Supporting Information

Supramolecular effect of aromaticity on the crystal packing of Furan/Thiophene carboxamide compounds

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10) Table S1. The binding energy (E_{calc} in kJ/mol) of the most stable tetramer fragments of compound *I*, along with contribution of cooperativity (E_{coop}), HB (E_{HB}) and π…π stacking ($E_{\pi\ldots\pi}$) energies as the magnitude (in kJ/mol) and percentage of total binding energy, as well as their weighted contributions. Page S46

11) Table S2.The binding energy (E_{calc} in kJ/mol) of the most stable tetramer fragments of compound *II*, along with contribution of cooperativity (E_{coop}), HB (E_{HB}) and π…π stacking ($E_{\pi\ldots\pi}$) energies as the magnitude (in kJ/mol) and percentage of total binding energy, as well as their weighted contributions. Page S47

1) The Cambridge Structural Database (CSD) analysis of C-H...π interactions in five-membered furan ring

The Cambridge Structural Database (CSD) search was carried out with help of Vista program (version 2.1) in the November 2013 release of the CSD version 5.35. The searches based on geometrical parameters of the H…Cg contact distance (d_{cent}), H…Pln(mean plane) distance (d_{pln}), C-H…Cg angle (alpha/°) and the displacement angle (beta/°) for CH···π interactions of furan ring are shown in Figures S1-S4. The Scattergrams for a correlation between d_{cent} /alpha angle and d_{pln}/alpha angle are depicted in Figure S5.

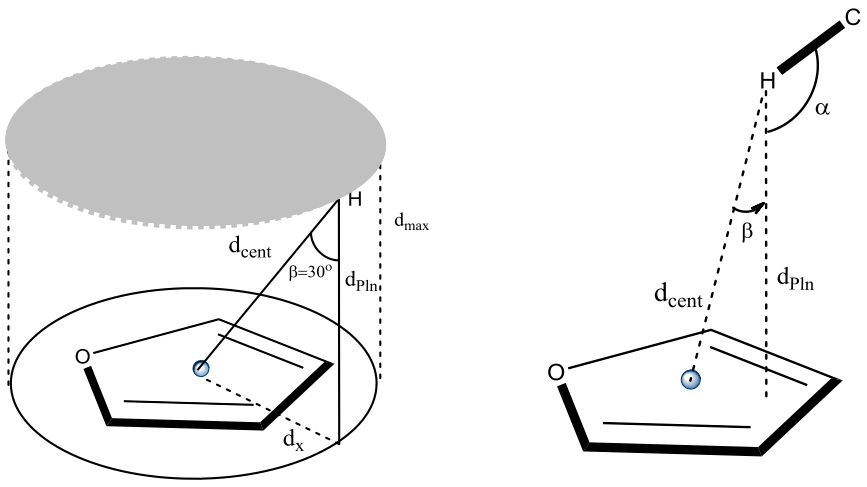


Figure S1. Representation of geometrical parameters related to CH···π interactions of furan ring in the database analysis. The restricted parameters are 0<β<30° and dpln=dmax=4.0 Å in which dx= 2 Å referred to the maximum radius of cylindrical space searchable.

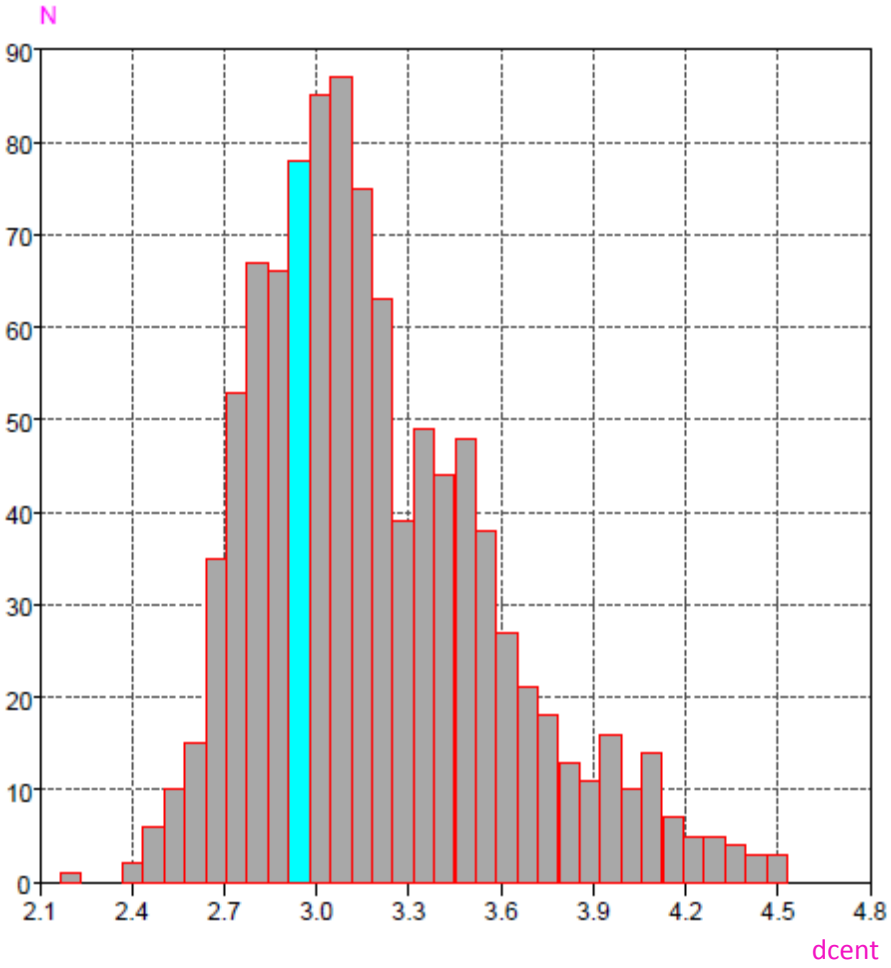


Figure S2. The Histogram for the H…Cg contact distance (d_{cent}), from a CSD search (592 hits) which was obtained between 2.1 Å to 4.5 Å. The blue column is related to the value of C9-H9...π_{Furan} interaction in compound I^{Furan}.

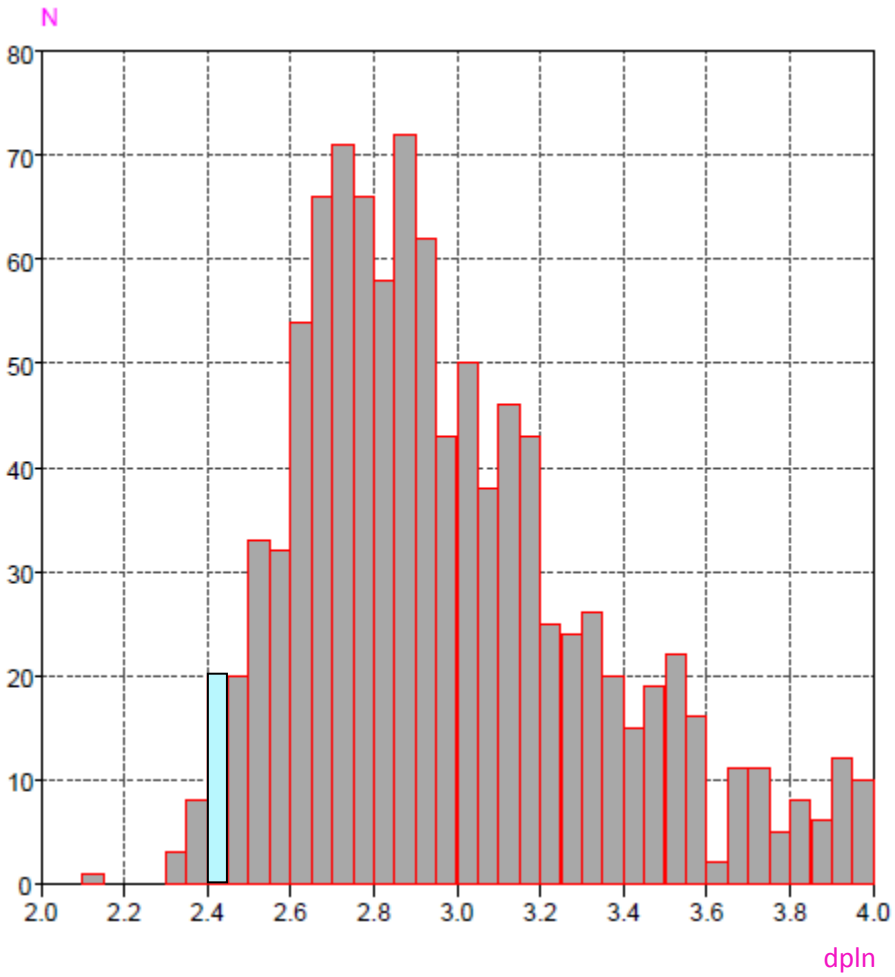


Figure S3. The Histogram for the H…Pln (mean plane) distance (d_{pln}) from a CSD search (592 hits) which was constrained between 2.0 Å and 4.0 Å.

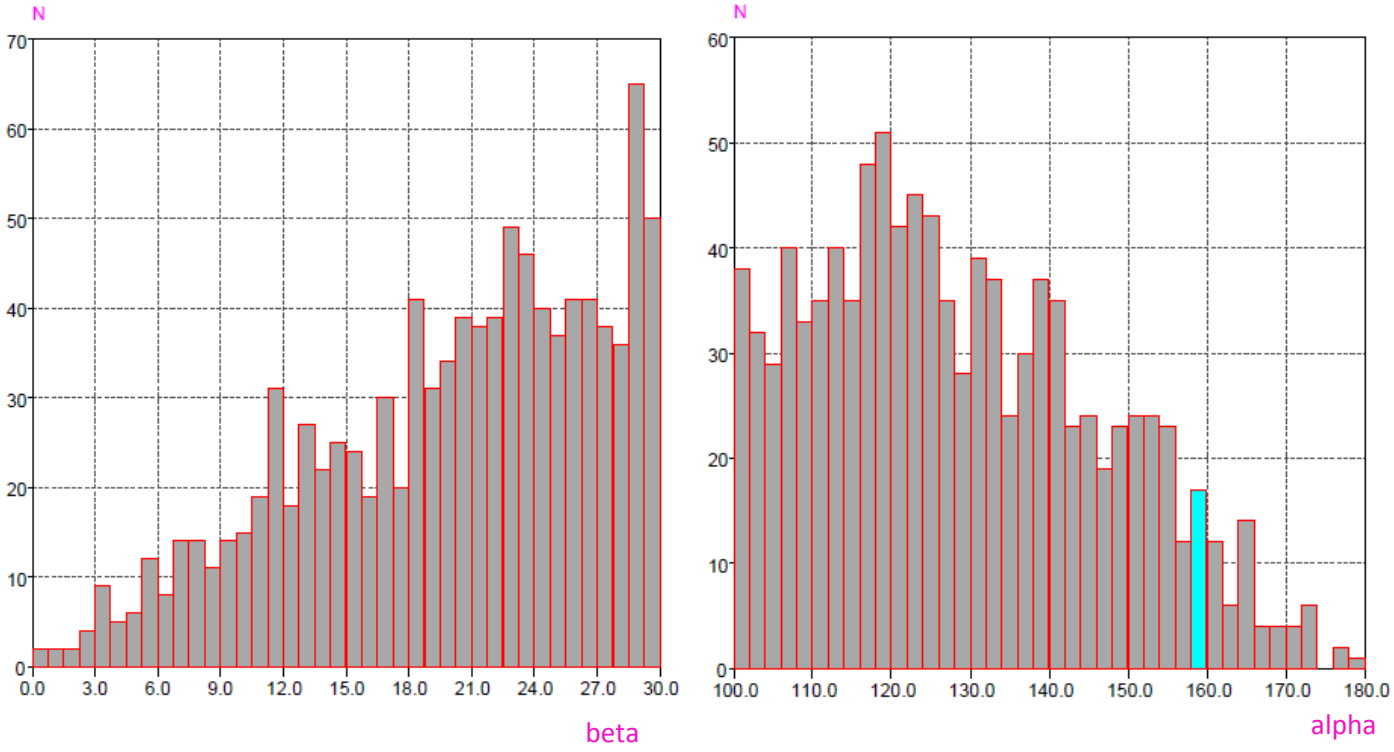


Figure S4. The Histograms for the C-H…Cg angle (alpha/˚) and the displacement angle (beta/˚) for CH···π interactions of furan ring from a CSD search (592 hits) which was constrained for α between 100° and 180° and for β between 0° and 30°.

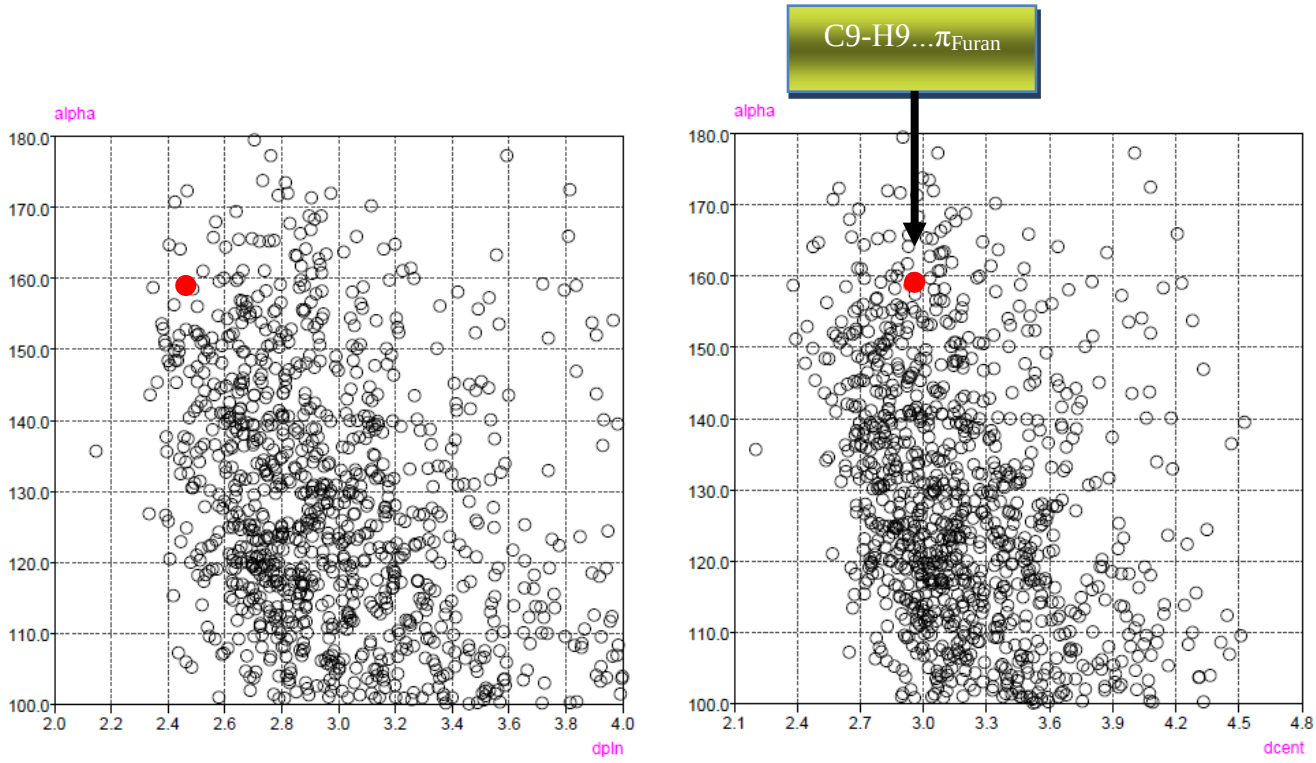


Figure S5. The Scattergrams for a correlation between d_{cent}/alpha angle (right) and d_{pln}/alpha angle (left). The red spots are related to the corresponding values of C9-H9...π_{Furan} interaction in compound I^{Furan}.

2) The Cambridge Structural Database (CSD) analysis of π···π interactions between furan rings ($\pi_{Furan}\cdots\pi_{Furan}$ interaction)

The Cambridge Structural Database (CSD) search was carried out with help of Vista program (version 2.1) in the November 2013 release of the CSD version 5.35. The searches based on geometrical parameters of the centroid–centroid distance (C–C/A˚) and the displacement angle (P–CC/˚) for π···π interactions between furan rings ($\pi_{Furan}\cdots\pi_{Furan}$ interaction) are shown in Figures S6 and S7. The Scattergram for a correlation between the centroid–centroid distance (C–C/A˚) and the displacement angle (P–CC/˚) of five memebred furan rings is depicted in Figure S8.

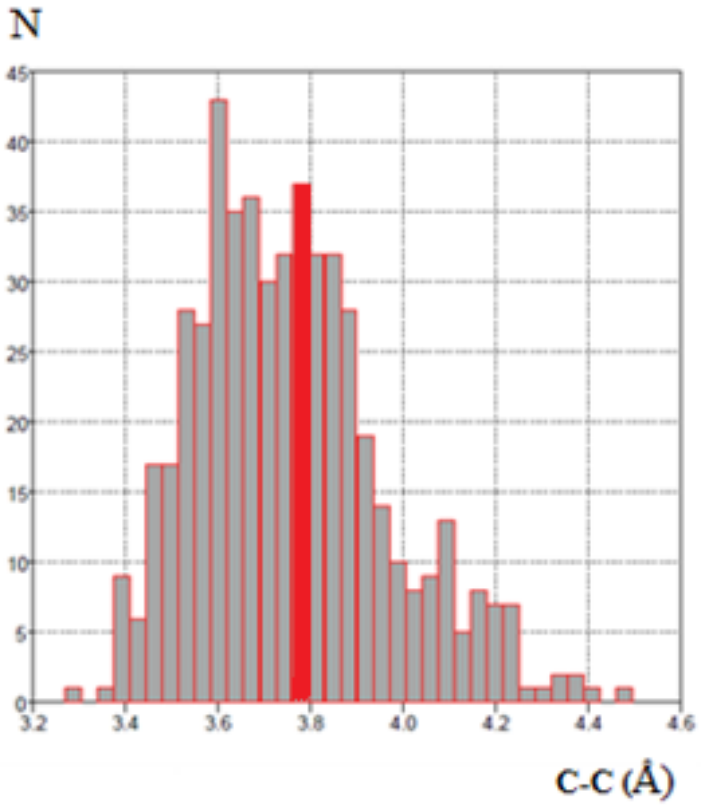


Figure S6. The Histogram for the centroid–centroid distance (C–C/Å) between furan rings from a CSD search (519 hits) which was constrained between 3.2 Å and 4.6 Å. The red column is related to the value of $\pi_{Furan}\cdots\pi_{Furan}$ interaction in compound I^{Furan}.

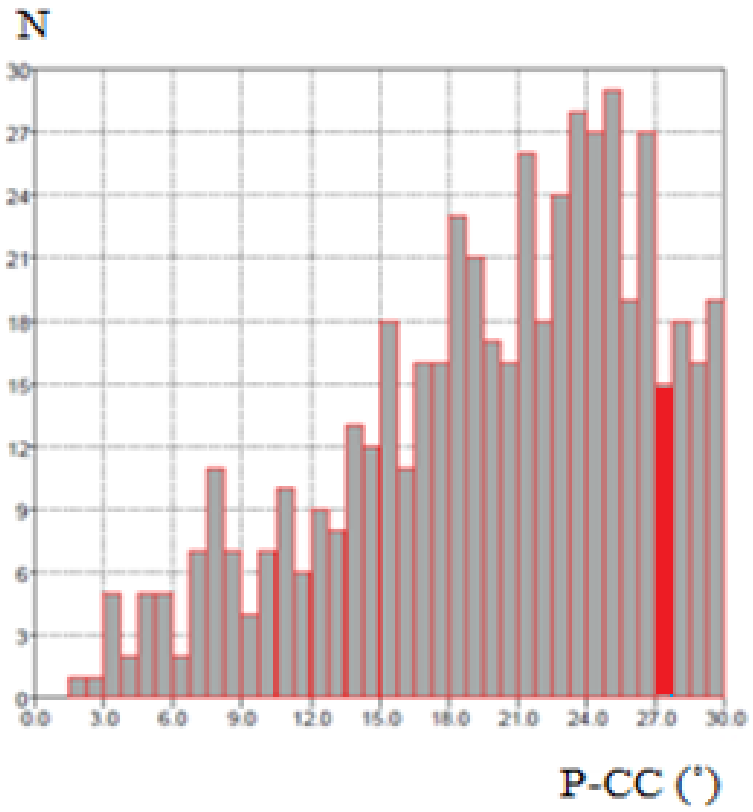


Figure S7. The Histogram for the displacement angle (P–CC/˚)between furan rings from a CSD search (519 hits) which was constrained between 0° and 30°. The red column is related to the value of $\pi_{\text{Furan}}\cdots\pi_{\text{Furan}}$ interaction in compound I^{Furan}.

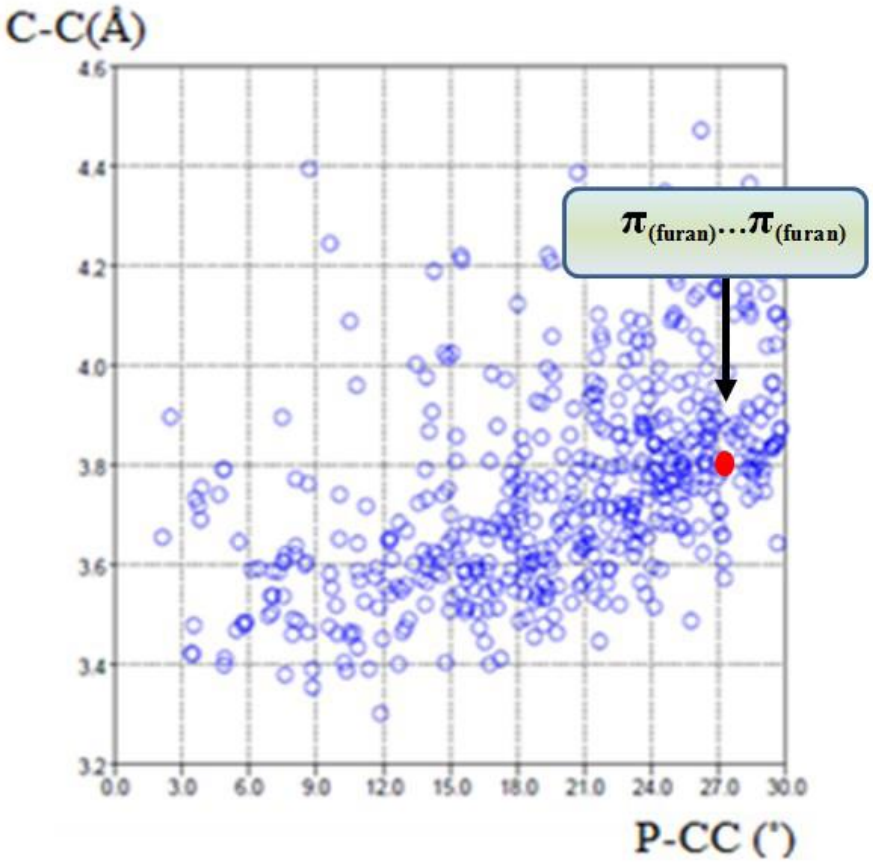


Figure S8. The Scattergram for a correlation between the centroid–centroid distance (C–C/A˚) and the displacement angle (P–CC/°). The red spot is related to the corresponding values of $\pi_{Furan}\cdots\pi_{Furan}$ interaction in compound I^{Furan}.

3) The Cambridge Structural Database (CSD) analysis of π···π interactions between pyrazine rings ($\pi_{pyz}\cdots\pi_{pyz}$ interaction)

The searches based on geometrical parameters of the centroid–centroid distance (C–C/A˚) and the displacement angle (P–CC/˚) for π···π interactions between pyrazine rings ($\pi_{Furan}\cdots\pi_{Furan}$ interaction) are shown in Figures S9 and S10. The Scattergram for a correlation between the centroid–centroid distance (C–C/A˚) and the displacement angle (P–CC/˚) of six memebred pyrazine rings is depicted in Figure S11.

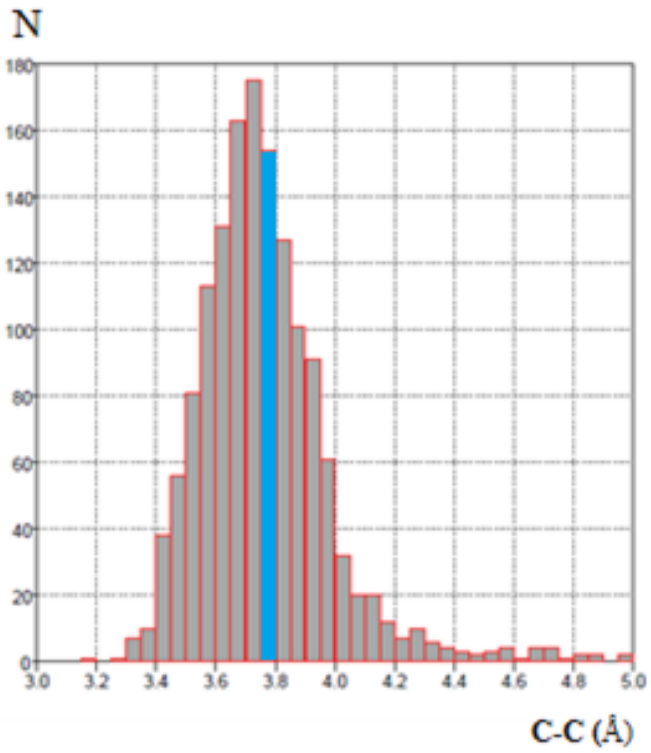


Figure S9. The Histogram for the centroid–centroid distance (C–C/Å) between pyrazine rings from a CSD search (1449 hits) which was constrained between 3.0 Å and 5.0 Å. The blue column is related to the value of $\pi_{pyz}\cdots\pi_{pyz}$ interaction in compound I^{Furan}.

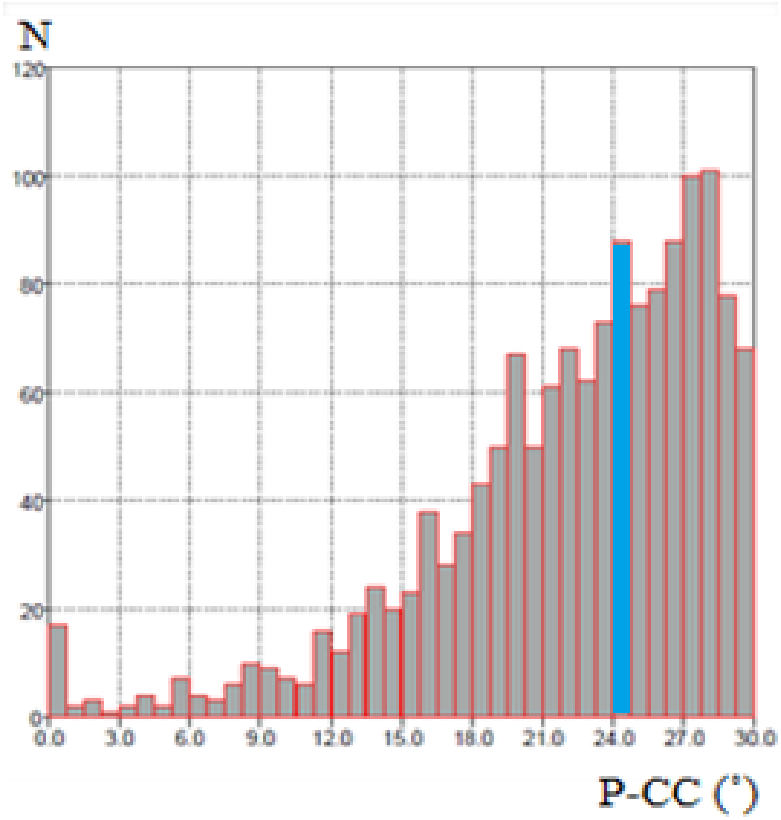


Figure S10. The Histogram for the displacement angle (P–CC/˚) between pyrazine rings from a CSD search (1449 hits) which was constrained between 0° and 30°. The blue column is related to the value of $\pi_{pyz}\cdots\pi_{pyz}$ interaction in compound I^{Furan}.

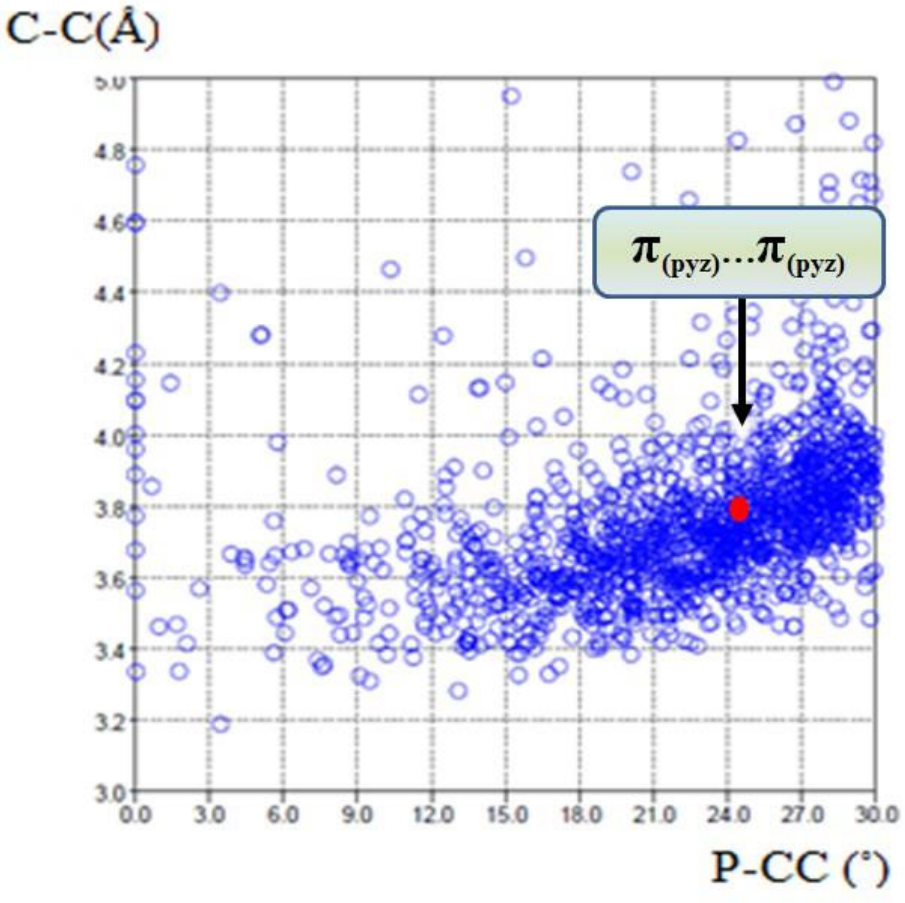


Figure S11. The Scattergram for a correlation between the centroid–centroid distance (C–C/A˚) and the displacement angle (P–CC/°). The red spot is related to the corresponding values of $\pi_{pyz}\cdots\pi_{pyz}$ interaction in compound I^{Furan}.

4) The Cambridge Structural Database (CSD) analysis of π···π interactions between thiophene rings (π_{Thio}··· π_{Thio} interaction)

The searches based on geometrical parameters of the centroid–centroid distance (C–C/A˚) and the displacement angle (P–CC/˚) for π···π interactions between thiophene rings (π_{Thio}··· π_{Thio} interaction) are shown in Figures S12 and S13. The Scattergram for a correlation between the centroid–centroid distance (C–C/A˚) and the displacement angle (P–CC/˚) of five memebred thiophene rings is depicted in Figure S14.

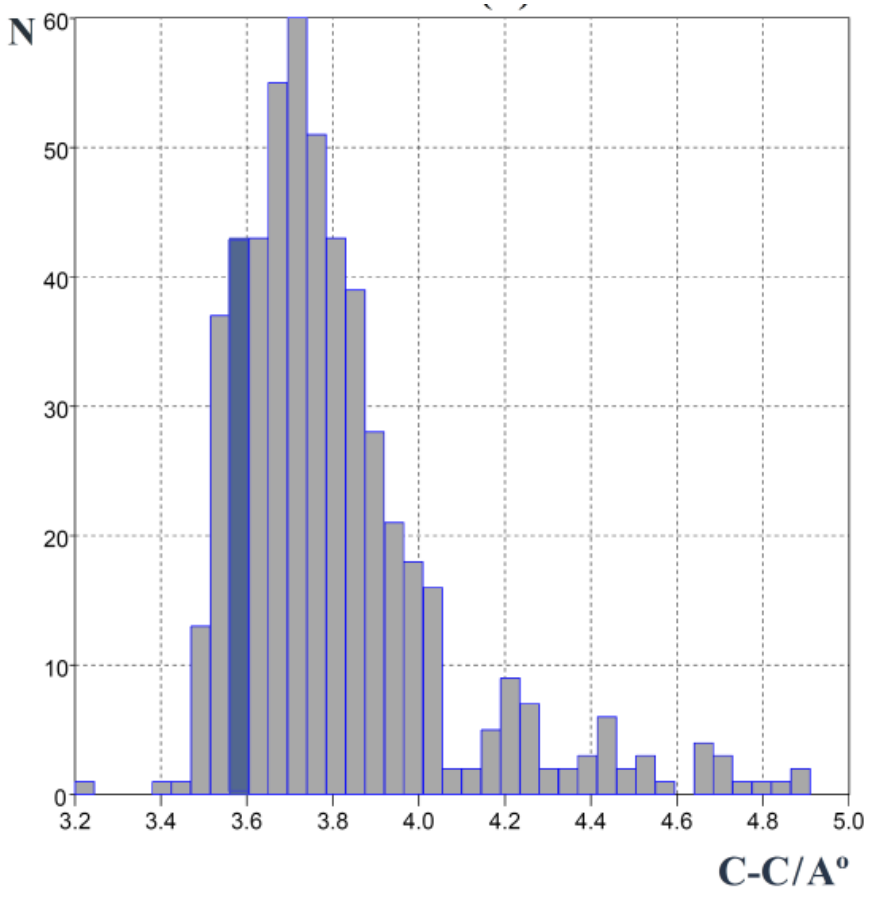


Figure S12. The Histogram for the centroid–centroid distance (C–C/Å) between thiophene rings from a CSD search (526 hits) which was constrained between 3.2 Å and 5.0 Å. The blue column is related to the value of π_{Thio}···π_{Thio} interaction in compound $II^{Thiophene}$.

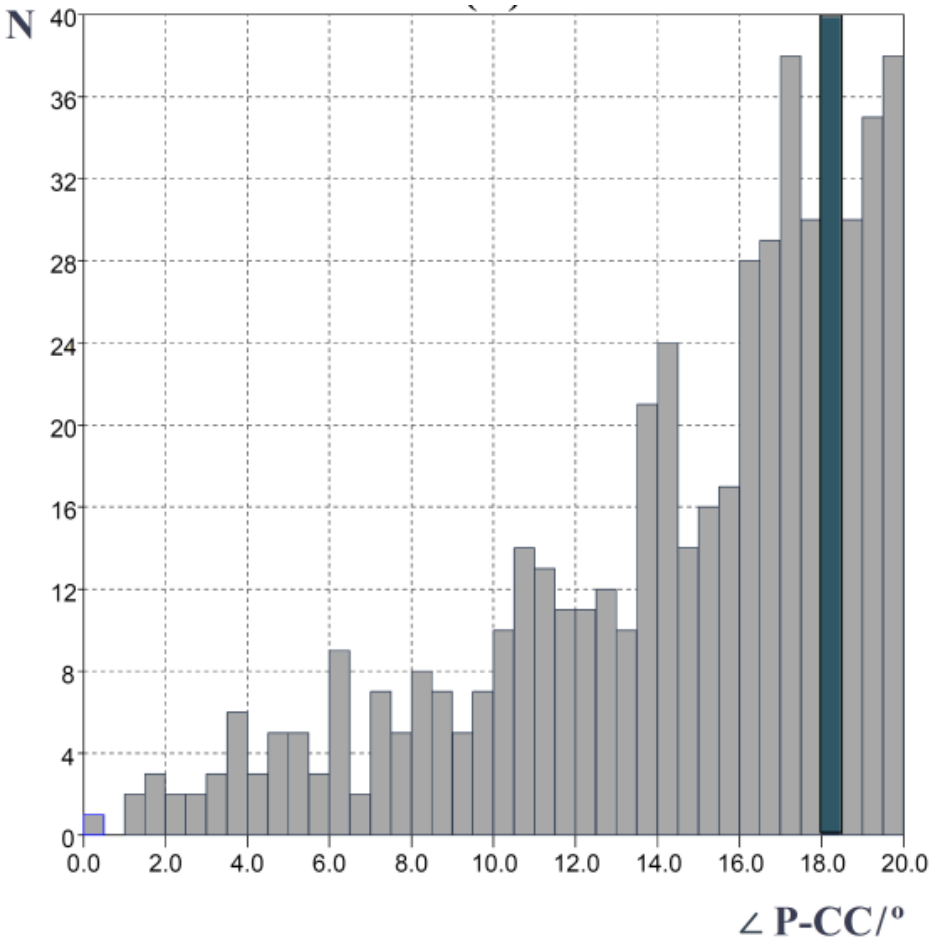


Figure S13. The Histogram for the displacement angle (P–CC/˚) between thiophene rings from a CSD search (526 hits) which was constrained between 0° and 20°. The blue column is related to the value of $\pi_{Thio}\cdots\pi_{Thio}$ interaction in compound $II^{Thiophene}$.

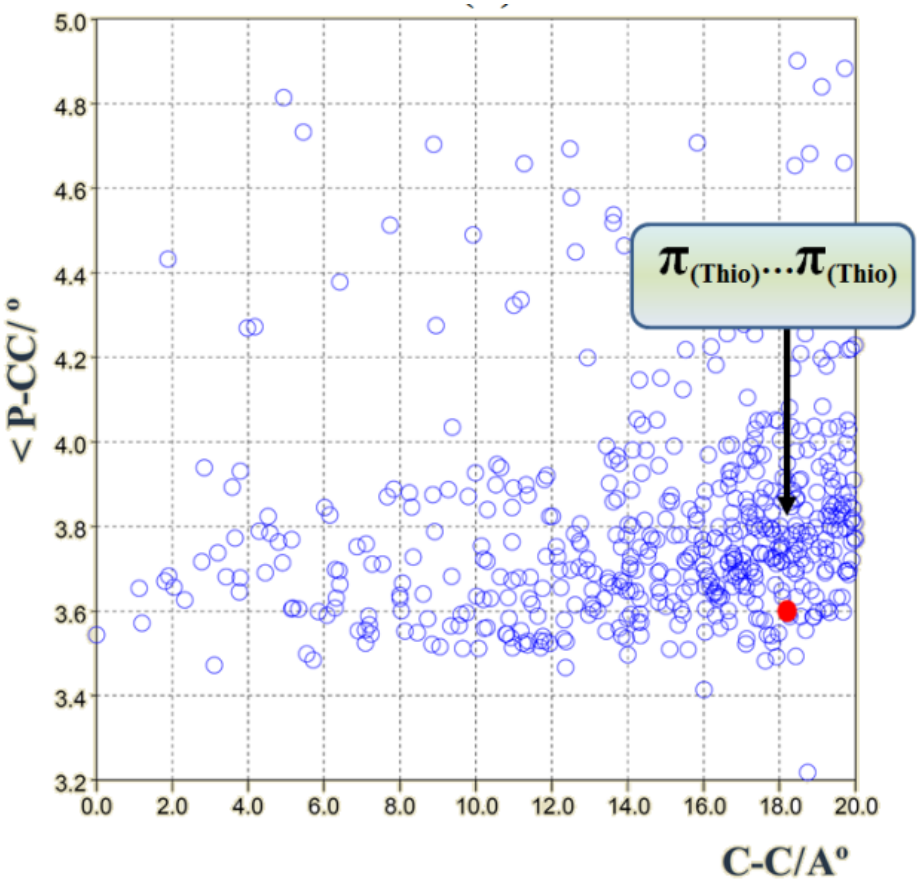


Figure S14. The Scattergram for a correlation between the centroid–centroid distance (C–C/A˚) and the displacement angle (P–CC/˚). The red spot is related to the corresponding values of $\pi_{Thio}\cdots\pi_{Thio}$ interaction in compound $II^{Thiophene}$.

5) **NMR and IR data of *I***

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.68 (d, J=1.6 Hz, 1*H*-pyrazine), 8.74 (s, 1*H*-Amide), 8.40 (d, J=2.4 Hz, 1*H*-pyrazine), 8.31 (dd, J=1.6, 0.8 Hz, 1*H*-pyrazine), 7.59 (dd, J=0.8, 0.4 Hz, 1*H*-furan), 7.35 (dd, J=2.8, 0.8 Hz, 1*H*-furan), 6.62 (dd, J=2.0, 1.6 Hz, 1*H*-furan). ^{13}C NMR (100.61 MHz, $CDCl_3$): δ 155.81 (C=O), 147.85 (C4-furan), 146.77 (C6-pyrazine), 145.16 (C1-furan), 142.23 (C9-pyrazine), 140.45 (C7-pyrazine), 137.11 (C8-pyrazine), 116.77 (C3-furan), 112.96 (C2-furan). Selected IR bands (KBr pellet, cm^{-1}): 3225 (b), 3124 (b), 1671 (s), 1545 (s), 1416 (s), 1307 (s), 723 (b).

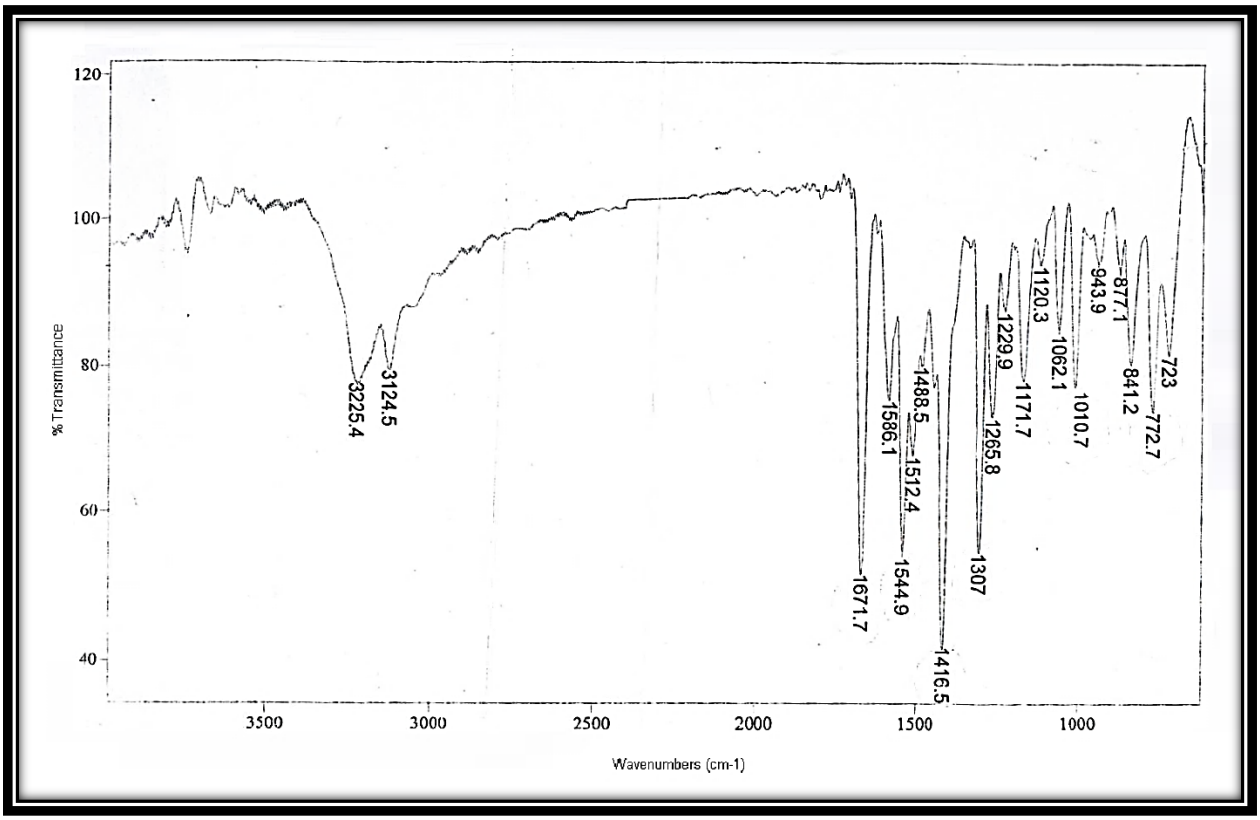


Figure S15.IR spectrum of I

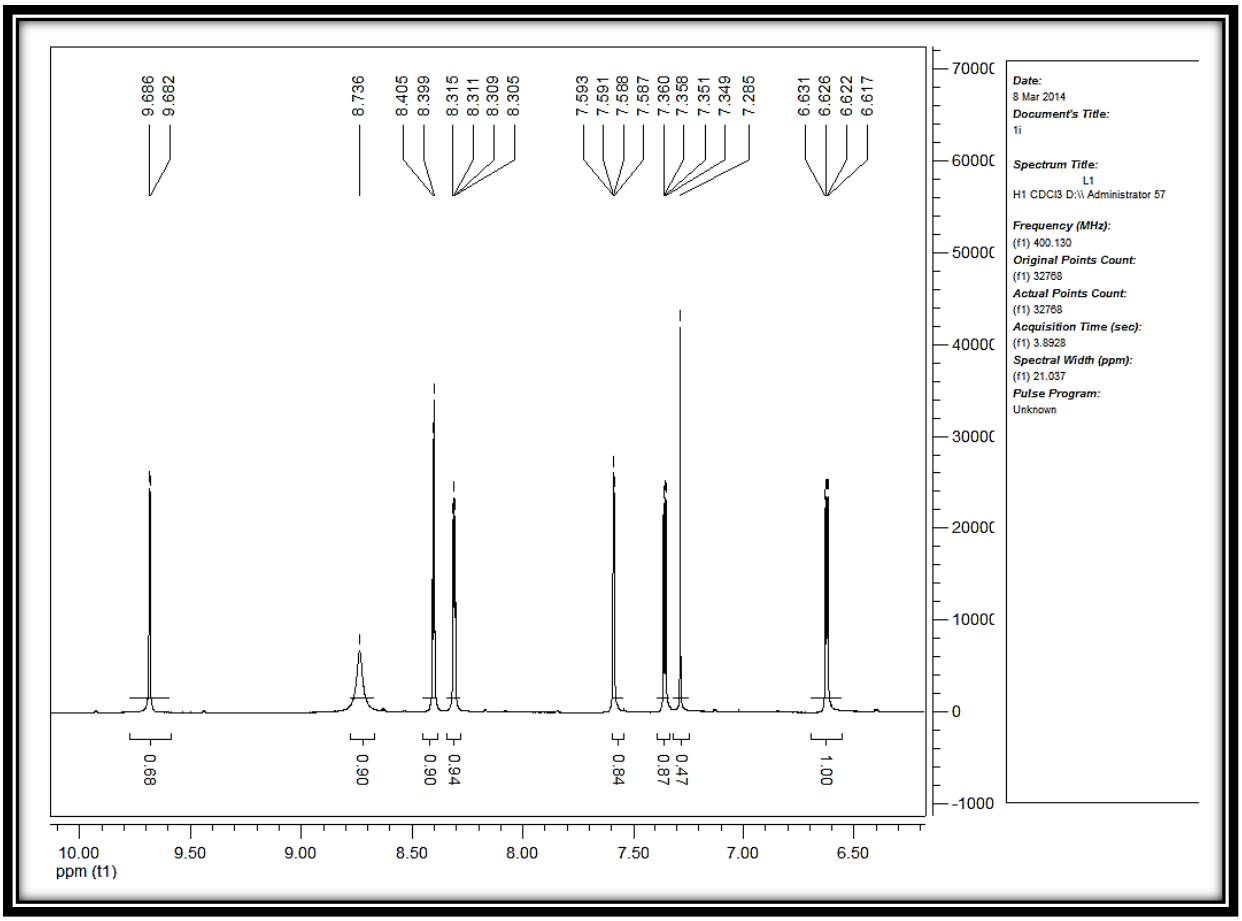


Figure S16.1H-NMR spectrum of I

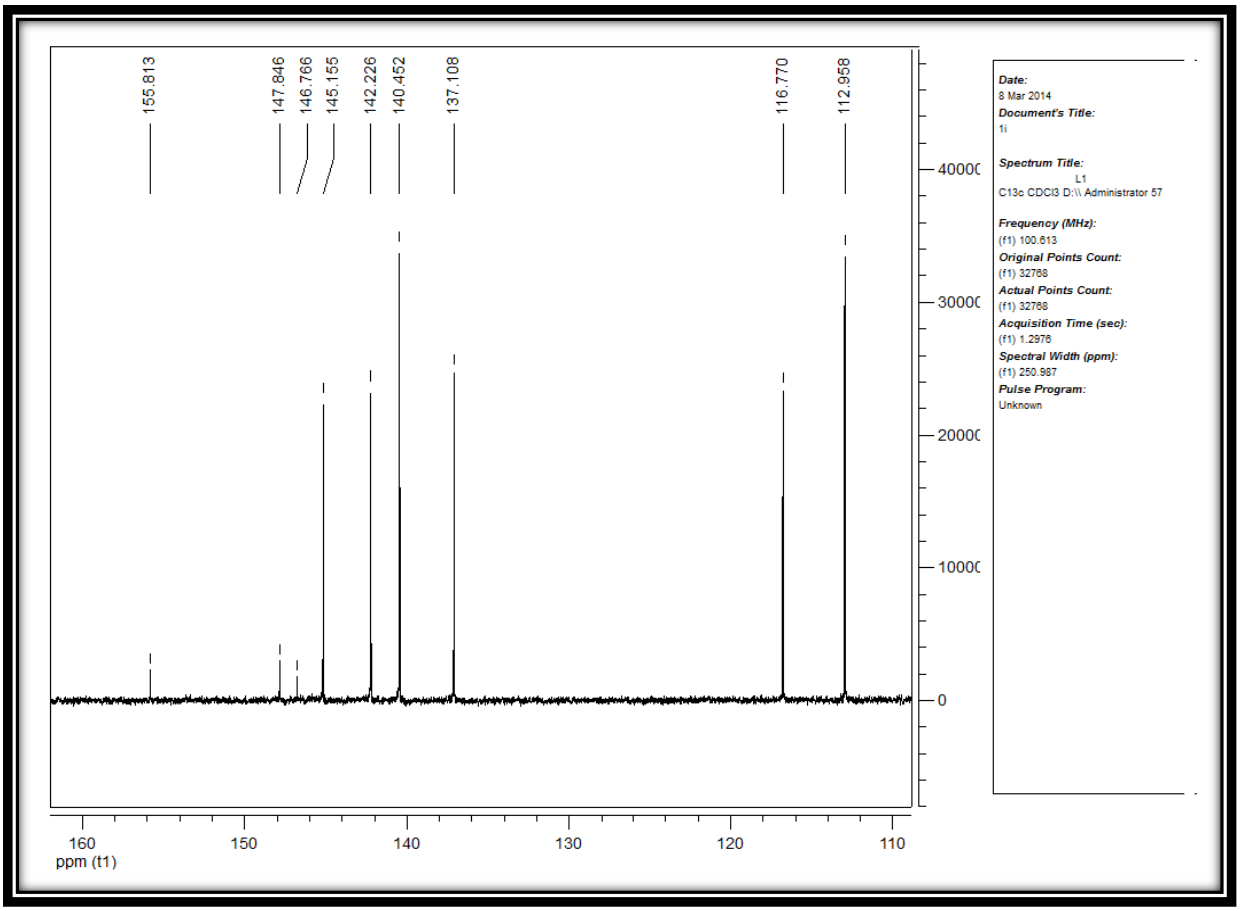


Figure S17.13C-NMR spectrum of I

6) **NMR and IR data of *II***

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.69 (s, 1*H*-pyrazine), 8.71 (s, 1*H*-Amide), 8.40 (d, J=1.6 Hz, 1*H*-pyrazine), 8.28 (s, 1*H*-pyrazine), 7.78 (dd, J=3.2, 0.8 Hz, 1*H*-thiophene), 7.66 (d, J=4.4 Hz, 1*H*-thiophene), 7.18 (d, J=4.4 Hz, 1*H*-thiophene). ^{13}C NMR (100.61 MHz, $CDCl_3$): δ 159.93 (C=O), 148.15 (C6-pyrazine), 141.99 (C4-furan), 140.31 (C9-pyrazine), 137.92 (C7-pyrazine), 137.39 (C8-pyrazine), 132.42 (C3-furan), 129.73 (C1-furan), 128.19 (C2-furan) .Selected IR bands (KBr pellet, cm^{-1}): 3215 (b), 3084 (b), 1653 (s), 1536 (s), 1411 (s), 1299 (s), 735 (b).

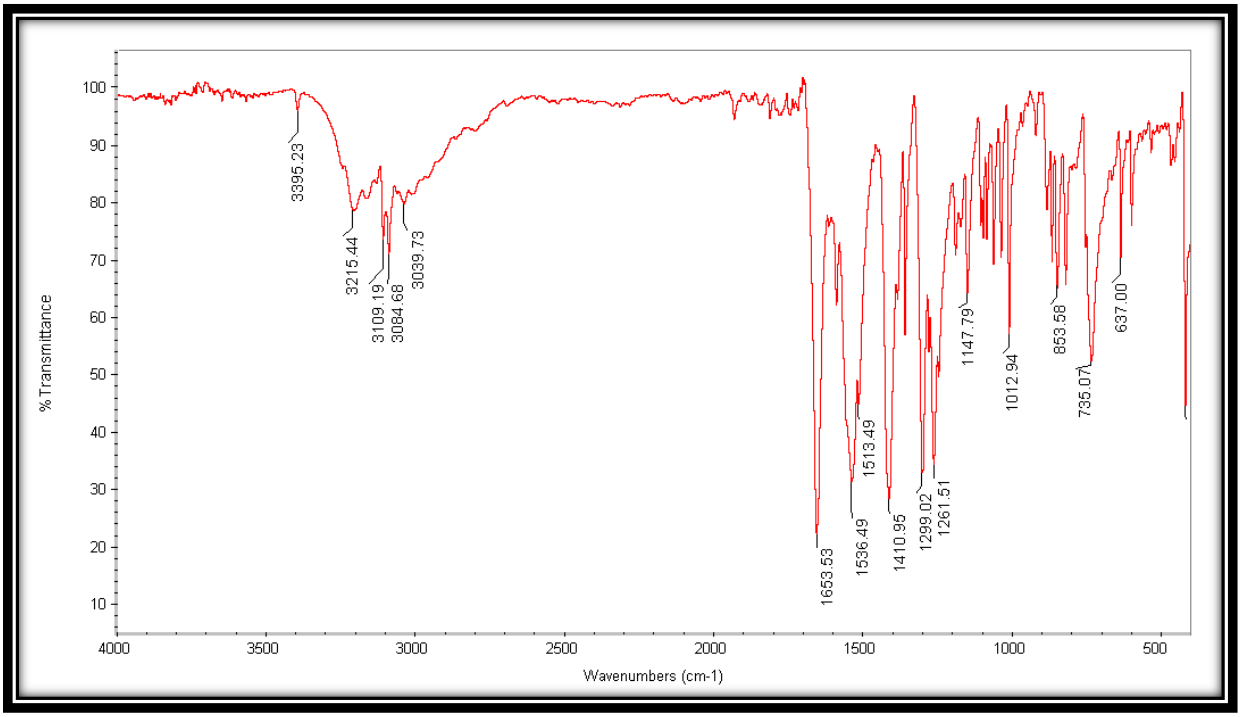


Figure S18.IR spectrum of II

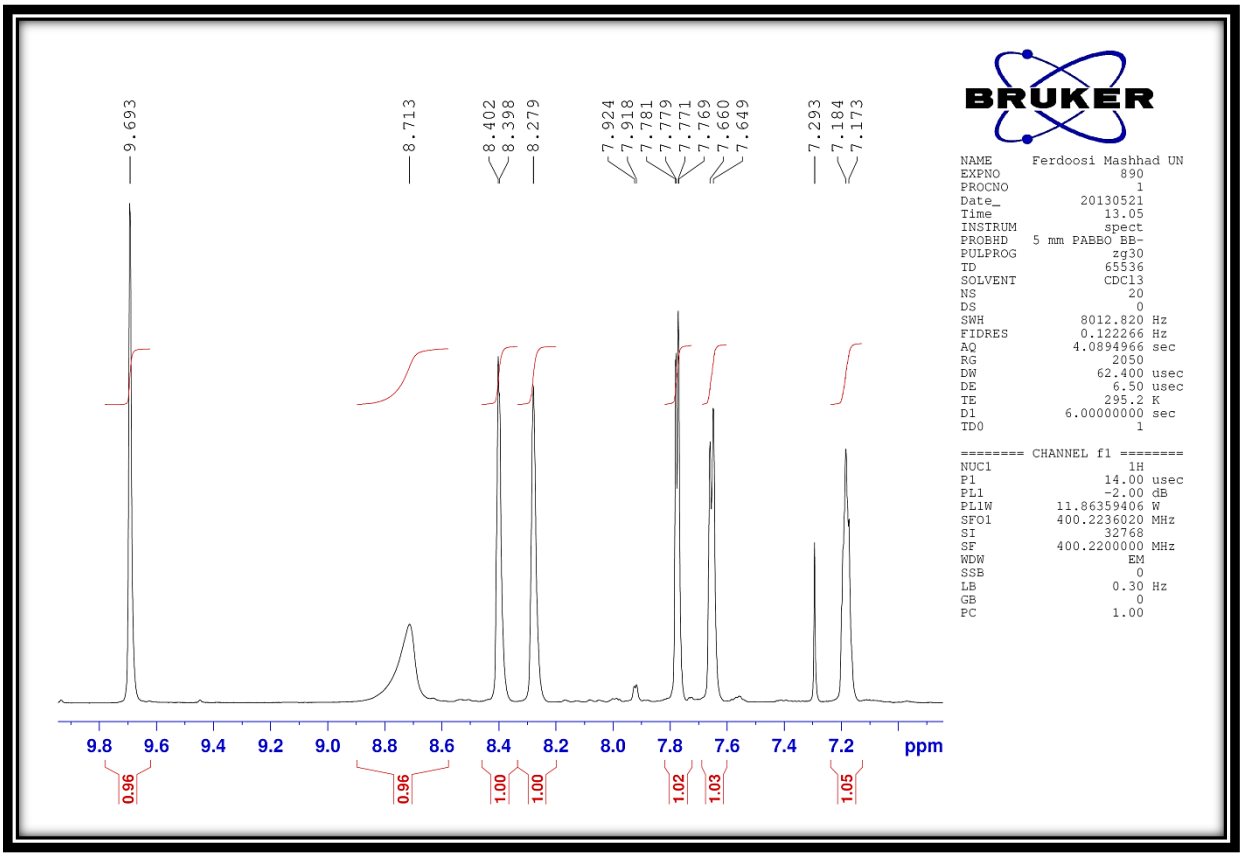


Figure S19.1H-NMR spectrum of II

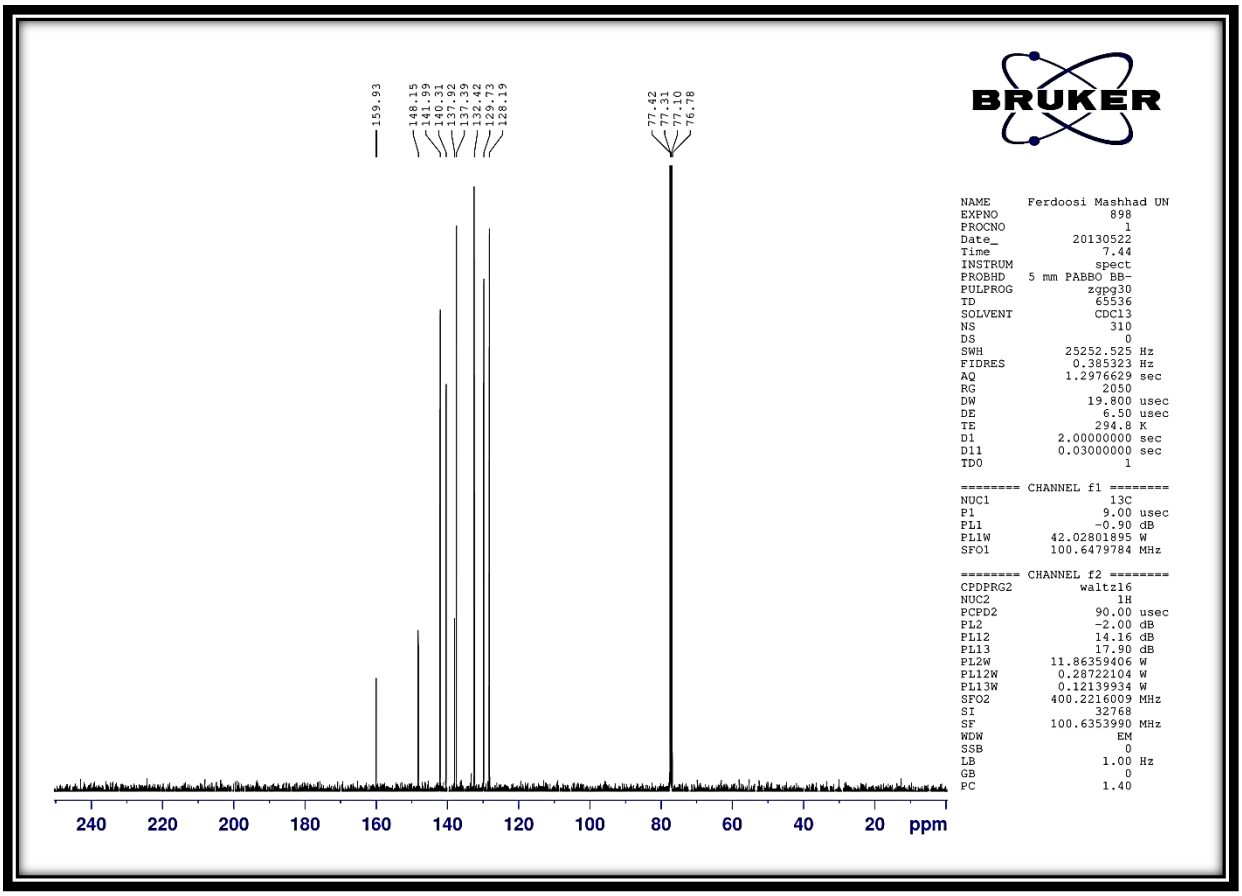


Figure S20.13C-NMR spectrum of II

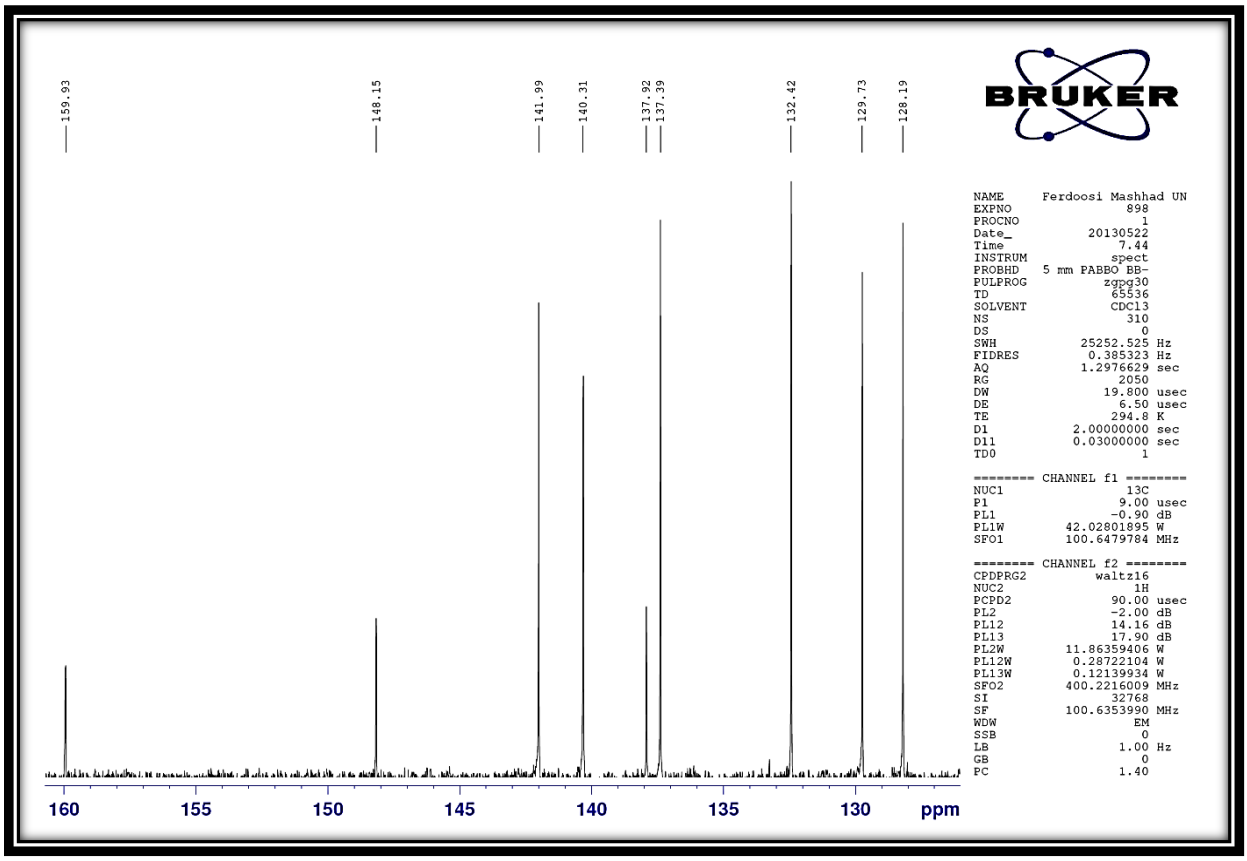


Figure S20.Extended 13C-NMR spectrum of II

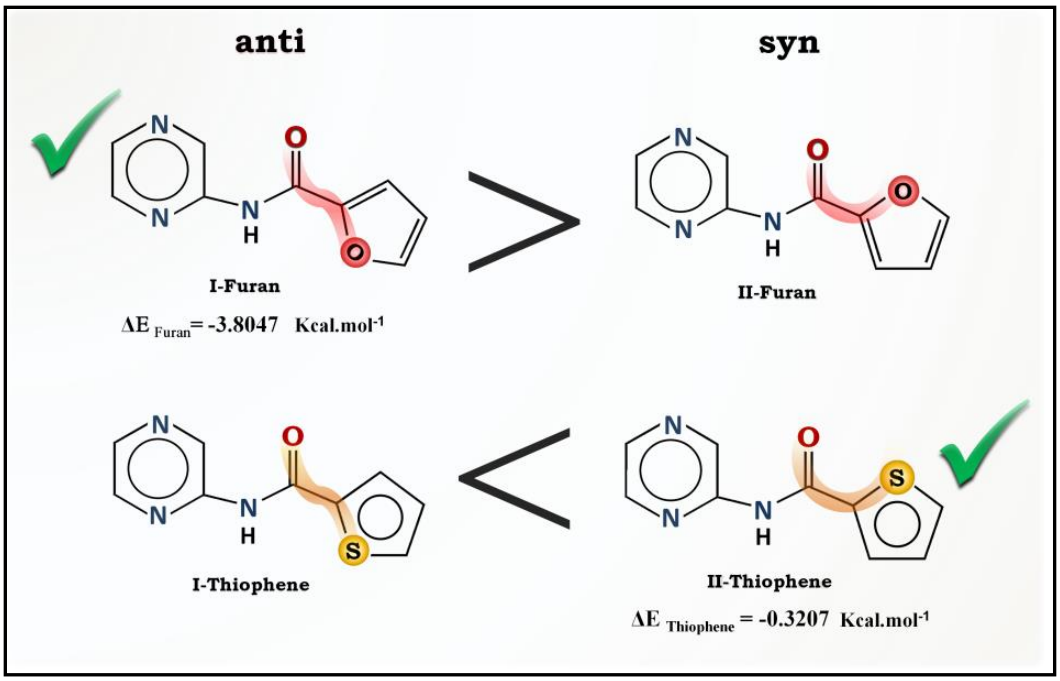
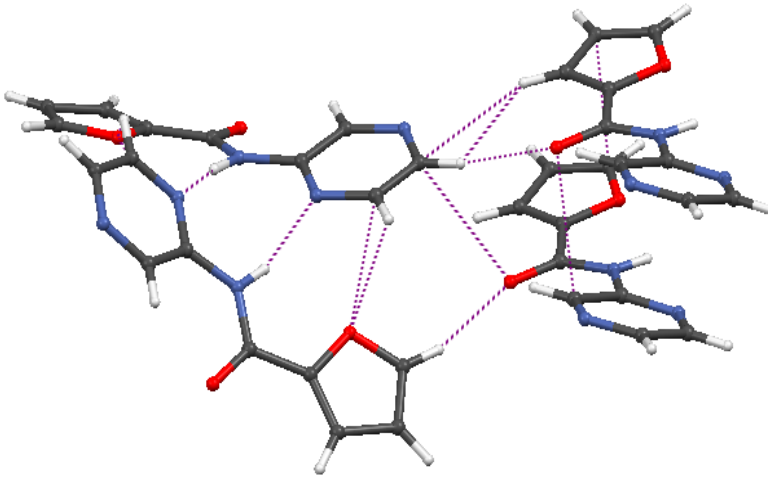
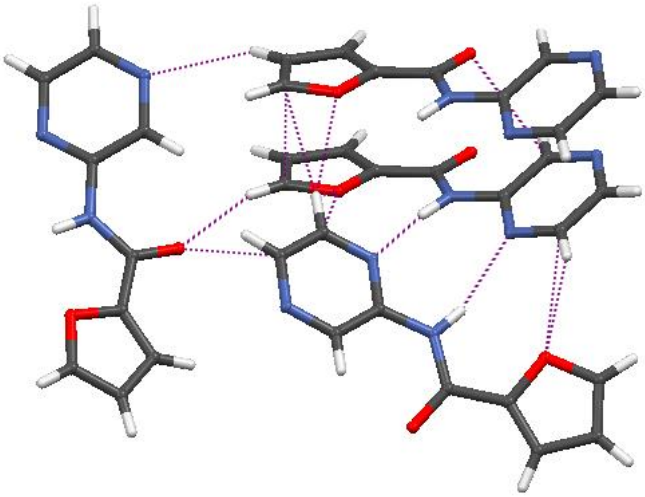


Figure S21. Independent view of titled compounds by two probable conformations for five-membered heterocyclic rings. The agreement with experimental result has been presented by thick mark.

Tet 1



Tet 1



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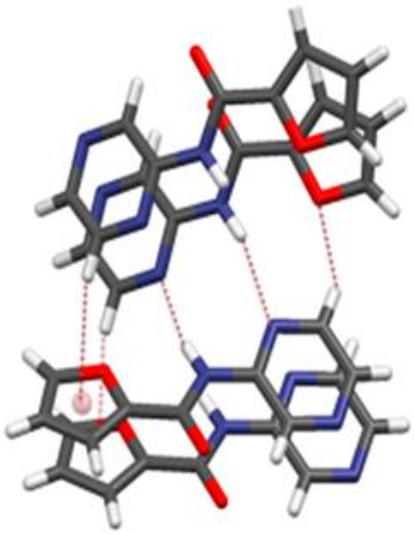

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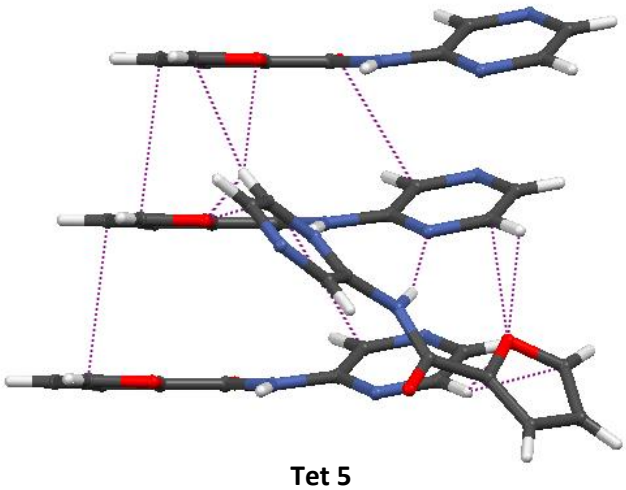

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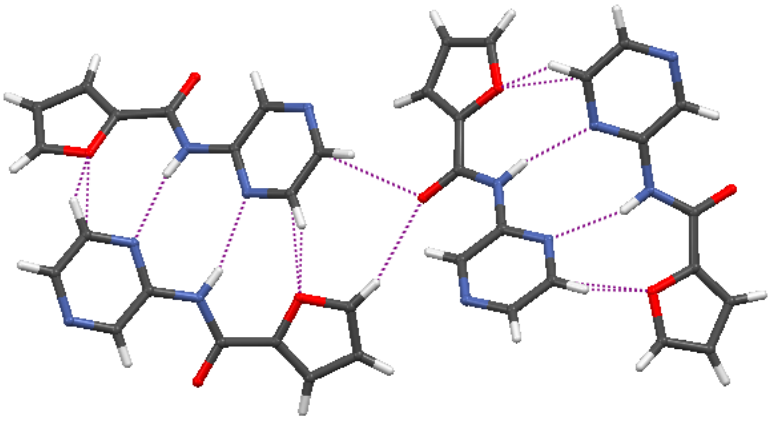

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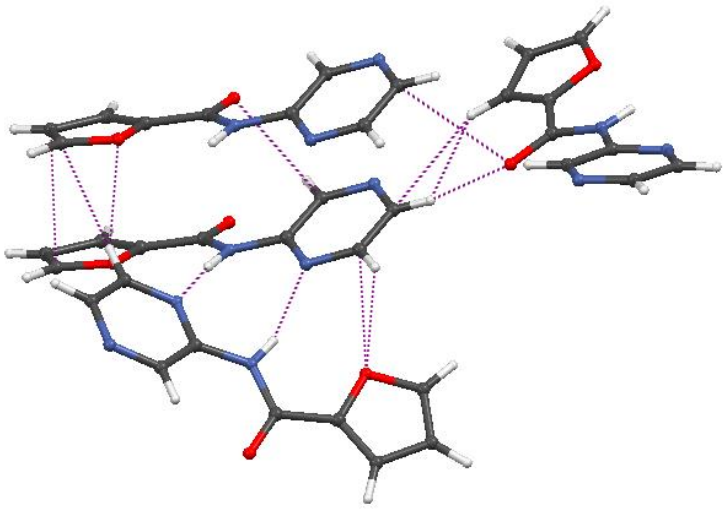

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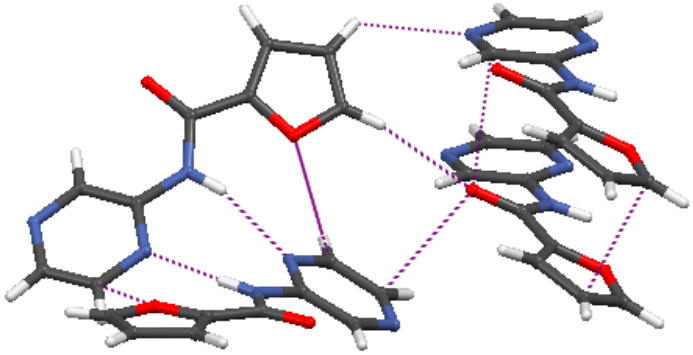
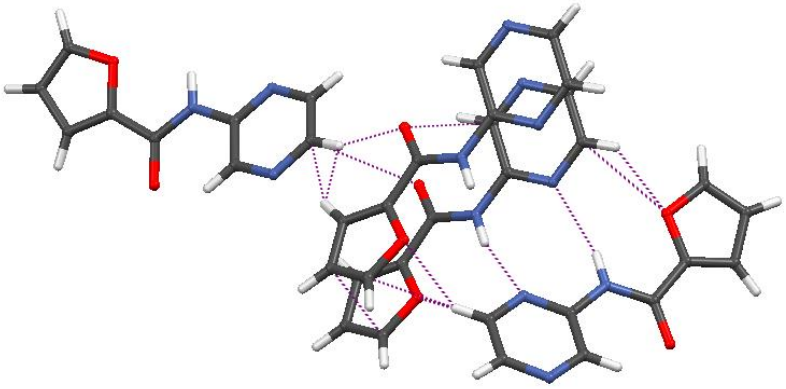


Tet 8



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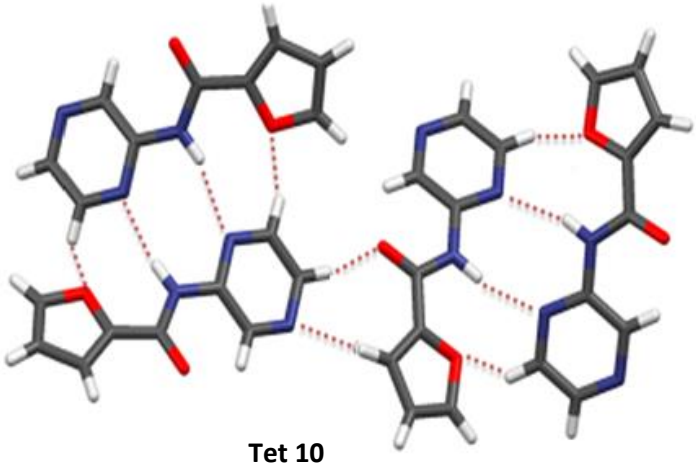

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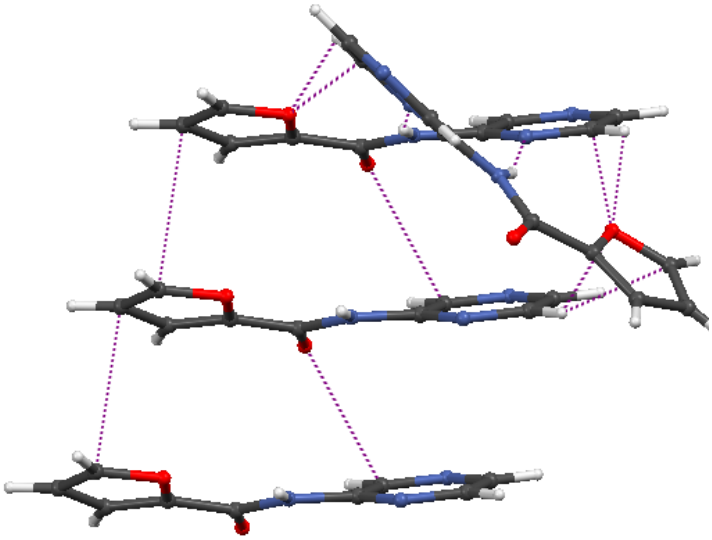

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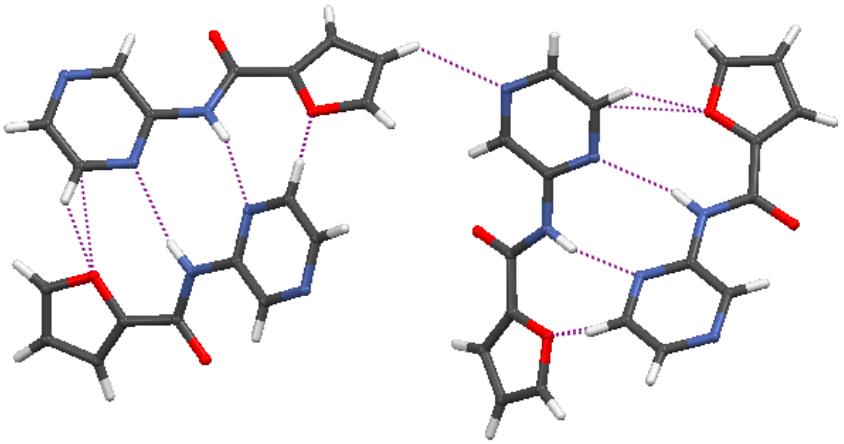
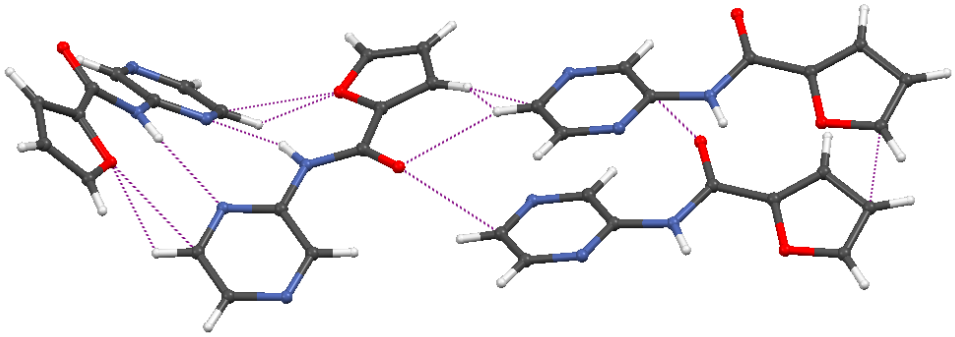


Tet 12



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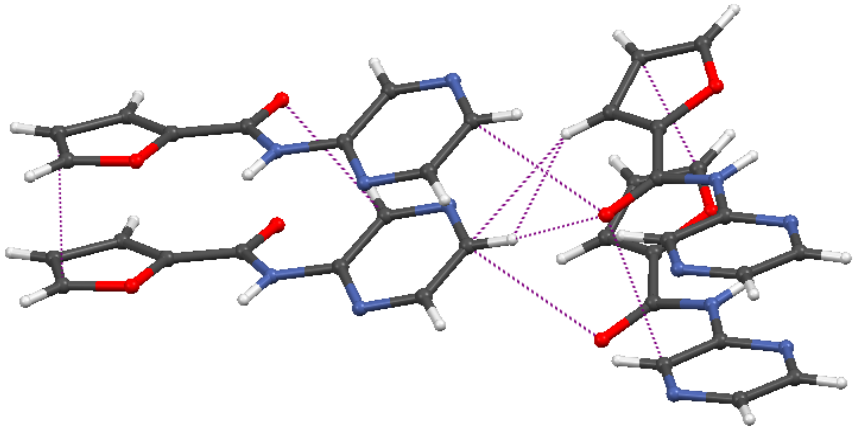
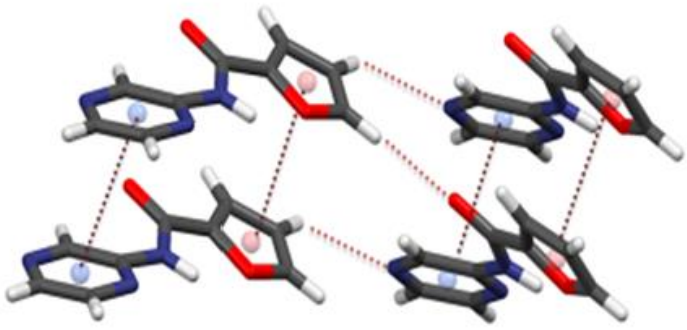


Tet 14



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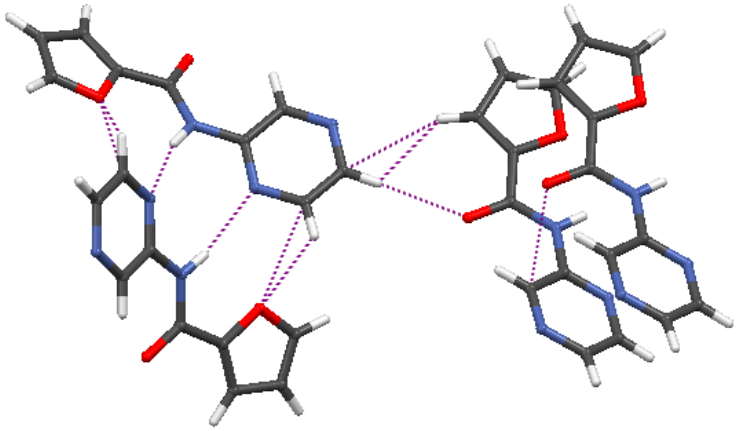

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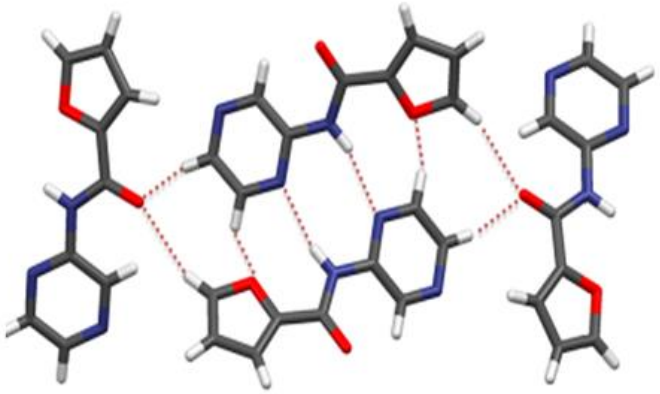

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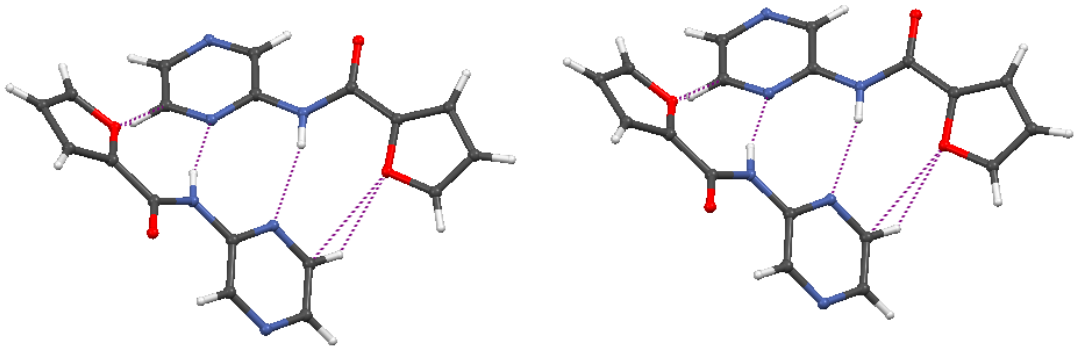

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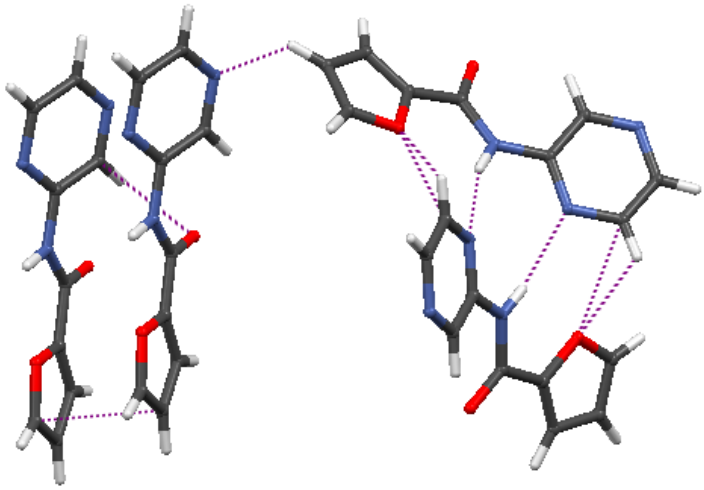

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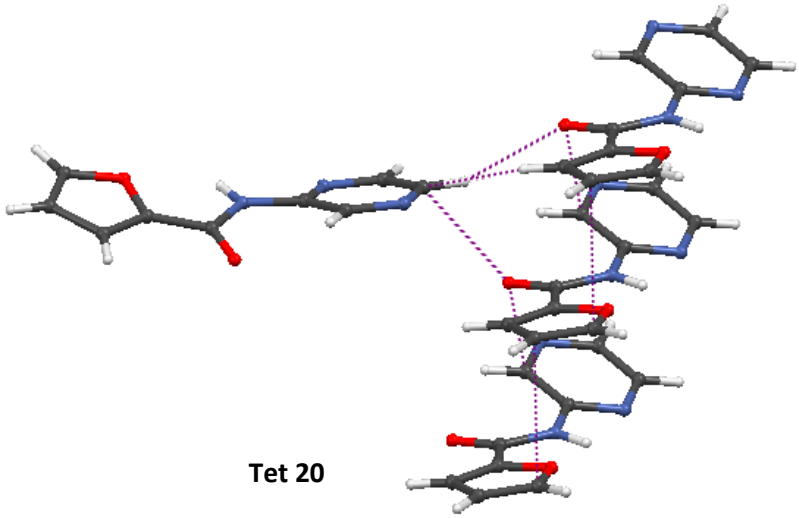

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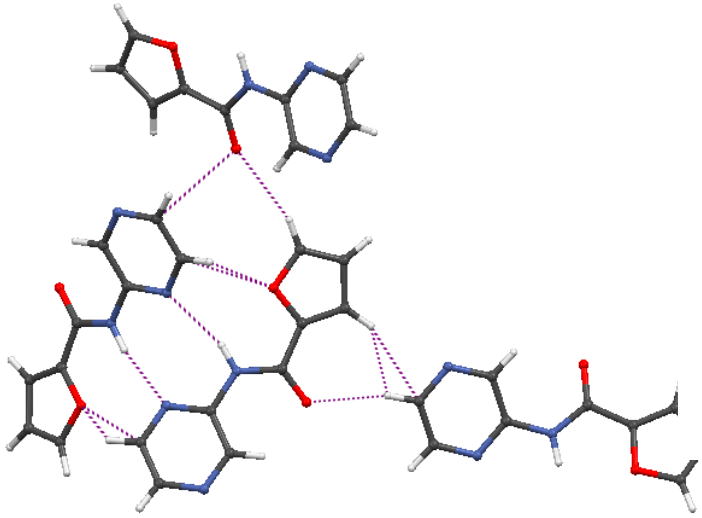

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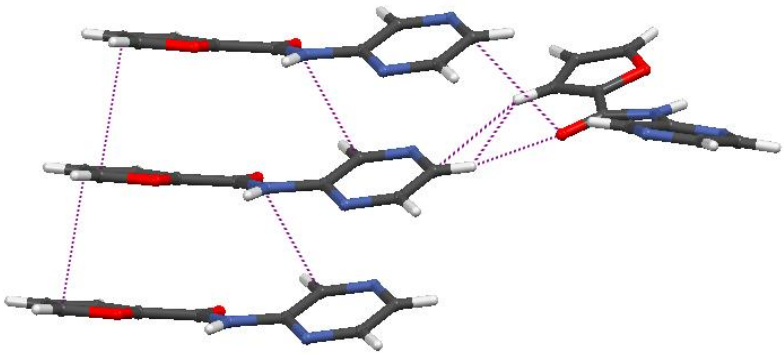

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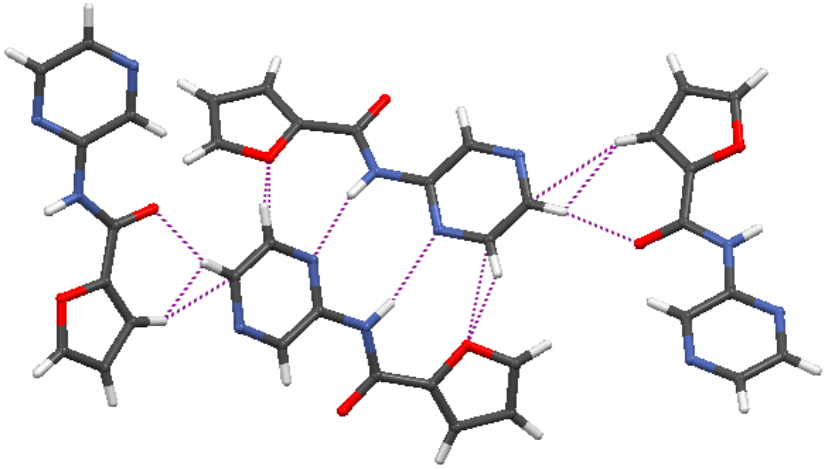

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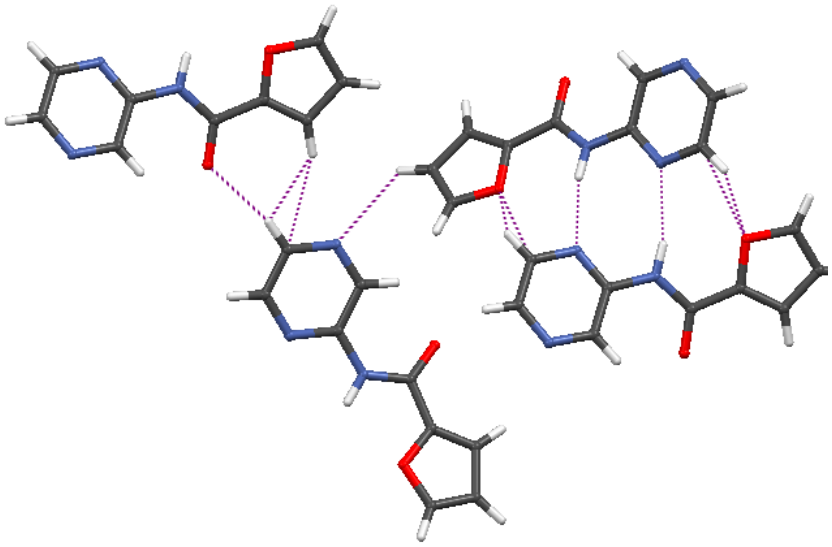

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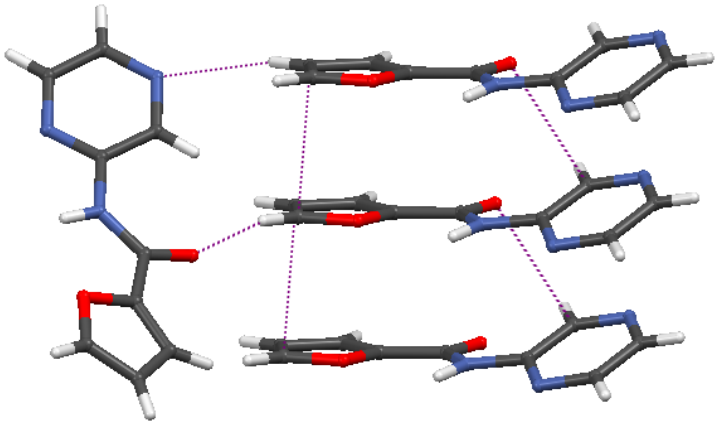

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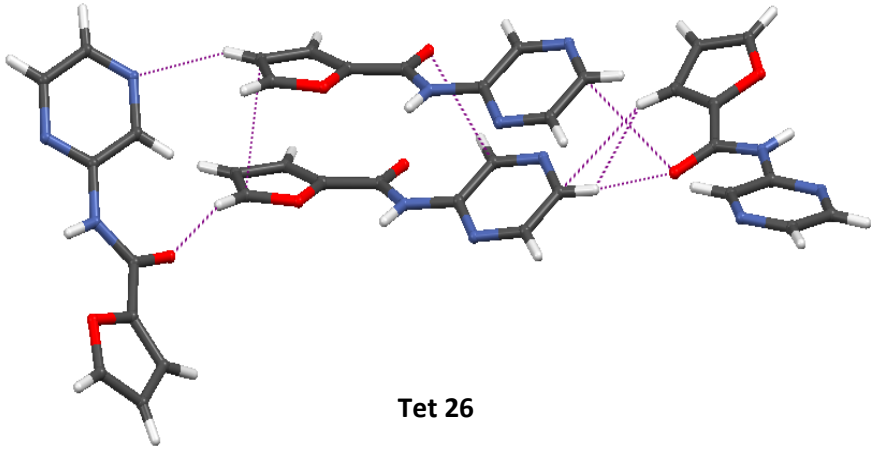

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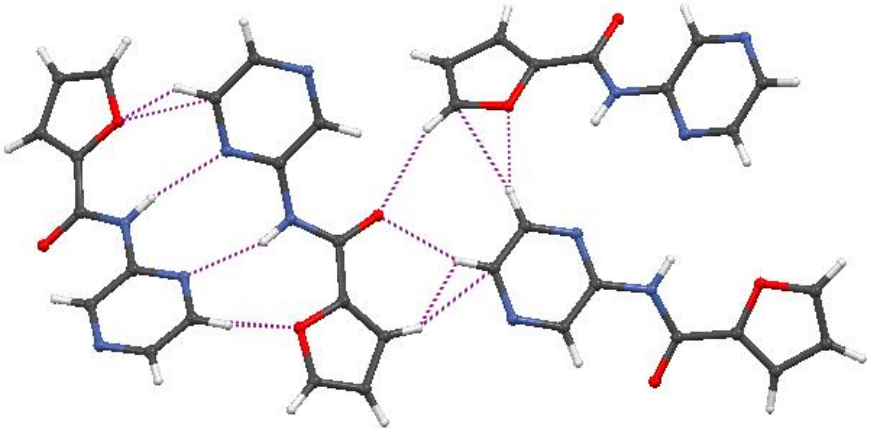

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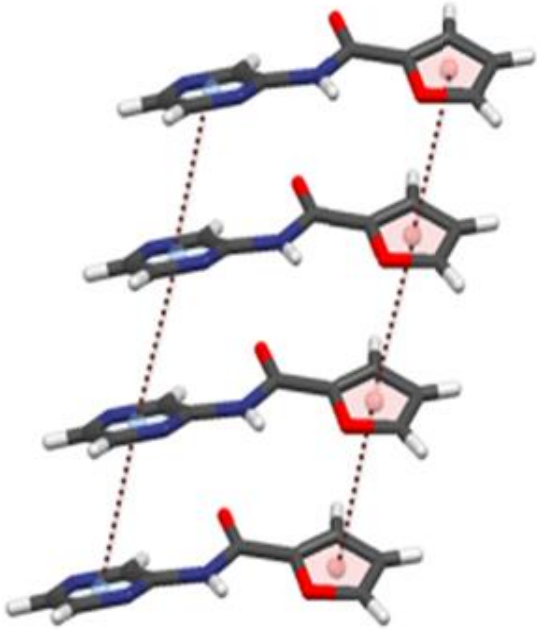

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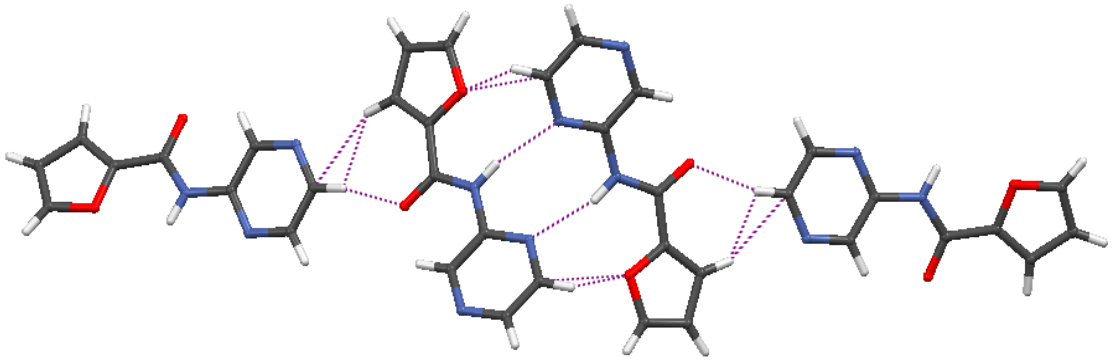

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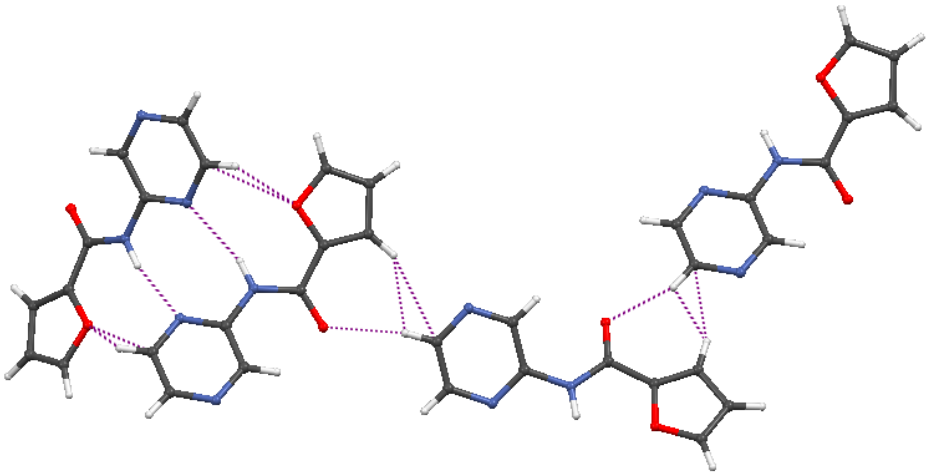

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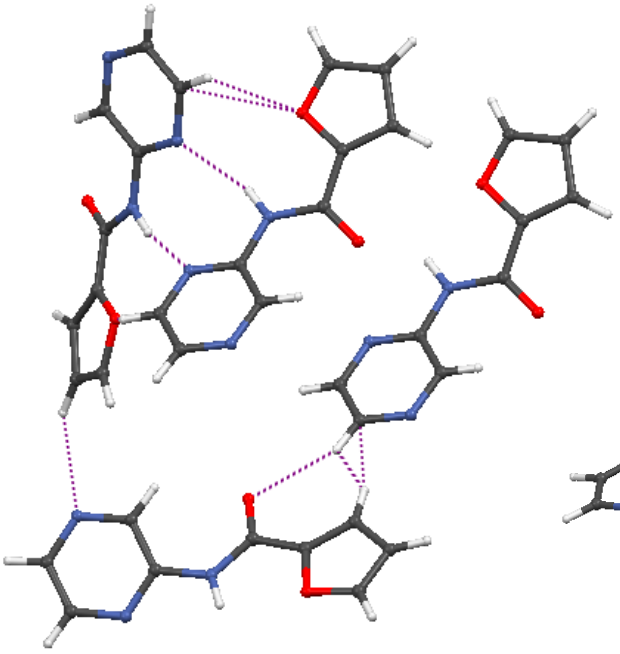

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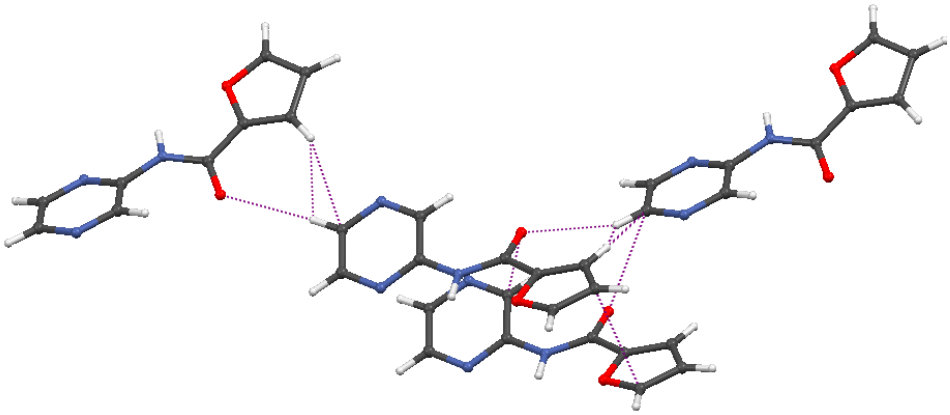

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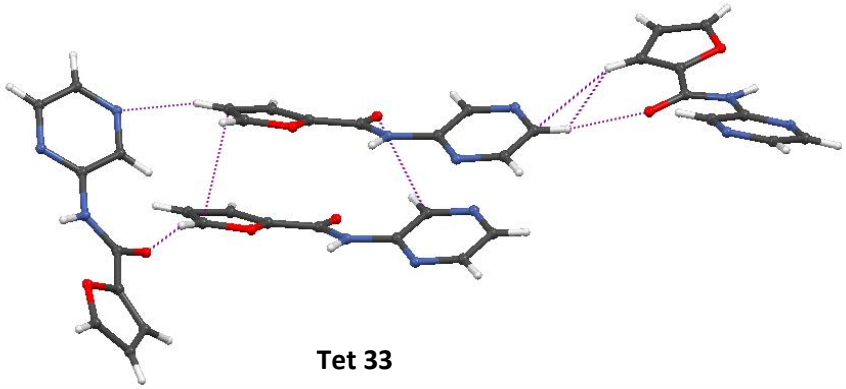

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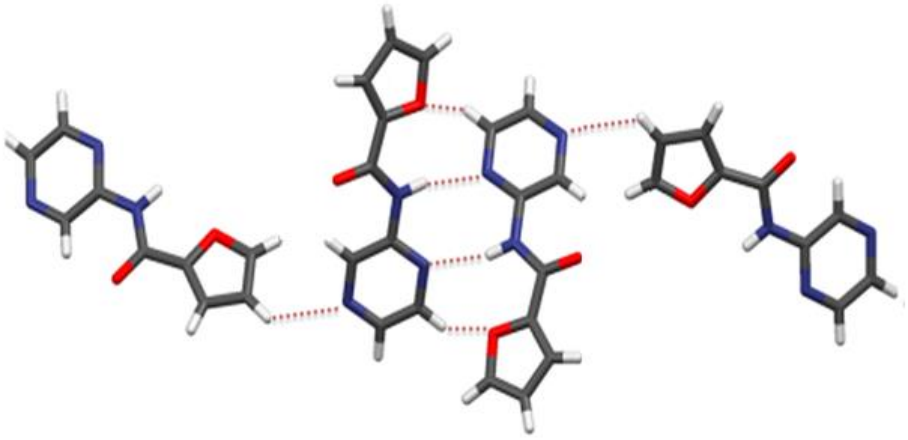

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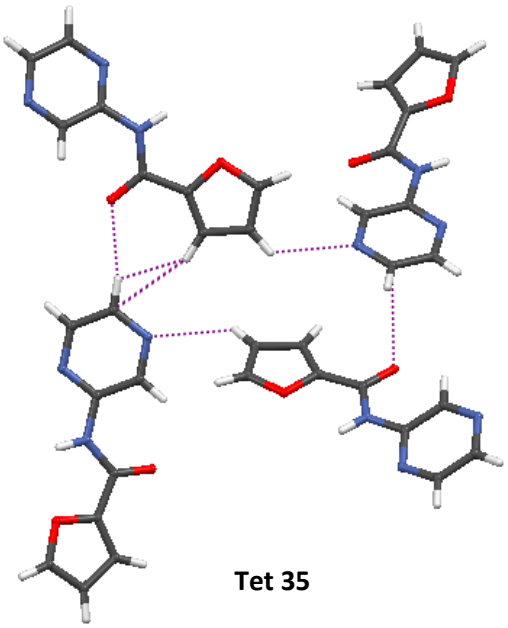

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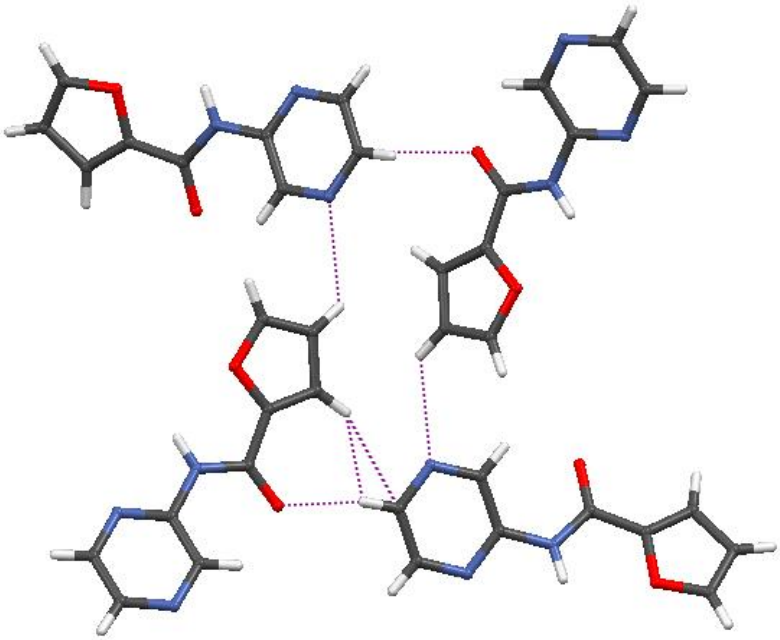

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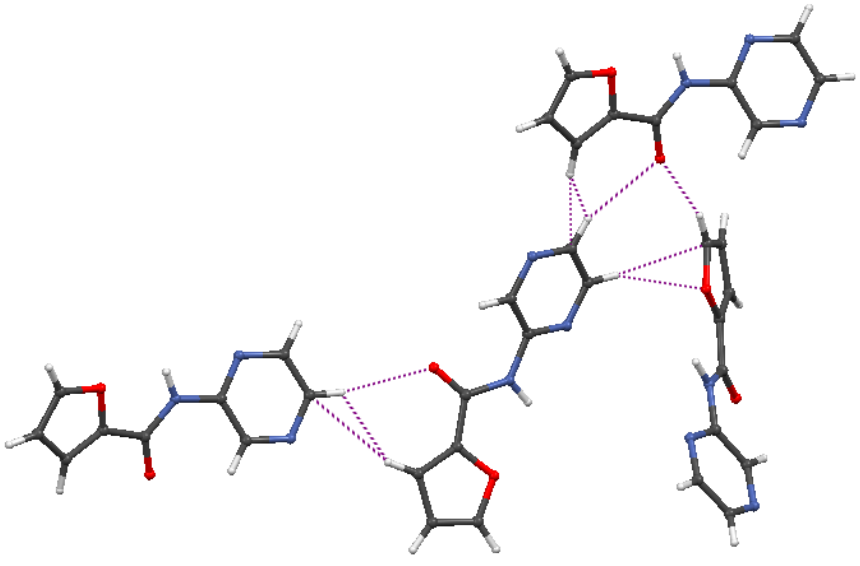

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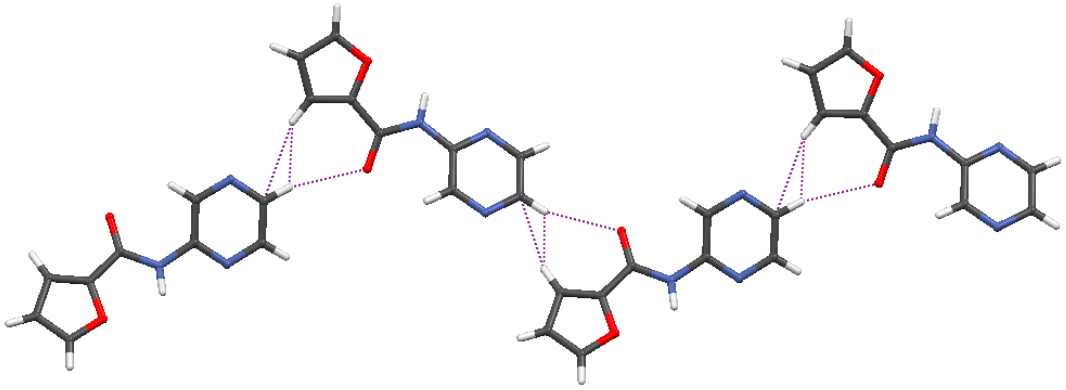

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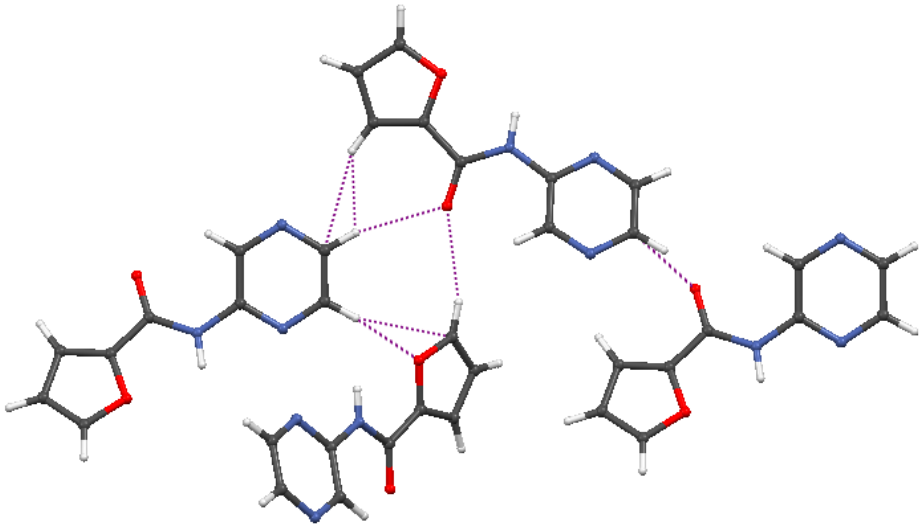

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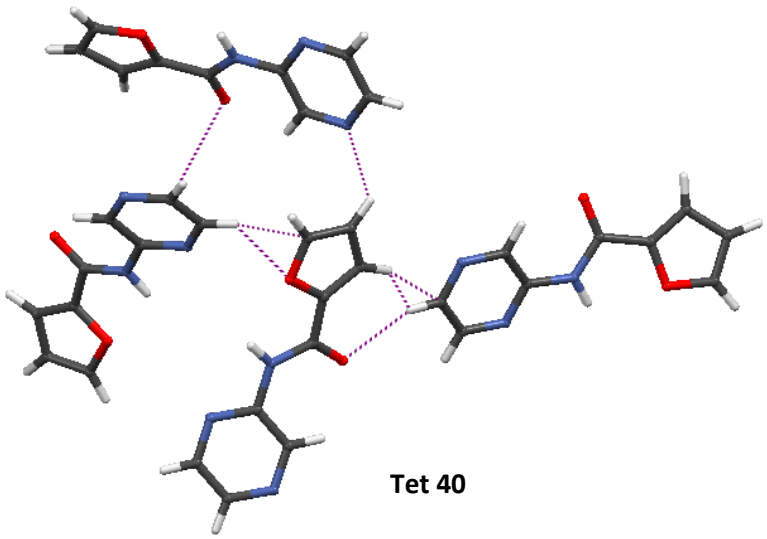
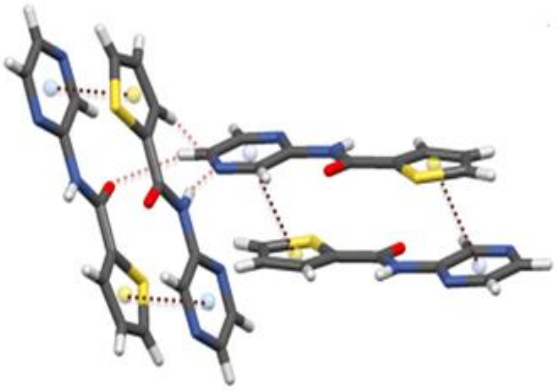


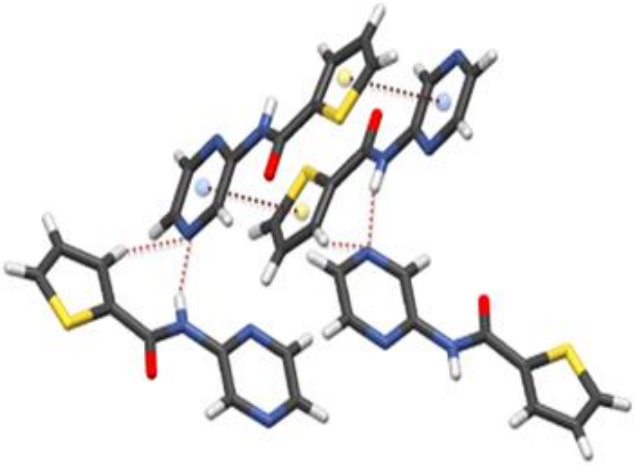
Tet 40

Figure S22.Representation of the most stable tetramer motifs of I which are labeled based on the interaction energy ranking



Tet1

Tet2



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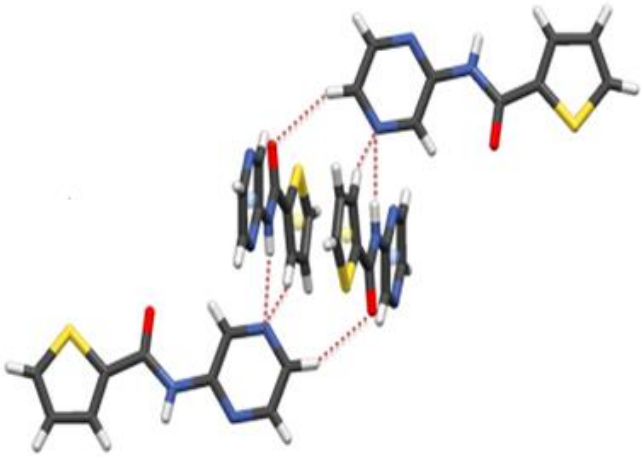

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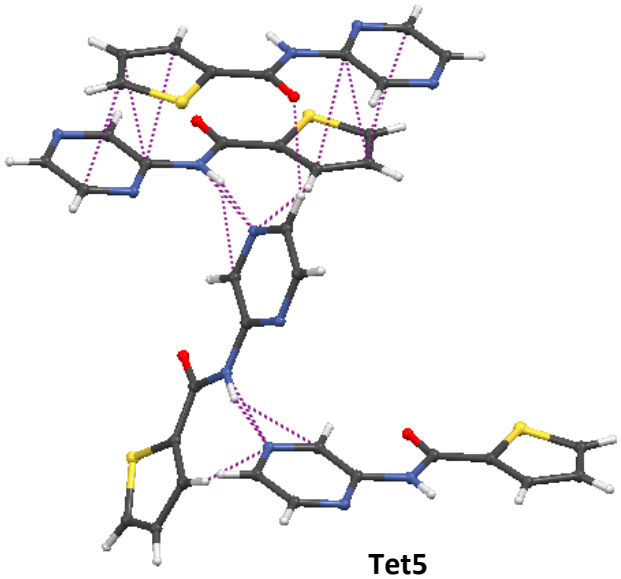

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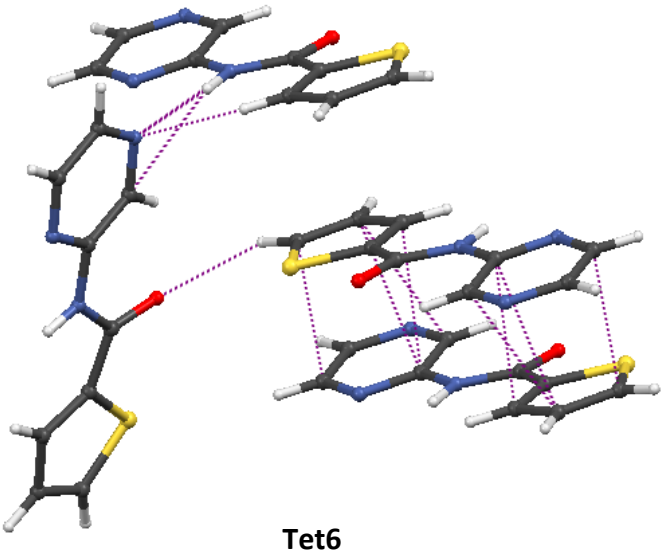

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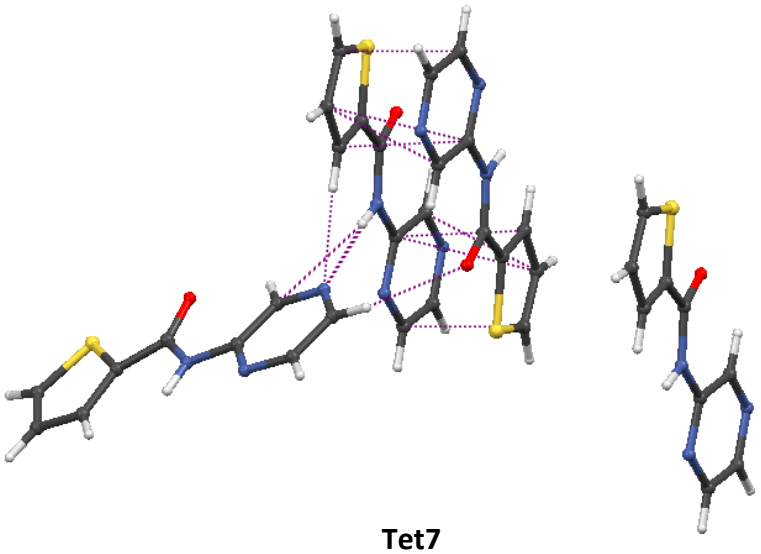

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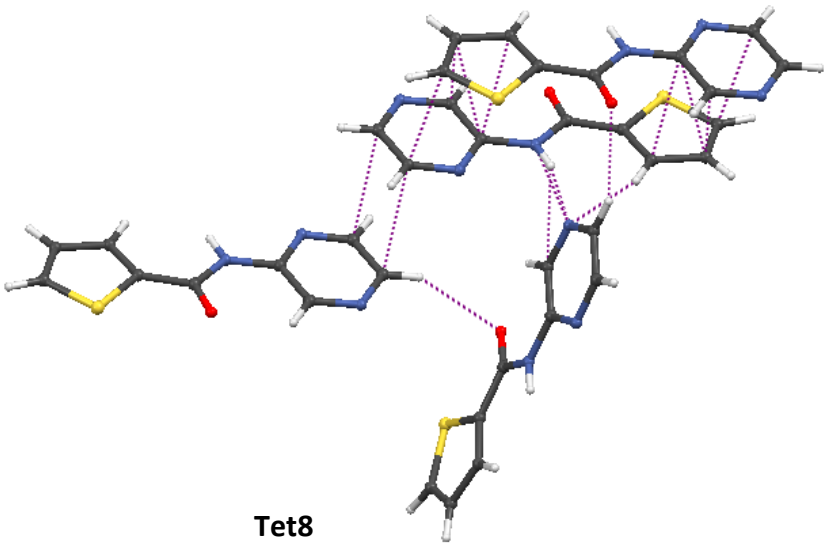

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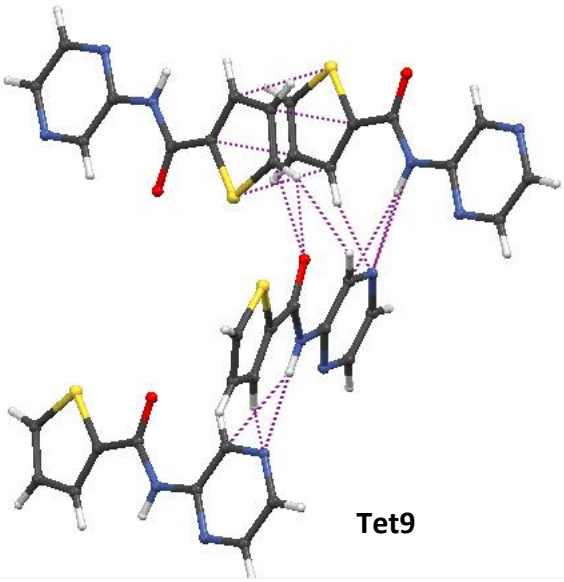

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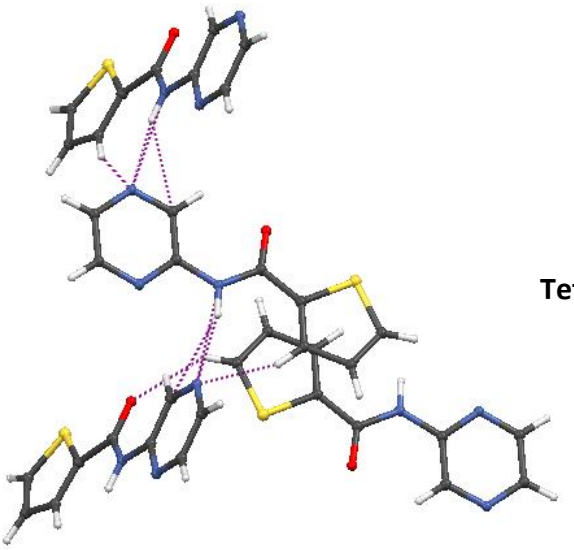

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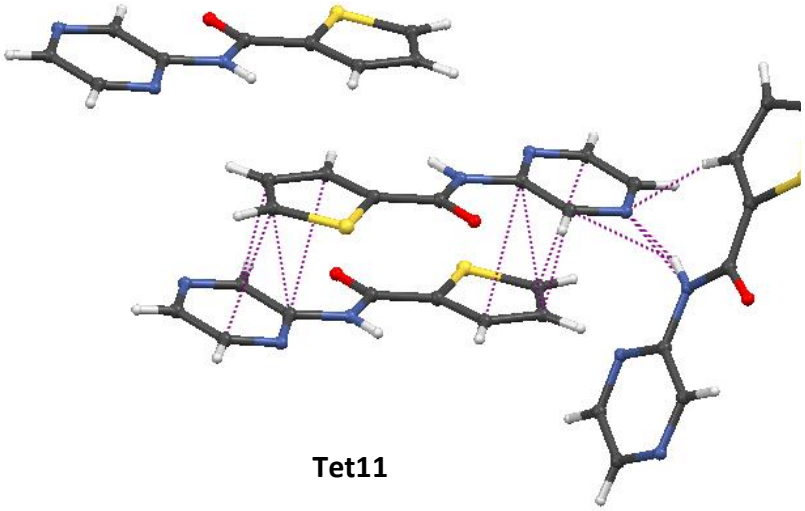

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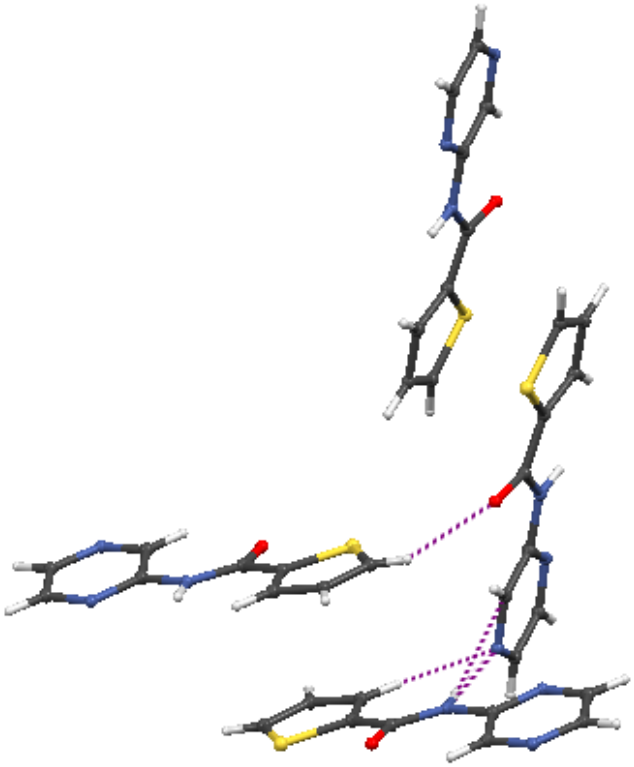

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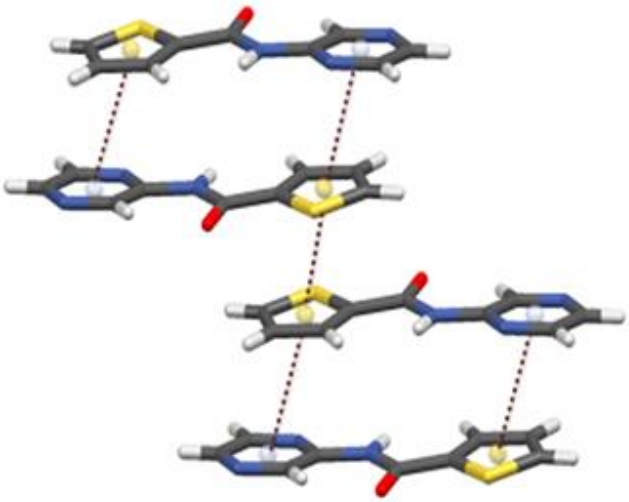

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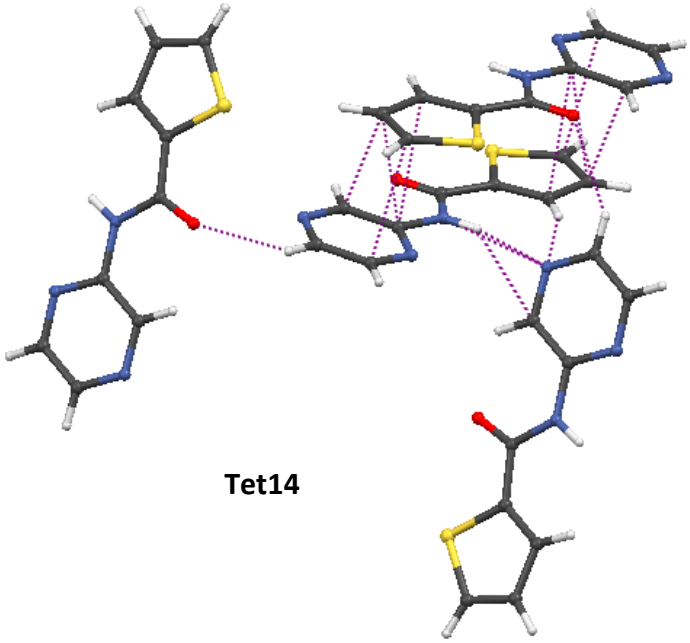

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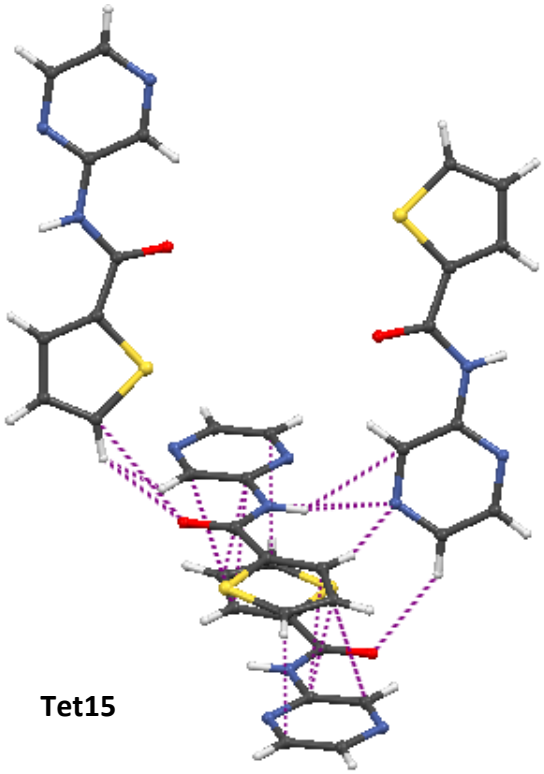

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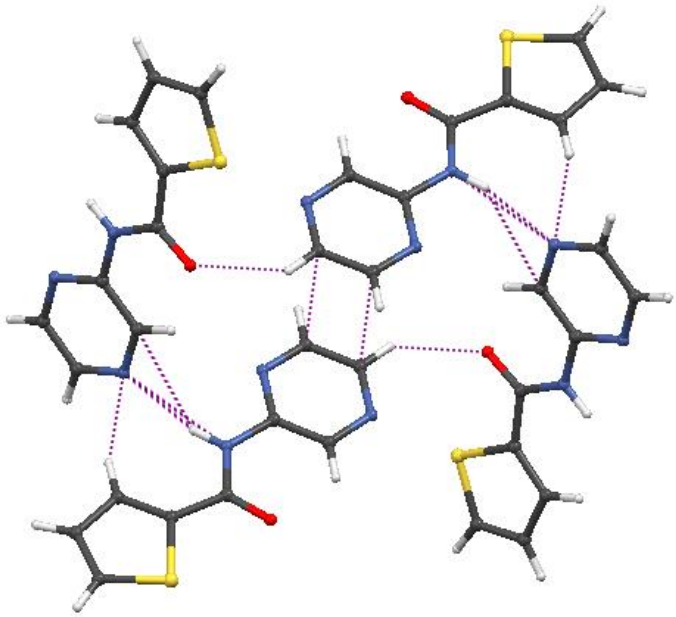

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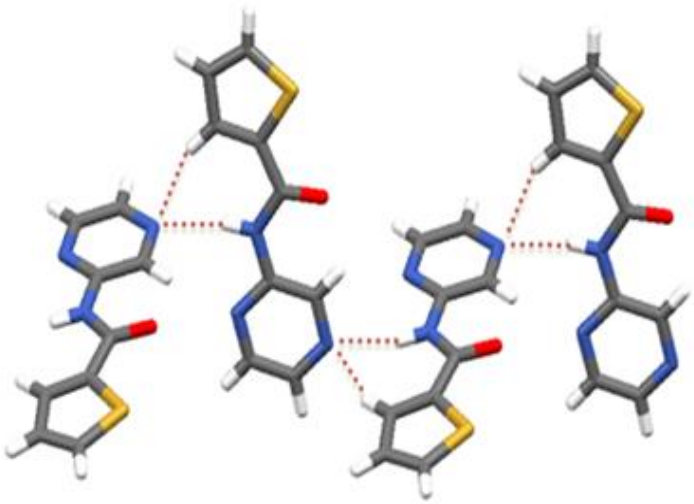

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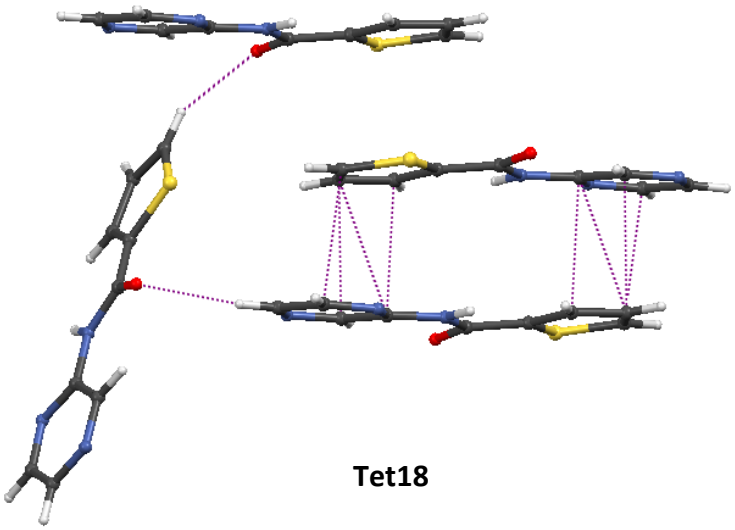

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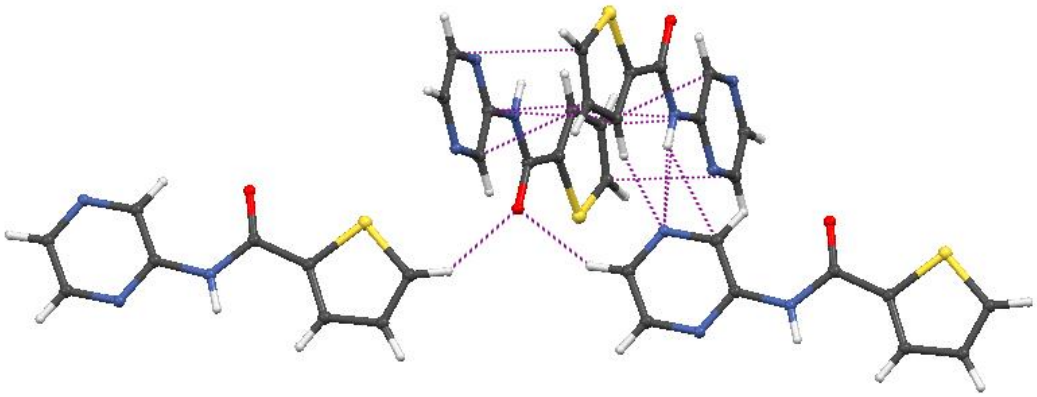

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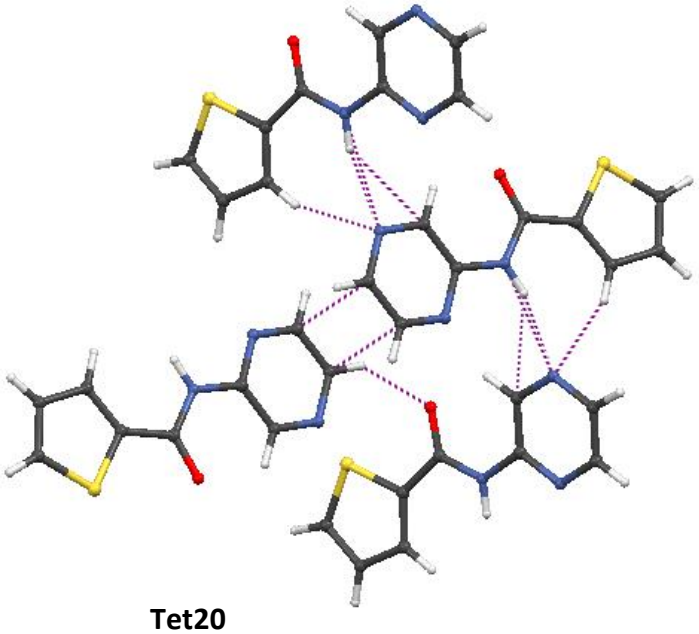

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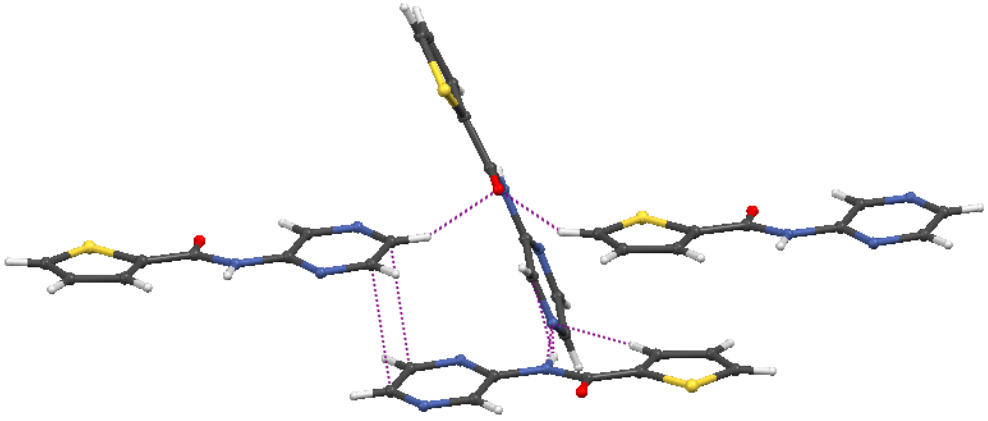

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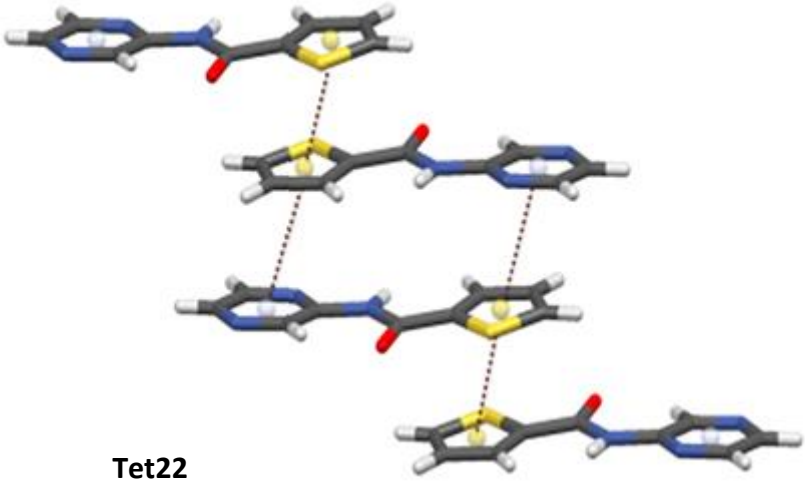

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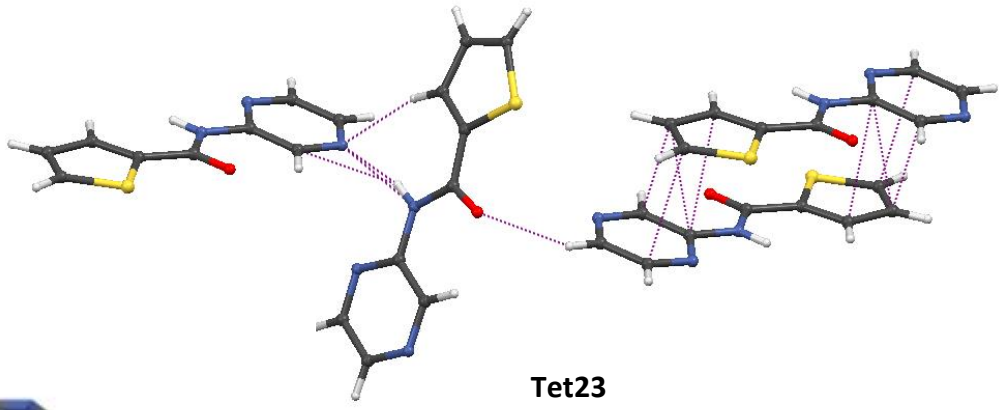

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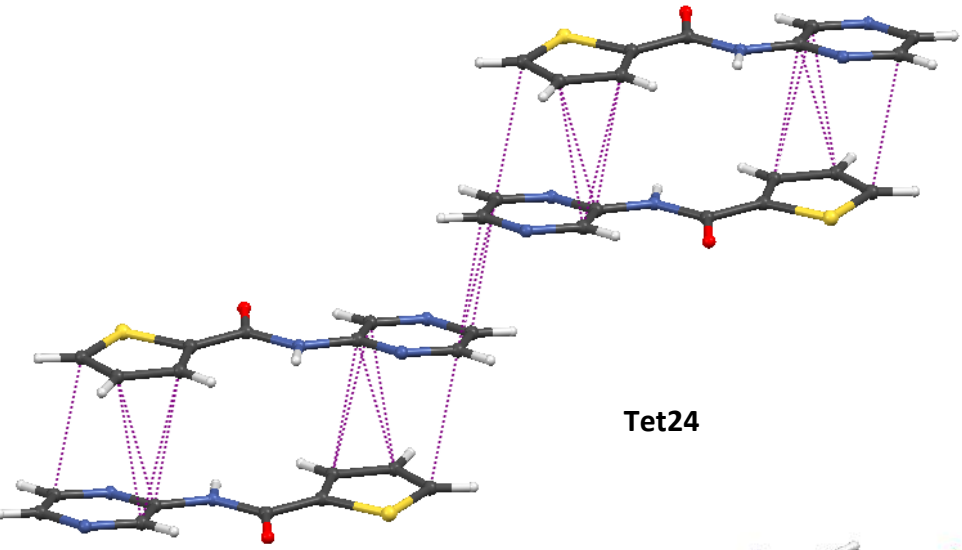

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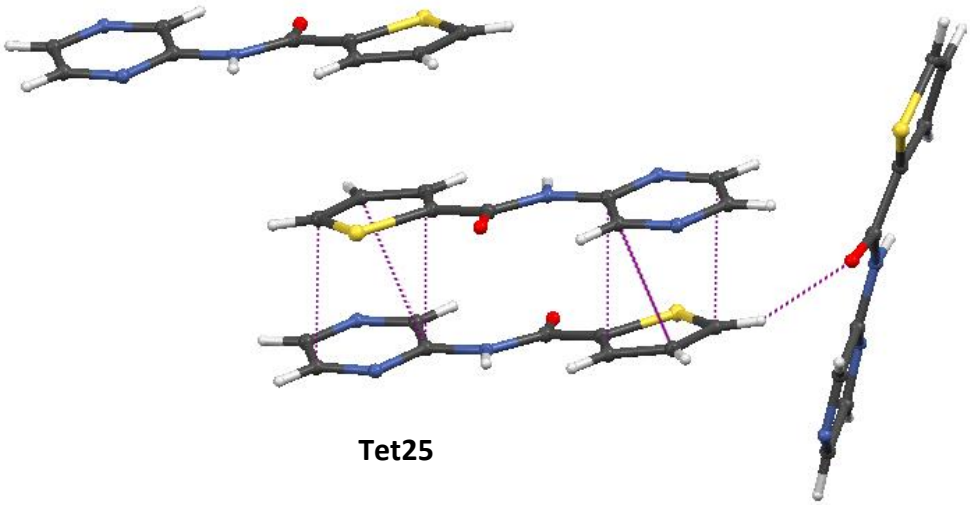

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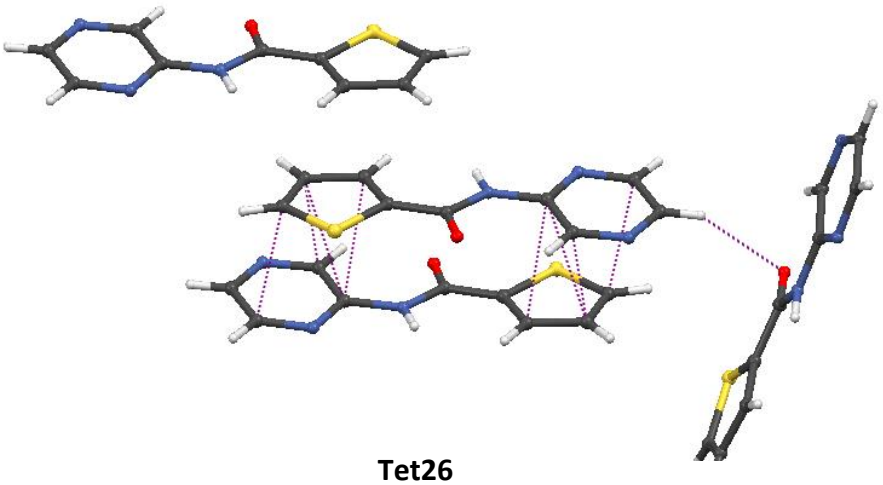

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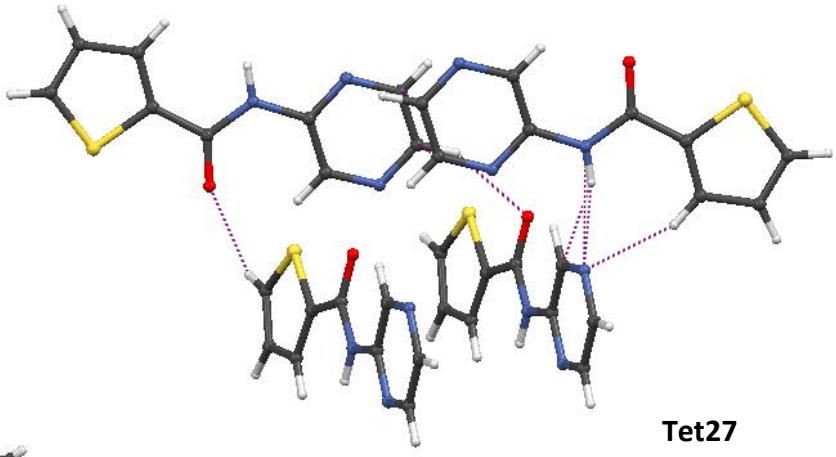

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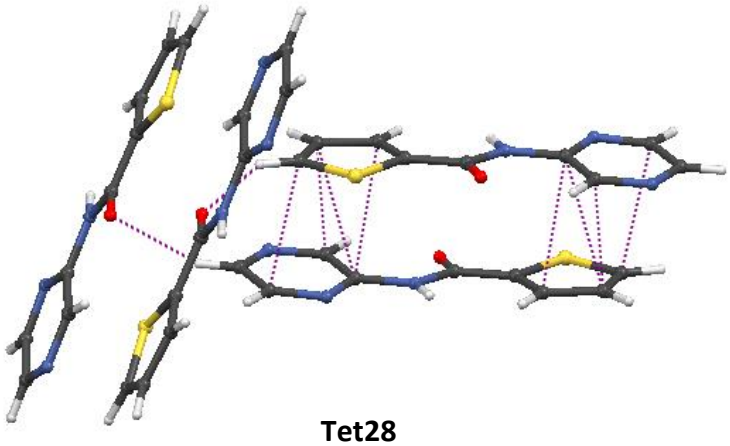

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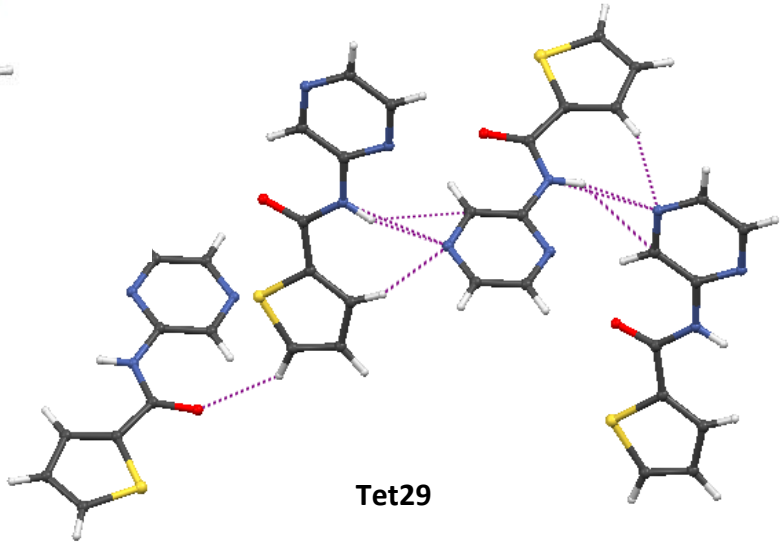

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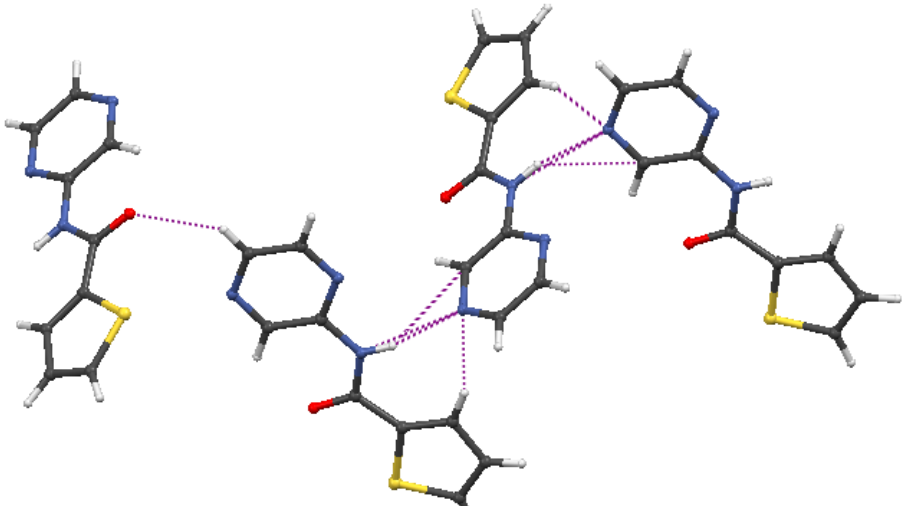

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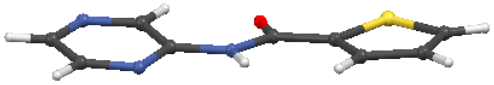

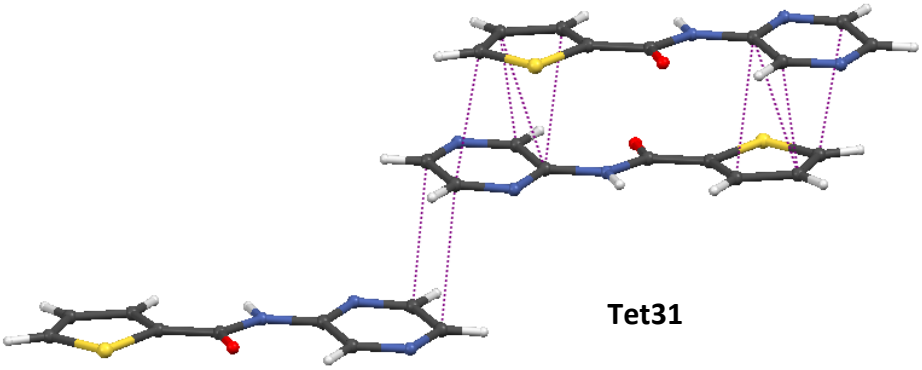

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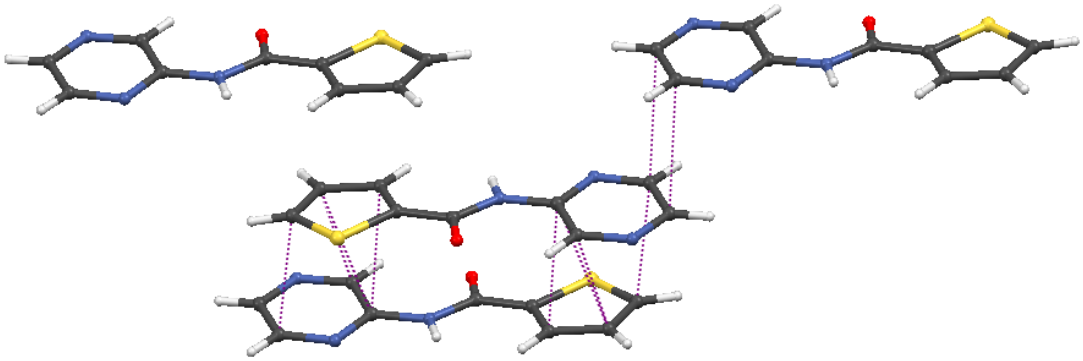
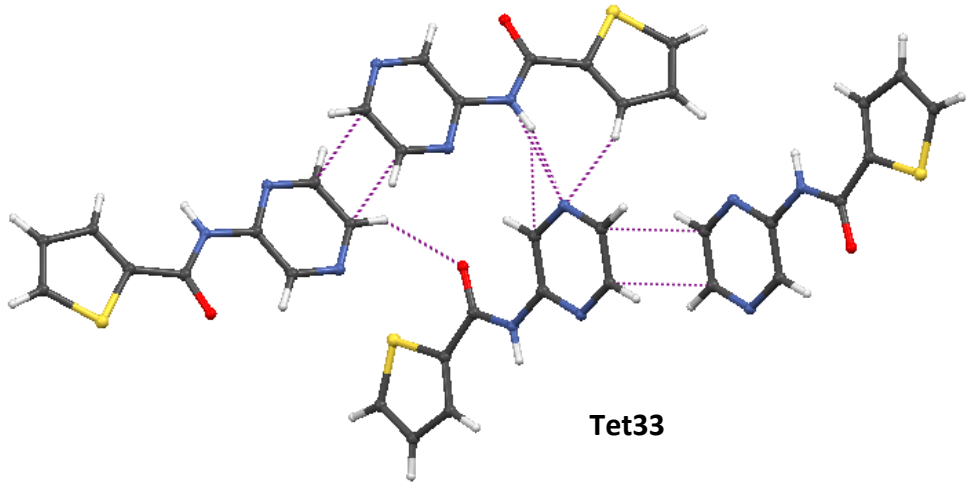


Tet32



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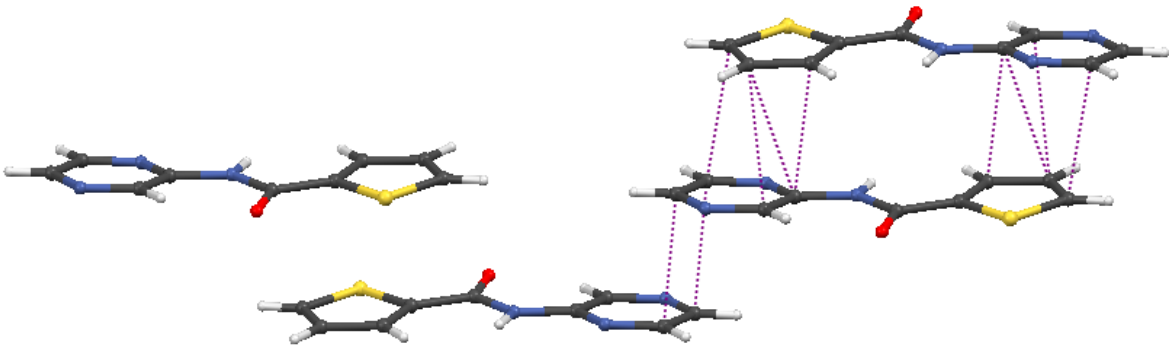

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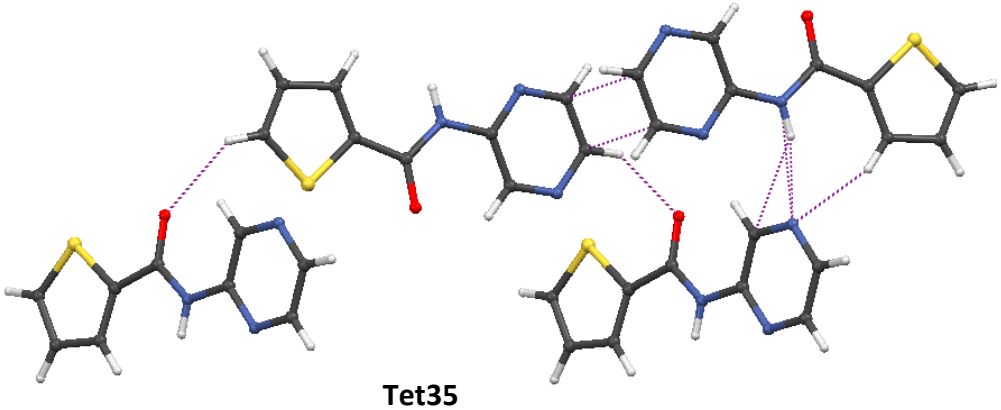

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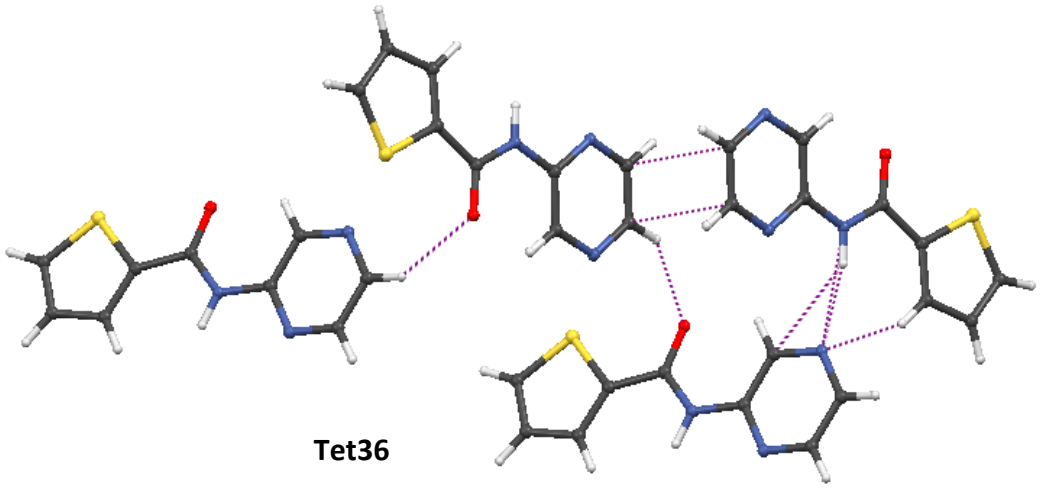
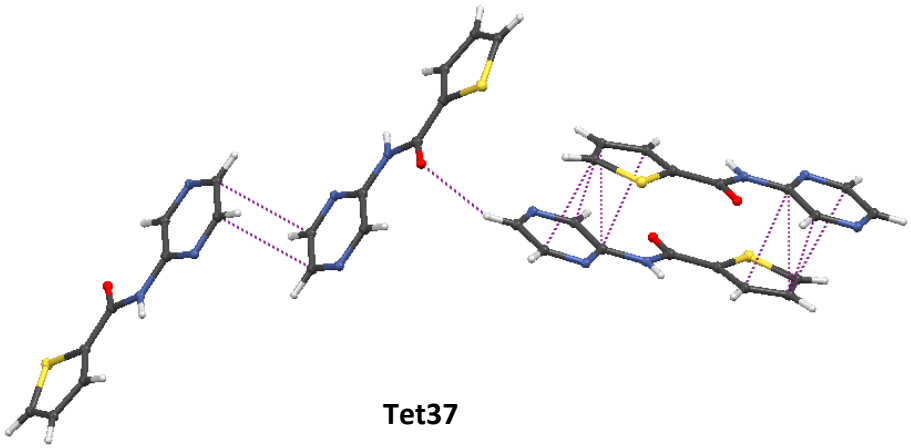


Tet36



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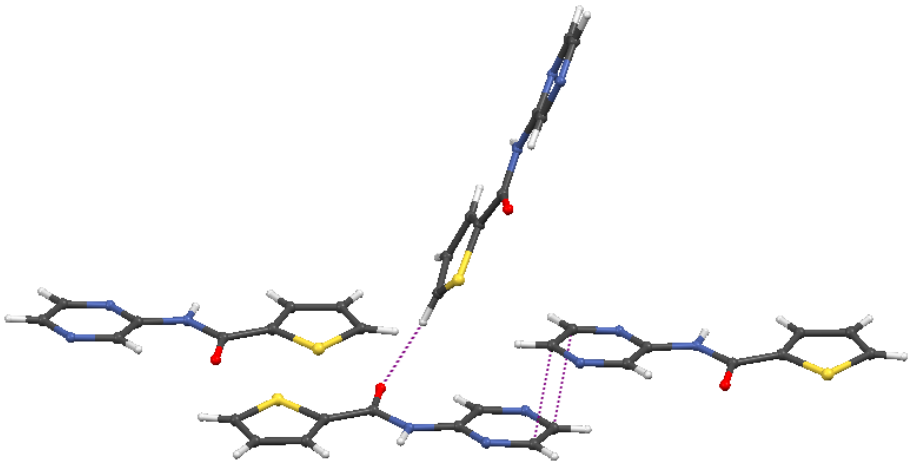
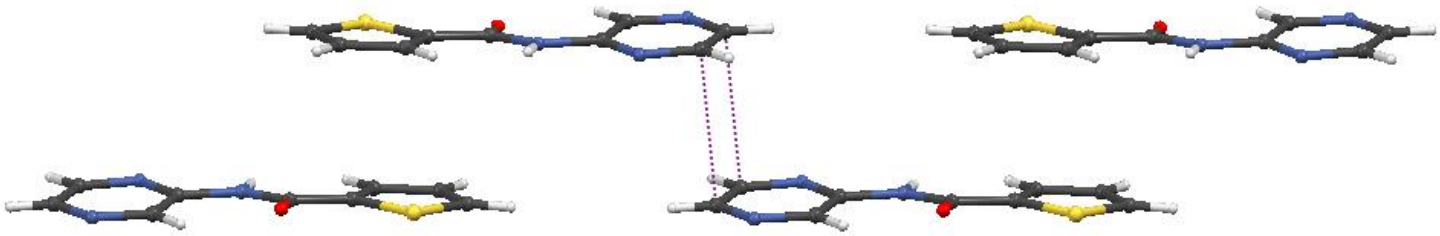
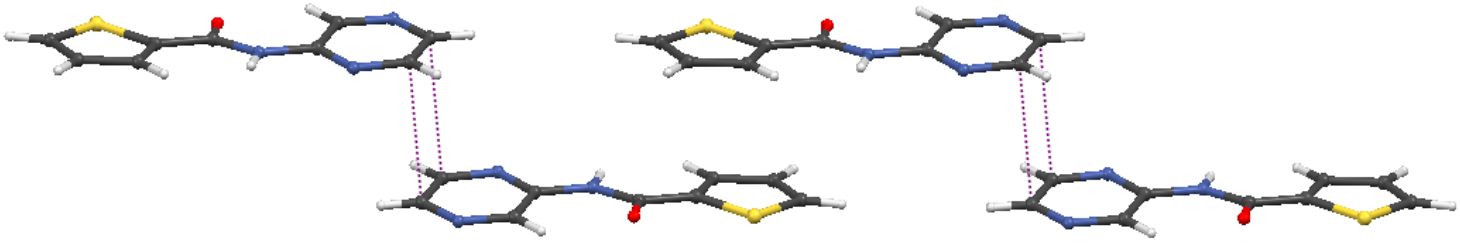


Tet38



Tet39



Tet40

Figure S23. Representation of the most stable tetramer motifs of *II* which are labeled based on the interaction energy ranking

Table S1.The binding energy (E_{calc} in kJ/mol) of the most stable tetramer fragments of compound *I*, along with contribution of cooperativity (E_{coop}), HB (E_{HB}) and π…π stacking ($E_{\pi\ldots\pi}$) energies as the magnitude (in kJ/mol) and percentage of total binding energy, as well as their weighted contributions.

	Furan	E_{Calc}	E_{coop}	% E_{coop}	%W E_{coop}	E_{HB}	%HB	%W HB	E π-based	% π-based	%W π-based
Tet1	2D1 (HB)+2D2 (π…π)+2D7 (HB)	-160.27	-1.18	0.74	0.03	-103.01	64.27	2.78	-56.08	34.99	1.52
Tet2	D1 (HB)+D2 (π…π)+D3 (HB)+D6 (HB)+D4 (HB)	-119.22	-1.95	1.64	0.05	-89.23	74.85	2.41	-28.04	23.52	0.76
Tet3	D1 (HB)+D2 (π…π)+D5 (HB)+D6 (HB)+D4 (HB)+D7 (HB)	-118.97	-0.51	0.43	0.01	-90.42	76.00	2.44	-28.04	23.57	0.76
Tet4	D1 (HB)+2D2 (π…π)+2D7 (HB)	-116.75	-1.85	1.59	0.05	-58.82	50.38	1.59	-56.08	48.03	1.52
Tet5	D1 (HB)+2D2 (π…π)+2D7 (HB)	-116.38	-1.48	1.28	0.04	-58.82	50.54	1.59	-56.08	48.19	1.52
Tet6	2D1 (HB)+D6 (HB)+D4 (HB)	-113.71	-0.16	0.14	0.00	-113.55	99.86	3.07	0.00	0.00	0.00
Tet7	D1 (HB)+D2 (π…π)+D3 (HB)+D6 (HB)+D7 (HB)	-112.72	0.77	-0.68	-0.02	-85.45	75.81	2.31	-28.04	24.87	0.76
Tet8	D1 (HB)+D2 (π…π)+D5 (HB)+D6 (HB)+D4 (HB)	-112.48	-1.33	1.18	0.04	-83.11	73.89	2.25	-28.04	24.93	0.76
Tet9	D1 (HB)+D2 (π…π)+D3 (HB)+D6 (HB)+D7 (HB)	-111.13	-0.30	0.27	0.01	-82.79	74.50	2.24	-28.04	25.23	0.76
Tet10	2D1 (HB)+D3 (HB)	-110.44	-2.17	1.96	0.06	-108.27	98.04	2.93	0.00	0.00	0.00
Tet11	D1 (HB)+2D2 (π…π)+D7 (HB)	-109.38	-1.79	1.64	0.05	-51.51	47.09	1.39	-56.08	51.27	1.52
Tet12	2D1 (HB)+D5 (HB)	-104.59	-2.45	2.34	0.07	-102.15	97.66	2.76	0.00	0.00	0.00
Tet13	D1 (HB)+D2 (π…π)+D3 (HB)+D6 (HB)	-103.14	0.38	-0.37	-0.01	-75.48	73.18	2.04	-28.04	27.19	0.76
Tet14	2D2 (π…π)+D3 (HB)+2D6 (HB)	-99.74	-0.98	0.98	0.03	-42.68	42.80	1.15	-56.08	56.22	1.52
Tet15	2D2 (π…π)+2D5 (HB)+D4 (HB)	-96.35	0.99	-1.03	-0.03	-41.26	42.83	1.12	-56.08	58.20	1.52
Tet16	D1 (HB)+D2 (π…π)+D3 (HB)	-96.03	-3.92	4.08	0.11	-64.08	66.72	1.73	-28.04	29.20	0.76
Tet17	D1 (HB)+2D6 (HB)+2D4 (HB)	-94.74	-0.23	0.24	0.01	-94.51	99.76	2.56	0.00	0.00	0.00
Tet18	2D1 (HB)+D8 (C-H…π)	-94.06	0.09	-0.10	0.00	-94.15	100.10	2.55	0.00	0.00	0.00
Tet19	D1 (HB)+D2 (π…π)+D5 (HB)	-90.64	-4.65	5.13	0.13	-57.95	63.94	1.57	-28.04	30.94	0.76
Tet20	2D2 (π…π)+D3 (HB)+D6 (HB)	-90.08	-2.72	3.02	0.07	-31.28	34.73	0.85	-56.08	62.26	1.52
Tet21	D1 (HB)+D3 (HB)+D6 (HB)+D4 (HB)	-89.10	0.14	-0.15	0.00	-89.23	100.15	2.41	0.00	0.00	0.00
Tet22	2D2 (π…π)+D3 (HB)+D6 (HB)	-88.82	-1.46	1.65	0.04	-31.28	35.22	0.85	-56.08	63.14	1.52
Tet23	D1 (HB)+2D3 (HB)	-87.93	-3.98	4.52	0.11	-83.96	95.48	2.27	0.00	0.00	0.00
Tet24	D1 (HB)+D3 (HB)+D5 (HB) +D8 (HB)	-86.27	-2.68	3.11	0.07	-83.59	96.89	2.26	0.00	0.00	0.00
Tet25	2D2 (π…π)+D5 (HB)+D4 (HB)	-85.73	-2.15	2.50	0.06	-27.51	32.09	0.74	-56.08	65.41	1.52
Tet26	D2 (π…π)+D3 (HB)+D5 (HB)+D6 (HB)+D4 (HB)	-85.56	1.28	-1.49	-0.03	-58.79	68.72	1.59	-28.04	32.77	0.76
Tet27	D1 (HB)+D3 (HB)+D4 (HB)+D7 (HB)	-85.27	-0.13	0.16	0.00	-85.14	99.85	2.30	0.00	0.00	0.00
Tet28	3D2 (π…π)	-84.99	-0.88	1.03	0.02	0.88	-1.03	-0.02	-84.99	100.00	2.30
Tet29	D1 (HB)+2D3 (HB)	-84.11	-0.15	0.18	0.00	-83.96	99.82	2.27	0.00	0.00	0.00
Tet30	D1 (HB)+2D3 (HB)	-83.86	0.10	-0.12	0.00	-83.96	100.12	2.27	0.00	0.00	0.00
Tet31	D1 (HB)+D3 (HB)+D5 (HB)	-81.09	-3.26	4.03	0.09	-77.83	95.98	2.10	0.00	0.00	0.00
Tet32	D2 (π…π)+2D3 (HB)+D6 (HB)	-80.49	-1.29	1.60	0.04	-51.16	63.57	1.38	-28.04	34.84	0.76
Tet33	D2 (HB)+D3 (HB)+D5 (HB)+D4 (HB)	-76.35	-0.93	1.21	0.03	-75.43	98.79	2.04	0.00	0.00	0.00
Tet34	D1 (HB)+2D5 (HB)	-70.26	1.45	-2.06	-0.04	-71.71	102.06	1.94	0.00	0.00	0.00
Tet35	D3 (HB)+2D5 (HB)+D6 (HB) +D8 (HB)	-64.29	0.26	-0.40	-0.01	-64.55	100.40	1.75	0.00	0.00	0.00
Tet36	D3 (HB)+2D5 (HB)+D6 (HB) +D8 (HB)	-64.15	0.40	-0.62	-0.01	-64.55	100.62	1.75	0.00	0.00	0.00
Tet37	2D3 (HB)+D4 (HB)+D7 (C-H…π)	-60.76	0.07	-0.11	0.00	-60.82	100.11	1.64	0.00	0.00	0.00
Tet38	3D3 (HB)	-59.36	0.28	-0.46	-0.01	-59.64	100.46	1.61	0.00	0.00	0.00
Tet39	D3 (HB)+D6 (HB)+D4 (HB)+D7 (HB)+D8 (HB)	-58.52	-0.42	0.71	0.01	-58.11	99.29	1.57	0.00	0.00	0.00
Tet40	D3 (HB)+D5 (HB)+D6 (HB)+D7 (HB)	-51.84	0.51	-0.98	-0.01	-52.35	100.98	1.42	0.00	0.00	0.00
∑*					**1.04**			**75.45**			**23.52**

*The summation of the percentage of weighted contribution of E_{coop}, E_{HB} and $E_{\pi\ldots\pi}$ in all of the tetramer fragments

Table S2.The binding energy (E_{calc} in kJ/mol) of the most stable tetramer fragments of compound *II*, along with contribution of cooperativity (E_{coop}), HB (E_{HB}) and π…π stacking ($E_{\pi\ldots\pi}$) energies as the magnitude (in kJ/mol) and percentage of total binding energy, as well as their weighted contributions.

	Thiophene	$E_{Calc.}$	E_{coop}	% E_{coop}	%W E_{coop}	E_{HB}	%HB	%WHB	$E_{\pi\text{-based}}$	%π-based	%Wπ-based
Tet1	2D1 (π…π)+D2 (HB)+D5 (HB)+D7 (HB)+D9 (HB)	-140.76	-2.39	1.70	0.06	-59.49	42.26	1.55	-78.88	56.04	2.06
Tet2	D1 (π…π)+2D2 (HB)+D5 (HB)+D6 (π…π)+D7 (HB)	-140.30	-3.55	2.53	0.09	-86.96	61.98	2.27	-49.79	35.49	1.30
Tet3	D1 (π…π)+2D2 (HB)+D5 (HB)+D6 (π…π)+D7 (HB)	-140.27	-3.52	2.51	0.09	-86.96	62.00	2.27	-49.79	35.50	1.30
Tet4	D1 (π…π)+2D2 (HB)+2D5 (HB)	-134.71	-3.58	2.66	0.09	-91.68	68.06	2.39	-39.44	29.28	1.03
Tet5	D1 (π…π)+2D2 (HB)+ D5 (HB)	-120.48	-3.13	2.60	0.08	-77.91	64.67	2.03	-39.44	32.74	1.03
Tet6	D1 (π…π)+D2 (HB)+D3 (π…π)+D4 (HB) +D8 (HB)	-119.78	1.03	-0.86	-0.03	-53.99	45.07	1.41	-66.82	55.79	1.74
Tet7	D1 (π…π)+ D2 (HB)+ D3 (π…π)+D5 (HB)	-113.26	-0.58	0.51	0.02	-11.48	10.14	0.30	-101.19	89.35	2.64
Tet8	D1 (π…π)+D2 (HB)+2D5 (HB)+D6 (π…π)	-111.82	-2.40	2.15	0.06	-59.63	53.33	1.56	-49.79	44.53	1.30
Tet9	2D2 (HB)+D3 (π…π)+D4 (HB)	-110.25	-3.04	2.76	0.08	-79.82	72.41	2.08	-27.38	24.83	0.71
Tet10	D2 (HB)+D2 (HB)+D3 (π…π)+D4 (HB)	-109.10	-1.90	1.74	0.05	-79.82	73.17	2.08	-27.38	25.10	0.71
Tet11	D1 (π…π)+D2 (HB)+D3 (π…π)+D7 (HB)	-109.01	-1.06	0.97	0.03	-41.14	37.74	1.07	-66.82	61.30	1.74
Tet12	D2 (HB)+2D3 (π…π)+D4 (HB)+D9 (HB)	-106.88	0.19	-0.18	-0.01	-52.32	48.95	1.37	-54.76	51.23	1.43
Tet13	2D1 (π…π)+D3 (π…π)	-106.56	-0.30	0.28	0.01	0.30	-0.28	-0.01	-106.56	100.00	2.78
Tet14	D1 (π…π)+D2 (HB)+2D5 (HB)+D9 (HB)	-104.32	-0.70	0.67	0.02	-64.18	61.52	1.68	-39.44	37.81	1.03
Tet15	D1 (π…π)+D2 (HB)+D4 (HB)+D5 (HB)	-103.10	-2.15	2.08	0.06	-61.51	59.66	1.61	-39.44	38.26	1.03
Tet16	2D2 (HB)+2D5 (HB)+D6 (π…π)	-102.53	-0.50	0.49	0.01	-91.68	89.42	2.39	-10.35	10.09	0.27
Tet17	3D2 (HB)	-102.00	-5.80	5.69	0.15	-96.20	94.31	2.51	0.00	0.00	0.00
Tet18	D1 (π…π)+D3 (π…π)+D4 (HB)+D5 (HB)+D9 (HB)	-100.77	0.05	-0.05	0.00	-34.00	33.74	0.89	-66.82	66.31	1.74
Tet19	D1 (π…π)+D2 (HB)+D4 (HB)+D5 (HB)	-100.69	0.29	-0.29	-0.01	-61.54	61.12	1.61	-39.44	39.17	1.03
Tet20	2D2 (HB)+D5 (HB)+D6 (π…π)+D7 (HB)	-100.29	-2.94	2.94	0.08	-86.99	86.75	2.27	-10.35	10.32	0.27
Tet21	D2 (HB)+D3 (π…π)+D4 (HB)+D5 (HB)+D6 (π…π)	-97.75	1.48	-1.51	-0.04	-61.51	62.92	1.61	-37.73	38.59	0.99
Tet22	D1 (π…π)+2D3 (π…π)	-94.03	0.17	-0.18	0.00	-0.17	0.18	0.00	-94.03	100.00	2.45
Tet23	D1 (π…π)+D2 (HB)+D5 (HB)+D9 (HB)	-90.97	-1.16	1.27	0.03	-50.37	55.37	1.32	-39.44	43.36	1.03
Tet24	2D1 (π…π)+D6 (π…π)	-90.22	-0.99	1.10	0.03	0.99	-1.10	-0.03	-90.22	100.00	2.36
Tet25	D1 (π…π)+D3 (π…π)+D4 (HB)+D8 (HB)	-89.22	-0.47	0.53	0.01	-21.93	24.58	0.57	-66.82	74.89	1.74
Tet26	D1 (π…π)+D3 (π…π)+D5 (HB) +D9 (HB)	-85.13	0.01	-0.01	0.00	-18.32	21.52	0.48	-66.82	78.49	1.74
Tet27	D2 (HB)+D4 (HB)+D5 (HB)+D6 (π…π)+D8 (HB)	-79.53	-1.42	1.79	0.04	-67.76	85.20	1.77	-10.35	13.01	0.27
Tet28	D1 (π…π)+D4 (HB)+D5 (HB)+D8 (HB)+D9 (HB)	-79.49	0.21	-0.26	-0.01	-40.25	50.64	1.05	-39.44	49.62	1.03
Tet29	2D2 (HB)+D4 (HB)	-79.25	0.58	-0.73	-0.02	-79.82	100.73	2.08	0.00	0.00	0.00
Tet30	2D2 (HB)+D5 (HB)	-79.06	-1.15	1.46	0.03	-77.91	98.54	2.03	0.00	0.00	0.00
Tet31	D1 (π…π)+D3 (π…π)+D6 (π…π)	-77.91	-0.75	0.96	0.02	0.75	-0.96	-0.02	-77.91	100.00	2.03
Tet32	D1 (π…π)+D3 (π…π)+D6 (π…π)	-76.56	0.61	-0.80	-0.02	-0.61	0.80	0.02	-76.56	100.00	2.00
Tet33	D2 (HB)+D5 (HB)+2D6 (π…π)+D7 (HB)	-76.24	-0.64	0.84	0.02	-54.91	72.01	1.43	-20.70	27.15	0.54
Tet34	D1 (π…π)+D3 (π…π)+D6 (π…π)	-76.16	1.01	-1.32	-0.03	-1.01	1.32	0.03	-76.16	100.00	1.99
Tet35	D2 (HB)+D4 (HB)+D5 (HB)+D6 (π…π)	-71.70	0.16	-0.23	0.00	-61.51	85.79	1.61	-10.35	14.43	0.27
Tet36	D2 (HB)+2D5 (HB)+D6 (π…π)	-71.00	-1.06	1.49	0.03	-59.60	83.94	1.56	-10.35	14.58	0.27
Tet37	D1 (π…π)+D5 (HB)+D6 (π…π)+D9 (HB)	-67.67	0.44	-0.65	-0.01	-18.32	27.07	0.48	-49.79	73.58	1.30
Tet38	D3 (π…π)+D4 (HB)+D6 (π…π)+D8 (HB)+D9 (HB)	-64.29	-0.08	0.12	0.00	-26.48	41.19	0.69	-37.73	58.69	0.99
Tet39	2D3 (π…π)+D6 (π…π)	-62.80	2.31	-3.67	-0.06	-2.31	3.67	0.06	-62.80	100.00	1.64
Tet40	D3 (π…π)+2D6 (π…π)	-46.04	2.03	-4.42	-0.05	-2.03	4.42	0.05	-46.04	100.00	1.20
∑*					**0.91**			**50.11**			**48.99**

***** The summation of the percentage of weighted contribution of E_{coop}, E_{HB} and $E_{\pi\ldots\pi}$ in all of the tetramer fragments