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Supporting Information For

Crystal and molecular structure of $[Ni(2\text{-}H_2NC(=O)C_5H_4N)_2(H_2O)_2][Ni(2,6\text{-}(O_2C)_2C_5H_3N)_2]\cdot 4.67H_2O$; DFT studies on hydrogen bonding energies in the crystal

Mohammad Chahkandi*, Abolfazl Keivanloo Shahrestanaki, Masoud Mirzaei*, Muhammad Nawaz Tahir and Joel T. Mague

Department of Chemistry, Hakim Sabzevari University, Sabzevar, 96179-76487, Iran

Department of Chemistry, Faculty of Science, Ferdowsi University of Mashhad, Mashhad, 917751436, Iran

Department of Physics, University of Sargodha, Sargodha, Pakistan

Department of Chemistry, Tulane University, New Orleans, LA, 70118, USA

*To whom correspondence should be addressed:

[a]E-mail: m.chahkandi@hsu.ac.ir;

[b]E-mail: mirzaeesh@um.ac.ir

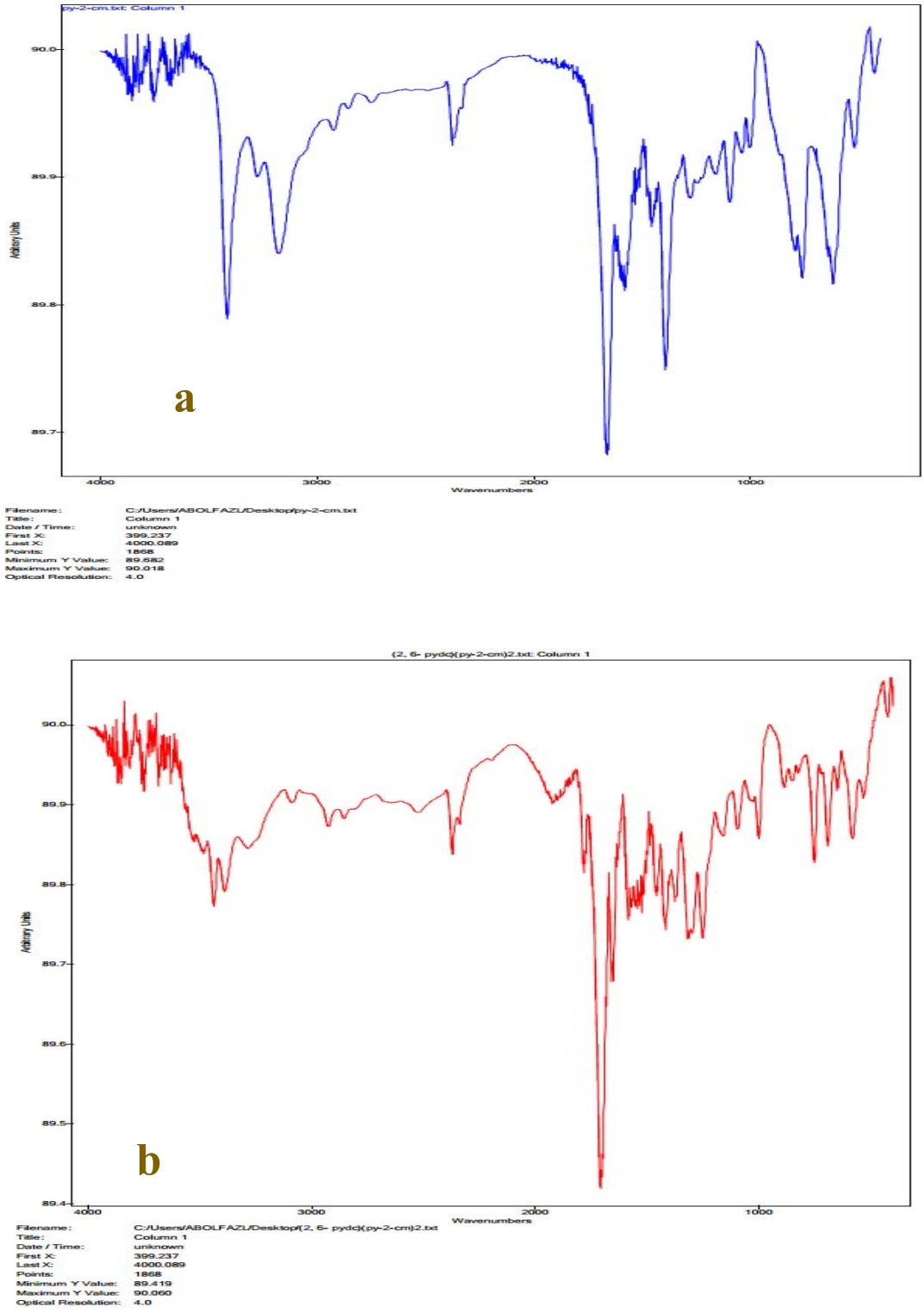

Figure 1S. FT-IR spectra of (a) py–2–cm and (b) 2,6–pydc(py–2–cm)$_2$.

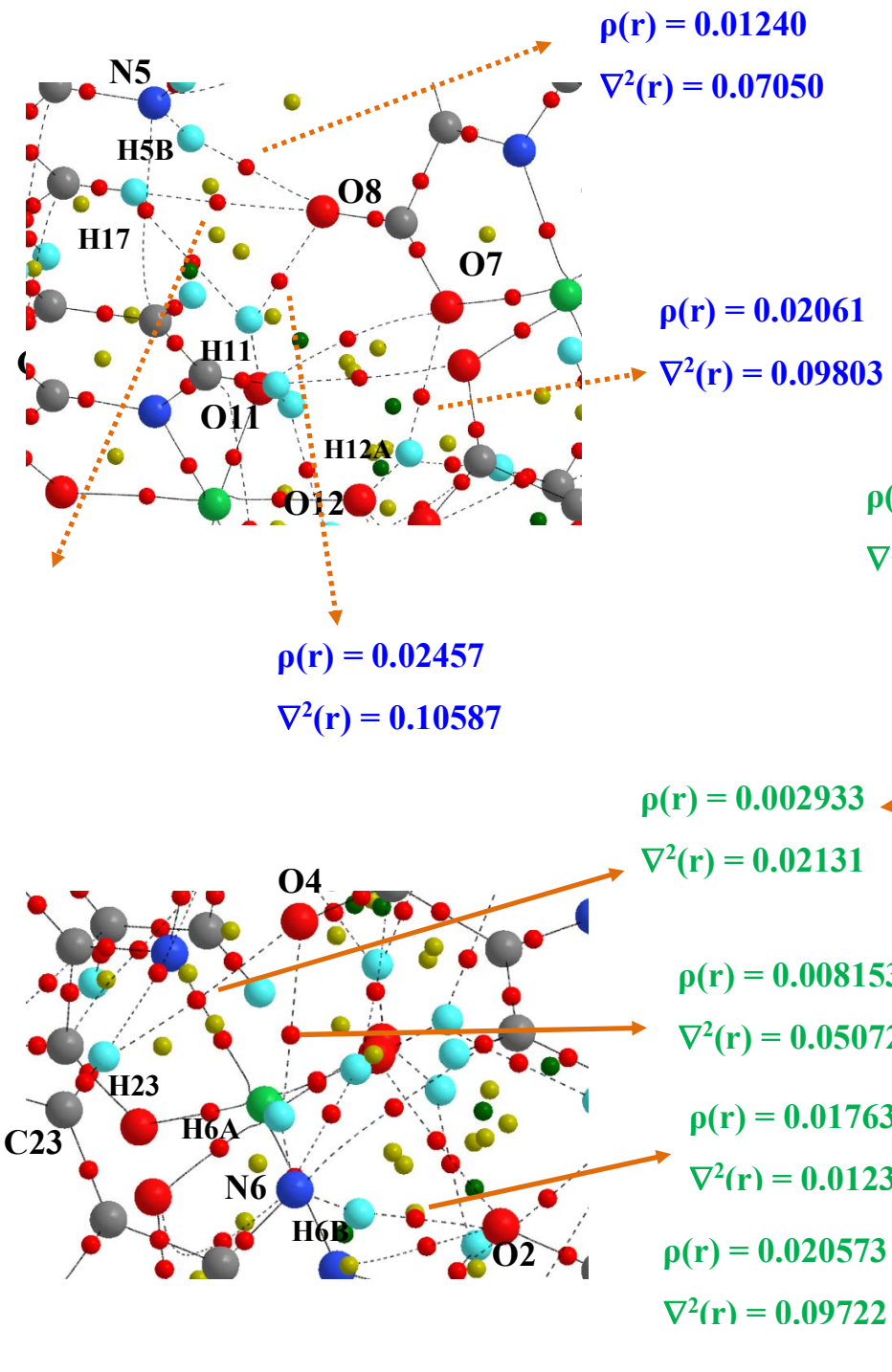

Figure 2S. (a). The calculated electron density and Laplacian values (in a.u.) for HBs in optimized 1−CN. The small red, yellow and green dots represent BCPs, RCP, and CCP, respectively.

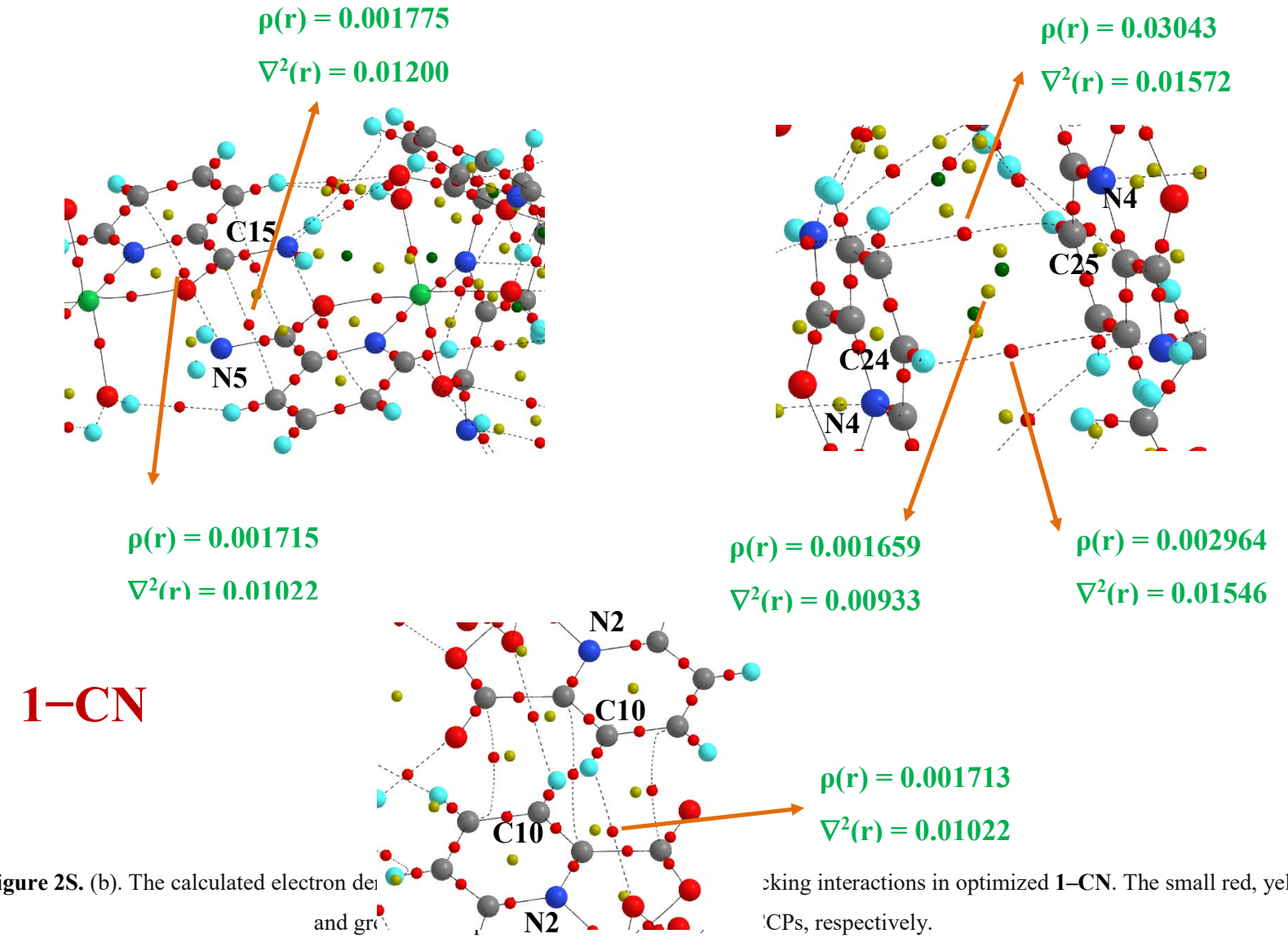

Figure 2S. (b). The calculated electron de[illegible]cking interactions in optimized **1–CN**. The small red, yellow, and gr[illegible]CPs, respectively.

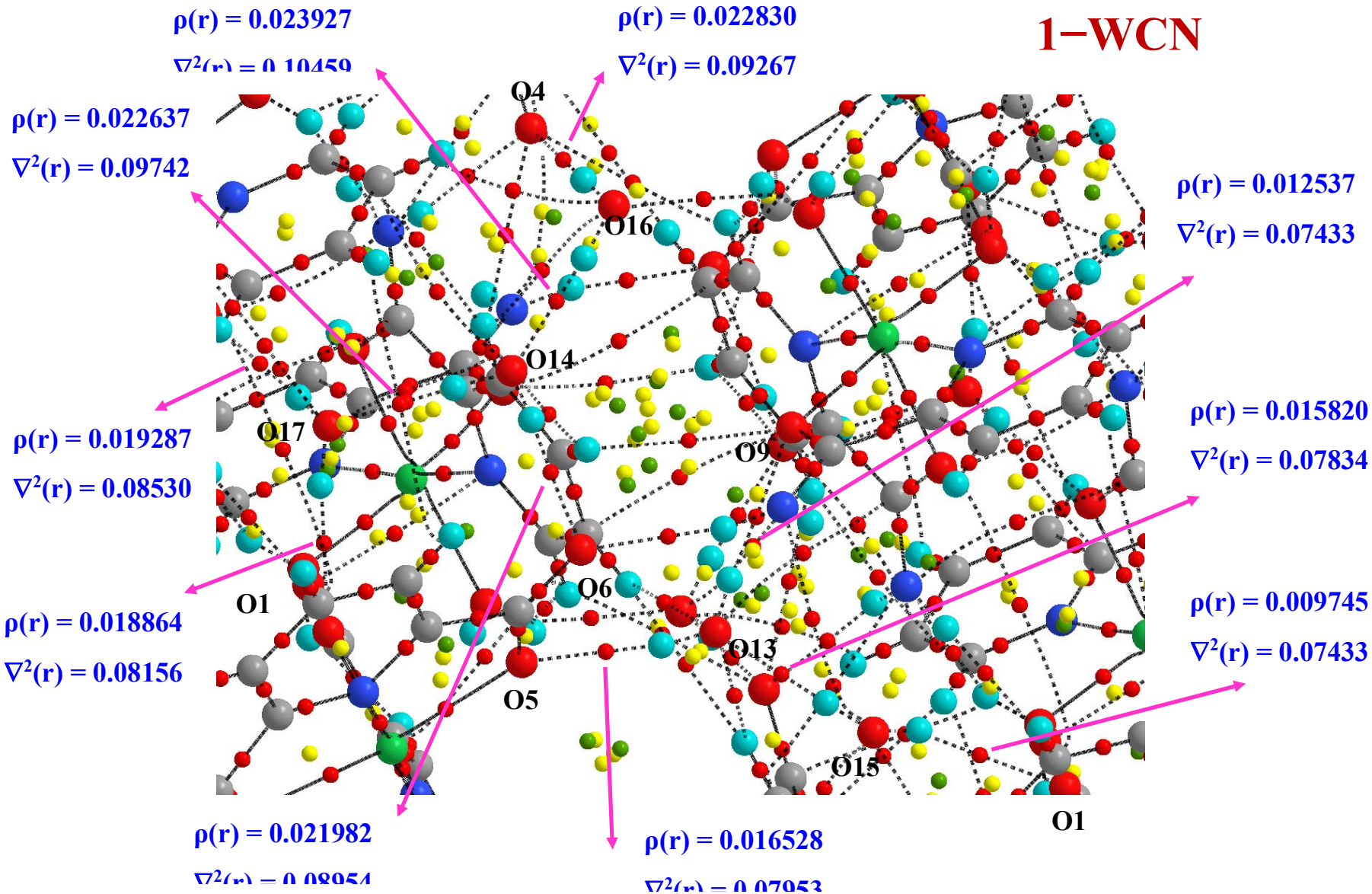
1−WCN
ρ(r) = 0.023927
∇²(r) = 0.10459
ρ(r) = 0.022830
∇²(r) = 0.09267
ρ(r) = 0.022637
∇²(r) = 0.09742
ρ(r) = 0.012537
∇²(r) = 0.07433
ρ(r) = 0.019287
∇²(r) = 0.08530
ρ(r) = 0.015820
∇²(r) = 0.07834
ρ(r) = 0.018864
∇²(r) = 0.08156
ρ(r) = 0.009745
∇²(r) = 0.07433
ρ(r) = 0.021982
∇²(r) = 0.08954
ρ(r) = 0.016528
∇²(r) = 0.07953
O4
O16
O14
O17
O9
O1
O6
O13
O5
O15
O1

Figure 3S. The calculated electron density and Laplacian values (in a.u) for water clustered HBs in optimized **1–WCN**. The small red, yellow, and green dots represent the BCPs, RCPs, and CCPs, respectively.

Table 1S. The calculated non–covalent interactions distances (Å), angles (º), and their binding energies (kJ mol^{-1}) of **1–CN** and **1–WCN**.

	d(H···A)	**< (DHA)**	**Binding Energy**	
		1–CN		**Interaction Types**
O_{11}–H_{11A}···O_8	1.893	143.56	−30.63	2 × (N5–H5A···O6 + O12–H12A···O7 + C23–H23···O4 + N6–H6B···O4) + N5–H5B···O8 + O11–H11A···O8 + C17–H17···O8 + N6–H6A···O2 + O11–H11A···O8 + N5–H5B···O8 + C17–H17···O8 + N5–H5A···$\pi_{(py)}$ + N5–H5B···$\pi_{(py)}$ + C25–H25···$\pi_{(py)}$ + C24–H24···$\pi_{(py)}$ + C10–H10···$\pi_{(py)}$ + $\pi_{(py)}$···$\pi_{(py)}$
O_{12}–H_{12A}···O_7	1.922	145.70	−29.95	
O_{11}–H_{11A}···O_8				
N_5–H_{5A}···O_6	1.965	142.59	−29.12	
N_6–H_{6A}···O_2	1.937	166.42	−22.17	
N_5–H_{5B}···O_8	1.996	165.27	−20.54	
N_5–H_{5B}···O_8	2.164	163.14	−18.95	
N_6–H_{6B}···O_4	2.171	162.83	−18.20	
C_{17}–H_{17}···O_8	2.353	155.44	−17.16	**ΔE_{CN} = –344.18 kJ mol^{-1}**
C_{17}–H_{17}···O_8	2.647	167.38	−10.58	
C_{23}–H_{23}···O_4	2.661	166.29	−9.73	
N_5–H_{5B}···$\pi_{(pyridine)}$	2.787	145.26	−9.05	
N_5–H_{5A}···$\pi_{(pyridine)}$	3.669	88.07	−6.45	
C_{24}–H_{24}···$\pi_{(pyridine)}$	3.970	72.21	−5.76	
C_{10}–H_{10}···$\pi_{(pyridine)}$	3.822	73.31	−4.59	
C_{25}–H_{25}···$\pi_{(pyridine)}$	3.917	88.73	−4.25	
$\pi_{(pyridine)}$···$\pi_{(pyridine)}$	3.976	68.29	−4.03	
	3.428	180	−3.64	

Table 1S. Continued.

	d(H···A)	< (DHA)	Binding Energy	
	1–WCN			**Interaction Types**
O_{11}–H_{11A}···O_8	1.868	139.20	−30.05	3 × (O_{16}–H_{16A}···O_{14}) + 2 × (O_{12}–H_{12A}···O_7 + O_{15}–H_{15A}···O_1 + O_{11}–H_{11A}···O_8 + O_{17}–H_{17B}···O_1 + O_{14}–H_{14A}···O_{17} + O_{17}–H_{17A}···O_{10} + O_{14}–H_{14B}···O_6 + N_5–H_{5A}···O_6 + N_6–H_{6A}···O_2 + N_6–H_{6B}···O_4 + C_{20}–H_{20}···O_3 + C_{24}–H_{24}···$\pi_{(pyridine)}$ + C_{25}–H_{25}···$\pi_{(pyridine)}$) + O_{16}–H_{16B}···O_4 + O_{13}–H_{13A}···O_5 + O_{15}–H_{15B}···O_{13} + O_{13}–H_{13B}···O_9 + $\pi_{(py)}$···$\pi_{(py)}$
O_{16}–H_{16A}···O_{14}	1.872	172.42	−29.87	
O_{11}–H_{11A}···O_8	1.873	141.85	−28.46	
O_{12}–H_{12A}···O_7	1.923	143.17	−27.83	
O_{16}–H_{16A}···O_{14}	1.939	165.66	−26.76	
O_{16}–H_{16B}···O_4	1.962	173.05	−25.55	
O_{14}–H_{14A}···O_{17}	1.965	168.39	−25.07	
O_{16}–H_{16A}···O_{14}	1.970	174.72	−24.71	
O_{14}–H_{14B}···O_6	2.013	170.40	−23.14	**ΔE_{WCN} = –627.75 kJ mol^{-1}**
O_{17}–H_{17B}···O_1	2.017	139.37	−22.83	
O_{14}–H_{14A}···O_{17}	2.027	167.13	−22.39	
O_{14}–H_{14B}···O_6	2.075	175.18	−21.82	
O_{17}–H_{17A}···O_{10}	2.086	173.95	−21.29	
O_{17}–H_{17B}···O_1	2.088	176.29	−21.08	
O_{13}–H_{13A}···O_5	2.104	171.53	−20.47	
O_{15}–H_{15B}···O_{13}	2.151	170.48	−19.63	
O_{17}–H_{17A}···O_{10}	2.183	175.97	−19.15	
O_{13}–H_{13B}···O_9	2.210	161.22	−17.74	
O_{15}–H_{15A}···O_1	2.330	164.64	−16.12	
N_5–H_{5A}···O_6	1.971	166.38	−18.29	
N_5–H_{5A}···O_6	1.977	166.49	−17.77	
N_6–H_{6A}···O_2	1.985	163.25	−17.02	
N_6–H_{6A}···O_2	2.007	165.20	−16.26	
N_6–H_{6B}···O_4	2.264	157.34	−15.67	
N_6–H_{6B}···O_4	2.327	159.57	−15.18	
C_{20}–H_{20}···O_3	2.617	158.94	−10.70	
C_{20}–H_{20}···O_3	2.644	157.83	−10.16	
C_{24}–H_{24}···$\pi_{(pyridine)}$	3.579	72.46	−4.17	
C_{25}–H_{25}···$\pi_{(pyridine)}$	3.662	71.81	−3.58	
$\pi_{(pyridine)}$···$\pi_{(pyridine)}$	3.428	180	−3.29	