Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Table S1. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for HIF-4. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C10	1404.0(14)	8867.8(19)	1822.1(13)	47.7(4)
C3	3433.8(15)	9882.5(19)	2668.0(14)	49.4(4)
C9	1614.8(15)	8949.7(19)	825.0(13)	48.4(4)
C1'	5422.7(15)	8958.8(19)	2662.6(13)	48.0(4)
O1	2561.7(11)	9652.7(15)	700.7(10)	60.5(4)
O2	2153.3(12)	9330.0(19)	3712.6(11)	77.0(5)
C2'	6299.4(15)	9565(2)	3548.5(14)	50.0(4)
O3	6044.0(14)	9717(2)	4489.1(12)	79.9(5)
C4	2305.9(15)	9379(2)	2818.6(14)	51.1(4)
C3'	7371.3(17)	9972(2)	3450.6(17)	59.8(5)
C11	4263.1(15)	8524(2)	2781.0(15)	53.6(4)
C6'	5660.4(19)	8786(2)	1691.2(16)	65.8(5)
C8	849.3(17)	8289(2)	-101.5(15)	63.0(5)
C5	379.3(16)	8163(2)	1856.2(17)	66.4(6)
C7	-126.1(19)	7589(3)	-39.3(19)	74.7(6)
C4'	7576(2)	9785(2)	2475(2)	73.5(6)
C5'	6727(2)	9196(3)	1591.6(19)	80.7(7)
C6	-383.6(18)	7525(3)	927(2)	78.8(7)
C2	3153.3(16)	10646(2)	1574.9(15)	56.9(5)

Table S2. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for HIF-4. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C10	39.9(9)	52(1)	48.1(9)	2.9(7)	9.3(7)	1.4(7)
C3	43.7(10)	48.1(9)	50.1(9)	-7.2(7)	5.9(7)	-4.1(7)
C9	45.1(10)	46.5(9)	49.2(9)	0.7(7)	8.9(7)	1.6(7)
C1'	48.5(10)	44.4(9)	49.0(9)	1.7(7)	12.5(7)	4.1(7)
O1	56.4(8)	75.0(9)	48.9(7)	2.9(6)	14.8(6)	-10.6(7)
O2	66.6(10)	117.0(13)	47.2(8)	-5.5(8)	17.8(6)	-6.1(9)
C2'	45.7(10)	52.8(10)	50.0(9)	-0.6(8)	12.8(7)	3.8(8)
O3	60.9(9)	125.5(14)	51.6(8)	-17.3(8)	15.4(7)	-5.7(9)
C4	48.3(10)	56.4(10)	46.5(9)	-0.9(8)	11.9(7)	1.8(8)
C3'	45.2(11)	51.7(11)	78.4(13)	-0.2(9)	13.8(9)	2.7(8)
C11	47.1(10)	48.5(10)	59.3(10)	3.6(8)	8.5(8)	-0.9(8)
C6'	71.3(14)	72.9(13)	51.1(10)	-2.4(9)	16.2(9)	7.6(11)
C8	60.7(13)	67.1(12)	51.6(10)	-7.2(9)	4.3(9)	3(1)
C5	46.8(11)	82.2(15)	67.5(13)	14.4(11)	14.3(9)	-2.7(10)
C7	60.9(14)	71.6(14)	74.1(14)	-5.0(11)	-3.4(10)	-7.5(11)
C4'	60.2(14)	70.4(14)	101.0(18)	16.8(13)	41.1(13)	3.9(11)
C5'	86.4(17)	99.4(18)	70.0(14)	8.9(13)	43.9(13)	13.1(14)
C6	42.6(12)	80.9(15)	99.5(18)	12.2(13)	3.5(11)	-16.4(10)
C2	49.7(11)	50.5(10)	65.6(11)	4.8(8)	11.4(8)	-6.0(8)

Table S3. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for HIF-4.

Atom	*x*	*y*	*z*	U(eq)
H3	3807.1	10610.63	3239.01	59
H3'	7949.56	10369.63	4045.4	72
H11A	4393.23	8063.55	3488.86	64
H11B	3891.6	7787.47	2228.73	64
H6'	5090.07	8385.38	1091.67	79
H8	1005.41	8326.52	-760.54	76
H5	209.97	8123.06	2508.88	80
H7	-631.78	7143.81	-660.18	90
H4'	8294.62	10059.96	2410.16	88
H5'	6869.05	9073.43	930.85	97
H6	-1063.02	7056.93	953.47	95
H2A	2663.81	11511.78	1562.11	68
H2B	3871.88	10993.8	1469.89	68
O3H	6690(20)	10030(30)	5070(20)	102(8)

Table S4. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for HIF-13. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O4'	3619(3)	2867.1(7)	8429(2)	68.5(6)
C1'	6603(4)	3480.9(8)	5669(3)	43.1(6)
O2	8603(3)	4027.9(7)	1943(3)	73.2(7)
C3'	3669(4)	3065.9(9)	5614(3)	42.7(7)
C2'	4701(4)	3275.8(8)	4748(3)	39.6(6)
C3	6973(4)	4180.4(9)	3828(3)	42.8(6)
C4	7834(4)	4321.7(10)	2554(3)	46.8(7)
C11	7741(4)	3688.7(9)	4711(3)	52.1(7)
C10	7634(3)	4839.4(10)	2063(3)	43.4(7)
C4'	4529(4)	3066.4(9)	7452(3)	47.7(7)
O1	6590(3)	5048.5(6)	4348(3)	61.2(6)
C9	6998(4)	5174.9(10)	2967(3)	48.3(7)
C2	7376(4)	4589.7(9)	5153(3)	53.1(7)
C6	7759(4)	5494.1(12)	180(4)	63.0(8)
C5'	6380(4)	3275.2(10)	8402(3)	54.6(8)
C7	7077(4)	5812.8(11)	1070(4)	65.6(9)
C13	1758(5)	2627.7(11)	7528(4)	71.6(9)
C8	6702(4)	5658.8(10)	2452(4)	59.6(8)
C5	8005(4)	5011.1(11)	659(4)	55.0(8)
O2'	3970(2)	3296.1(6)	2943(2)	51.7(5)
C12	2015(4)	3110.6(11)	1908(3)	64.2(8)
C6'	7376(4)	3475.3(10)	7498(4)	55.8(8)

Table S5. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for HIF-13. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O4'	88.1(16)	72.3(14)	46.0(12)	0.7(10)	29.9(12)	-22.0(12)
C1'	40.3(15)	32.7(14)	50.0(17)	4.5(12)	13.6(13)	3.3(12)
O2	96.3(17)	56.0(14)	84.7(16)	-2.0(11)	55.4(14)	13.9(11)
C3'	44.6(16)	36.8(15)	42.7(16)	-1.1(11)	15.0(13)	-3.2(12)
C2'	41.5(15)	33.5(14)	36.6(15)	1.9(11)	10.1(12)	2.6(12)
C3	30.8(14)	42.0(16)	52.5(16)	1.3(12)	15.2(12)	-0.6(11)
C4	40.2(16)	45.0(18)	52.9(17)	-7.6(13)	17.9(14)	-1.0(13)
C11	37.1(15)	42.4(17)	71.9(19)	6.2(14)	19.0(14)	-0.9(12)
C10	30.8(14)	47.4(17)	52.9(17)	-0.3(13)	19.1(13)	-1.7(12)
C4'	62.2(19)	36.6(15)	42.8(17)	4.5(12)	21.2(15)	0.5(13)
O1	79.0(14)	43.3(12)	84.4(14)	9.3(10)	57.1(12)	7(1)
C9	38.8(15)	46.2(17)	63.6(19)	7.3(14)	25.6(14)	-4.1(13)
C2	59.5(18)	43.4(17)	65.5(19)	8.3(14)	35.6(16)	3.1(14)
C6	48.4(18)	74(2)	64(2)	19.8(17)	21.6(16)	0.6(16)
C5'	57.5(19)	50.2(18)	38.9(16)	1.8(13)	4.7(14)	-4.7(14)
C7	47.9(19)	55(2)	87(2)	20.4(18)	23.0(17)	0.0(15)
C13	86(2)	67(2)	69(2)	-5.4(16)	40.4(19)	-25.9(18)
C8	55.8(19)	45.0(19)	86(2)	6.3(15)	38.1(17)	2.4(14)
C5	44.8(17)	64(2)	57.4(18)	0.6(15)	23.7(14)	-2.5(14)
O2'	50.3(12)	61.1(12)	39.6(11)	-2.0(8)	15.7(9)	-10.9(9)
C12	59.3(19)	82(2)	39.5(16)	-2.5(14)	10.0(14)	-14.7(16)
C6'	45.1(17)	42.6(17)	62(2)	3.7(14)	6.2(15)	-3.6(13)

Table S6. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for HIF-13.

Atom	*x*	*y*	*z*	U(eq)
H3'	2412.43	2925.89	4970.68	51
H3	5513.44	4153.32	3146.25	51
H11A	7682.49	3456.77	3811.5	62
H11B	9139.41	3724.23	5548.3	62
H2A	6789.86	4505.06	5953.84	64
H2B	8815.45	4620.87	5852.05	64
H6	8048.74	5605.09	-734.65	76
H5'	6950.68	3281.17	9634.9	65
H7	6867.47	6139.26	724.15	79
H13A	771.83	2857.79	6783.49	107
H13B	1340.04	2493.43	8375.63	107
H13C	1895.84	2368.87	6812.63	107
H8	6248.6	5879.7	3044.13	72
H5	8427.65	4792.65	37.17	66
H12A	1972.86	2769.62	2165.78	96
H12B	1685.94	3150.22	672.66	96
H12C	1061.55	3286.38	2185.77	96
H6'	8632.8	3613.95	8150.54	67

Table S7. Molecular pairs and interaction energies (kJ/mole) obtained from energy framework calculations for seven 3-benzylchroman-4-one structures. N is the number of pairs, and R is the distance between molecular centroids (Å). E_{ele}, E_{pol}, E_{disp}, and E_{rep} represent the energy components of electrostatic, polarization, dispersion, and exchange-repulsion, respectively, and E_{tot} is calculated as $E_{tot} = k_{ele}E_{ele} + k_{pol}E_{pol} + k_{disp}E_{disp} + k_{rep}E_{rep}$. Total energies are reported only for two benchmarked energy models, are the sum of the four energy components, scaled appropriately. The energy model CE-B3LYP … B3LYP /6-31G (d, p) is used to compare electron densities with the scale factors 1.057 (k_{ele}), 0.740 (k_{pol}), 0.871 (k_{disp}), and 0.618 (k_{rep}).

N	Symop	R	E_ele	E_pol	E_dis	E_rep	E_tot
HIF-4							
1	-x, -y, -z	7.36	-100.5	-26.0	-25.7	100.9	-85.5
1	-x, y+1/2, -z+1/2	5.59	-11.9	-1.7	-52.0	31.6	-39.6
0	-x, -y, -z	8.68	-0.8	-0.7	-31.2	15.2	-19.1
0	-x, -y, -z	7.56	-4.1	-1.0	-20.1	12.1	-15.1
1	x, -y+1/2, z+1/2	7.08	-0.5	-1.8	-14.4	6.4	-10.4
HIF-13							
N	-x, -y, -z	5.78	-17.0	-2.6	-54.5	37.8	-44.0
1	-x, -y, -z	8.38	-5.2	-1.6	-51.5	25.2	-35.9
1	-x, -y, -z	7.57	-9.2	-1.5	-48.2	31.2	-33.6
1	x, y, z	7.39	-7.9	-2.3	-17.8	8.3	-20.4
1	-x, -y, -z	12.15	-7.2	-1.2	-15.2	12.0	-14.3
1	x, y, z	8.36	-1.7	-2.5	-17.7	8.6	-13.8
AFAYIR							
2	x+1/2, -y+1/2, z+1/2	9.69	-56.8	-18.0	-17.7	55.8	-54.3
1	-x, -y, -z	5.20	-16.1	-5.3	-55.1	28.1	-51.6
2	x, y, z	5.26	-45.8	-6.4	-61.7	126.9	-28.4
1	-x, -y, -z	5.66	-7.3	-1.6	-43.6	34.3	-25.6
2	-x+1/2, y+1/2, -z+1/2	9.35	-4.8	-1.1	-16.2	7.0	-15.6
2	x+1/2, -y+1/2, z+1/2	9.13	-12.6	-3.1	-24.6	38.1	-13.5
AFEWAL							
1	-x, -y, -z	6.90	-20.1	-8.4	-59.5	59.5	-42.6

1	x, y, z	6.58	-12.5	-8.0	-41.9	31.9	-35.9
1	-x, -y, -z	5.78	-7.1	-1.5	-51.8	33.1	-33.4
2	-x+1/2, y+1/2, -z+1/2	10.52	-3.3	-0.9	-11.2	5.4	-10.5
LERYEO							
2	x, y, z	5.45	-11.3	-3.0	-51.9	26.2	-43.2
1	-x+1/2, -y+1/2, -z	5.85	-12.9	-2.4	-48.1	36.5	-34.7
1	-x+1/2, -y+1/2, -z	5.76	-8.3	-1.1	-42.6	20.5	-34.0
2	-x+1/2, y+1/2, -z+1/2	6.30	-10.5	-4.5	-37.1	23.0	-32.5
1	-x, -y, -z	12.01	-3.9	-2.1	-14.2	4.0	-15.5
ECUFUG							
2	x, y, z	4.65	-9.3	-2.4	-57.5	30.6	-42.8
2	x+1/2, -y+1/2, z+1/2	5.50	-5.9	-1.3	-35.0	17.9	-26.6
2	x+1/2, -y+1/2, z+1/2	6.38	-7.1	-2.8	-22.4	13.6	-20.6
ECUFOA							
1	-x, -y, -z	6.66	-25.5	-6.1	-44.0	34.5	-48.5
1	-x, -y, -z	5.22	-15.5	-3.2	-59.7	43.8	-43.6
2	-x+1/2, y+1/2, -z+1/2	10.38	-38.0	-8.8	-16.5	36.2	-38.7
1	-x, -y, -z	5.85	-12.5	-2.6	-53.7	38.6	-38.0
1	-x, -y, -z	7.17	-9.4	-4.0	-44.1	25.6	-35.4
2	x, y, z	6.48	-11.0	-4.7	-38.4	24.5	-33.5

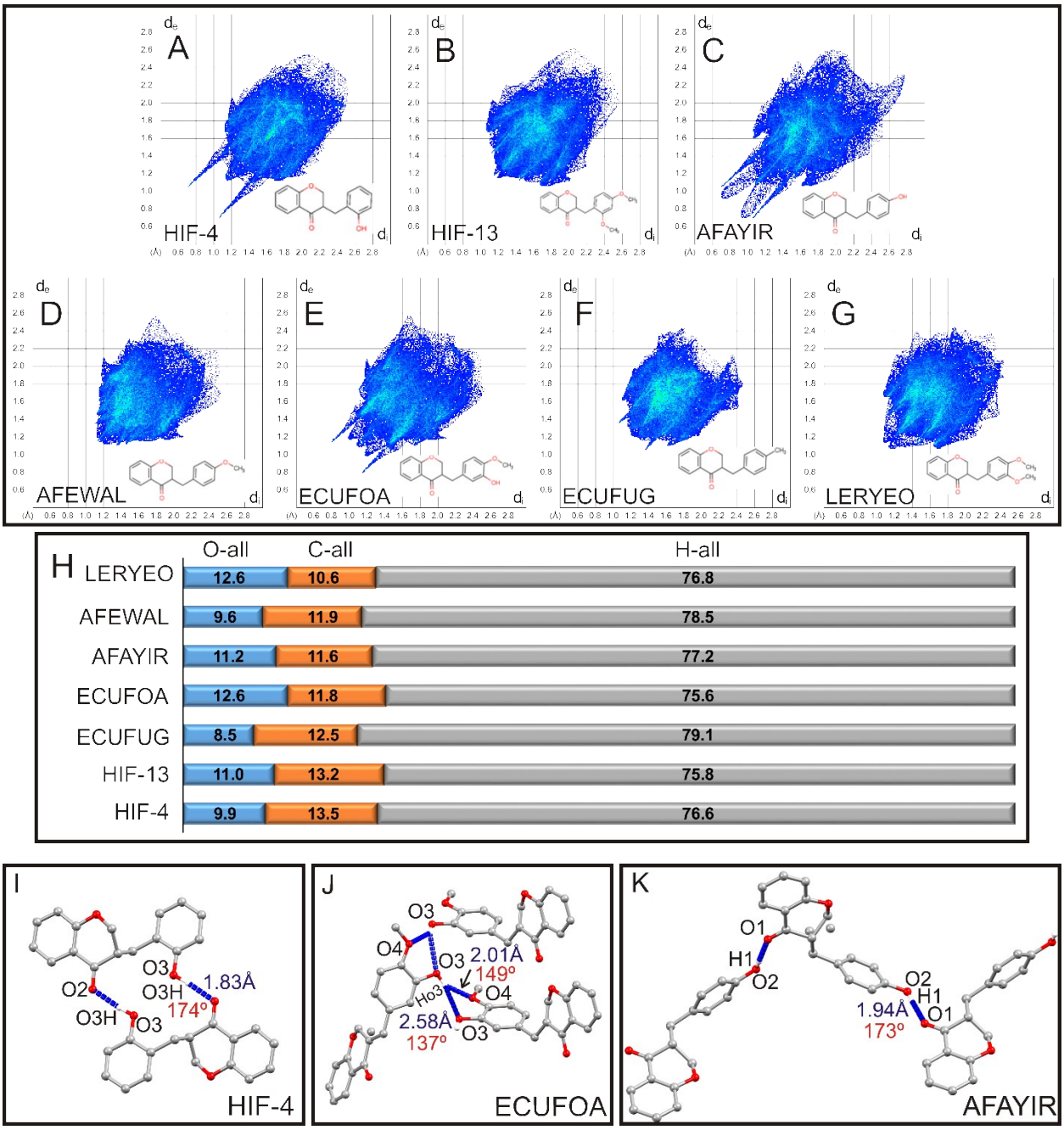

Figure S1. Intermolecular interactions of 3-benzylchroman-4-ones. 2D finger plot of full for (A) HIF-4, (B) HIF-13, (C) AFAYIR, (D) AFEWAL (E) ECUFOA, (F) ECUFUG, and (G) LERYEO. The chemical diagram of each structure is shown in the inset. (H) Percentage of contribution to the Hirshfeld surface area for carbon, oxygen, and hydrogen contacts for seven 3-benzylchroman-4-ones structures. O-H…O intermolecular interactions of HIF-4 (I), ECUFOA (J), and AFAYIR (K) are shown. The hydrogen bonds are shown in dotted lines, and the corresponding atoms, distance, and angles are marked. The hydrogen atoms, which are not involved in the O-H…O interactions, are omitted for clarity.

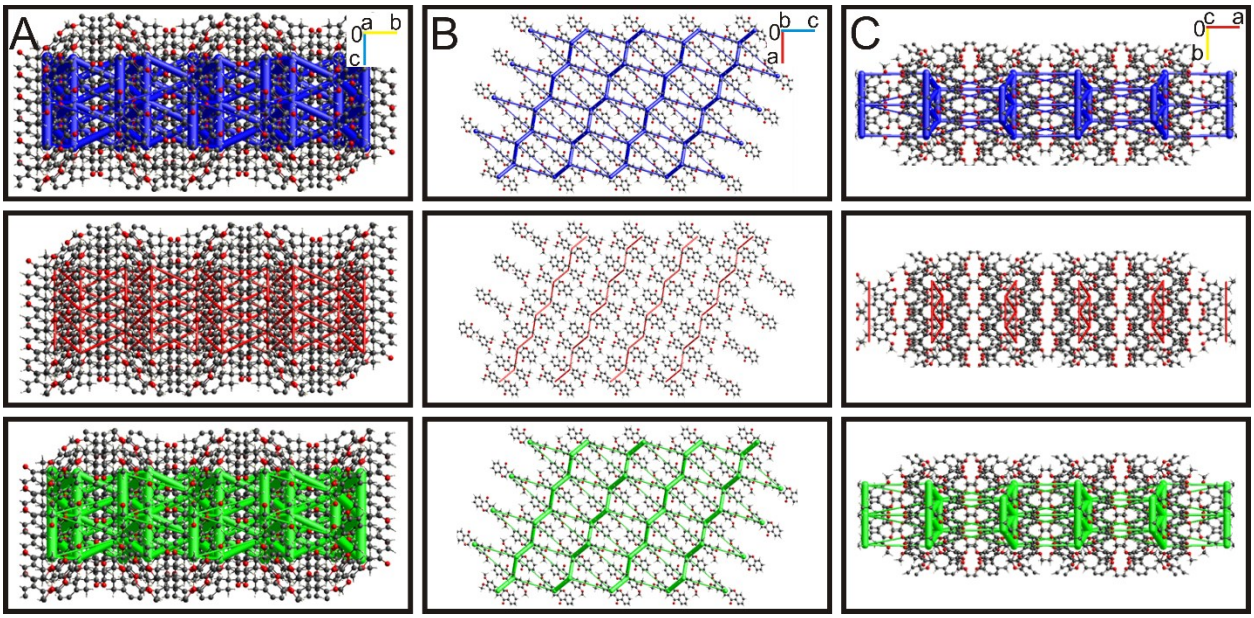

Figure S2. Energy frameworks for LERYEO. The molecular arrangement of LERYEO is viewed down the *a* (A, D, and G), *b* (B, E, and H), and *c* (C, F, and I) directions. The models are shown in ball-and-stick representation. The total interaction energies (A-C), electrostatic terms (D-F), and dispersion energy terms (G-I) are shown in blue, red, and green colors, respectively.

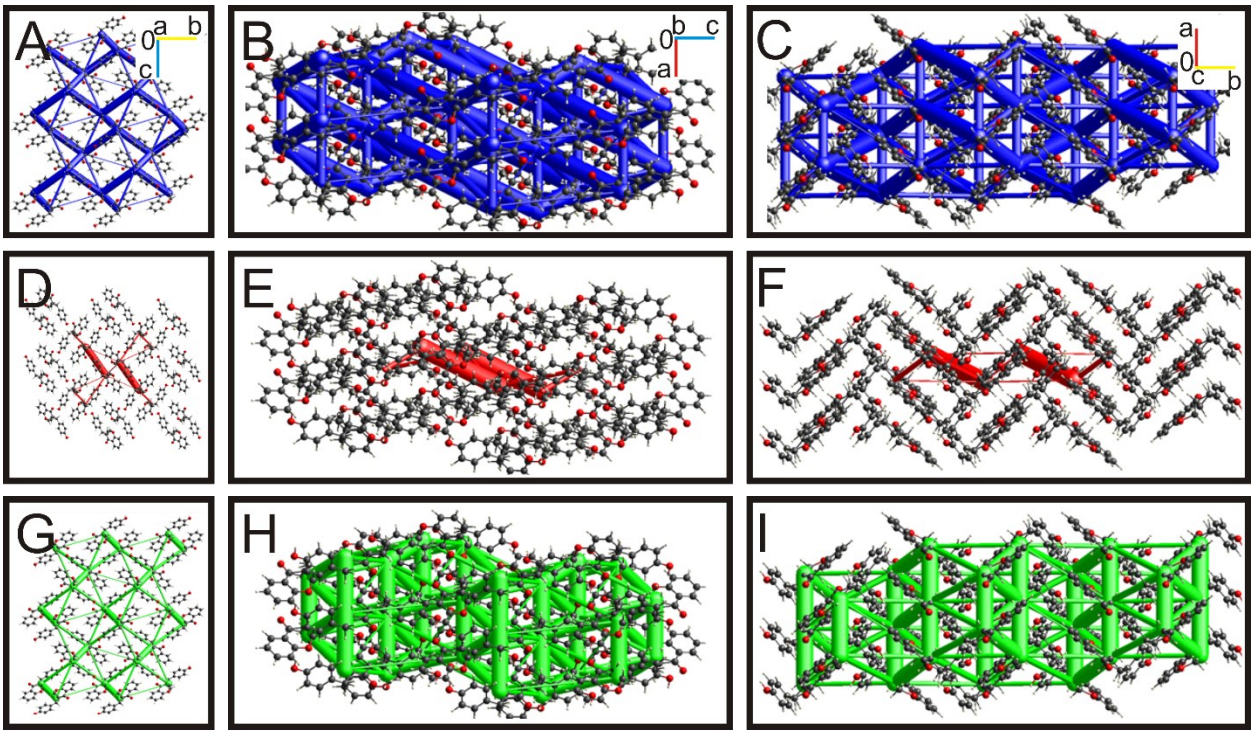

Figure S3. Energy frameworks for AFAYIR. The molecular arrangement of AFAYIR is viewed down the *a* (A, D, and G), *b* (B, E, and H), and *c* (C, F, and I) directions. The models are shown in ball-and-stick representation. The total interaction energies (A-C), electrostatic terms (D-F), and dispersion energy terms (G-I) are shown in blue, red, and green colors, respectively.

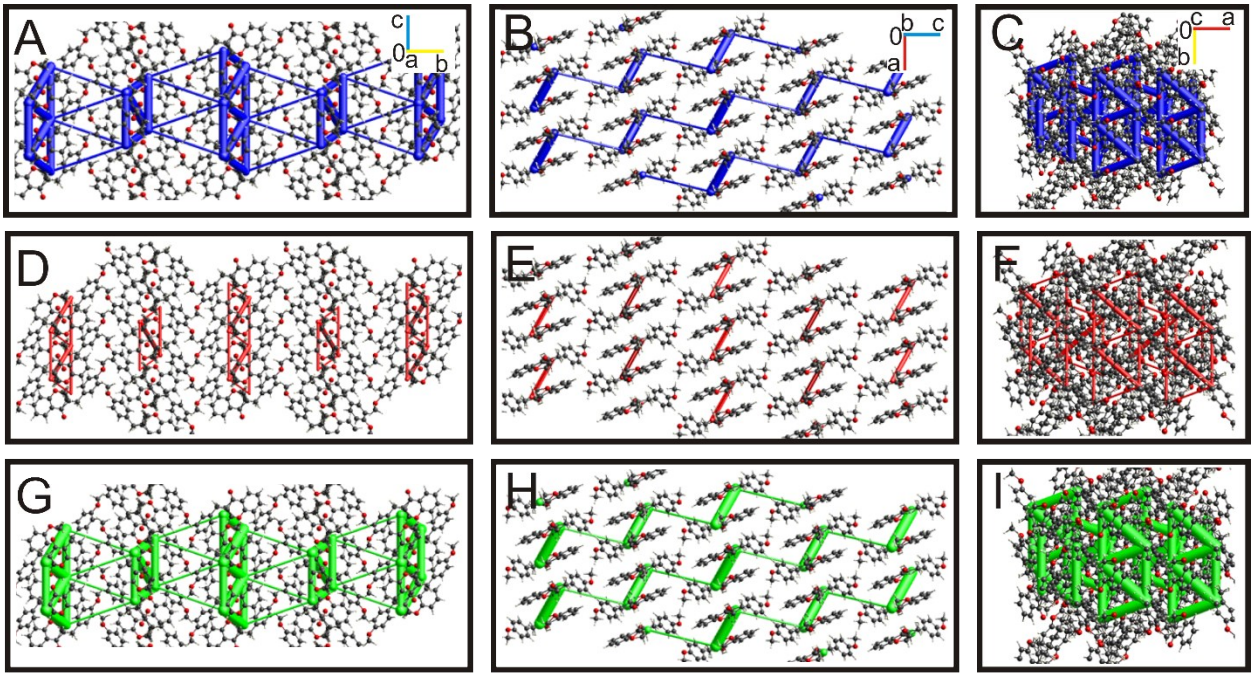

Figure S4. Energy frameworks for AFEWAL. The molecular arrangement of AFEWAL is viewed down the *a* (A, D, and G), *b* (B, E, and H), and *c* (C, F, and I) directions. The models are shown in ball-and-stick representation. The total interaction energies (A-C), electrostatic terms (D-F), and dispersion energy terms (G-I) are shown in blue, red, and green colors, respectively.

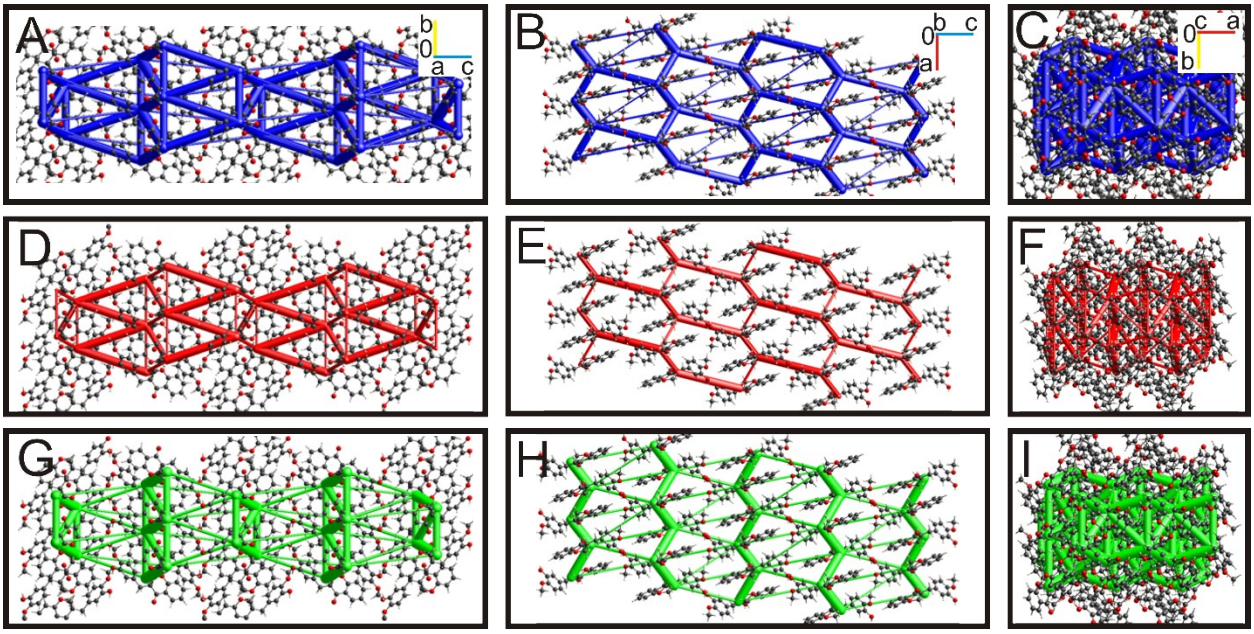

Figure S5. Energy frameworks for ECUFOA. The molecular arrangement of ECUFOA is viewed down the *a* (A, D, and G), *b* (B, E, and H), and *c* (C, F, and I) directions. The models are shown

in ball-and-stick representation. The total interaction energies (A-C), electrostatic terms (D-F), and dispersion energy terms (G-I) are shown in blue, red, and green colors, respectively.

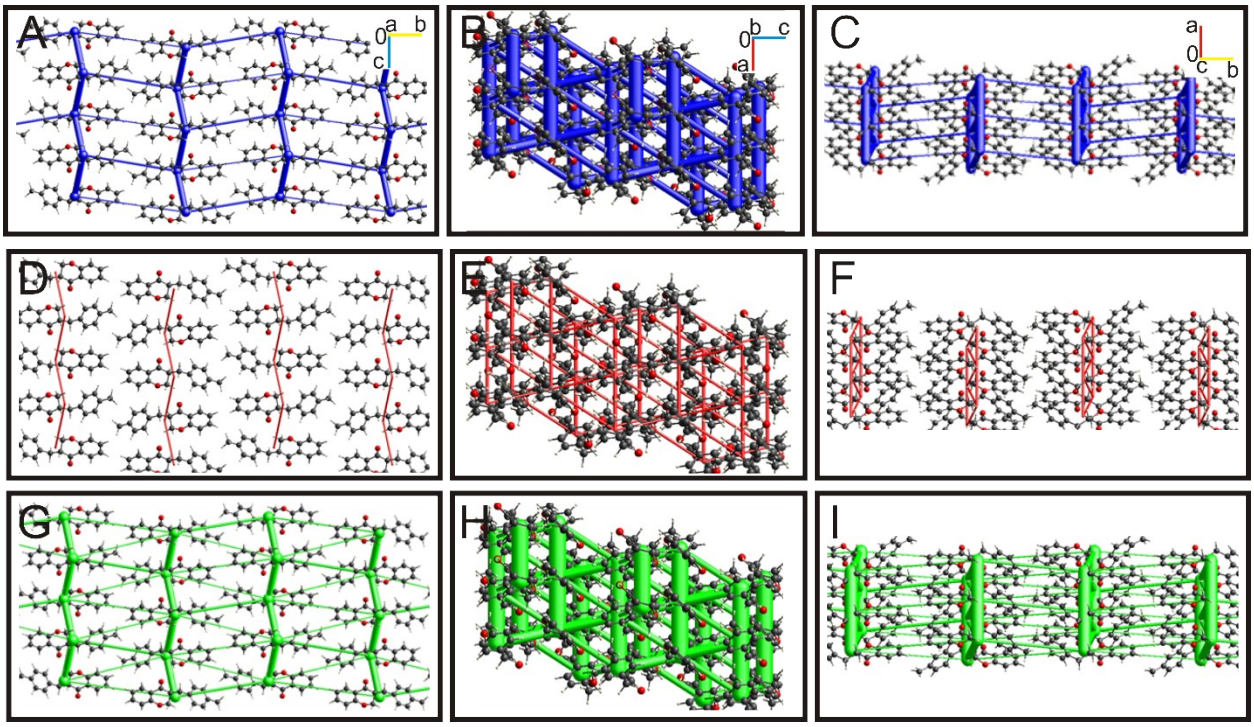

Figure S6. Energy frameworks for ECUFUG. The molecular arrangement of ECUFUG is viewed down the *a* (A, D, and G), *b* (B, E, and H), and *c* (C, F, and I) directions. The models are shown in ball-and-stick representation. The total interaction energies (A-C), electrostatic terms (D-F), and dispersion energy terms (G-I) are shown in blue, red, and green colors, respectively.