Supporting Information for "Probing Non-covalent Interactions Driving Molecular Assembly in Organo-electronic Building Blocks"

Sarah N. Johnson,[a] Thomas L. Ellington,[a] Duong Ngo,[a] Jorge Nevarez,[a] Nicholas Sparks,[a] Arnold L. Rheingold,[b] and Davita L. Watkins,[a] Gregory S. Tschumper[a]*

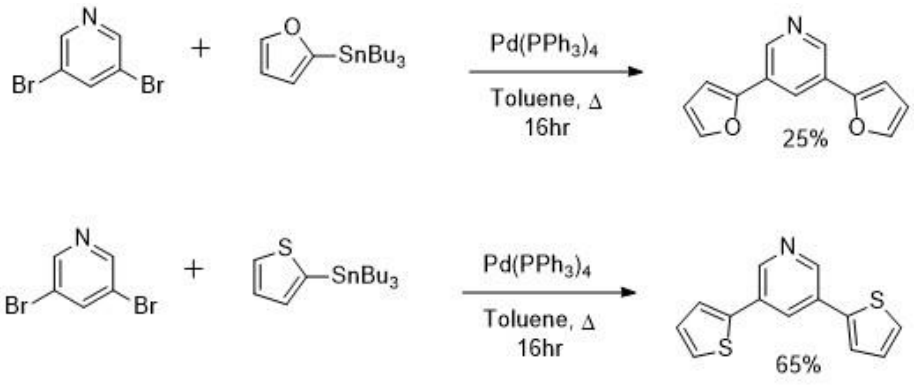
[a] Department of Chemistry and Biochemistry, University of Mississippi, University, MS 38677-1848, USA

[b] Department of Chemistry, University of California, San Diego, La Jolla, CA 92093-0358, USA

*To whom correspondence should be addressed:

Table of Contents Pages

General Summary: Reagents and solvents were purchased from commercial sources and used without further purification unless otherwise specified. DMF was degassed in 20 L drums and passed through two sequential purification columns (activated alumina; molecular sieves for DMF) under a positive argon atmosphere. Thin layer chromatography (TLC) was performed on SiO_2-60 F254 aluminum plates with visualization by UV light or staining. Flash column chromatography was performed using Purasil SiO_2-60, 230–400 mesh from Fisher. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker Avance-300 (300 MHz), Bruker Avance DRX-500 (500 MHz spectrometer and are reported in ppm using solvent as an internal standard ($CDCl_3$ at 7.26 ppm). Data reported as: s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, m = multiplet, b = broad, ap = apparent; coupling constant(s) in Hz; integration.



Scheme S1. Synthesis of pyridine XB acceptors

Synthesis of 3,5-di(furan-2-yl)pyridine. To a flame dried RBF equipped with a stir bar, 1 equivalence (8.44 mmol) of 3,5-dibromopyridine was added followed by 0.05 equivalence (0.422 mmol) of $Pd(PPh_3)_4$. The RBF was then put under an inert atmosphere of N_2. The solid reagents were then dissolved in dry toluene after which 2.2 equivalence (18.57 mmol) of 2-(tributylstannyl)furan was added. The reaction was allowed to run for 12 hours at the reflux temperature of 110 ºC. After 12 hours, the reaction mixture was cooled to room temperature and 100 mL of $NaHCO_3$ was added to quench the reaction. Ethyl acetate was used to extract the compound and the organic layer was then washed with 100 mL of DI water three times. The organic layer was then separated and dried over Na_2SO_4. The organic solvent was then removed by rotary evaporation to afford a yellow solid. The compound was then purified by column chromatography using silica gel as the stationary phase and a 1:1 mixture of hexanes and ethyl acetate as the mobile phase to afford 0.444 grams (25% yield) of pure 3,5-di(furan-2-yl)pyridine. ^{1}H NMR (500 MHz-$CDCl_3$) δ= 8.81 (s, 2H), 8.18 (s, 1H), 7.55 (d, 2H), 6.80 (d, 2H), 6.53 (t, 2H); ^{13}C NMR (300 MHz-$CDCl_3$) δ= 150.84, 143.79, 143.18, 126.74, 125.38, 111.94, 106.84

Synthesis of 3,5-di(thiophen-2-yl)pyridine. To a flame dried RBF equipped with a stir bar, 1 equivalence (4.51 mmol) of 3,5-dibromopyridine was added followed by 0.1 equivalence (0.451 mmol) of $Pd(PPh_3)_4$. The RBF was then put under an inert atmosphere of N_2. The solid reagents were then dissolved in dry toluene after which 2.2 equivalence (9.92 mmol) of 2-(tributylstannyl)thiophene was added. The reaction was allowed to run for 12 hours at the reflux temperature of 110 ºC. After 12 hours, the reaction mixture was cooled to room temperature and 100 mL of $NaHCO_3$ was added to quench the reaction. Ethyl acetate was used to extract the compound and the organic layer was then washed with 100 mL of DI water three times. The organic

layer was then separated and dried over Na_2SO_4. The organic solvent was then removed by rotary evaporation to afford a yellow solid. The compound was then purified by column chromatography using silica gel as the stationary phase and a 1:1 mixture of hexanes and ethyl acetate as the mobile phase to afford 0.7149 grams (65% yield) of pure 3,5-di(thiophen-2-yl)pyridine. ^{1}H NMR (500 MHz-$CDCl_3$) δ= 8.78 (s, 2H), 8.02 (s, 1H), 7.41 (d, 2H), 7.39 (d, 2H), 7.15 (t, 2H); ^{13}C NMR (300 MHz-$CDCl_3$) δ= 145.58, 139.88, 130.37, 129.88, 128.28, 126.25, 124.54

Preliminary Investigation of Co-crystals

Table S1. Summary of preliminary investigation of co-crystals

	Infrared (cm^{-1})			Thermal (^{o}C)		
	XB donor C≡ C_{sp}-I	**Co-crystal**	**Shift Δ**	**Melting**	**DTA**	**Weight Loss**
F_5BAI- PyrThio$_2$	2185	2167	-18	124.5 – 130.8	128.4	107.5
F_5BAI- PyrFur$_2$	2185	2168	-17	112.3 – 113.8	111.5	111.0

Spectroscopic Analysis Infrared Spectroscopy

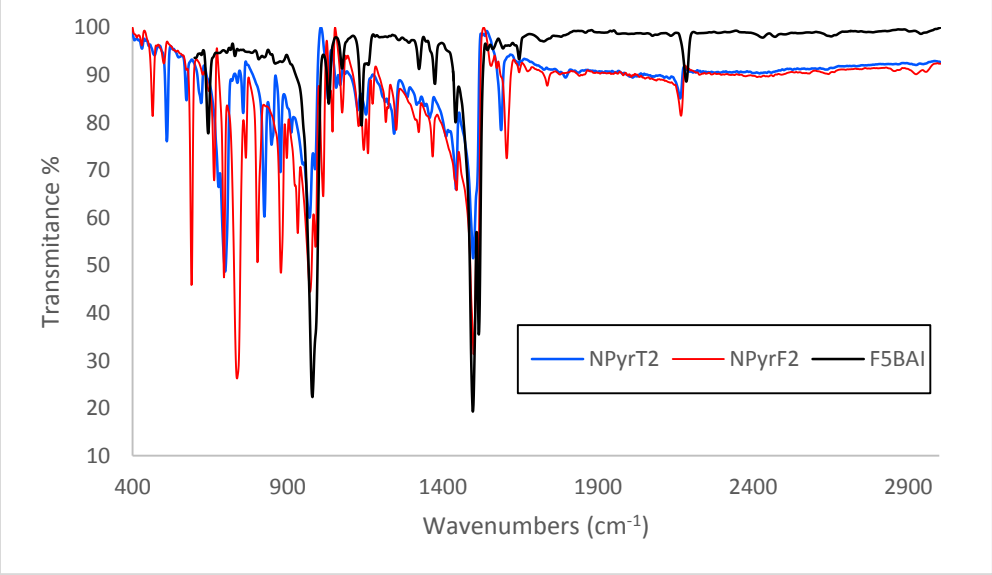


Figure S1. Infrared spectra of F_5BAI and co-crystals

Thermal Analysis

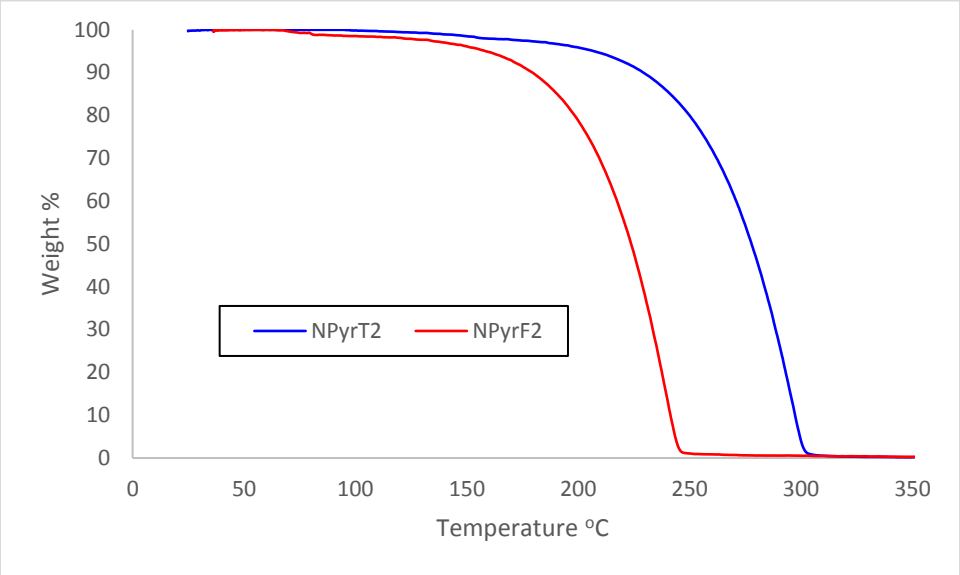


Figure S2. TGA of neat XB acceptors

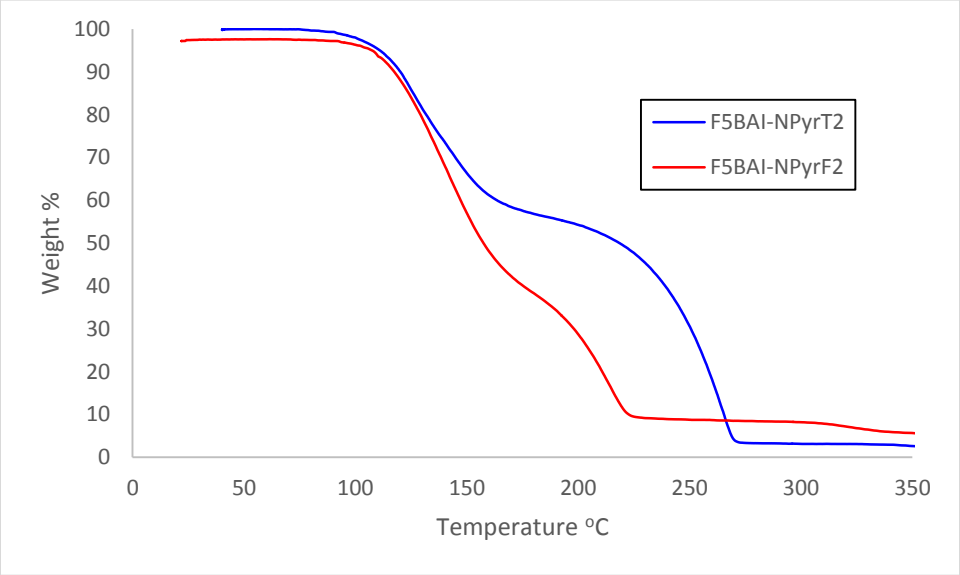


Figure S3. TGA of co-crystals

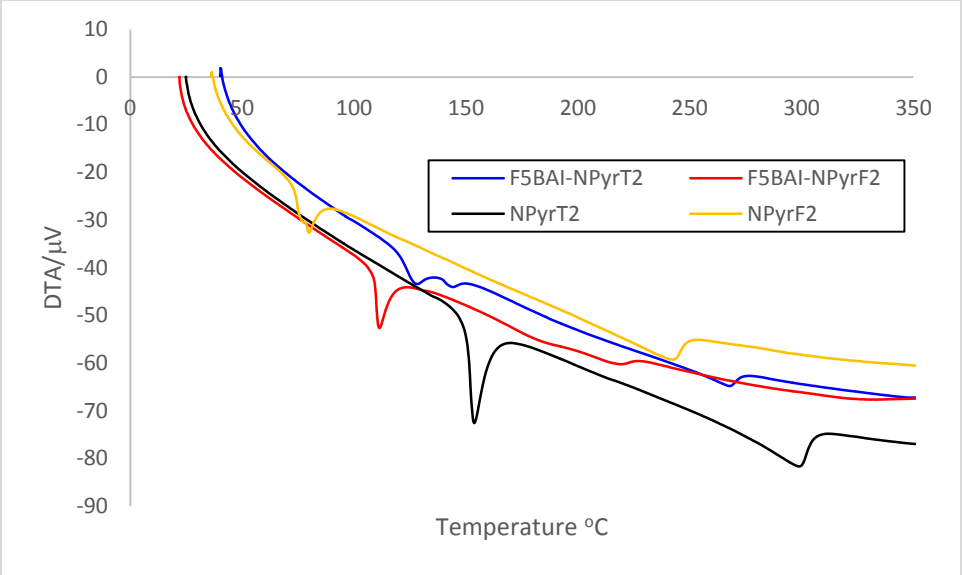


Figure S4. DTA of co-crystals and neat XB acceptors

Computational Results

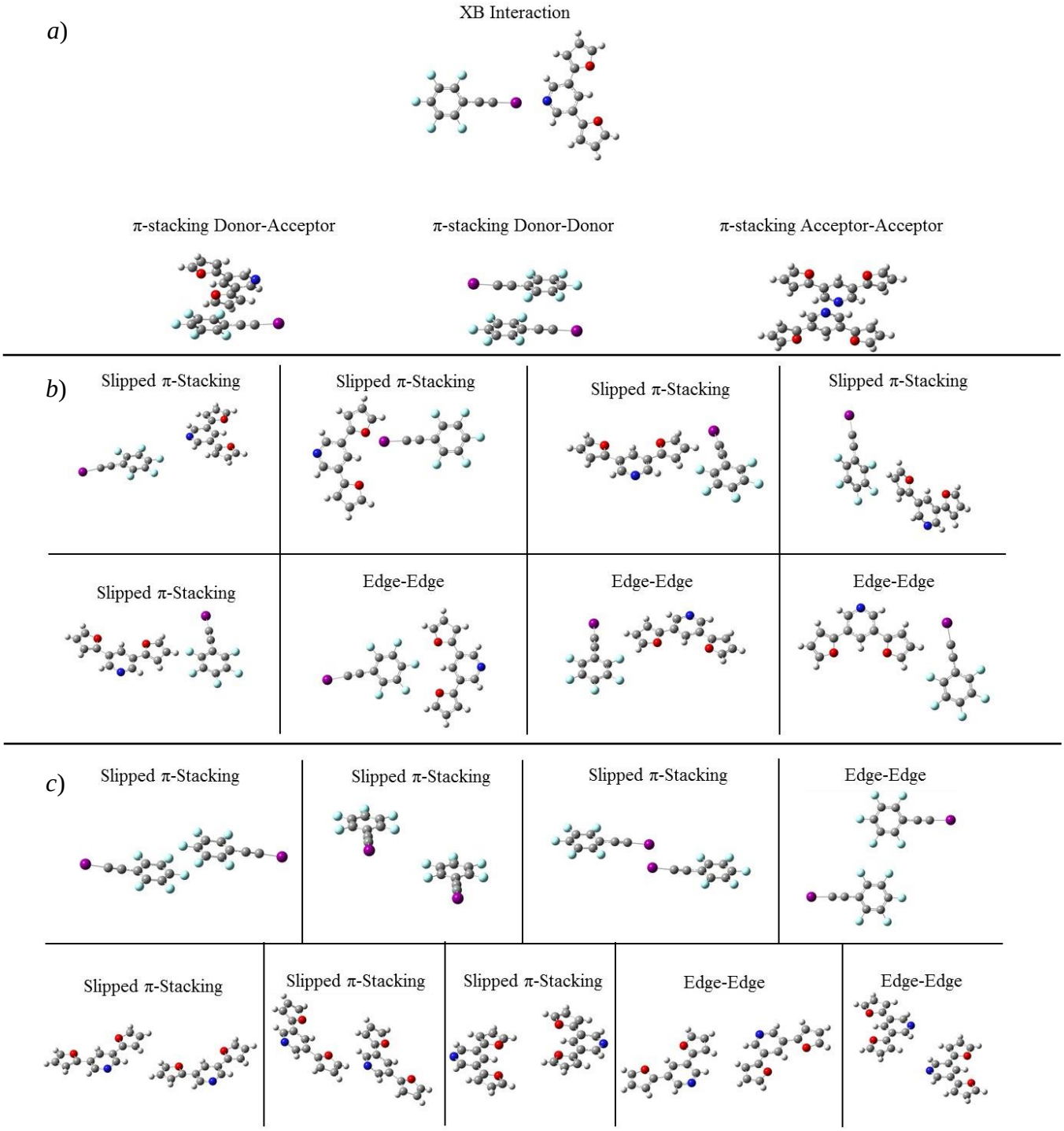


Figure S5. Pictorial representations of all pair-wise contacts characterized in the **F_5BAI-PyrFur$_2$** co-crystal, where the dominant interactions are shown in *a*, minor heterogeneous interactions in *b* and minor homogeneous interactions in *c*.

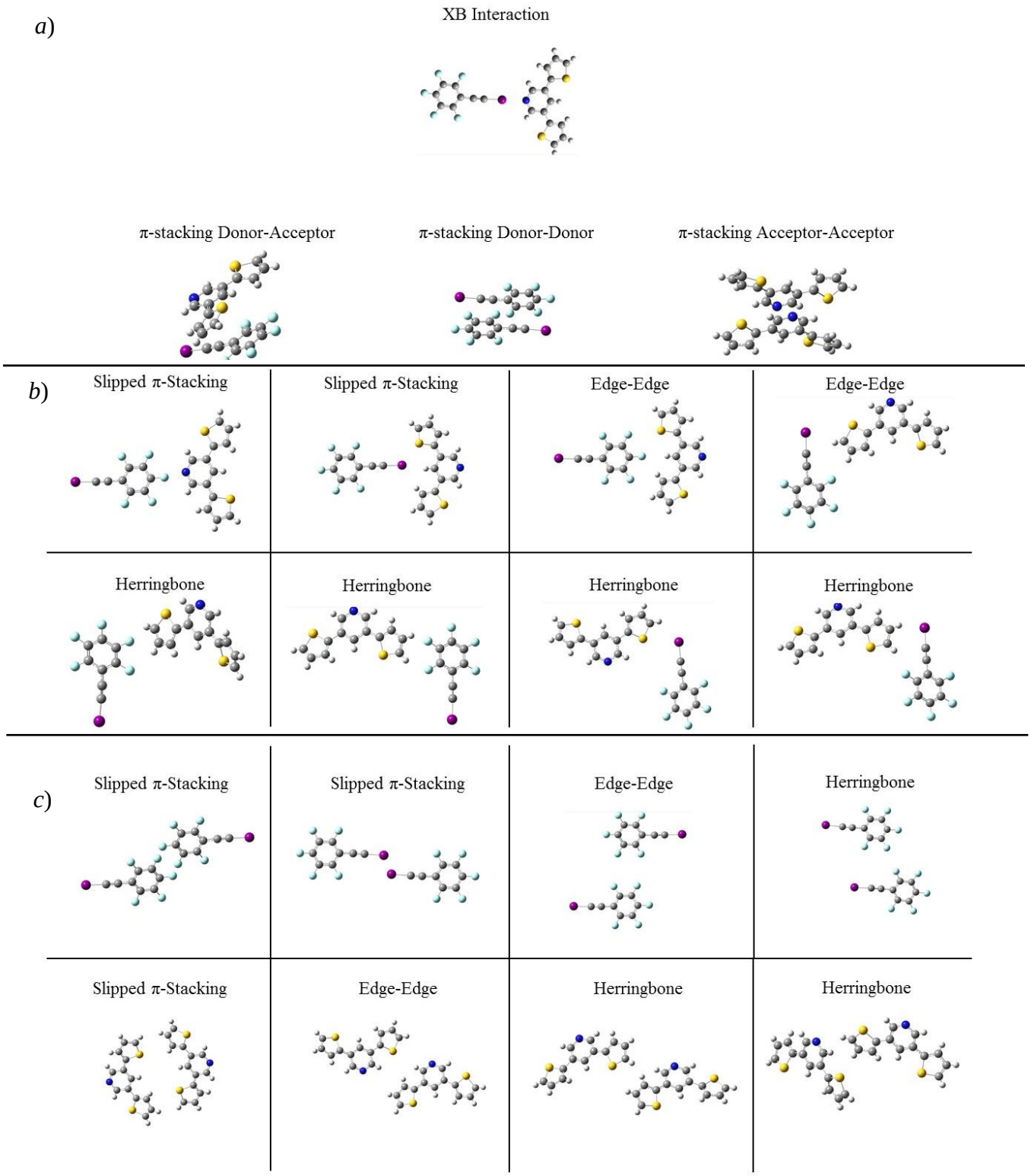


Figure S6. Pictorial representations of all pair-wise contacts characterized in the **F_5BAI-PyrThio$_2$** co-crystal with torsional angles $\tau_\alpha = 171°$ and $\tau_\beta = -25°$, where the dominant interactions are shown in *a*, minor heterogeneous interactions in *b* and minor homogeneous interactions in *c*.

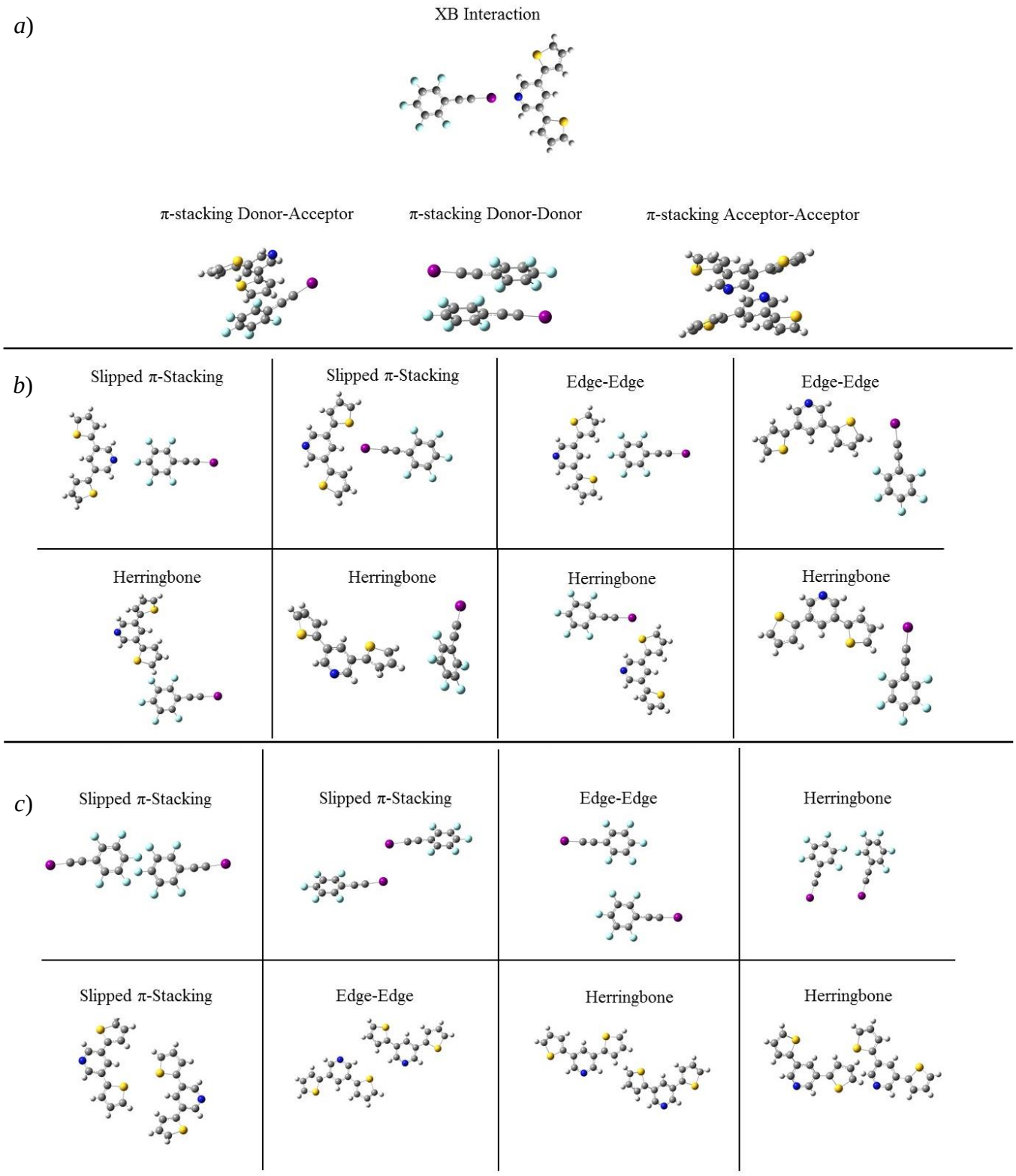


Figure S7. Pictorial representations of all pair-wise contacts characterized in the **F_5BAI-PyrThio$_2$** co-crystal with torsional angles τ_α = 166° and τ_β = 24°, where the dominant interactions are shown in *a*, minor heterogeneous interactions in *b* and minor homogeneous interactions in *c*.

Figure S8. Pictorial representations of all pair-wise contacts characterized in the **F_5BAI-PyrThio$_2$** co-crystal with torsional angles τ_α = 166° and τ_β = −163°, where the dominant interactions are shown in *a*, minor heterogeneous interactions in *b* and minor homogeneous interactions in *c*.

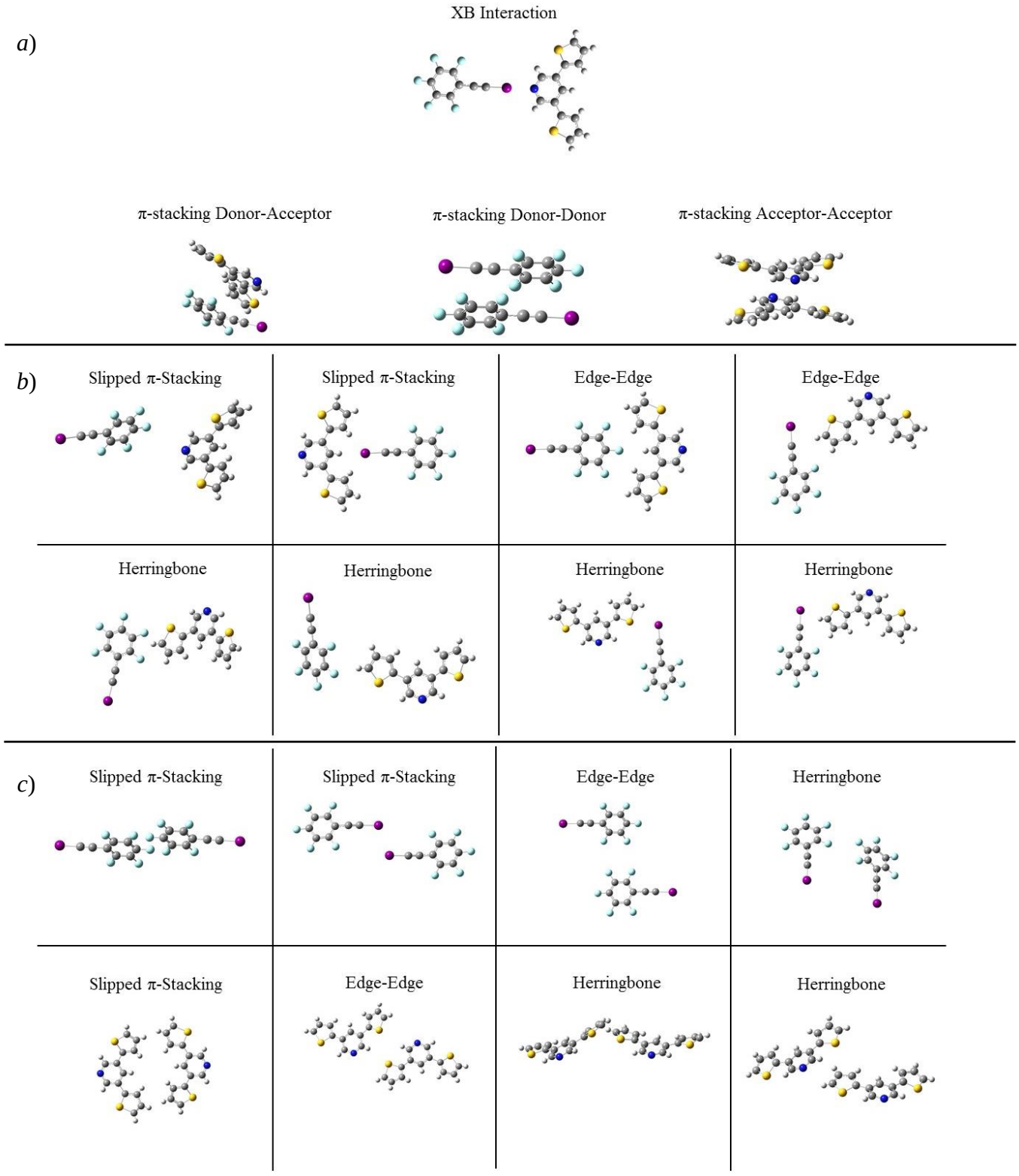


Figure S9. Pictorial representations of all pair-wise contacts characterized in the **F_5BAI-PyrThio$_2$** co-crystal with torsional angles $\tau_\alpha = -166°$ and $\tau_\beta = 163°$, where the dominant interactions are shown in *a*, minor heterogeneous interactions in *b* and minor homogeneous interactions in *c*.

Table S2. Summary of interaction energies (in kcal mol^{-1}) observed in the **F_5BAI-PyrFur$_2$** co-crystal (Figure S5).

Type	Identity	E_{int}	Eint (CP)	Average
Donor-Acceptor	XB	−7.6	−7.5	−7.6
Donor-Acceptor	π-Stacking	−7.3	−6.3	−6.8
Donor-Donor	π-Stacking	−7.7	−6.6	−7.2
Acceptor-Acceptor	π-Stacking	−8.7	−7.9	−8.3
Donor-Acceptor	Slipped π-Stacking	−2.1	−1.6	−1.8
Donor-Acceptor	Slipped π-Stacking	−1.1	−1.0	−1.0
Donor-Acceptor	Slipped π-Stacking	−0.4	−0.3	−0.3
Donor-Acceptor	Slipped π-Stacking	−0.1	−0.1	−0.1
Donor-Acceptor	Slipped π-Stacking	−0.1	0.0	0.0
Donor-Acceptor	Edge-Edge	−1.7	−1.5	−1.6
Donor-Acceptor	Edge-Edge	−1.4	−1.1	−1.3
Donor-Acceptor	Edge-Edge	−0.9	−0.7	−0.8
Donor-Donor	Slipped π-Stacking	−2.4	−1.8	−2.1
Donor-Donor	Slipped π-Stacking	−0.1	−0.1	−0.1
Donor-Donor	Slipped π-Stacking	−0.1	0.0	−0.1
Donor-Donor	Edge-Edge	−0.5	−0.3	−0.4
Acceptor-Acceptor	Slipped π-Stacking	−1.9	−1.7	−1.8
Acceptor-Acceptor	Slipped π-Stacking	−0.9	−0.8	−0.9
Acceptor-Acceptor	Slipped π-Stacking	−0.1	0.0	−0.1
Acceptor-Acceptor	Edge-Edge	−0.6	−0.5	−0.6
Acceptor-Acceptor	Edge-Edge	−0.4	−0.3	−0.3

CP = Boys-Bernardi procedure

Table S3. Summary of interaction energies (in kcal mol^{-1}) observed in the **F_5BAI-PyrThio$_2$** co-crystal with torsional angles τ_α = 171° and τ_β = −25° (Figure S6).

Type	Identity	E_{int}	Eint (CP)	Average
Donor-Acceptor	XB	−7.5	−7.4	−7.4
Donor-Acceptor	π-Stacking	−9.5	−8.3	−8.9
Donor-Donor	π-Stacking	−8.7	−7.5	−8.1
Acceptor-Acceptor	π-Stacking	−11.7	−10.9	−11.3
Donor-Acceptor	Slipped π-Stacking	−0.7	−0.7	−0.7
Donor-Acceptor	Slipped π-Stacking	−0.3	−0.2	−0.3
Donor-Acceptor	Edge-Edge	−1.8	−1.5	−1.7
Donor-Acceptor	Edge-Edge	−1.2	−1.0	−1.1
Donor-Acceptor	Herringbone	−1.4	−1.2	−1.3
Donor-Acceptor	Herringbone	−0.9	−0.6	−0.8
Donor-Acceptor	Herringbone	−0.5	−0.3	−0.4
Donor-Acceptor	Herringbone	−0.3	−0.3	−0.3
Donor-Donor	Slipped π-Stacking	−2.3	−1.8	−2.1
Donor-Donor	Slipped π-Stacking	−0.2	−0.1	−0.1
Donor-Donor	Edge-Edge	−0.2	−0.1	−0.1
Donor-Donor	Herringbone	−0.1	0.0	−0.1
Acceptor-Acceptor	Slipped π-Stacking	−0.1	0.0	0.0
Acceptor-Acceptor	Edge-Edge	−1.1	−1.0	−1.0
Acceptor-Acceptor	Herringbone	−2.1	−1.9	−2.0
Acceptor-Acceptor	Herringbone	−1.0	−0.8	−0.9

CP = Boys-Bernardi procedure

Table S4. Summary of interaction energies (in kcal mol^{-1}) observed in the **F_5BAI-PyrThio$_2$** co-crystal with torsional angles τ_α = 166° and τ_β = 24° (Figure S7).

Type	Identity	E_{int}	Eint (CP)	Average
Donor-Acceptor	XB	−7.5	−7.3	−7.4
Donor-Acceptor	π-Stacking	−9.2	−8.1	−8.6
Donor-Donor	π-Stacking	−8.7	−7.6	−8.1
Acceptor-Acceptor	π-Stacking	−11.3	−10.5	−10.9
Donor-Acceptor	Slipped π-Stacking	−0.8	−0.7	−0.7
Donor-Acceptor	Slipped π-Stacking	−0.3	−0.2	−0.3
Donor-Acceptor	Edge-Edge	−1.9	−1.5	−1.7
Donor-Acceptor	Edge-Edge	−1.8	−1.6	−1.7
Donor-Acceptor	Herringbone	−1.4	−1.2	−1.3
Donor-Acceptor	Herringbone	−0.5	−0.3	−0.4
Donor-Acceptor	Herringbone	−0.5	−0.3	−0.4
Donor-Acceptor	Herringbone	−0.3	−0.2	−0.3
Donor-Donor	Slipped π-Stacking	−2.3	−1.8	−2.1
Donor-Donor	Slipped π-Stacking	−0.2	−0.1	−0.1
Donor-Donor	Edge-Edge	−0.2	−0.1	−0.1
Donor-Donor	Herringbone	−0.1	0.0	−0.1
Acceptor-Acceptor	Slipped π-Stacking	−0.2	−0.1	−0.1
Acceptor-Acceptor	Edge-Edge	−1.2	−1.0	−1.1
Acceptor-Acceptor	Herringbone	−1.8	−1.5	−1.6
Acceptor-Acceptor	Herringbone	−1.0	−0.8	−0.9

CP = Boys-Bernardi procedure

Table S5. Summary of interaction energies (in kcal mol^{-1}) observed in the **F_5BAI-PyrThio$_2$** co-crystal with torsional angles τ_α = 166° and τ_β = −163° (Figure S8).

Type	Identity	E_{int}	Eint (CP)	Average
Donor-Acceptor	XB	−7.4	−7.2	−7.3
Donor-Acceptor	π-Stacking	−8.8	−7.7	−8.3
Donor-Donor	π-Stacking	−8.7	−7.5	−8.1
Acceptor-Acceptor	π-Stacking	−12.4	−11.6	−12.0
Donor-Acceptor	Slipped π-Stacking	−0.8	−0.7	−0.7
Donor-Acceptor	Slipped π-Stacking	−0.3	−0.2	−0.2
Donor-Acceptor	Edge-Edge	−2.2	−1.8	−2.0
Donor-Acceptor	Edge-Edge	−1.8	−1.6	−1.7
Donor-Acceptor	Herringbone	−1.5	−1.3	−1.4
Donor-Acceptor	Herringbone	−0.5	−0.3	−0.4
Donor-Acceptor	Herringbone	−0.4	−0.1	−0.2
Donor-Acceptor	Herringbone	−0.3	−0.2	−0.2
Donor-Donor	Slipped π-Stacking	−2.3	−1.8	−2.1
Donor-Donor	Slipped π-Stacking	−0.2	−0.1	−0.1
Donor-Donor	Edge-Edge	−0.2	−0.1	−0.1
Donor-Donor	Herringbone	−0.1	0.0	−0.1
Acceptor-Acceptor	Slipped π-Stacking	−0.2	−0.2	−0.2
Acceptor-Acceptor	Edge-Edge	−1.2	−1.1	−1.1
Acceptor-Acceptor	Herringbone	−1.7	−1.5	−1.6
Acceptor-Acceptor	Herringbone	−0.4	−0.3	−0.4

CP = Boys-Bernardi procedure

Table S6. Summary of interaction energies (in kcal mol^{-1}) observed in the **F_5BAI-PyrThio$_2$** co-crystal with torsional angles $\tau_\alpha = -166°$ and $\tau_\beta = 163°$ (Figure S9).

Type	Identity	E_{int}	Eint (CP)	Average
Donor-Acceptor	XB	−7.4	−7.2	−7.3
Donor-Acceptor	π-Stacking	−8.8	−7.7	−8.3
Donor-Donor	π-Stacking	−8.7	−7.5	−8.1
Acceptor-Acceptor	π-Stacking	−12.4	−11.6	−12.0
Donor-Acceptor	Slipped π-Stacking	−0.8	−0.7	−0.7
Donor-Acceptor	Slipped π-Stacking	−0.3	−0.2	−0.2
Donor-Acceptor	Edge-Edge	−2.2	−1.8	−2.0
Donor-Acceptor	Edge-Edge	−1.8	−1.6	−1.7
Donor-Acceptor	Herringbone	−1.5	−1.3	−1.4
Donor-Acceptor	Herringbone	−0.5	−0.3	−0.4
Donor-Acceptor	Herringbone	−0.4	−0.1	−0.2
Donor-Acceptor	Herringbone	−0.3	−0.2	−0.2
Donor-Donor	Slipped π-Stacking	−2.3	−1.8	−2.1
Donor-Donor	Slipped π-Stacking	−0.2	−0.1	−0.1
Donor-Donor	Edge-Edge	−0.2	−0.1	−0.1
Donor-Donor	Herringbone	−0.1	0.0	−0.1
Acceptor-Acceptor	Slipped π-Stacking	−0.2	−0.2	−0.2
Acceptor-Acceptor	Edge-Edge	−1.8	−1.6	−1.7
Acceptor-Acceptor	Herringbone	−1.7	−1.5	−1.6
Acceptor-Acceptor	Herringbone	−0.4	−0.3	−0.4

CP = Boys-Bernardi procedure

Table S7: Summary of intermolecular distances (Å) for the dominant interactions depicted in Figures S5(*a*) – S9(*a*).

	XB	Donor-Acceptor π-Stacking	Donor-Donor π-Stacking	Acceptor-Acceptor π-Stacking
F_5BAI-PyrFur$_2$	2.74	4.18	5.01	3.53
F_5BAI-PyrThio$_2$ **($\tau_\alpha = 171°$ & $\tau_\beta = -25°$)**	2.70	3.81	4.97	3.52
F_5BAI-PyrThio$_2$ **($\tau_\alpha = 166°$ & $\tau_\beta = 24°$)**	2.70	3.81	4.97	3.52
F_5BAI-PyrThio$_2$ **($\tau_\alpha = 166°$ & $\tau_\beta = -163°$)**	2.70	3.80	4.97	3.52
F_5BAI-PyrThio$_2$ **($\tau_\alpha = -166°$ & $\tau_\beta = 163°$)**	2.70	3.80	4.97	3.52

Table S8: Relative Energies (ΔE in kcal mol^{-1}) for the three different optimized (M06-2X/aug-cc-pVTZ-PP) conformations for PyrFur$_2$ and PyrThio$_2$, where τ_α and τ_β are defined in Figure 1 of the main article.

PyrFur$_2$			PyrThio$_2$		
τ_α	τ_β	ΔE (kcal mol^{-1})	τ_α	τ_β	ΔE (kcal mol^{-1})
0°	0°	0.00	27°	27°	0.00
180°	0°	+0.15	154°	27°	+0.05
180°	180°	+0.64	153°	153°	+0.20

Table S9: Summary of select interaction energies (in kcal mol^{-1}) observed in the **F_5BAI-PyrFur$_2$** co-crystal at the M06-2X/aug-cc-pVDZ-PP level of theory.

Type	Identity	E_{int}	Eint (CP)	Average
Donor-Acceptor	XB	−8.6	−7.8	−8.2
Donor-Acceptor	π-Stacking	−9.1	−6.7	−7.9
Donor-Donor	π-Stacking	-	-	-
Acceptor-Acceptor	π-Stacking	−12.0	−8.7	−10.4
Donor-Acceptor	Slipped π-Stacking	−2.7	−1.7	−2.2
Donor-Acceptor	Slipped π-Stacking	−1.5	−1.1	−1.3
Donor-Acceptor	Slipped π-Stacking	−0.7	−0.4	−0.5
Donor-Acceptor	Slipped π-Stacking	−0.2	−0.1	−0.2
Donor-Acceptor	Slipped π-Stacking	−0.1	0.0	−0.1
Donor-Acceptor	Edge-Edge	−2.6	−1.7	−2.1
Donor-Acceptor	Edge-Edge	−1.9	−1.1	−1.5
Donor-Acceptor	Edge-Edge	−1.4	−0.7	−1.1
Donor-Donor	Slipped π-Stacking	-	-	-
Donor-Donor	Slipped π-Stacking	-	-	-
Donor-Donor	Slipped π-Stacking	-	-	-
Donor-Donor	Edge-Edge	-	-	-
Acceptor-Acceptor	Slipped π-Stacking	−2.8	−1.9	−2.3
Acceptor-Acceptor	Slipped π-Stacking	−1.5	−0.9	−1.2
Acceptor-Acceptor	Slipped π-Stacking	−0.2	−0.1	−0.2
Acceptor-Acceptor	Edge-Edge	−0.9	−0.5	−0.7
Acceptor-Acceptor	Edge-Edge	−0.6	−0.3	−0.4

CP = Boys-Bernardi procedure

Table S10: Summary of select interaction energies (in kcal mol^{-1}) after optimizing the hydrogen atoms at the M06-2X/aug-cc-pVDZ-PP level of theory for the **F_5BAI-PyrFur$_2$** co-crystal.

Type	Identity	E_{int}	Eint (CP)	Average
Donor-Acceptor	XB	−8.8	−7.9	−8.3
Donor-Acceptor	π-Stacking	−9.1	−6.8	−7.9
Donor-Donor	π-Stacking	-	-	-
Acceptor-Acceptor	π-Stacking	−12.2	−9.4	−10.8
Donor-Acceptor	Slipped π-Stacking	−2.8	−1.8	−2.3
Donor-Acceptor	Slipped π-Stacking	−1.6	−1.2	−1.4
Donor-Acceptor	Slipped π-Stacking	−0.7	−0.5	−0.6
Donor-Acceptor	Slipped π-Stacking	−0.2	−0.1	−0.1
Donor-Acceptor	Slipped π-Stacking	−0.1	0.0	−0.1
Donor-Acceptor	Edge-Edge	−2.5	−1.7	−2.1
Donor-Acceptor	Edge-Edge	−1.9	−1.1	−1.5
Donor-Acceptor	Edge-Edge	−1.2	−0.6	−0.9
Donor-Donor	Slipped π-Stacking	-	-	-
Donor-Donor	Slipped π-Stacking	-	-	-
Donor-Donor	Slipped π-Stacking	-	-	-
Donor-Donor	Edge-Edge	-	-	-
Acceptor-Acceptor	Slipped π-Stacking	−2.8	−2.1	−2.4
Acceptor-Acceptor	Slipped π-Stacking	−1.4	−1.0	−1.2
Acceptor-Acceptor	Slipped π-Stacking	−0.3	−0.2	−0.2
Acceptor-Acceptor	Edge-Edge	−0.8	−0.5	−0.6
Acceptor-Acceptor	Edge-Edge	−0.7	0.0	−0.4

CP = Boys-Bernardi procedure

Table S11: Comparison of select average interaction energies (in kcal mol^{-1}) between the pair-wise contacts observed in the **F_5BAI-PyrFur$_2$** co-crystal and after the hydrogens were optimized at the M06-2X/aug-cc-pVDZ-PP level of theory (|Δ|) as well as the relative deviations from the Avg (SP) values.

Type	Identity	Avg (SP)	Avg (H-Opt)	|Δ|	Relative Deviation
Donor-Acceptor	XB	−8.2	−8.3	0.17	2.0
Donor-Acceptor	π-Stacking	−7.9	−7.9	0.03	0.3
Donor-Donor	π-Stacking	-	-	-	-
Acceptor-Acceptor	π-Stacking	−10.4	−10.8	0.41	3.9
Donor-Acceptor	Slipped π-Stacking	−2.2	−2.3	0.10	4.3
Donor-Acceptor	Slipped π-Stacking	−1.3	−1.4	0.06	4.6
Donor-Acceptor	Slipped π-Stacking	−0.5	−0.6	0.05	9.3
Donor-Acceptor	Slipped π-Stacking	−0.2	−0.1	0.04	19.4
Donor-Acceptor	Slipped π-Stacking	−0.1	−0.1	0.01	12.5
Donor-Acceptor	Edge-Edge	−2.1	−2.1	0.02	0.9
Donor-Acceptor	Edge-Edge	−1.5	−1.5	0.00	0.0
Donor-Acceptor	Edge-Edge	−1.1	−0.9	0.18	17.1
Donor-Donor	Slipped π-Stacking	-	-	-	-
Donor-Donor	Slipped π-Stacking	-	-	-	-
Donor-Donor	Slipped π-Stacking	-	-	-	-
Donor-Donor	Edge-Edge	-	-	-	-
Acceptor-Acceptor	Slipped π-Stacking	−2.3	−2.4	0.10	4.1
Acceptor-Acceptor	Slipped π-Stacking	−1.2	−1.2	0.04	2.9
Acceptor-Acceptor	Slipped π-Stacking	−0.2	−0.2	0.03	15.8
Acceptor-Acceptor	Edge-Edge	−0.7	−0.6	0.10	11.6
Acceptor-Acceptor	Edge-Edge	−0.4	−0.4	0.08	18.6
----------Average----------				0.09	8.0

Table S12: Summary of select interaction energies (in kcal mol^{-1}) observed in the **F_5BAI-PyrThio$_2$** co-crystal with torsional angles $\tau_\alpha = 171°$ and $\tau_\beta = -25°$ at the M06-2X/aug-cc-pVDZ-PP level of theory.

Type	Identity	E_{int}	Eint (CP)	Average
Donor-Acceptor	XB	−8.6	−7.6	−8.1
Donor-Acceptor	π-Stacking	−11.9	−8.9	−10.4
Donor-Donor	π-Stacking	-	-	-
Acceptor-Acceptor	π-Stacking	−16.2	−12.0	−14.1
Donor-Acceptor	Slipped π-Stacking	−1.1	−0.8	−0.9
Donor-Acceptor	Slipped π-Stacking	−0.4	−0.2	−0.3
Donor-Acceptor	Edge-Edge	−2.3	−1.5	−1.9
Donor-Acceptor	Edge-Edge	−1.9	−1.2	−1.5
Donor-Acceptor	Herringbone	−2.1	−1.4	−1.7
Donor-Acceptor	Herringbone	−1.2	−0.7	−0.9
Donor-Acceptor	Herringbone	−0.5	−0.3	−0.4
Donor-Acceptor	Herringbone	−0.8	−0.5	−0.6
Donor-Donor	Slipped π-Stacking	-	-	-
Donor-Donor	Slipped π-Stacking	-	-	-
Donor-Donor	Edge-Edge	-	-	-
Donor-Donor	Herringbone	-	-	-
Acceptor-Acceptor	Slipped π-Stacking	−0.3	−0.1	−0.2
Acceptor-Acceptor	Edge-Edge	−1.8	−1.0	−1.4
Acceptor-Acceptor	Herringbone	−3.4	−2.1	−2.7
Acceptor-Acceptor	Herringbone	−1.9	−1.1	−1.5

CP = Boys-Bernardi procedure

Table S13: Summary of select interaction energies (in kcal mol^{-1}) after optimizing the hydrogen atoms at the M06-2X/aug-cc-pVDZ-PP level of theory for the **F_5BAI-PyrThio$_2$** co-crystal with torsional angles $\tau_\alpha = 171°$ and $\tau_\beta = -25°$.

Type	Identity	E_{int}	Eint (CP)	Average
Donor-Acceptor	XB	−8.7	−7.7	−8.2
Donor-Acceptor	π-Stacking	−11.8	−9.1	−10.4
Donor-Donor	π-Stacking	-	-	-
Acceptor-Acceptor	π-Stacking	−15.8	−12.1	−14.0
Donor-Acceptor	Slipped π-Stacking	−1.1	−0.8	−1.0
Donor-Acceptor	Slipped π-Stacking	−0.4	−0.2	−0.3
Donor-Acceptor	Edge-Edge	−2.3	−1.5	−1.9
Donor-Acceptor	Edge-Edge	−1.6	−1.0	−1.3
Donor-Acceptor	Herringbone	−2.0	−1.3	−1.6
Donor-Acceptor	Herringbone	−1.2	−0.7	−0.9
Donor-Acceptor	Herringbone	−0.5	−0.3	−0.4
Donor-Acceptor	Herringbone	−0.7	−0.4	−0.6
Donor-Donor	Slipped π-Stacking	-	-	-
Donor-Donor	Slipped π-Stacking	-	-	-
Donor-Donor	Edge-Edge	-	-	-
Donor-Donor	Herringbone	-	-	-
Acceptor-Acceptor	Slipped π-Stacking	−0.3	−0.1	−0.2
Acceptor-Acceptor	Edge-Edge	−1.8	−1.2	−1.5
Acceptor-Acceptor	Herringbone	−3.3	−2.3	−2.8
Acceptor-Acceptor	Herringbone	−1.9	−1.3	−1.6

CP = Boys-Bernardi procedure

Table S14: Comparison of select average interaction energies (in kcal mol^{-1}) between the pair-wise contacts observed in the **F_5BAI-PyrThio$_2$** co-crystal (with torsional angles $\tau_\alpha = 171°$ and $\tau_\beta = -25°$) and after the hydrogens were optimized at the M06-2X/aug-cc-pVDZ-PP level of theory (|Δ|) as well as the relative deviations from the Avg (SP) values.

Type	Identity	Avg-SP	Avg-Hopt	|Δ|	Percent (From SP)
Donor-Acceptor	XB	−8.1	−8.2	0.12	1.4
Donor-Acceptor	π-Stacking	−10.4	−10.4	0.05	0.5
Donor-Donor	π-Stacking	-	-	-	-
Acceptor-Acceptor	π-Stacking	−14.1	−14.0	0.12	0.8
Donor-Acceptor	Slipped π-Stacking	−0.9	−1.0	0.04	4.2
Donor-Acceptor	Slipped π-Stacking	−0.3	−0.3	0.02	6.5
Donor-Acceptor	Edge-Edge	−1.9	−1.9	0.01	0.3
Donor-Acceptor	Edge-Edge	−1.5	−1.3	0.23	14.8
Donor-Acceptor	Herringbone	−1.7	−1.6	0.06	3.5
Donor-Acceptor	Herringbone	−0.9	−0.9	0.01	1.1
Donor-Acceptor	Herringbone	−0.4	−0.4	0.01	2.6
Donor-Acceptor	Herringbone	−0.6	−0.6	0.04	5.6
Donor-Donor	Slipped π-Stacking	-	-	-	-
Donor-Donor	Slipped π-Stacking	-	-	-	-
Donor-Donor	Edge-Edge	-	-	-	-
Donor-Donor	Herringbone	-	-	-	-
Acceptor-Acceptor	Slipped π-Stacking	−0.2	−0.2	0.02	10.8
Acceptor-Acceptor	Edge-Edge	−1.4	−1.5	0.05	3.5
Acceptor-Acceptor	Herringbone	−2.7	−2.8	0.12	4.4
Acceptor-Acceptor	Herringbone	−1.5	−1.6	0.13	8.6
----------Average----------				0.07	4.6

Crystal Data and Structure Refinement

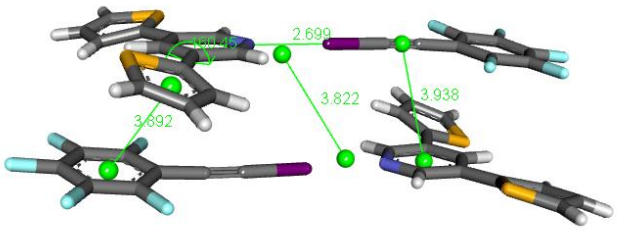


Figure S10. Centroid to centroid stacking distances (in Å) and the S-C-C-C torsional angle (in º) in the **F_5BAI-PyrThio$_2$** crystal structure.

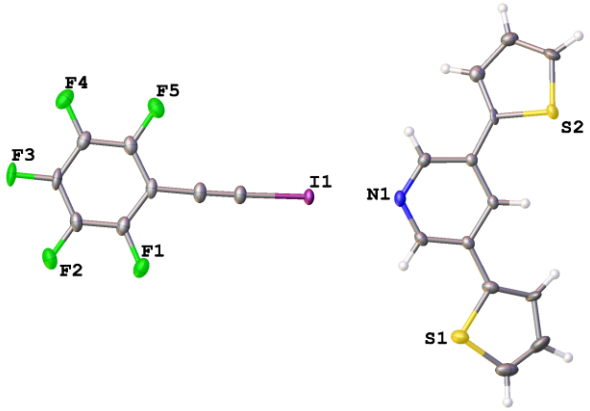


Table S15. Crystal data and structure refinement for **F_5BAI-PyrThio$_2$**.

Identification code	JLN071417	
Empirical formula	C21 H9 F5 I N S2	
Formula weight	561.31	
Temperature	100.0 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 11.921(3) Å	α = 90 °
	b = 16.418(4) Å	β = 104.408(5) °
	c = 10.642(2) Å	γ = 90 °
Volume	2017.3(8) Å^3	
Z	4	
Density (calculated)	1.848 Mg/m^3	
Absorption coefficient	1.848 mm^{-1}	
F(000)	1088	
Crystal size	0.29 x 0.2 x 0.16 mm^3	
Theta range for data collection	3.045 to 28.289°.	
Index ranges	-15<=h<=12, -21<=k<=21, -13<=l<=14	
Reflections collected	13126	
Independent reflections	4976 [R(int) = 0.0240]	
Completeness to theta = 25.242°	99.8 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.3790 and 0.3418
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4976 / 312 / 355
Goodness-of-fit on F^2	1.029
Final R indices [I>2sigma(I)]	R1 = 0.0234, wR2 = 0.0500
R indices (all data)	R1 = 0.0306, wR2 = 0.0526
Extinction coefficient	n/a
Largest diff. peak and hole	0.423 and -0.340 e.Å^{-3}

Table S16. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for F_5BAI-PyrThio$_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
I(001)	6595(1)	5333(1)	6212(1)	17(1)
S(003)	4606(5)	7592(2)	9602(7)	31(1)
F(005)	11241(1)	5300(1)	977(1)	30(1)
F(006)	10081(1)	3944(1)	1363(1)	33(1)
F(007)	9794(1)	6706(1)	4075(1)	31(1)
F(008)	8703(1)	3978(1)	3028(1)	31(1)
F(009)	11113(1)	6678(1)	2347(1)	34(1)
N(00A)	5050(2)	5274(1)	7681(2)	19(1)
C(00B)	3675(2)	4542(1)	8555(2)	14(1)
C(00C)	7751(2)	5366(1)	5093(2)	21(1)
C(00D)	9975(2)	4630(1)	2007(2)	23(1)
C(00E)	3444(2)	5254(1)	9155(2)	14(1)
C(00F)	10512(2)	6020(1)	2519(2)	24(1)
C(00G)	10575(2)	5319(2)	1830(2)	24(1)
C(00H)	4008(2)	5980(1)	9011(2)	15(1)
C(00I)	4503(2)	4585(1)	7830(2)	18(1)
C(00J)	4808(2)	5951(1)	8248(2)	18(1)
C(00K)	9171(2)	5354(1)	3566(2)	20(1)
C(00M)	8412(2)	5371(1)	4419(2)	23(1)
C(00N)	9819(2)	6025(1)	3386(2)	22(1)
C(00O)	9280(2)	4653(1)	2863(2)	22(1)
C(00P)	3753(2)	6736(1)	9619(2)	20(1)
C(00R)	3722(15)	8156(4)	10356(7)	33(2)

C(00T)	2786(9)	6902(4)	10097(11)	25(2)
C(00U)	2867(11)	7724(7)	10526(12)	38(2)
S(0AA)	2369(3)	3580(3)	9790(4)	20(1)
C(2)	2902(18)	3120(9)	7731(16)	22(2)
C(3)	3061(16)	3781(9)	8575(16)	15(2)
C(2AA)	2242(8)	2486(5)	8040(7)	25(1)
C(1AA)	1883(7)	2651(4)	9123(7)	23(1)
C(3A)	3050(30)	3774(13)	8770(20)	15(3)
S(0AB)	3006(8)	2983(4)	7746(8)	29(1)
C(1AB)	2092(10)	2469(7)	8478(12)	26(2)
C(2AB)	1839(11)	2890(6)	9456(12)	24(2)
C(2A)	2360(20)	3645(18)	9600(20)	24(3)
S(0)	4139(11)	7683(2)	9268(5)	42(1)
C(0AA)	3156(8)	6804(4)	10610(10)	21(1)
C(00V)	3059(10)	7624(6)	11024(10)	30(2)
C(00S)	3340(40)	8120(20)	10360(30)	25(4)

Table S17. Bond lengths [Å] and angles [°] for F_5BAI-PyrThio$_2$.

I(001)-C(00C)	2.034(2)	C(00D)-C(00O)	1.376(3)
S(003)-C(00P)	1.739(3)	C(00E)-H(00E)	0.9500
S(003)-C(00R)	1.741(13)	C(00E)-C(00H)	1.397(3)
F(005)-C(00G)	1.347(2)	C(00F)-C(00G)	1.377(3)
F(006)-C(00D)	1.340(3)	C(00F)-C(00N)	1.383(3)
F(007)-C(00N)	1.341(3)	C(00H)-C(00J)	1.399(3)
F(008)-C(00O)	1.340(3)	C(00H)-C(00P)	1.465(3)
F(009)-C(00F)	1.333(3)	C(00I)-H(00I)	0.9500
N(00A)-C(00I)	1.334(3)	C(00J)-H(00J)	0.9500
N(00A)-C(00J)	1.331(3)	C(00K)-C(00M)	1.433(3)
C(00B)-C(00E)	1.392(3)	C(00K)-C(00N)	1.387(3)
C(00B)-C(00I)	1.397(3)	C(00K)-C(00O)	1.396(3)
C(00B)-C(3)	1.451(12)	C(00P)-C(00T)	1.397(7)
C(00B)-C(3A)	1.508(18)	C(00P)-S(0)	1.691(3)
C(00C)-C(00M)	1.190(3)	C(00P)-C(0AA)	1.415(7)
C(00D)-C(00G)	1.375(3)	C(00R)-H(00R)	0.9500

C(00R)-C(00U)	1.291(19)	F(006)-C(00D)-C(00O)	120.7(2)
C(00T)-H(00T)	0.9500	C(00G)-C(00D)-C(00O)	119.2(2)
C(00T)-C(00U)	1.421(11)	C(00B)-C(00E)-H(00E)	119.6
C(00U)-H(00U)	0.9500	C(00B)-C(00E)-C(00H)	120.73(19)
S(0AA)-C(3)	1.729(10)	C(00H)-C(00E)-H(00E)	119.6
S(0AA)-C(1AA)	1.721(7)	F(009)-C(00F)-C(00G)	120.13(19)
C(2)-H(2)	0.9500	F(009)-C(00F)-C(00N)	121.1(2)
C(2)-C(3)	1.392(15)	C(00G)-C(00F)-C(00N)	118.8(2)
C(2)-C(2AA)	1.393(17)	F(005)-C(00G)-C(00D)	119.2(2)
C(2AA)-H(2AA)	0.9500	F(005)-C(00G)-C(00F)	119.8(2)
C(2AA)-C(1AA)	1.352(7)	C(00D)-C(00G)-C(00F)	121.0(2)
C(1AA)-H(1AA)	0.9500	C(00E)-C(00H)-C(00J)	116.82(18)
C(3A)-S(0AB)	1.684(18)	C(00E)-C(00H)-C(00P)	121.06(18)
C(3A)-C(2A)	1.371(18)	C(00J)-C(00H)-C(00P)	122.11(18)
S(0AB)-C(1AB)	1.710(13)	N(00A)-C(00I)-C(00B)	122.80(18)
C(1AB)-H(1AB)	0.9500	N(00A)-C(00I)-H(00I)	118.6
C(1AB)-C(2AB)	1.344(11)	C(00B)-C(00I)-H(00I)	118.6
C(2AB)-H(2AB)	0.9500	N(00A)-C(00J)-C(00H)	123.20(19)
C(2AB)-C(2A)	1.38(3)	N(00A)-C(00J)-H(00J)	118.4
C(2A)-H(2A)	0.9500	C(00H)-C(00J)-H(00J)	118.4
S(0)-C(00S)	1.82(4)	C(00N)-C(00K)-C(00M)	122.3(2)
C(0AA)-H(0AA)	0.9500	C(00N)-C(00K)-C(00O)	116.83(19)
C(0AA)-C(00V)	1.430(11)	C(00O)-C(00K)-C(00M)	120.9(2)
C(00V)-H(00V)	0.9500	C(00C)-C(00M)-C(00K)	177.3(3)
C(00V)-C(00S)	1.18(5)	F(007)-C(00N)-C(00F)	118.0(2)
C(00S)-H(00S)	0.9500	F(007)-C(00N)-C(00K)	119.82(19)
		C(00F)-C(00N)-C(00K)	122.2(2)
C(00P)-S(003)-C(00R)	90.1(4)	F(008)-C(00O)-C(00D)	118.5(2)
C(00J)-N(00A)-C(00I)	119.12(18)	F(008)-C(00O)-C(00K)	119.54(19)
C(00E)-C(00B)-C(00I)	117.31(18)	C(00D)-C(00O)-C(00K)	122.0(2)
C(00E)-C(00B)-C(3)	123.9(5)	C(00H)-C(00P)-S(003)	119.58(19)
C(00E)-C(00B)-C(3A)	118.2(7)	C(00H)-C(00P)-S(0)	125.7(2)
C(00I)-C(00B)-C(3)	118.7(5)	C(00T)-C(00P)-S(003)	112.5(3)
C(00I)-C(00B)-C(3A)	124.4(8)	C(00T)-C(00P)-C(00H)	127.4(3)
C(00M)-C(00C)-I(001)	178.4(2)	C(0AA)-C(00P)-C(00H)	126.5(3)
F(006)-C(00D)-C(00G)	120.1(2)	C(0AA)-C(00P)-S(0)	107.9(3)

S(003)-C(00R)-H(00R)	124.4
C(00U)-C(00R)-S(003)	111.2(6)
C(00U)-C(00R)-H(00R)	124.4
C(00P)-C(00T)-H(00T)	126.1
C(00P)-C(00T)-C(00U)	107.9(7)
C(00U)-C(00T)-H(00T)	126.1
C(00R)-C(00U)-C(00T)	118.0(9)
C(00R)-C(00U)-H(00U)	121.0
C(00T)-C(00U)-H(00U)	121.0
C(1AA)-S(0AA)-C(3)	92.1(6)
C(3)-C(2)-H(2)	122.5
C(3)-C(2)-C(2AA)	115.0(12)
C(2AA)-C(2)-H(2)	122.5
C(00B)-C(3)-S(0AA)	120.8(8)
C(2)-C(3)-C(00B)	130.5(10)
C(2)-C(3)-S(0AA)	108.7(10)
C(2)-C(2AA)-H(2AA)	124.1
C(1AA)-C(2AA)-C(2)	111.7(8)
C(1AA)-C(2AA)-H(2AA)	124.1
S(0AA)-C(1AA)-H(1AA)	123.8
C(2AA)-C(1AA)-S(0AA)	112.5(6)
C(2AA)-C(1AA)-H(1AA)	123.8
C(00B)-C(3A)-S(0AB)	119.1(11)
C(2A)-C(3A)-C(00B)	128.6(18)
C(2A)-C(3A)-S(0AB)	111.7(17)
C(3A)-S(0AB)-C(1AB)	90.5(8)
S(0AB)-C(1AB)-H(1AB)	123.5
C(2AB)-C(1AB)-S(0AB)	113.0(9)
C(2AB)-C(1AB)-H(1AB)	123.5
C(1AB)-C(2AB)-H(2AB)	124.3
C(1AB)-C(2AB)-C(2A)	111.5(14)
C(2A)-C(2AB)-H(2AB)	124.3
C(3A)-C(2A)-C(2AB)	113(2)
C(3A)-C(2A)-H(2A)	123.4
C(2AB)-C(2A)-H(2A)	123.4
C(00P)-S(0)-C(00S)	90.4(14)
C(00P)-C(0AA)-H(0AA)	123.3
C(00P)-C(0AA)-C(00V)	113.5(6)
C(00V)-C(0AA)-H(0AA)	123.3
C(0AA)-C(00V)-H(00V)	123.0
C(00S)-C(00V)-C(0AA)	114.0(17)
C(00S)-C(00V)-H(00V)	123.0
S(0)-C(00S)-H(00S)	123.8
C(00V)-C(00S)-S(0)	112(2)
C(00V)-C(00S)-H(00S)	123.8

Symmetry transformations used to generate equivalent atoms:

Table S18. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for F_5BAI-Pyr$Thio_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
I(001)	13(1)	23(1)	16(1)	2(1)	7(1)	1(1)
S(003)	36(2)	20(1)	41(2)	-5(1)	15(1)	-6(1)
F(005)	25(1)	50(1)	21(1)	5(1)	16(1)	9(1)
F(006)	36(1)	36(1)	27(1)	-2(1)	9(1)	13(1)
F(007)	27(1)	39(1)	29(1)	-7(1)	11(1)	2(1)
F(008)	28(1)	33(1)	34(1)	10(1)	11(1)	1(1)
F(009)	28(1)	41(1)	36(1)	4(1)	16(1)	-5(1)
N(00A)	18(1)	24(1)	18(1)	2(1)	8(1)	0(1)
C(00B)	12(1)	15(1)	12(1)	2(1)	2(1)	1(1)
C(00C)	17(1)	30(1)	16(1)	4(1)	5(1)	3(1)
C(00D)	20(1)	33(1)	16(1)	1(1)	4(1)	10(1)
C(00E)	12(1)	18(1)	13(1)	3(1)	4(1)	1(1)
C(00F)	16(1)	35(1)	20(1)	6(1)	6(1)	2(1)
C(00G)	19(1)	42(1)	13(1)	6(1)	9(1)	10(1)
C(00H)	14(1)	16(1)	14(1)	3(1)	2(1)	0(1)
C(00I)	19(1)	20(1)	15(1)	-1(1)	5(1)	3(1)
C(00J)	17(1)	19(1)	19(1)	5(1)	4(1)	-2(1)
C(00K)	12(1)	36(1)	13(1)	6(1)	3(1)	8(1)
C(00M)	16(1)	37(1)	17(1)	6(1)	4(1)	5(1)
C(00N)	16(1)	33(1)	18(1)	1(1)	4(1)	6(1)
C(00O)	16(1)	32(1)	18(1)	8(1)	3(1)	4(1)
C(00P)	20(1)	16(1)	23(1)	-1(1)	1(1)	-2(1)
C(00R)	51(6)	17(2)	26(2)	-3(1)	0(3)	-2(2)
C(00T)	23(4)	15(3)	41(5)	-14(3)	16(4)	-4(2)
C(00U)	45(5)	34(4)	37(6)	-20(4)	14(5)	2(3)
S(0AA)	22(1)	22(1)	19(1)	1(1)	10(1)	-5(1)
C(2)	24(4)	24(5)	18(4)	4(3)	3(3)	4(4)
C(3)	14(3)	22(3)	9(4)	9(2)	5(3)	3(2)

C(2AA)	32(3)	19(2)	23(4)	-3(2)	5(2)	1(2)
C(1AA)	28(3)	12(3)	29(5)	3(2)	8(3)	-5(3)
C(3A)	20(6)	7(4)	11(7)	-3(4)	-7(4)	-1(3)
S(0AB)	30(2)	19(2)	39(2)	-12(2)	9(2)	0(2)
C(1AB)	26(5)	13(3)	39(9)	-5(5)	6(5)	-3(3)
C(2AB)	24(4)	21(5)	25(5)	5(3)	5(4)	-3(4)
C(2A)	31(6)	20(6)	15(7)	-1(4)	-4(4)	-6(4)
S(0)	76(4)	19(1)	33(1)	1(1)	20(2)	-10(1)
C(0AA)	20(4)	13(2)	30(4)	-5(2)	8(3)	0(2)
C(00V)	38(4)	27(3)	22(4)	-16(3)	2(4)	5(3)
C(00S)	19(13)	17(6)	30(8)	-10(5)	-7(8)	3(7)

Table S19. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for F_5BAI-PyrThio$_2$.

	x	y	z	U(eq)
H(00E)	2896	5245	9668	17
H(00I)	4684	4103	7426	21
H(00J)	5198	6439	8130	22
H(00R)	3852	8710	10608	40
H(00T)	2182	6531	10128	30
H(00U)	2308	7949	10927	46
H(2)	3221	3102	6997	27
H(2AA)	2065	1999	7551	30
H(1AA)	1414	2293	9476	28
H(1AB)	1795	1942	8220	32
H(2AB)	1359	2691	9980	28
H(2A)	2253	4036	10219	28
H(0AA)	2850	6349	10965	25
H(00V)	2794	7758	11769	36
H(00S)	3164	8683	10383	29

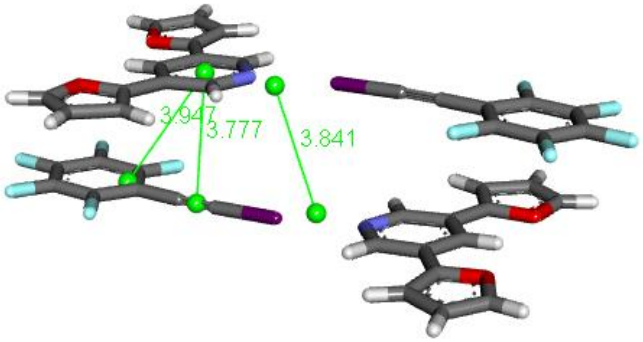


Figure S11. Centroid to centroid stacking distances (in Å) in the **F_5BAI-PyrThio$_2$** crystal structure.

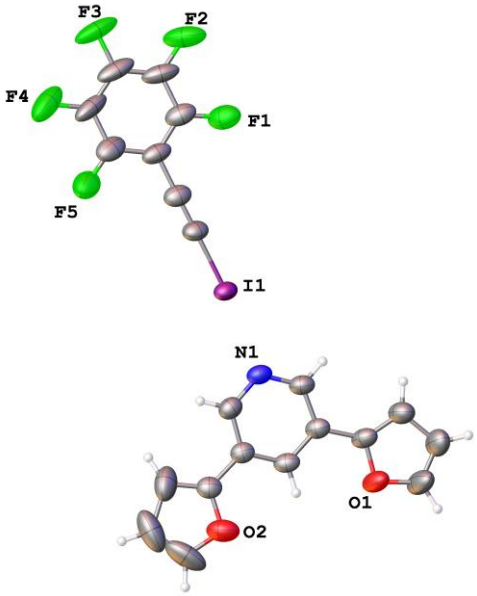


Table S20. Crystal data and structure refinement for **F_5BAI-PyrFur$_2$**.

Identification code	JLN071417	
Empirical formula	C21 H9 F5 I N O2	
Formula weight	529.19	
Temperature	200 K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.6980(15) Å	α = 86.922(7) °
	b = 10.4998(15) Å	β = 70.756(6) °
	c = 12.215(2) Å	γ = 68.527(4) °
Volume	977.2(3) Å^3	
Z	2	
Density (calculated)	1.798 Mg/m^3	
Absorption coefficient	13.480 mm^{-1}	
F(000)	512	
Crystal size	0.24 x 0.22 x 0.07 mm^3	

Theta range for data collection	3.844 to 68.418°.
Index ranges	-10<=h<=10, -12<=k<=12, -14<=l<=13
Reflections collected	12356
Independent reflections	3504 [R(int) = 0.0432]
Completeness to theta = 67.679°	98.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.3201 and 0.1434
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3504 / 0 / 271
Goodness-of-fit on F^2	1.038
Final R indices [I>2sigma(I)]	R1 = 0.0381, wR2 = 0.1012
R indices (all data)	R1 = 0.0407, wR2 = 0.1040
Extinction coefficient	n/a
Largest diff. peak and hole	0.998 and -0.563 e.Å^{-3}

Table S21. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for F_5BAI-PyrFur$_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
I(1)	3332(1)	6323(1)	6461(1)	49(1)
F(1)	-1589(5)	4644(4)	9051(3)	79(1)
F(2)	-2794(7)	2871(5)	10415(3)	103(2)
F(3)	-570(8)	723(4)	11139(3)	107(2)
F(4)	2864(8)	302(4)	10452(4)	119(2)
F(5)	4090(6)	2073(4)	9071(4)	95(1)
C(1)	2435(7)	5077(5)	7626(4)	54(1)
C(2)	1920(7)	4322(5)	8269(4)	56(1)
C(3)	1283(8)	3407(5)	9016(4)	56(1)
C(4)	-467(9)	3578(6)	9380(4)	61(1)
C(5)	-1090(10)	2679(7)	10082(5)	74(2)
C(6)	28(12)	1590(7)	10451(5)	81(2)
C(7)	1778(11)	1378(6)	10099(5)	81(2)
C(8)	2405(9)	2279(6)	9401(5)	71(2)
O(1)	4684(6)	11522(5)	2349(4)	78(1)
O(2)	10239(6)	8439(5)	2784(4)	82(1)
N(1)	4799(5)	7812(4)	4833(3)	51(1)
C(9)	6541(7)	7444(5)	4533(4)	50(1)
C(10)	7484(6)	8134(5)	3768(4)	45(1)

C(11)	6569(6)	9264(5)	3287(4)	46(1)
C(12)	4749(6)	9666(5)	3576(4)	46(1)
C(13)	3939(7)	8898(5)	4356(4)	50(1)
C(14)	9383(6)	7684(5)	3488(4)	50(1)
C(15)	10455(10)	6584(7)	3795(6)	87(2)
C(16)	12203(11)	6714(11)	3227(9)	113(3)
C(17)	11968(10)	7773(13)	2651(8)	111(3)
C(18)	3751(7)	10865(6)	3107(4)	53(1)
C(19)	2021(7)	11557(6)	3297(5)	64(1)
C(20)	1886(9)	12702(7)	2615(6)	75(2)
C(21)	3484(10)	12632(8)	2085(7)	90(2)

Table S22. Bond lengths [Å] and angles [°] for F_5BAI-PyrFur_2.

		N(1)-C(13)	1.338(7)
I(1)-C(1)	2.040(5)	C(9)-H(9)	0.9500
F(1)-C(4)	1.333(7)	C(9)-C(10)	1.389(7)
F(2)-C(5)	1.339(8)	C(10)-C(11)	1.388(7)
F(3)-C(6)	1.334(7)	C(10)-C(14)	1.464(7)
F(4)-C(7)	1.338(9)	C(11)-H(11)	0.9500
F(5)-C(8)	1.321(8)	C(11)-C(12)	1.402(7)
C(1)-C(2)	1.186(7)	C(12)-C(13)	1.395(7)
C(2)-C(3)	1.423(7)	C(12)-C(18)	1.454(7)
C(3)-C(4)	1.382(8)	C(13)-H(13)	0.9500
C(3)-C(8)	1.404(9)	C(14)-C(15)	1.319(8)
C(4)-C(5)	1.379(8)	C(15)-H(15)	0.9500
C(5)-C(6)	1.370(11)	C(15)-C(16)	1.502(14)
C(6)-C(7)	1.372(11)	C(16)-H(16)	0.9500
C(7)-C(8)	1.380(8)	C(16)-C(17)	1.272(14)
O(1)-C(18)	1.356(6)	C(17)-H(17)	0.9500
O(1)-C(21)	1.357(8)	C(18)-C(19)	1.355(8)
O(2)-C(14)	1.363(7)	C(19)-H(19)	0.9500
O(2)-C(17)	1.363(10)	C(19)-C(20)	1.417(8)
N(1)-C(9)	1.342(6)	C(20)-H(20)	0.9500

C(20)-C(21)	1.301(10)	C(10)-C(11)-C(12)	119.8(4)
C(21)-H(21)	0.9500	C(12)-C(11)-H(11)	120.1
		C(11)-C(12)-C(18)	120.9(4)
C(2)-C(1)-I(1)	177.6(4)	C(13)-C(12)-C(11)	117.3(4)
C(1)-C(2)-C(3)	178.3(6)	C(13)-C(12)-C(18)	121.7(4)
C(4)-C(3)-C(2)	121.3(6)	N(1)-C(13)-C(12)	123.7(4)
C(4)-C(3)-C(8)	117.1(5)	N(1)-C(13)-H(13)	118.1
C(8)-C(3)-C(2)	121.6(6)	C(12)-C(13)-H(13)	118.1
F(1)-C(4)-C(3)	119.3(5)	O(2)-C(14)-C(10)	118.6(5)
F(1)-C(4)-C(5)	118.9(6)	C(15)-C(14)-O(2)	112.6(6)
C(5)-C(4)-C(3)	121.7(6)	C(15)-C(14)-C(10)	128.8(6)
F(2)-C(5)-C(4)	120.3(7)	C(14)-C(15)-H(15)	128.8
F(2)-C(5)-C(6)	119.6(5)	C(14)-C(15)-C(16)	102.4(7)
C(6)-C(5)-C(4)	120.2(6)	C(16)-C(15)-H(15)	128.8
F(3)-C(6)-C(5)	120.4(7)	C(15)-C(16)-H(16)	126.1
F(3)-C(6)-C(7)	119.8(7)	C(17)-C(16)-C(15)	107.8(7)
C(5)-C(6)-C(7)	119.8(5)	C(17)-C(16)-H(16)	126.1
F(4)-C(7)-C(6)	119.4(6)	O(2)-C(17)-H(17)	124.4
F(4)-C(7)-C(8)	120.4(8)	C(16)-C(17)-O(2)	111.3(8)
C(6)-C(7)-C(8)	120.2(7)	C(16)-C(17)-H(17)	124.4
F(5)-C(8)-C(3)	119.2(5)	O(1)-C(18)-C(12)	116.4(4)
F(5)-C(8)-C(7)	119.8(6)	C(19)-C(18)-O(1)	109.2(5)
C(7)-C(8)-C(3)	121.0(7)	C(19)-C(18)-C(12)	134.3(5)
C(18)-O(1)-C(21)	105.8(5)	C(18)-C(19)-H(19)	126.7
C(17)-O(2)-C(14)	105.9(7)	C(18)-C(19)-C(20)	106.7(5)
C(13)-N(1)-C(9)	117.7(4)	C(20)-C(19)-H(19)	126.7
N(1)-C(9)-H(9)	118.2	C(19)-C(20)-H(20)	127.0
N(1)-C(9)-C(10)	123.5(4)	C(21)-C(20)-C(19)	106.0(6)
C(10)-C(9)-H(9)	118.2	C(21)-C(20)-H(20)	127.0
C(9)-C(10)-C(14)	120.7(4)	O(1)-C(21)-H(21)	123.8
C(11)-C(10)-C(9)	118.0(4)	C(20)-C(21)-O(1)	112.3(6)
C(11)-C(10)-C(14)	121.3(4)	C(20)-C(21)-H(21)	123.8
C(10)-C(11)-H(11)	120.1		

Symmetry transformations used to generate equivalent atoms:

Table S23. Anisotropic displacement parameters ($Å^2$ x 10^3) for F_5BAI-PyrFur_2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
I(1)	50(1)	49(1)	42(1)	7(1)	-4(1)	-23(1)
F(1)	94(3)	106(3)	60(2)	24(2)	-31(2)	-61(2)
F(2)	130(4)	155(4)	67(2)	24(2)	-23(2)	-113(3)
F(3)	194(5)	84(2)	54(2)	14(2)	-4(2)	-97(3)
F(4)	166(5)	59(2)	78(3)	20(2)	-4(3)	-17(3)
F(5)	84(3)	78(2)	83(3)	17(2)	4(2)	-13(2)
C(1)	57(3)	58(3)	41(2)	3(2)	-2(2)	-27(2)
C(2)	70(3)	59(3)	36(2)	-2(2)	-5(2)	-31(3)
C(3)	84(4)	52(3)	34(2)	0(2)	-4(2)	-40(3)
C(4)	93(4)	70(3)	35(2)	5(2)	-16(3)	-50(3)
C(5)	115(5)	91(4)	39(3)	5(3)	-6(3)	-79(4)
C(6)	145(7)	67(4)	32(3)	3(2)	1(3)	-68(4)
C(7)	136(6)	45(3)	43(3)	8(2)	0(3)	-39(3)
C(8)	90(4)	60(3)	42(3)	-3(2)	4(3)	-27(3)
O(1)	71(2)	101(3)	92(3)	58(3)	-48(2)	-55(2)
O(2)	74(3)	105(3)	77(3)	15(2)	-15(2)	-54(3)
N(1)	56(2)	55(2)	44(2)	7(2)	-10(2)	-31(2)
C(9)	61(3)	48(2)	42(2)	5(2)	-15(2)	-23(2)
C(10)	54(2)	51(2)	34(2)	0(2)	-13(2)	-25(2)
C(11)	58(3)	61(3)	31(2)	4(2)	-13(2)	-35(2)
C(12)	56(3)	58(3)	37(2)	6(2)	-19(2)	-32(2)
C(13)	54(3)	60(3)	42(2)	6(2)	-12(2)	-32(2)
C(14)	56(3)	59(3)	35(2)	-2(2)	-11(2)	-26(2)
C(15)	93(5)	62(4)	70(4)	2(3)	-24(4)	7(3)
C(16)	70(5)	125(7)	118(7)	-37(6)	-48(5)	15(5)
C(17)	54(4)	170(9)	110(7)	-44(7)	-10(4)	-52(5)
C(18)	63(3)	69(3)	48(3)	19(2)	-26(2)	-42(3)
C(19)	61(3)	81(4)	63(3)	21(3)	-25(3)	-38(3)
C(20)	72(4)	84(4)	88(4)	33(3)	-49(3)	-34(3)
C(21)	84(4)	112(5)	111(5)	70(5)	-63(4)	-60(4)

Table S24. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for F_5BAI-PyrFur$_2$.

	x	y	z	U(eq)
H(9)	7163	6668	4862	60
H(11)	7173	9763	2765	56
H(13)	2706	9161	4559	60
H(15)	10190	5887	4257	104
H(16)	13291	6112	3288	136
H(17)	12879	8062	2188	133
H(19)	1080	11321	3792	76
H(20)	842	13382	2556	90
H(21)	3777	13283	1572	107

NMR Analysis

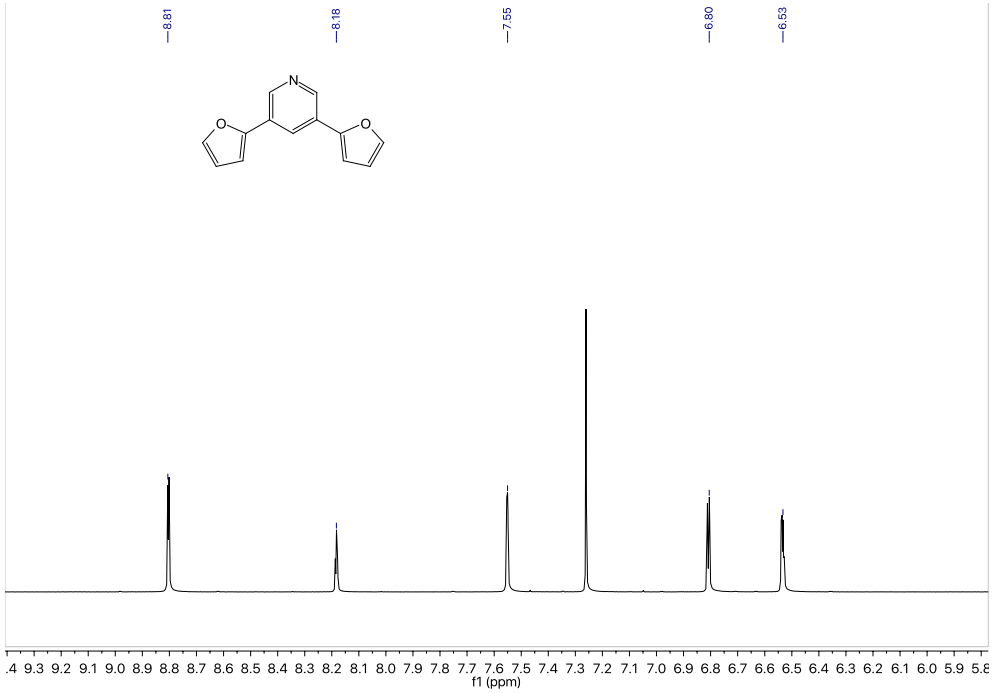


Figure S12. ^{1}H NMR of 3,5-di(furan-2-yl)pyridine

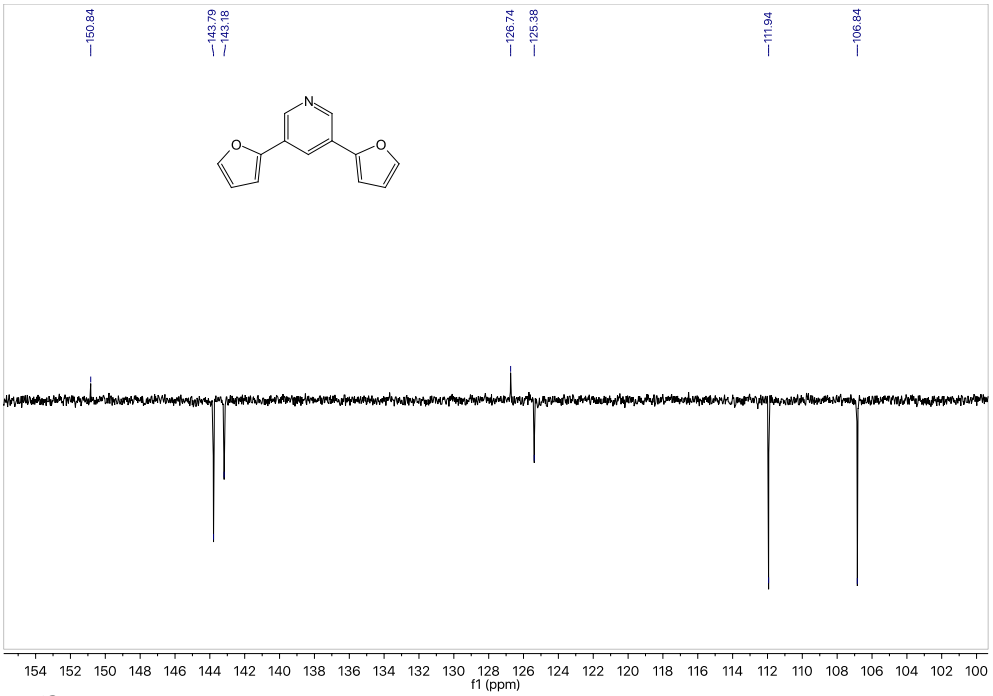


Figure S13. ^{13}C NMR of 3,5-di(furan-2-yl)pyridine

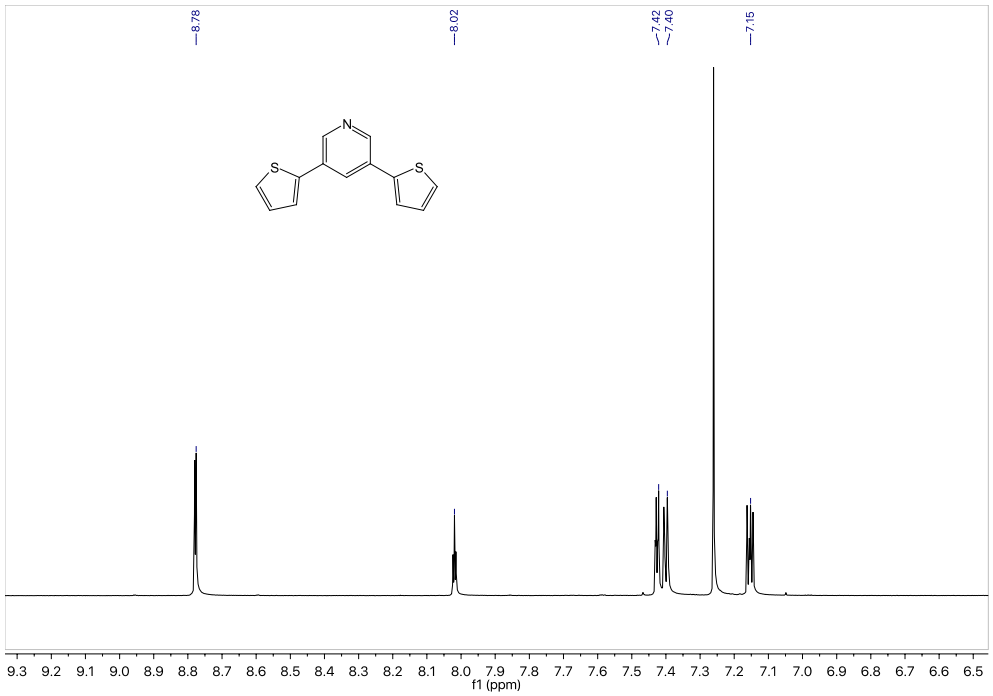


Figure S14. ^{1}H NMR of 3,5-di(thiophen-2-yl)pyridine

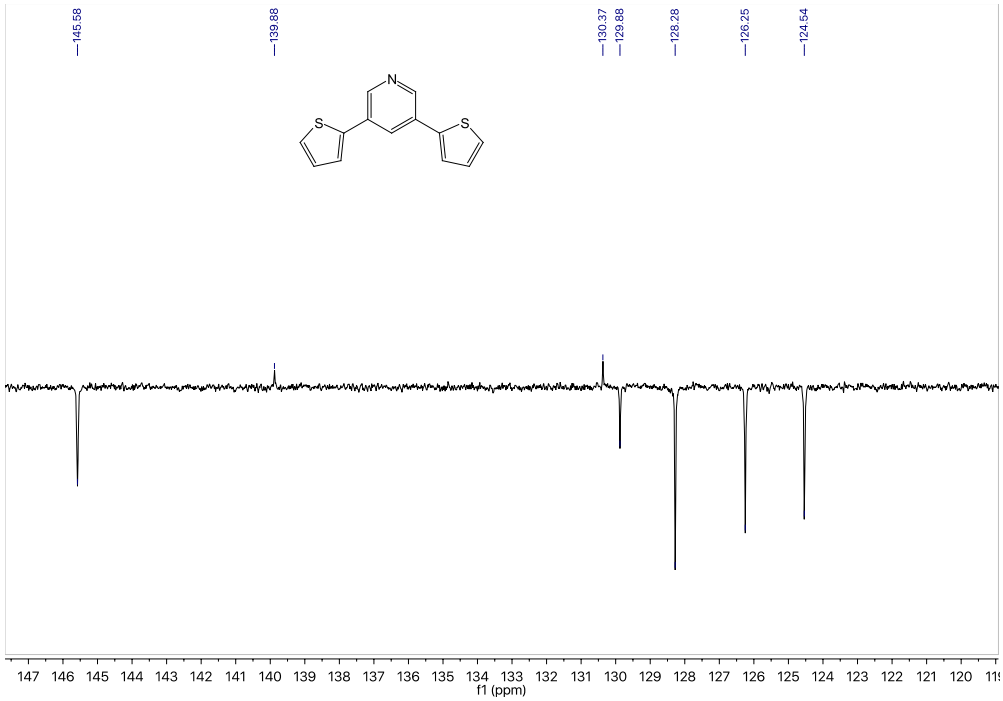


Figure S15. ^{13}C NMR of 3,5-di(thiophen-2-yl)pyridine

Table S24: Cartesian coordinates (Å) for the XB contact in the **F_5BAI-PyrFur$_2$** co crystal.

atom	*x*	*y*	*z*
I	-13.43010	2.40270	15.56790
F	-9.54720	4.27110	12.59020
F	-8.36680	6.12340	11.02170
F	-9.76710	8.28580	10.18920
F	-12.31560	8.63680	10.97920
F	-13.50670	6.78500	12.56720
C	-12.64000	3.72280	14.22880
C	-12.16080	4.51700	13.48940
C	-11.55580	5.47670	12.63040
C	-10.24590	5.34160	12.21190
C	-9.64110	6.28170	11.40460
C	-10.34350	7.37820	10.98030
C	-11.64250	7.55440	11.38510
C	-12.25310	6.61270	12.18770
O	-14.94890	-3.03840	20.29680
O	-18.77080	0.01220	19.79660
N	-14.62300	0.80490	17.44040
C	-15.87600	1.13810	17.78540
H	-16.25150	1.92480	17.40750
C	-16.65340	0.39670	18.66510
C	-16.09820	-0.74970	19.21820
H	-16.60530	-1.28340	19.81840
C	-14.78610	-1.11710	18.88580
C	-14.10040	-0.29810	17.98890
H	-13.21120	-0.53700	17.75510
C	-18.01950	0.81180	18.98700
C	-18.65270	1.91360	18.63400
H	-18.34020	2.63520	18.10240
C	-19.99440	1.73660	19.28720
H	-20.73350	2.33000	19.21730
C	-19.96520	0.65130	19.94950
H	-20.68200	0.32820	20.48210
C	-14.19000	-2.32990	19.42510
C	-13.02770	-2.98930	19.20670
H	-12.31770	-2.71490	18.63770
C	-13.07580	-4.16800	19.99090
H	-12.40540	-4.83730	20.05860
C	-14.22550	-4.14620	20.60030
H	-14.52420	-4.82790	21.19030

Table S25: Cartesian coordinates (Å) for the Donor-Acceptor π-Stacking contact in the **F_5BAI-PyrFur$_2$** co crystal.

atom	*x*	*y*	*z*
O	31.51650	11.93060	-8.79780
O	35.33830	8.87990	-8.29760
N	31.19060	8.08720	-5.94150
C	32.44350	7.75400	-6.28650
H	32.81900	6.96730	-5.90850
C	33.22100	8.49550	-7.16610
C	32.66580	9.64180	-7.71920
H	33.17280	10.17560	-8.31950
C	31.35360	10.00920	-7.38690
C	30.66790	9.19030	-6.49000
H	29.77870	9.42920	-6.25620
C	34.58700	8.08040	-7.48810
C	35.22030	6.97860	-7.13510
H	34.90770	6.25690	-6.60350
C	36.56200	7.15550	-7.78820
H	37.30100	6.56210	-7.71830
C	36.53270	8.24090	-8.45060
H	37.24950	8.56400	-8.98320
C	30.75760	11.22200	-7.92620
C	29.59530	11.88150	-7.70770
H	28.88520	11.60700	-7.13880
C	29.64340	13.06020	-8.49200
H	28.97290	13.72950	-8.55970
C	30.79310	13.03840	-9.10140
H	31.09170	13.72000	-9.69140
I	30.70600	4.16050	-7.42990
F	34.58880	6.02880	-10.40770
F	35.76930	7.88110	-11.97610
F	34.36900	10.04350	-12.80870
F	31.82050	10.39450	-12.01870
F	30.62940	8.54270	-10.43070
C	31.49600	5.48050	-8.76910
C	31.97530	6.27470	-9.50850
C	32.58030	7.23440	-10.36740
C	33.89020	7.09930	-10.78600
C	34.49500	8.03940	-11.59320
C	33.79260	9.13590	-12.01750
C	32.49360	9.31210	-11.61280
C	31.88300	8.37040	-10.81010

Table S26: Cartesian coordinates (Å) for the Donor-Donor π-Stacking contact in the **F_5BAI-PyrFur$_2$** co crystal.

atom	*x*	*y*	*z*
I	21.48200	-4.16050	7.42990
F	17.59920	-6.02880	10.40770
F	16.41870	-7.88110	11.97610
F	17.81900	-10.04350	12.80870
F	20.36750	-10.39450	12.01870
F	21.55860	-8.54270	10.43070
C	20.69200	-5.48050	8.76910
C	20.21270	-6.27470	9.50850
C	19.60770	-7.23440	10.36740
C	18.29780	-7.09930	10.78600
C	17.69300	-8.03940	11.59320
C	18.39540	-9.13590	12.01750
C	19.69440	-9.31210	11.61280
C	20.30500	-8.37040	10.81010
I	17.51830	-7.36830	15.56790
F	21.40120	-5.49990	12.59020
F	22.58160	-3.64770	11.02170
F	21.18130	-1.48520	10.18920
F	18.63280	-1.13420	10.97920
F	17.44170	-2.98600	12.56720
C	18.30840	-6.04830	14.22880
C	18.78760	-5.25400	13.48940
C	19.39270	-4.29430	12.63040
C	20.70250	-4.42940	12.21190
C	21.30730	-3.48930	11.40460
C	20.60490	-2.39280	10.98030
C	19.30600	-2.21660	11.38510
C	18.69530	-3.15830	12.18770

Table S27: Cartesian coordinates (Å) for the Acceptor-Acceptor π-Stacking contact in the **F_5BAI-PyrFur$_2$** co crystal.

atom	*x*	*y*	*z*
O	17.96400	21.70160	-8.79780
O	21.78590	18.65100	-8.29760
N	17.63810	17.85820	-5.94150
C	18.89110	17.52500	-6.28650
H	19.26660	16.73830	-5.90850
C	19.66860	18.26650	-7.16610
C	19.11340	19.41290	-7.71920
H	19.62040	19.94660	-8.31950
C	17.80120	19.78030	-7.38690
C	17.11550	18.96130	-6.49000
H	16.22630	19.20020	-6.25620
C	21.03460	17.85140	-7.48810
C	21.66790	16.74960	-7.13510
H	21.35530	16.02800	-6.60350
C	23.00960	16.92650	-7.78820
H	23.74860	16.33310	-7.71830
C	22.98030	18.01190	-8.45060
H	23.69710	18.33500	-8.98320
C	17.20520	20.99300	-7.92620
C	16.04290	21.65250	-7.70770
H	15.33280	21.37810	-7.13880
C	16.09100	22.83120	-8.49200
H	15.42050	23.50050	-8.55970
C	17.24060	22.80940	-9.10140
H	17.53930	23.49100	-9.69140
O	19.47830	18.26130	-2.70110
O	15.65640	21.31200	-3.20130
N	19.80420	22.10470	-5.55740
C	18.55130	22.43790	-5.21250
H	18.17580	23.22460	-5.59040
C	17.77380	21.69640	-4.33280
C	18.32900	20.55010	-3.77970
H	17.82200	20.01630	-3.17940
C	19.64120	20.18270	-4.11200
C	20.32690	21.00160	-5.00890
H	21.21610	20.76270	-5.24270
C	16.40780	22.11150	-4.01080
C	15.77450	23.21330	-4.36380
H	16.08700	23.93500	-4.89540
C	14.43280	23.03640	-3.71070
H	13.69370	23.62980	-3.78060
C	14.46210	21.95100	-3.04840
H	13.74530	21.62790	-2.51580
C	20.23720	18.96990	-3.57270
C	21.39950	18.31040	-3.79120
H	22.10960	18.58490	-4.36020
C	21.35140	17.13170	-3.00700
H	22.02190	16.46240	-2.93920
C	20.20170	17.15350	-2.39750
H	19.90310	16.47190	-1.80750

Table S28: Cartesian coordinates (Å) for the Donor-Acceptor Slipped π-Stacking contact in the **F_5BAI-PyrFur$_2$** co crystal.

atom	*x*	*y*	*z*
I	29.99770	6.48940	-4.06900
F	26.11480	4.62110	-1.09120
F	24.93430	2.76880	0.47720
F	26.33470	0.60630	1.30970
F	28.88320	0.25540	0.51980
F	30.07420	2.10720	-1.06830
C	29.20760	5.16940	-2.72980
C	28.72830	4.37520	-1.99050
C	28.12330	3.41550	-1.13150
C	26.81340	3.55060	-0.71290
C	26.20860	2.61040	0.09430
C	26.91110	1.51400	0.51860
C	28.21000	1.33770	0.11380
C	28.82070	2.27950	-0.68880
O	31.69880	1.28070	2.70110
O	35.52070	-1.76990	3.20130
N	31.37290	-2.56270	5.55740
C	32.62590	-2.89590	5.21250
H	33.00140	-3.68260	5.59040
C	33.40340	-2.15440	4.33280
C	32.84820	-1.00800	3.77970
H	33.35520	-0.47430	3.17940
C	31.53600	-0.64060	4.11200
C	30.85030	-1.45960	5.00890
H	29.96110	-1.22070	5.24270
C	34.76940	-2.56950	4.01080
C	35.40260	-3.67130	4.36380
H	35.09010	-4.39290	4.89540
C	36.74430	-3.49440	3.71070
H	37.48340	-4.08780	3.78060
C	36.71510	-2.40900	3.04840
H	37.43190	-2.08590	2.51580
C	30.94000	0.57210	3.57270
C	29.77770	1.23160	3.79120
H	29.06760	0.95720	4.36020
C	29.82580	2.41030	3.00700
H	29.15530	3.07960	2.93920
C	30.97540	2.38850	2.39750
H	31.27410	3.07020	1.80750

Table S29: Cartesian coordinates (Å) for the Donor-Acceptor Slipped π-Stacking contact in the **F_5BAI-PyrFur$_2$** co crystal.

atom	*x*	*y*	*z*
I	29.99770	6.48940	-4.06900
F	26.11480	4.62110	-1.09120
F	24.93430	2.76880	0.47720
F	26.33470	0.60630	1.30970
F	28.88320	0.25540	0.51980
F	30.07420	2.10720	-1.06830
C	29.20760	5.16940	-2.72980
C	28.72830	4.37520	-1.99050
C	28.12330	3.41550	-1.13150
C	26.81340	3.55060	-0.71290
C	26.20860	2.61040	0.09430
C	26.91110	1.51400	0.51860
C	28.21000	1.33770	0.11380
C	28.82070	2.27950	-0.68880
O	18.14640	11.05170	2.70110
O	21.96830	8.00110	3.20130
N	17.82050	7.20840	5.55740
C	19.07350	6.87510	5.21250
H	19.44900	6.08840	5.59040
C	19.85090	7.61660	4.33280
C	19.29570	8.76300	3.77970
H	19.80280	9.29670	3.17940
C	17.98360	9.13040	4.11200
C	17.29790	8.31140	5.00890
H	16.40870	8.55030	5.24270
C	21.21700	7.20150	4.01080
C	21.85020	6.09970	4.36380
H	21.53770	5.37810	4.89540
C	23.19190	6.27660	3.71070
H	23.93100	5.68320	3.78060
C	23.16270	7.36200	3.04840
H	23.87950	7.68510	2.51580
C	17.38750	10.34310	3.57270
C	16.22530	11.00260	3.79120
H	15.51520	10.72820	4.36020
C	16.27340	12.18130	3.00700
H	15.60290	12.85060	2.93920
C	17.42300	12.15950	2.39750
H	17.72170	12.84120	1.80750

Table S30: Cartesian coordinates (Å) for the Donor-Acceptor Slipped π-Stacking contact in the **F_5BAI-PyrFur$_2$** co crystal.

atom	*x*	*y*	*z*
O	31.51650	11.93060	-8.79780
O	35.33830	8.87990	-8.29760
N	31.19060	8.08720	-5.94150
C	32.44350	7.75400	-6.28650
H	32.81900	6.96730	-5.90850
C	33.22100	8.49550	-7.16610
C	32.66580	9.64180	-7.71920
H	33.17280	10.17560	-8.31950
C	31.35360	10.00920	-7.38690
C	30.66790	9.19030	-6.49000
H	29.77870	9.42920	-6.25620
C	34.58700	8.08040	-7.48810
C	35.22030	6.97860	-7.13510
H	34.90770	6.25690	-6.60350
C	36.56200	7.15550	-7.78820
H	37.30100	6.56210	-7.71830
C	36.53270	8.24090	-8.45060
H	37.24950	8.56400	-8.98320
C	30.75760	11.22200	-7.92620
C	29.59530	11.88150	-7.70770
H	28.88520	11.60700	-7.13880
C	29.64340	13.06020	-8.49200
H	28.97290	13.72950	-8.55970
C	30.79310	13.03840	-9.10140
H	31.09170	13.72000	-9.69140
I	34.54950	13.93150	-7.42990
F	38.43240	15.79980	-10.40770
F	39.61290	17.65210	-11.97610
F	38.21250	19.81450	-12.80870
F	35.66410	20.16550	-12.01870
F	34.47300	18.31370	-10.43070
C	35.33960	15.25150	-8.76910
C	35.81890	16.04570	-9.50850
C	36.42390	17.00540	-10.36740
C	37.73380	16.87030	-10.78600
C	38.33860	17.81040	-11.59320
C	37.63620	18.90690	-12.01750
C	36.33720	19.08310	-11.61280
C	35.72650	18.14140	-10.81010

Table S31: Cartesian coordinates (Å) for the Donor-Acceptor Slipped π-Stacking contact in the **F_5BAI-PyrFur$_2$** co crystal.

atom	*x*	*y*	*z*
I	30.18000	-4.16050	7.42990
F	26.29720	-6.02880	10.40770
F	25.11670	-7.88110	11.97610
F	26.51700	-10.04350	12.80870
F	29.06550	-10.39450	12.01870
F	30.25660	-8.54270	10.43070
C	29.39000	-5.48050	8.76910
C	28.91070	-6.27470	9.50850
C	28.30570	-7.23440	10.36740
C	26.99580	-7.09930	10.78600
C	26.39100	-8.03940	11.59320
C	27.09340	-9.13590	12.01750
C	28.39240	-9.31210	11.61280
C	29.00300	-8.37040	10.81010
O	23.00080	1.28070	2.70110
O	26.82270	-1.76990	3.20130
N	22.67490	-2.56270	5.55740
C	23.92790	-2.89590	5.21250
H	24.30340	-3.68260	5.59040
C	24.70540	-2.15440	4.33280
C	24.15020	-1.00800	3.77970
H	24.65720	-0.47430	3.17940
C	22.83800	-0.64060	4.11200
C	22.15230	-1.45960	5.00890
H	21.26310	-1.22070	5.24270
C	26.07140	-2.56950	4.01080
C	26.70460	-3.67130	4.36380
H	26.39210	-4.39290	4.89540
C	28.04630	-3.49440	3.71070
H	28.78540	-4.08780	3.78060
C	28.01710	-2.40900	3.04840
H	28.73390	-2.08590	2.51580
C	22.24200	0.57210	3.57270
C	21.07970	1.23160	3.79120
H	20.36960	0.95720	4.36020
C	21.12780	2.41030	3.00700
H	20.45730	3.07960	2.93920
C	22.27740	2.38850	2.39750
H	22.57610	3.07020	1.80750

Table S32: Cartesian coordinates (Å) for the Donor-Acceptor Slipped π-Stacking contact in the **F_5BAI-PyrFur$_2$** co crystal.

atom	*x*	*y*	*z*
I	16.26290	26.91030	-15.56790
F	12.38000	25.04200	-12.59020
F	11.19960	23.18970	-11.02170
F	12.59990	21.02720	-10.18920
F	15.14840	20.67620	-10.97920
F	16.33950	22.52810	-12.56720
C	15.47280	25.59030	-14.22880
C	14.99350	24.79610	-13.48940
C	14.38850	23.83640	-12.63040
C	13.07860	23.97140	-12.21190
C	12.47380	23.03130	-11.40460
C	13.17630	21.93480	-10.98030
C	14.47520	21.75860	-11.38510
C	15.08590	22.70030	-12.18770
O	10.78030	18.26130	-2.70110
O	6.95840	21.31200	-3.20130
N	11.10620	22.10470	-5.55740
C	9.85330	22.43790	-5.21250
H	9.47780	23.22460	-5.59040
C	9.07580	21.69640	-4.33280
C	9.63100	20.55010	-3.77970
H	9.12400	20.01630	-3.17940
C	10.94320	20.18270	-4.11200
C	11.62890	21.00160	-5.00890
H	12.51810	20.76270	-5.24270
C	7.70980	22.11150	-4.01080
C	7.07650	23.21330	-4.36380
H	7.38900	23.93500	-4.89540
C	5.73480	23.03640	-3.71070
H	4.99570	23.62980	-3.78060
C	5.76410	21.95100	-3.04840
H	5.04730	21.62790	-2.51580
C	11.53920	18.96990	-3.57270
C	12.70150	18.31040	-3.79120
H	13.41160	18.58490	-4.36020
C	12.65340	17.13170	-3.00700
H	13.32390	16.46240	-2.93920
C	11.50370	17.15350	-2.39750
H	11.20510	16.47190	-1.80750

Table S33: Cartesian coordinates (Å) for the Donor-Acceptor Edge-Edge contact in the **F_5BAI-PyrFur$_2$** co crystal.

atom	*x*	*y*	*z*
I	29.99770	6.48940	-4.06900
F	26.11480	4.62110	-1.09120
F	24.93430	2.76880	0.47720
F	26.33470	0.60630	1.30970
F	28.88320	0.25540	0.51980
F	30.07420	2.10720	-1.06830
C	29.20760	5.16940	-2.72980
C	28.72830	4.37520	-1.99050
C	28.12330	3.41550	-1.13150
C	26.81340	3.55060	-0.71290
C	26.20860	2.61040	0.09430
C	26.91110	1.51400	0.51860
C	28.21000	1.33770	0.11380
C	28.82070	2.27950	-0.68880
O	24.33270	8.49030	-2.70110
O	20.51090	11.54090	-3.20130
N	24.65860	12.33370	-5.55740
C	23.40570	12.66690	-5.21250
H	23.03020	13.45360	-5.59040
C	22.62820	11.92540	-4.33280
C	23.18340	10.77900	-3.77970
H	22.67640	10.24530	-3.17940
C	24.49560	10.41160	-4.11200
C	25.18130	11.23060	-5.00890
H	26.07050	10.99170	-5.24270
C	21.26220	12.34050	-4.01080
C	20.62890	13.44230	-4.36380
H	20.94150	14.16390	-4.89540
C	19.28720	13.26540	-3.71070
H	18.54820	13.85880	-3.78060
C	19.31650	12.18000	-3.04840
H	18.59970	11.85690	-2.51580
C	25.09160	9.19890	-3.57270
C	26.25390	8.53940	-3.79120
H	26.96400	8.81380	-4.36020
C	26.20580	7.36070	-3.00700
H	26.87630	6.69140	-2.93920
C	25.05620	7.38250	-2.39750
H	24.75750	6.70090	-1.80750

Table S34: Cartesian coordinates (Å) for the Donor-Acceptor Edge-Edge contact in the **F_5BAI-PyrFur$_2$** co crystal.

atom	*x*	*y*	*z*
I	25.14320	16.26040	-4.06900
F	21.26040	14.39210	-1.09120
F	20.07990	12.53980	0.47720
F	21.48020	10.37740	1.30970
F	24.02870	10.02640	0.51980
F	25.21980	11.87820	-1.06830
C	24.35320	14.94040	-2.72980
C	23.87390	14.14620	-1.99050
C	23.26890	13.18650	-1.13150
C	21.95900	13.32160	-0.71290
C	21.35420	12.38150	0.09430
C	22.05660	11.28500	0.51860
C	23.35560	11.10880	0.11380
C	23.96630	12.05050	-0.68880
O	33.03070	8.49030	-2.70110
O	29.20890	11.54090	-3.20130
N	33.35660	12.33370	-5.55740
C	32.10370	12.66690	-5.21250
H	31.72820	13.45360	-5.59040
C	31.32620	11.92540	-4.33280
C	31.88140	10.77900	-3.77970
H	31.37440	10.24530	-3.17940
C	33.19360	10.41160	-4.11200
C	33.87930	11.23060	-5.00890
H	34.76850	10.99170	-5.24270
C	29.96020	12.34050	-4.01080
C	29.32690	13.44230	-4.36380
H	29.63950	14.16390	-4.89540
C	27.98520	13.26540	-3.71070
H	27.24620	13.85880	-3.78060
C	28.01450	12.18000	-3.04840
H	27.29770	11.85690	-2.51580
C	33.78960	9.19890	-3.57270
C	34.95190	8.53940	-3.79120
H	35.66200	8.81380	-4.36020
C	34.90380	7.36070	-3.00700
H	35.57430	6.69140	-2.93920
C	33.75420	7.38250	-2.39750
H	33.45550	6.70090	-1.80750

Table S35: Cartesian coordinates (Å) for the Donor-Acceptor Edge-Edge contact in the **F_5BAI-PyrFur$_2$** co crystal.

atom	*x*	*y*	*z*
O	19.47830	18.26130	-2.70110
O	15.65640	21.31200	-3.20130
N	19.80420	22.10470	-5.55740
C	18.55130	22.43790	-5.21250
H	18.17580	23.22460	-5.59040
C	17.77380	21.69640	-4.33280
C	18.32900	20.55010	-3.77970
H	17.82200	20.01630	-3.17940
C	19.64120	20.18270	-4.11200
C	20.32690	21.00160	-5.00890
H	21.21610	20.76270	-5.24270
C	16.40780	22.11150	-4.01080
C	15.77450	23.21330	-4.36380
H	16.08700	23.93500	-4.89540
C	14.43280	23.03640	-3.71070
H	13.69370	23.62980	-3.78060
C	14.46210	21.95100	-3.04840
H	13.74530	21.62790	-2.51580
C	20.23720	18.96990	-3.57270
C	21.39950	18.31040	-3.79120
H	22.10960	18.58490	-4.36020
C	21.35140	17.13170	-3.00700
H	22.02190	16.46240	-2.93920
C	20.20170	17.15350	-2.39750
H	19.90310	16.47190	-1.80750
I	12.48150	13.05260	4.06900
F	16.36440	14.92100	1.09120
F	17.54480	16.77320	-0.47720
F	16.14450	18.93570	-1.30970
F	13.59600	19.28670	-0.51980
F	12.40490	17.43480	1.06830
C	13.27160	14.37260	2.72980
C	13.75090	15.16690	1.99050
C	14.35590	16.12660	1.13150
C	15.66570	15.99150	0.71290
C	16.27050	16.93160	-0.09430
C	15.56810	18.02810	-0.51860
C	14.26920	18.20430	-0.11380
C	13.65850	17.26260	0.68880

Table S36: Cartesian coordinates (Å) for the Donor-Donor Slipped π-Stacking contact in the **F_5BAI-PyrFur$_2$** co crystal.

atom	*x*	*y*	*z*
I	25.14320	16.26040	-4.06900
F	21.26040	14.39210	-1.09120
F	20.07990	12.53980	0.47720
F	21.48020	10.37740	1.30970
F	24.02870	10.02640	0.51980
F	25.21980	11.87820	-1.06830
C	24.35320	14.94040	-2.72980
C	23.87390	14.14620	-1.99050
C	23.26890	13.18650	-1.13150
C	21.95900	13.32160	-0.71290
C	21.35420	12.38150	0.09430
C	22.05660	11.28500	0.51860
C	23.35560	11.10880	0.11380
C	23.96630	12.05050	-0.68880
I	17.33590	3.28160	4.06900
F	21.21880	5.14990	1.09120
F	22.39920	7.00220	-0.47720
F	20.99890	9.16470	-1.30970
F	18.45040	9.51570	-0.51980
F	17.25930	7.66380	1.06830
C	18.12600	4.60160	2.72980
C	18.60530	5.39580	1.99050
C	19.21030	6.35550	1.13150
C	20.52020	6.22050	0.71290
C	21.12500	7.16060	-0.09430
C	20.42250	8.25710	-0.51860
C	19.12360	8.43330	-0.11380
C	18.51290	7.49160	0.68880

Table S37: Cartesian coordinates (Å) for the Donor-Donor Slipped π-Stacking contact in the **F_5BAI-PyrFur$_2$** co crystal.

atom	*x*	*y*	*z*
I	21.48200	-4.16050	7.42990
F	17.59920	-6.02880	10.40770
F	16.41870	-7.88110	11.97610
F	17.81900	-10.04350	12.80870
F	20.36750	-10.39450	12.01870
F	21.55860	-8.54270	10.43070
C	20.69200	-5.48050	8.76910
C	20.21270	-6.27470	9.50850
C	19.60770	-7.23440	10.36740
C	18.29780	-7.09930	10.78600
C	17.69300	-8.03940	11.59320
C	18.39540	-9.13590	12.01750
C	19.69440	-9.31210	11.61280
C	20.30500	-8.37040	10.81010
I	22.19030	-6.48940	4.06900
F	26.07320	-4.62110	1.09120
F	27.25370	-2.76880	-0.47720
F	25.85330	-0.60630	-1.30970
F	23.30480	-0.25540	-0.51980
F	22.11380	-2.10720	1.06830
C	22.98040	-5.16940	2.72980
C	23.45970	-4.37520	1.99050
C	24.06470	-3.41550	1.13150
C	25.37460	-3.55060	0.71290
C	25.97940	-2.61040	-0.09430
C	25.27690	-1.51400	-0.51860
C	23.97800	-1.33770	-0.11380
C	23.36730	-2.27950	0.68880

Table S38: Cartesian coordinates (Å) for the Donor-Donor Slipped π-Stacking contact in the **F_5BAI-PyrFur$_2$** co crystal.

atom	*x*	*y*	*z*
I	12.96640	-14.81040	18.92890
F	9.08350	-16.67870	21.90660
F	7.90310	-18.53100	23.47510
F	9.30340	-20.69340	24.30760
F	11.85190	-21.04440	23.51760
F	13.04300	-19.19260	21.92960
C	12.17630	-16.13040	20.26800
C	11.69710	-16.92460	21.00740
C	11.09210	-17.88430	21.86640
C	9.78220	-17.74920	22.28490
C	9.17740	-18.68930	23.09220
C	9.87980	-19.78580	23.51650
C	11.17880	-19.96200	23.11170
C	11.78940	-19.02030	22.30910
I	4.26840	-14.81040	18.92890
F	0.38550	-16.67870	21.90660
F	-0.79490	-18.53100	23.47510
F	0.60540	-20.69340	24.30760
F	3.15390	-21.04440	23.51760
F	4.34500	-19.19260	21.92960
C	3.47830	-16.13040	20.26800
C	2.99910	-16.92460	21.00740
C	2.39410	-17.88430	21.86640
C	1.08420	-17.74920	22.28490
C	0.47940	-18.68930	23.09220
C	1.18180	-19.78580	23.51650
C	2.48080	-19.96200	23.11170
C	3.09140	-19.02030	22.30910

Table S39: Cartesian coordinates (Å) for the Donor-Donor Edge-Edge contact in the **F_5BAI-PyrFur$_2$** co crystal.

atom	*x*	*y*	*z*
I	21.29970	6.48940	-4.06900
F	17.41680	4.62110	-1.09120
F	16.23630	2.76880	0.47720
F	17.63670	0.60630	1.30970
F	20.18520	0.25540	0.51980
F	21.37620	2.10720	-1.06830
C	20.50960	5.16940	-2.72980
C	20.03030	4.37520	-1.99050
C	19.42530	3.41550	-1.13150
C	18.11540	3.55060	-0.71290
C	17.51060	2.61040	0.09430
C	18.21310	1.51400	0.51860
C	19.51200	1.33770	0.11380
C	20.12270	2.27950	-0.68880
I	22.19030	-6.48940	4.06900
F	26.07320	-4.62110	1.09120
F	27.25370	-2.76880	-0.47720
F	25.85330	-0.60630	-1.30970
F	23.30480	-0.25540	-0.51980
F	22.11380	-2.10720	1.06830
C	22.98040	-5.16940	2.72980
C	23.45970	-4.37520	1.99050
C	24.06470	-3.41550	1.13150
C	25.37460	-3.55060	0.71290
C	25.97940	-2.61040	-0.09430
C	25.27690	-1.51400	-0.51860
C	23.97800	-1.33770	-0.11380
C	23.36730	-2.27950	0.68880

Table S40: Cartesian coordinates (Å) for the Acceptor-Acceptor Slipped π-Stacking contact in the **F_5BAI-PyrFur$_2$** co crystal.

atom	*x*	*y*	*z*
O	31.51650	11.93060	-8.79780
O	35.33830	8.87990	-8.29760
N	31.19060	8.08720	-5.94150
C	32.44350	7.75400	-6.28650
H	32.81900	6.96730	-5.90850
C	33.22100	8.49550	-7.16610
C	32.66580	9.64180	-7.71920
H	33.17280	10.17560	-8.31950
C	31.35360	10.00920	-7.38690
C	30.66790	9.19030	-6.49000
H	29.77870	9.42920	-6.25620
C	34.58700	8.08040	-7.48810
C	35.22030	6.97860	-7.13510
H	34.90770	6.25690	-6.60350
C	36.56200	7.15550	-7.78820
H	37.30100	6.56210	-7.71830
C	36.53270	8.24090	-8.45060
H	37.24950	8.56400	-8.98320
C	30.75760	11.22200	-7.92620
C	29.59530	11.88150	-7.70770
H	28.88520	11.60700	-7.13880
C	29.64340	13.06020	-8.49200
H	28.97290	13.72950	-8.55970
C	30.79310	13.03840	-9.10140
H	31.09170	13.72000	-9.69140
O	26.66200	21.70160	-8.79780
O	30.48390	18.65100	-8.29760
N	26.33610	17.85820	-5.94150
C	27.58910	17.52500	-6.28650
H	27.96460	16.73830	-5.90850
C	28.36660	18.26650	-7.16610
C	27.81140	19.41290	-7.71920
H	28.31840	19.94660	-8.31950
C	26.49920	19.78030	-7.38690
C	25.81350	18.96130	-6.49000
H	24.92430	19.20020	-6.25620
C	29.73260	17.85140	-7.48810
C	30.36590	16.74960	-7.13510
H	30.05330	16.02800	-6.60350
C	31.70760	16.92650	-7.78820
H	32.44660	16.33310	-7.71830
C	31.67830	18.01190	-8.45060
H	32.39510	18.33500	-8.98320
C	25.90320	20.99300	-7.92620
C	24.74090	21.65250	-7.70770
H	24.03080	21.37810	-7.13880
C	24.78900	22.83120	-8.49200
H	24.11850	23.50050	-8.55970
C	25.93860	22.80940	-9.10140
H	26.23730	23.49100	-9.69140

Table S41: Cartesian coordinates (Å) for the Acceptor-Acceptor Slipped π-Stacking contact in the **F_5BAI-PyrFur$_2$** co crystal.

atom	*x*	*y*	*z*
O	31.51650	11.93060	-8.79780
O	35.33830	8.87990	-8.29760
N	31.19060	8.08720	-5.94150
C	32.44350	7.75400	-6.28650
H	32.81900	6.96730	-5.90850
C	33.22100	8.49550	-7.16610
C	32.66580	9.64180	-7.71920
H	33.17280	10.17560	-8.31950
C	31.35360	10.00920	-7.38690
C	30.66790	9.19030	-6.49000
H	29.77870	9.42920	-6.25620
C	34.58700	8.08040	-7.48810
C	35.22030	6.97860	-7.13510
H	34.90770	6.25690	-6.60350
C	36.56200	7.15550	-7.78820
H	37.30100	6.56210	-7.71830
C	36.53270	8.24090	-8.45060
H	37.24950	8.56400	-8.98320
C	30.75760	11.22200	-7.92620
C	29.59530	11.88150	-7.70770
H	28.88520	11.60700	-7.13880
C	29.64340	13.06020	-8.49200
H	28.97290	13.72950	-8.55970
C	30.79310	13.03840	-9.10140
H	31.09170	13.72000	-9.69140
O	26.66200	21.70160	-8.79780
O	30.48390	18.65100	-8.29760
N	26.33610	17.85820	-5.94150
C	27.58910	17.52500	-6.28650
H	27.96460	16.73830	-5.90850
C	28.36660	18.26650	-7.16610
C	27.81140	19.41290	-7.71920
H	28.31840	19.94660	-8.31950
C	26.49920	19.78030	-7.38690
C	25.81350	18.96130	-6.49000
H	24.92430	19.20020	-6.25620
C	29.73260	17.85140	-7.48810
C	30.36590	16.74960	-7.13510
H	30.05330	16.02800	-6.60350
C	31.70760	16.92650	-7.78820
H	32.44660	16.33310	-7.71830
C	31.67830	18.01190	-8.45060
H	32.39510	18.33500	-8.98320
C	25.90320	20.99300	-7.92620
C	24.74090	21.65250	-7.70770
H	24.03080	21.37810	-7.13880
C	24.78900	22.83120	-8.49200
H	24.11850	23.50050	-8.55970
C	25.93860	22.80940	-9.10140
H	26.23730	23.49100	-9.69140

Table S42: Cartesian coordinates (Å) for the Acceptor-Acceptor Slipped π-Stacking contact in the **F_5BAI-PyrFur$_2$** co crystal.

atom	*x*	*y*	*z*
O	18.14640	11.05170	2.70110
O	21.96830	8.00110	3.20130
N	17.82050	7.20840	5.55740
C	19.07350	6.87510	5.21250
H	19.44900	6.08840	5.59040
C	19.85090	7.61660	4.33280
C	19.29570	8.76300	3.77970
H	19.80280	9.29670	3.17940
C	17.98360	9.13040	4.11200
C	17.29790	8.31140	5.00890
H	16.40870	8.55030	5.24270
C	21.21700	7.20150	4.01080
C	21.85020	6.09970	4.36380
H	21.53770	5.37810	4.89540
C	23.19190	6.27660	3.71070
H	23.93100	5.68320	3.78060
C	23.16270	7.36200	3.04840
H	23.87950	7.68510	2.51580
C	17.38750	10.34310	3.57270
C	16.22530	11.00260	3.79120
H	15.51520	10.72820	4.36020
C	16.27340	12.18130	3.00700
H	15.60290	12.85060	2.93920
C	17.42300	12.15950	2.39750
H	17.72170	12.84120	1.80750
O	24.33270	8.49030	-2.70110
O	20.51090	11.54090	-3.20130
N	24.65860	12.33370	-5.55740
C	23.40570	12.66690	-5.21250
H	23.03020	13.45360	-5.59040
C	22.62820	11.92540	-4.33280
C	23.18340	10.77900	-3.77970
H	22.67640	10.24530	-3.17940
C	24.49560	10.41160	-4.11200
C	25.18130	11.23060	-5.00890
H	26.07050	10.99170	-5.24270
C	21.26220	12.34050	-4.01080
C	20.62890	13.44230	-4.36380
H	20.94150	14.16390	-4.89540
C	19.28720	13.26540	-3.71070
H	18.54820	13.85880	-3.78060
C	19.31650	12.18000	-3.04840
H	18.59970	11.85690	-2.51580
C	25.09160	9.19890	-3.57270
C	26.25390	8.53940	-3.79120
H	26.96400	8.81380	-4.36020
C	26.20580	7.36070	-3.00700
H	26.87630	6.69140	-2.93920
C	25.05620	7.38250	-2.39750
H	24.75750	6.70090	-1.80750

Table S43: Cartesian coordinates (Å) for the Acceptor-Acceptor Edge-Edge contact in the **F_5BAI-PyrFur$_2$** co crystal.

atom	*x*	*y*	*z*
O	22.81850	11.93060	-8.79780
O	26.64030	8.87990	-8.29760
N	22.49260	8.08720	-5.94150
C	23.74550	7.75400	-6.28650
H	24.12100	6.96730	-5.90850
C	24.52300	8.49550	-7.16610
C	23.96780	9.64180	-7.71920
H	24.47480	10.17560	-8.31950
C	22.65560	10.00920	-7.38690
C	21.96990	9.19030	-6.49000
H	21.08070	9.42920	-6.25620
C	25.88900	8.08040	-7.48810
C	26.52230	6.97860	-7.13510
H	26.20970	6.25690	-6.60350
C	27.86400	7.15550	-7.78820
H	28.60300	6.56210	-7.71830
C	27.83470	8.24090	-8.45060
H	28.55150	8.56400	-8.98320
C	22.05960	11.22200	-7.92620
C	20.89730	11.88150	-7.70770
H	20.18720	11.60700	-7.13880
C	20.94540	13.06020	-8.49200
H	20.27490	13.72950	-8.55970
C	22.09510	13.03840	-9.10140
H	22.39370	13.72000	-9.69140
O	29.18720	-1.28070	-2.70110
O	25.36530	1.76990	-3.20130
N	29.51310	2.56270	-5.55740
C	28.26010	2.89590	-5.21250
H	27.88460	3.68260	-5.59040
C	27.48260	2.15440	-4.33280
C	28.03780	1.00800	-3.77970
H	27.53080	0.47430	-3.17940
C	29.35000	0.64060	-4.11200
C	30.03570	1.45960	-5.00890
H	30.92490	1.22070	-5.24270
C	26.11660	2.56950	-4.01080
C	25.48340	3.67130	-4.36380
H	25.79590	4.39290	-4.89540
C	24.14170	3.49440	-3.71070
H	23.40260	4.08780	-3.78060
C	24.17090	2.40900	-3.04840
H	23.45410	2.08590	-2.51580
C	29.94600	-0.57210	-3.57270
C	31.10830	-1.23160	-3.79120
H	31.81840	-0.95720	-4.36020
C	31.06020	-2.41030	-3.00700
H	31.73070	-3.07960	-2.93920
C	29.91060	-2.38850	-2.39750
H	29.61190	-3.07020	-1.80750

Table S44: Cartesian coordinates (Å) for the Acceptor-Acceptor Edge-Edge contact in the **F_5BAI-PyrFur$_2$** co crystal.

atom	*x*	*y*	*z*
O	17.96400	21.70160	-8.79780
O	21.78590	18.65100	-8.29760
N	17.63810	17.85820	-5.94150
C	18.89110	17.52500	-6.28650
H	19.26660	16.73830	-5.90850
C	19.66860	18.26650	-7.16610
C	19.11340	19.41290	-7.71920
H	19.62040	19.94660	-8.31950
C	17.80120	19.78030	-7.38690
C	17.11550	18.96130	-6.49000
H	16.22630	19.20020	-6.25620
C	21.03460	17.85140	-7.48810
C	21.66790	16.74960	-7.13510
H	21.35530	16.02800	-6.60350
C	23.00960	16.92650	-7.78820
H	23.74860	16.33310	-7.71830
C	22.98030	18.01190	-8.45060
H	23.69710	18.33500	-8.98320
C	17.20520	20.99300	-7.92620
C	16.04290	21.65250	-7.70770
H	15.33280	21.37810	-7.13880
C	16.09100	22.83120	-8.49200
H	15.42050	23.50050	-8.55970
C	17.24060	22.80940	-9.10140
H	17.53930	23.49100	-9.69140
O	10.78030	18.26130	-2.70110
O	6.95840	21.31200	-3.20130
N	11.10620	22.10470	-5.55740
C	9.85330	22.43790	-5.21250
H	9.47780	23.22460	-5.59040
C	9.07580	21.69640	-4.33280
C	9.63100	20.55010	-3.77970
H	9.12400	20.01630	-3.17940
C	10.94320	20.18270	-4.11200
C	11.62890	21.00160	-5.00890
H	12.51810	20.76270	-5.24270
C	7.70980	22.11150	-4.01080
C	7.07650	23.21330	-4.36380
H	7.38900	23.93500	-4.89540
C	5.73480	23.03640	-3.71070
H	4.99570	23.62980	-3.78060
C	5.76410	21.95100	-3.04840
H	5.04730	21.62790	-2.51580
C	11.53920	18.96990	-3.57270
C	12.70150	18.31040	-3.79120
H	13.41160	18.58490	-4.36020
C	12.65340	17.13170	-3.00700
H	13.32390	16.46240	-2.93920
C	11.50370	17.15350	-2.39750
H	11.20510	16.47190	-1.80750

Table S45: Cartesian coordinates (Å) for the XB contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles τ_α = 171° and τ_β = −25°.

atom	*x*	*y*	*z*
I	-17.62480	8.75630	6.40230
F	-10.70010	8.70190	1.00660
F	-12.18590	6.47610	1.40470
F	-13.24600	11.01040	4.19970
F	-14.26900	6.53030	3.12080
F	-11.21620	10.96330	2.41910
C	-15.95040	8.81060	5.24950
C	-12.48230	7.60190	2.06870
C	-11.97720	9.88310	2.59640
C	-11.72010	8.73210	1.88620
C	-13.85360	8.79070	3.67560
C	-14.98420	8.81890	4.55480
C	-13.03290	9.89270	3.48900
C	-13.53780	7.64010	2.95100
S	-20.89290	12.46450	9.89810
N	-19.85610	8.65850	7.91670
C	-21.72620	7.45690	8.81770
C	-22.16120	8.62500	9.43610
H	-22.95010	8.61070	9.96500
C	-21.45050	9.81850	9.28770
C	-20.54760	7.52780	8.07060
H	-20.22480	6.73730	7.65420
C	-20.29430	9.77100	8.50150
H	-19.79780	10.57160	8.37980
C	-21.91570	11.05850	9.91560
C	-22.18770	13.38720	10.66910
H	-22.12140	14.30170	10.92160
C	-23.19810	11.33170	10.40730
H	-23.92470	10.72100	10.44230
C	-23.22230	12.66650	10.84020
H	-23.99750	13.02600	11.25450
S	-23.60750	5.87600	10.08470
C	-22.42880	5.12240	7.96960
H	-21.85230	5.08470	7.21510
C	-22.45900	6.22240	8.82510
C	-23.29550	4.07990	8.29020
H	-23.37310	3.27700	7.78920
C	-24.01250	4.35570	9.40130
H	-24.66840	3.77120	9.76410

Table S46: Cartesian coordinates (Å) for the Donor-Acceptor π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 171°$ and $\tau_\beta = -25°$.

atom	*x*	*y*	*z*
S	6.92110	28.58050	-5.56280
N	7.95790	32.38650	-7.54420
C	6.08780	33.58810	-6.64330
C	5.65280	32.42000	-6.02480
H	4.86390	32.43430	-5.49600
C	6.36350	31.22650	-6.17320
C	7.26640	33.51720	-7.39030
H	7.58920	34.30770	-7.80670
C	7.51970	31.27400	-6.95950
H	8.01620	30.47340	-7.08110
C	5.89830	29.98650	-5.54530
C	5.62630	27.65780	-4.79190
H	5.69260	26.74330	-4.53930
C	4.61590	29.71330	-5.05370
H	3.88930	30.32400	-5.01860
C	4.59170	28.37850	-4.62080
H	3.81650	28.01900	-4.20640
S	4.20650	35.16900	-5.37630
C	5.38520	35.92260	-7.49130
H	5.96170	35.96030	-8.24580
C	5.35500	34.82260	-6.63580
C	4.51850	36.96510	-7.17080
H	4.44090	37.76800	-7.67170
C	3.80150	36.68930	-6.05970
H	3.14560	37.27380	-5.69680
I	7.02780	33.38330	-11.55600
F	0.10310	33.32890	-6.16030
F	1.58890	31.10310	-6.55830
F	2.64900	35.63740	-9.35340
F	3.67200	31.15730	-8.27450
F	0.61920	35.59030	-7.57280
C	5.35340	33.43760	-10.40320
C	1.88530	32.22890	-7.22230
C	1.38020	34.51010	-7.75010
C	1.12310	33.35910	-7.03990
C	3.25660	33.41770	-8.82920
C	4.38720	33.44590	-9.70840
C	2.43590	34.51970	-8.64270
C	2.94080	32.26710	-8.10460

Table S47: Cartesian coordinates (Å) for the Donor-Donor π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 171°$ and $\tau_\beta = -25°$.

atom	*x*	*y*	*z*
I	10.18920	15.87070	-9.05860
F	17.11390	15.92510	-14.45430
F	15.62810	18.15090	-14.05630
F	14.56800	13.61660	-11.26120
F	13.54500	18.09670	-12.34010
F	16.59780	13.66370	-13.04180
C	11.86360	15.81640	-10.21140
C	15.33170	17.02510	-13.39230
C	15.83680	14.74390	-12.86450
C	16.09390	15.89490	-13.57470
C	13.96030	15.83630	-11.78540
C	12.82980	15.80810	-10.90610
C	14.78110	14.73430	-11.97190
C	14.27620	16.98690	-12.51000
I	18.94880	16.96530	-11.55600
F	12.02410	16.91090	-6.16030
F	13.50990	14.68510	-6.55830
F	14.57000	19.21940	-9.35340
F	15.59300	14.73930	-8.27450
F	12.54020	19.17230	-7.57280
C	17.27440	17.01960	-10.40320
C	13.80630	15.81090	-7.22230
C	13.30120	18.09210	-7.75010
C	13.04410	16.94110	-7.03990
C	15.17760	16.99970	-8.82920
C	16.30820	17.02790	-9.70840
C	14.35690	18.10170	-8.64270
C	14.86180	15.84910	-8.10460

Table S48: Cartesian coordinates (Å) for the Acceptor-Acceptor π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 171°$ and $\tau_\beta = -25°$.

atom	*x*	*y*	*z*
S	-7.64790	-4.25550	4.74440
N	-6.61110	-0.44950	2.76310
C	-8.48120	0.75210	3.66400
C	-8.91620	-0.41600	4.28250
H	-9.70510	-0.40170	4.81130
C	-8.20550	-1.60950	4.13400
C	-7.30260	0.68120	2.91700
H	-6.97980	1.47170	2.50050
C	-7.04930	-1.56200	3.34780
H	-6.55280	-2.36260	3.22620
C	-8.67070	-2.84950	4.76200
C	-8.94270	-5.17820	5.51540
H	-8.87640	-6.09270	5.76800
C	-9.95310	-3.12270	5.25360
H	-10.67970	-2.51200	5.28870
C	-9.97730	-4.45750	5.68650
H	-10.75250	-4.81700	6.10090
S	-10.36250	2.33300	4.93100
C	-9.18380	3.08660	2.81600
H	-8.60730	3.12430	2.06150
C	-9.21400	1.98660	3.67150
C	-10.05050	4.12910	3.13650
H	-10.12810	4.93200	2.63560
C	-10.76750	3.85330	4.24760
H	-11.42340	4.43780	4.61050
S	-4.20650	-2.33300	5.37630
C	-5.38520	-3.08660	7.49130
H	-5.96170	-3.12430	8.24580
C	-5.35500	-1.98660	6.63580
C	-4.51850	-4.12910	7.17080
H	-4.44090	-4.93200	7.67170
C	-3.80150	-3.85330	6.05970
H	-3.14560	-4.43780	5.69680
S	-6.92110	4.25550	5.56280
N	-7.95790	0.44950	7.54420
C	-6.08780	-0.75210	6.64330
C	-5.65280	0.41600	6.02480
H	-4.86390	0.40170	5.49600
C	-6.36350	1.60950	6.17320
C	-7.26640	-0.68120	7.39030
H	-7.58920	-1.47170	7.80670
C	-7.51970	1.56200	6.95950
H	-8.01620	2.36260	7.08110
C	-5.89830	2.84950	5.54530
C	-5.62630	5.17820	4.79190
H	-5.69260	6.09270	4.53930
C	-4.61590	3.12270	5.05370
H	-3.88930	2.51200	5.01860
C	-4.59170	4.45750	4.62080
H	-3.81650	4.81700	4.20640

Table S49: Cartesian coordinates (Å) for the Donor-Acceptor Slipped π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 171°$ and $\tau_\beta = -25°$.

atom	*x*	*y*	*z*
S	6.92110	28.58050	-5.56280
N	7.95790	32.38650	-7.54420
C	6.08780	33.58810	-6.64330
C	5.65280	32.42000	-6.02480
H	4.86390	32.43430	-5.49600
C	6.36350	31.22650	-6.17320
C	7.26640	33.51720	-7.39030
H	7.58920	34.30770	-7.80670
C	7.51970	31.27400	-6.95950
H	8.01620	30.47340	-7.08110
C	5.89830	29.98650	-5.54530
C	5.62630	27.65780	-4.79190
H	5.69260	26.74330	-4.53930
C	4.61590	29.71330	-5.05370
H	3.88930	30.32400	-5.01860
C	4.59170	28.37850	-4.62080
H	3.81650	28.01900	-4.20640
S	4.20650	35.16900	-5.37630
C	5.38520	35.92260	-7.49130
H	5.96170	35.96030	-8.24580
C	5.35500	34.82260	-6.63580
C	4.51850	36.96510	-7.17080
H	4.44090	37.76800	-7.67170
C	3.80150	36.68930	-6.05970
H	3.14560	37.27380	-5.69680
I	4.37980	33.38330	-1.24870
F	-2.54490	33.32890	4.14700
F	-1.05910	31.10310	3.74900
F	0.00100	35.63740	0.95390
F	1.02400	31.15730	2.03280
F	-2.02880	35.59030	2.73450
C	2.70540	33.43760	-0.09590
C	-0.76270	32.22890	3.08500
C	-1.26780	34.51010	2.55720
C	-1.52490	33.35910	3.26740
C	0.60860	33.41770	1.47810
C	1.73920	33.44590	0.59890
C	-0.21210	34.51970	1.66460
C	0.29280	32.26710	2.20270

Table S50: Cartesian coordinates (Å) for the Donor-Acceptor Slipped π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 171°$ and $\tau_\beta = -25°$.

atom	*x*	*y*	*z*
I	10.18920	15.87070	-9.05860
F	17.11390	15.92510	-14.45430
F	15.62810	18.15090	-14.05630
F	14.56800	13.61660	-11.26120
F	13.54500	18.09670	-12.34010
F	16.59780	13.66370	-13.04180
C	11.86360	15.81640	-10.21140
C	15.33170	17.02510	-13.39230
C	15.83680	14.74390	-12.86450
C	16.09390	15.89490	-13.57470
C	13.96030	15.83630	-11.78540
C	12.82980	15.80810	-10.90610
C	14.78110	14.73430	-11.97190
C	14.27620	16.98690	-12.51000
S	22.21690	20.67350	-15.05170
N	21.18010	16.86750	-13.07040
C	23.05020	15.66590	-13.97130
C	23.48520	16.83400	-14.58980
H	24.27410	16.81970	-15.11860
C	22.77450	18.02750	-14.44130
C	21.87160	15.73680	-13.22430
H	21.54880	14.94630	-12.80780
C	21.61830	17.98000	-13.65510
H	21.12180	18.78060	-13.53350
C	23.23970	19.26750	-15.06930
C	23.51170	21.59620	-15.82270
H	23.44540	22.51070	-16.07530
C	24.52210	19.54070	-15.56090
H	25.24870	18.93000	-15.59600
C	24.54630	20.87550	-15.99380
H	25.32150	21.23500	-16.40820
S	24.93150	14.08500	-15.23830
C	23.75280	13.33140	-13.12320
H	23.17630	13.29370	-12.36880
C	23.78300	14.43140	-13.97870
C	24.61950	12.28890	-13.44380
H	24.69710	11.48600	-12.94290
C	25.33650	12.56470	-14.55490
H	25.99240	11.98020	-14.91770

Table S51: Cartesian coordinates (Å) for the Donor-Acceptor Edge-Edge contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 171°$ and $\tau_\beta = -25°$.

atom	*x*	*y*	*z*
S	6.92110	28.58050	-5.56280
N	7.95790	32.38650	-7.54420
C	6.08780	33.58810	-6.64330
C	5.65280	32.42000	-6.02480
H	4.86390	32.43430	-5.49600
C	6.36350	31.22650	-6.17320
C	7.26640	33.51720	-7.39030
H	7.58920	34.30770	-7.80670
C	7.51970	31.27400	-6.95950
H	8.01620	30.47340	-7.08110
C	5.89830	29.98650	-5.54530
C	5.62630	27.65780	-4.79190
H	5.69260	26.74330	-4.53930
C	4.61590	29.71330	-5.05370
H	3.88930	30.32400	-5.01860
C	4.59170	28.37850	-4.62080
H	3.81650	28.01900	-4.20640
S	4.20650	35.16900	-5.37630
C	5.38520	35.92260	-7.49130
H	5.96170	35.96030	-8.24580
C	5.35500	34.82260	-6.63580
C	4.51850	36.96510	-7.17080
H	4.44090	37.76800	-7.67170
C	3.80150	36.68930	-6.05970
H	3.14560	37.27380	-5.69680
I	-4.37980	32.28870	1.24870
F	2.54490	32.34310	-4.14700
F	1.05910	34.56890	-3.74900
F	-0.00100	30.03460	-0.95390
F	-1.02400	34.51470	-2.03280
F	2.02880	30.08170	-2.73450
C	-2.70540	32.23440	0.09590
C	0.76270	33.44310	-3.08500
C	1.26780	31.16190	-2.55720
C	1.52490	32.31290	-3.26740
C	-0.60860	32.25430	-1.47810
C	-1.73920	32.22610	-0.59890
C	0.21210	31.15230	-1.66460
C	-0.29280	33.40490	-2.20270

Table S52: Cartesian coordinates (Å) for the Donor-Acceptor Edge-Edge contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 171°$ and $\tau_\beta = -25°$.

atom	*x*	*y*	*z*
S	-7.64790	12.16250	4.74440
N	-6.61110	15.96850	2.76310
C	-8.48120	17.17010	3.66400
C	-8.91620	16.00200	4.28250
H	-9.70510	16.01630	4.81130
C	-8.20550	14.80850	4.13400
C	-7.30260	17.09920	2.91700
H	-6.97980	17.88970	2.50050
C	-7.04930	14.85600	3.34780
H	-6.55280	14.05540	3.22620
C	-8.67070	13.56850	4.76200
C	-8.94270	11.23980	5.51540
H	-8.87640	10.32530	5.76800
C	-9.95310	13.29530	5.25360
H	-10.67970	13.90600	5.28870
C	-9.97730	11.96050	5.68650
H	-10.75250	11.60100	6.10090
S	-10.36250	18.75100	4.93100
C	-9.18380	19.50460	2.81600
H	-8.60730	19.54230	2.06150
C	-9.21400	18.40460	3.67150
C	-10.05050	20.54710	3.13650
H	-10.12810	21.35000	2.63560
C	-10.76750	20.27130	4.24760
H	-11.42340	20.85580	4.61050
I	-8.86520	7.66170	3.90500
F	-15.78990	7.71610	9.30070
F	-14.30410	9.94190	8.90260
F	-13.24400	5.40760	6.10760
F	-12.22100	9.88770	7.18650
F	-15.27380	5.45470	7.88820
C	-10.53960	7.60740	5.05780
C	-14.00770	8.81610	8.23860
C	-14.51280	6.53490	7.71090
C	-14.76990	7.68590	8.42110
C	-12.63640	7.62730	6.63170
C	-11.50580	7.59910	5.75250
C	-13.45710	6.52530	6.81830
C	-12.95220	8.77790	7.35630

Table S53: Cartesian coordinates (Å) for the Donor-Acceptor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 171°$ and $\tau_\beta = -25°$.

atom	*x*	*y*	*z*
S	6.92110	28.58050	-5.56280
N	7.95790	32.38650	-7.54420
C	6.08780	33.58810	-6.64330
C	5.65280	32.42000	-6.02480
H	4.86390	32.43430	-5.49600
C	6.36350	31.22650	-6.17320
C	7.26640	33.51720	-7.39030
H	7.58920	34.30770	-7.80670
C	7.51970	31.27400	-6.95950
H	8.01620	30.47340	-7.08110
C	5.89830	29.98650	-5.54530
C	5.62630	27.65780	-4.79190
H	5.69260	26.74330	-4.53930
C	4.61590	29.71330	-5.05370
H	3.88930	30.32400	-5.01860
C	4.59170	28.37850	-4.62080
H	3.81650	28.01900	-4.20640
S	4.20650	35.16900	-5.37630
C	5.38520	35.92260	-7.49130
H	5.96170	35.96030	-8.24580
C	5.35500	34.82260	-6.63580
C	4.51850	36.96510	-7.17080
H	4.44090	37.76800	-7.67170
C	3.80150	36.68930	-6.05970
H	3.14560	37.27380	-5.69680
I	-3.05580	25.17430	-3.90500
F	3.86890	25.11990	-9.30070
F	2.38310	22.89410	-8.90260
F	1.32300	27.42840	-6.10760
F	0.30000	22.94830	-7.18650
F	3.35280	27.38130	-7.88820
C	-1.38140	25.22860	-5.05780
C	2.08670	24.01990	-8.23860
C	2.59180	26.30110	-7.71090
C	2.84890	25.15010	-8.42110
C	0.71540	25.20870	-6.63170
C	-0.41520	25.23690	-5.75250
C	1.53610	26.31070	-6.81830
C	1.03120	24.05810	-7.35630

Table S54: Cartesian coordinates (Å) for the Donor-Acceptor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 171°$ and $\tau_\beta = -25°$.

atom	*x*	*y*	*z*
S	-7.64790	12.16250	4.74440
N	-6.61110	15.96850	2.76310
C	-8.48120	17.17010	3.66400
C	-8.91620	16.00200	4.28250
H	-9.70510	16.01630	4.81130
C	-8.20550	14.80850	4.13400
C	-7.30260	17.09920	2.91700
H	-6.97980	17.88970	2.50050
C	-7.04930	14.85600	3.34780
H	-6.55280	14.05540	3.22620
C	-8.67070	13.56850	4.76200
C	-8.94270	11.23980	5.51540
H	-8.87640	10.32530	5.76800
C	-9.95310	13.29530	5.25360
H	-10.67970	13.90600	5.28870
C	-9.97730	11.96050	5.68650
H	-10.75250	11.60100	6.10090
S	-10.36250	18.75100	4.93100
C	-9.18380	19.50460	2.81600
H	-8.60730	19.54230	2.06150
C	-9.21400	18.40460	3.67150
C	-10.05050	20.54710	3.13650
H	-10.12810	21.35000	2.63560
C	-10.76750	20.27130	4.24760
H	-11.42340	20.85580	4.61050
I	-8.86520	24.07970	3.90500
F	-15.78990	24.13410	9.30070
F	-14.30410	26.35990	8.90260
F	-13.24400	21.82560	6.10760
F	-12.22100	26.30570	7.18650
F	-15.27380	21.87270	7.88820
C	-10.53960	24.02540	5.05780
C	-14.00770	25.23410	8.23860
C	-14.51280	22.95290	7.71090
C	-14.76990	24.10390	8.42110
C	-12.63640	24.04530	6.63170
C	-11.50580	24.01710	5.75250
C	-13.45710	22.94330	6.81830
C	-12.95220	25.19590	7.35630

Table S55: Cartesian coordinates (Å) for the Donor-Acceptor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 171°$ and $\tau_\beta = -25°$.

atom	*x*	*y*	*z*
S	-7.64790	12.16250	4.74440
N	-6.61110	15.96850	2.76310
C	-8.48120	17.17010	3.66400
C	-8.91620	16.00200	4.28250
H	-9.70510	16.01630	4.81130
C	-8.20550	14.80850	4.13400
C	-7.30260	17.09920	2.91700
H	-6.97980	17.88970	2.50050
C	-7.04930	14.85600	3.34780
H	-6.55280	14.05540	3.22620
C	-8.67070	13.56850	4.76200
C	-8.94270	11.23980	5.51540
H	-8.87640	10.32530	5.76800
C	-9.95310	13.29530	5.25360
H	-10.67970	13.90600	5.28870
C	-9.97730	11.96050	5.68650
H	-10.75250	11.60100	6.10090
S	-10.36250	18.75100	4.93100
C	-9.18380	19.50460	2.81600
H	-8.60730	19.54230	2.06150
C	-9.21400	18.40460	3.67150
C	-10.05050	20.54710	3.13650
H	-10.12810	21.35000	2.63560
C	-10.76750	20.27130	4.24760
H	-11.42340	20.85580	4.61050
I	-5.70380	8.75630	6.40230
F	1.22090	8.70190	1.00660
F	-0.26490	6.47610	1.40470
F	-1.32500	11.01040	4.19970
F	-2.34800	6.53030	3.12080
F	0.70480	10.96330	2.41910
C	-4.02940	8.81060	5.24950
C	-0.56130	7.60190	2.06870
C	-0.05620	9.88310	2.59640
C	0.20090	8.73210	1.88620
C	-1.93260	8.79070	3.67560
C	-3.06320	8.81890	4.55480
C	-1.11190	9.89270	3.48900
C	-1.61680	7.64010	2.95100

Table S56: Cartesian coordinates (Å) for the Donor-Acceptor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 171°$ and $\tau_\beta = -25°$.

atom	*x*	*y*	*z*
S	-7.64790	12.16250	4.74440
N	-6.61110	15.96850	2.76310
C	-8.48120	17.17010	3.66400
C	-8.91620	16.00200	4.28250
H	-9.70510	16.01630	4.81130
C	-8.20550	14.80850	4.13400
C	-7.30260	17.09920	2.91700
H	-6.97980	17.88970	2.50050
C	-7.04930	14.85600	3.34780
H	-6.55280	14.05540	3.22620
C	-8.67070	13.56850	4.76200
C	-8.94270	11.23980	5.51540
H	-8.87640	10.32530	5.76800
C	-9.95310	13.29530	5.25360
H	-10.67970	13.90600	5.28870
C	-9.97730	11.96050	5.68650
H	-10.75250	11.60100	6.10090
S	-10.36250	18.75100	4.93100
C	-9.18380	19.50460	2.81600
H	-8.60730	19.54230	2.06150
C	-9.21400	18.40460	3.67150
C	-10.05050	20.54710	3.13650
H	-10.12810	21.35000	2.63560
C	-10.76750	20.27130	4.24760
H	-11.42340	20.85580	4.61050
I	-17.62480	25.17430	6.40230
F	-10.70010	25.11990	1.00660
F	-12.18590	22.89410	1.40470
F	-13.24600	27.42840	4.19970
F	-14.26900	22.94830	3.12080
F	-11.21620	27.38130	2.41910
C	-15.95040	25.22860	5.24950
C	-12.48230	24.01990	2.06870
C	-11.97720	26.30110	2.59640
C	-11.72010	25.15010	1.88620
C	-13.85360	25.20870	3.67560
C	-14.98420	25.23690	4.55480
C	-13.03290	26.31070	3.48900
C	-13.53780	24.05810	2.95100

Table S57: Cartesian coordinates (Å) for the Donor-Donor Slipped π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 171°$ and $\tau_\beta = -25°$.

atom	*x*	*y*	*z*
I	10.18920	32.28870	-9.05860
F	17.11390	32.34310	-14.45430
F	15.62810	34.56890	-14.05630
F	14.56800	30.03460	-11.26120
F	13.54500	34.51470	-12.34010
F	16.59780	30.08170	-13.04180
C	11.86360	32.23440	-10.21140
C	15.33170	33.44310	-13.39230
C	15.83680	31.16190	-12.86450
C	16.09390	32.31290	-13.57470
C	13.96030	32.25430	-11.78540
C	12.82980	32.22610	-10.90610
C	14.78110	31.15230	-11.97190
C	14.27620	33.40490	-12.51000
I	7.02780	33.38330	-11.55600
F	0.10310	33.32890	-6.16030
F	1.58890	31.10310	-6.55830
F	2.64900	35.63740	-9.35340
F	3.67200	31.15730	-8.27450
F	0.61920	35.59030	-7.57280
C	5.35340	33.43760	-10.40320
C	1.88530	32.22890	-7.22230
C	1.38020	34.51010	-7.75010
C	1.12310	33.35910	-7.03990
C	3.25660	33.41770	-8.82920
C	4.38720	33.44590	-9.70840
C	2.43590	34.51970	-8.64270
C	2.94080	32.26710	-8.10460

Table S58: Cartesian coordinates (Å) for the Donor-Donor Slipped π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 171°$ and $\tau_\beta = -25°$.

atom	*x*	*y*	*z*
I	-4.37980	32.28870	1.24870
F	2.54490	32.34310	-4.14700
F	1.05910	34.56890	-3.74900
F	-0.00100	30.03460	-0.95390
F	-1.02400	34.51470	-2.03280
F	2.02880	30.08170	-2.73450
C	-2.70540	32.23440	0.09590
C	0.76270	33.44310	-3.08500
C	1.26780	31.16190	-2.55720
C	1.52490	32.31290	-3.26740
C	-0.60860	32.25430	-1.47810
C	-1.73920	32.22610	-0.59890
C	0.21210	31.15230	-1.66460
C	-0.29280	33.40490	-2.20270
I	7.02780	33.38330	-11.55600
F	0.10310	33.32890	-6.16030
F	1.58890	31.10310	-6.55830
F	2.64900	35.63740	-9.35340
F	3.67200	31.15730	-8.27450
F	0.61920	35.59030	-7.57280
C	5.35340	33.43760	-10.40320
C	1.88530	32.22890	-7.22230
C	1.38020	34.51010	-7.75010
C	1.12310	33.35910	-7.03990
C	3.25660	33.41770	-8.82920
C	4.38720	33.44590	-9.70840
C	2.43590	34.51970	-8.64270
C	2.94080	32.26710	-8.10460

Table S59: Cartesian coordinates (Å) for the Donor-Donor Edge-Edge contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 171°$ and $\tau_\beta = -25°$.

atom	*x*	*y*	*z*
I	-4.37980	-0.54730	1.24870
F	2.54490	-0.49290	-4.14700
F	1.05910	1.73290	-3.74900
F	-0.00100	-2.80140	-0.95390
F	-1.02400	1.67870	-2.03280
F	2.02880	-2.75430	-2.73450
C	-2.70540	-0.60160	0.09590
C	0.76270	0.60710	-3.08500
C	1.26780	-1.67410	-2.55720
C	1.52490	-0.52310	-3.26740
C	-0.60860	-0.58170	-1.47810
C	-1.73920	-0.60990	-0.59890
C	0.21210	-1.68370	-1.66460
C	-0.29280	0.56890	-2.20270
I	5.70380	7.66170	-6.40230
F	-1.22090	7.71610	-1.00660
F	0.26490	9.94190	-1.40470
F	1.32500	5.40760	-4.19970
F	2.34800	9.88770	-3.12080
F	-0.70480	5.45470	-2.41910
C	4.02940	7.60740	-5.24950
C	0.56130	8.81610	-2.06870
C	0.05620	6.53490	-2.59640
C	-0.20090	7.68590	-1.88620
C	1.93260	7.62730	-3.67560
C	3.06320	7.59910	-4.55480
C	1.11190	6.52530	-3.48900
C	1.61680	8.77790	-2.95100

Table S60: Cartesian coordinates (Å) for the Donor-Donor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 171°$ and $\tau_\beta = -25°$.

atom	*x*	*y*	*z*
I	-18.94880	15.87070	11.55600
F	-12.02410	15.92510	6.16030
F	-13.50990	18.15090	6.55830
F	-14.57000	13.61660	9.35340
F	-15.59300	18.09670	8.27450
F	-12.54020	13.66370	7.57280
C	-17.27440	15.81640	10.40320
C	-13.80630	17.02510	7.22230
C	-13.30120	14.74390	7.75010
C	-13.04410	15.89490	7.03990
C	-15.17760	15.83630	8.82920
C	-16.30820	15.80810	9.70840
C	-14.35690	14.73430	8.64270
C	-14.86180	16.98690	8.10460
I	-17.62480	8.75630	6.40230
F	-10.70010	8.70190	1.00660
F	-12.18590	6.47610	1.40470
F	-13.24600	11.01040	4.19970
F	-14.26900	6.53030	3.12080
F	-11.21620	10.96330	2.41910
C	-15.95040	8.81060	5.24950
C	-12.48230	7.60190	2.06870
C	-11.97720	9.88310	2.59640
C	-11.72010	8.73210	1.88620
C	-13.85360	8.79070	3.67560
C	-14.98420	8.81890	4.55480
C	-13.03290	9.89270	3.48900
C	-13.53780	7.64010	2.95100

Table S61: Cartesian coordinates (Å) for the Acceptor-Acceptor Slipped π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 171°$ and $\tau_\beta = -25°$.

atom	*x*	*y*	*z*
S	6.92110	28.58050	-5.56280
N	7.95790	32.38650	-7.54420
C	6.08780	33.58810	-6.64330
C	5.65280	32.42000	-6.02480
H	4.86390	32.43430	-5.49600
C	6.36350	31.22650	-6.17320
C	7.26640	33.51720	-7.39030
H	7.58920	34.30770	-7.80670
C	7.51970	31.27400	-6.95950
H	8.01620	30.47340	-7.08110
C	5.89830	29.98650	-5.54530
C	5.62630	27.65780	-4.79190
H	5.69260	26.74330	-4.53930
C	4.61590	29.71330	-5.05370
H	3.88930	30.32400	-5.01860
C	4.59170	28.37850	-4.62080
H	3.81650	28.01900	-4.20640
S	4.20650	35.16900	-5.37630
C	5.38520	35.92260	-7.49130
H	5.96170	35.96030	-8.24580
C	5.35500	34.82260	-6.63580
C	4.51850	36.96510	-7.17080
H	4.44090	37.76800	-7.67170
C	3.80150	36.68930	-6.05970
H	3.14560	37.27380	-5.69680
S	-4.27310	37.09150	-4.74440
N	-5.30990	33.28550	-2.76310
C	-3.43980	32.08390	-3.66400
C	-3.00480	33.25200	-4.28250
H	-2.21590	33.23770	-4.81130
C	-3.71550	34.44550	-4.13400
C	-4.61840	32.15480	-2.91700
H	-4.94120	31.36430	-2.50050
C	-4.87170	34.39800	-3.34780
H	-5.36820	35.19860	-3.22620
C	-3.25030	35.68550	-4.76200
C	-2.97830	38.01420	-5.51540
H	-3.04460	38.92870	-5.76800
C	-1.96790	35.95870	-5.25360
H	-1.24130	35.34800	-5.28870
C	-1.94370	37.29350	-5.68650
H	-1.16850	37.65300	-6.10090
S	-1.55850	30.50300	-4.93100
C	-2.73720	29.74940	-2.81600
H	-3.31370	29.71170	-2.06150
C	-2.70700	30.84940	-3.67150
C	-1.87050	28.70690	-3.13650
H	-1.79290	27.90400	-2.63560
C	-1.15350	28.98270	-4.24760
H	-0.49760	28.39820	-4.61050

Table S62: Cartesian coordinates (Å) for the Acceptor-Acceptor Edge-Edge contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 171°$ and $\tau_\beta = -25°$.

atom	*x*	*y*	*z*
S	6.92110	28.58050	-5.56280
N	7.95790	32.38650	-7.54420
C	6.08780	33.58810	-6.64330
C	5.65280	32.42000	-6.02480
H	4.86390	32.43430	-5.49600
C	6.36350	31.22650	-6.17320
C	7.26640	33.51720	-7.39030
H	7.58920	34.30770	-7.80670
C	7.51970	31.27400	-6.95950
H	8.01620	30.47340	-7.08110
C	5.89830	29.98650	-5.54530
C	5.62630	27.65780	-4.79190
H	5.69260	26.74330	-4.53930
C	4.61590	29.71330	-5.05370
H	3.88930	30.32400	-5.01860
C	4.59170	28.37850	-4.62080
H	3.81650	28.01900	-4.20640
S	4.20650	35.16900	-5.37630
C	5.38520	35.92260	-7.49130
H	5.96170	35.96030	-8.24580
C	5.35500	34.82260	-6.63580
C	4.51850	36.96510	-7.17080
H	4.44090	37.76800	-7.67170
C	3.80150	36.68930	-6.05970
H	3.14560	37.27380	-5.69680
S	8.97190	20.37150	-9.89810
N	7.93510	24.17750	-7.91670
C	9.80520	25.37910	-8.81770
C	10.24020	24.21100	-9.43610
H	11.02910	24.22530	-9.96500
C	9.52950	23.01750	-9.28770
C	8.62660	25.30820	-8.07060
H	8.30380	26.09870	-7.65420
C	8.37330	23.06500	-8.50150
H	7.87680	22.26440	-8.37980
C	9.99470	21.77750	-9.91560
C	10.26670	19.44880	-10.66910
H	10.20040	18.53430	-10.92160
C	11.27710	21.50430	-10.40730
H	12.00370	22.11500	-10.44230
C	11.30130	20.16950	-10.84020
H	12.07650	19.81000	-11.25450
S	11.68650	26.96000	-10.08470
C	10.50780	27.71360	-7.96960
H	9.93130	27.75130	-7.21510
C	10.53800	26.61360	-8.82510
C	11.37450	28.75610	-8.29020
H	11.45210	29.55900	-7.78920
C	12.09150	28.48030	-9.40130
H	12.74740	29.06480	-9.76410

Table S63: Cartesian coordinates (Å) for the Acceptor-Acceptor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 171°$ and $\tau_\beta = -25°$.

atom	*x*	*y*	*z*
S	6.92110	12.16250	-5.56280
N	7.95790	15.96850	-7.54420
C	6.08780	17.17010	-6.64330
C	5.65280	16.00200	-6.02480
H	4.86390	16.01630	-5.49600
C	6.36350	14.80850	-6.17320
C	7.26640	17.09920	-7.39030
H	7.58920	17.88970	-7.80670
C	7.51970	14.85600	-6.95950
H	8.01620	14.05540	-7.08110
C	5.89830	13.56850	-5.54530
C	5.62630	11.23980	-4.79190
H	5.69260	10.32530	-4.53930
C	4.61590	13.29530	-5.05370
H	3.88930	13.90600	-5.01860
C	4.59170	11.96050	-4.62080
H	3.81650	11.60100	-4.20640
S	4.20650	18.75100	-5.37630
C	5.38520	19.50460	-7.49130
H	5.96170	19.54230	-8.24580
C	5.35500	18.40460	-6.63580
C	4.51850	20.54710	-7.17080
H	4.44090	21.35000	-7.67170
C	3.80150	20.27130	-6.05970
H	3.14560	20.85580	-5.69680
S	8.24510	12.46450	-10.71650
N	9.28190	8.65850	-12.69790
C	7.41180	7.45690	-11.79690
C	6.97680	8.62500	-11.17850
H	6.18790	8.61070	-10.64960
C	7.68750	9.81850	-11.32690
C	8.59040	7.52780	-12.54400
H	8.91310	6.73730	-12.96040
C	8.84370	9.77100	-12.11310
H	9.34020	10.57160	-12.23480
C	7.22230	11.05850	-10.69900
C	6.95030	13.38720	-9.94550
H	7.01660	14.30170	-9.69300
C	5.93990	11.33170	-10.20730
H	5.21330	10.72100	-10.17230
C	5.91570	12.66650	-9.77440
H	5.14050	13.02600	-9.36010
S	5.53050	5.87600	-10.52990
C	6.70920	5.12240	-12.64500
H	7.28570	5.08470	-13.39950
C	6.67900	6.22240	-11.78950
C	5.84250	4.07990	-12.32440
H	5.76490	3.27700	-12.82540
C	5.12550	4.35570	-11.21330
H	4.46960	3.77120	-10.85050

Table S64: Cartesian coordinates (Å) for the Acceptor-Acceptor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 171°$ and $\tau_\beta = -25°$.

atom	*x*	*y*	*z*
S	-7.64790	12.16250	4.74440
N	-6.61110	15.96850	2.76310
C	-8.48120	17.17010	3.66400
C	-8.91620	16.00200	4.28250
H	-9.70510	16.01630	4.81130
C	-8.20550	14.80850	4.13400
C	-7.30260	17.09920	2.91700
H	-6.97980	17.88970	2.50050
C	-7.04930	14.85600	3.34780
H	-6.55280	14.05540	3.22620
C	-8.67070	13.56850	4.76200
C	-8.94270	11.23980	5.51540
H	-8.87640	10.32530	5.76800
C	-9.95310	13.29530	5.25360
H	-10.67970	13.90600	5.28870
C	-9.97730	11.96050	5.68650
H	-10.75250	11.60100	6.10090
S	-10.36250	18.75100	4.93100
C	-9.18380	19.50460	2.81600
H	-8.60730	19.54230	2.06150
C	-9.21400	18.40460	3.67150
C	-10.05050	20.54710	3.13650
H	-10.12810	21.35000	2.63560
C	-10.76750	20.27130	4.24760
H	-11.42340	20.85580	4.61050
S	-8.97190	28.88250	9.89810
N	-7.93510	25.07650	7.91670
C	-9.80520	23.87490	8.81770
C	-10.24020	25.04300	9.43610
H	-11.02910	25.02870	9.96500
C	-9.52950	26.23650	9.28770
C	-8.62660	23.94580	8.07060
H	-8.30380	23.15530	7.65420
C	-8.37330	26.18900	8.50150
H	-7.87680	26.98960	8.37980
C	-9.99470	27.47650	9.91560
C	-10.26670	29.80520	10.66910
H	-10.20040	30.71970	10.92160
C	-11.27710	27.74970	10.40730
H	-12.00370	27.13900	10.44230
C	-11.30130	29.08450	10.84020
H	-12.07650	29.44400	11.25450
S	-11.68650	22.29400	10.08470
C	-10.50780	21.54040	7.96960
H	-9.93130	21.50270	7.21510
C	-10.53800	22.64040	8.82510
C	-11.37450	20.49790	8.29020
H	-11.45210	19.69500	7.78920
C	-12.09150	20.77370	9.40130
H	-12.74740	20.18920	9.76410

Table S65: Cartesian coordinates (Å) for the XB contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles τ_α = 166° and τ_β = 24°.

atom	*x*	*y*	*z*
I	17.62480	24.07960	-6.40240
F	10.70000	24.13400	-1.00660
F	12.18580	26.35990	-1.40470
F	13.24610	21.82560	-4.19980
F	14.26910	26.30570	-3.12090
F	11.21620	21.87270	-2.41910
C	15.95050	24.02530	-5.24950
C	12.48230	25.23410	-2.06870
C	11.97710	22.95300	-2.59640
C	11.72010	24.10390	-1.88620
C	13.85360	24.04550	-3.67560
C	14.98370	24.01720	-4.55480
C	13.03300	22.94350	-3.49000
C	13.53760	25.19600	-2.95100
N	19.85600	24.17760	-7.91660
C	21.72620	25.37910	-8.81770
C	22.16110	24.21080	-9.43620
H	22.94990	24.22510	-9.96550
C	21.45060	23.01750	-9.28760
C	20.54780	25.30850	-8.07060
H	20.22520	26.09910	-7.65420
C	20.29450	23.06520	-8.50150
H	19.79800	22.26440	-8.37980
C	21.91540	21.77770	-9.91460
S	23.61030	26.95840	-10.09080
C	22.42970	27.71360	-7.96860
H	21.85460	27.74240	-7.21200
C	22.46360	26.62840	-8.83850
C	23.29830	28.75450	-8.28710
H	23.37990	29.55460	-7.78320
C	24.01300	28.48360	-9.40330
H	24.66540	29.07090	-9.76740
S	21.36210	20.22210	-9.55280
C	22.88930	21.66520	-10.93600
H	23.34850	22.41220	-11.30200
C	23.11450	20.31890	-11.36280
H	23.62780	20.09940	-12.13090
C	22.60370	19.50460	-10.67840
H	22.81900	18.58050	-10.70190

Table S66: Cartesian coordinates (Å) for the Donor-Acceptor π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles τ_α = 166° and τ_β = 24°.

atom	*x*	*y*	*z*
I	20.78620	25.17440	-3.90490
F	27.71100	25.12000	-9.30070
F	26.22520	22.89410	-8.90260
F	25.16490	27.42840	-6.10750
F	24.14190	22.94830	-7.18630
F	27.19480	27.38130	-7.88820
C	22.46050	25.22870	-5.05780
C	25.92870	24.01990	-8.23860
C	26.43390	26.30100	-7.71090
C	26.69090	25.15010	-8.42110
C	24.55740	25.20850	-6.63170
C	23.42730	25.23680	-5.75250
C	25.37800	26.31050	-6.81720
C	24.87340	24.05800	-7.35630
N	19.85600	24.17760	-7.91660
C	21.72620	25.37910	-8.81770
C	22.16110	24.21080	-9.43620
H	22.94990	24.22510	-9.96550
C	21.45060	23.01750	-9.28760
C	20.54780	25.30850	-8.07060
H	20.22520	26.09910	-7.65420
C	20.29450	23.06520	-8.50150
H	19.79800	22.26440	-8.37980
C	21.91540	21.77770	-9.91460
S	23.61030	26.95840	-10.09080
C	22.42970	27.71360	-7.96860
H	21.85460	27.74240	-7.21200
C	22.46360	26.62840	-8.83850
C	23.29830	28.75450	-8.28710
H	23.37990	29.55460	-7.78320
C	24.01300	28.48360	-9.40330
H	24.66540	29.07090	-9.76740
S	21.36210	20.22210	-9.55280
C	22.88930	21.66520	-10.93600
H	23.34850	22.41220	-11.30200
C	23.11450	20.31890	-11.36280
H	23.62780	20.09940	-12.13090
C	22.60370	19.50460	-10.67840
H	22.81900	18.58050	-10.70190

Table S67: Cartesian coordinates (Å) for the Donor-Donor π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles τ_α = 166° and τ_β = 24°.

atom	*x*	*y*	*z*
I	16.30080	0.54740	-1.24870
F	9.37600	0.49300	4.14700
F	10.86180	-1.73290	3.74900
F	11.92210	2.80140	0.95380
F	12.94510	-1.67870	2.03270
F	9.89220	2.75430	2.73450
C	14.62650	0.60170	-0.09590
C	11.15830	-0.60710	3.08500
C	10.65310	1.67400	2.55720
C	10.39610	0.52310	3.26740
C	12.52960	0.58150	1.47810
C	13.65970	0.60980	0.59890
C	11.70900	1.68350	1.66360
C	12.21360	-0.56900	2.20270
I	7.54120	-0.54740	1.24870
F	14.46600	-0.49300	-4.14700
F	12.98020	1.73290	-3.74900
F	11.91990	-2.80140	-0.95380
F	10.89690	1.67870	-2.03270
F	13.94980	-2.75430	-2.73450
C	9.21550	-0.60170	0.09590
C	12.68370	0.60710	-3.08500
C	13.18890	-1.67400	-2.55720
C	13.44590	-0.52310	-3.26740
C	11.31240	-0.58150	-1.47810
C	10.18230	-0.60980	-0.59890
C	12.13300	-1.68350	-1.66360
C	11.62840	0.56900	-2.20270

Table S68: Cartesian coordinates (Å) for the Acceptor-Acceptor π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles τ_α = 166° and τ_β = 24°.

atom	*x*	*y*	*z*
N	18.53200	16.86740	-2.76300
C	20.40220	15.66590	-3.66400
C	20.83710	16.83420	-4.28260
H	21.62590	16.81990	-4.81180
C	20.12660	18.02750	-4.13390
C	19.22380	15.73650	-2.91700
H	18.90120	14.94590	-2.50050
C	18.97050	17.97980	-3.34780
H	18.47400	18.78060	-3.22620
C	20.59140	19.26730	-4.76090
S	22.28630	14.08660	-4.93720
C	21.10570	13.33140	-2.81490
H	20.53060	13.30260	-2.05840
C	21.13960	14.41660	-3.68490
C	21.97430	12.29050	-3.13340
H	22.05590	11.49040	-2.62960
C	22.68900	12.56140	-4.24970
H	23.34140	11.97410	-4.61380
S	20.03810	20.82290	-4.39920
C	21.56530	19.37980	-5.78240
H	22.02450	18.63280	-6.14840
C	21.79050	20.72610	-6.20910
H	22.30380	20.94560	-6.97720
C	21.27970	21.54040	-5.52470
H	21.49500	22.46450	-5.54830
N	19.87900	15.96860	-7.54430
C	18.00880	17.17010	-6.64330
C	17.57390	16.00180	-6.02470
H	16.78510	16.01610	-5.49550
C	18.28440	14.80850	-6.17330
C	19.18720	17.09950	-7.39030
H	19.50980	17.89010	-7.80680
C	19.44050	14.85620	-6.95950
H	19.93700	14.05540	-7.08110
C	17.81960	13.56870	-5.54640
S	16.12470	18.74940	-5.37010
C	17.30530	19.50460	-7.49240
H	17.88040	19.53340	-8.24890
C	17.27140	18.41940	-6.62240
C	16.43670	20.54550	-7.17390
H	16.35510	21.34560	-7.67770
C	15.72200	20.27460	-6.05760
H	15.06960	20.86190	-5.69350
S	18.37290	12.01310	-5.90810
C	16.84570	13.45620	-4.52490
H	16.38650	14.20320	-4.15890
C	16.62050	12.10990	-4.09820
H	16.10720	11.89040	-3.33010
C	17.13130	11.29560	-4.78260
H	16.91600	10.37150	-4.75900

Table S69: Cartesian coordinates (Å) for the Donor-Acceptor Slipped π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles τ_α = 166° and τ_β = 24°.

atom	*x*	*y*	*z*
I	20.78620	25.17440	-3.90490
F	27.71100	25.12000	-9.30070
F	26.22520	22.89410	-8.90260
F	25.16490	27.42840	-6.10750
F	24.14190	22.94830	-7.18630
F	27.19480	27.38130	-7.88820
C	22.46050	25.22870	-5.05780
C	25.92870	24.01990	-8.23860
C	26.43390	26.30100	-7.71090
C	26.69090	25.15010	-8.42110
C	24.55740	25.20850	-6.63170
C	23.42730	25.23680	-5.75250
C	25.37800	26.31050	-6.81720
C	24.87340	24.05800	-7.35630
N	17.20800	24.17760	2.39070
C	19.07820	25.37910	1.48960
C	19.51310	24.21080	0.87110
H	20.30190	24.22510	0.34180
C	18.80260	23.01750	1.01970
C	17.89980	25.30850	2.23670
H	17.57720	26.09910	2.65310
C	17.64650	23.06520	1.80580
H	17.15000	22.26440	1.92750
C	19.26740	21.77770	0.39270
S	20.96230	26.95840	0.21650
C	19.78170	27.71360	2.33870
H	19.20660	27.74240	3.09530
C	19.81560	26.62840	1.46880
C	20.65030	28.75450	2.02020
H	20.73190	29.55460	2.52410
C	21.36500	28.48360	0.90390
H	22.01740	29.07090	0.53990
S	18.71410	20.22210	0.75450
C	20.24130	21.66520	-0.62870
H	20.70050	22.41220	-0.99470
C	20.46650	20.31890	-1.05550
H	20.97980	20.09940	-1.82360
C	19.95570	19.50460	-0.37110
H	20.17100	18.58050	-0.39460

Table S70: Cartesian coordinates (Å) for the Donor-Acceptor Slipped π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles τ_α = 166° and τ_β = 24°.

atom	*x*	*y*	*z*
I	1.73180	33.38340	9.05860
F	-5.19300	33.32900	14.45430
F	-3.70720	31.10310	14.05630
F	-2.64690	35.63740	11.26110
F	-1.62390	31.15730	12.34000
F	-4.67680	35.59030	13.04180
C	0.05750	33.43770	10.21140
C	-3.41070	32.22890	13.39230
C	-3.91590	34.51000	12.86450
C	-4.17290	33.35910	13.57470
C	-2.03930	33.41750	11.78540
C	-0.90930	33.44580	10.90610
C	-2.86000	34.51950	11.97090
C	-2.35540	32.26700	12.51000
N	-9.25900	32.38660	13.07030
C	-11.12920	33.58810	13.97130
C	-11.56410	32.41980	14.58990
H	-12.35290	32.43410	15.11910
C	-10.85360	31.22650	14.44120
C	-9.95080	33.51750	13.22430
H	-9.62820	34.30810	12.80780
C	-9.69740	31.27420	13.65510
H	-9.20100	30.47340	13.53340
C	-11.31840	29.98670	15.06820
S	-13.01330	35.16740	15.24450
C	-11.83270	35.92260	13.12220
H	-11.25760	35.95140	12.36570
C	-11.86660	34.83740	13.99210
C	-12.70130	36.96350	13.44070
H	-12.78290	37.76360	12.93680
C	-13.41600	36.69260	14.55700
H	-14.06840	37.27990	14.92110
S	-10.76510	28.43110	14.70640
C	-12.29230	29.87420	16.08970
H	-12.75150	30.62120	16.45570
C	-12.51750	28.52790	16.51640
H	-13.03080	28.30840	17.28450
C	-12.00670	27.71360	15.83200
H	-12.22200	26.78950	15.85560

Table S71: Cartesian coordinates (Å) for the Donor-Acceptor Edge-Edge contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles τ_α = 166° and τ_β = 24°.

atom	*x*	*y*	*z*
I	20.78620	25.17440	-3.90490
F	27.71100	25.12000	-9.30070
F	26.22520	22.89410	-8.90260
F	25.16490	27.42840	-6.10750
F	24.14190	22.94830	-7.18630
F	27.19480	27.38130	-7.88820
C	22.46050	25.22870	-5.05780
C	25.92870	24.01990	-8.23860
C	26.43390	26.30100	-7.71090
C	26.69090	25.15010	-8.42110
C	24.55740	25.20850	-6.63170
C	23.42730	25.23680	-5.75250
C	25.37800	26.31050	-6.81720
C	24.87340	24.05800	-7.35630
N	18.53200	16.86740	-2.76300
C	20.40220	15.66590	-3.66400
C	20.83710	16.83420	-4.28260
H	21.62590	16.81990	-4.81180
C	20.12660	18.02750	-4.13390
C	19.22380	15.73650	-2.91700
H	18.90120	14.94590	-2.50050
C	18.97050	17.97980	-3.34780
H	18.47400	18.78060	-3.22620
C	20.59140	19.26730	-4.76090
S	22.28630	14.08660	-4.93720
C	21.10570	13.33140	-2.81490
H	20.53060	13.30260	-2.05840
C	21.13960	14.41660	-3.68490
C	21.97430	12.29050	-3.13340
H	22.05590	11.49040	-2.62960
C	22.68900	12.56140	-4.24970
H	23.34140	11.97410	-4.61380
S	20.03810	20.82290	-4.39920
C	21.56530	19.37980	-5.78240
H	22.02450	18.63280	-6.14840
C	21.79050	20.72610	-6.20910
H	22.30380	20.94560	-6.97720
C	21.27970	21.54040	-5.52470
H	21.49500	22.46450	-5.54830

Table S72: Cartesian coordinates (Å) for the Donor-Acceptor Edge-Edge contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles τ_α = 166° and τ_β = 24°.

atom	*x*	*y*	*z*
I	1.73180	33.38340	9.05860
F	-5.19300	33.32900	14.45430
F	-3.70720	31.10310	14.05630
F	-2.64690	35.63740	11.26110
F	-1.62390	31.15730	12.34000
F	-4.67680	35.59030	13.04180
C	0.05750	33.43770	10.21140
C	-3.41070	32.22890	13.39230
C	-3.91590	34.51000	12.86450
C	-4.17290	33.35910	13.57470
C	-2.03930	33.41750	11.78540
C	-0.90930	33.44580	10.90610
C	-2.86000	34.51950	11.97090
C	-2.35540	32.26700	12.51000
N	-10.60600	33.28540	17.85160
C	-8.73580	32.08390	16.95050
C	-8.30090	33.25220	16.33200
H	-7.51210	33.23790	15.80280
C	-9.01140	34.44550	16.48060
C	-9.91420	32.15450	17.69760
H	-10.23680	31.36390	18.11410
C	-10.16750	34.39780	17.26680
H	-10.66400	35.19860	17.38840
C	-8.54660	35.68530	15.85360
S	-6.85170	30.50460	15.67740
C	-8.03230	29.74940	17.79970
H	-8.60740	29.72060	18.55620
C	-7.99840	30.83460	16.92970
C	-7.16370	28.70850	17.48120
H	-7.08210	27.90840	17.98500
C	-6.44890	28.97940	16.36490
H	-5.79660	28.39210	16.00080
S	-9.09990	37.24090	16.21540
C	-7.57270	35.79780	14.83220
H	-7.11350	35.05080	14.46620
C	-7.34750	37.14410	14.40550
H	-6.83420	37.36360	13.63740
C	-7.85830	37.95840	15.08990
H	-7.64300	38.88250	15.06630

Table S73: Cartesian coordinates (Å) for the Donor-Acceptor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles τ_α = 166° and τ_β = 24°.

atom	*x*	*y*	*z*
I	20.78620	25.17440	-3.90490
F	27.71100	25.12000	-9.30070
F	26.22520	22.89410	-8.90260
F	25.16490	27.42840	-6.10750
F	24.14190	22.94830	-7.18630
F	27.19480	27.38130	-7.88820
C	22.46050	25.22870	-5.05780
C	25.92870	24.01990	-8.23860
C	26.43390	26.30100	-7.71090
C	26.69090	25.15010	-8.42110
C	24.55740	25.20850	-6.63170
C	23.42730	25.23680	-5.75250
C	25.37800	26.31050	-6.81720
C	24.87340	24.05800	-7.35630
N	18.53200	33.28540	-2.76300
C	20.40220	32.08390	-3.66400
C	20.83710	33.25220	-4.28260
H	21.62590	33.23790	-4.81180
C	20.12660	34.44550	-4.13390
C	19.22380	32.15450	-2.91700
H	18.90120	31.36390	-2.50050
C	18.97050	34.39780	-3.34780
H	18.47400	35.19860	-3.22620
C	20.59140	35.68530	-4.76090
S	22.28630	30.50460	-4.93720
C	21.10570	29.74940	-2.81490
H	20.53060	29.72060	-2.05840
C	21.13960	30.83460	-3.68490
C	21.97430	28.70850	-3.13340
H	22.05590	27.90840	-2.62960
C	22.68900	28.97940	-4.24970
H	23.34140	28.39210	-4.61380
S	20.03810	37.24090	-4.39920
C	21.56530	35.79780	-5.78240
H	22.02450	35.05080	-6.14840
C	21.79050	37.14410	-6.20910
H	22.30380	37.36360	-6.97720
C	21.27970	37.95840	-5.52470
H	21.49500	38.88250	-5.54830

Table S74: Cartesian coordinates (Å) for the Donor-Acceptor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles τ_α = 166° and τ_β = 24°.

atom	*x*	*y*	*z*
I	1.73180	16.96540	9.05860
F	-5.19300	16.91100	14.45430
F	-3.70720	14.68510	14.05630
F	-2.64690	19.21940	11.26110
F	-1.62390	14.73930	12.34000
F	-4.67680	19.17230	13.04180
C	0.05750	17.01970	10.21140
C	-3.41070	15.81090	13.39230
C	-3.91590	18.09200	12.86450
C	-4.17290	16.94110	13.57470
C	-2.03930	16.99950	11.78540
C	-0.90930	17.02780	10.90610
C	-2.86000	18.10150	11.97090
C	-2.35540	15.84900	12.51000
N	-9.28200	24.17760	12.69800
C	-7.41180	25.37910	11.79690
C	-6.97690	24.21080	11.17840
H	-6.18810	24.22510	10.64910
C	-7.68740	23.01750	11.32700
C	-8.59020	25.30850	12.54400
H	-8.91280	26.09910	12.96040
C	-8.84350	23.06520	12.11310
H	-9.34000	22.26440	12.23480
C	-7.22260	21.77770	10.70000
S	-5.52770	26.95840	10.52370
C	-6.70830	27.71360	12.64600
H	-7.28340	27.74240	13.40260
C	-6.67440	26.62840	11.77610
C	-5.83970	28.75450	12.32750
H	-5.75810	29.55460	12.83140
C	-5.12500	28.48360	11.21120
H	-4.47260	29.07090	10.84720
S	-7.77590	20.22210	11.06180
C	-6.24870	21.66520	9.67850
H	-5.78950	22.41220	9.31260
C	-6.02350	20.31890	9.25180
H	-5.51020	20.09940	8.48370
C	-6.53430	19.50460	9.93620
H	-6.31900	18.58050	9.91270

Table S75: Cartesian coordinates (Å) for the Donor-Acceptor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles τ_α = 166° and τ_β = 24°.

atom	*x*	*y*	*z*
N	3.96300	16.86740	7.54430
C	5.83320	15.66590	6.64330
C	6.26810	16.83420	6.02470
H	7.05690	16.81990	5.49550
C	5.55760	18.02750	6.17330
C	4.65480	15.73650	7.39030
H	4.33220	14.94590	7.80680
C	4.40150	17.97980	6.95950
H	3.90500	18.78060	7.08110
C	6.02240	19.26730	5.54640
S	7.71730	14.08660	5.37010
C	6.53670	13.33140	7.49240
H	5.96160	13.30260	8.24890
C	6.57060	14.41660	6.62240
C	7.40530	12.29050	7.17390
H	7.48690	11.49040	7.67770
C	8.12000	12.56140	6.05760
H	8.77240	11.97410	5.69350
S	5.46910	20.82290	5.90810
C	6.99630	19.37980	4.52490
H	7.45550	18.63280	4.15890
C	7.22150	20.72610	4.09820
H	7.73480	20.94560	3.33010
C	6.71070	21.54040	4.78260
H	6.92600	22.46450	4.75900
I	14.97680	7.66160	3.90490
F	8.05200	7.71600	9.30070
F	9.53780	9.94190	8.90260
F	10.59810	5.40760	6.10750
F	11.62110	9.88770	7.18630
F	8.56820	5.45470	7.88820
C	13.30250	7.60730	5.05780
C	9.83430	8.81610	8.23860
C	9.32910	6.53500	7.71090
C	9.07210	7.68590	8.42110
C	11.20560	7.62750	6.63170
C	12.33570	7.59920	5.75250
C	10.38500	6.52550	6.81720
C	10.88960	8.77800	7.35630

Table S76: Cartesian coordinates (Å) for the Donor-Acceptor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles τ_α = 166° and τ_β = 24°.

atom	*x*	*y*	*z*
N	3.96300	16.86740	7.54430
C	5.83320	15.66590	6.64330
C	6.26810	16.83420	6.02470
H	7.05690	16.81990	5.49550
C	5.55760	18.02750	6.17330
C	4.65480	15.73650	7.39030
H	4.33220	14.94590	7.80680
C	4.40150	17.97980	6.95950
H	3.90500	18.78060	7.08110
C	6.02240	19.26730	5.54640
S	7.71730	14.08660	5.37010
C	6.53670	13.33140	7.49240
H	5.96160	13.30260	8.24890
C	6.57060	14.41660	6.62240
C	7.40530	12.29050	7.17390
H	7.48690	11.49040	7.67770
C	8.12000	12.56140	6.05760
H	8.77240	11.97410	5.69350
S	5.46910	20.82290	5.90810
C	6.99630	19.37980	4.52490
H	7.45550	18.63280	4.15890
C	7.22150	20.72610	4.09820
H	7.73480	20.94560	3.33010
C	6.71070	21.54040	4.78260
H	6.92600	22.46450	4.75900
I	3.05580	24.07960	3.90490
F	-3.86900	24.13400	9.30070
F	-2.38320	26.35990	8.90260
F	-1.32290	21.82560	6.10750
F	-0.29990	26.30570	7.18630
F	-3.35280	21.87270	7.88820
C	1.38150	24.02530	5.05780
C	-2.08670	25.23410	8.23860
C	-2.59190	22.95300	7.71090
C	-2.84890	24.10390	8.42110
C	-0.71540	24.04550	6.63170
C	0.41470	24.01720	5.75250
C	-1.53600	22.94350	6.81720
C	-1.03140	25.19600	7.35630

Table S77: Cartesian coordinates (Å) for the Donor-Donor Slipped π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles τ_α = 166° and τ_β = 24°.

atom	*x*	*y*	*z*
I	20.78620	25.17440	-3.90490
F	27.71100	25.12000	-9.30070
F	26.22520	22.89410	-8.90260
F	25.16490	27.42840	-6.10750
F	24.14190	22.94830	-7.18630
F	27.19480	27.38130	-7.88820
C	22.46050	25.22870	-5.05780
C	25.92870	24.01990	-8.23860
C	26.43390	26.30100	-7.71090
C	26.69090	25.15010	-8.42110
C	24.55740	25.20850	-6.63170
C	23.42730	25.23680	-5.75250
C	25.37800	26.31050	-6.81720
C	24.87340	24.05800	-7.35630
I	17.62480	24.07960	-6.40240
F	10.70000	24.13400	-1.00660
F	12.18580	26.35990	-1.40470
F	13.24610	21.82560	-4.19980
F	14.26910	26.30570	-3.12090
F	11.21620	21.87270	-2.41910
C	15.95050	24.02530	-5.24950
C	12.48230	25.23410	-2.06870
C	11.97710	22.95300	-2.59640
C	11.72010	24.10390	-1.88620
C	13.85360	24.04550	-3.67560
C	14.98370	24.01720	-4.55480
C	13.03300	22.94350	-3.49000
C	13.53760	25.19600	-2.95100

Table S78: Cartesian coordinates (Å) for the Donor-Donor Slipped π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles τ_α = 166° and τ_β = 24°.

atom	*x*	*y*	*z*
I	6.21720	25.17440	6.40240
F	13.14200	25.12000	1.00660
F	11.65620	22.89410	1.40470
F	10.59590	27.42840	4.19980
F	9.57290	22.94830	3.12090
F	12.62580	27.38130	2.41910
C	7.89150	25.22870	5.24950
C	11.35970	24.01990	2.06870
C	11.86490	26.30100	2.59640
C	12.12190	25.15010	1.88620
C	9.98840	25.20850	3.67560
C	8.85830	25.23680	4.55480
C	10.80900	26.31050	3.49000
C	10.30440	24.05800	2.95100
I	17.62480	24.07960	-6.40240
F	10.70000	24.13400	-1.00660
F	12.18580	26.35990	-1.40470
F	13.24610	21.82560	-4.19980
F	14.26910	26.30570	-3.12090
F	11.21620	21.87270	-2.41910
C	15.95050	24.02530	-5.24950
C	12.48230	25.23410	-2.06870
C	11.97710	22.95300	-2.59640
C	11.72010	24.10390	-1.88620
C	13.85360	24.04550	-3.67560
C	14.98370	24.01720	-4.55480
C	13.03300	22.94350	-3.49000
C	13.53760	25.19600	-2.95100

Table S79: Cartesian coordinates (Å) for the Donor-Donor Edge-Edge contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles τ_α = 166° and τ_β = 24°.

atom	*x*	*y*	*z*
I	0.40780	-8.75640	14.21220
F	-6.51700	-8.70200	19.60800
F	-5.03120	-6.47610	19.20990
F	-3.97090	-11.01040	16.41480
F	-2.94790	-6.53030	17.49360
F	-6.00080	-10.96330	18.19550
C	-1.26650	-8.81070	15.36510
C	-4.73470	-7.60190	18.54590
C	-5.23990	-9.88300	18.01820
C	-5.49690	-8.73210	18.72840
C	-3.36330	-8.79050	16.93900
C	-2.23330	-8.81880	16.05980
C	-4.18400	-9.89250	17.12450
C	-3.67940	-7.64000	17.66360
I	-9.67580	-0.54740	21.86330
F	-2.75100	-0.49300	16.46750
F	-4.23680	1.73290	16.86560
F	-5.29710	-2.80140	19.66070
F	-6.32010	1.67870	18.58190
F	-3.26710	-2.75430	17.88010
C	-8.00150	-0.60170	20.71040
C	-4.53330	0.60710	17.52960
C	-4.02810	-1.67400	18.05730
C	-3.77110	-0.52310	17.34720
C	-5.90460	-0.58150	19.13650
C	-7.03470	-0.60980	20.01570
C	-5.08400	-1.68350	18.95100
C	-5.58850	0.56900	18.41190

Table S80: Cartesian coordinates (Å) for the Donor-Donor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles τ_α = 166° and τ_β = 24°.

atom	*x*	*y*	*z*
I	20.78620	25.17440	-3.90490
F	27.71100	25.12000	-9.30070
F	26.22520	22.89410	-8.90260
F	25.16490	27.42840	-6.10750
F	24.14190	22.94830	-7.18630
F	27.19480	27.38130	-7.88820
C	22.46050	25.22870	-5.05780
C	25.92870	24.01990	-8.23860
C	26.43390	26.30100	-7.71090
C	26.69090	25.15010	-8.42110
C	24.55740	25.20850	-6.63170
C	23.42730	25.23680	-5.75250
C	25.37800	26.31050	-6.81720
C	24.87340	24.05800	-7.35630
I	19.46220	32.28860	1.24870
F	26.38700	32.34300	-4.14700
F	24.90120	34.56890	-3.74900
F	23.84090	30.03460	-0.95380
F	22.81790	34.51470	-2.03270
F	25.87080	30.08170	-2.73450
C	21.13650	32.23430	0.09590
C	24.60470	33.44310	-3.08500
C	25.10990	31.16200	-2.55720
C	25.36690	32.31290	-3.26740
C	23.23340	32.25450	-1.47810
C	22.10330	32.22620	-0.59890
C	24.05400	31.15250	-1.66360
C	23.54940	33.40500	-2.20270

Table S81: Cartesian coordinates (Å) for the Acceptor-Acceptor Slipped π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles τ_α = 166° and τ_β = 24°.

atom	*x*	*y*	*z*
N	18.55500	25.07640	-2.39070
C	16.68480	23.87490	-1.48960
C	16.24990	25.04320	-0.87110
H	15.46110	25.02890	-0.34180
C	16.96040	26.23650	-1.01970
C	17.86320	23.94550	-2.23670
H	18.18580	23.15490	-2.65310
C	18.11650	26.18880	-1.80580
H	18.61300	26.98960	-1.92750
C	16.49560	27.47630	-0.39270
S	14.80070	22.29560	-0.21650
C	15.98130	21.54040	-2.33870
H	16.55640	21.51160	-3.09530
C	15.94740	22.62560	-1.46880
C	15.11270	20.49950	-2.02020
H	15.03110	19.69940	-2.52410
C	14.39800	20.77040	-0.90390
H	13.74560	20.18310	-0.53990
S	17.04890	29.03190	-0.75450
C	15.52170	27.58880	0.62870
H	15.06250	26.84180	0.99470
C	15.29650	28.93510	1.05550
H	14.78320	29.15460	1.82360
C	15.80730	29.74940	0.37110
H	15.59200	30.67350	0.39460
N	5.28700	24.17760	2.39070
C	7.15720	25.37910	1.48960
C	7.59210	24.21080	0.87110
H	8.38090	24.22510	0.34180
C	6.88160	23.01750	1.01970
C	5.97880	25.30850	2.23670
H	5.65620	26.09910	2.65310
C	5.72550	23.06520	1.80580
H	5.22900	22.26440	1.92750
C	7.34640	21.77770	0.39270
S	9.04130	26.95840	0.21650
C	7.86070	27.71360	2.33870
H	7.28560	27.74240	3.09530
C	7.89460	26.62840	1.46880
C	8.72930	28.75450	2.02020
H	8.81090	29.55460	2.52410
C	9.44400	28.48360	0.90390
H	10.09640	29.07090	0.53990
S	6.79310	20.22210	0.75450
C	8.32030	21.66520	-0.62870
H	8.77950	22.41220	-0.99470
C	8.54550	20.31890	-1.05550
H	9.05880	20.09940	-1.82360
C	8.03470	19.50460	-0.37110
H	8.25000	18.58050	-0.39460

Table S82: Cartesian coordinates (Å) for the Acceptor-Acceptor Edge-Edge contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles τ_α = 166° and τ_β = 24°.

atom	*x*	*y*	*z*
N	19.85600	24.17760	-7.91660
C	21.72620	25.37910	-8.81770
C	22.16110	24.21080	-9.43620
H	22.94990	24.22510	-9.96550
C	21.45060	23.01750	-9.28760
C	20.54780	25.30850	-8.07060
H	20.22520	26.09910	-7.65420
C	20.29450	23.06520	-8.50150
H	19.79800	22.26440	-8.37980
C	21.91540	21.77770	-9.91460
S	23.61030	26.95840	-10.09080
C	22.42970	27.71360	-7.96860
H	21.85460	27.74240	-7.21200
C	22.46360	26.62840	-8.83850
C	23.29830	28.75450	-8.28710
H	23.37990	29.55460	-7.78320
C	24.01300	28.48360	-9.40330
H	24.66540	29.07090	-9.76740
S	21.36210	20.22210	-9.55280
C	22.88930	21.66520	-10.93600
H	23.34850	22.41220	-11.30200
C	23.11450	20.31890	-11.36280
H	23.62780	20.09940	-12.13090
C	22.60370	19.50460	-10.67840
H	22.81900	18.58050	-10.70190
N	19.87900	32.38660	-7.54430
C	18.00880	33.58810	-6.64330
C	17.57390	32.41980	-6.02470
H	16.78510	32.43410	-5.49550
C	18.28440	31.22650	-6.17330
C	19.18720	33.51750	-7.39030
H	19.50980	34.30810	-7.80680
C	19.44050	31.27420	-6.95950
H	19.93700	30.47340	-7.08110
C	17.81960	29.98670	-5.54640
S	16.12470	35.16740	-5.37010
C	17.30530	35.92260	-7.49240
H	17.88040	35.95140	-8.24890
C	17.27140	34.83740	-6.62240
C	16.43670	36.96350	-7.17390
H	16.35510	37.76360	-7.67770
C	15.72200	36.69260	-6.05760
H	15.06960	37.27990	-5.69350
S	18.37290	28.43110	-5.90810
C	16.84570	29.87420	-4.52490
H	16.38650	30.62120	-4.15890
C	16.62050	28.52790	-4.09820
H	16.10720	28.30840	-3.33010
C	17.13130	27.71360	-4.78260
H	16.91600	26.78950	-4.75900

Table S83: Cartesian coordinates (Å) for the Acceptor-Acceptor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles τ_α = 166° and τ_β = 24°.

atom	*x*	*y*	*z*
N	18.55500	25.07640	-2.39070
C	16.68480	23.87490	-1.48960
C	16.24990	25.04320	-0.87110
H	15.46110	25.02890	-0.34180
C	16.96040	26.23650	-1.01970
C	17.86320	23.94550	-2.23670
H	18.18580	23.15490	-2.65310
C	18.11650	26.18880	-1.80580
H	18.61300	26.98960	-1.92750
C	16.49560	27.47630	-0.39270
S	14.80070	22.29560	-0.21650
C	15.98130	21.54040	-2.33870
H	16.55640	21.51160	-3.09530
C	15.94740	22.62560	-1.46880
C	15.11270	20.49950	-2.02020
H	15.03110	19.69940	-2.52410
C	14.39800	20.77040	-0.90390
H	13.74560	20.18310	-0.53990
S	17.04890	29.03190	-0.75450
C	15.52170	27.58880	0.62870
H	15.06250	26.84180	0.99470
C	15.29650	28.93510	1.05550
H	14.78320	29.15460	1.82360
C	15.80730	29.74940	0.37110
H	15.59200	30.67350	0.39460
N	19.87900	32.38660	-7.54430
C	18.00880	33.58810	-6.64330
C	17.57390	32.41980	-6.02470
H	16.78510	32.43410	-5.49550
C	18.28440	31.22650	-6.17330
C	19.18720	33.51750	-7.39030
H	19.50980	34.30810	-7.80680
C	19.44050	31.27420	-6.95950
H	19.93700	30.47340	-7.08110
C	17.81960	29.98670	-5.54640
S	16.12470	35.16740	-5.37010
C	17.30530	35.92260	-7.49240
H	17.88040	35.95140	-8.24890
C	17.27140	34.83740	-6.62240
C	16.43670	36.96350	-7.17390
H	16.35510	37.76360	-7.67770
C	15.72200	36.69260	-6.05760
H	15.06960	37.27990	-5.69350
S	18.37290	28.43110	-5.90810
C	16.84570	29.87420	-4.52490
H	16.38650	30.62120	-4.15890
C	16.62050	28.52790	-4.09820
H	16.10720	28.30840	-3.33010
C	17.13130	27.71360	-4.78260
H	16.91600	26.78950	-4.75900

Table S84: Cartesian coordinates (Å) for the Acceptor-Acceptor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles τ_α = 166° and τ_β = 24°.

atom	*x*	*y*	*z*
N	18.55500	25.07640	-2.39070
C	16.68480	23.87490	-1.48960
C	16.24990	25.04320	-0.87110
H	15.46110	25.02890	-0.34180
C	16.96040	26.23650	-1.01970
C	17.86320	23.94550	-2.23670
H	18.18580	23.15490	-2.65310
C	18.11650	26.18880	-1.80580
H	18.61300	26.98960	-1.92750
C	16.49560	27.47630	-0.39270
S	14.80070	22.29560	-0.21650
C	15.98130	21.54040	-2.33870
H	16.55640	21.51160	-3.09530
C	15.94740	22.62560	-1.46880
C	15.11270	20.49950	-2.02020
H	15.03110	19.69940	-2.52410
C	14.39800	20.77040	-0.90390
H	13.74560	20.18310	-0.53990
S	17.04890	29.03190	-0.75450
C	15.52170	27.58880	0.62870
H	15.06250	26.84180	0.99470
C	15.29650	28.93510	1.05550
H	14.78320	29.15460	1.82360
C	15.80730	29.74940	0.37110
H	15.59200	30.67350	0.39460
N	19.87900	15.96860	-7.54430
C	18.00880	17.17010	-6.64330
C	17.57390	16.00180	-6.02470
H	16.78510	16.01610	-5.49550
C	18.28440	14.80850	-6.17330
C	19.18720	17.09950	-7.39030
H	19.50980	17.89010	-7.80680
C	19.44050	14.85620	-6.95950
H	19.93700	14.05540	-7.08110
C	17.81960	13.56870	-5.54640
S	16.12470	18.74940	-5.37010
C	17.30530	19.50460	-7.49240
H	17.88040	19.53340	-8.24890
C	17.27140	18.41940	-6.62240
C	16.43670	20.54550	-7.17390
H	16.35510	21.34560	-7.67770
C	15.72200	20.27460	-6.05760
H	15.06960	20.86190	-5.69350
S	18.37290	12.01310	-5.90810
C	16.84570	13.45620	-4.52490
H	16.38650	14.20320	-4.15890
C	16.62050	12.10990	-4.09820
H	16.10720	11.89040	-3.33010
C	17.13130	11.29560	-4.78260
H	16.91600	10.37150	-4.75900

Table S85: Cartesian coordinates (Å) for the XB contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 166°$ and $\tau_\beta = -163°$.

atom	*x*	*y*	*z*
I	22.11020	15.87060	-9.05860
F	29.03500	15.92500	-14.45430
F	27.54920	18.15090	-14.05630
F	26.48890	13.61660	-11.26110
F	25.46590	18.09670	-12.34000
F	28.51880	13.66370	-13.04180
C	23.78450	15.81630	-10.21140
C	27.25270	17.02510	-13.39230
C	27.75790	14.74400	-12.86450
C	28.01490	15.89490	-13.57470
C	25.88130	15.83650	-11.78540
C	24.75130	15.80820	-10.90610
C	26.70200	14.73450	-11.97090
C	26.19740	16.98700	-12.51000
N	19.87900	15.96860	-7.54430
C	18.00880	17.17010	-6.64330
C	17.57390	16.00180	-6.02470
H	16.78510	16.01610	-5.49550
C	18.28440	14.80850	-6.17330
C	19.18720	17.09950	-7.39030
H	19.50980	17.89010	-7.80680
C	19.44050	14.85620	-6.95950
H	19.93700	14.05540	-7.08110
C	17.81960	13.56870	-5.54640
C	17.20660	18.43080	-6.42140
S	17.42530	19.72950	-7.47690
C	16.14190	20.57340	-6.72240
H	15.85640	21.43870	-6.98840
C	15.58130	19.88220	-5.71440
H	14.87050	20.20820	-5.17440
C	16.16430	18.64260	-5.56590
H	15.87280	18.00070	-4.92820
S	18.37290	12.01310	-5.90810
C	16.84570	13.45620	-4.52490
H	16.38650	14.20320	-4.15890
C	16.62050	12.10990	-4.09820
H	16.10720	11.89040	-3.33010
C	17.13130	11.29560	-4.78260
H	16.91600	10.37150	-4.75900

Table S86: Cartesian coordinates (Å) for the Donor-Acceptor π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 166°$ and $\tau_\beta = -163°$.

atom	*x*	*y*	*z*
N	19.87900	15.96860	-7.54430
C	18.00880	17.17010	-6.64330
C	17.57390	16.00180	-6.02470
H	16.78510	16.01610	-5.49550
C	18.28440	14.80850	-6.17330
C	19.18720	17.09950	-7.39030
H	19.50980	17.89010	-7.80680
C	19.44050	14.85620	-6.95950
H	19.93700	14.05540	-7.08110
C	17.81960	13.56870	-5.54640
C	17.20660	18.43080	-6.42140
S	17.42530	19.72950	-7.47690
C	16.14190	20.57340	-6.72240
H	15.85640	21.43870	-6.98840
C	15.58130	19.88220	-5.71440
H	14.87050	20.20820	-5.17440
C	16.16430	18.64260	-5.56590
H	15.87280	18.00070	-4.92820
S	18.37290	12.01310	-5.90810
C	16.84570	13.45620	-4.52490
H	16.38650	14.20320	-4.15890
C	16.62050	12.10990	-4.09820
H	16.10720	11.89040	-3.33010
C	17.13130	11.29560	-4.78260
H	16.91600	10.37150	-4.75900
I	18.94880	16.96540	-11.55600
F	12.02400	16.91100	-6.16030
F	13.50980	14.68510	-6.55830
F	14.57010	19.21940	-9.35350
F	15.59310	14.73930	-8.27460
F	12.54020	19.17230	-7.57280
C	17.27450	17.01970	-10.40320
C	13.80630	15.81090	-7.22230
C	13.30110	18.09200	-7.75010
C	13.04410	16.94110	-7.03990
C	15.17760	16.99950	-8.82920
C	16.30770	17.02780	-9.70840
C	14.35700	18.10150	-8.64370
C	14.86160	15.84900	-8.10460

Table S87: Cartesian coordinates (Å) for the Donor-Donor π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 166°$ and $\tau_\beta = -163°$.

atom	*x*	*y*	*z*
I	10.18920	15.87060	-9.05860
F	17.11400	15.92500	-14.45430
F	15.62820	18.15090	-14.05630
F	14.56790	13.61660	-11.26110
F	13.54490	18.09670	-12.34000
F	16.59780	13.66370	-13.04180
C	11.86350	15.81630	-10.21140
C	15.33170	17.02510	-13.39230
C	15.83690	14.74400	-12.86450
C	16.09390	15.89490	-13.57470
C	13.96030	15.83650	-11.78540
C	12.83030	15.80820	-10.90610
C	14.78100	14.73450	-11.97090
C	14.27640	16.98700	-12.51000
I	18.94880	16.96540	-11.55600
F	12.02400	16.91100	-6.16030
F	13.50980	14.68510	-6.55830
F	14.57010	19.21940	-9.35350
F	15.59310	14.73930	-8.27460
F	12.54020	19.17230	-7.57280
C	17.27450	17.01970	-10.40320
C	13.80630	15.81090	-7.22230
C	13.30110	18.09200	-7.75010
C	13.04410	16.94110	-7.03990
C	15.17760	16.99950	-8.82920
C	16.30770	17.02780	-9.70840
C	14.35700	18.10150	-8.64370
C	14.86160	15.84900	-8.10460

Table S88: Cartesian coordinates (Å) for the Acceptor-Acceptor π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 166°$ and $\tau_\beta = -163°$.

atom	*x*	*y*	*z*
N	7.95800	32.38660	-7.54430
C	6.08780	33.58810	-6.64330
C	5.65290	32.41980	-6.02470
H	4.86410	32.43410	-5.49550
C	6.36340	31.22650	-6.17330
C	7.26620	33.51750	-7.39030
H	7.58880	34.30810	-7.80680
C	7.51950	31.27420	-6.95950
H	8.01600	30.47340	-7.08110
C	5.89860	29.98670	-5.54640
C	5.28560	34.84880	-6.42140
S	5.50430	36.14750	-7.47690
C	4.22090	36.99140	-6.72240
H	3.93540	37.85670	-6.98840
C	3.66030	36.30020	-5.71440
H	2.94950	36.62620	-5.17440
C	4.24330	35.06060	-5.56590
H	3.95180	34.41870	-4.92820
S	6.45190	28.43110	-5.90810
C	4.92470	29.87420	-4.52490
H	4.46550	30.62120	-4.15890
C	4.69950	28.52790	-4.09820
H	4.18620	28.30840	-3.33010
C	5.21030	27.71360	-4.78260
H	4.99500	26.78950	-4.75900
N	6.61100	33.28540	-2.76300
C	8.48120	32.08390	-3.66400
C	8.91610	33.25220	-4.28260
H	9.70490	33.23790	-4.81180
C	8.20560	34.44550	-4.13390
C	7.30280	32.15450	-2.91700
H	6.98020	31.36390	-2.50050
C	7.04950	34.39780	-3.34780
H	6.55300	35.19860	-3.22620
C	8.67040	35.68530	-4.76090
C	9.28340	30.82320	-3.88580
S	9.06470	29.52450	-2.83040
C	10.34810	28.68060	-3.58490
H	10.63360	27.81530	-3.31890
C	10.90870	29.37180	-4.59290
H	11.61950	29.04580	-5.13290
C	10.32570	30.61140	-4.74140
H	10.61720	31.25330	-5.37910
S	8.11710	37.24090	-4.39920
C	9.64430	35.79780	-5.78240
H	10.10350	35.05080	-6.14840
C	9.86950	37.14410	-6.20910
H	10.38280	37.36360	-6.97720
C	9.35870	37.95840	-5.52470
H	9.57400	38.88250	-5.54830

Table S89: Cartesian coordinates (Å) for the Donor-Acceptor Slipped π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 166°$ and $\tau_\beta = -163°$.

atom	*x*	*y*	*z*
I	10.18920	32.28860	-9.05860
F	17.11400	32.34300	-14.45430
F	15.62820	34.56890	-14.05630
F	14.56790	30.03460	-11.26110
F	13.54490	34.51470	-12.34000
F	16.59780	30.08170	-13.04180
C	11.86350	32.23430	-10.21140
C	15.33170	33.44310	-13.39230
C	15.83690	31.16200	-12.86450
C	16.09390	32.31290	-13.57470
C	13.96030	32.25450	-11.78540
C	12.83030	32.22620	-10.90610
C	14.78100	31.15250	-11.97090
C	14.27640	33.40500	-12.51000
N	6.61100	33.28540	-2.76300
C	8.48120	32.08390	-3.66400
C	8.91610	33.25220	-4.28260
H	9.70490	33.23790	-4.81180
C	8.20560	34.44550	-4.13390
C	7.30280	32.15450	-2.91700
H	6.98020	31.36390	-2.50050
C	7.04950	34.39780	-3.34780
H	6.55300	35.19860	-3.22620
C	8.67040	35.68530	-4.76090
C	9.28340	30.82320	-3.88580
S	9.06470	29.52450	-2.83040
C	10.34810	28.68060	-3.58490
H	10.63360	27.81530	-3.31890
C	10.90870	29.37180	-4.59290
H	11.61950	29.04580	-5.13290
C	10.32570	30.61140	-4.74140
H	10.61720	31.25330	-5.37910
S	8.11710	37.24090	-4.39920
C	9.64430	35.79780	-5.78240
H	10.10350	35.05080	-6.14840
C	9.86950	37.14410	-6.20910
H	10.38280	37.36360	-6.97720
C	9.35870	37.95840	-5.52470
H	9.57400	38.88250	-5.54830

Table S90: Cartesian coordinates (Å) for the Donor-Acceptor Slipped π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 166°$ and $\tau_\beta = -163°$.

atom	*x*	*y*	*z*
I	10.18920	15.87060	-9.05860
F	17.11400	15.92500	-14.45430
F	15.62820	18.15090	-14.05630
F	14.56790	13.61660	-11.26110
F	13.54490	18.09670	-12.34000
F	16.59780	13.66370	-13.04180
C	11.86350	15.81630	-10.21140
C	15.33170	17.02510	-13.39230
C	15.83690	14.74400	-12.86450
C	16.09390	15.89490	-13.57470
C	13.96030	15.83650	-11.78540
C	12.83030	15.80820	-10.90610
C	14.78100	14.73450	-11.97090
C	14.27640	16.98700	-12.51000
N	21.18000	16.86740	-13.07030
C	23.05020	15.66590	-13.97130
C	23.48510	16.83420	-14.58990
H	24.27390	16.81990	-15.11910
C	22.77460	18.02750	-14.44120
C	21.87180	15.73650	-13.22430
H	21.54920	14.94590	-12.80780
C	21.61840	17.97980	-13.65510
H	21.12200	18.78060	-13.53340
C	23.23940	19.26730	-15.06820
C	23.85240	14.40520	-14.19310
S	23.63370	13.10650	-13.13770
C	24.91710	12.26260	-13.89220
H	25.20260	11.39730	-13.62610
C	25.47770	12.95380	-14.90020
H	26.18850	12.62780	-15.44020
C	24.89470	14.19340	-15.04860
H	25.18620	14.83530	-15.68640
S	22.68610	20.82290	-14.70640
C	24.21330	19.37980	-16.08970
H	24.67250	18.63280	-16.45570
C	24.43850	20.72610	-16.51640
H	24.95180	20.94560	-17.28450
C	23.92770	21.54040	-15.83200
H	24.14300	22.46450	-15.85560

Table S91: Cartesian coordinates (Å) for the Donor-Acceptor Edge-Edge contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 166°$ and $\tau_\beta = -163°$.

atom	*x*	*y*	*z*
I	22.11020	15.87060	-9.05860
F	29.03500	15.92500	-14.45430
F	27.54920	18.15090	-14.05630
F	26.48890	13.61660	-11.26110
F	25.46590	18.09670	-12.34000
F	28.51880	13.66370	-13.04180
C	23.78450	15.81630	-10.21140
C	27.25270	17.02510	-13.39230
C	27.75790	14.74400	-12.86450
C	28.01490	15.89490	-13.57470
C	25.88130	15.83650	-11.78540
C	24.75130	15.80820	-10.90610
C	26.70200	14.73450	-11.97090
C	26.19740	16.98700	-12.51000
N	19.85600	24.17760	-7.91660
C	21.72620	25.37910	-8.81770
C	22.16110	24.21080	-9.43620
H	22.94990	24.22510	-9.96550
C	21.45060	23.01750	-9.28760
C	20.54780	25.30850	-8.07060
H	20.22520	26.09910	-7.65420
C	20.29450	23.06520	-8.50150
H	19.79800	22.26440	-8.37980
C	21.91540	21.77770	-9.91460
C	22.52840	26.63980	-9.03950
S	22.30970	27.93850	-7.98400
C	23.59310	28.78240	-8.73850
H	23.87860	29.64770	-8.47250
C	24.15370	28.09120	-9.74660
H	24.86450	28.41720	-10.28660
C	23.57070	26.85160	-9.89500
H	23.86220	26.20970	-10.53270
S	21.36210	20.22210	-9.55280
C	22.88930	21.66520	-10.93600
H	23.34850	22.41220	-11.30200
C	23.11450	20.31890	-11.36280
H	23.62780	20.09940	-12.13090
C	22.60370	19.50460	-10.67840
H	22.81900	18.58050	-10.70190

Table S92: Cartesian coordinates (Å) for the Donor-Acceptor Edge-Edge contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 166°$ and $\tau_\beta = -163°$.

atom	*x*	*y*	*z*
N	19.87900	15.96860	-7.54430
C	18.00880	17.17010	-6.64330
C	17.57390	16.00180	-6.02470
H	16.78510	16.01610	-5.49550
C	18.28440	14.80850	-6.17330
C	19.18720	17.09950	-7.39030
H	19.50980	17.89010	-7.80680
C	19.44050	14.85620	-6.95950
H	19.93700	14.05540	-7.08110
C	17.81960	13.56870	-5.54640
C	17.20660	18.43080	-6.42140
S	17.42530	19.72950	-7.47690
C	16.14190	20.57340	-6.72240
H	15.85640	21.43870	-6.98840
C	15.58130	19.88220	-5.71440
H	14.87050	20.20820	-5.17440
C	16.16430	18.64260	-5.56590
H	15.87280	18.00070	-4.92820
S	18.37290	12.01310	-5.90810
C	16.84570	13.45620	-4.52490
H	16.38650	14.20320	-4.15890
C	16.62050	12.10990	-4.09820
H	16.10720	11.89040	-3.33010
C	17.13130	11.29560	-4.78260
H	16.91600	10.37150	-4.75900
I	7.54120	15.87060	1.24870
F	14.46600	15.92500	-4.14700
F	12.98020	18.15090	-3.74900
F	11.91990	13.61660	-0.95380
F	10.89690	18.09670	-2.03270
F	13.94980	13.66370	-2.73450
C	9.21550	15.81630	0.09590
C	12.68370	17.02510	-3.08500
C	13.18890	14.74400	-2.55720
C	13.44590	15.89490	-3.26740
C	11.31240	15.83650	-1.47810
C	10.18230	15.80820	-0.59890
C	12.13300	14.73450	-1.66360
C	11.62840	16.98700	-2.20270

Table S93: Cartesian coordinates (Å) for the Donor-Acceptor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 166°$ and $\tau_\beta = -163°$.

atom	*x*	*y*	*z*
N	19.87900	15.96860	-7.54430
C	18.00880	17.17010	-6.64330
C	17.57390	16.00180	-6.02470
H	16.78510	16.01610	-5.49550
C	18.28440	14.80850	-6.17330
C	19.18720	17.09950	-7.39030
H	19.50980	17.89010	-7.80680
C	19.44050	14.85620	-6.95950
H	19.93700	14.05540	-7.08110
C	17.81960	13.56870	-5.54640
C	17.20660	18.43080	-6.42140
S	17.42530	19.72950	-7.47690
C	16.14190	20.57340	-6.72240
H	15.85640	21.43870	-6.98840
C	15.58130	19.88220	-5.71440
H	14.87050	20.20820	-5.17440
C	16.16430	18.64260	-5.56590
H	15.87280	18.00070	-4.92820
S	18.37290	12.01310	-5.90810
C	16.84570	13.45620	-4.52490
H	16.38650	14.20320	-4.15890
C	16.62050	12.10990	-4.09820
H	16.10720	11.89040	-3.33010
C	17.13130	11.29560	-4.78260
H	16.91600	10.37150	-4.75900
I	17.62480	24.07960	-6.40240
F	10.70000	24.13400	-1.00660
F	12.18580	26.35990	-1.40470
F	13.24610	21.82560	-4.19980
F	14.26910	26.30570	-3.12090
F	11.21620	21.87270	-2.41910
C	15.95050	24.02530	-5.24950
C	12.48230	25.23410	-2.06870
C	11.97710	22.95300	-2.59640
C	11.72010	24.10390	-1.88620
C	13.85360	24.04550	-3.67560
C	14.98370	24.01720	-4.55480
C	13.03300	22.94350	-3.49000
C	13.53760	25.19600	-2.95100

Table S94: Cartesian coordinates (Å) for the Donor-Acceptor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 166°$ and $\tau_\beta = -163°$.

atom	*x*	*y*	*z*
N	19.87900	15.96860	-7.54430
C	18.00880	17.17010	-6.64330
C	17.57390	16.00180	-6.02470
H	16.78510	16.01610	-5.49550
C	18.28440	14.80850	-6.17330
C	19.18720	17.09950	-7.39030
H	19.50980	17.89010	-7.80680
C	19.44050	14.85620	-6.95950
H	19.93700	14.05540	-7.08110
C	17.81960	13.56870	-5.54640
C	17.20660	18.43080	-6.42140
S	17.42530	19.72950	-7.47690
C	16.14190	20.57340	-6.72240
H	15.85640	21.43870	-6.98840
C	15.58130	19.88220	-5.71440
H	14.87050	20.20820	-5.17440
C	16.16430	18.64260	-5.56590
H	15.87280	18.00070	-4.92820
S	18.37290	12.01310	-5.90810
C	16.84570	13.45620	-4.52490
H	16.38650	14.20320	-4.15890
C	16.62050	12.10990	-4.09820
H	16.10720	11.89040	-3.33010
C	17.13130	11.29560	-4.78260
H	16.91600	10.37150	-4.75900
I	8.86520	25.17440	-3.90490
F	15.79000	25.12000	-9.30070
F	14.30420	22.89410	-8.90260
F	13.24390	27.42840	-6.10750
F	12.22090	22.94830	-7.18630
F	15.27380	27.38130	-7.88820
C	10.53950	25.22870	-5.05780
C	14.00770	24.01990	-8.23860
C	14.51290	26.30100	-7.71090
C	14.76990	25.15010	-8.42110
C	12.63640	25.20850	-6.63170
C	11.50630	25.23680	-5.75250
C	13.45700	26.31050	-6.81720
C	12.95240	24.05800	-7.35630

Table S95: Cartesian coordinates (Å) for the Donor-Acceptor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 166°$ and $\tau_\beta = -163°$.

atom	*x*	*y*	*z*
N	19.87900	15.96860	-7.54430
C	18.00880	17.17010	-6.64330
C	17.57390	16.00180	-6.02470
H	16.78510	16.01610	-5.49550
C	18.28440	14.80850	-6.17330
C	19.18720	17.09950	-7.39030
H	19.50980	17.89010	-7.80680
C	19.44050	14.85620	-6.95950
H	19.93700	14.05540	-7.08110
C	17.81960	13.56870	-5.54640
C	17.20660	18.43080	-6.42140
S	17.42530	19.72950	-7.47690
C	16.14190	20.57340	-6.72240
H	15.85640	21.43870	-6.98840
C	15.58130	19.88220	-5.71440
H	14.87050	20.20820	-5.17440
C	16.16430	18.64260	-5.56590
H	15.87280	18.00070	-4.92820
S	18.37290	12.01310	-5.90810
C	16.84570	13.45620	-4.52490
H	16.38650	14.20320	-4.15890
C	16.62050	12.10990	-4.09820
H	16.10720	11.89040	-3.33010
C	17.13130	11.29560	-4.78260
H	16.91600	10.37150	-4.75900
I	8.86520	8.75640	-3.90490
F	15.79000	8.70200	-9.30070
F	14.30420	6.47610	-8.90260
F	13.24390	11.01040	-6.10750
F	12.22090	6.53030	-7.18630
F	15.27380	10.96330	-7.88820
C	10.53950	8.81070	-5.05780
C	14.00770	7.60190	-8.23860
C	14.51290	9.88300	-7.71090
C	14.76990	8.73210	-8.42110
C	12.63640	8.79050	-6.63170
C	11.50630	8.81880	-5.75250
C	13.45700	9.89250	-6.81720
C	12.95240	7.64000	-7.35630

Table S96: Cartesian coordinates (Å) for the Donor-Acceptor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 166°$ and $\tau_\beta = -163°$.

atom	*x*	*y*	*z*
I	7.54120	32.28860	1.24870
F	14.46600	32.34300	-4.14700
F	12.98020	34.56890	-3.74900
F	11.91990	30.03460	-0.95380
F	10.89690	34.51470	-2.03270
F	13.94980	30.08170	-2.73450
C	9.21550	32.23430	0.09590
C	12.68370	33.44310	-3.08500
C	13.18890	31.16200	-2.55720
C	13.44590	32.31290	-3.26740
C	11.31240	32.25450	-1.47810
C	10.18230	32.22620	-0.59890
C	12.13300	31.15250	-1.66360
C	11.62840	33.40500	-2.20270
N	6.63400	25.07640	-2.39070
C	4.76380	23.87490	-1.48960
C	4.32890	25.04320	-0.87110
H	3.54010	25.02890	-0.34180
C	5.03940	26.23650	-1.01970
C	5.94220	23.94550	-2.23670
H	6.26480	23.15490	-2.65310
C	6.19550	26.18880	-1.80580
H	6.69200	26.98960	-1.92750
C	4.57460	27.47630	-0.39270
C	3.96160	22.61420	-1.26780
S	4.18030	21.31550	-2.32330
C	2.89690	20.47160	-1.56880
H	2.61140	19.60630	-1.83480
C	2.33630	21.16280	-0.56070
H	1.62550	20.83680	-0.02070
C	2.91930	22.40240	-0.41230
H	2.62780	23.04430	0.22540
S	5.12790	29.03190	-0.75450
C	3.60070	27.58880	0.62870
H	3.14150	26.84180	0.99470
C	3.37550	28.93510	1.05550
H	2.86220	29.15460	1.82360
C	3.88630	29.74940	0.37110
H	3.67100	30.67350	0.39460

Table S97: Cartesian coordinates (Å) for the Donor-Donor Slipped π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 166°$ and $\tau_\beta = -163°$.

atom	*x*	*y*	*z*
I	22.11020	15.87060	-9.05860
F	29.03500	15.92500	-14.45430
F	27.54920	18.15090	-14.05630
F	26.48890	13.61660	-11.26110
F	25.46590	18.09670	-12.34000
F	28.51880	13.66370	-13.04180
C	23.78450	15.81630	-10.21140
C	27.25270	17.02510	-13.39230
C	27.75790	14.74400	-12.86450
C	28.01490	15.89490	-13.57470
C	25.88130	15.83650	-11.78540
C	24.75130	15.80820	-10.90610
C	26.70200	14.73450	-11.97090
C	26.19740	16.98700	-12.51000
I	18.94880	16.96540	-11.55600
F	12.02400	16.91100	-6.16030
F	13.50980	14.68510	-6.55830
F	14.57010	19.21940	-9.35350
F	15.59310	14.73930	-8.27460
F	12.54020	19.17230	-7.57280
C	17.27450	17.01970	-10.40320
C	13.80630	15.81090	-7.22230
C	13.30110	18.09200	-7.75010
C	13.04410	16.94110	-7.03990
C	15.17760	16.99950	-8.82920
C	16.30770	17.02780	-9.70840
C	14.35700	18.10150	-8.64370
C	14.86160	15.84900	-8.10460

Table S98: Cartesian coordinates (Å) for the Donor-Donor Slipped π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 166°$ and $\tau_\beta = -163°$.

atom	*x*	*y*	*z*
I	7.54120	15.87060	1.24870
F	14.46600	15.92500	-4.14700
F	12.98020	18.15090	-3.74900
F	11.91990	13.61660	-0.95380
F	10.89690	18.09670	-2.03270
F	13.94980	13.66370	-2.73450
C	9.21550	15.81630	0.09590
C	12.68370	17.02510	-3.08500
C	13.18890	14.74400	-2.55720
C	13.44590	15.89490	-3.26740
C	11.31240	15.83650	-1.47810
C	10.18230	15.80820	-0.59890
C	12.13300	14.73450	-1.66360
C	11.62840	16.98700	-2.20270
I	18.94880	16.96540	-11.55600
F	12.02400	16.91100	-6.16030
F	13.50980	14.68510	-6.55830
F	14.57010	19.21940	-9.35350
F	15.59310	14.73930	-8.27460
F	12.54020	19.17230	-7.57280
C	17.27450	17.01970	-10.40320
C	13.80630	15.81090	-7.22230
C	13.30110	18.09200	-7.75010
C	13.04410	16.94110	-7.03990
C	15.17760	16.99950	-8.82920
C	16.30770	17.02780	-9.70840
C	14.35700	18.10150	-8.64370
C	14.86160	15.84900	-8.10460

Table S99: Cartesian coordinates (Å) for the Donor-Donor Edge-Edge contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 166°$ and $\tau_\beta = -163°$.

atom	*x*	*y*	*z*
I	7.54120	32.28860	1.24870
F	14.46600	32.34300	-4.14700
F	12.98020	34.56890	-3.74900
F	11.91990	30.03460	-0.95380
F	10.89690	34.51470	-2.03270
F	13.94980	30.08170	-2.73450
C	9.21550	32.23430	0.09590
C	12.68370	33.44310	-3.08500
C	13.18890	31.16200	-2.55720
C	13.44590	32.31290	-3.26740
C	11.31240	32.25450	-1.47810
C	10.18230	32.22620	-0.59890
C	12.13300	31.15250	-1.66360
C	11.62840	33.40500	-2.20270
I	17.62480	24.07960	-6.40240
F	10.70000	24.13400	-1.00660
F	12.18580	26.35990	-1.40470
F	13.24610	21.82560	-4.19980
F	14.26910	26.30570	-3.12090
F	11.21620	21.87270	-2.41910
C	15.95050	24.02530	-5.24950
C	12.48230	25.23410	-2.06870
C	11.97710	22.95300	-2.59640
C	11.72010	24.10390	-1.88620
C	13.85360	24.04550	-3.67560
C	14.98370	24.01720	-4.55480
C	13.03300	22.94350	-3.49000
C	13.53760	25.19600	-2.95100

Table S100: Cartesian coordinates (Å) for the Donor-Donor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 166°$ and $\tau_\beta = -163°$.

atom	*x*	*y*	*z*
I	10.18920	15.87060	-9.05860
F	17.11400	15.92500	-14.45430
F	15.62820	18.15090	-14.05630
F	14.56790	13.61660	-11.26110
F	13.54490	18.09670	-12.34000
F	16.59780	13.66370	-13.04180
C	11.86350	15.81630	-10.21140
C	15.33170	17.02510	-13.39230
C	15.83690	14.74400	-12.86450
C	16.09390	15.89490	-13.57470
C	13.96030	15.83650	-11.78540
C	12.83030	15.80820	-10.90610
C	14.78100	14.73450	-11.97090
C	14.27640	16.98700	-12.51000
I	8.86520	8.75640	-3.90490
F	15.79000	8.70200	-9.30070
F	14.30420	6.47610	-8.90260
F	13.24390	11.01040	-6.10750
F	12.22090	6.53030	-7.18630
F	15.27380	10.96330	-7.88820
C	10.53950	8.81070	-5.05780
C	14.00770	7.60190	-8.23860
C	14.51290	9.88300	-7.71090
C	14.76990	8.73210	-8.42110
C	12.63640	8.79050	-6.63170
C	11.50630	8.81880	-5.75250
C	13.45700	9.89250	-6.81720
C	12.95240	7.64000	-7.35630

Table S101: Cartesian coordinates (Å) for the Acceptor-Acceptor Slipped π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 166°$ and $\tau_\beta = -163°$.

atom	*x*	*y*	*z*
N	5.31000	32.38660	2.76300
C	3.43980	33.58810	3.66400
C	3.00490	32.41980	4.28260
H	2.21610	32.43410	4.81180
C	3.71540	31.22650	4.13390
C	4.61820	33.51750	2.91700
H	4.94080	34.30810	2.50050
C	4.87150	31.27420	3.34780
H	5.36800	30.47340	3.22620
C	3.25060	29.98670	4.76090
C	2.63760	34.84880	3.88580
S	2.85630	36.14750	2.83040
C	1.57290	36.99140	3.58490
H	1.28740	37.85670	3.31890
C	1.01230	36.30020	4.59290
H	0.30150	36.62620	5.13290
C	1.59530	35.06060	4.74140
H	1.30380	34.41870	5.37910
S	3.80390	28.43110	4.39920
C	2.27670	29.87420	5.78240
H	1.81750	30.62120	6.14840
C	2.05150	28.52790	6.20910
H	1.53820	28.30840	6.97720
C	2.56230	27.71360	5.52470
H	2.34700	26.78950	5.54830
N	-7.95800	33.28540	7.54430
C	-6.08780	32.08390	6.64330
C	-5.65290	33.25220	6.02470
H	-4.86410	33.23790	5.49550
C	-6.36340	34.44550	6.17330
C	-7.26620	32.15450	7.39030
H	-7.58880	31.36390	7.80680
C	-7.51950	34.39780	6.95950
H	-8.01600	35.19860	7.08110
C	-5.89860	35.68530	5.54640
C	-5.28560	30.82320	6.42140
S	-5.50430	29.52450	7.47690
C	-4.22090	28.68060	6.72240
H	-3.93540	27.81530	6.98840
C	-3.66030	29.37180	5.71440
H	-2.94950	29.04580	5.17440
C	-4.24330	30.61140	5.56590
H	-3.95180	31.25330	4.92820
S	-6.45190	37.24090	5.90810
C	-4.92470	35.79780	4.52490
H	-4.46550	35.05080	4.15890
C	-4.69950	37.14410	4.09820
H	-4.18620	37.36360	3.33010
C	-5.21030	37.95840	4.78260
H	-4.99500	38.88250	4.75900

Table S102: Cartesian coordinates (Å) for the Acceptor-Acceptor Edge-Edge contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 166°$ and $\tau_\beta = -163°$.

atom	*x*	*y*	*z*
N	19.87900	15.96860	-7.54430
C	18.00880	17.17010	-6.64330
C	17.57390	16.00180	-6.02470
H	16.78510	16.01610	-5.49550
C	18.28440	14.80850	-6.17330
C	19.18720	17.09950	-7.39030
H	19.50980	17.89010	-7.80680
C	19.44050	14.85620	-6.95950
H	19.93700	14.05540	-7.08110
C	17.81960	13.56870	-5.54640
C	17.20660	18.43080	-6.42140
S	17.42530	19.72950	-7.47690
C	16.14190	20.57340	-6.72240
H	15.85640	21.43870	-6.98840
C	15.58130	19.88220	-5.71440
H	14.87050	20.20820	-5.17440
C	16.16430	18.64260	-5.56590
H	15.87280	18.00070	-4.92820
S	18.37290	12.01310	-5.90810
C	16.84570	13.45620	-4.52490
H	16.38650	14.20320	-4.15890
C	16.62050	12.10990	-4.09820
H	16.10720	11.89040	-3.33010
C	17.13130	11.29560	-4.78260
H	16.91600	10.37150	-4.75900
N	19.85600	24.17760	-7.91660
C	21.72620	25.37910	-8.81770
C	22.16110	24.21080	-9.43620
H	22.94990	24.22510	-9.96550
C	21.45060	23.01750	-9.28760
C	20.54780	25.30850	-8.07060
H	20.22520	26.09910	-7.65420
C	20.29450	23.06520	-8.50150
H	19.79800	22.26440	-8.37980
C	21.91540	21.77770	-9.91460
C	22.52840	26.63980	-9.03950
S	22.30970	27.93850	-7.98400
C	23.59310	28.78240	-8.73850
H	23.87860	29.64770	-8.47250
C	24.15370	28.09120	-9.74660
H	24.86450	28.41720	-10.28660
C	23.57070	26.85160	-9.89500
H	23.86220	26.20970	-10.53270
S	21.36210	20.22210	-9.55280
C	22.88930	21.66520	-10.93600
H	23.34850	22.41220	-11.30200
C	23.11450	20.31890	-11.36280
H	23.62780	20.09940	-12.13090
C	22.60370	19.50460	-10.67840
H	22.81900	18.58050	-10.70190

Table S103: Cartesian coordinates (Å) for the Acceptor-Acceptor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 166°$ and $\tau_\beta = -163°$.

atom	*x*	*y*	*z*
N	7.95800	32.38660	-7.54430
C	6.08780	33.58810	-6.64330
C	5.65290	32.41980	-6.02470
H	4.86410	32.43410	-5.49550
C	6.36340	31.22650	-6.17330
C	7.26620	33.51750	-7.39030
H	7.58880	34.30810	-7.80680
C	7.51950	31.27420	-6.95950
H	8.01600	30.47340	-7.08110
C	5.89860	29.98670	-5.54640
C	5.28560	34.84880	-6.42140
S	5.50430	36.14750	-7.47690
C	4.22090	36.99140	-6.72240
H	3.93540	37.85670	-6.98840
C	3.66030	36.30020	-5.71440
H	2.94950	36.62620	-5.17440
C	4.24330	35.06060	-5.56590
H	3.95180	34.41870	-4.92820
S	6.45190	28.43110	-5.90810
C	4.92470	29.87420	-4.52490
H	4.46550	30.62120	-4.15890
C	4.69950	28.52790	-4.09820
H	4.18620	28.30840	-3.33010
C	5.21030	27.71360	-4.78260
H	4.99500	26.78950	-4.75900
N	6.63400	41.49440	-2.39070
C	4.76380	40.29290	-1.48960
C	4.32890	41.46120	-0.87110
H	3.54010	41.44690	-0.34180
C	5.03940	42.65450	-1.01970
C	5.94220	40.36350	-2.23670
H	6.26480	39.57290	-2.65310
C	6.19550	42.60680	-1.80580
H	6.69200	43.40760	-1.92750
C	4.57460	43.89430	-0.39270
C	3.96160	39.03220	-1.26780
S	4.18030	37.73350	-2.32330
C	2.89690	36.88960	-1.56880
H	2.61140	36.02430	-1.83480
C	2.33630	37.58080	-0.56070
H	1.62550	37.25480	-0.02070
C	2.91930	38.82040	-0.41230
H	2.62780	39.46230	0.22540
S	5.12790	45.44990	-0.75450
C	3.60070	44.00680	0.62870
H	3.14150	43.25980	0.99470
C	3.37550	45.35310	1.05550
H	2.86220	45.57260	1.82360
C	3.88630	46.16740	0.37110
H	3.67100	47.09150	0.39460

Table S104: Cartesian coordinates (Å) for the Acceptor-Acceptor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = 166°$ and $\tau_\beta = -163°$.

atom	*x*	*y*	*z*
N	7.95800	32.38660	-7.54430
C	6.08780	33.58810	-6.64330
C	5.65290	32.41980	-6.02470
H	4.86410	32.43410	-5.49550
C	6.36340	31.22650	-6.17330
C	7.26620	33.51750	-7.39030
H	7.58880	34.30810	-7.80680
C	7.51950	31.27420	-6.95950
H	8.01600	30.47340	-7.08110
C	5.89860	29.98670	-5.54640
C	5.28560	34.84880	-6.42140
S	5.50430	36.14750	-7.47690
C	4.22090	36.99140	-6.72240
H	3.93540	37.85670	-6.98840
C	3.66030	36.30020	-5.71440
H	2.94950	36.62620	-5.17440
C	4.24330	35.06060	-5.56590
H	3.95180	34.41870	-4.92820
S	6.45190	28.43110	-5.90810
C	4.92470	29.87420	-4.52490
H	4.46550	30.62120	-4.15890
C	4.69950	28.52790	-4.09820
H	4.18620	28.30840	-3.33010
C	5.21030	27.71360	-4.78260
H	4.99500	26.78950	-4.75900
N	6.63400	25.07640	-2.39070
C	4.76380	23.87490	-1.48960
C	4.32890	25.04320	-0.87110
H	3.54010	25.02890	-0.34180
C	5.03940	26.23650	-1.01970
C	5.94220	23.94550	-2.23670
H	6.26480	23.15490	-2.65310
C	6.19550	26.18880	-1.80580
H	6.69200	26.98960	-1.92750
C	4.57460	27.47630	-0.39270
C	3.96160	22.61420	-1.26780
S	4.18030	21.31550	-2.32330
C	2.89690	20.47160	-1.56880
H	2.61140	19.60630	-1.83480
C	2.33630	21.16280	-0.56070
H	1.62550	20.83680	-0.02070
C	2.91930	22.40240	-0.41230
H	2.62780	23.04430	0.22540
S	5.12790	29.03190	-0.75450
C	3.60070	27.58880	0.62870
H	3.14150	26.84180	0.99470
C	3.37550	28.93510	1.05550
H	2.86220	29.15460	1.82360
C	3.88630	29.74940	0.37110
H	3.67100	30.67350	0.39460

Table S105: Cartesian coordinates (Å) for the XB contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = -166°$ and $\tau_\beta = 163°$.

atom	*x*	*y*	*z*
I	20.78620	25.17440	-3.90490
F	27.71100	25.12000	-9.30070
F	26.22520	22.89410	-8.90260
F	25.16490	27.42840	-6.10750
F	24.14190	22.94830	-7.18630
F	27.19480	27.38130	-7.88820
C	22.46050	25.22870	-5.05780
C	25.92870	24.01990	-8.23860
C	26.43390	26.30100	-7.71090
C	26.69090	25.15010	-8.42110
C	24.55740	25.20850	-6.63170
C	23.42730	25.23680	-5.75250
C	25.37800	26.31050	-6.81720
C	24.87340	24.05800	-7.35630
N	18.55500	25.07640	-2.39070
C	16.68480	23.87490	-1.48960
C	16.24990	25.04320	-0.87110
H	15.46110	25.02890	-0.34180
C	16.96040	26.23650	-1.01970
C	17.86320	23.94550	-2.23670
H	18.18580	23.15490	-2.65310
C	18.11650	26.18880	-1.80580
H	18.61300	26.98960	-1.92750
C	16.49560	27.47630	-0.39270
C	15.88260	22.61420	-1.26780
S	16.10130	21.31550	-2.32330
C	14.81790	20.47160	-1.56880
H	14.53240	19.60630	-1.83480
C	14.25730	21.16280	-0.56070
H	13.54650	20.83680	-0.02070
C	14.84030	22.40240	-0.41230
H	14.54880	23.04430	0.22540
S	17.04890	29.03190	-0.75450
C	15.52170	27.58880	0.62870
H	15.06250	26.84180	0.99470
C	15.29650	28.93510	1.05550
H	14.78320	29.15460	1.82360
C	15.80730	29.74940	0.37110
H	15.59200	30.67350	0.39460

Table S106: Cartesian coordinates (Å) for the Donor-Acceptor π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = -166°$ and $\tau_\beta = 163°$.

atom	*x*	*y*	*z*
I	20.78620	25.17440	-3.90490
F	27.71100	25.12000	-9.30070
F	26.22520	22.89410	-8.90260
F	25.16490	27.42840	-6.10750
F	24.14190	22.94830	-7.18630
F	27.19480	27.38130	-7.88820
C	22.46050	25.22870	-5.05780
C	25.92870	24.01990	-8.23860
C	26.43390	26.30100	-7.71090
C	26.69090	25.15010	-8.42110
C	24.55740	25.20850	-6.63170
C	23.42730	25.23680	-5.75250
C	25.37800	26.31050	-6.81720
C	24.87340	24.05800	-7.35630
N	19.85600	24.17760	-7.91660
C	21.72620	25.37910	-8.81770
C	22.16110	24.21080	-9.43620
H	22.94990	24.22510	-9.96550
C	21.45060	23.01750	-9.28760
C	20.54780	25.30850	-8.07060
H	20.22520	26.09910	-7.65420
C	20.29450	23.06520	-8.50150
H	19.79800	22.26440	-8.37980
C	21.91540	21.77770	-9.91460
C	22.52840	26.63980	-9.03950
S	22.30970	27.93850	-7.98400
C	23.59310	28.78240	-8.73850
H	23.87860	29.64770	-8.47250
C	24.15370	28.09120	-9.74660
H	24.86450	28.41720	-10.28660
C	23.57070	26.85160	-9.89500
H	23.86220	26.20970	-10.53270
S	21.36210	20.22210	-9.55280
C	22.88930	21.66520	-10.93600
H	23.34850	22.41220	-11.30200
C	23.11450	20.31890	-11.36280
H	23.62780	20.09940	-12.13090
C	22.60370	19.50460	-10.67840
H	22.81900	18.58050	-10.70190

Table S107: Cartesian coordinates (Å) for the Donor-Donor π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = -166°$ and $\tau_\beta = 163°$.

atom	*x*	*y*	*z*
I	6.21720	8.75640	6.40240
F	13.14200	8.70200	1.00660
F	11.65620	6.47610	1.40470
F	10.59590	11.01040	4.19980
F	9.57290	6.53030	3.12090
F	12.62580	10.96330	2.41910
C	7.89150	8.81070	5.24950
C	11.35970	7.60190	2.06870
C	11.86490	9.88300	2.59640
C	12.12190	8.73210	1.88620
C	9.98840	8.79050	3.67560
C	8.85830	8.81880	4.55480
C	10.80900	9.89250	3.49000
C	10.30440	7.64000	2.95100
I	14.97680	7.66160	3.90490
F	8.05200	7.71600	9.30070
F	9.53780	9.94190	8.90260
F	10.59810	5.40760	6.10750
F	11.62110	9.88770	7.18630
F	8.56820	5.45470	7.88820
C	13.30250	7.60730	5.05780
C	9.83430	8.81610	8.23860
C	9.32910	6.53500	7.71090
C	9.07210	7.68590	8.42110
C	11.20560	7.62750	6.63170
C	12.33570	7.59920	5.75250
C	10.38500	6.52550	6.81720
C	10.88960	8.77800	7.35630

Table S108: Cartesian coordinates (Å) for the Acceptor-Acceptor π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = -166°$ and $\tau_\beta = 163°$.

atom	*x*	*y*	*z*
N	18.55500	25.07640	-2.39070
C	16.68480	23.87490	-1.48960
C	16.24990	25.04320	-0.87110
H	15.46110	25.02890	-0.34180
C	16.96040	26.23650	-1.01970
C	17.86320	23.94550	-2.23670
H	18.18580	23.15490	-2.65310
C	18.11650	26.18880	-1.80580
H	18.61300	26.98960	-1.92750
C	16.49560	27.47630	-0.39270
C	15.88260	22.61420	-1.26780
S	16.10130	21.31550	-2.32330
C	14.81790	20.47160	-1.56880
H	14.53240	19.60630	-1.83480
C	14.25730	21.16280	-0.56070
H	13.54650	20.83680	-0.02070
C	14.84030	22.40240	-0.41230
H	14.54880	23.04430	0.22540
S	17.04890	29.03190	-0.75450
C	15.52170	27.58880	0.62870
H	15.06250	26.84180	0.99470
C	15.29650	28.93510	1.05550
H	14.78320	29.15460	1.82360
C	15.80730	29.74940	0.37110
H	15.59200	30.67350	0.39460
N	17.20800	24.17760	2.39070
C	19.07820	25.37910	1.48960
C	19.51310	24.21080	0.87110
H	20.30190	24.22510	0.34180
C	18.80260	23.01750	1.01970
C	17.89980	25.30850	2.23670
H	17.57720	26.09910	2.65310
C	17.64650	23.06520	1.80580
H	17.15000	22.26440	1.92750
C	19.26740	21.77770	0.39270
C	19.88040	26.63980	1.26780
S	19.66170	27.93850	2.32330
C	20.94510	28.78240	1.56880
H	21.23060	29.64770	1.83480
C	21.50570	28.09120	0.56070
H	22.21650	28.41720	0.02070
C	20.92270	26.85160	0.41230
H	21.21420	26.20970	-0.22540
S	18.71410	20.22210	0.75450
C	20.24130	21.66520	-0.62870
H	20.70050	22.41220	-0.99470
C	20.46650	20.31890	-1.05550
H	20.97980	20.09940	-1.82360
C	19.95570	19.50460	-0.37110
H	20.17100	18.58050	-0.39460

Table S109: Cartesian coordinates (Å) for the Donor-Acceptor Slipped π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = -166°$ and $\tau_\beta = 163°$.

atom	*x*	*y*	*z*
I	20.78620	25.17440	-3.90490
F	27.71100	25.12000	-9.30070
F	26.22520	22.89410	-8.90260
F	25.16490	27.42840	-6.10750
F	24.14190	22.94830	-7.18630
F	27.19480	27.38130	-7.88820
C	22.46050	25.22870	-5.05780
C	25.92870	24.01990	-8.23860
C	26.43390	26.30100	-7.71090
C	26.69090	25.15010	-8.42110
C	24.55740	25.20850	-6.63170
C	23.42730	25.23680	-5.75250
C	25.37800	26.31050	-6.81720
C	24.87340	24.05800	-7.35630
N	17.20800	24.17760	2.39070
C	19.07820	25.37910	1.48960
C	19.51310	24.21080	0.87110
H	20.30190	24.22510	0.34180
C	18.80260	23.01750	1.01970
C	17.89980	25.30850	2.23670
H	17.57720	26.09910	2.65310
C	17.64650	23.06520	1.80580
H	17.15000	22.26440	1.92750
C	19.26740	21.77770	0.39270
C	19.88040	26.63980	1.26780
S	19.66170	27.93850	2.32330
C	20.94510	28.78240	1.56880
H	21.23060	29.64770	1.83480
C	21.50570	28.09120	0.56070
H	22.21650	28.41720	0.02070
C	20.92270	26.85160	0.41230
H	21.21420	26.20970	-0.22540
S	18.71410	20.22210	0.75450
C	20.24130	21.66520	-0.62870
H	20.70050	22.41220	-0.99470
C	20.46650	20.31890	-1.05550
H	20.97980	20.09940	-1.82360
C	19.95570	19.50460	-0.37110
H	20.17100	18.58050	-0.39460

Table S110: Cartesian coordinates (Å) for the Donor-Acceptor Slipped π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = -166°$ and $\tau_\beta = 163°$.

atom	*x*	*y*	*z*
I	6.21720	8.75640	6.40240
F	13.14200	8.70200	1.00660
F	11.65620	6.47610	1.40470
F	10.59590	11.01040	4.19980
F	9.57290	6.53030	3.12090
F	12.62580	10.96330	2.41910
C	7.89150	8.81070	5.24950
C	11.35970	7.60190	2.06870
C	11.86490	9.88300	2.59640
C	12.12190	8.73210	1.88620
C	9.98840	8.79050	3.67560
C	8.85830	8.81880	4.55480
C	10.80900	9.89250	3.49000
C	10.30440	7.64000	2.95100
N	17.20800	7.75960	2.39070
C	19.07820	8.96110	1.48960
C	19.51310	7.79280	0.87110
H	20.30190	7.80710	0.34180
C	18.80260	6.59950	1.01970
C	17.89980	8.89050	2.23670
H	17.57720	9.68110	2.65310
C	17.64650	6.64720	1.80580
H	17.15000	5.84640	1.92750
C	19.26740	5.35970	0.39270
C	19.88040	10.22180	1.26780
S	19.66170	11.52050	2.32330
C	20.94510	12.36440	1.56880
H	21.23060	13.22970	1.83480
C	21.50570	11.67320	0.56070
H	22.21650	11.99920	0.02070
C	20.92270	10.43360	0.41230
H	21.21420	9.79170	-0.22540
S	18.71410	3.80410	0.75450
C	20.24130	5.24720	-0.62870
H	20.70050	5.99420	-0.99470
C	20.46650	3.90090	-1.05550
H	20.97980	3.68140	-1.82360
C	19.95570	3.08660	-0.37110
H	20.17100	2.16250	-0.39460

Table S111: Cartesian coordinates (Å) for the Donor-Acceptor Edge-Edge contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = -166°$ and $\tau_\beta = 163°$.

atom	*x*	*y*	*z*
I	20.78620	25.17440	-3.90490
F	27.71100	25.12000	-9.30070
F	26.22520	22.89410	-8.90260
F	25.16490	27.42840	-6.10750
F	24.14190	22.94830	-7.18630
F	27.19480	27.38130	-7.88820
C	22.46050	25.22870	-5.05780
C	25.92870	24.01990	-8.23860
C	26.43390	26.30100	-7.71090
C	26.69090	25.15010	-8.42110
C	24.55740	25.20850	-6.63170
C	23.42730	25.23680	-5.75250
C	25.37800	26.31050	-6.81720
C	24.87340	24.05800	-7.35630
N	18.53200	16.86740	-2.76300
C	20.40220	15.66590	-3.66400
C	20.83710	16.83420	-4.28260
H	21.62590	16.81990	-4.81180
C	20.12660	18.02750	-4.13390
C	19.22380	15.73650	-2.91700
H	18.90120	14.94590	-2.50050
C	18.97050	17.97980	-3.34780
H	18.47400	18.78060	-3.22620
C	20.59140	19.26730	-4.76090
C	21.20440	14.40520	-3.88580
S	20.98570	13.10650	-2.83040
C	22.26910	12.26260	-3.58490
H	22.55460	11.39730	-3.31890
C	22.82970	12.95380	-4.59290
H	23.54050	12.62780	-5.13290
C	22.24670	14.19340	-4.74140
H	22.53820	14.83530	-5.37910
S	20.03810	20.82290	-4.39920
C	21.56530	19.37980	-5.78240
H	22.02450	18.63280	-6.14840
C	21.79050	20.72610	-6.20910
H	22.30380	20.94560	-6.97720
C	21.27970	21.54040	-5.52470
H	21.49500	22.46450	-5.54830

Table S112: Cartesian coordinates (Å) for the Donor-Acceptor Edge-Edge contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = -166°$ and $\tau_\beta = 163°$.

atom	*x*	*y*	*z*
N	18.55500	25.07640	-2.39070
C	16.68480	23.87490	-1.48960
C	16.24990	25.04320	-0.87110
H	15.46110	25.02890	-0.34180
C	16.96040	26.23650	-1.01970
C	17.86320	23.94550	-2.23670
H	18.18580	23.15490	-2.65310
C	18.11650	26.18880	-1.80580
H	18.61300	26.98960	-1.92750
C	16.49560	27.47630	-0.39270
C	15.88260	22.61420	-1.26780
S	16.10130	21.31550	-2.32330
C	14.81790	20.47160	-1.56880
H	14.53240	19.60630	-1.83480
C	14.25730	21.16280	-0.56070
H	13.54650	20.83680	-0.02070
C	14.84030	22.40240	-0.41230
H	14.54880	23.04430	0.22540
S	17.04890	29.03190	-0.75450
C	15.52170	27.58880	0.62870
H	15.06250	26.84180	0.99470
C	15.29650	28.93510	1.05550
H	14.78320	29.15460	1.82360
C	15.80730	29.74940	0.37110
H	15.59200	30.67350	0.39460
I	6.21720	25.17440	6.40240
F	13.14200	25.12000	1.00660
F	11.65620	22.89410	1.40470
F	10.59590	27.42840	4.19980
F	9.57290	22.94830	3.12090
F	12.62580	27.38130	2.41910
C	7.89150	25.22870	5.24950
C	11.35970	24.01990	2.06870
C	11.86490	26.30100	2.59640
C	12.12190	25.15010	1.88620
C	9.98840	25.20850	3.67560
C	8.85830	25.23680	4.55480
C	10.80900	26.31050	3.49000
C	10.30440	24.05800	2.95100

Table S113: Cartesian coordinates (Å) for the Donor-Acceptor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = -166°$ and $\tau_\beta = 163°$.

atom	*x*	*y*	*z*
N	18.55500	25.07640	-2.39070
C	16.68480	23.87490	-1.48960
C	16.24990	25.04320	-0.87110
H	15.46110	25.02890	-0.34180
C	16.96040	26.23650	-1.01970
C	17.86320	23.94550	-2.23670
H	18.18580	23.15490	-2.65310
C	18.11650	26.18880	-1.80580
H	18.61300	26.98960	-1.92750
C	16.49560	27.47630	-0.39270
C	15.88260	22.61420	-1.26780
S	16.10130	21.31550	-2.32330
C	14.81790	20.47160	-1.56880
H	14.53240	19.60630	-1.83480
C	14.25730	21.16280	-0.56070
H	13.54650	20.83680	-0.02070
C	14.84030	22.40240	-0.41230
H	14.54880	23.04430	0.22540
S	17.04890	29.03190	-0.75450
C	15.52170	27.58880	0.62870
H	15.06250	26.84180	0.99470
C	15.29650	28.93510	1.05550
H	14.78320	29.15460	1.82360
C	15.80730	29.74940	0.37110
H	15.59200	30.67350	0.39460
I	16.30080	16.96540	-1.24870
F	9.37600	16.91100	4.14700
F	10.86180	14.68510	3.74900
F	11.92210	19.21940	0.95380
F	12.94510	14.73930	2.03270
F	9.89220	19.17230	2.73450
C	14.62650	17.01970	-0.09590
C	11.15830	15.81090	3.08500
C	10.65310	18.09200	2.55720
C	10.39610	16.94110	3.26740
C	12.52960	16.99950	1.47810
C	13.65970	17.02780	0.59890
C	11.70900	18.10150	1.66360
C	12.21360	15.84900	2.20270

Table S114: Cartesian coordinates (Å) for the Donor-Acceptor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = -166°$ and $\tau_\beta = 163°$.

atom	*x*	*y*	*z*
I	6.21720	8.75640	6.40240
F	13.14200	8.70200	1.00660
F	11.65620	6.47610	1.40470
F	10.59590	11.01040	4.19980
F	9.57290	6.53030	3.12090
F	12.62580	10.96330	2.41910
C	7.89150	8.81070	5.24950
C	11.35970	7.60190	2.06870
C	11.86490	9.88300	2.59640
C	12.12190	8.73210	1.88620
C	9.98840	8.79050	3.67560
C	8.85830	8.81880	4.55480
C	10.80900	9.89250	3.49000
C	10.30440	7.64000	2.95100
N	17.23100	15.96860	2.76300
C	15.36080	17.17010	3.66400
C	14.92590	16.00180	4.28260
H	14.13710	16.01610	4.81180
C	15.63640	14.80850	4.13390
C	16.53920	17.09950	2.91700
H	16.86180	17.89010	2.50050
C	16.79250	14.85620	3.34780
H	17.28900	14.05540	3.22620
C	15.17160	13.56870	4.76090
C	14.55860	18.43080	3.88580
S	14.77730	19.72950	2.83040
C	13.49390	20.57340	3.58490
H	13.20840	21.43870	3.31890
C	12.93330	19.88220	4.59290
H	12.22250	20.20820	5.13290
C	13.51630	18.64260	4.74140
H	13.22480	18.00070	5.37910
S	15.72490	12.01310	4.39920
C	14.19770	13.45620	5.78240
H	13.73850	14.20320	6.14840
C	13.97250	12.10990	6.20910
H	13.45920	11.89040	6.97720
C	14.48330	11.29560	5.52470
H	14.26800	10.37150	5.54830

Table S115: Cartesian coordinates (Å) for the Donor-Acceptor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = -166°$ and $\tau_\beta = 163°$.

atom	*x*	*y*	*z*
I	6.21720	8.75640	6.40240
F	13.14200	8.70200	1.00660
F	11.65620	6.47610	1.40470
F	10.59590	11.01040	4.19980
F	9.57290	6.53030	3.12090
F	12.62580	10.96330	2.41910
C	7.89150	8.81070	5.24950
C	11.35970	7.60190	2.06870
C	11.86490	9.88300	2.59640
C	12.12190	8.73210	1.88620
C	9.98840	8.79050	3.67560
C	8.85830	8.81880	4.55480
C	10.80900	9.89250	3.49000
C	10.30440	7.64000	2.95100
N	17.23100	-0.44940	2.76300
C	15.36080	0.75210	3.66400
C	14.92590	-0.41620	4.28260
H	14.13710	-0.40190	4.81180
C	15.63640	-1.60950	4.13390
C	16.53920	0.68150	2.91700
H	16.86180	1.47210	2.50050
C	16.79250	-1.56180	3.34780
H	17.28900	-2.36260	3.22620
C	15.17160	-2.84930	4.76090
C	14.55860	2.01280	3.88580
S	14.77730	3.31150	2.83040
C	13.49390	4.15540	3.58490
H	13.20840	5.02070	3.31890
C	12.93330	3.46420	4.59290
H	12.22250	3.79020	5.13290
C	13.51630	2.22460	4.74140
H	13.22480	1.58270	5.37910
S	15.72490	-4.40490	4.39920
C	14.19770	-2.96180	5.78240
H	13.73850	-2.21480	6.14840
C	13.97250	-4.30810	6.20910
H	13.45920	-4.52760	6.97720
C	14.48330	-5.12240	5.52470
H	14.26800	-6.04650	5.54830

Table S116: Cartesian coordinates (Å) for the Donor-Acceptor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = -166°$ and $\tau_\beta = 163°$.

atom	*x*	*y*	*z*
I	6.21720	8.75640	6.40240
F	13.14200	8.70200	1.00660
F	11.65620	6.47610	1.40470
F	10.59590	11.01040	4.19980
F	9.57290	6.53030	3.12090
F	12.62580	10.96330	2.41910
C	7.89150	8.81070	5.24950
C	11.35970	7.60190	2.06870
C	11.86490	9.88300	2.59640
C	12.12190	8.73210	1.88620
C	9.98840	8.79050	3.67560
C	8.85830	8.81880	4.55480
C	10.80900	9.89250	3.49000
C	10.30440	7.64000	2.95100
N	5.31000	15.96860	2.76300
C	3.43980	17.17010	3.66400
C	3.00490	16.00180	4.28260
H	2.21610	16.01610	4.81180
C	3.71540	14.80850	4.13390
C	4.61820	17.09950	2.91700
H	4.94080	17.89010	2.50050
C	4.87150	14.85620	3.34780
H	5.36800	14.05540	3.22620
C	3.25060	13.56870	4.76090
C	2.63760	18.43080	3.88580
S	2.85630	19.72950	2.83040
C	1.57290	20.57340	3.58490
H	1.28740	21.43870	3.31890
C	1.01230	19.88220	4.59290
H	0.30150	20.20820	5.13290
C	1.59530	18.64260	4.74140
H	1.30380	18.00070	5.37910
S	3.80390	12.01310	4.39920
C	2.27670	13.45620	5.78240
H	1.81750	14.20320	6.14840
C	2.05150	12.10990	6.20910
H	1.53820	11.89040	6.97720
C	2.56230	11.29560	5.52470
H	2.34700	10.37150	5.54830

Table S117: Cartesian coordinates (Å) for the Donor-Donor Slipped π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = -166°$ and $\tau_\beta = 163°$.

atom	*x*	*y*	*z*
I	20.78620	25.17440	-3.90490
F	27.71100	25.12000	-9.30070
F	26.22520	22.89410	-8.90260
F	25.16490	27.42840	-6.10750
F	24.14190	22.94830	-7.18630
F	27.19480	27.38130	-7.88820
C	22.46050	25.22870	-5.05780
C	25.92870	24.01990	-8.23860
C	26.43390	26.30100	-7.71090
C	26.69090	25.15010	-8.42110
C	24.55740	25.20850	-6.63170
C	23.42730	25.23680	-5.75250
C	25.37800	26.31050	-6.81720
C	24.87340	24.05800	-7.35630
I	17.62480	24.07960	-6.40240
F	10.70000	24.13400	-1.00660
F	12.18580	26.35990	-1.40470
F	13.24610	21.82560	-4.19980
F	14.26910	26.30570	-3.12090
F	11.21620	21.87270	-2.41910
C	15.95050	24.02530	-5.24950
C	12.48230	25.23410	-2.06870
C	11.97710	22.95300	-2.59640
C	11.72010	24.10390	-1.88620
C	13.85360	24.04550	-3.67560
C	14.98370	24.01720	-4.55480
C	13.03300	22.94350	-3.49000
C	13.53760	25.19600	-2.95100

Table S118: Cartesian coordinates (Å) for the Donor-Donor Slipped π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = -166°$ and $\tau_\beta = 163°$.

atom	*x*	*y*	*z*
I	6.21720	8.75640	6.40240
F	13.14200	8.70200	1.00660
F	11.65620	6.47610	1.40470
F	10.59590	11.01040	4.19980
F	9.57290	6.53030	3.12090
F	12.62580	10.96330	2.41910
C	7.89150	8.81070	5.24950
C	11.35970	7.60190	2.06870
C	11.86490	9.88300	2.59640
C	12.12190	8.73210	1.88620
C	9.98840	8.79050	3.67560
C	8.85830	8.81880	4.55480
C	10.80900	9.89250	3.49000
C	10.30440	7.64000	2.95100
I	17.62480	7.66160	-6.40240
F	10.70000	7.71600	-1.00660
F	12.18580	9.94190	-1.40470
F	13.24610	5.40760	-4.19980
F	14.26910	9.88770	-3.12090
F	11.21620	5.45470	-2.41910
C	15.95050	7.60730	-5.24950
C	12.48230	8.81610	-2.06870
C	11.97710	6.53500	-2.59640
C	11.72010	7.68590	-1.88620
C	13.85360	7.62750	-3.67560
C	14.98370	7.59920	-4.55480
C	13.03300	6.52550	-3.49000
C	13.53760	8.77800	-2.95100

Table S119: Cartesian coordinates (Å) for the Donor-Donor Edge-Edge contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = -166°$ and $\tau_\beta = 163°$.

atom	*x*	*y*	*z*
I	6.21720	8.75640	6.40240
F	13.14200	8.70200	1.00660
F	11.65620	6.47610	1.40470
F	10.59590	11.01040	4.19980
F	9.57290	6.53030	3.12090
F	12.62580	10.96330	2.41910
C	7.89150	8.81070	5.24950
C	11.35970	7.60190	2.06870
C	11.86490	9.88300	2.59640
C	12.12190	8.73210	1.88620
C	9.98840	8.79050	3.67560
C	8.85830	8.81880	4.55480
C	10.80900	9.89250	3.49000
C	10.30440	7.64000	2.95100
I	16.30080	0.54740	-1.24870
F	9.37600	0.49300	4.14700
F	10.86180	-1.73290	3.74900
F	11.92210	2.80140	0.95380
F	12.94510	-1.67870	2.03270
F	9.89220	2.75430	2.73450
C	14.62650	0.60170	-0.09590
C	11.15830	-0.60710	3.08500
C	10.65310	1.67400	2.55720
C	10.39610	0.52310	3.26740
C	12.52960	0.58150	1.47810
C	13.65970	0.60980	0.59890
C	11.70900	1.68350	1.66360
C	12.21360	-0.56900	2.20270

Table S120: Cartesian coordinates (Å) for the Donor-Donor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = -166°$ and $\tau_\beta = 163°$.

atom	*x*	*y*	*z*
I	6.21720	8.75640	6.40240
F	13.14200	8.70200	1.00660
F	11.65620	6.47610	1.40470
F	10.59590	11.01040	4.19980
F	9.57290	6.53030	3.12090
F	12.62580	10.96330	2.41910
C	7.89150	8.81070	5.24950
C	11.35970	7.60190	2.06870
C	11.86490	9.88300	2.59640
C	12.12190	8.73210	1.88620
C	9.98840	8.79050	3.67560
C	8.85830	8.81880	4.55480
C	10.80900	9.89250	3.49000
C	10.30440	7.64000	2.95100
I	7.54120	15.87060	1.24870
F	14.46600	15.92500	-4.14700
F	12.98020	18.15090	-3.74900
F	11.91990	13.61660	-0.95380
F	10.89690	18.09670	-2.03270
F	13.94980	13.66370	-2.73450
C	9.21550	15.81630	0.09590
C	12.68370	17.02510	-3.08500
C	13.18890	14.74400	-2.55720
C	13.44590	15.89490	-3.26740
C	11.31240	15.83650	-1.47810
C	10.18230	15.80820	-0.59890
C	12.13300	14.73450	-1.66360
C	11.62840	16.98700	-2.20270

Table S121: Cartesian coordinates (Å) for the Acceptor-Acceptor Slipped π-Stacking contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = -166°$ and $\tau_\beta = 163°$.

atom	*x*	*y*	*z*
N	18.55500	25.07640	-2.39070
C	16.68480	23.87490	-1.48960
C	16.24990	25.04320	-0.87110
H	15.46110	25.02890	-0.34180
C	16.96040	26.23650	-1.01970
C	17.86320	23.94550	-2.23670
H	18.18580	23.15490	-2.65310
C	18.11650	26.18880	-1.80580
H	18.61300	26.98960	-1.92750
C	16.49560	27.47630	-0.39270
C	15.88260	22.61420	-1.26780
S	16.10130	21.31550	-2.32330
C	14.81790	20.47160	-1.56880
H	14.53240	19.60630	-1.83480
C	14.25730	21.16280	-0.56070
H	13.54650	20.83680	-0.02070
C	14.84030	22.40240	-0.41230
H	14.54880	23.04430	0.22540
S	17.04890	29.03190	-0.75450
C	15.52170	27.58880	0.62870
H	15.06250	26.84180	0.99470
C	15.29650	28.93510	1.05550
H	14.78320	29.15460	1.82360
C	15.80730	29.74940	0.37110
H	15.59200	30.67350	0.39460
N	5.28700	24.17760	2.39070
C	7.15720	25.37910	1.48960
C	7.59210	24.21080	0.87110
H	8.38090	24.22510	0.34180
C	6.88160	23.01750	1.01970
C	5.97880	25.30850	2.23670
H	5.65620	26.09910	2.65310
C	5.72550	23.06520	1.80580
H	5.22900	22.26440	1.92750
C	7.34640	21.77770	0.39270
C	7.95940	26.63980	1.26780
S	7.74070	27.93850	2.32330
C	9.02410	28.78240	1.56880
H	9.30960	29.64770	1.83480
C	9.58470	28.09120	0.56070
H	10.29550	28.41720	0.02070
C	9.00170	26.85160	0.41230
H	9.29320	26.20970	-0.22540
S	6.79310	20.22210	0.75450
C	8.32030	21.66520	-0.62870
H	8.77950	22.41220	-0.99470
C	8.54550	20.31890	-1.05550
H	9.05880	20.09940	-1.82360
C	8.03470	19.50460	-0.37110
H	8.25000	18.58050	-0.39460

Table S122: Cartesian coordinates (Å) for the Acceptor-Acceptor Edge-Edge contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = -166°$ and $\tau_\beta = 163°$.

atom	*x*	*y*	*z*
N	18.55500	25.07640	-2.39070
C	16.68480	23.87490	-1.48960
C	16.24990	25.04320	-0.87110
H	15.46110	25.02890	-0.34180
C	16.96040	26.23650	-1.01970
C	17.86320	23.94550	-2.23670
H	18.18580	23.15490	-2.65310
C	18.11650	26.18880	-1.80580
H	18.61300	26.98960	-1.92750
C	16.49560	27.47630	-0.39270
C	15.88260	22.61420	-1.26780
S	16.10130	21.31550	-2.32330
C	14.81790	20.47160	-1.56880
H	14.53240	19.60630	-1.83480
C	14.25730	21.16280	-0.56070
H	13.54650	20.83680	-0.02070
C	14.84030	22.40240	-0.41230
H	14.54880	23.04430	0.22540
S	17.04890	29.03190	-0.75450
C	15.52170	27.58880	0.62870
H	15.06250	26.84180	0.99470
C	15.29650	28.93510	1.05550
H	14.78320	29.15460	1.82360
C	15.80730	29.74940	0.37110
H	15.59200	30.67350	0.39460
N	18.53200	16.86740	-2.76300
C	20.40220	15.66590	-3.66400
C	20.83710	16.83420	-4.28260
H	21.62590	16.81990	-4.81180
C	20.12660	18.02750	-4.13390
C	19.22380	15.73650	-2.91700
H	18.90120	14.94590	-2.50050
C	18.97050	17.97980	-3.34780
H	18.47400	18.78060	-3.22620
C	20.59140	19.26730	-4.76090
C	21.20440	14.40520	-3.88580
S	20.98570	13.10650	-2.83040
C	22.26910	12.26260	-3.58490
H	22.55460	11.39730	-3.31890
C	22.82970	12.95380	-4.59290
H	23.54050	12.62780	-5.13290
C	22.24670	14.19340	-4.74140
H	22.53820	14.83530	-5.37910
S	20.03810	20.82290	-4.39920
C	21.56530	19.37980	-5.78240
H	22.02450	18.63280	-6.14840
C	21.79050	20.72610	-6.20910
H	22.30380	20.94560	-6.97720
C	21.27970	21.54040	-5.52470
H	21.49500	22.46450	-5.54830

Table S123: Cartesian coordinates (Å) for the Acceptor-Acceptor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = -166°$ and $\tau_\beta = 163°$.

atom	*x*	*y*	*z*
N	18.55500	25.07640	-2.39070
C	16.68480	23.87490	-1.48960
C	16.24990	25.04320	-0.87110
H	15.46110	25.02890	-0.34180
C	16.96040	26.23650	-1.01970
C	17.86320	23.94550	-2.23670
H	18.18580	23.15490	-2.65310
C	18.11650	26.18880	-1.80580
H	18.61300	26.98960	-1.92750
C	16.49560	27.47630	-0.39270
C	15.88260	22.61420	-1.26780
S	16.10130	21.31550	-2.32330
C	14.81790	20.47160	-1.56880
H	14.53240	19.60630	-1.83480
C	14.25730	21.16280	-0.56070
H	13.54650	20.83680	-0.02070
C	14.84030	22.40240	-0.41230
H	14.54880	23.04430	0.22540
S	17.04890	29.03190	-0.75450
C	15.52170	27.58880	0.62870
H	15.06250	26.84180	0.99470
C	15.29650	28.93510	1.05550
H	14.78320	29.15460	1.82360
C	15.80730	29.74940	0.37110
H	15.59200	30.67350	0.39460
N	17.23100	15.96860	2.76300
C	15.36080	17.17010	3.66400
C	14.92590	16.00180	4.28260
H	14.13710	16.01610	4.81180
C	15.63640	14.80850	4.13390
C	16.53920	17.09950	2.91700
H	16.86180	17.89010	2.50050
C	16.79250	14.85620	3.34780
H	17.28900	14.05540	3.22620
C	15.17160	13.56870	4.76090
C	14.55860	18.43080	3.88580
S	14.77730	19.72950	2.83040
C	13.49390	20.57340	3.58490
H	13.20840	21.43870	3.31890
C	12.93330	19.88220	4.59290
H	12.22250	20.20820	5.13290
C	13.51630	18.64260	4.74140
H	13.22480	18.00070	5.37910
S	15.72490	12.01310	4.39920
C	14.19770	13.45620	5.78240
H	13.73850	14.20320	6.14840
C	13.97250	12.10990	6.20910
H	13.45920	11.89040	6.97720
C	14.48330	11.29560	5.52470
H	14.26800	10.37150	5.54830

Table S124: Cartesian coordinates (Å) for the Acceptor-Acceptor Herringbone contact in the **F_5BAI-PyrThio$_2$** co crystal with a torsional angles $\tau_\alpha = -166°$ and $\tau_\beta = 163°$.

atom	*x*	*y*	*z*
N	3.98600	25.07640	7.91660
C	2.11580	23.87490	8.81770
C	1.68090	25.04320	9.43620
H	0.89210	25.02890	9.96550
C	2.39140	26.23650	9.28760
C	3.29420	23.94550	8.07060
H	3.61680	23.15490	7.65420
C	3.54750	26.18880	8.50150
H	4.04400	26.98960	8.37980
C	1.92660	27.47630	9.91460
C	1.31360	22.61420	9.03950
S	1.53230	21.31550	7.98400
C	0.24890	20.47160	8.73850
H	-0.03660	19.60630	8.47250
C	-0.31170	21.16280	9.74660
H	-1.02250	20.83680	10.28660
C	0.27130	22.40240	9.89500
H	-0.02020	23.04430	10.53270
S	2.47990	29.03190	9.55280
C	0.95270	27.58880	10.93600
H	0.49350	26.84180	11.30200
C	0.72750	28.93510	11.36280
H	0.21420	29.15460	12.13090
C	1.23830	29.74940	10.67840
H	1.02300	30.67350	10.70190
N	5.31000	32.38660	2.76300
C	3.43980	33.58810	3.66400
C	3.00490	32.41980	4.28260
H	2.21610	32.43410	4.81180
C	3.71540	31.22650	4.13390
C	4.61820	33.51750	2.91700
H	4.94080	34.30810	2.50050
C	4.87150	31.27420	3.34780
H	5.36800	30.47340	3.22620
C	3.25060	29.98670	4.76090
C	2.63760	34.84880	3.88580
S	2.85630	36.14750	2.83040
C	1.57290	36.99140	3.58490
H	1.28740	37.85670	3.31890
C	1.01230	36.30020	4.59290
H	0.30150	36.62620	5.13290
C	1.59530	35.06060	4.74140
H	1.30380	34.41870	5.37910
S	3.80390	28.43110	4.39920
C	2.27670	29.87420	5.78240
H	1.81750	30.62120	6.14840
C	2.05150	28.52790	6.20910
H	1.53820	28.30840	6.97720
C	2.56230	27.71360	5.52470
H	2.34700	26.78950	5.54830