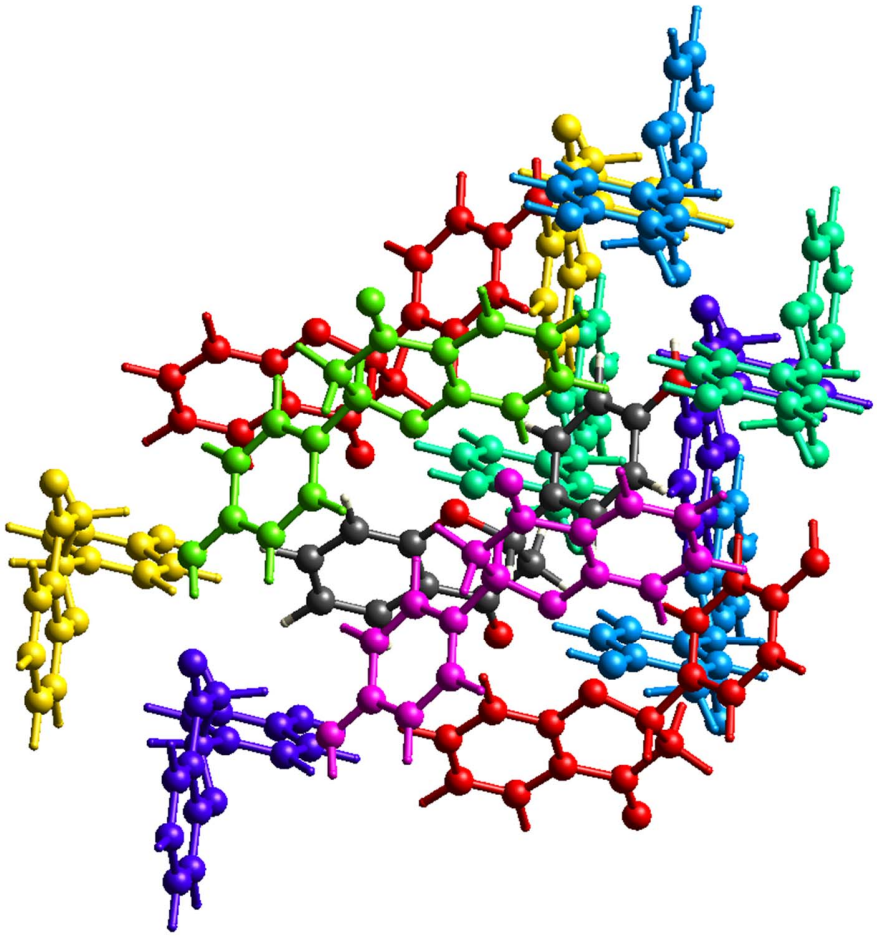
	1	-	12.93	-2.6	-0.6	-14.5	8.9	-10.3	
	1	-	12.62	-1.7	-0.4	-7.1	1.6	-7.3	
	2	x, y, z	8.04	-3.4	-2.3	-7.6	3.9	-9.5	
	1	-	9.04	-11.5	-2.6	-33.7	25.4	-27.8	C-H…π
	1	-	12.34	-7.4	-2.1	-10.7	10.5	-12.2	
	1	-	9.07	0.1	-0.2	-5.4	1.0	-4.0	
	1	-	9.93	0.2	-0.1	-2.6	0.0	-2.1	
	2	x, y, z	8.04	-7.6	-3.1	-9.6	9.4	-12.8	
	2	-x+1/2, y+1/2, -z+1/2	7.17	-11.1	-3.2	-40.0	31.1	-29.7	all C-H…O
	1	-x, -y, -z	5.41	-11.6	-1.6	-54.8	30.6	-42.3	C-H..π
							Sum	-405.9	Elatt=-202.95

Fig. S7. Output of interaction energy calculations for flavanone **FL3** using CrystalExplorer. In table there is row with sum of the total energy and Elatt energy.



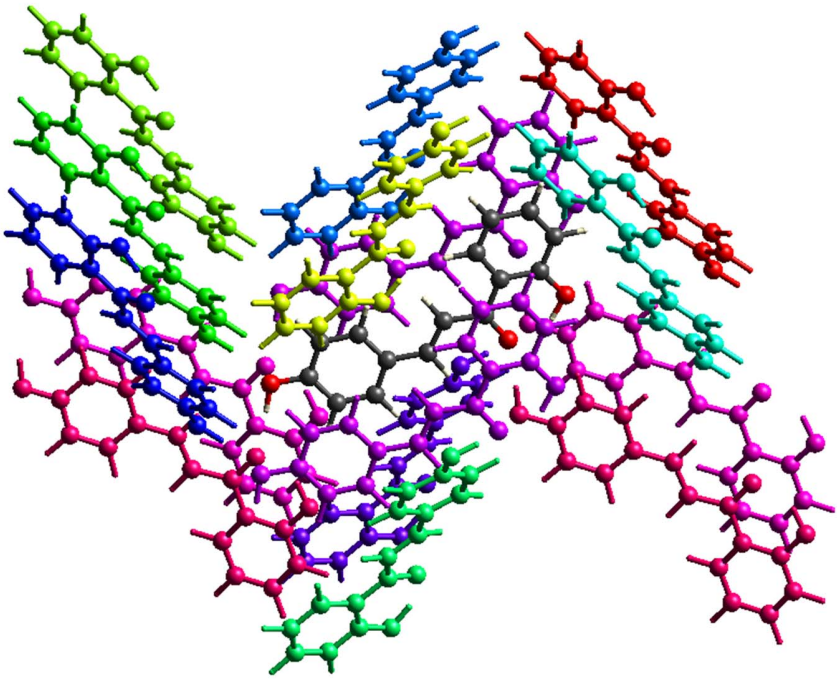
	N	**CH3**	R	E_ele	E_pol	E_dis	E_rep	E_tot	
	1	-x, -y, -z	10.01	-6.6	-1.1	-32.1	19.3	-23.8	C-H…O
	2	x, y, z	15.45	0.9	-0.6	-8.0	4.1	-3.9	
	2	-x, y+1/2, -z+1/2	9.88	-2.0	-0.9	-15.2	6.9	-11.8	
	1	-x, -y, -z	5.97	-10.4	-1.3	-43.0	22.5	-35.6	C1-H1…O1
	2	x, -y+1/2, z+1/2	7.54	-10.5	-3.4	-19.0	15.2	-20.8	C-H…π
	2	-x, y+1/2, -z+1/2	9.91	-0.3	-0.1	-4.2	1.1	-3.3	
	1	-x, -y, -z	7.22	-7.3	-2.0	-51.3	29.5	-35.6	π…π
	2	x, -y+1/2, z+1/2	8.35	-6.0	-1.8	-16.6	13.8	-13.7	
	2	-x, y+1/2, -z+1/2	12.63	0.6	-0.3	-4.1	1.2	-2.4	
	2	-x, y+1/2, -z+1/2	8.31	-7.7	-1.6	-10.2	6.0	-14.5	
	1	-x, -y, -z	11.93	-9.3	-1.6	-26.1	18.4	-22.4	C17-H15…π
							Sum	-258.2	Elatt=-129.1

Fig. S8. Output of interaction energy calculations for flavanone **CH3** using CrystalExplorer. In table there is row with sum of the total energy and Elatt energy.



	N	**FL4**	R	E_ele	E_pol	E_dis	E_rep	E_tot	
	2	x, y, z	5.25	-5.3	-2.6	-41.4	23.1	-29.3	
	2	-x, y+1/2, -z+1/2	9.66	-0.0	-0.4	-8.5	3.3	-5.8	
	1	-x, -y, -z	5.67	-11.5	-1.5	-37.9	25.9	-30.3	C-H…π
	2	x, -y+1/2, z+1/2	9.06	-7.2	-1.9	-16.2	11.3	-16.1	C-H…O
	2	x, -y+1/2, z+1/2	9.62	-57.9	-13.8	-12.5	65.5	-41.9	O3-H9…O2
	2	-x, y+1/2, -z+1/2	8.38	-6.3	-0.7	-20.8	11.5	-18.1	C-H…π
	1	-x, -y, -z	5.10	-13.4	-1.4	-46.2	33.0	-35.0	C-H…π
							Sum	-287.7	Elatt=-143.85

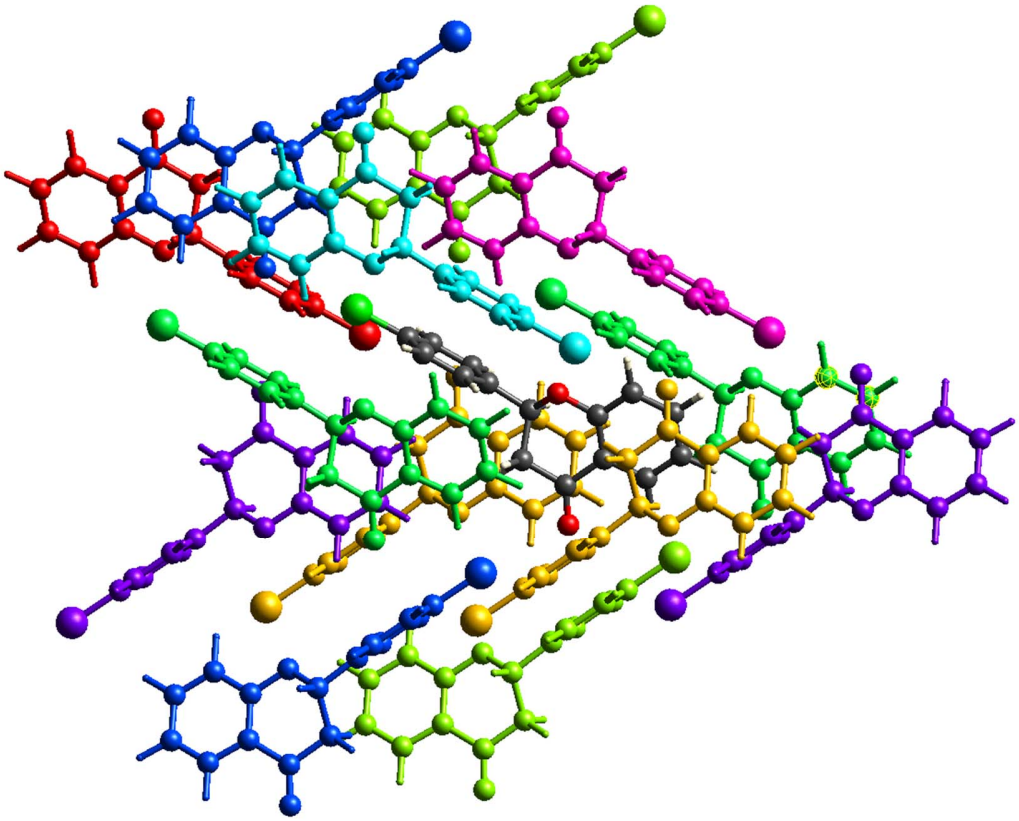
Fig. S9. Output of interaction energy calculations for flavanone **FL4** using CrystalExplorer. In table there is row with sum of the total energy and Elatt energy.



x 2	N	**CH4**	R	E_ele	E_pol	E_dis	E_rep	E_tot	
	1	-	9.23	-1.4	-0.9	-15.2	8.1	-10.4	
	2	x, y, z	3.94	-0.6	-2.5	-63.3	36.5	-35.0	π…π
	2	-x, y+1/2, -z	9.12	-3.8	-1.0	-11.7	10.0	-8.7	
	1	-	7.50	-5.5	-2.1	-18.0	10.2	-16.8	
	1	-	11.96	0.2	-0.3	-1.6	0.1	-1.3	
	1	-	11.39	-35.0	-8.2	-12.5	43.4	-27.2	O-H…O
	1	-	10.67	-8.4	-1.5	-13.5	13.3	-13.6	
	1	-	8.47	-8.4	-2.2	-22.4	16.6	-19.8	C-H…π
	2	-x, y+1/2, -z	9.33	-3.4	-0.5	-9.7	6.5	-8.4	
	1	-	7.63	-8.5	-2.2	-22.3	18.2	-18.8	2nd molecule
	1	-	12.14	2.1	-0.3	-2.7	0.2	-0.3	
	1	-	10.25	-5.0	-0.9	-10.4	5.0	-12.0	
	2	x, y, z	3.94	-0.3	-2.4	-64.0	32.8	-37.6	π…π

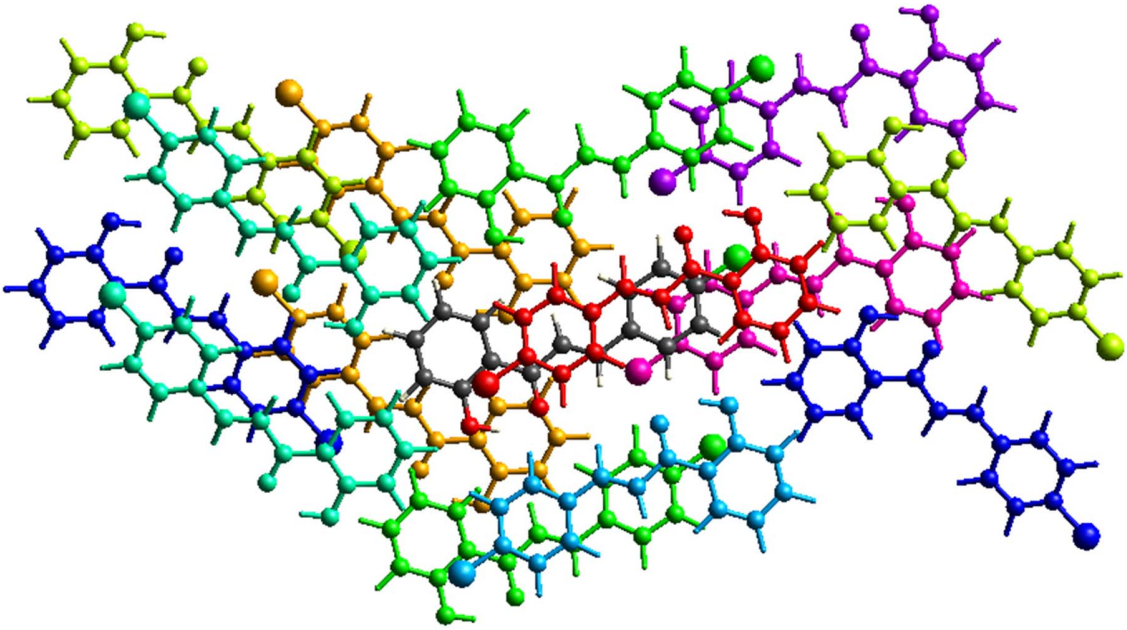
	2	-x, y+1/2, -z	10.21	-2.9	-1.5	-11.0	5.5	-10.3	
	2	-x, y+1/2, -z	10.73	-45.0	-10.4	-13.7	46.9	-38.2	O3-H31…O2
							Sum	-396.6	Elatt=-198.3

Fig. S10. Output of interaction energy calculations for flavanone **CH4** using CrystalExplorer. In table there is row with sum of the total energy and Elatt energy.



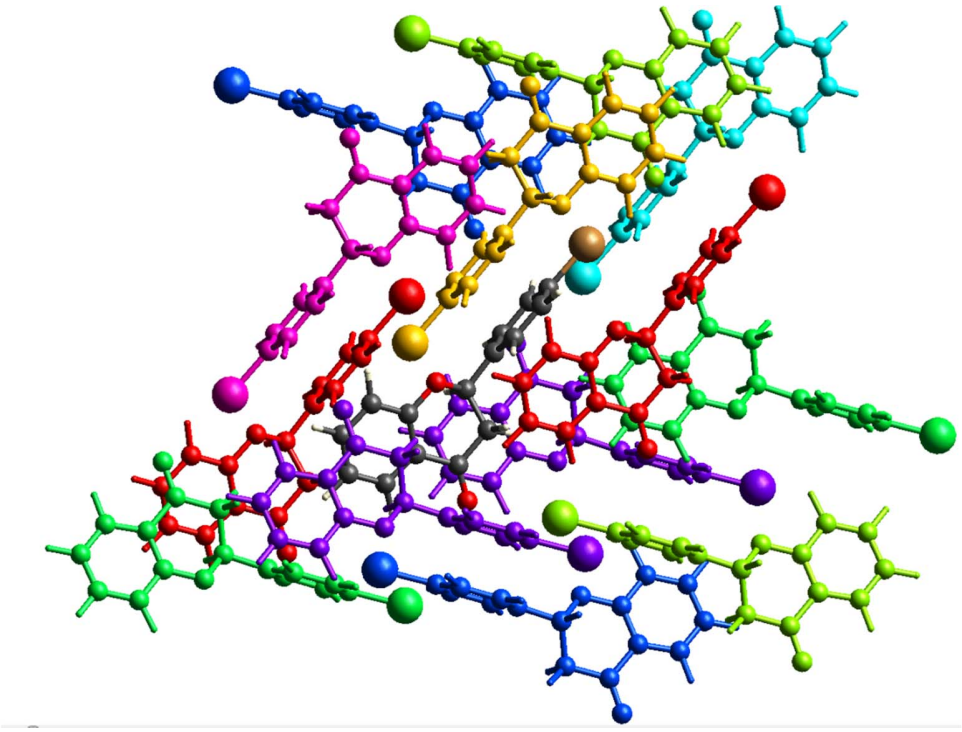
	N	**FL5**	R	E_ele	E_pol	E_dis	E_rep	E_tot	
	1	-x, -y, -z	12.18	-4.6	-0.4	-7.0	6.3	-7.4	
	2	x, -y+1/2, z+1/2	6.73	-14.4	-3.4	-35.8	24.8	-33.5	C-H…π (C17-H17…Cg2)
	2	-x, y+1/2, -z+1/2	9.06	-4.2	-1.5	-6.9	3.3	-9.5	
	2	x, y, z	6.48	-10.0	-1.6	-35.4	24.1	-27.7	C13-H13…π(Cg2)
	1	-x, -y, -z	6.78	-6.4	-0.7	-22.6	11.4	-19.9	
	2	-x, y+1/2, -z+1/2	10.31	-3.7	-1.0	-7.2	10.2	-4.7	C15-Cl1…O4
	2	x, -y+1/2, z+1/2	9.88	-1.9	-0.8	-21.2	13.0	-13.1	C7-H7…π(Cg3)
	1	-x, -y, -z	5.66	-11.2	-1.3	-38.7	31.4	-27.1	C8-H8…Cl1
							Sum	-231.4	Elatt=115.7

Fig. S11. Output of interaction energy calculations for flavanone **FL5** using CrystalExplorer. In table there is row with sum of the total energy and Elatt energy.



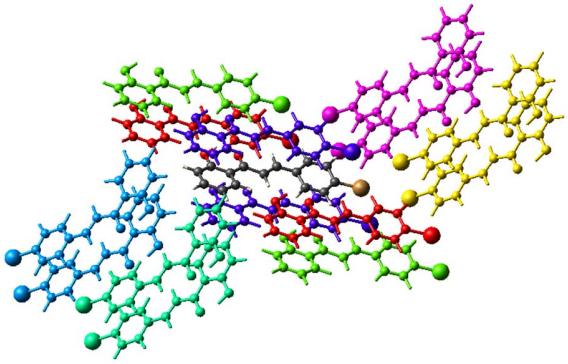
	N	**CH5**	R	E_ele	E_pol	E_dis	E_rep	E_tot	
	1	-x, -y, -z	4.27	-10.5	-1.4	-78.6	61.1	-42.9	C13- Cl1…π(Cg2) C…C
	2	-x, y+1/2, -z+1/2	7.45	-3.9	-1.7	-34.3	19.2	-23.4	π…π
	2	x, -y+1/2, z+1/2	14.43	-1.3	-0.1	-5.6	4.6	-3.5	
	2	x, y, z	6.81	-7.8	-2.9	-22.8	15.2	-20.9	C-H…O1
	2	-x, y+1/2, -z+1/2	12.15	-1.9	-0.6	-10.4	4.7	-8.6	
	1	-x, -y, -z	6.35	-13.3	-2.2	-22.7	14.8	-26.3	C-H…O2
	2	x, -y+1/2, z+1/2	13.56	-0.2	-0.7	-9.6	7.9	-4.1	
	1	-x, -y, -z	12.00	-7.4	-0.6	-10.1	15.2	-7.7	
	1	-x, -y, -z	8.56	-2.4	-0.4	-32.9	19.5	-19.5	π…π
							Sum	-217.4	Elatt=-108.7

Fig. S12. Output of interaction energy calculations for flavanone **CH5** using CrystalExplorer. In table there is row with sum of the total energy and Elatt energy.

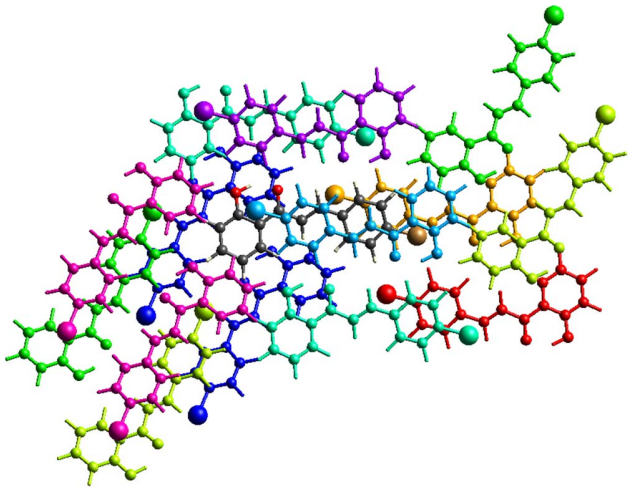


	N	**FL6**	R	E_ele	E_pol	E_dis	E_rep	E_tot	Br…Br 4.721
	2	x, y, z	6.64	-9.7	-1.6	-35.2	22.4	-28.3	C-H…pi
	1	-x, -y, -z	5.89	-4.9	-0.5	-23.1	9.0	-20.1	C-H…Br
	2	-x, y+1/2, -z+1/2	9.64	-7.0	-1.3	-9.1	11.8	-8.9	
	2	x, -y+1/2, z+1/2	10.38	-0.8	-0.7	-19.2	8.5	-12.8	
	1	-x, -y, -z	10.74	-3.5	-0.3	-9.1	6.0	-8.3	
	2	-x, y+1/2, -z+1/2	9.13	-4.4	-1.3	-7.0	2.6	-10.1	
	2	x, -y+1/2, z+1/2	7.26	-11.1	-2.8	-32.6	18.8	-30.6	C-H…O
	1	-x, -y, -z	6.00	-9.0	-1.0	-37.3	24.1	-27.8	C-H…Br
							Sum	-237.6	Elatt=-118.8

Fig. S13. Output of interaction energy calculations for flavanone **FL6** using CrystalExplorer. In table there is row with sum of the total energy and Elatt energy.



IKOFAR



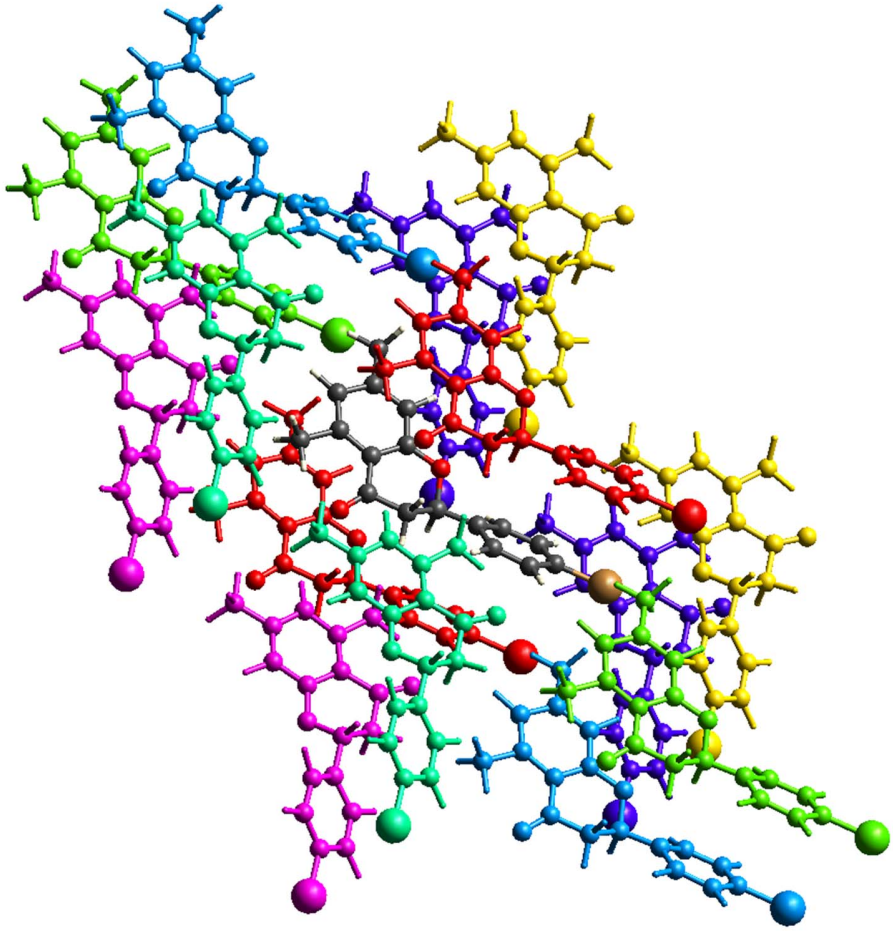
IKOFAR01

	N	**CH6 IKOFAR**	R	E_ele	E_pol	E_dis	E_rep	E_tot	Br…Br 4.002
	2	x, y, z	6.95	-10.6	-3.0	-23.3	15.6	-24.1	C-H…O
	2	-x, y+1/2, -z	13.12	-2.3	-0.1	-5.2	5.0	-4.0	
	2	x, y, z	8.02	-4.2	-1.2	-16.8	8.9	-14.5	C-H…Br
	2	-x, y+1/2, -z	13.18	-0.4	-0.3	-6.8	3.6	-4.4	
	2	-x, y+1/2, -z	15.03	-2.6	-0.5	-9.0	5.2	-7.7	
	2	x, y, z	4.00	-3.0	-1.4	-71.4	35.8	-44.3	π...π
	2	-x, y+1/2, -z	10.07	-3.5	-0.5	-11.4	6.8	-9.7	
							Sum	-217.4	Elatt=-108.7

	N	**CH6 IKOFAR01**	R	E_ele	E_pol	E_dis	E_rep	E_tot	
	1	-x, -y, -z	10.48	-5.5	-0.5	-12.3	12.8	-9.0	
	1	-x, -y, -z	7.09	-2.6	-0.3	-33.8	15.0	-23.2	. π …π
	2	x, -y+1/2, z+1/2	14.24	-0.7	-0.2	-6.8	4.1	-4.3	
	2	x, -y+1/2, z+1/2	13.80	-0.5	-0.5	-9.3	6.7	-4.9	

	2	x, y, z	6.87	-7.6	-2.7	-22.8	13.5	-21.6	C-H…O
	1	-x, -y, -z	3.54	-7.4	-1.2	-75.9	44.8	-47.1	. π …π
	2	-x, y+1/2, -z+1/2	8.76	-2.3	-1.4	-30.2	12.7	-22.0	C-H…π
	1	-x, -y, -z	6.89	-11.2	-2.1	-21.3	11.2	-25.1	.C…O
	2	-x, y+1/2, -z+1/2	13.81	-1.3	-0.4	-7.9	2.0	-7.3	
							Sum	-224.6	Elatt=-112.3

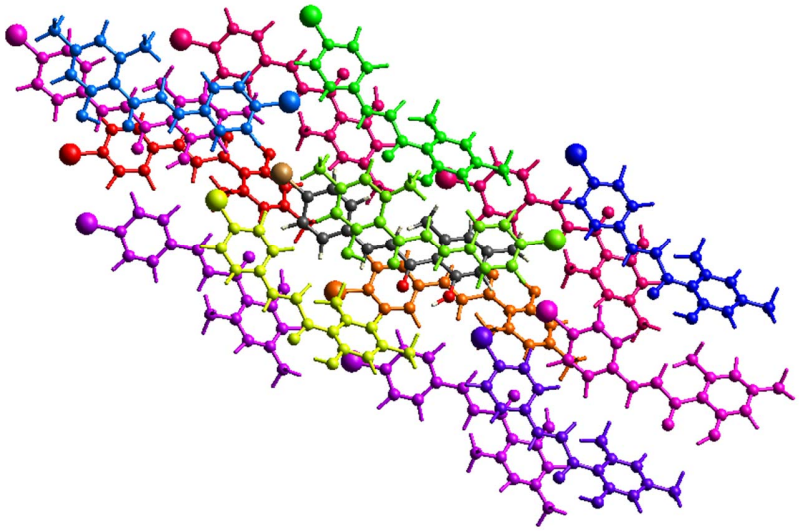
Fig. S14. Output of interaction energy calculations for flavanone **CH6** using CrystalExplorer. In table there is row with sum of the total energy and Elatt energy.



	N	**FL7 YIVREA**	R	E_ele	E_pol	E_dis	E_rep	E_tot	

	2	x, y, z	4.19	-11.5	-3.0	-80.0	43.2	-57.4	pi…pi
	2	-x, y+1/2, -z	9.31	-1.8	-0.4	-14.7	6.5	-11.0	
	2	x, y, z	13.80	-0.1	-0.1	-4.2	1.0	-3.2	
	2	-x, y+1/2, -z	9.91	-20.6	-4.7	-24.8	84.2	5.1	Br…Br 4.194
	2	x, y, z	13.15	-1.9	-0.2	-9.8	7.1	-6.3	
	2	-x, y+1/2, -z	8.72	-3.0	-0.7	-21.0	14.0	-13.3	
	2	-x, y+1/2, -z	11.23	-6.4	-1.5	-11.5	8.2	-12.8	
							Sum	-197.8	Elatt=-98.9

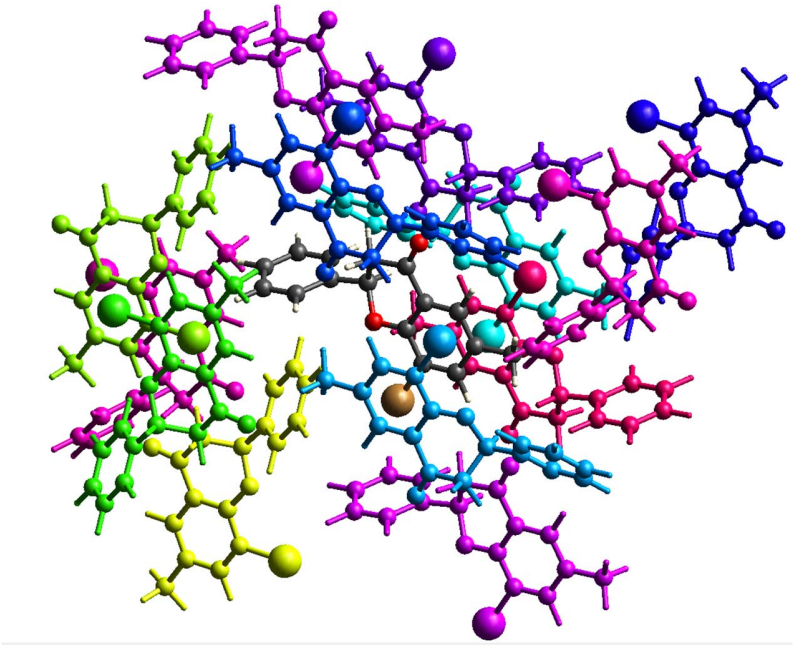
Fig. S15. Output of interaction energy calculations for flavanone **FL7** using CrystalExplorer. In table there is row with sum of the total energy and Elatt energy.



	N	**CH7 YIVPUO**	R	E_ele	E_pol	E_dis	E_rep	E_tot	Br…Br 4.367
	1	-	11.67	-3.9	-0.5	-24.3	17.9	-14.7	
	1	-	6.46	-6.0	-1.4	-50.3	20.4	-38.7	. C-H…pi
	2	-x, y+1/2, -z+1/2	11.03	-0.6	-0.2	-3.9	0.5	-3.8	
	1	-	6.62	-7.8	-2.3	-32.4	24.4	-23.1	

	1	-	5.00	-5.4	-2.7	-76.0	32.1	-54.1	. C-H…π, π…π
	1	-	7.03	-11.5	-2.5	-36.5	25.1	-30.4	. C-H…π, π..pi
	2	x, y, z	16.01	0.0	-0.1	-4.8	1.8	-3.2	
	2	-x+1/2, -y, z+1/2	11.64	-2.4	-0.3	-7.3	6.0	-5.4	
	2	-x+1/2, -y, z+1/2	8.96	-8.8	-4.3	-22.9	17.8	-21.5	C-H…O
	1	-	13.21	-0.5	-0.1	-5.4	1.2	-4.5	
	1	-	14.53	0.8	-0.2	-3.6	0.8	-1.9	
	1	-	14.34	-4.5	-0.5	-6.6	6.0	-7.2	
	2	-x, y+1/2, -z+1/2	10.45	-6.3	-1.0	-10.6	6.5	-12.5	
	2	x, y, z	16.01	-1.0	-0.1	-7.1	5.0	-4.2	
	2	-x, y+1/2, -z+1/2	10.17	-1.8	-0.2	-19.0	8.0	-13.7	
							Sum	-303.2	Elatt=-151.6

Fig. S16. Output of interaction energy calculations for flavanone **CH7** using CrystalExplorer. In table there is row with sum of the total energy and Elatt energy.

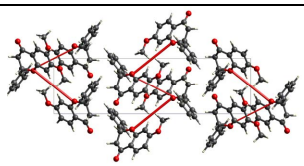
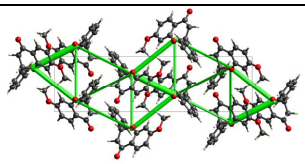
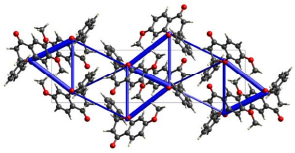
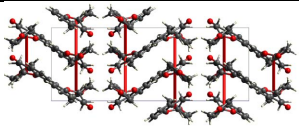
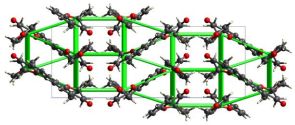
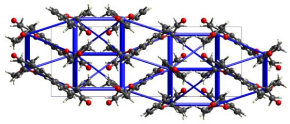
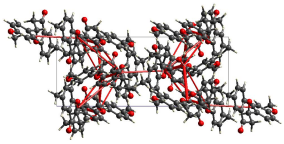
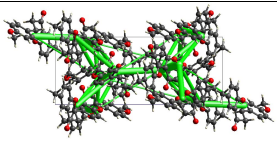
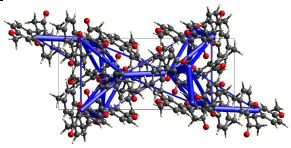
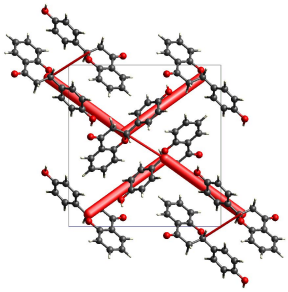
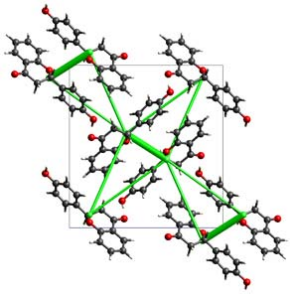
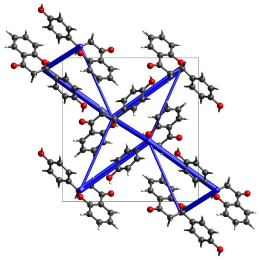
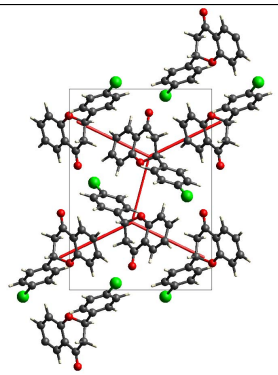
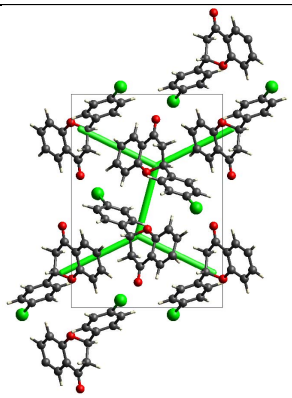
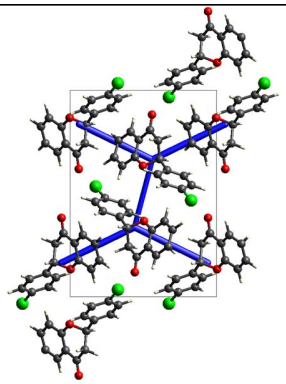
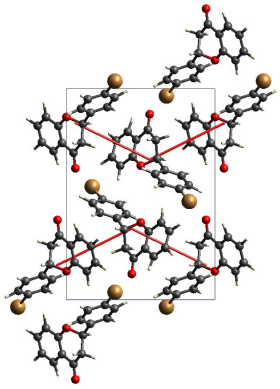
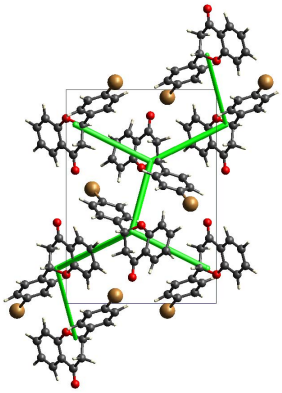
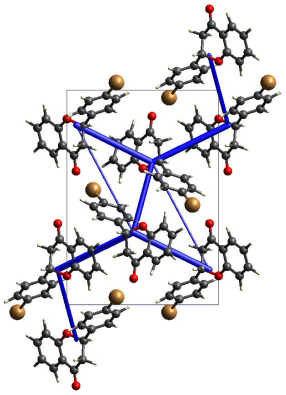


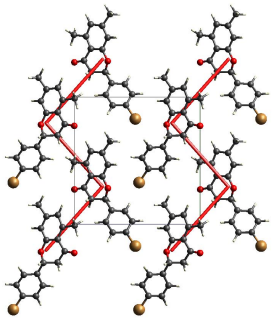
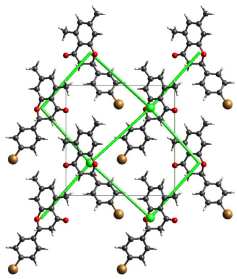
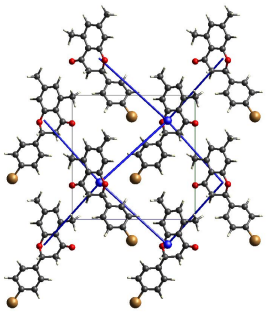
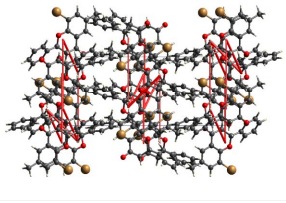
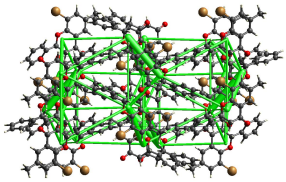
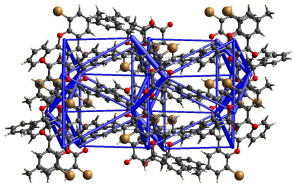
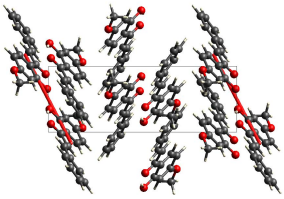
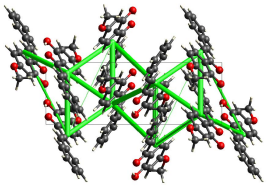
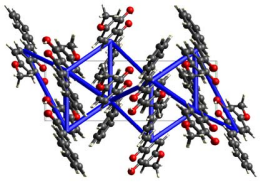
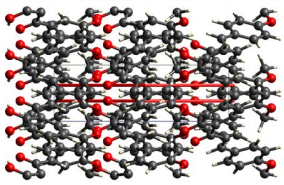
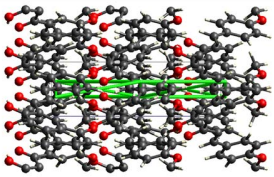
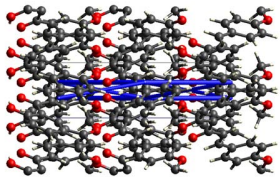
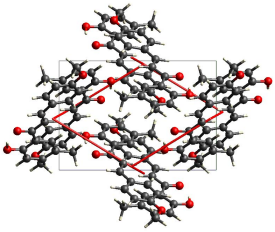
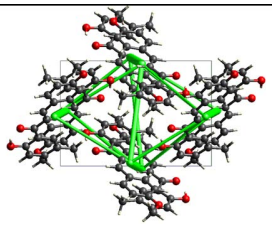
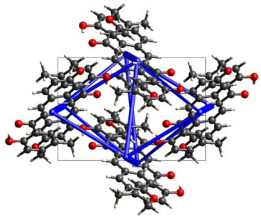
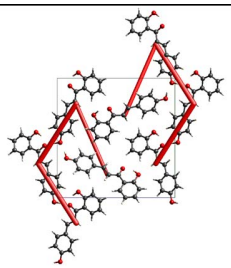
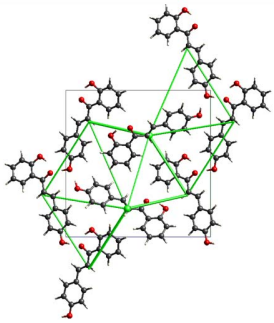
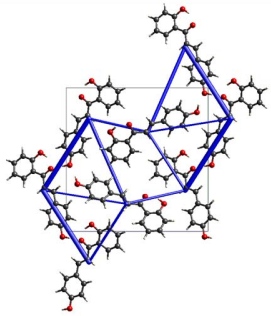
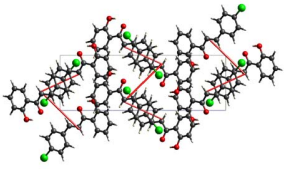
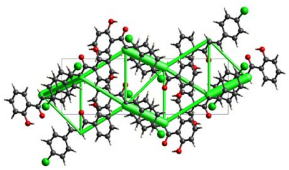
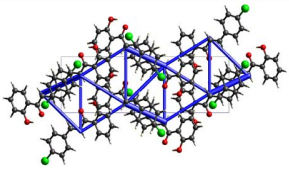
	N	**FL8**	R	E_ele	E_pol	E_dis	E_rep	E_tot	
	1	-x, -y, -z	5.03	-1.6	-1.3	-39.7	15.2	-27.9	C-H… π
	1	-x, -y, -z	7.10	-8.4	-1.7	-33.3	18.7	-27.6	C-H… π
	2	x+1/2, -y+1/2, z+1/2	12.67	0.7	-0.1	-3.5	0.7	-2.0	
	1	-	9.49	-7.5	-1.3	-23.0	16.6	-18.6	
	1	-	9.38	-4.6	-0.9	-21.1	13.7	-15.4	
	1	-	8.51	-1.9	-0.6	-18.9	9.3	-13.2	
	2	x, y, z	8.76	-12.2	-1.6	-20.4	19.4	-19.8	
	2	-x+1/2, y+1/2, -z+1/2	11.89	-2.3	-1.2	-9.0	6.0	-7.5	
	1	-	6.76	2.1	-0.5	-11.6	4.0	-5.8	
	1	-	6.10	-4.0	-2.0	-58.6	31.6	-37.2	π…π
	1	-	7.77	-16.1	-4.4	-21.5	15.6	-29.4	C-H…O
	1	-	12.55	0.5	-0.1	-2.7	0.2	-1.7	
	1	-x, -y, -z	7.35	-18.4	-5.2	-28.2	17.6	-37.0	C-H…O
	2	x, y, z	8.76	-9.9	-1.5	-16.4	12.5	-18.1	
	2	x+1/2, -y+1/2, z+1/2	12.65	-0.2	-0.2	-6.7	4.5	-3.4	
	1	-x, -y, -z	5.74	-7.2	-2.8	-66.8	36.8	-45.2	π…π
							Sum	-360.6	Elatt=-180.3

Fig. S17. Output of interaction energy calculations for flavanone **FL8** using CrystalExplorer. In table there is row with sum of the total energy and Elatt energy.

Table S4. The energy framework diagrams for separate electrostatic (red) and dispersion (green) components, and the total interaction energy (blue) for all compounds. All diagrams use the same energy tube scale factor of 80 and the energy threshold of 10 kJ/mol

view along *a* axis

FL1			
FL2			
FL3			
FL4			
FL5			
FL6			

FL7			
FL8			
CH1			
CH2			
CH3			
CH4			
CH5			

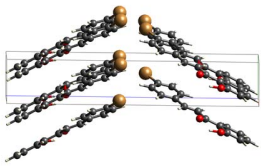
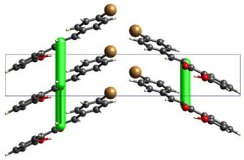
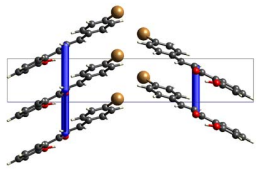
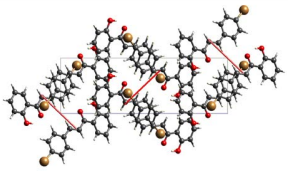
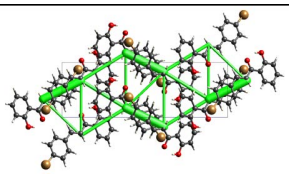
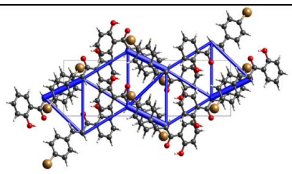
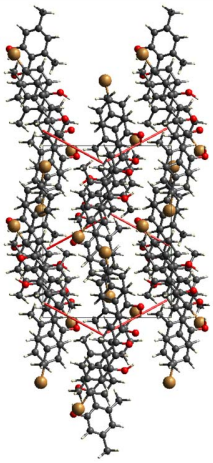
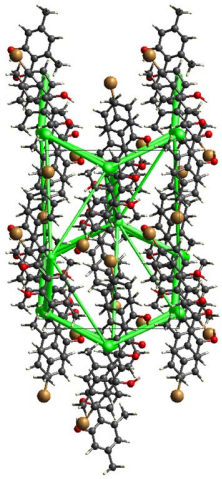
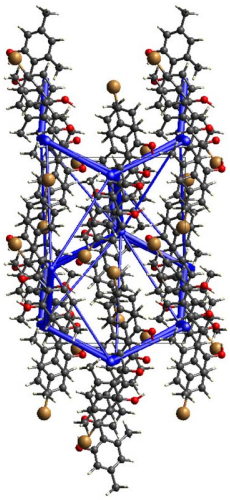
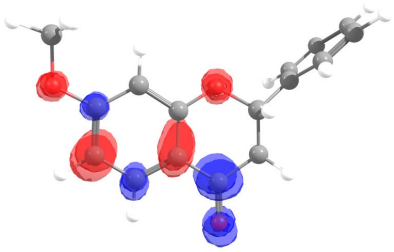
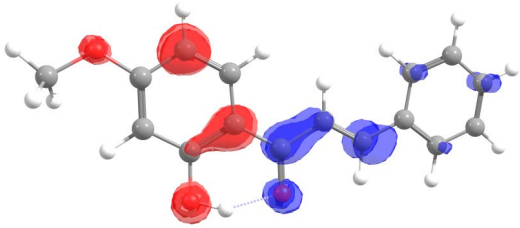
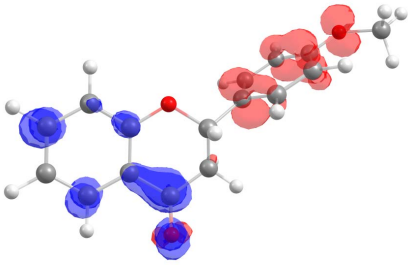
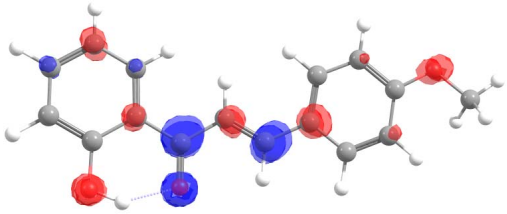
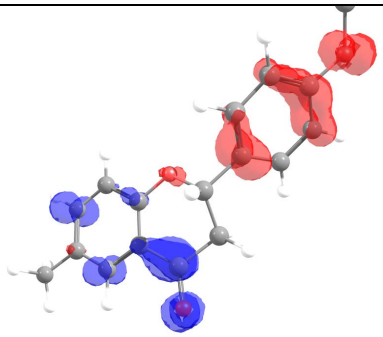
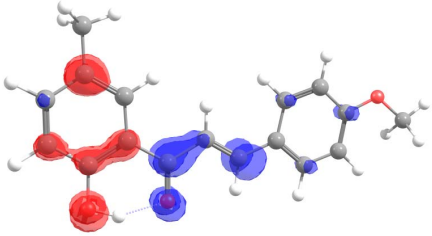
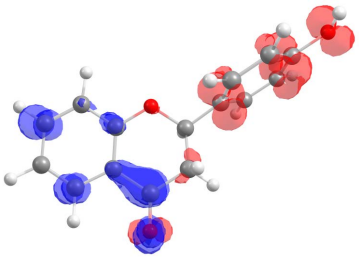
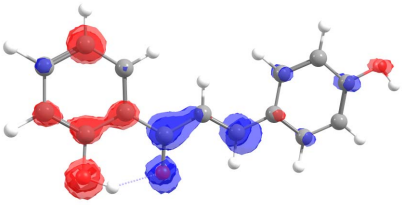
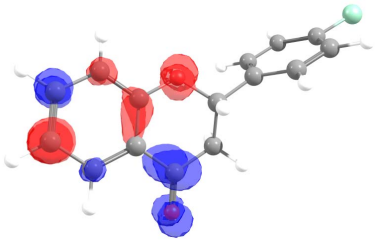
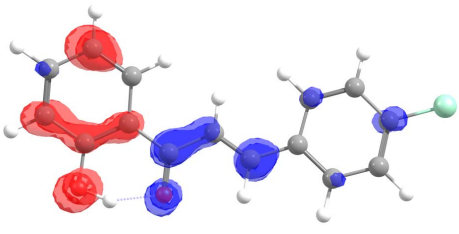
CH6A			
CH6B			
CH7			

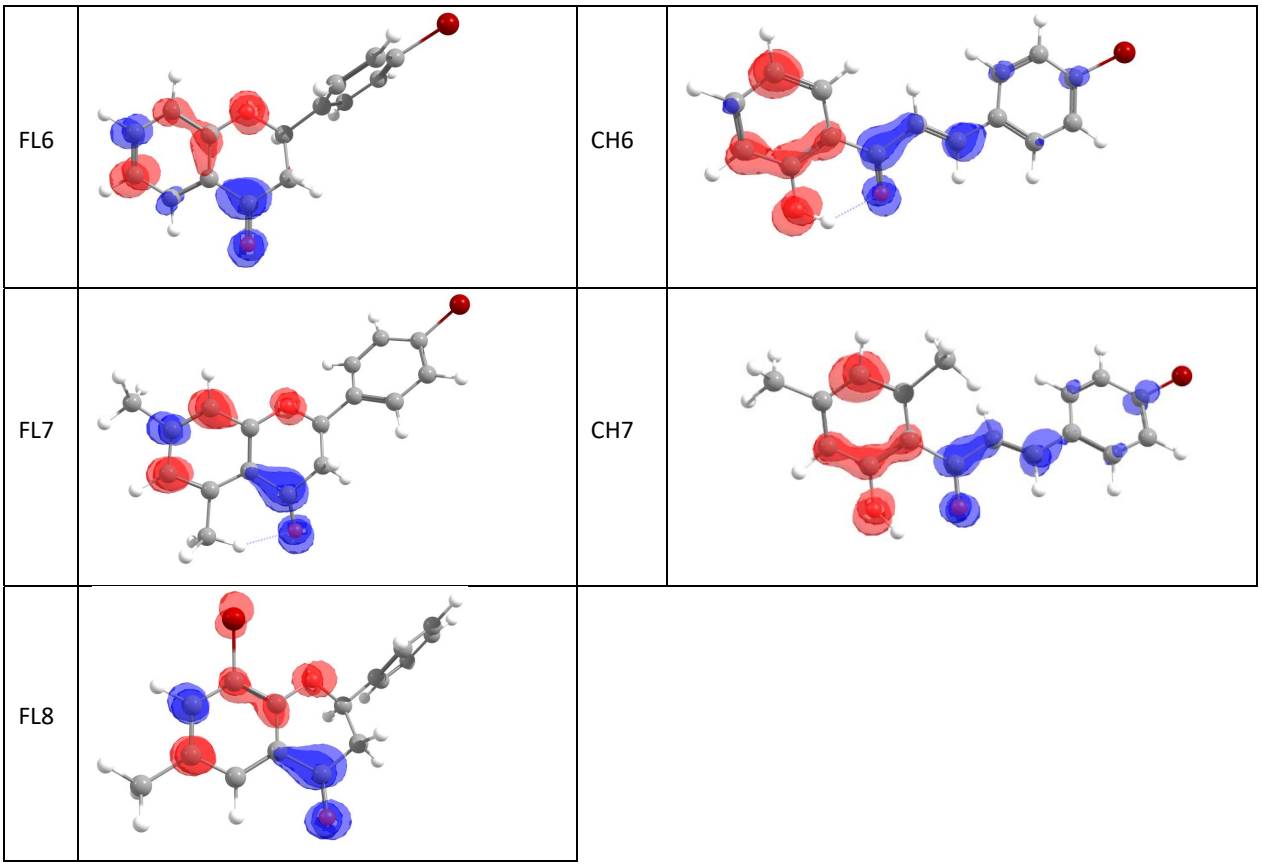
Table S5. The values of frontier molecular orbital energy (E_{HOMO}, E_{LUMO}), energy gap (E_g) and global reactivity descriptors

Code	E_{HOMO} (eV)	E_{LUMO} (eV)	E_g (eV)	Chemical hardness (eV)	Chemical softness (eV)	Chemical potential (eV)	Electrophilicity (eV)
FL1	-6.043	-1.259	4.788	2.394	0.209	-3.653	2.787
FL2	-6.079	-1.437	4.606	2.303	0.217	-3.776	3.096
FL3	-6.021	-1.427	4.594	2.297	0.218	-3.724	3.019
FL4	-6.167	-1.477	4.690	2.345	0.213	-3.822	3.115
FL5	-6.438	-1.675	4.763	2.382	0.210	-4.057	3.455
FL6	-6.482	-1.646	4.836	2.418	0.207	-4.064	3.415
FL7	-6.419	-1.558	4.861	2.431	0.206	-3.989	3.273
FL8	-6.271	-1.740	4.531	2.266	0.221	-4.006	3.541
CH1	-5.944	-2.040	3.904	1.952	0.256	-3.992	4.082
CH2	-5.875	-2.147	3.728	1.864	0.268	-4.011	4.315
CH3	-5.730	-2.035	3.695	1.848	0.271	-3.883	4.080
CH4	-5.920	-2.210	3.710	1.855	0.270	-4.065	4.454

CH5	-6.147	-2.416	3.731	1.866	0.268	-4.282	4.913
CH6	-6.243	-2.286	3.957	1.979	0.253	-4.265	4.596
CH7	-5.976	-2.068	3.908	1.954	0.256	-4.022	4.139

Table S6. The electron density difference between LUMO and HOMO orbitals. Blue color represents the electron acceptor groups in the molecule and red color represents the electron donor groups.

Flavanones (ρ_{LUMO}-ρ_{HOMO})		Chalcones (ρ_{LUMO}-ρ_{HOMO})	
FL1		CH1	
FL2		CH2	
FL3		CH3	
FL4		CH4	
FL5		CH5	



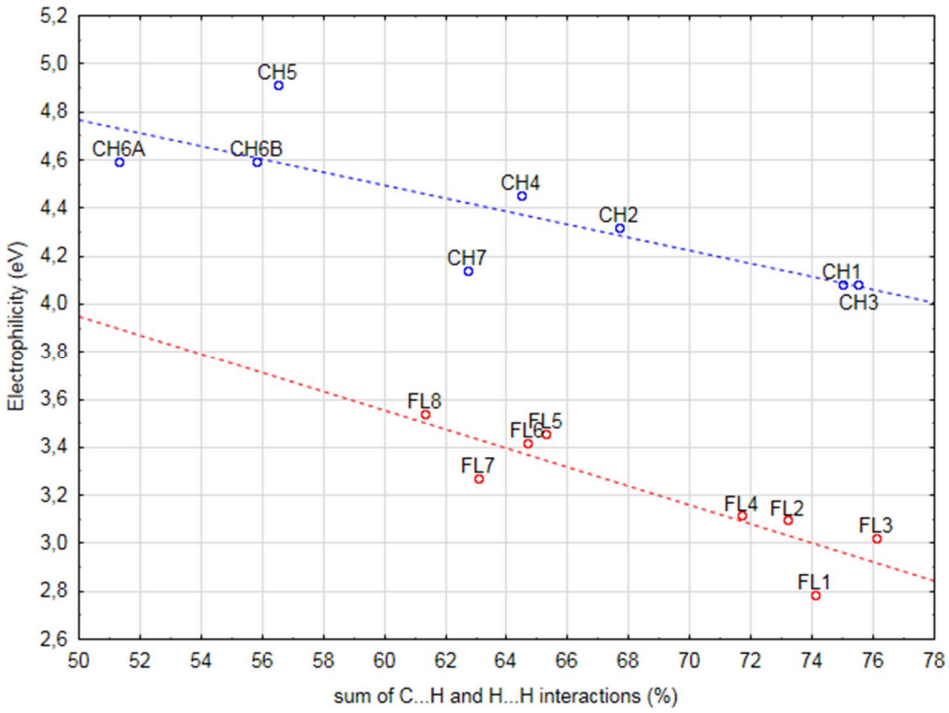


Fig. S18. Relationship between electrophilicity index and sum of C…H and H…H interactions derived from Hirshfeld surface analysis for flavanones and chalcones.

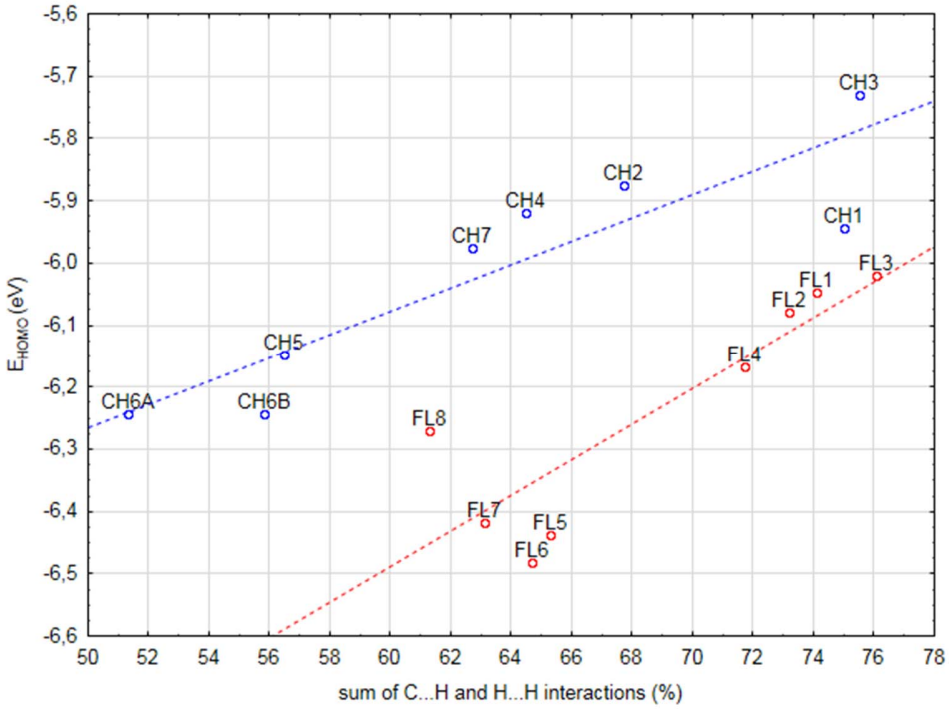


Fig. S19. Relationship between energy of frontier orbital E_{HOMO} (HOMO – highest occupied molecular orbital) and sum of C…H and H…H interactions derived from Hirshfeld surface analysis for flavanones and chalcones.

Fig. S20. Fragment of molecular structure for FL7 (a): Br1 atoms are arrayed one above the others along a axis, but in the direction [0-11] Br1 is directed to other molecule to H3 atom with C5-H3…Br1 contact; energy frameworks showing total energy in FL7 structure; blue large cylinder are directed along a axis (b); the packing arrangement of CH6A structure, with short Br1…Br1 contact: along the direction [010] molecules array “head-to-tail” fashion (c), while along [100] direction molecules create zigzag chains (d).

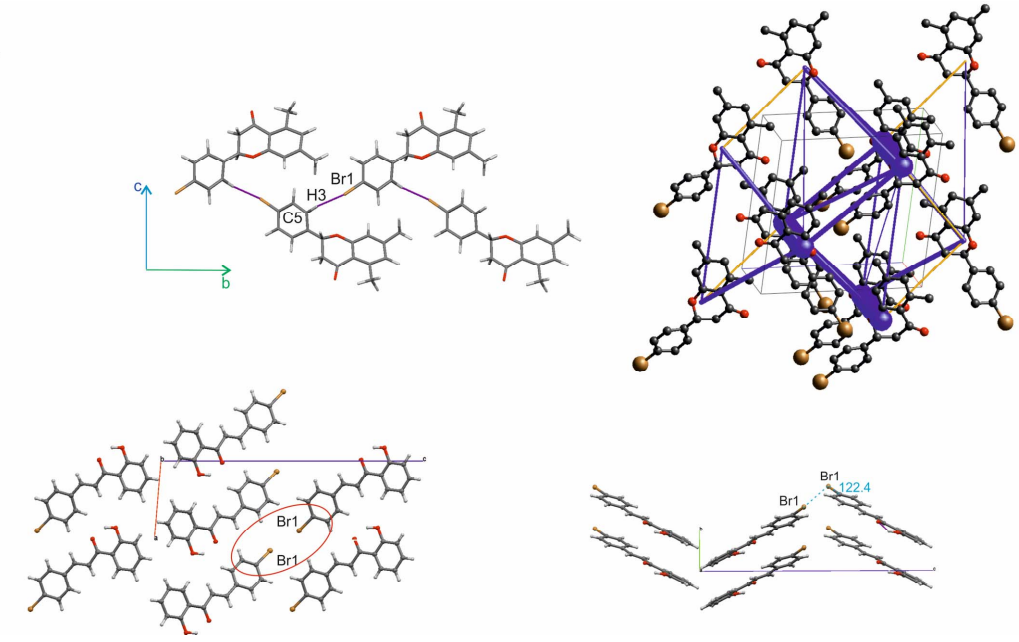


Fig. S21. Electrostatic potential surface showing the location of σ- hole on bromine atom of FL7.

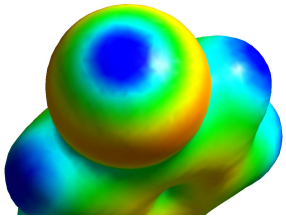


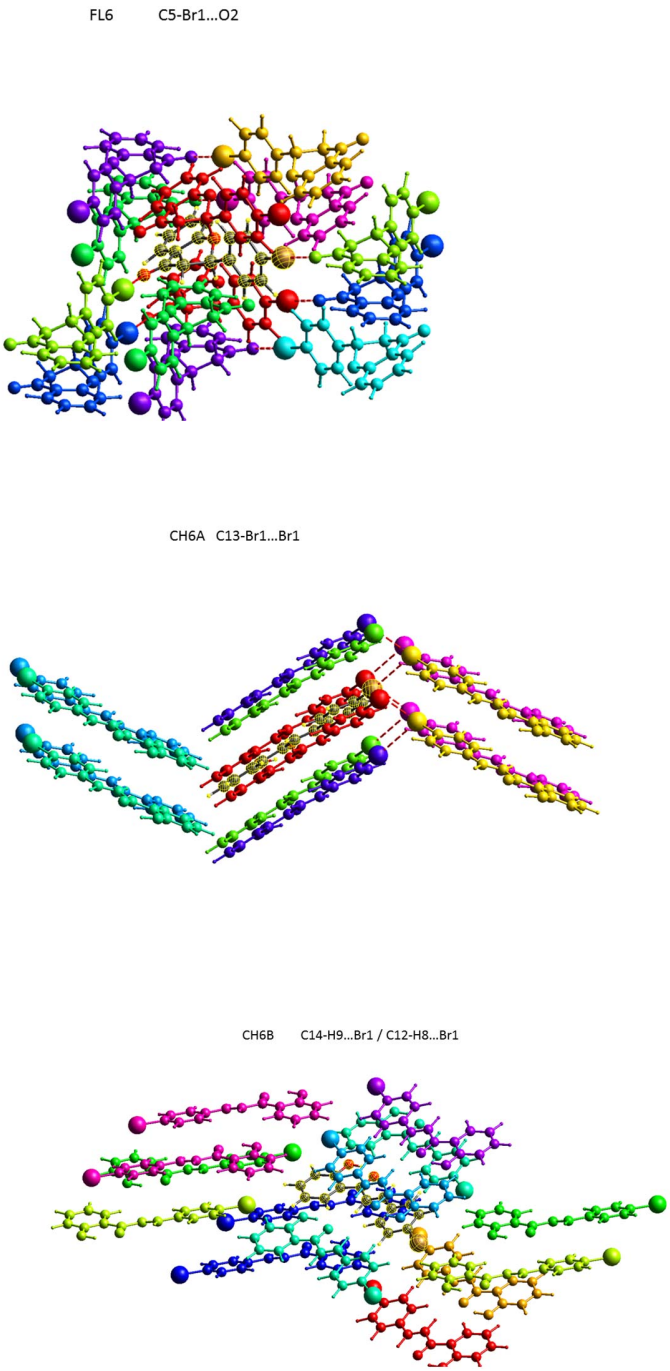
Table S7. Lattice energy including cell dipole energies for polar space group(20 Å 25Å.)

Lattice Energy with cell dipole energies for polar space group

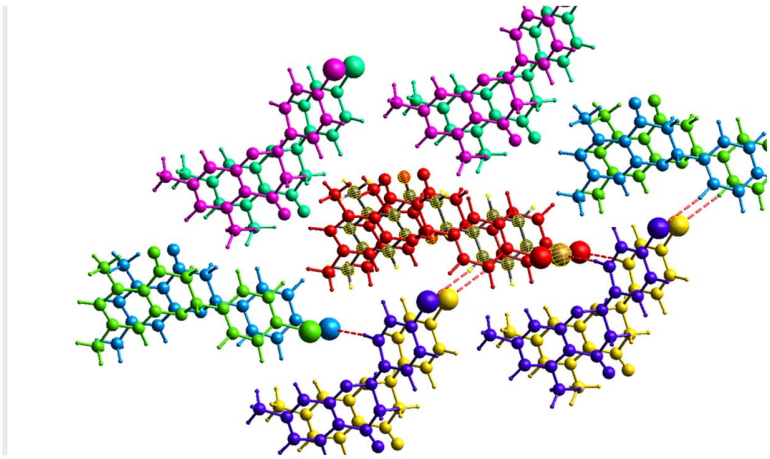
	CH1	CH2	CH3	CH4 x2	CH5	CH6a	CH6b	CH7 x2
Σ Etot*N	-251,7	-264,2	-275,5	-440,5	-257,4	-247,4	-257,7	-351,3
E lat	-125,85	-132,1	-137,75	-220,25	-128,7	-123,7	-128,85	-175,65
pcell		6,9746		1,2942		1,2942		
Z		4		4		2		
Vcell		1293,9		1176,1		633,553		
Ecell dipole		-1,18549		-0,04491		-0,16673		
Elat new	-125,85	-130,915	-137,75	-220,205	-128,7	-123,533	-128,85	-175,65

	FL1	FL2	FL3 x 2	FL4	FL5	FL6	FL7	FL8 x2
Σ Etot*N	-272,4	-267,6	437,9	-308,6	-248,2	-254,8	-225,6	401,8
E lat	-136,2	-133,8	218,95	-154,3	-124,1	-127,4	-112,8	200,9
pcell							4,3346	
Z							2	
Vcell							716,219	
Ecell dipole							-1,6544	
Elat new	-136,2	-133,8	218,95	-154,3	-124,1	-127,4	-111,146	200,9

Fig **S22**. The energy frameworks for FL6, CH6A/B Fl7 and CH7 with interactions to Br atoms



FL7 C5-H3...Br1



CH7 C18-Br2...O1