

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

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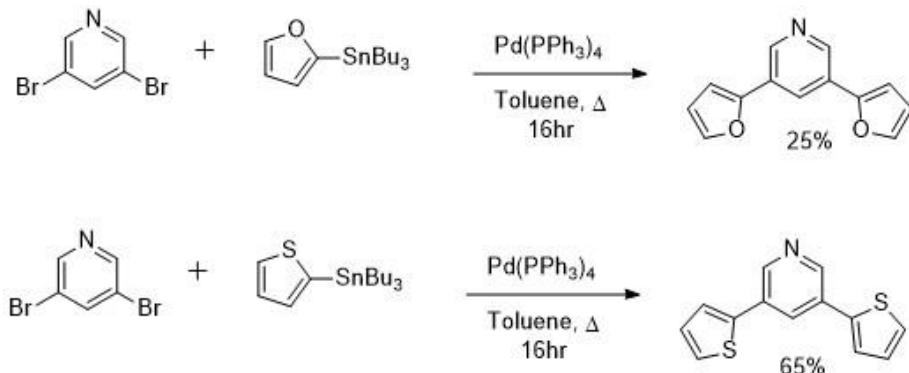
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General Summary: Reagents and solvents were purchased from commercial sources and used without further purification unless otherwise specified. DMF was degassed in 20 L drums and passed through two sequential purification columns (activated alumina; molecular sieves for DMF) under a positive argon atmosphere. Thin layer chromatography (TLC) was performed on SiO₂-60 F254 aluminum plates with visualization by UV light or staining. Flash column chromatography was performed using Purasil SiO₂-60, 230–400 mesh from Fisher. ¹H and ¹³C 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 (CDCl₃ 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(PPh₃)₄. The RBF was then put under an inert atmosphere of N₂. 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 °C. After 12 hours, the reaction mixture was cooled to room temperature and 100 mL of NaHCO₃ 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 Na₂SO₄. 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. ¹H NMR (500 MHz-CDCl₃) δ= 8.81 (s, 2H), 8.18 (s, 1H), 7.55 (d, 2H), 6.80 (d, 2H), 6.53 (t, 2H); ¹³C NMR (300 MHz-CDCl₃) 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(PPh₃)₄. The RBF was then put under an inert atmosphere of N₂. 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 °C. After 12 hours, the reaction mixture was cooled to room temperature and 100 mL of NaHCO₃ 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. ^1H 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 ($^{\circ}\text{C}$)		
	XB donor $\text{C} \equiv \text{C}_{\text{sp}-\text{I}}$	Co-crystal	Shift Δ	Melting	DTA	Weight Loss
F ₅ BAI- PyrThio ₂	2185	2167	-18	124.5 – 130.8	128.4	107.5
F ₅ BAI- PyrFur ₂	2185	2168	-17	112.3 – 113.8	111.5	111.0

Spectroscopic Analysis Infrared Spectroscopy

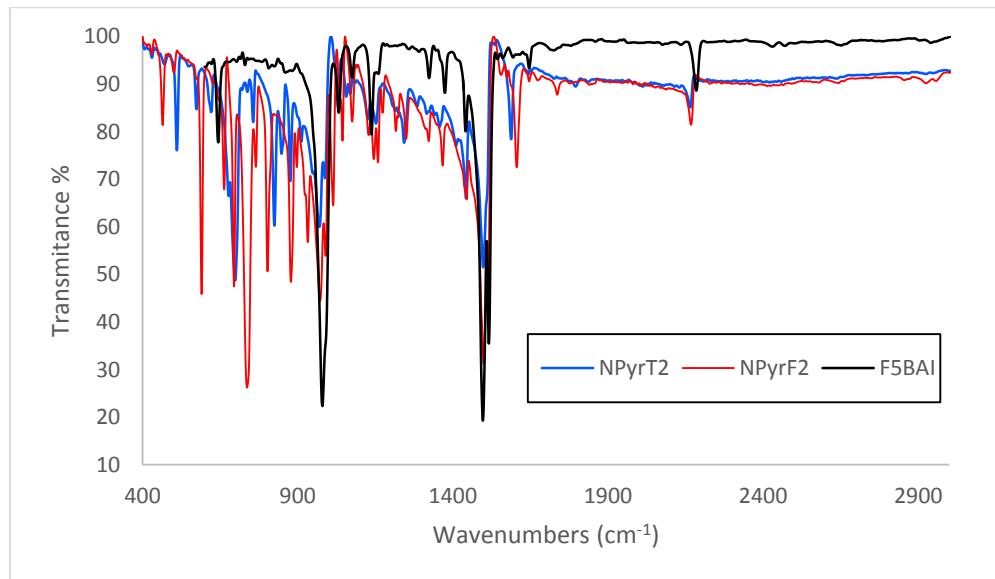


Figure S1. Infrared spectra of F₅BAI and co-crystals

Thermal Analysis

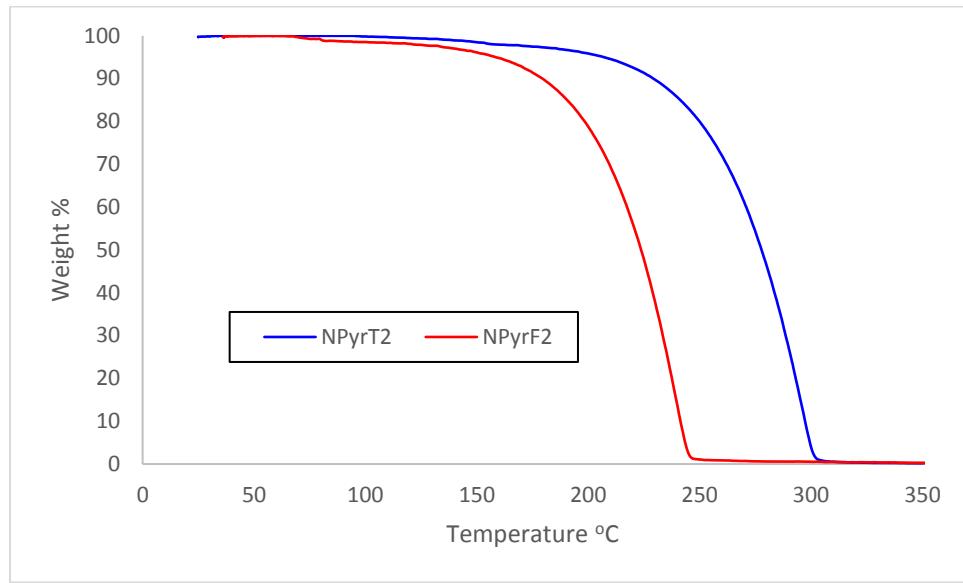


Figure S2. TGA of neat XB acceptors

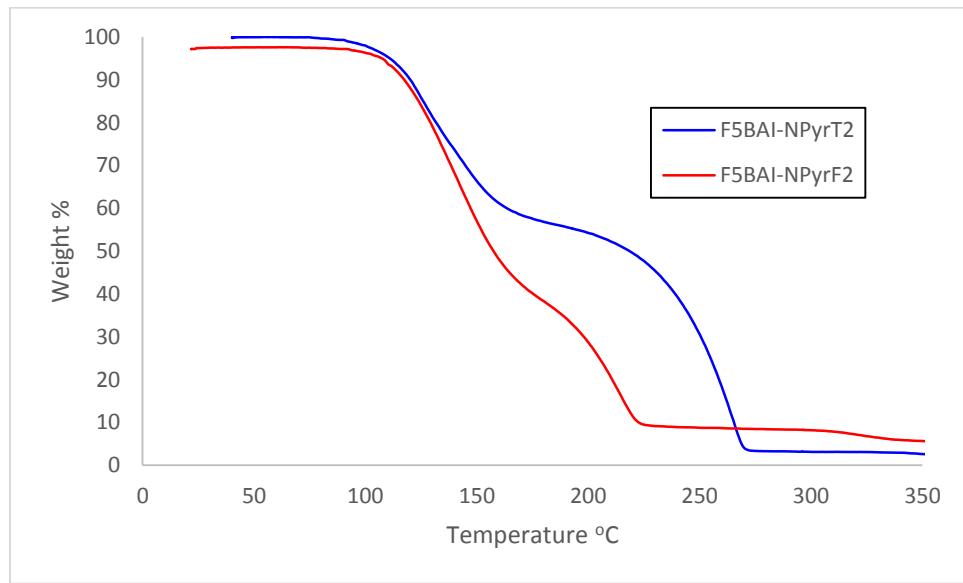


Figure S3. TGA of co-crystals

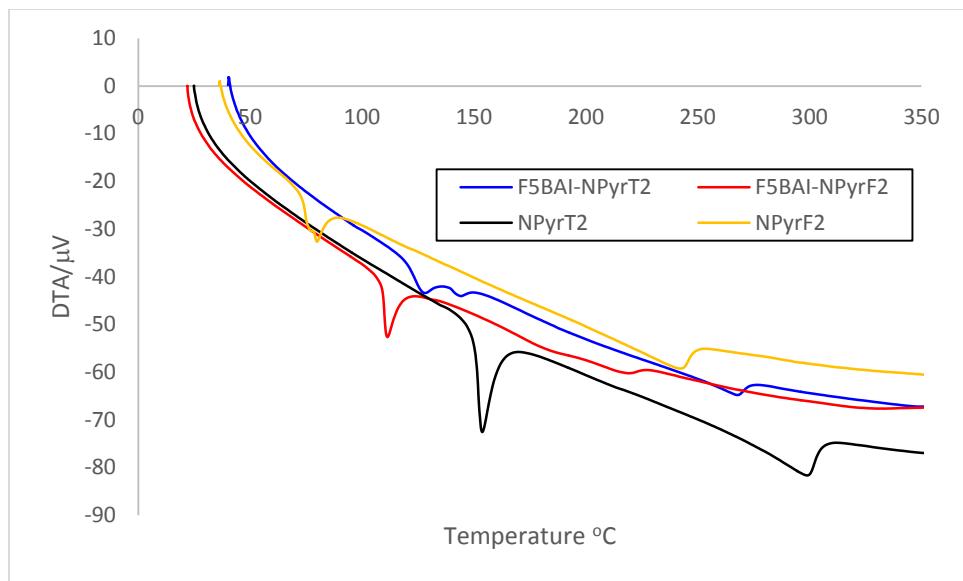
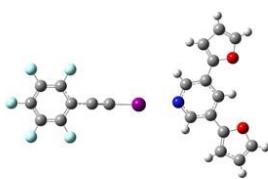


Figure S4. DTA of co-crystals and neat XB acceptors

Computational Results

a)

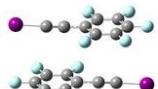
XB Interaction



π -stacking Donor-Acceptor



π -stacking Donor-Donor



π -stacking Acceptor-Acceptor

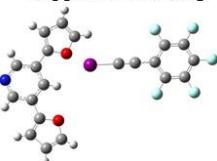


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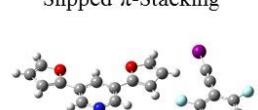
Slipped π -Stacking



Slipped π -Stacking



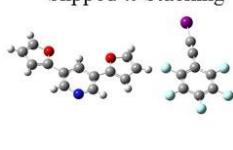
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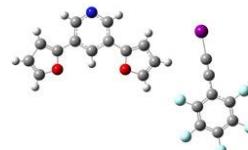
Edge-Edge



Edge-Edge



Edge-Edge



c)

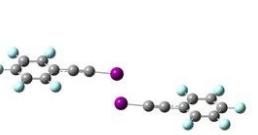
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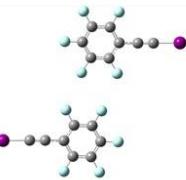
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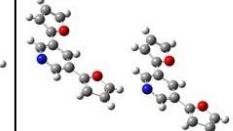
Edge-Edge



Slipped π -Stacking



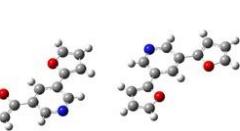
Slipped π -Stacking



Slipped π -Stacking



Edge-Edge



Edge-Edge



Figure S5. Pictorial representations of all pair-wise contacts characterized in the **F₅BAI-PyrFur₂** co-crystal, where the dominant interactions are shown in *a*, minor heterogeneous interactions in *b* and minor homogeneous interactions in *c*.

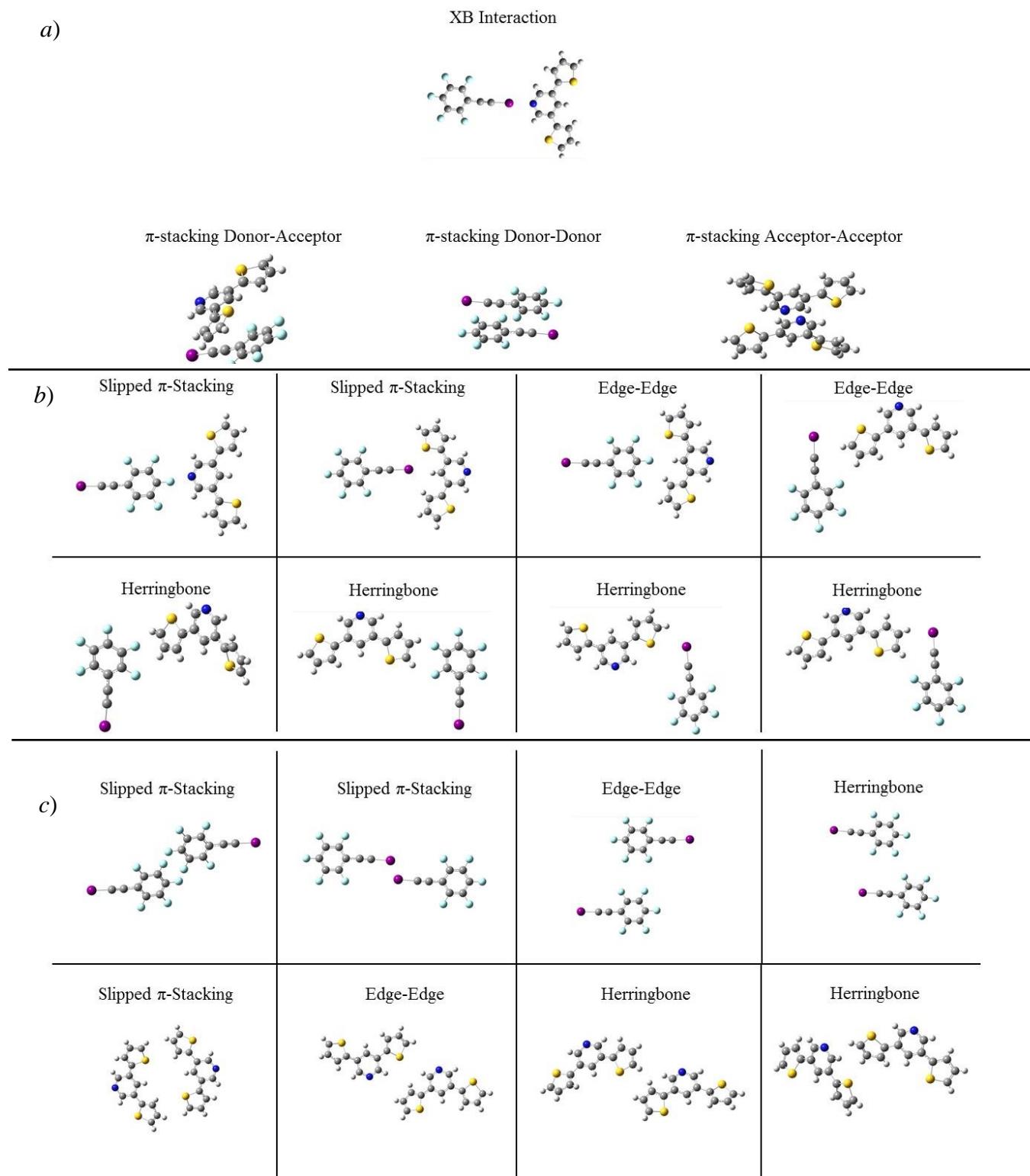


Figure S6. Pictorial representations of all pair-wise contacts characterized in the **F₅BAI-PyrThio₂** co-crystal with torsional angles $\tau_\alpha = 171^\circ$ and $\tau_\beta = -25^\circ$, where the dominant interactions are shown in *a*, minor heterogeneous interactions in *b* and minor homogeneous interactions in *c*.

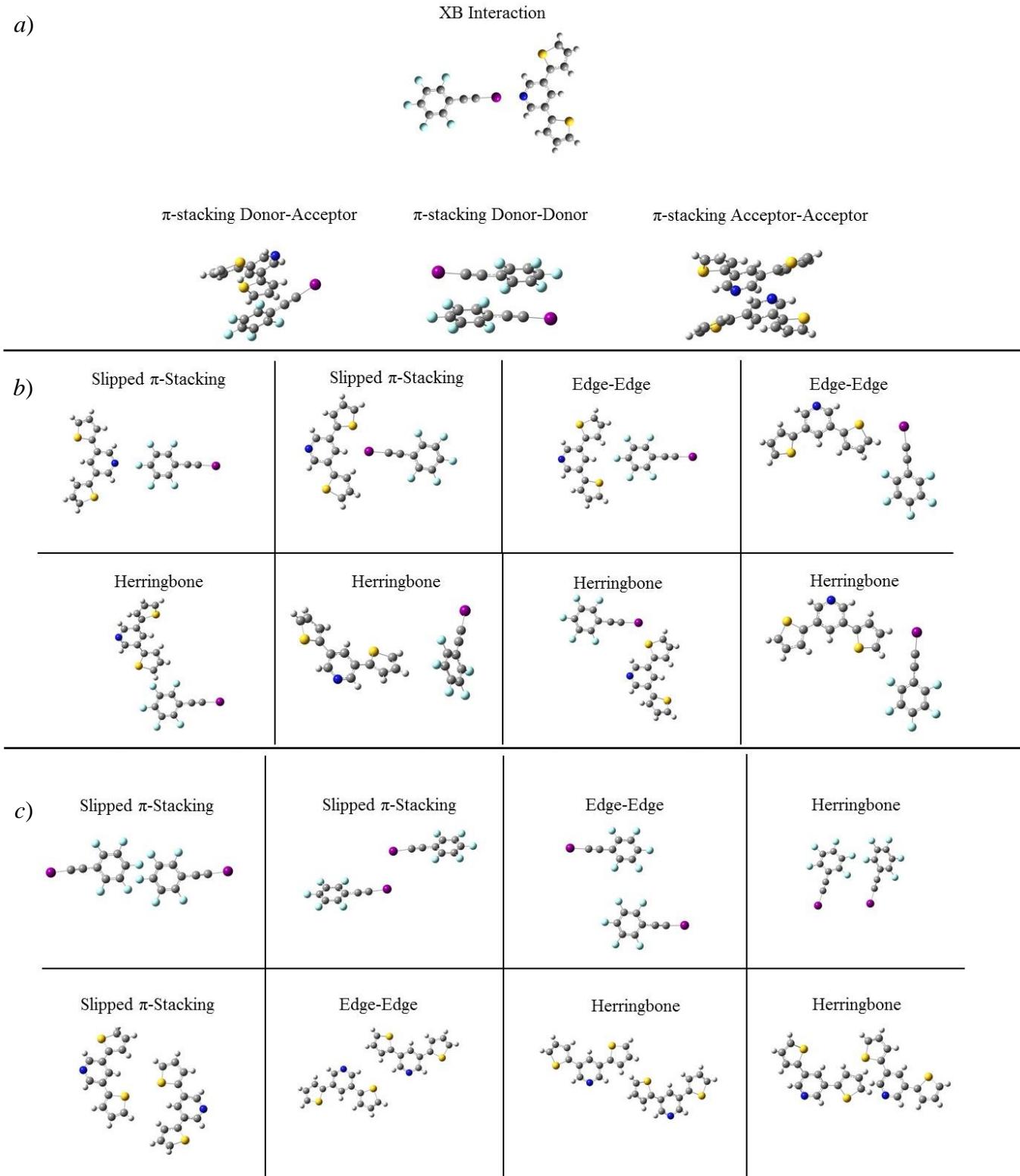
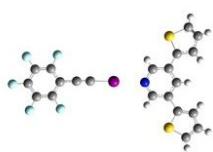


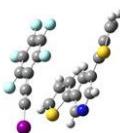
Figure S7. Pictorial representations of all pair-wise contacts characterized in the **F₅BAI-PyrThio₂** co-crystal with torsional angles $\tau_{\alpha} = 166^\circ$ and $\tau_{\beta} = 24^\circ$, where the dominant interactions are shown in *a*, minor heterogeneous interactions in *b* and minor homogeneous interactions in *c*.

a)

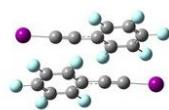
XB Interaction



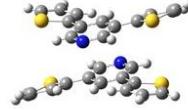
π -stacking Donor-Acceptor



π -stacking Donor-Donor

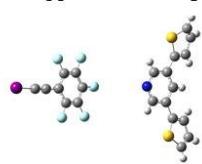


π -stacking Acceptor-Acceptor

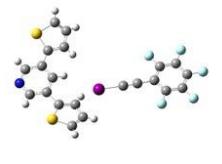


b)

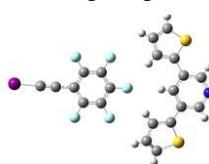
Slipped π -Stacking



Slipped π -Stacking



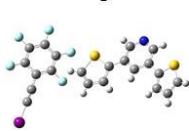
Edge-Edge



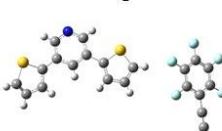
Edge-Edge



Herringbone



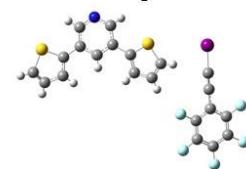
Herringbone



Herringbone



Herringbone

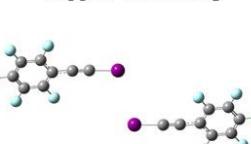


c)

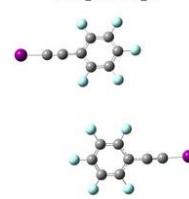
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Slipped π -Stacking



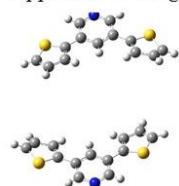
Edge-Edge



Herringbone



Slipped π -Stacking



Edge-Edge



Herringbone



Herringbone

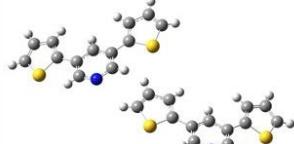


Figure S8. Pictorial representations of all pair-wise contacts characterized in the **F₅BAI-PyrThio₂** co-crystal with torsional angles $\tau_a = 166^\circ$ and $\tau_b = -163^\circ$, where the dominant interactions are shown in *a*, minor heterogeneous interactions in *b* and minor homogeneous interactions in *c*.

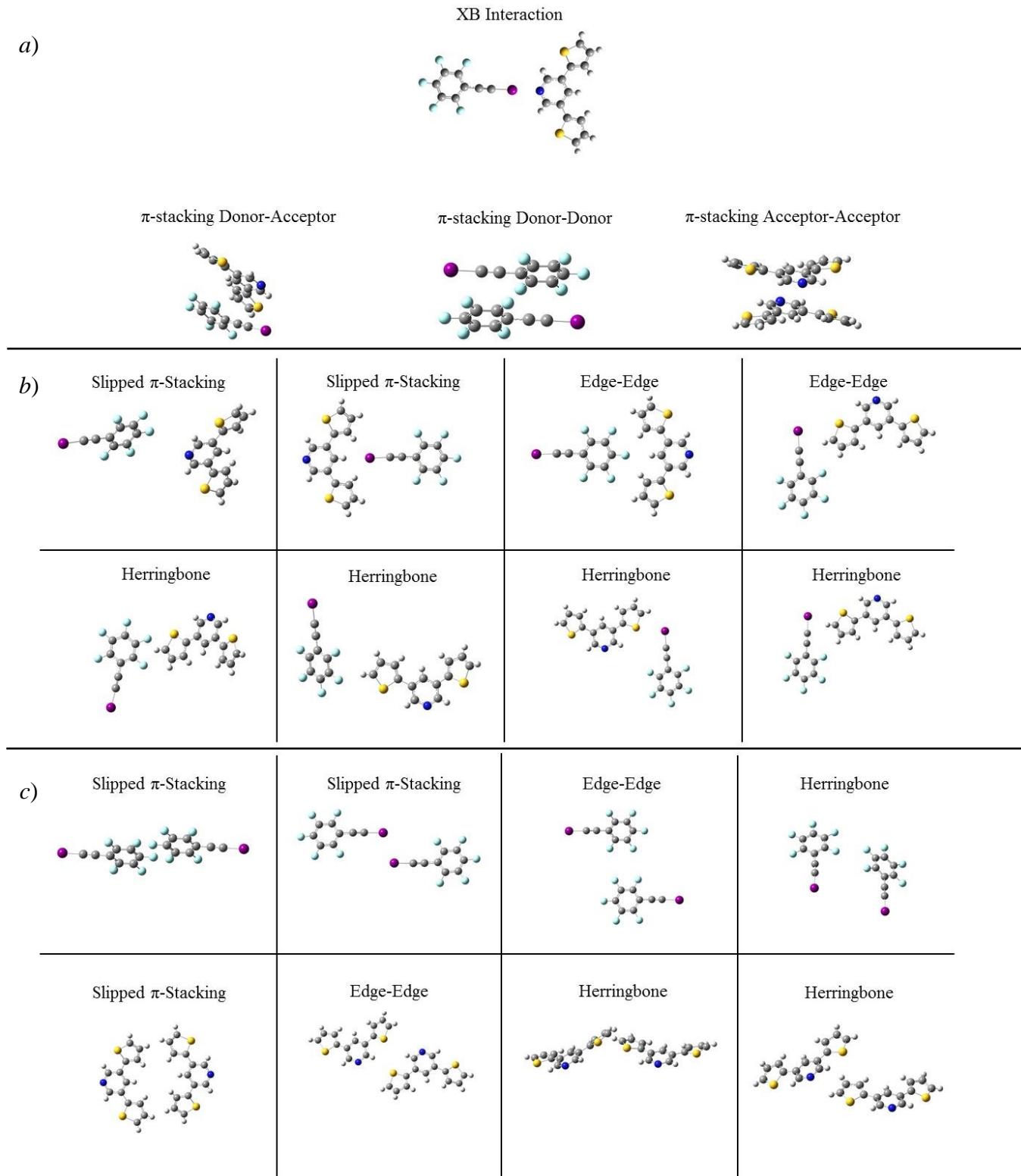


Figure S9. Pictorial representations of all pair-wise contacts characterized in the **F₅BAI-PyrThio₂** co-crystal with torsional angles $\tau_\alpha = -166^\circ$ and $\tau_\beta = 163^\circ$, where the dominant interactions are shown in *a*, minor heterogeneous interactions in *b* and minor homogeneous interactions in *c*.

Table S2. Summary of interaction energies (in kcal mol⁻¹) observed in the **F₅BAI-PyrFur₂** 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 **F₅BAI-PyrThio₂** co-crystal with torsional angles $\tau_\alpha = 171^\circ$ and $\tau_\beta = -25^\circ$ (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 **F₅BAI-PyrThio₂** co-crystal with torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = 24^\circ$ (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 **F₅BAI-PyrThio₂** co-crystal with torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = -163^\circ$ (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 **F₅BAI-PyrThio₂** co-crystal with torsional angles $\tau_\alpha = -166^\circ$ and $\tau_\beta = 163^\circ$ (Figure S9).

Type	Identity	E _{int}	E _{int} (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 (\AA) for the dominant interactions depicted in Figures S5(a) – S9(a).

	XB	Donor-Acceptor π -Stacking	Donor-Donor π -Stacking	Acceptor-Acceptor π -Stacking
F₅BAI-PyrFur₂	2.74	4.18	5.01	3.53
F₅BAI-PyrThio₂ ($\tau_\alpha = 171^\circ$ & $\tau_\beta = -25^\circ$)	2.70	3.81	4.97	3.52
F₅BAI-PyrThio₂ ($\tau_\alpha = 166^\circ$ & $\tau_\beta = 24^\circ$)	2.70	3.81	4.97	3.52
F₅BAI-PyrThio₂ ($\tau_\alpha = 166^\circ$ & $\tau_\beta = -163^\circ$)	2.70	3.80	4.97	3.52
F₅BAI-PyrThio₂ ($\tau_\alpha = -166^\circ$ & $\tau_\beta = 163^\circ$)	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 PyrFur₂ and PyrThio₂, 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 **F₅BAI-PyrFur₂** 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 **F₅BAI-PyrFur₂** 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 **F₅BAI-PyrFur₂** co-crystal and after the hydrogens were optimized at the M06-2X/aug-cc-pVDZ-PP level of theory ($|\Delta|$) as well as the relative deviations from the Avg (SP) values.

Type	Identity	Avg (SP)	Avg (H-Opt)	$ \Delta $	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 **F₅BAI-PyrThio₂** co-crystal with torsional angles $\tau_\alpha = 171^\circ$ and $\tau_\beta = -25^\circ$ at the M06-2X/aug-cc-pVDZ-PP level of theory.

Type	Identity	E _{int}	E _{int} (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 **F₅BAI-PyrThio₂** co-crystal with torsional angles $\tau_\alpha = 171^\circ$ and $\tau_\beta = -25^\circ$.

Type	Identity	E _{int}	E _{int} (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 **F₅BAI-PyrThio₂** co-crystal (with torsional angles $\tau_\alpha = 171^\circ$ and $\tau_\beta = -25^\circ$) and after the hydrogens were optimized at the M06-2X/aug-cc-pVDZ-PP level of theory ($|\Delta|$) as well as the relative deviations from the Avg (SP) values.

Type	Identity	Avg-SP	Avg-Hopt	$ \Delta $	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

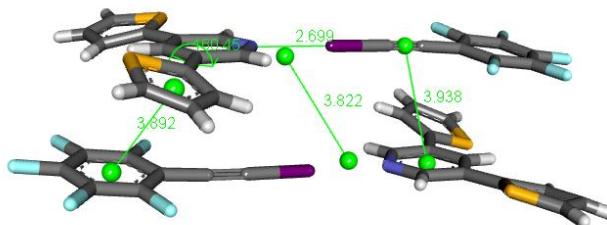


Figure S10. Centroid to centroid stacking distances (in Å) and the S-C-C-C torsional angle (in °) in the F₅BAI-PyrThio₂ crystal structure.

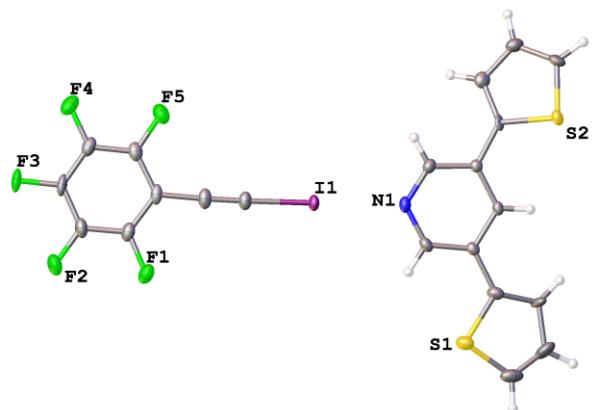


Table S15. Crystal data and structure refinement for F₅BAI-PyrThio₂.

Identification code	JLN071417					
Empirical formula	C ₂₁ H ₉ F ₅ I N S ₂					
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 [$I > 2\text{sigma}(I)$]	$R_1 = 0.0234$, $wR_2 = 0.0500$
R indices (all data)	$R_1 = 0.0306$, $wR_2 = 0.0526$
Extinction coefficient	n/a
Largest diff. peak and hole	0.423 and -0.340 e. \AA^{-3}

Table S16. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{F}_5\text{BAI-PyrThio}_2$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
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 F₅BAI-PyrThio₂.

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(00P)-C(0AA)-H(0AA)	123.3
C(00U)-C(00R)-S(003)	111.2(6)	C(00P)-C(0AA)-C(00V)	113.5(6)
C(00U)-C(00R)-H(00R)	124.4	C(00V)-C(0AA)-H(0AA)	123.3
C(00P)-C(00T)-H(00T)	126.1	C(0AA)-C(00V)-H(00V)	123.0
C(00P)-C(00T)-C(00U)	107.9(7)	C(00S)-C(00V)-C(0AA)	114.0(17)
C(00U)-C(00T)-H(00T)	126.1	C(00S)-C(00V)-H(00V)	123.0
C(00R)-C(00U)-C(00T)	118.0(9)	S(0)-C(00S)-H(00S)	123.8
C(00R)-C(00U)-H(00U)	121.0	C(00V)-C(00S)-S(0)	112(2)
C(00T)-C(00U)-H(00U)	121.0	C(00V)-C(00S)-H(00S)	123.8
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)		

Symmetry transformations used to generate equivalent atoms:

Table S18. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for F₅BAI-PyrThio₂. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^{*} b^{*} U^{12}]$

	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 ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{F}_5\text{BAI-PyrThio}_2$.

	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

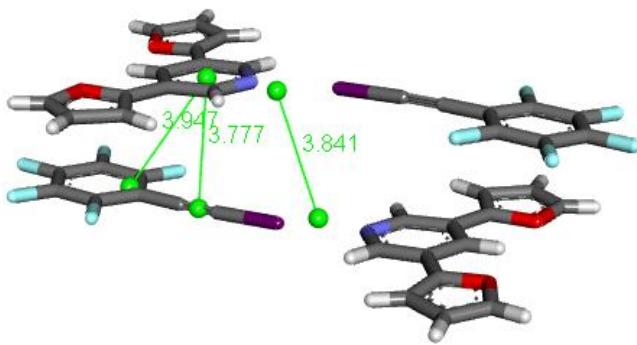


Figure S11. Centroid to centroid stacking distances (in Å) in the **F₅BAI-PyrThio₂** crystal structure.

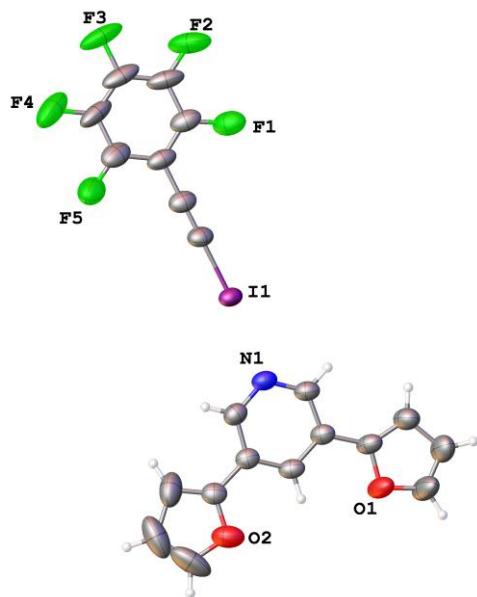


Table S20. Crystal data and structure refinement for **F₅BAI-PyrFur₂**.

Identification code	JLN071417		
Empirical formula	C ₂₁ H ₉ F ₅ I N O ₂		
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 10⁴) and equivalent isotropic displacement parameters (Å²x 10³) for F₅BAI-PyrFur₂. 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 F₅BAI-PyrFur₂.

I(1)-C(1)	2.040(5)	N(1)-C(13)	1.338(7)
F(1)-C(4)	1.333(7)	C(9)-H(9)	0.9500
F(2)-C(5)	1.339(8)	C(9)-C(10)	1.389(7)
F(3)-C(6)	1.334(7)	C(10)-C(11)	1.388(7)
F(4)-C(7)	1.338(9)	C(10)-C(14)	1.464(7)
F(5)-C(8)	1.321(8)	C(11)-H(11)	0.9500
C(1)-C(2)	1.186(7)	C(11)-C(12)	1.402(7)
C(2)-C(3)	1.423(7)	C(12)-C(13)	1.395(7)
C(3)-C(4)	1.382(8)	C(12)-C(18)	1.454(7)
C(3)-C(8)	1.404(9)	C(13)-H(13)	0.9500
C(4)-C(5)	1.379(8)	C(14)-C(15)	1.319(8)
C(5)-C(6)	1.370(11)	C(15)-H(15)	0.9500
C(6)-C(7)	1.372(11)	C(15)-C(16)	1.502(14)
C(7)-C(8)	1.380(8)	C(16)-H(16)	0.9500
O(1)-C(18)	1.356(6)	C(16)-C(17)	1.272(14)
O(1)-C(21)	1.357(8)	C(17)-H(17)	0.9500
O(2)-C(14)	1.363(7)	C(18)-C(19)	1.355(8)
O(2)-C(17)	1.363(10)	C(19)-H(19)	0.9500
N(1)-C(9)	1.342(6)	C(19)-C(20)	1.417(8)
		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 ($\text{\AA}^2 \times 10^3$) for $\text{F}_5\text{BAI-PyrFur}_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^{*} b^{*} U^{12}]$

	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 ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for F₅BAI-PyrFur₂.

	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

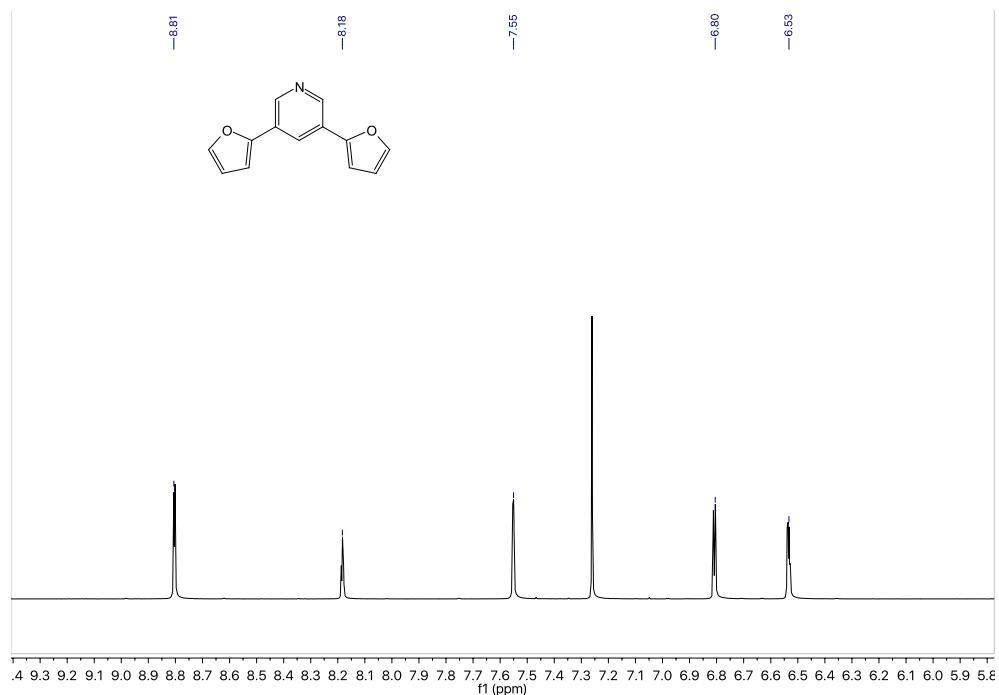


Figure S12. ¹H NMR of 3,5-di(furan-2-yl)pyridine

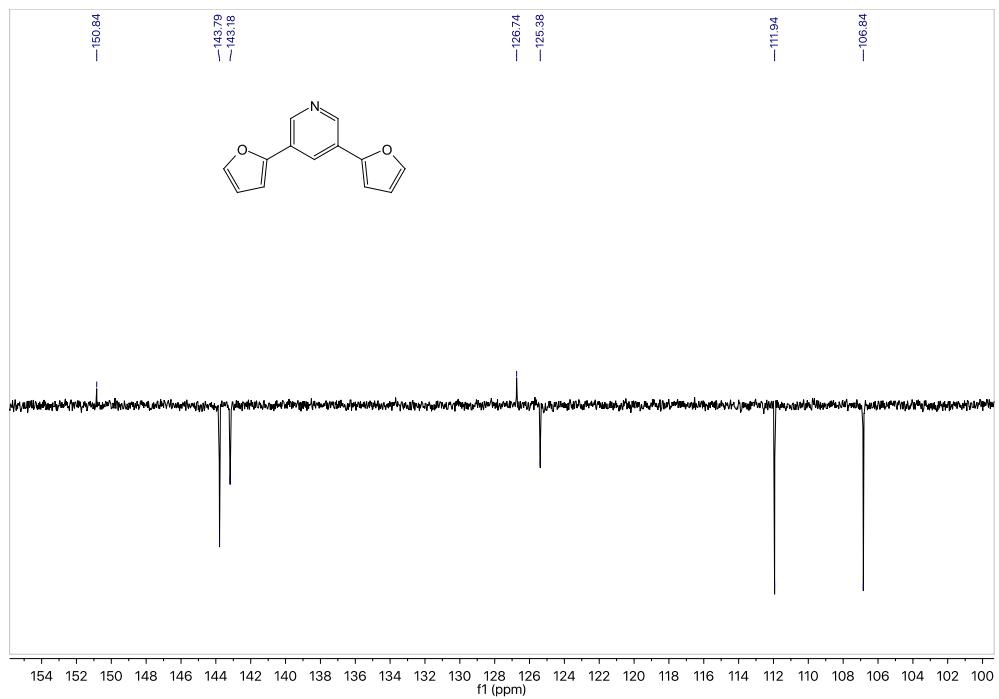


Figure S13. ¹³C NMR of 3,5-di(furan-2-yl)pyridine

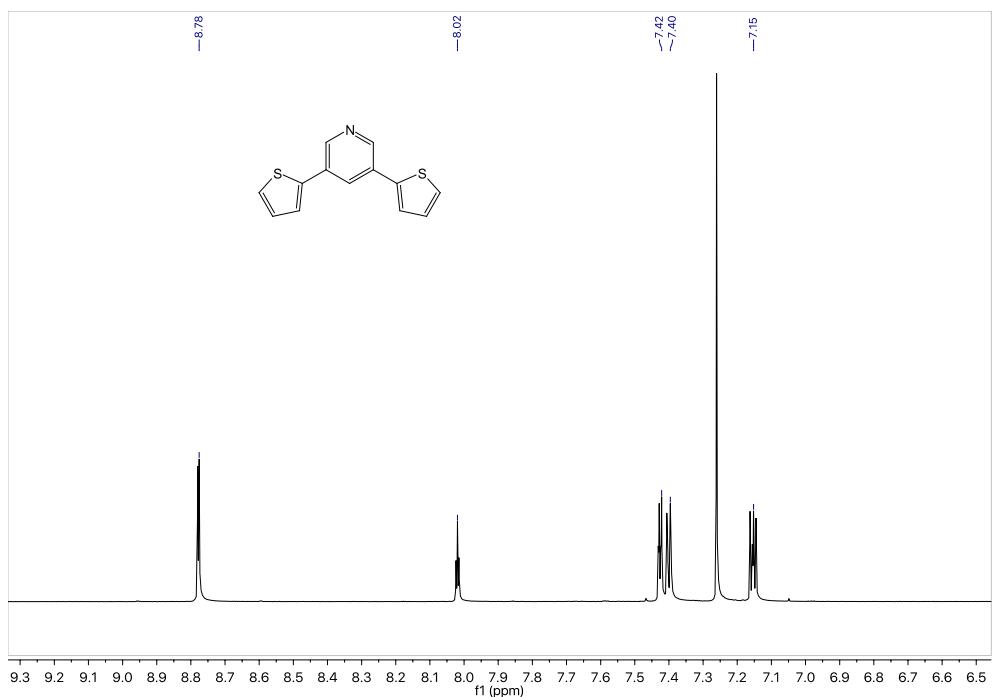


Figure S14. ¹H NMR of 3,5-di(thiophen-2-yl)pyridine

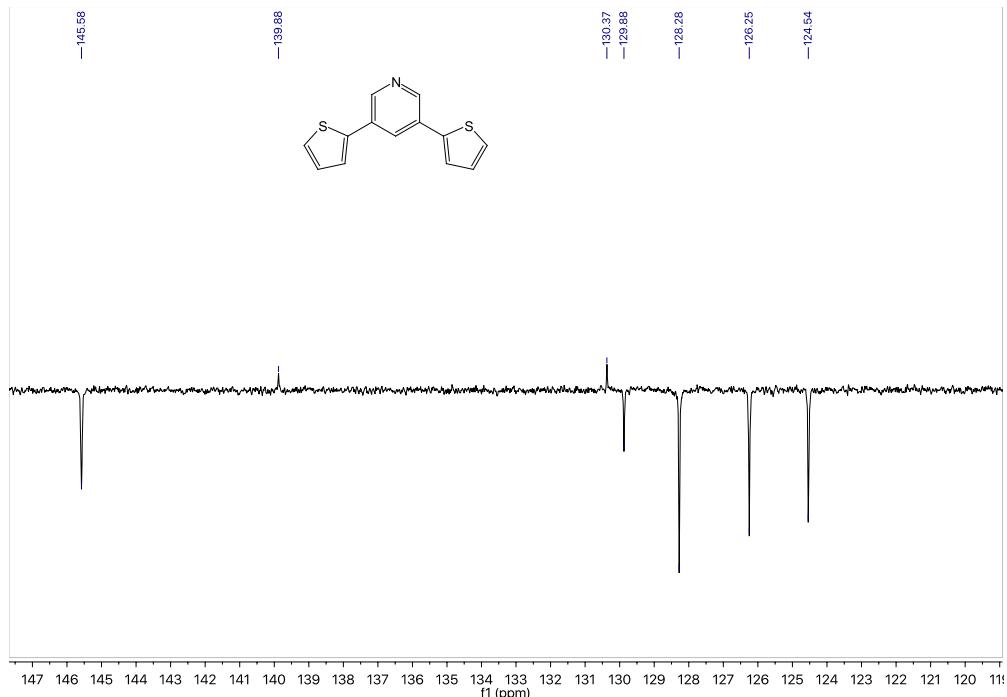


Figure S15. ¹³C NMR of 3,5-di(thiophen-2-yl)pyridine

Table S24: Cartesian coordinates (\AA) for the XB contact in the **F₅BAI-PyrFur₂** co crystal.

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

Table S25: Cartesian coordinates (\AA) for the Donor-Acceptor π -Stacking contact in the **F₅BAI-PyrFur₂** co crystal.

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

Table S26: Cartesian coordinates (\AA) for the Donor-Donor π -Stacking contact in the **F₅BAI-PyrFur₂** co crystal.

<i>atom</i>	<i>x</i>	<i>y</i>	<i>z</i>
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 (\AA) for the Acceptor-Acceptor π -Stacking contact in the $\text{F}_5\text{BAI-PyrFur}_2$ co crystal.

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

Table S28: Cartesian coordinates (\AA) for the Donor-Acceptor Slipped π -Stacking contact in the $\text{F}_5\text{BAI-PyrFur}_2$ co crystal.

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

Table S29: Cartesian coordinates (\AA) for the Donor-Acceptor Slipped π -Stacking contact in the $\text{F}_5\text{BAI-PyrFur}_2$ co crystal.

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

Table S30: Cartesian coordinates (Å) for the Donor-Acceptor Slipped π -Stacking contact in the F₅BAI-PyrFur₂ co crystal.

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

Table S31: Cartesian coordinates (\AA) for the Donor-Acceptor Slipped π -Stacking contact in the $\text{F}_5\text{BAI-PyrFur}_2$ co crystal.

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

Table S32: Cartesian coordinates (\AA) for the Donor-Acceptor Slipped π -Stacking contact in the $\text{F}_5\text{BAI-PyrFur}_2$ co crystal.

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

Table S33: Cartesian coordinates (Å) for the Donor-Acceptor Edge-Edge contact in the **F₅BAI-PyrFur₂** co crystal.

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

Table S34: Cartesian coordinates (Å) for the Donor-Acceptor Edge-Edge contact in the **F₅BAI-PyrFur₂** co crystal.

atom	x	y	z				
I	25.14320	16.26040	-4.06900	C	31.32620	11.92540	-4.33280
F	21.26040	14.39210	-1.09120	C	31.88140	10.77900	-3.77970
F	20.07990	12.53980	0.47720	H	31.37440	10.24530	-3.17940
F	21.48020	10.37740	1.30970	C	33.19360	10.41160	-4.11200
F	24.02870	10.02640	0.51980	C	33.87930	11.23060	-5.00890
F	25.21980	11.87820	-1.06830	H	34.76850	10.99170	-5.24270
C	24.35320	14.94040	-2.72980	C	29.96020	12.34050	-4.01080
C	23.87390	14.14620	-1.99050	C	29.32690	13.44230	-4.36380
C	23.26890	13.18650	-1.13150	H	29.63950	14.16390	-4.89540
C	21.95900	13.32160	-0.71290	C	27.98520	13.26540	-3.71070
C	21.35420	12.38150	0.09430	H	27.24620	13.85880	-3.78060
C	22.05660	11.28500	0.51860	C	28.01450	12.18000	-3.04840
C	23.35560	11.10880	0.11380	H	27.29770	11.85690	-2.51580
C	23.96630	12.05050	-0.68880	C	33.78960	9.19890	-3.57270
O	33.03070	8.49030	-2.70110	C	34.95190	8.53940	-3.79120
O	29.20890	11.54090	-3.20130	H	35.66200	8.81380	-4.36020
N	33.35660	12.33370	-5.55740	C	34.90380	7.36070	-3.00700
C	32.10370	12.66690	-5.21250	H	35.57430	6.69140	-2.93920
H	31.72820	13.45360	-5.59040	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 **F₅BAI-PyrFur₂** co crystal.

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

Table S36: Cartesian coordinates (\AA) for the Donor-Donor Slipped π -Stacking contact in the $\text{F}_5\text{BAI-PyrFur}_2$ co crystal.

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

Table S37: Cartesian coordinates (\AA) for the Donor-Donor Slipped π -Stacking contact in the $\text{F}_5\text{BAI-PyrFur}_2$ co crystal.

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

Table S38: Cartesian coordinates (Å) for the Donor-Donor Slipped π -Stacking contact in the **F₅BAI-PyrFur₂** co crystal.

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

Table S39: Cartesian coordinates (\AA) for the Donor-Donor Edge-Edge contact in the **F₅BAI-PyrFur₂** co crystal.

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

Table S40: Cartesian coordinates (Å) for the Acceptor-Acceptor Slipped π -Stacking contact in the **F₅BAI-PyrFur₂** co crystal.

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

Table S41: Cartesian coordinates (\AA) for the Acceptor-Acceptor Slipped π -Stacking contact in the **F₅BAI-PyrFur₂** co crystal.

atom	x	y	z				
O	31.51650	11.93060	-8.79780	H	31.09170	13.72000	-9.69140
O	35.33830	8.87990	-8.29760	O	26.66200	21.70160	-8.79780
N	31.19060	8.08720	-5.94150	O	30.48390	18.65100	-8.29760
C	32.44350	7.75400	-6.28650	N	26.33610	17.85820	-5.94150
H	32.81900	6.96730	-5.90850	C	27.58910	17.52500	-6.28650
C	33.22100	8.49550	-7.16610	H	27.96460	16.73830	-5.90850
C	32.66580	9.64180	-7.71920	C	28.36660	18.26650	-7.16610
H	33.17280	10.17560	-8.31950	C	27.81140	19.41290	-7.71920
C	31.35360	10.00920	-7.38690	H	28.31840	19.94660	-8.31950
C	30.66790	9.19030	-6.49000	C	26.49920	19.78030	-7.38690
H	29.77870	9.42920	-6.25620	H	24.92430	19.20020	-6.25620
C	34.58700	8.08040	-7.48810	C	29.73260	17.85140	-7.48810
C	35.22030	6.97860	-7.13510	C	30.36590	16.74960	-7.13510
H	34.90770	6.25690	-6.60350	H	30.05330	16.02800	-6.60350
C	36.56200	7.15550	-7.78820	C	31.70760	16.92650	-7.78820
H	37.30100	6.56210	-7.71830	H	32.44660	16.33310	-7.71830
C	36.53270	8.24090	-8.45060	C	31.67830	18.01190	-8.45060
H	37.24950	8.56400	-8.98320	H	32.39510	18.33500	-8.98320
C	30.75760	11.22200	-7.92620	C	25.90320	20.99300	-7.92620
C	29.59530	11.88150	-7.70770	C	24.74090	21.65250	-7.70770
H	28.88520	11.60700	-7.13880	H	24.03080	21.37810	-7.13880
C	29.64340	13.06020	-8.49200	C	24.78900	22.83120	-8.49200
H	28.97290	13.72950	-8.55970	H	24.11850	23.50050	-8.55970
C	30.79310	13.03840	-9.10140	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 **F₅BAI-PyrFur₂** co crystal.

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

Table S43: Cartesian coordinates (\AA) for the Acceptor-Acceptor Edge-Edge contact in the $\text{F}_5\text{BAI-PyrFur}_2$ co crystal.

atom	x	y	z				
O	22.81850	11.93060	-8.79780	H	22.39370	13.72000	-9.69140
O	26.64030	8.87990	-8.29760	O	29.18720	-1.28070	-2.70110
N	22.49260	8.08720	-5.94150	O	25.36530	1.76990	-3.20130
C	23.74550	7.75400	-6.28650	N	29.51310	2.56270	-5.55740
H	24.12100	6.96730	-5.90850	C	28.26010	2.89590	-5.21250
C	24.52300	8.49550	-7.16610	H	27.88460	3.68260	-5.59040
C	23.96780	9.64180	-7.71920	C	27.48260	2.15440	-4.33280
H	24.47480	10.17560	-8.31950	C	28.03780	1.00800	-3.77970
C	22.65560	10.00920	-7.38690	H	27.53080	0.47430	-3.17940
C	21.96990	9.19030	-6.49000	C	29.35000	0.64060	-4.11200
H	21.08070	9.42920	-6.25620	H	30.92490	1.22070	-5.24270
C	25.88900	8.08040	-7.48810	C	26.11660	2.56950	-4.01080
C	26.52230	6.97860	-7.13510	C	25.48340	3.67130	-4.36380
H	26.20970	6.25690	-6.60350	H	25.79590	4.39290	-4.89540
C	27.86400	7.15550	-7.78820	C	24.14170	3.49440	-3.71070
H	28.60300	6.56210	-7.71830	H	23.40260	4.08780	-3.78060
C	27.83470	8.24090	-8.45060	C	24.17090	2.40900	-3.04840
H	28.55150	8.56400	-8.98320	H	23.45410	2.08590	-2.51580
C	22.05960	11.22200	-7.92620	C	29.94600	-0.57210	-3.57270
C	20.89730	11.88150	-7.70770	C	31.10830	-1.23160	-3.79120
H	20.18720	11.60700	-7.13880	H	31.81840	-0.95720	-4.36020
C	20.94540	13.06020	-8.49200	C	31.06020	-2.41030	-3.00700
H	20.27490	13.72950	-8.55970	H	31.73070	-3.07960	-2.93920
C	22.09510	13.03840	-9.10140	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 F₅BAI-PyrFur₂ co crystal.

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

Table S45: Cartesian coordinates (\AA) for the XB contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 171^\circ$ and $\tau_\beta = -25^\circ$.

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

Table S46: Cartesian coordinates (\AA) for the Donor-Acceptor π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 171^\circ$ and $\tau_\beta = -25^\circ$.

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

Table S47: Cartesian coordinates (Å) for the Donor-Donor π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 171^\circ$ and $\tau_\beta = -25^\circ$.

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

Table S48: Cartesian coordinates (\AA) for the Acceptor-Acceptor π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_{\alpha} = 171^\circ$ and $\tau_{\beta} = -25^\circ$.

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

Table S49: Cartesian coordinates (\AA) for the Donor-Acceptor Slipped π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 171^\circ$ and $\tau_\beta = -25^\circ$.

atom	x	y	z				
S	6.92110	28.58050	-5.56280	H	5.96170	35.96030	-8.24580
N	7.95790	32.38650	-7.54420	C	5.35500	34.82260	-6.63580
C	6.08780	33.58810	-6.64330	C	4.51850	36.96510	-7.17080
C	5.65280	32.42000	-6.02480	H	4.44090	37.76800	-7.67170
H	4.86390	32.43430	-5.49600	C	3.80150	36.68930	-6.05970
C	6.36350	31.22650	-6.17320	H	3.14560	37.27380	-5.69680
C	7.26640	33.51720	-7.39030	I	4.37980	33.38330	-1.24870
H	7.58920	34.30770	-7.80670	F	-2.54490	33.32890	4.14700
C	7.51970	31.27400	-6.95950	F	-1.05910	31.10310	3.74900
H	8.01620	30.47340	-7.08110	F	0.00100	35.63740	0.95390
C	5.89830	29.98650	-5.54530	F	1.02400	31.15730	2.03280
C	5.62630	27.65780	-4.79190	F	-2.02880	35.59030	2.73450
H	5.69260	26.74330	-4.53930	C	2.70540	33.43760	-0.09590
C	4.61590	29.71330	-5.05370	C	-0.76270	32.22890	3.08500
H	3.88930	30.32400	-5.01860	C	-1.26780	34.51010	2.55720
C	4.59170	28.37850	-4.62080	C	-1.52490	33.35910	3.26740
H	3.81650	28.01900	-4.20640	C	0.60860	33.41770	1.47810
S	4.20650	35.16900	-5.37630	C	1.73920	33.44590	0.59890
C	5.38520	35.92260	-7.49130	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 **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 171^\circ$ and $\tau_\beta = -25^\circ$.

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

Table S51: Cartesian coordinates (\AA) for the Donor-Acceptor Edge-Edge contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_a = 171^\circ$ and $\tau_b = -25^\circ$.

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

Table S52: Cartesian coordinates (\AA) for the Donor-Acceptor Edge-Edge contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 171^\circ$ and $\tau_\beta = -25^\circ$.

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

Table S53: Cartesian coordinates (\AA) for the Donor-Acceptor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 171^\circ$ and $\tau_\beta = -25^\circ$.

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

Table S54: Cartesian coordinates (\AA) for the Donor-Acceptor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 171^\circ$ and $\tau_\beta = -25^\circ$.

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

Table S55: Cartesian coordinates (\AA) for the Donor-Acceptor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 171^\circ$ and $\tau_\beta = -25^\circ$.

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

Table S56: Cartesian coordinates (\AA) for the Donor-Acceptor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 171^\circ$ and $\tau_\beta = -25^\circ$.

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

Table S57: Cartesian coordinates (\AA) for the Donor-Donor Slipped π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 171^\circ$ and $\tau_\beta = -25^\circ$.

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

Table S58: Cartesian coordinates (\AA) for the Donor-Donor Slipped π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 171^\circ$ and $\tau_\beta = -25^\circ$.

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

Table S59: Cartesian coordinates (\AA) for the Donor-Donor Edge-Edge contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 171^\circ$ and $\tau_\beta = -25^\circ$.

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

Table S60: Cartesian coordinates (\AA) for the Donor-Donor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 171^\circ$ and $\tau_\beta = -25^\circ$.

<i>atom</i>	<i>x</i>	<i>y</i>	<i>z</i>
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 (\AA) for the Acceptor-Acceptor Slipped π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 171^\circ$ and $\tau_\beta = -25^\circ$.

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

Table S62: Cartesian coordinates (\AA) for the Acceptor-Acceptor Edge-Edge contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 171^\circ$ and $\tau_\beta = -25^\circ$.

atom	x	y	z				
S	6.92110	28.58050	-5.56280	H	3.14560	37.27380	-5.69680
N	7.95790	32.38650	-7.54420	S	8.97190	20.37150	-9.89810
C	6.08780	33.58810	-6.64330	N	7.93510	24.17750	-7.91670
C	5.65280	32.42000	-6.02480	C	9.80520	25.37910	-8.81770
H	4.86390	32.43430	-5.49600	C	10.24020	24.21100	-9.43610
C	6.36350	31.22650	-6.17320	H	11.02910	24.22530	-9.96500
C	7.26640	33.51720	-7.39030	C	9.52950	23.01750	-9.28770
H	7.58920	34.30770	-7.80670	C	8.62660	25.30820	-8.07060
C	7.51970	31.27400	-6.95950	H	8.30380	26.09870	-7.65420
H	8.01620	30.47340	-7.08110	C	8.37330	23.06500	-8.50150
C	5.89830	29.98650	-5.54530	H	7.87680	22.26440	-8.37980
C	5.62630	27.65780	-4.79190	C	9.99470	21.77750	-9.91560
H	5.69260	26.74330	-4.53930	C	10.26670	19.44880	-10.66910
C	4.61590	29.71330	-5.05370	H	10.20040	18.53430	-10.92160
H	3.88930	30.32400	-5.01860	C	11.27710	21.50430	-10.40730
C	4.59170	28.37850	-4.62080	H	12.00370	22.11500	-10.44230
H	3.81650	28.01900	-4.20640	C	11.30130	20.16950	-10.84020
S	4.20650	35.16900	-5.37630	H	12.07650	19.81000	-11.25450
C	5.38520	35.92260	-7.49130	S	11.68650	26.96000	-10.08470
H	5.96170	35.96030	-8.24580	C	10.50780	27.71360	-7.96960
C	5.35500	34.82260	-6.63580	H	9.93130	27.75130	-7.21510
C	4.51850	36.96510	-7.17080	C	10.53800	26.61360	-8.82510
H	4.44090	37.76800	-7.67170	C	11.37450	28.75610	-8.29020
C	3.80150	36.68930	-6.05970	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 (\AA) for the Acceptor-Acceptor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 171^\circ$ and $\tau_\beta = -25^\circ$.

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

Table S64: Cartesian coordinates (\AA) for the Acceptor-Acceptor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 171^\circ$ and $\tau_\beta = -25^\circ$.

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

Table S65: Cartesian coordinates (\AA) for the XB contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = 24^\circ$.

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

Table S66: Cartesian coordinates (\AA) for the Donor-Acceptor π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = 24^\circ$.

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

Table S67: Cartesian coordinates (\AA) for the Donor-Donor π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = 24^\circ$.

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

Table S68: Cartesian coordinates (\AA) for the Acceptor-Acceptor π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_a = 166^\circ$ and $\tau_b = 24^\circ$.

atom	x	y	z				
N	18.53200	16.86740	-2.76300	H	21.49500	22.46450	-5.54830
C	20.40220	15.66590	-3.66400	N	19.87900	15.96860	-7.54430
C	20.83710	16.83420	-4.28260	C	18.00880	17.17010	-6.64330
H	21.62590	16.81990	-4.81180	C	17.57390	16.00180	-6.02470
C	20.12660	18.02750	-4.13390	H	16.78510	16.01610	-5.49550
C	19.22380	15.73650	-2.91700	C	18.28440	14.80850	-6.17330
H	18.90120	14.94590	-2.50050	C	19.18720	17.09950	-7.39030
C	18.97050	17.97980	-3.34780	H	19.50980	17.89010	-7.80680
H	18.47400	18.78060	-3.22620	C	19.44050	14.85620	-6.95950
C	20.59140	19.26730	-4.76090	H	19.93700	14.05540	-7.08110
S	22.28630	14.08660	-4.93720	C	17.81960	13.56870	-5.54640
C	21.10570	13.33140	-2.81490	S	16.12470	18.74940	-5.37010
H	20.53060	13.30260	-2.05840	C	17.30530	19.50460	-7.49240
C	21.13960	14.41660	-3.68490	H	17.88040	19.53340	-8.24890
C	21.97430	12.29050	-3.13340	C	17.27140	18.41940	-6.62240
H	22.05590	11.49040	-2.62960	C	16.43670	20.54550	-7.17390
C	22.68900	12.56140	-4.24970	H	16.35510	21.34560	-7.67770
H	23.34140	11.97410	-4.61380	C	15.72200	20.27460	-6.05760
S	20.03810	20.82290	-4.39920	H	15.06960	20.86190	-5.69350
C	21.56530	19.37980	-5.78240	S	18.37290	12.01310	-5.90810
H	22.02450	18.63280	-6.14840	C	16.84570	13.45620	-4.52490
C	21.79050	20.72610	-6.20910	H	16.38650	14.20320	-4.15890
H	22.30380	20.94560	-6.97720	C	16.62050	12.10990	-4.09820
C	21.27970	21.54040	-5.52470	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 (\AA) for the Donor-Acceptor Slipped π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = 24^\circ$.

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

Table S70: Cartesian coordinates (\AA) for the Donor-Acceptor Slipped π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = 24^\circ$.

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

Table S71: Cartesian coordinates (\AA) for the Donor-Acceptor Edge-Edge contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = 24^\circ$.

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

Table S72: Cartesian coordinates (\AA) for the Donor-Acceptor Edge-Edge contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = 24^\circ$.

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

Table S73: Cartesian coordinates (\AA) for the Donor-Acceptor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = 24^\circ$.

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

Table S74: Cartesian coordinates (\AA) for the Donor-Acceptor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = 24^\circ$.

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

Table S75: Cartesian coordinates (\AA) for the Donor-Acceptor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = 24^\circ$.

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

Table S76: Cartesian coordinates (\AA) for the Donor-Acceptor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = 24^\circ$.

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

Table S77: Cartesian coordinates (\AA) for the Donor-Donor Slipped π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = 24^\circ$.

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

Table S78: Cartesian coordinates (Å) for the Donor-Donor Slipped π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = 24^\circ$.

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

Table S79: Cartesian coordinates (\AA) for the Donor-Donor Edge-Edge contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = 24^\circ$.

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

Table S80: Cartesian coordinates (\AA) for the Donor-Donor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = 24^\circ$.

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

Table S81: Cartesian coordinates (\AA) for the Acceptor-Acceptor Slipped π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = 24^\circ$.

atom	x	y	z				
N	18.55500	25.07640	-2.39070	H	15.59200	30.67350	0.39460
C	16.68480	23.87490	-1.48960	N	5.28700	24.17760	2.39070
C	16.24990	25.04320	-0.87110	C	7.15720	25.37910	1.48960
H	15.46110	25.02890	-0.34180	C	7.59210	24.21080	0.87110
C	16.96040	26.23650	-1.01970	H	8.38090	24.22510	0.34180
C	17.86320	23.94550	-2.23670	C	6.88160	23.01750	1.01970
H	18.18580	23.15490	-2.65310	C	5.97880	25.30850	2.23670
C	18.11650	26.18880	-1.80580	H	5.65620	26.09910	2.65310
H	18.61300	26.98960	-1.92750	C	5.72550	23.06520	1.80580
C	16.49560	27.47630	-0.39270	H	5.22900	22.26440	1.92750
S	14.80070	22.29560	-0.21650	C	7.34640	21.77770	0.39270
C	15.98130	21.54040	-2.33870	S	9.04130	26.95840	0.21650
H	16.55640	21.51160	-3.09530	C	7.86070	27.71360	2.33870
C	15.94740	22.62560	-1.46880	H	7.28560	27.74240	3.09530
C	15.11270	20.49950	-2.02020	C	7.89460	26.62840	1.46880
H	15.03110	19.69940	-2.52410	C	8.72930	28.75450	2.02020
C	14.39800	20.77040	-0.90390	H	8.81090	29.55460	2.52410
H	13.74560	20.18310	-0.53990	C	9.44400	28.48360	0.90390
S	17.04890	29.03190	-0.75450	H	10.09640	29.07090	0.53990
C	15.52170	27.58880	0.62870	S	6.79310	20.22210	0.75450
H	15.06250	26.84180	0.99470	C	8.32030	21.66520	-0.62870
C	15.29650	28.93510	1.05550	H	8.77950	22.41220	-0.99470
H	14.78320	29.15460	1.82360	C	8.54550	20.31890	-1.05550
C	15.80730	29.74940	0.37110	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 (\AA) for the Acceptor-Acceptor Edge-Edge contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = 24^\circ$.

atom	x	y	z				
N	19.85600	24.17760	-7.91660	H	22.81900	18.58050	-10.70190
C	21.72620	25.37910	-8.81770	N	19.87900	32.38660	-7.54430
C	22.16110	24.21080	-9.43620	C	18.00880	33.58810	-6.64330
H	22.94990	24.22510	-9.96550	C	17.57390	32.41980	-6.02470
C	21.45060	23.01750	-9.28760	H	16.78510	32.43410	-5.49550
C	20.54780	25.30850	-8.07060	C	18.28440	31.22650	-6.17330
H	20.22520	26.09910	-7.65420	C	19.18720	33.51750	-7.39030
C	20.29450	23.06520	-8.50150	H	19.50980	34.30810	-7.80680
H	19.79800	22.26440	-8.37980	C	19.44050	31.27420	-6.95950
C	21.91540	21.77770	-9.91460	H	19.93700	30.47340	-7.08110
S	23.61030	26.95840	-10.09080	C	17.81960	29.98670	-5.54640
C	22.42970	27.71360	-7.96860	S	16.12470	35.16740	-5.37010
H	21.85460	27.74240	-7.21200	C	17.30530	35.92260	-7.49240
C	22.46360	26.62840	-8.83850	H	17.88040	35.95140	-8.24890
C	23.29830	28.75450	-8.28710	C	17.27140	34.83740	-6.62240
H	23.37990	29.55460	-7.78320	C	16.43670	36.96350	-7.17390
C	24.01300	28.48360	-9.40330	H	16.35510	37.76360	-7.67770
H	24.66540	29.07090	-9.76740	C	15.72200	36.69260	-6.05760
S	21.36210	20.22210	-9.55280	H	15.06960	37.27990	-5.69350
C	22.88930	21.66520	-10.93600	S	18.37290	28.43110	-5.90810
H	23.34850	22.41220	-11.30200	C	16.84570	29.87420	-4.52490
C	23.11450	20.31890	-11.36280	H	16.38650	30.62120	-4.15890
H	23.62780	20.09940	-12.13090	C	16.62050	28.52790	-4.09820
C	22.60370	19.50460	-10.67840	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 (\AA) for the Acceptor-Acceptor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = 24^\circ$.

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

Table S84: Cartesian coordinates (\AA) for the Acceptor-Acceptor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = 24^\circ$.

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

Table S85: Cartesian coordinates (\AA) for the XB contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = -163^\circ$.

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

Table S86: Cartesian coordinates (\AA) for the Donor-Acceptor π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = -163^\circ$.

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

Table S87: Cartesian coordinates (\AA) for the Donor-Donor π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = -163^\circ$.

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

Table S88: Cartesian coordinates (\AA) for the Acceptor-Acceptor π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_{\alpha} = 166^\circ$ and $\tau_{\beta} = -163^\circ$.

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

Table S89: Cartesian coordinates (\AA) for the Donor-Acceptor Slipped π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_a = 166^\circ$ and $\tau_b = -163^\circ$.

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

Table S90: Cartesian coordinates (\AA) for the Donor-Acceptor Slipped π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_{\alpha} = 166^\circ$ and $\tau_{\beta} = -163^\circ$.

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

Table S91: Cartesian coordinates (\AA) for the Donor-Acceptor Edge-Edge contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = -163^\circ$.

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

Table S92: Cartesian coordinates (\AA) for the Donor-Acceptor Edge-Edge contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = -163^\circ$.

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

Table S93: Cartesian coordinates (\AA) for the Donor-Acceptor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = -163^\circ$.

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

Table S94: Cartesian coordinates (\AA) for the Donor-Acceptor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = -163^\circ$.

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

Table S95: Cartesian coordinates (\AA) for the Donor-Acceptor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = -163^\circ$.

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

Table S96: Cartesian coordinates (\AA) for the Donor-Acceptor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = -163^\circ$.

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

Table S97: Cartesian coordinates (\AA) for the Donor-Donor Slipped π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_{\alpha} = 166^\circ$ and $\tau_{\beta} = -163^\circ$.

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

Table S98: Cartesian coordinates (Å) for the Donor-Donor Slipped π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = -163^\circ$.

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

Table S99: Cartesian coordinates (\AA) for the Donor-Donor Edge-Edge contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = -163^\circ$.

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

Table S100: Cartesian coordinates (\AA) for the Donor-Donor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = -163^\circ$.

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

Table S101: Cartesian coordinates (\AA) for the Acceptor-Acceptor Slipped π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_{\alpha} = 166^\circ$ and $\tau_{\beta} = -163^\circ$.

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

Table S102: Cartesian coordinates (\AA) for the Acceptor-Acceptor Edge-Edge contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = -163^\circ$.

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

Table S103: Cartesian coordinates (\AA) for the Acceptor-Acceptor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = -163^\circ$.

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

Table S104: Cartesian coordinates (\AA) for the Acceptor-Acceptor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = 166^\circ$ and $\tau_\beta = -163^\circ$.

atom	x	y	z				
N	7.95800	32.38660	-7.54430	H	4.99500	26.78950	-4.75900
C	6.08780	33.58810	-6.64330	N	6.63400	25.07640	-2.39070
C	5.65290	32.41980	-6.02470	C	4.76380	23.87490	-1.48960
H	4.86410	32.43410	-5.49550	C	4.32890	25.04320	-0.87110
C	6.36340	31.22650	-6.17330	H	3.54010	25.02890	-0.34180
C	7.26620	33.51750	-7.39030	C	5.03940	26.23650	-1.01970
H	7.58880	34.30810	-7.80680	C	5.94220	23.94550	-2.23670
C	7.51950	31.27420	-6.95950	H	6.26480	23.15490	-2.65310
H	8.01600	30.47340	-7.08110	C	6.19550	26.18880	-1.80580
C	5.89860	29.98670	-5.54640	H	6.69200	26.98960	-1.92750
C	5.28560	34.84880	-6.42140	C	4.57460	27.47630	-0.39270
S	5.50430	36.14750	-7.47690	C	3.96160	22.61420	-1.26780
C	4.22090	36.99140	-6.72240	S	4.18030	21.31550	-2.32330
H	3.93540	37.85670	-6.98840	C	2.89690	20.47160	-1.56880
C	3.66030	36.30020	-5.71440	H	2.61140	19.60630	-1.83480
H	2.94950	36.62620	-5.17440	C	2.33630	21.16280	-0.56070
C	4.24330	35.06060	-5.56590	H	1.62550	20.83680	-0.02070
H	3.95180	34.41870	-4.92820	C	2.91930	22.40240	-0.41230
S	6.45190	28.43110	-5.90810	H	2.62780	23.04430	0.22540
C	4.92470	29.87420	-4.52490	S	5.12790	29.03190	-0.75450
H	4.46550	30.62120	-4.15890	C	3.60070	27.58880	0.62870
C	4.69950	28.52790	-4.09820	H	3.14150	26.84180	0.99470
H	4.18620	28.30840	-3.33010	C	3.37550	28.93510	1.05550
C	5.21030	27.71360	-4.78260	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 (\AA) for the XB contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = -166^\circ$ and $\tau_\beta = 163^\circ$.

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

Table S106: Cartesian coordinates (\AA) for the Donor-Acceptor π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = -166^\circ$ and $\tau_\beta = 163^\circ$.

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

Table S107: Cartesian coordinates (\AA) for the Donor-Donor π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = -166^\circ$ and $\tau_\beta = 163^\circ$.

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

Table S108: Cartesian coordinates (\AA) for the Acceptor-Acceptor π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = -166^\circ$ and $\tau_\beta = 163^\circ$.

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

Table S109: Cartesian coordinates (\AA) for the Donor-Acceptor Slipped π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_{\alpha} = -166^\circ$ and $\tau_{\beta} = 163^\circ$.

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

Table S110: Cartesian coordinates (Å) for the Donor-Acceptor Slipped π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = -166^\circ$ and $\tau_\beta = 163^\circ$.

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

Table S111: Cartesian coordinates (\AA) for the Donor-Acceptor Edge-Edge contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = -166^\circ$ and $\tau_\beta = 163^\circ$.

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

Table S112: Cartesian coordinates (\AA) for the Donor-Acceptor Edge-Edge contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = -166^\circ$ and $\tau_\beta = 163^\circ$.

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

Table S113: Cartesian coordinates (\AA) for the Donor-Acceptor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = -166^\circ$ and $\tau_\beta = 163^\circ$.

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

Table S114: Cartesian coordinates (\AA) for the Donor-Acceptor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_{\alpha} = -166^\circ$ and $\tau_{\beta} = 163^\circ$.

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

Table S115: Cartesian coordinates (\AA) for the Donor-Acceptor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = -166^\circ$ and $\tau_\beta = 163^\circ$.

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

Table S116: Cartesian coordinates (\AA) for the Donor-Acceptor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = -166^\circ$ and $\tau_\beta = 163^\circ$.

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

Table S117: Cartesian coordinates (\AA) for the Donor-Donor Slipped π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = -166^\circ$ and $\tau_\beta = 163^\circ$.

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

Table S118: Cartesian coordinates (\AA) for the Donor-Donor Slipped π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_{\alpha} = -166^\circ$ and $\tau_{\beta} = 163^\circ$.

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

Table S119: Cartesian coordinates (\AA) for the Donor-Donor Edge-Edge contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = -166^\circ$ and $\tau_\beta = 163^\circ$.

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

Table S120: Cartesian coordinates (\AA) for the Donor-Donor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = -166^\circ$ and $\tau_\beta = 163^\circ$.

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

Table S121: Cartesian coordinates (\AA) for the Acceptor-Acceptor Slipped π -Stacking contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_{\alpha} = -166^\circ$ and $\tau_{\beta} = 163^\circ$.

atom	x	y	z				
N	18.55500	25.07640	-2.39070	H	15.59200	30.67350	0.39460
C	16.68480	23.87490	-1.48960	N	5.28700	24.17760	2.39070
C	16.24990	25.04320	-0.87110	C	7.15720	25.37910	1.48960
H	15.46110	25.02890	-0.34180	C	7.59210	24.21080	0.87110
C	16.96040	26.23650	-1.01970	H	8.38090	24.22510	0.34180
C	17.86320	23.94550	-2.23670	C	6.88160	23.01750	1.01970
H	18.18580	23.15490	-2.65310	C	5.97880	25.30850	2.23670
C	18.11650	26.18880	-1.80580	H	5.65620	26.09910	2.65310
H	18.61300	26.98960	-1.92750	C	5.72550	23.06520	1.80580
C	16.49560	27.47630	-0.39270	H	5.22900	22.26440	1.92750
C	15.88260	22.61420	-1.26780	C	7.34640	21.77770	0.39270
S	16.10130	21.31550	-2.32330	C	7.95940	26.63980	1.26780
C	14.81790	20.47160	-1.56880	S	7.74070	27.93850	2.32330
H	14.53240	19.60630	-1.83480	C	9.02410	28.78240	1.56880
C	14.25730	21.16280	-0.56070	H	9.30960	29.64770	1.83480
H	13.54650	20.83680	-0.02070	C	9.58470	28.09120	0.56070
C	14.84030	22.40240	-0.41230	H	10.29550	28.41720	0.02070
H	14.54880	23.04430	0.22540	C	9.00170	26.85160	0.41230
S	17.04890	29.03190	-0.75450	H	9.29320	26.20970	-0.22540
C	15.52170	27.58880	0.62870	S	6.79310	20.22210	0.75450
H	15.06250	26.84180	0.99470	C	8.32030	21.66520	-0.62870
C	15.29650	28.93510	1.05550	H	8.77950	22.41220	-0.99470
H	14.78320	29.15460	1.82360	C	8.54550	20.31890	-1.05550
C	15.80730	29.74940	0.37110	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 (\AA) for the Acceptor-Acceptor Edge-Edge contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = -166^\circ$ and $\tau_\beta = 163^\circ$.

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

Table S123: Cartesian coordinates (\AA) for the Acceptor-Acceptor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = -166^\circ$ and $\tau_\beta = 163^\circ$.

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

Table S124: Cartesian coordinates (\AA) for the Acceptor-Acceptor Herringbone contact in the **F₅BAI-PyrThio₂** co crystal with a torsional angles $\tau_\alpha = -166^\circ$ and $\tau_\beta = 163^\circ$.

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