Electronic Supplementary Material (ESI) for CrystEngComm.

What are the prospects of [1,2,5]oxadiazolo[3,4-c]cinnoline 5-oxides, 1,5-dioxides and their nitro derivatives as high-energy-density materials? Synthesis, experimental and predicted crystal structures, and calculated explosive properties

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Additional information on crystal structure calculations for compounds 1–8

Table S1 The comparison of various charge models of molecules. MK –Merzh-Kollman; AC – atom centered charge; SC – shifted charge model (XX, YY, ZZ, XY, XZ, YZ – quadrupole moments; RMSD – root mean square deviation; RRMSD – relative root mean square deviation)

Compound	Model	Dipole moment	XX	YY	ZZ	XY	XZ	YZ	RMSD, kcal mol^{-1}	RRMSD, %
1	MK	6.3309	–1.99	–0.34	2.33	–6.01	0.00	0.00	0.21	3.51
	AC	6.3569	–2.07	–0.42	2.49	–5.94	0.00	0.00	0.19	3.19
	SC	6.3773	–2.17	–0.42	2.59	–5.93	0.00	0.00	0.04	0.60
	QM	6.3731	–2.17	–0.41	2.58	–5.92	0.00	0.00	—	—
2	MK	6.7394	6.55	–10.50	3.95	9.93	0.00	0.00	0.25	3.53
	AC	6.7685	6.43	–10.80	4.37	9.80	0.00	0.00	0.21	2.97
	SC	6.78	6.44	–11.00	4.56	9.82	0.00	0.00	0.05	0.66
	QM	6.7756	6.43	–10.97	4.54	9.81	0.00	0.00	—	—
3	MK	3.4974	–17.82	3.69	14.13	–1.95	0.00	0.00	0.24	4.35
	AC	3.5095	–17.98	3.81	14.17	–1.98	0.00	0.00	0.19	3.50
	SC	3.5116	–18.28	3.88	14.40	–2.06	0.00	0.00	0.05	0.82
	QM	3.5113	–18.24	3.88	14.37	–2.06	0.00	0.00	—	—
4	MK	2.3017	–18.93	4.84	14.08	3.98	0.00	0.00	0.26	5.17
	AC	2.4078	–18.83	4.75	14.09	4.20	0.00	0.00	0.20	4.01
	SC	2.4262	–18.97	4.69	14.28	4.29	0.00	0.00	0.04	0.83
	QM	2.4289	–18.95	4.70	14.25	4.28	0.00	0.00	—	—
5	MK	5.7968	–10.50	3.65	6.85	13.12	1.07	0.37	0.27	4.33
	AC	5.8664	–10.32	3.57	6.74	12.93	1.14	0.24	0.20	3.24
	SC	5.8923	–10.30	3.44	6.86	12.89	1.09	0.28	0.05	0.87
	QM	5.8893	–10.29	3.44	6.85	12.86	1.08	0.29	—	—
6	MK	1.2696	–9.25	–8.32	17.58	–0.91	–1.46	0.62	0.27	5.11
	AC	1.3592	–9.39	–8.21	17.60	–0.98	–1.38	0.76	0.21	3.94
	SC	1.3807	–9.72	–8.11	17.83	–1.07	–1.36	0.69	0.04	0.83
	QM	1.381	–9.71	–8.09	17.80	–1.07	–1.36	0.68	—	—
7	MK	5.9936	–6.73	2.75	3.99	–7.80	0.00	0.00	0.16	2.78
	AC	6.0132	–6.51	2.52	3.99	–7.67	0.00	0.00	0.14	2.43
	SC	6.0261	–6.49	2.49	4.00	–7.65	0.00	0.00	0.04	0.64

	QM	6.0225	–6.48	2.49	3.98	–7.63	0.00	0.00	—	—
8	MK	2.8656	–10.09	–5.89	15.99	8.56	0.00	0.00	0.17	3.21
	AC	2.8894	–10.27	–5.71	15.98	8.63	0.00	0.00	0.15	2.73
	SC	2.8938	–10.40	–5.70	16.10	8.76	0.00	0.00	0.05	0.84
	QM	2.8935	–10.37	–5.69	16.06	8.76	0.00	0.00	—	—

Fig. S1 Illustration of atomic charge model AC (left) and SC (right)

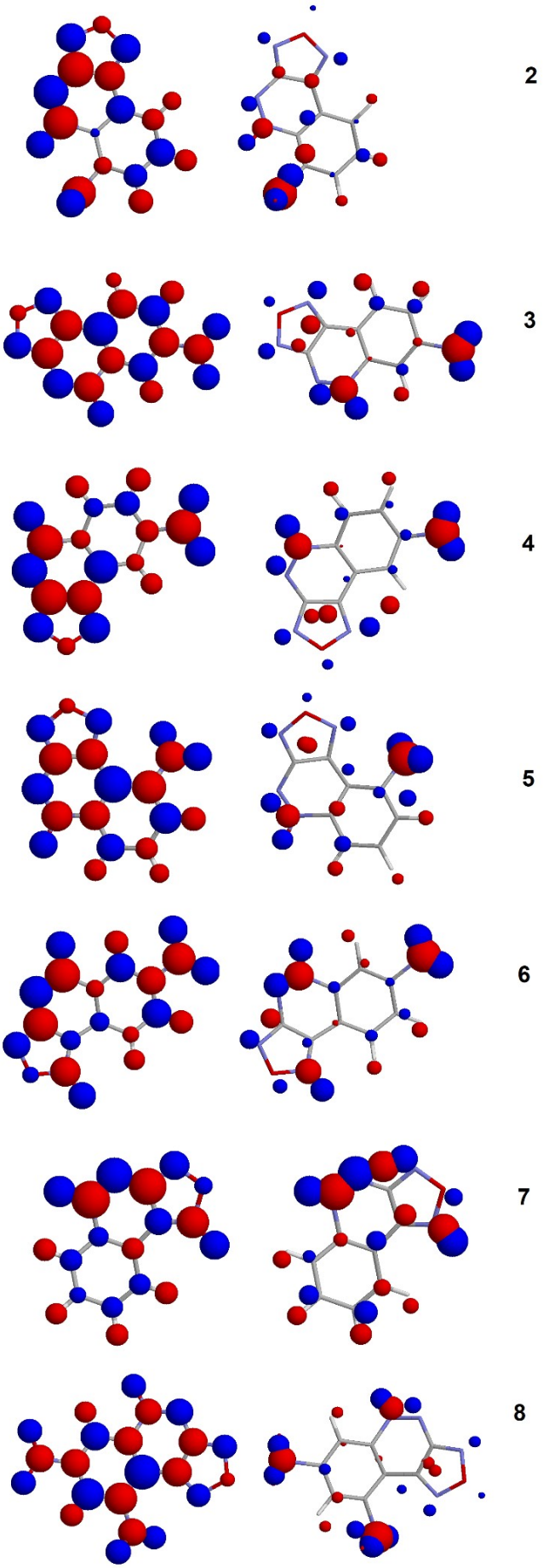


Fig. S2 Cluster of 13 molecules of compound **1**

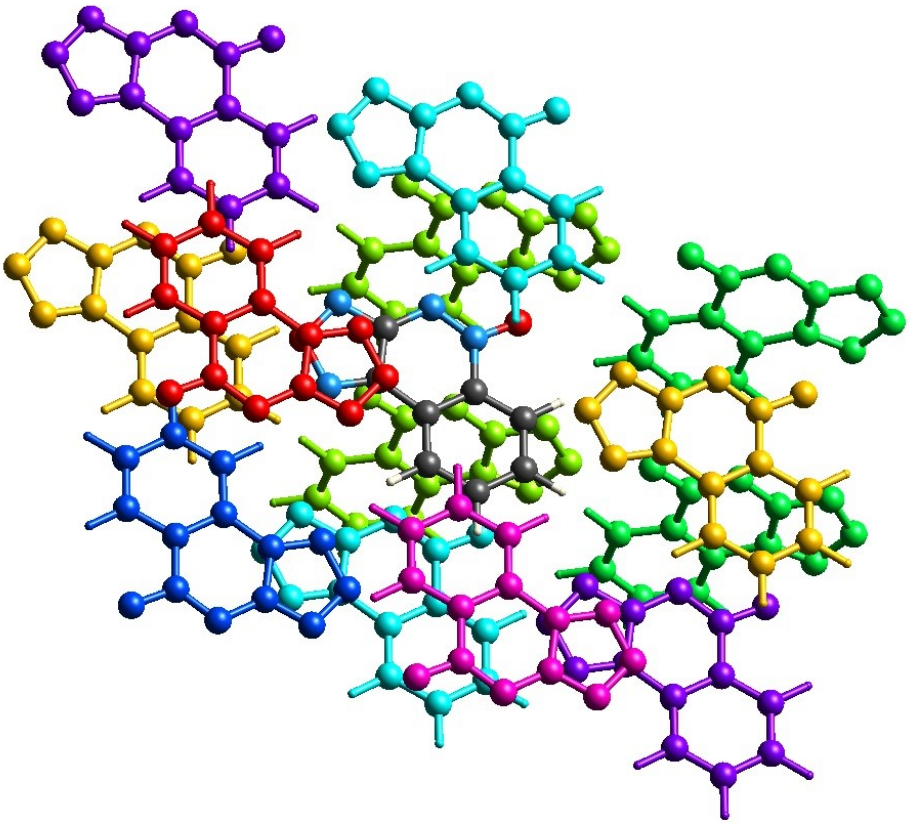


Table S2 Intermolecular interaction energy of 13 molecules cluster of compound **1**[a]

	N	Symop	R	E_ele, kcal·mol^{-1}	E_pol, kcal·mol^{-1}	E_dis, kcal·mol^{-1}	E_rep, kcal·mol^{-1}	E_tot, kcal·mol^{-1}
	1	–x, –y, –z	5.78	–3.35	–0.38	–5.38	3.39	–6.41
	2	x, y, z	7.74	0.24	–0.48	–5.31	2.92	–2.96
	2	–x, y+1/2, –z+1/2	5.09	–5.54	–2.06	–11.62	9.99	–11.33
	2	–x, y+1/2, –z+1/2	8.32	–3.54	–1.29	–5.59	5.98	–5.88
	2	x, y, z	5.37	0.91	–1.20	–12.19	6.36	–6.64
	1	–x, –y, –z	7.16	–5.74	–0.84	–2.82	5.14	–5.98
	2	x, y, z	9.43	–5.78	–1.00	–3.68	4.73	–7.12
	1	–x, –y, –z	8.42	0.53	–0.33	–2.51	1.53	–0.96
Total energy of cluster, kcal·mol^{-1}				–22.28	–7.58	–49.09	40.03	–47.28

[a] **Hereinafter:** Calculations were performed by B3LYP/6-31G(d,p) functional; N – number of interacting molecules; Symop – symmetry operations relating that particular colour coded molecule with the central molecule; R – distance between molecules center of mass; E_ele –energy of electrostatic interaction; E_pol – energy of polarization interaction; E_dis – energy of dispersion interaction; E_tot – total interaction energy.

Fig. S3 Cluster of 13 molecules of compound **7** asymmetric unit molecule A

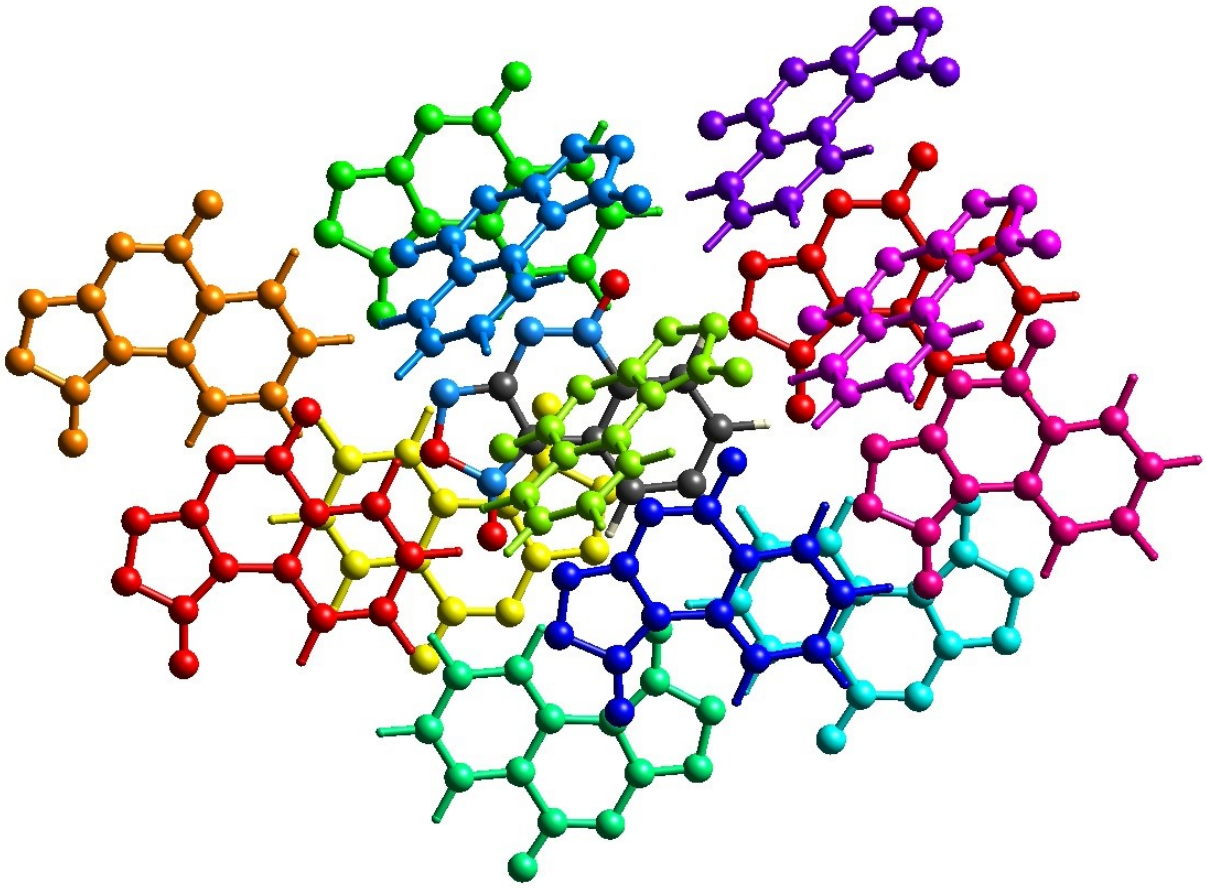


Table S3 Intermolecular interaction energy of 13 molecules cluster of compound **7** asymmetric unit molecule A

	N	Symop	R	E_ele, kcal·mol^{-1}	E_pol, kcal·mol^{-1}	E_dis, kcal·mol^{-1}	E_rep, kcal·mol^{-1}	E_tot, kcal·mol^{-1}
	2	x, y, z	8.1	0.05	–0.48	–5.11	2.68	–3.11
	1	—	9.58	–2.70	–0.43	–1.58	2.39	–3.06
	1	–x, –y, –z	4.79	–3.04	–0.65	–8.82	5.04	–8.25
	1	—	5.04	–3.08	–1.12	–7.24	6.26	–6.52
	1	—	5.68	0.07	–0.60	–5.43	2.92	–3.27
	1	—	7.52	–4.83	–0.79	–3.25	4.18	–5.93
	1	—	9.61	0.98	–0.29	–1.53	0.79	–0.02
	1	—	5.21	–2.01	–0.91	–6.02	4.37	–5.33

	1	—	5.25	0.29	–0.67	–7.29	3.73	–4.25
	1	—	8.96	–1.15	–0.45	–2.06	1.27	–2.56
	1	—	8.67	–1.79	–0.60	–2.65	2.68	–3.01
	1	—	9.79	–2.34	–0.33	–1.39	1.70	–2.87
Total energy of cluster, kcal·mol^{-1}				–19.55	–7.31	–52.37	38.00	–48.18

Fig. S4 Cluster of 13 molecules of compound **7** asymmetric unit molecule B

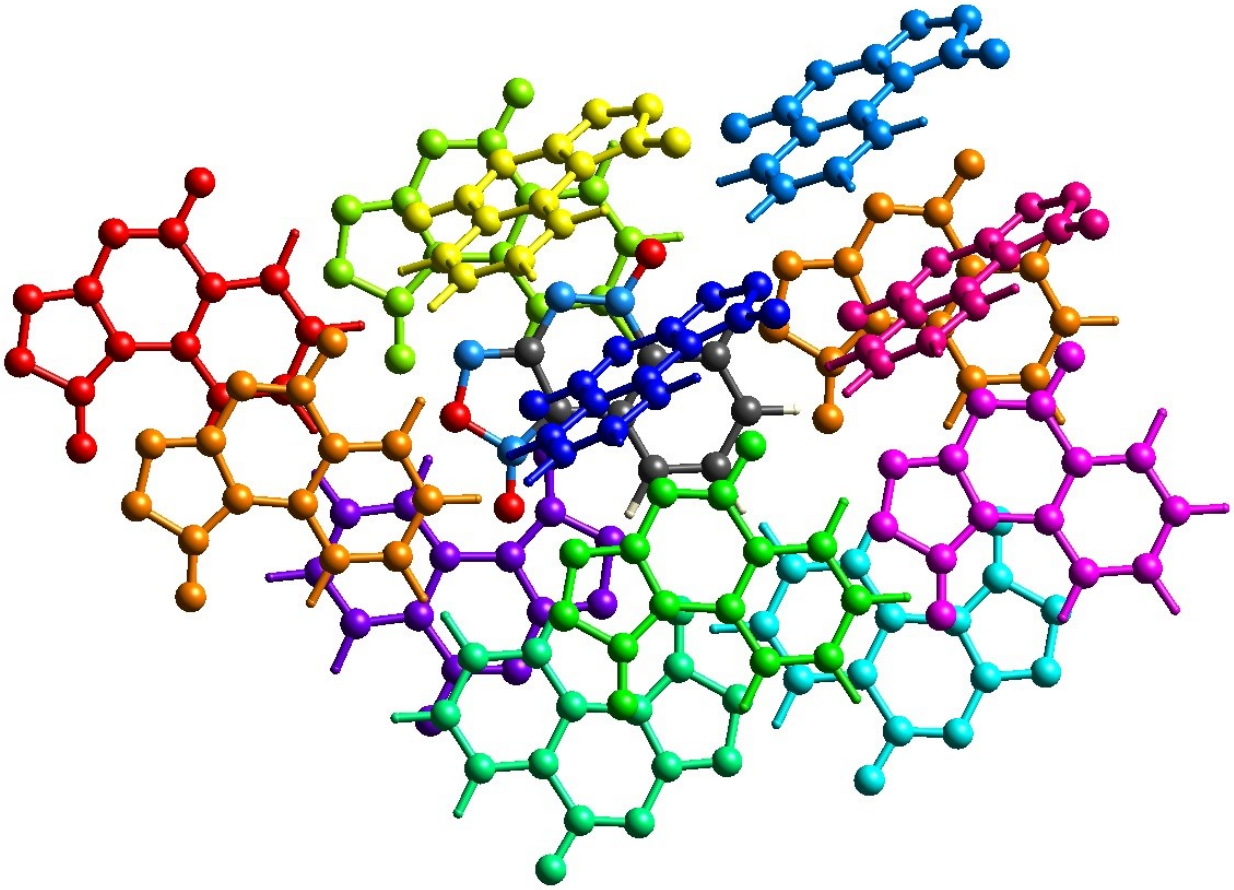


Table S4 Intermolecular interaction energy of 13 molecules cluster of compound **7** asymmetric unit molecule B

	N	Symop	R	E_ele, kcal·mol^{-1}	E_pol, kcal·mol^{-1}	E_dis, kcal·mol^{-1}	E_rep, kcal·mol^{-1}	E_tot, kcal·mol^{-1}
	1	—	9.71	–2.58	–0.36	–1.58	2.15	–3.04
	2	x, y, z	8.1	0.00	–0.48	–5.21	2.68	–3.25
	1	—	5.04	–3.08	–1.12	–7.24	6.26	–6.52
	1	—	5.02	–0.45	–0.76	–8.58	5.33	–5.23

	1	—	5.68	0.07	–0.60	–5.43	2.92	–3.27
	1	—	7.52	–4.83	–0.79	–3.25	4.18	–5.93
	1	—	9.61	0.98	–0.29	–1.53	0.79	–0.02
	1	—	8.67	–1.79	–0.60	–2.65	2.68	–3.01
	1	—	5.08	–3.80	–1.20	–7.36	7.03	–6.98
	1	—	5.69	–3.90	–0.60	–6.52	4.66	–7.34
	1	—	9.58	–2.70	–0.43	–1.58	2.39	–3.06
	1	—	8.54	–2.39	–0.69	–3.04	3.94	–3.25
Total energy of cluster, kcal·mol^{-1}				–24.47	–7.91	–53.97	45.00	–50.91

Fig. S4 Cluster of 13 molecules of compound **7** asymmetric unit molecule B

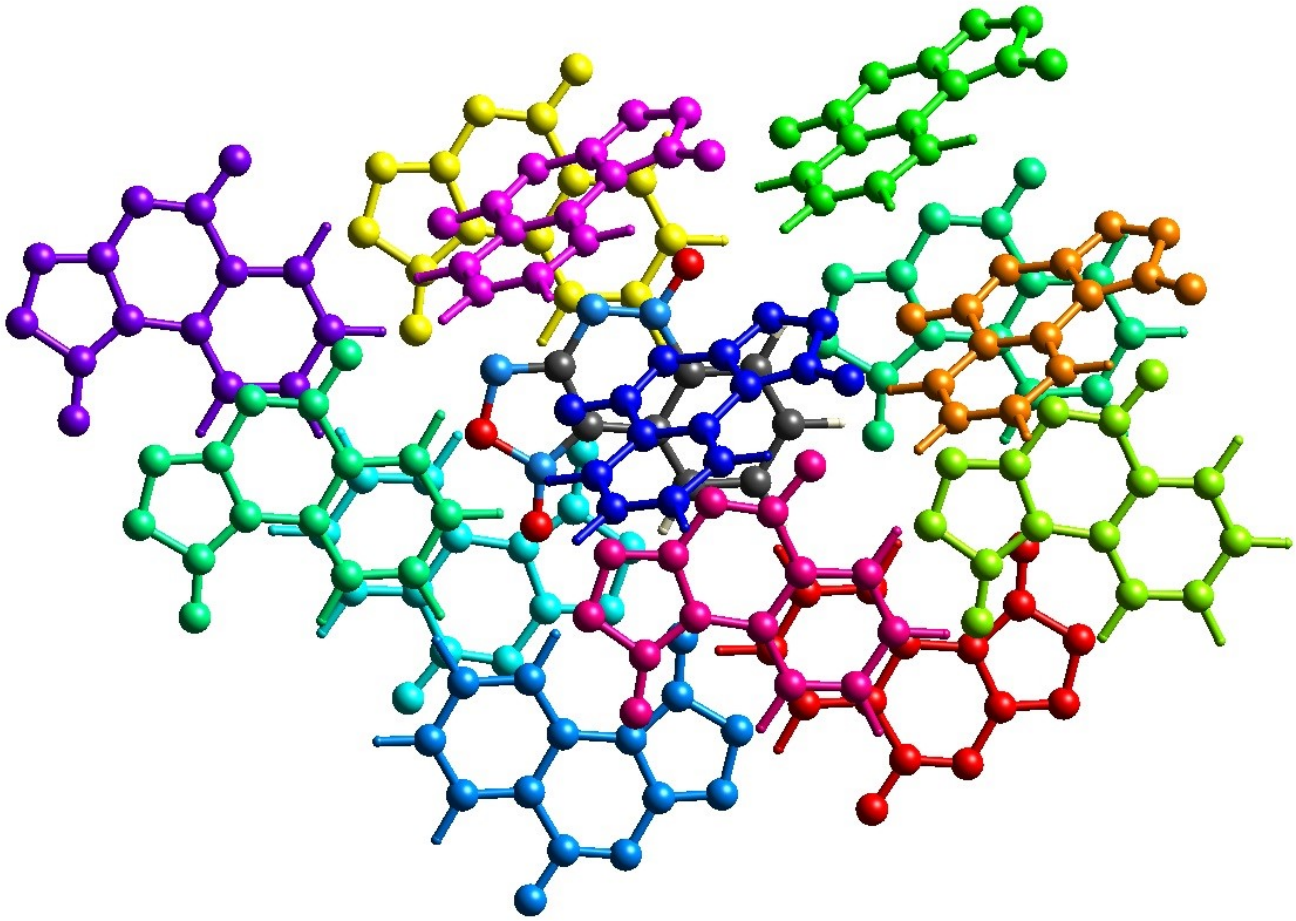


Fig. S5 Cluster of 13 molecules of compound **7** asymmetric unit molecule C

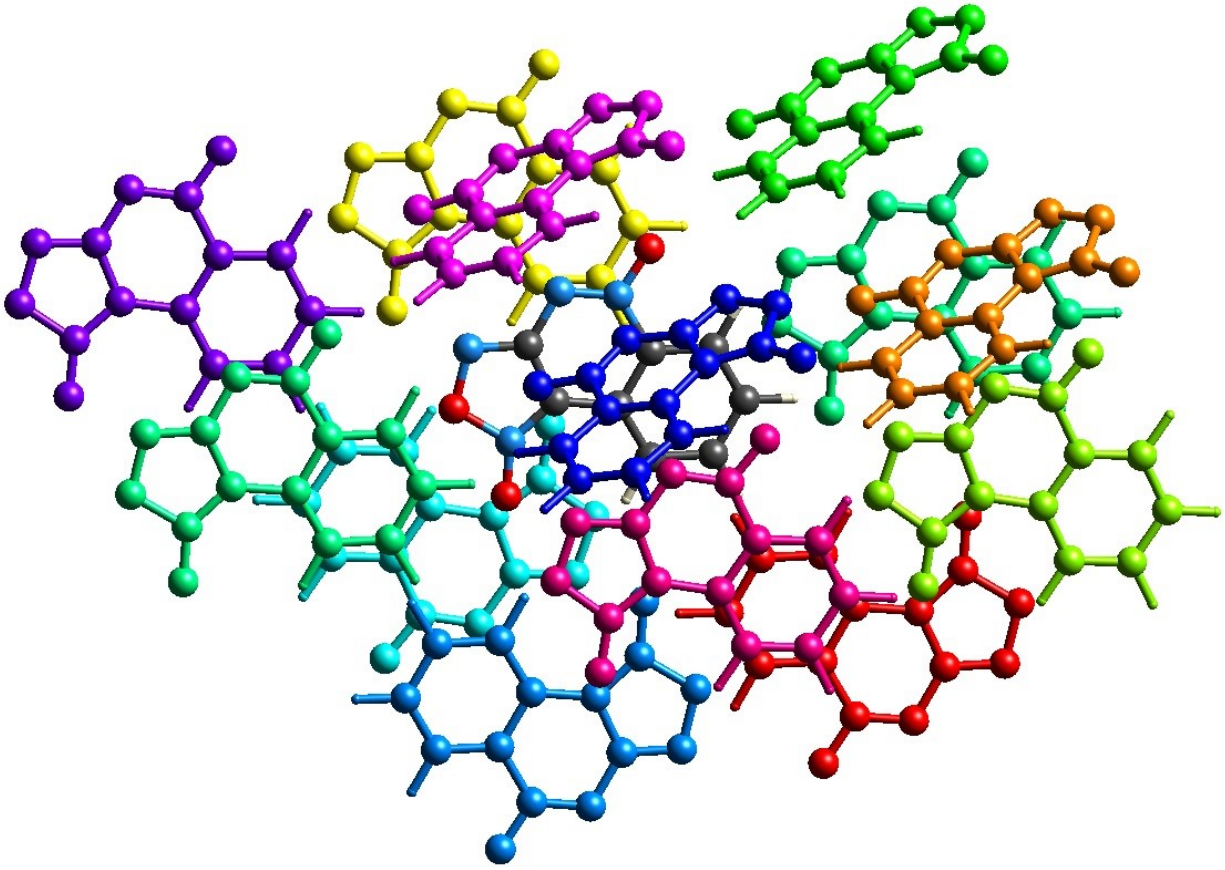


Table S5 Intermolecular interaction energy of 13 molecules cluster of compound **7** asymmetric unit molecule C

	N	Symop	R	E_ele, kcal·mol^{-1}	E_pol, kcal·mol^{-1}	E_dis, kcal·mol^{-1}	E_rep, kcal·mol^{-1}	E_tot, kcal·mol^{-1}
	1	–x, –y, –z	9.73	0.96	–0.24	–1.10	0.38	0.12
	1	—	8.96	–1.15	-0.45	–2.06	1.27	–2.56
	1	—	5.25	0.29	–0.67	–7.29	3.73	–4.25
	1	—	9.71	–2.58	–0.36	–1.58	2.15	–3.04
	1	—	8.54	–2.39	–0.69	–3.04	3.94	–3.25
	2	x, y, z	8.1	-0.05	–0.48	–5.26	2.82	–3.25
	1	—	5.69	–3.90	–0.60	–6.52	4.66	–7.34
	1	–x, –y, –z	7.62	–4.92	–0.67	–2.56	4.33	–5.26
	1	—	5.21	–2.01	–0.91	–6.02	4.37	–5.33

	1	—	9.79	–2.34	–0.33	–1.39	1.70	–2.87
	1	—	5.08	–3.80	–1.20	–7.36	7.03	–6.98
	1	—	5.02	–0.45	–0.76	–8.58	5.33	–5.23
Total energy of cluster, kcal·mol^{-1}				–22.35	–7.36	–52.75	41.71	–49.24

Fig. S6 Cluster of 14 molecules of compound **6**

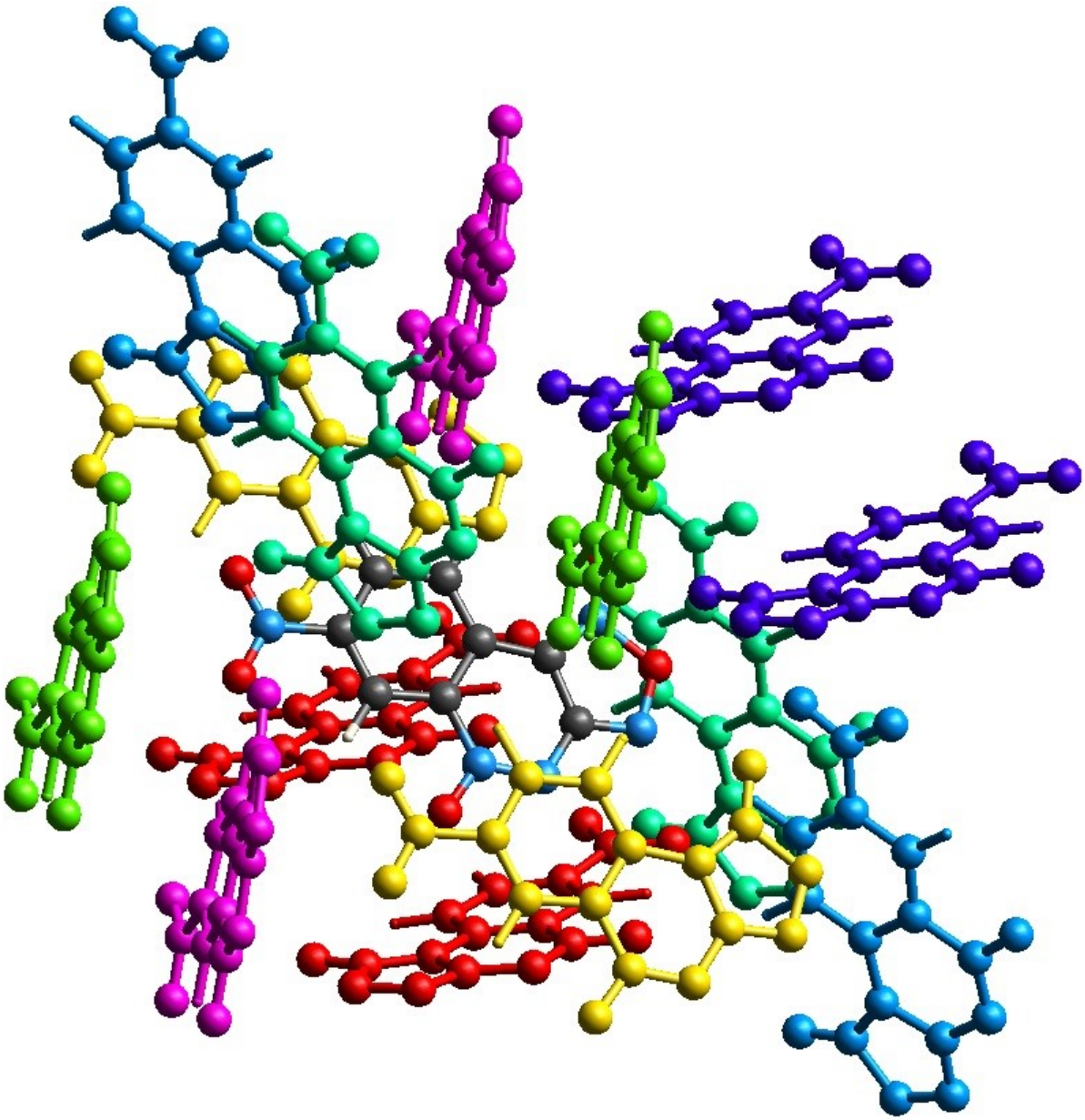


Table S6 Intermolecular interaction energy of 14 molecules cluster of compound **6**

	N	Symop	R	E_ele, kcal·mol^{-1}	E_pol, kcal·mol^{-1}	E_dis, kcal·mol^{-1}	E_rep, kcal·mol^{-1}	E_tot, kcal·mol^{-1}
	2	–x, -y, z+1/2	5.10	–6.74	–2.25	–15.49	14.05	–13.58
	2	x, y, z	6.14	–1.24	–1.53	–11.57	7.41	–7.98
	2	–x+1/2, y+1/2, z+1/2	7.42	–7.31	–1.48	–9.99	10.76	–10.90
	2	x+1/2, -y+1/2, z	7.58	–1.43	–0.62	–7.07	5.31	–4.88
	2	x+1/2, -y+1/2, z	9.76	–2.87	–0.48	–3.35	2.63	–4.64
	2	–x, -y, z+1/2	8.71	–3.25	–0.33	–3.78	1.29	–6.17
	2	–x+1/2, y+1/2, z+1/2	7.42	–4.35	–1.00	–6.17	6.55	–6.69
Total energy of cluster, kcal·mol^{-1}				–27.20	–7.70	–57.41	47.99	–54.83

Fig. S7 Cluster of 14 molecules of compound **3**

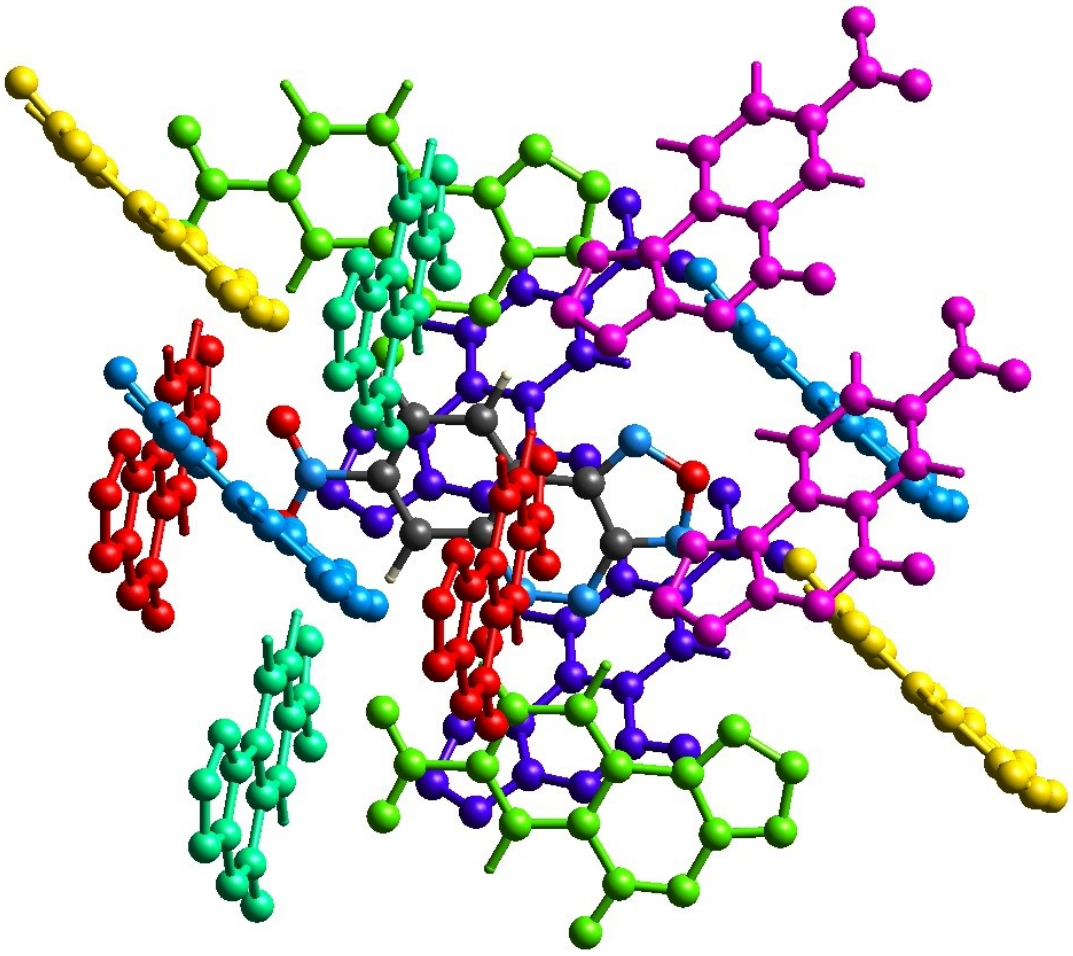


Table S7 Intermolecular interaction energy of 14 molecules cluster of compounds **3**

	N	Symop	R	E_ele, kcal·mol^{-1}	E_pol, kcal·mol^{-1}	E_dis, kcal·mol^{-1}	E_rep, kcal·mol^{-1}	E_tot, kcal·mol^{-1}
	2	-x+1/2, y+1/2, z+1/2	7.18	–5.83	–1.29	–9.32	9.18	–9.61
	2	x+1/2, -y+1/2, z	9.91	–2.49	-0.53	–3.25	3.35	–3.82
	2	x, y, z	6.39	–0.76	-1.39	–9.42	5.50	–6.64
	2	–x+1/2, y+1/2, z+1/2	7.18	–4.25	-1.00	–6.31	6.45	–6.74
	2	x+1/2, -y+1/2, z	7.57	–1.91	-0.62	–6.64	4.21	–5.64
	2	–x, –y, z+1/2	5.10	–5.98	-2.15	–14.96	13.15	–12.81
	2	–x, –y, z+1/2	8.74	–2.01	-0.29	–2.49	0.33	–4.35
Total energy of cluster, kcal·mol^{-1}				–23.23	-7.27	–52.39	42.16	–49.62

Fig. S8 Cluster of 12 molecules of compound **5**

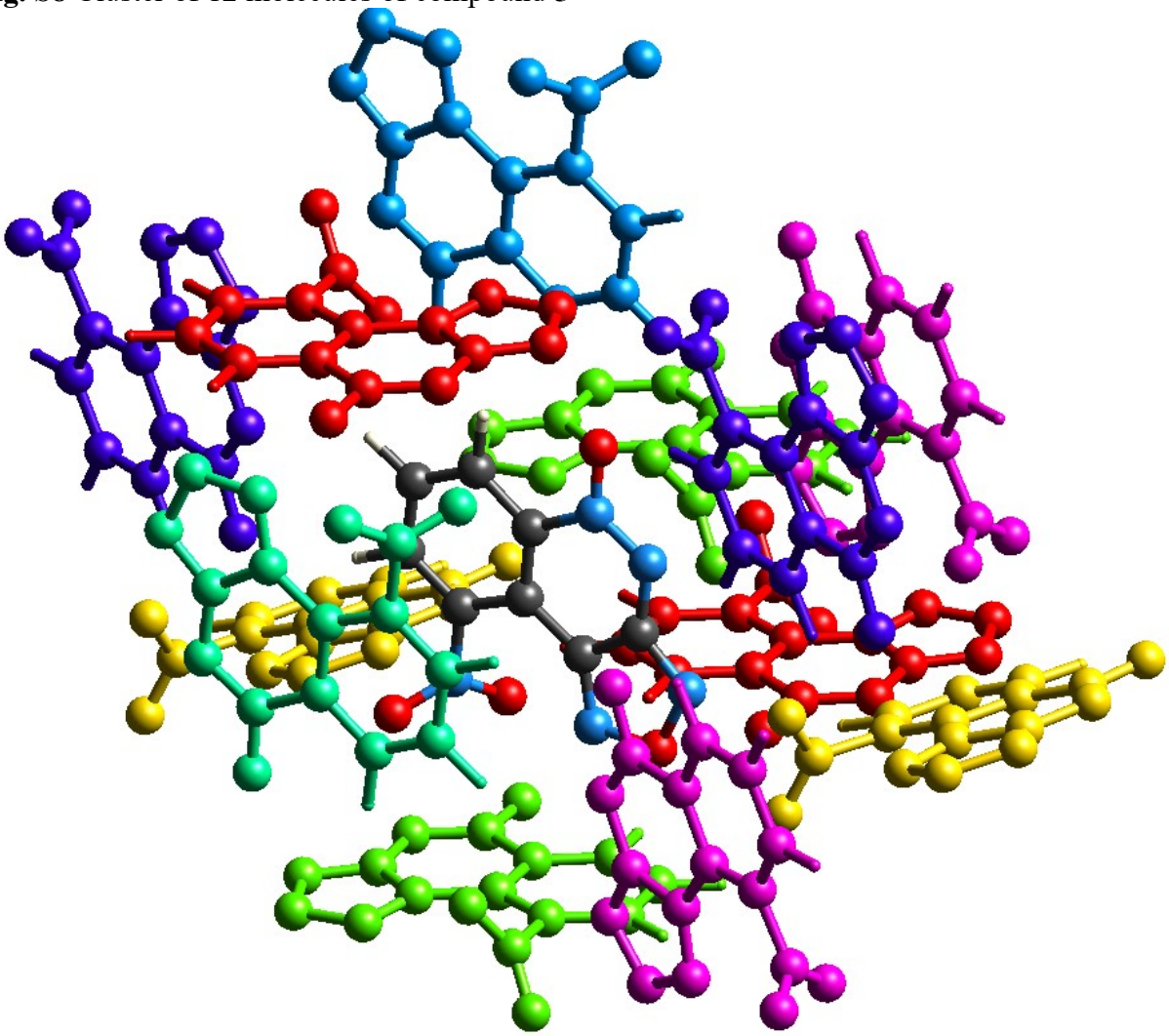


Table S8 Energy of 12 molecules cluster of compounds **5**

	N	Symop	R	E_ele, kcal·mol^{-1}	E_pol, kcal·mol^{-1}	E_dis, kcal·mol^{-1}	E_rep, kcal·mol^{-1}	E_tot, kcal·mol^{-1}
	2	–x+1/2, y+1/2, z	6.79	–2.58	–1.39	–7.84	6.31	–6.69
	2	x, –y+1/2, z+1/2	8.29	–3.87	–1.10	–5.74	7.89	–5.07
	2	x+1/2, –y+1/2, –z	5.44	–9.94	–1.91	–14.10	11.81	–16.92
	1	–x, –y, –z	4.33	–1.91	–1.74	–13.86	10.13	–9.13
	1	–x, –y, –z	7.76	–1.53	–0.74	–4.33	3.32	–3.92
	2	–x+1/2, –y, z+1/2	8.87	–8.32	–1.63	–5.31	6.17	–10.85
	2	x+1/2, y, –z+1/2	7.5	–2.49	–0.53	–5.11	1.82	–6.31
Total energy of cluster, kcal·mol^{-1}				–30.64	–9.03	–56.29	47.44	–58.89

Fig. S9 Relationship "Lattice energy–Density" and "Lattice energy–Energy of electrostatic interactions" for the 50 deepest minima obtained as a result of scanning PES compounds **2**, **4**, **8**

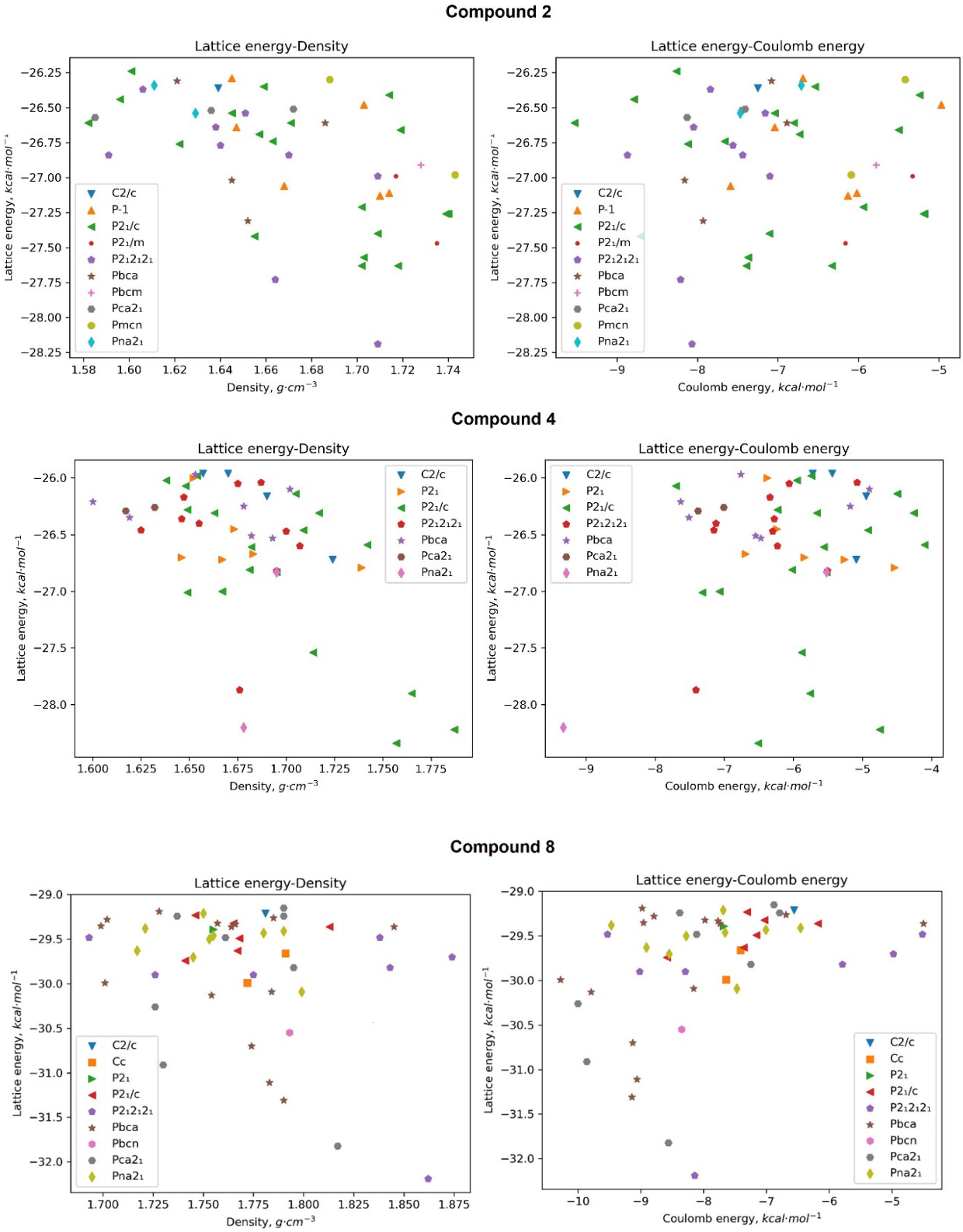


Fig. S10 2D fingerprint plots of Hirshfeld surface of main close contacts for compound **1**.

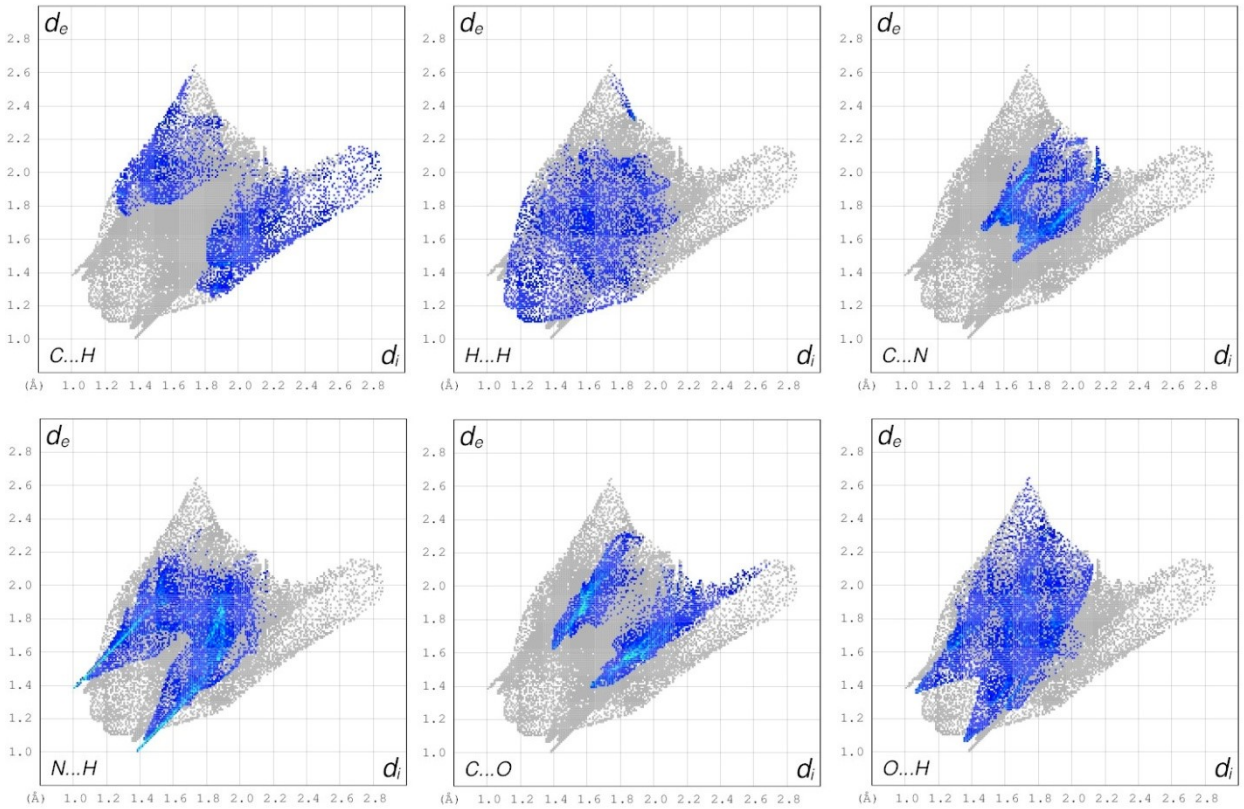


Fig. S11 2D fingerprint plots of Hirshfeld surface of main close contacts for compound **3**.

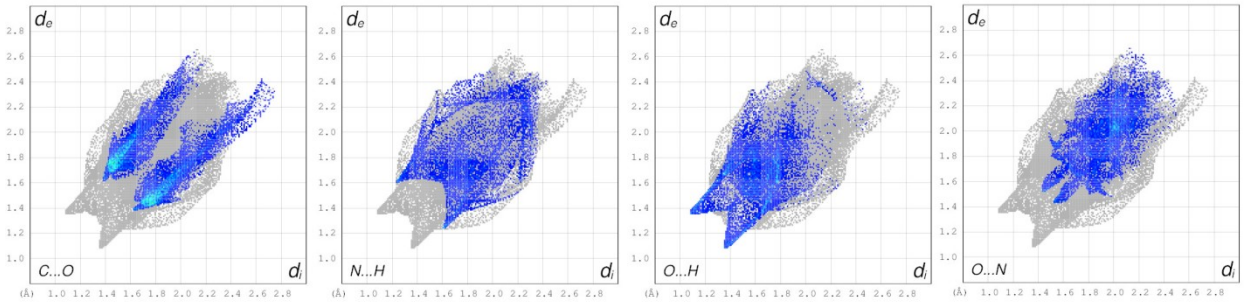


Fig. S12 2D fingerprint plots of Hirshfeld surface of main close contacts for compound **6**.

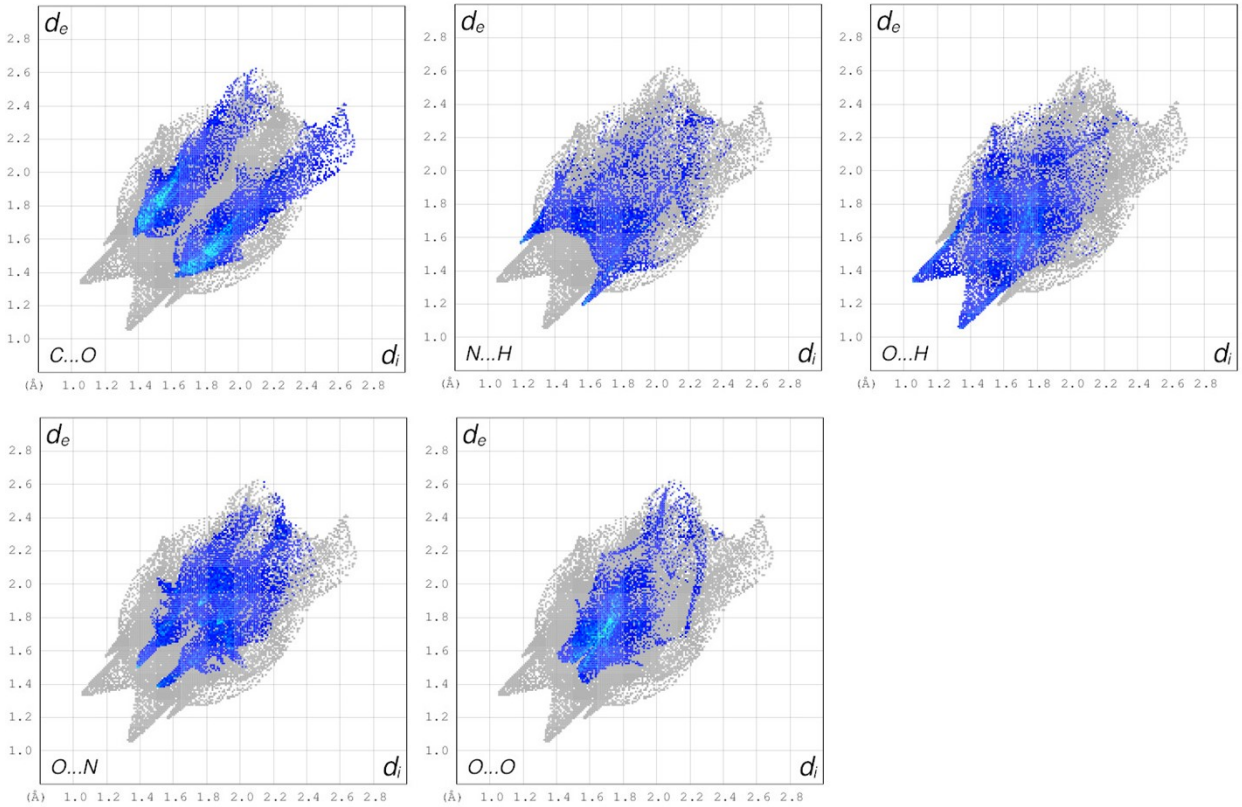


Fig. S13 2D fingerprint plots of Hirshfeld surface of main close contacts for compound **5**.

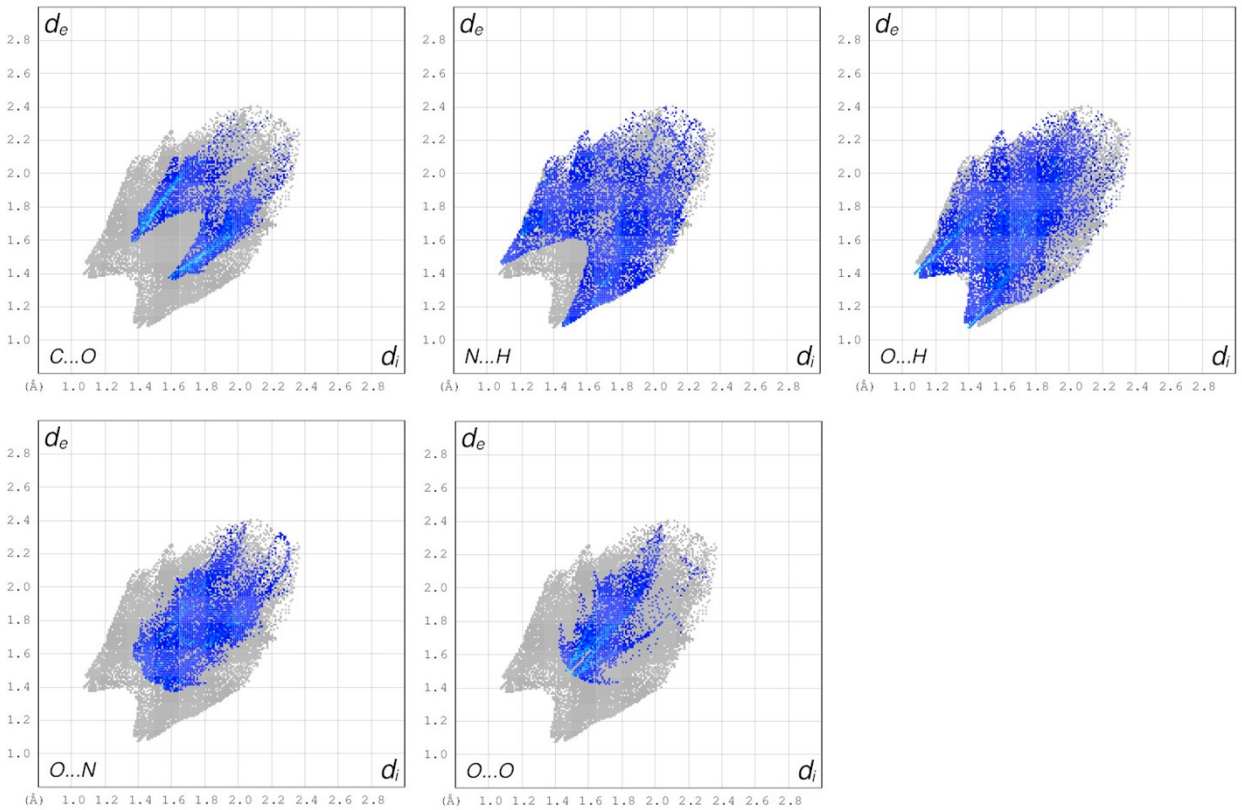
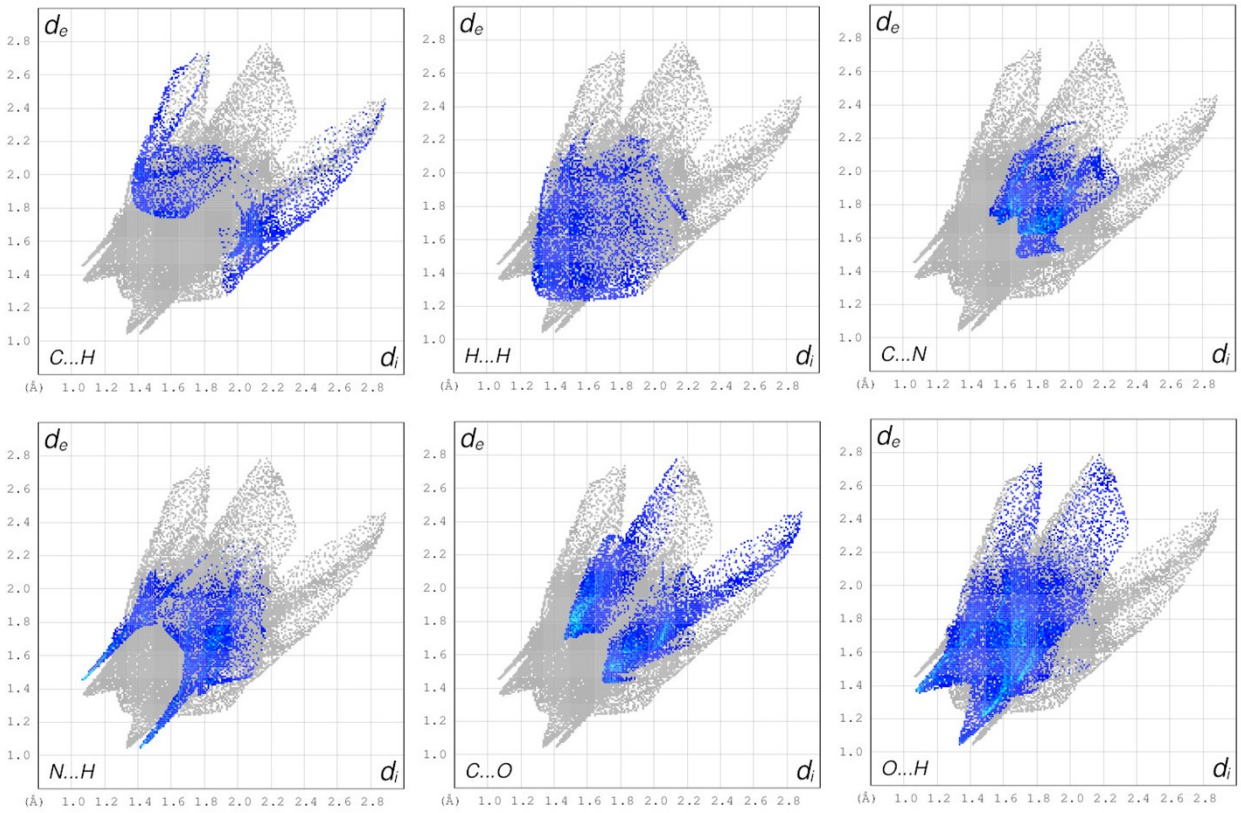
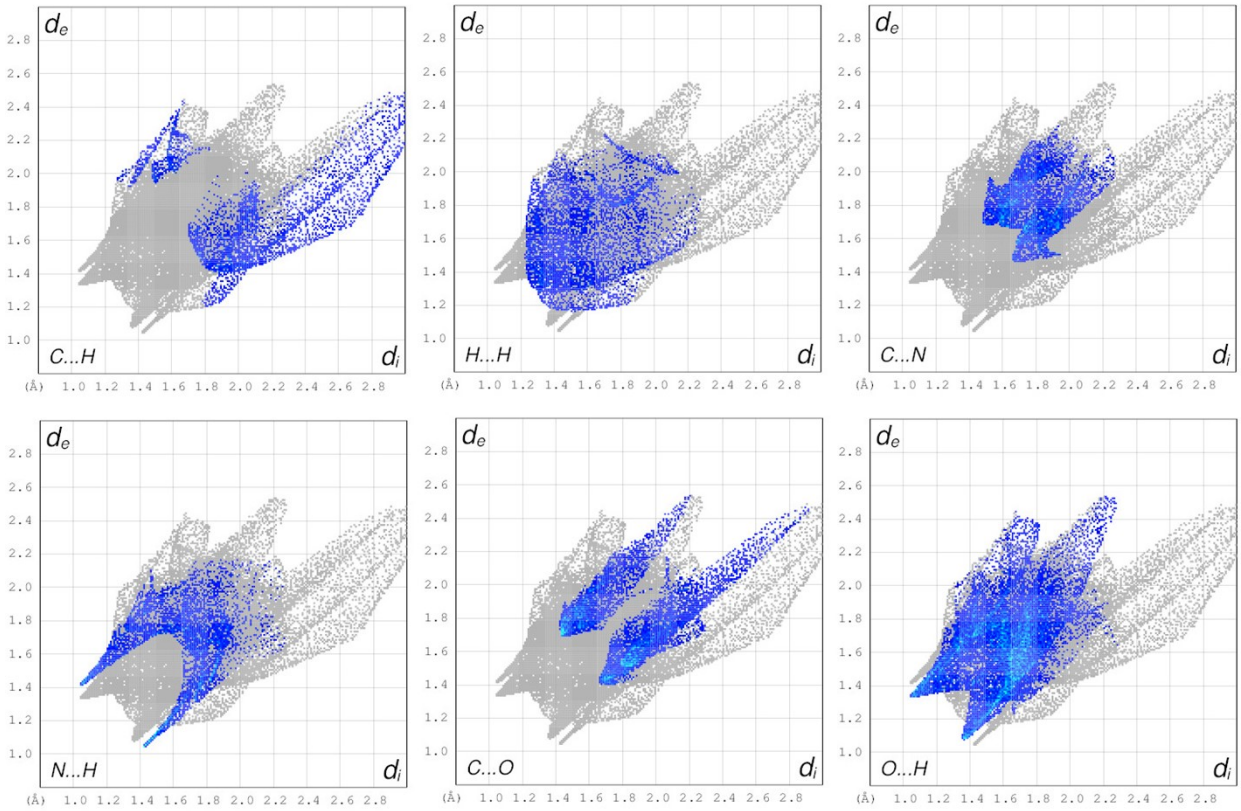


Fig. S14 2D fingerprint plots of Hirshfeld surface of main close contacts for compound **7**.

A



B



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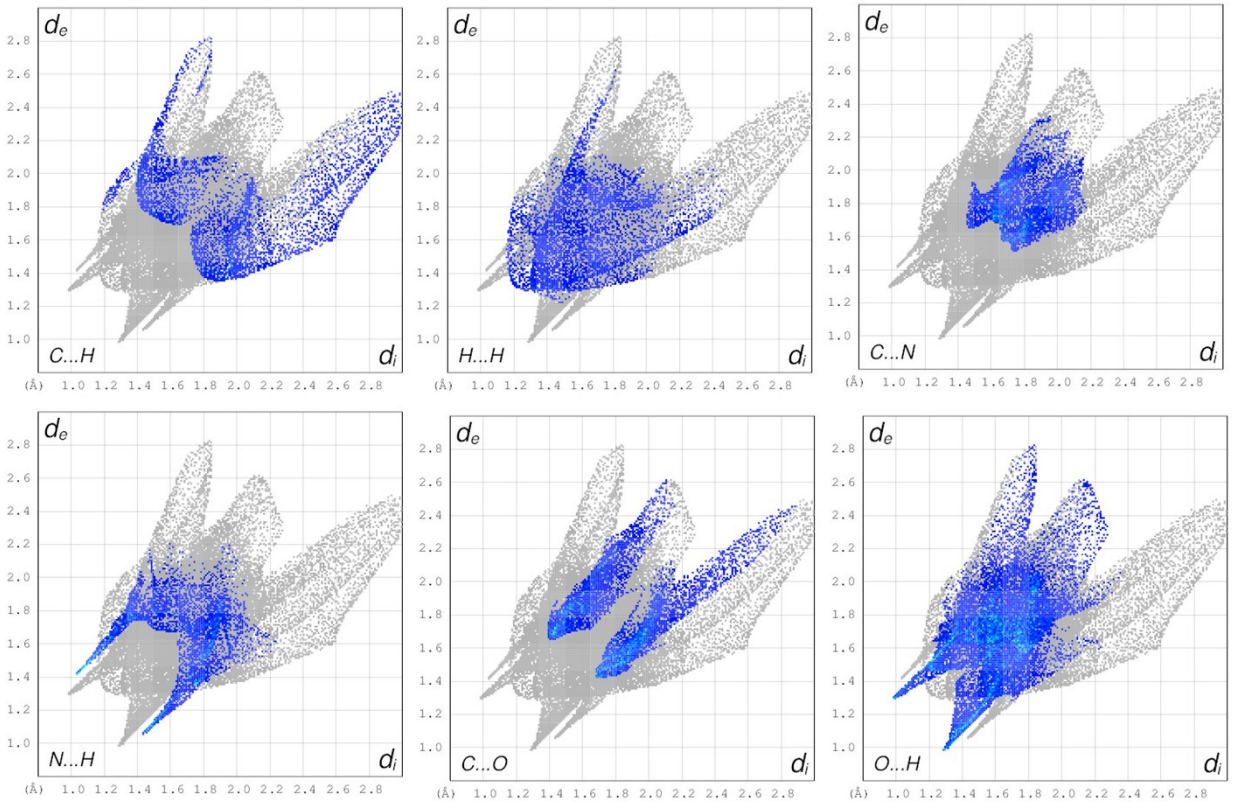
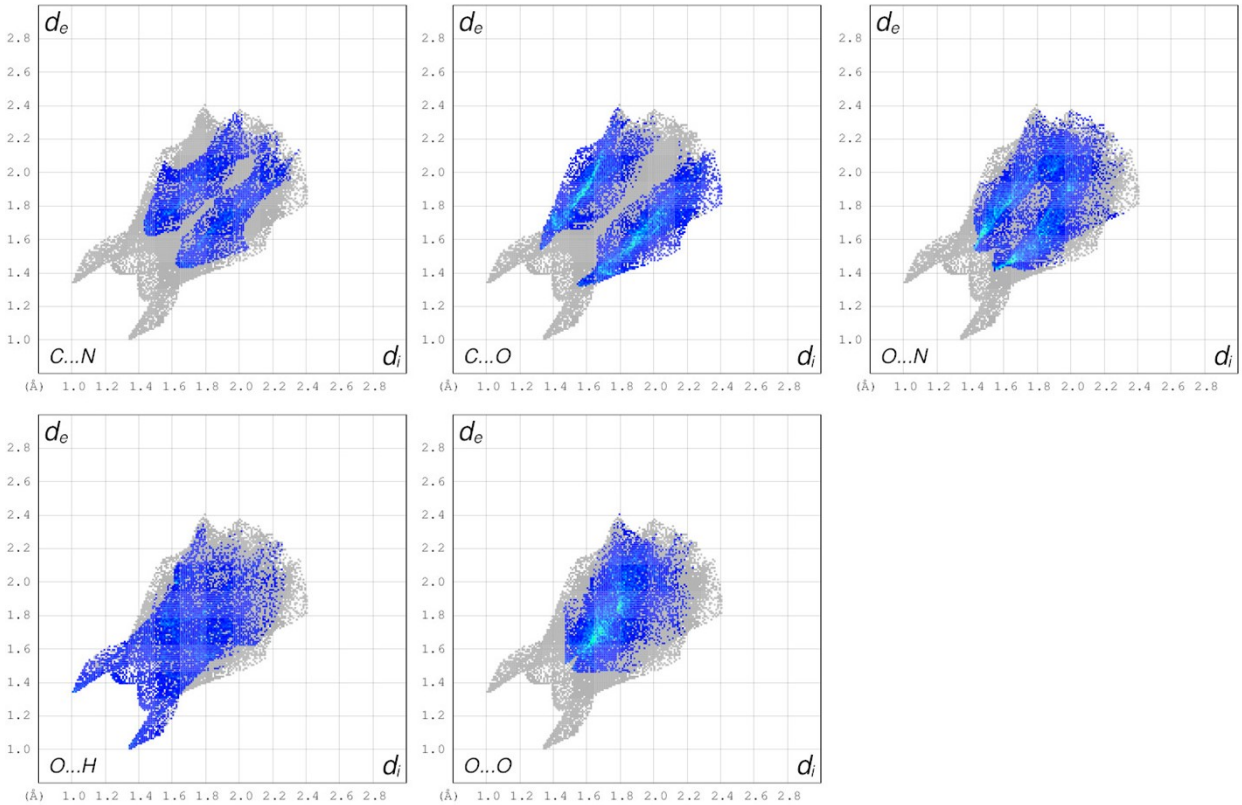


Fig. S15 2D fingerprint plots of Hirshfeld surface of main close contacts for compound **8**.



Experimental section

X-ray diffraction data were collected at 100K on a four-circle Rigaku Synergy S diffractometer equipped with a HyPix6000HE area-detector (kappa geometry, shutterless ω-scan technique), using graphite monochromatized Cu K_α-radiation. The intensity data were integrated and corrected for absorption and decay by the CrysAlisPro program[1]. The structure was solved by direct methods using SHELXT[2] and refined on F^2 using SHELXL-2018[3] in the OLEX2 program[4] . All non-hydrogen atoms were refined with individual anisotropic displacement parameters. All hydrogen atoms were placed in ideal calculated positions and refined as riding atoms with relative isotropic displacement parameters. The Mercury program suite[5] was used for molecular graphics. Detailed crystallographic information is given in Table S9.

^{1}H, ^{14}N and ^{13}C spectra were recorded on a Bruker AM300 spectrometer, operating at 300.13, 21.69 MHz, and 75.47 MHz, respectively. Chemical shifts are reported in delta (δ) units, parts per million (ppm) downfield from external Me_4Si (^{1}H, ^{13}C) or CH_3NO_2 (^{14}N negative values of δ_N correspond to upfield shifts).

[1,2,5]Oxadiazolo[3,4-*c*]cinnoline 1,5-dioxide **7** was prepared by the known method.[6]

[1,2,5]Oxadiazolo[3,4-*c*]cinnoline 5-oxide (1).

A. A solutions of HNO_3 (63 mg, 1 mmol) in Ac_2O (1 mL) and 93% H_2SO_4 (200 mg, 2 mmol) in Ac_2O (1 mL) was added successively and quickly to a solution of 3-amino-4-phenylfurazan (**9**) (161 mg, 1 mmol) in Ac_2O (2 mL) at 0 °C with vigorous stirring. Cooling was removed, the reaction mixture was stirred at 20–25 °C for 30 min and poured into ice water (40 mL). The mixture was stirred for 30 min to complete the hydrolysis of Ac_2O and extracted with CH_2Cl_2 (3×5 mL). The combined organic extracts were dried ($MgSO_4$) and evaporated *in vacuo*. Cinnoline 5-oxide **1** was isolated by preparative chromatography (silica gel, $CHCl_3$ as eluent) and obtained in a yield of 96 mg (51 %), m.p. 165 °C (lit. 167–169 °C[7]), and its NMR ^{1}H, ^{13}C, ^{14}N spectra are identical to the earlier synthesized compound **1**[7].

B. A 93% H_2SO_4 (0.5 g, 5 mmol) was dissolved in $(CF_3CO)_2O$ (6 mL) at room temperature for 2.5 h. Then a solution of 3-nitramino-4-phenylfurazan (**11**) (412 mg, 2 mmol) in CH_2Cl_2 (5 mL) was added to acid mixture at 15–20 °C with vigorous stirring. The reaction mixture was stirred at 20–25 °C for 20 min, the organic layer was separated from the acid by decantation, and poured into ice water (20 ml). The reaction mixture was extracted with CH_2Cl_2 (3×5 mL), the combined organic extracts were dried ($MgSO_4$) and evaporated *in vacuo*. Cinnoline 5-oxide **1** was obtained in a yield of 157 mg (42 %).

Nitration of [1,2,5]oxadiazolo[3,4-*c*]cinnoline 5-oxide (1).

Compound **1** (273 mg, 1.45 mmol) was added at mixing under argon to a solution of $(NO_2)_2S_2O_7$ (3.54 g, 13 mmol) in HNO_3 (1.5 g·cm^{-3}, 8 mL) at 20 °C. The reaction mixture, equipped with a $CaCl_2$ tube, was refluxed at 100–105 °C for 100 h and poured into ice water (100 mL). The residue was filtered, washed with H_2O (2×20 mL). The mixture of nitrocinnoline 5-oxides **3**, **5** and **8** was separated by preparative chromatography (silica gel, $CHCl_3$ as eluent). 7-Nitrocinnoline 5-oxide **3** and 9-nitrocinnoline 5-oxide **5** were isolated in a yields of 50 mg (15 %) and 67 mg (20 %), respectively. The resulting mixture of compounds **5** and **8** was further separated by TLC (silica gel, benzene as eluent), and compound **8** was obtained (2 mg, 1 %). ^{1}H NMR, δ, ppm: (acetone-d_6) 9.51 (s, 1H), 9.63 (s, 1H); (CD_3OD) 9.34 (s, 1H), 9.55 (s, 1H); ^{14}N NMR, δ, ppm (CD_3OD): –18; –22 ($2NO_2$), –55 (N→O).

Nitration of 9-nitro-[1,2,5]oxadiazolo[3,4-*c*]cinnoline 5-oxide (5).

Compound **5** (62 mg, 0.3 mmol) was added at mixing under argon to a solution of $(NO_2)_2S_2O_7$ (1.06 g, 4 mmol) in HNO_3 (1.5 g·cm^{-3}, 1 mL) at 20 °C. The reaction mixture, equipped with a $CaCl_2$ tube, was refluxed at 80–85 °C for 120 h and poured into ice water (10 mL). The residue was filtered, washed with H_2O (3×2 mL) and dried. The resulting crystals were a mixture of compounds **5** (main) and **8** (traces) according TLC ($CHCl_3$). The residue was washed with CD_3OD (0.5 mL) with heating to give a solution of a mixture of compounds **5** and **8** with a ratio ~1 : 1 (^{1}H NMR). Evaporation of CD_3OD in *vacuo* gave 0.4 mg of the mixture. The crystals obtained after washing the precipitate with CD_3OD were pure compound **5** (60 mg) according TLC ($CHCl_3$).

SXRD experiments

Table S9 Crystallographic data for structures **1**, **3**, and **5**–**8**

Compound	**1**	**3**	**5**	**6**	**7**	**8**
CCDC	2288834	2288835	2288836	2288837	2288838	2295832
Formula	$C_8H_4N_4O_2$	$C_8H_3N_5O_4$	$C_8H_3N_5O_4$	$C_8H_3N_5O_5$	$C_8H_4N_4O_3$	$C_8H_2N_6O_6$
M, g cm^{-3}	188.15	233.15	233.15	249.15	204.15	278.16
T, K	100					
Crystal	monoclinic	orthorhombic	orthorhombic	orthorhombic	monoclinic	orthorhombic
Space group	$P2_1/c$	$Pna2_1$	$Pbca$	$Pna2_1$	$P2_1/c$	$Pca2_1$
Z/Z'	4 / 1	4 / 1	8 / 1	4 / 1	12 / 3	4 / 1
a, Å	7.74397(15)	14.2846(2)	8.6598(2)	14.40027(12)	8.09790(10)	12.53304(19)
b, Å	5.37413(10)	9.99780(10)	12.7026(3)	10.46252(9)	15.91000(10)	8.30693(13)
c, Å	18.7390(3)	6.38630(10)	15.5750(4)	6.13809(5)	18.71190(10)	9.61288(13)
β, °	99.3886(18)	90	90	90	95.2870(10)	90

V, Å^3	769.42(2)	912.06(2)	1713.28(7)	924.783(13)	2400.54(4)	1000.81(3)
d_{calc},g cm^{-3}	1.624	1.698	1.808	1.790	1.695	1.846
μ, см$^{-1}$	10.51	12.29	13.08	13.44	11.63	14.32
$2\theta_{max}$, °	155.2	155.6	155.3	155.4	155.7	159.6
Collected reflns.	8675	6846	10416	11803	32530	12518
Independent reflns.	1627	1472	1824	1716	5114	1908
Reflns with. I>2s(I)	1531	1441	1680	1703	4842	1884
R_1	0.0382	0.0238	0.0439	0.0308	0.0357	0.0322
wR_2	0.1047	0.0625	0.1247	0.0831	0.0983	0.0882
GOF	1.041	1.075	1.059	1.077	1.034	1.058
Residual density, e Å^{-3}(d_{max}/d_{min})	0.212/–0.333	0.129/–0.154	0.485/–0.318	0.194/–0.203	0.266/–0.303	0.262/–0.202

X-ray experiment details for compound 1

Table S10 Atomic coordinates (x10^4) and equivalent isotropic displacement parameters (Å^{2}x10^3) for CCDC 2288834. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(2)	2618(1)	4976(2)	4341(1)	34(1)
O(6)	7275(1)	6906(2)	2472(1)	31(1)
N(6)	6524(1)	5995(2)	2952(1)	24(1)
N(5)	5069(1)	7003(2)	3067(1)	27(1)
N(1)	3930(1)	3183(2)	4463(1)	29(1)
N(3)	2880(2)	6634(2)	3806(1)	32(1)
C(12)	6604(2)	2681(2)	3882(1)	22(1)
C(7)	7373(2)	3864(2)	3346(1)	22(1)
C(13)	4977(2)	3750(2)	4007(1)	23(1)
C(11)	7447(2)	656(2)	4254(1)	25(1)
C(4)	4332(2)	5864(2)	3600(1)	25(1)
C(8)	8970(2)	3059(2)	3180(1)	26(1)
C(10)	9026(2)	-154(2)	4083(1)	27(1)
C(9)	9782(2)	1053(3)	3551(1)	28(1)

Table S11 Bond lengths [Å] and angles [°] for CCDC 2288834.

O(2)-N(1)	1.3918(15)

O(2)-N(3)	1.3815(15)
O(6)-N(6)	1.2483(13)
N(6)-N(5)	1.2995(15)
N(6)-C(7)	1.4603(15)
N(5)-C(4)	1.3721(17)
N(1)-C(13)	1.3056(16)
N(3)-C(4)	1.3140(17)
C(12)-C(7)	1.4014(16)
C(12)-C(13)	1.4382(17)
C(12)-C(11)	1.3954(17)
C(7)-C(8)	1.3922(17)
C(13)-C(4)	1.4141(17)
C(11)-H(11)	0.9500
C(11)-C(10)	1.3831(18)
C(8)-H(8)	0.9500
C(8)-C(9)	1.3778(18)
C(10)-H(10)	0.9500
C(10)-C(9)	1.3967(18)
C(9)-H(9)	0.9500
N(3)-O(2)-N(1)	112.05(9)
O(6)-N(6)-N(5)	118.34(10)
O(6)-N(6)-C(7)	116.64(10)
N(5)-N(6)-C(7)	125.02(10)
N(6)-N(5)-C(4)	114.20(10)
C(13)-N(1)-O(2)	104.26(10)
C(4)-N(3)-O(2)	104.17(10)
C(7)-C(12)-C(13)	114.93(11)
C(11)-C(12)-C(7)	119.49(11)
C(11)-C(12)-C(13)	125.57(11)
C(12)-C(7)-N(6)	120.65(11)
C(8)-C(7)-N(6)	118.25(11)
C(8)-C(7)-C(12)	121.10(11)
N(1)-C(13)-C(12)	131.84(12)
N(1)-C(13)-C(4)	109.77(11)
C(4)-C(13)-C(12)	118.35(11)
C(12)-C(11)-H(11)	120.3
C(10)-C(11)-C(12)	119.31(12)
C(10)-C(11)-H(11)	120.3
N(5)-C(4)-C(13)	126.81(11)
N(3)-C(4)-N(5)	123.44(12)

N(3)-C(4)-C(13)	109.75(11)
C(7)-C(8)-H(8)	120.7
C(9)-C(8)-C(7)	118.63(11)
C(9)-C(8)-H(8)	120.7
C(11)-C(10)-H(10)	119.7
C(11)-C(10)-C(9)	120.55(12)
C(9)-C(10)-H(10)	119.7
C(8)-C(9)-C(10)	120.92(11)
C(8)-C(9)-H(9)	119.5
C(10)-C(9)-H(9)	119.5

Table S12 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for CCDC 2288834. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(2)	26(1)	42(1)	34(1)	-5(1)	10(1)	5(1)
O(6)	36(1)	31(1)	26(1)	7(1)	7(1)	-4(1)
N(6)	26(1)	24(1)	22(1)	1(1)	3(1)	-2(1)
N(5)	28(1)	24(1)	27(1)	0(1)	1(1)	3(1)
N(1)	25(1)	37(1)	28(1)	-3(1)	8(1)	2(1)
N(3)	27(1)	34(1)	35(1)	-5(1)	4(1)	6(1)
C(12)	23(1)	25(1)	18(1)	-3(1)	3(1)	0(1)
C(7)	24(1)	22(1)	20(1)	-2(1)	2(1)	0(1)
C(13)	24(1)	26(1)	20(1)	-3(1)	4(1)	-1(1)
C(11)	30(1)	26(1)	20(1)	0(1)	4(1)	1(1)
C(4)	24(1)	26(1)	25(1)	-5(1)	1(1)	2(1)
C(8)	26(1)	32(1)	22(1)	-1(1)	6(1)	0(1)
C(10)	31(1)	26(1)	22(1)	-2(1)	-1(1)	7(1)
C(9)	25(1)	35(1)	24(1)	-5(1)	4(1)	6(1)

Table S13 Hydrogen coordinates ($x10^4$) and isotropic displacement parameters ($Å^2 x\ 10^3$) for CCDC 2288834.

	x	y	z	U(eq)
H(11)	6943	-159	4620	30
H(8)	9488	3876	2818	32

H(10)	9600	-1543	4330	33
H(9)	10872	484	3443	34

Table S14 Torsion angles [°] for CCDC 2288834.

O(2)-N(1)-C(13)-C(12)	177.34(12)
O(2)-N(1)-C(13)-C(4)	-0.39(13)
O(2)-N(3)-C(4)-N(5)	179.80(10)
O(2)-N(3)-C(4)-C(13)	-0.40(13)
O(6)-N(6)-N(5)-C(4)	179.45(10)
O(6)-N(6)-C(7)-C(12)	-178.41(10)
O(6)-N(6)-C(7)-C(8)	2.14(16)
N(6)-N(5)-C(4)-N(3)	178.63(11)
N(6)-N(5)-C(4)-C(13)	-1.13(18)
N(6)-C(7)-C(8)-C(9)	179.84(10)
N(5)-N(6)-C(7)-C(12)	2.07(18)
N(5)-N(6)-C(7)-C(8)	-177.38(11)
N(1)-O(2)-N(3)-C(4)	0.17(13)
N(1)-C(13)-C(4)-N(5)	-179.68(11)
N(1)-C(13)-C(4)-N(3)	0.53(15)
N(3)-O(2)-N(1)-C(13)	0.15(13)
C(12)-C(7)-C(8)-C(9)	0.39(18)
C(12)-C(13)-C(4)-N(5)	2.24(19)
C(12)-C(13)-C(4)-N(3)	-177.55(10)
C(12)-C(11)-C(10)-C(9)	0.69(19)
C(7)-N(6)-N(5)-C(4)	-1.04(17)
C(7)-C(12)-C(13)-N(1)	-178.63(12)
C(7)-C(12)-C(13)-C(4)	-1.06(16)
C(7)-C(12)-C(11)-C(10)	-0.29(18)
C(7)-C(8)-C(9)-C(10)	0.01(18)
C(13)-C(12)-C(7)-N(6)	-0.83(16)
C(13)-C(12)-C(7)-C(8)	178.60(10)
C(13)-C(12)-C(11)-C(10)	-179.01(11)
C(11)-C(12)-C(7)-N(6)	-179.68(10)
C(11)-C(12)-C(7)-C(8)	-0.25(18)
C(11)-C(12)-C(13)-N(1)	0.1(2)
C(11)-C(12)-C(13)-C(4)	177.72(11)
C(11)-C(10)-C(9)-C(8)	-0.56(19)

X-ray experiment details for compound 7

Table S15 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for CCDC 2288838. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1A)	7601(1)	4020(1)	2701(1)	30(1)
O(1B)	7869(1)	696(1)	2317(1)	24(1)
O(1C)	2584(1)	2378(1)	2650(1)	26(1)
O(2A)	2107(1)	4634(1)	4188(1)	27(1)
O(2B)	2551(1)	1012(1)	3966(1)	26(1)
O(2C)	7702(1)	2987(1)	944(1)	26(1)
O(3A)	2999(1)	5858(1)	4771(1)	29(1)
O(3B)	3518(1)	2127(1)	4682(1)	27(1)
O(3C)	6556(1)	4114(1)	291(1)	29(1)
N(1A)	6635(1)	4337(1)	3107(1)	22(1)
N(1B)	6956(1)	928(1)	2782(1)	20(1)
N(1C)	3443(1)	2687(1)	2195(1)	20(1)
N(2A)	5228(1)	3960(1)	3173(1)	24(1)
N(2B)	5534(1)	554(1)	2807(1)	21(1)
N(2C)	4880(1)	2351(1)	2120(1)	21(1)
N(3A)	2743(1)	4070(1)	3727(1)	27(1)
N(3B)	3122(1)	541(1)	3419(1)	25(1)
N(3C)	7234(1)	2464(1)	1477(1)	25(1)
N(4A)	3337(1)	5295(1)	4354(1)	23(1)
N(4B)	3802(1)	1643(1)	4192(1)	21(1)
N(4C)	6367(1)	3594(1)	765(1)	22(1)
C(1A)	7186(1)	5111(1)	3482(1)	21(1)
C(1B)	7584(1)	1604(1)	3263(1)	19(1)
C(1C)	2727(1)	3397(1)	1780(1)	20(1)
C(2A)	8730(2)	5434(1)	3364(1)	24(1)
C(2B)	9164(1)	1913(1)	3194(1)	22(1)
C(2C)	1165(1)	3681(1)	1917(1)	24(1)
C(3A)	9260(2)	6165(1)	3717(1)	26(1)
C(3B)	9751(1)	2559(1)	3647(1)	23(1)
C(3C)	461(2)	4336(1)	1507(1)	26(1)
C(4A)	8266(2)	6567(1)	4185(1)	24(1)
C(4B)	8777(1)	2896(1)	4154(1)	23(1)
C(4C)	1295(2)	4698(1)	963(1)	26(1)

C(5A)	6723(1)	6246(1)	4300(1)	22(1)
C(5B)	7205(1)	2584(1)	4224(1)	21(1)
C(5C)	2861(2)	4421(1)	831(1)	24(1)
C(6A)	6168(1)	5514(1)	3943(1)	20(1)
C(6B)	6604(1)	1929(1)	3777(1)	19(1)
C(6C)	3594(1)	3770(1)	1246(1)	20(1)
C(7A)	4608(1)	5107(1)	3996(1)	21(1)
C(7B)	5030(1)	1525(1)	3789(1)	20(1)
C(7C)	5199(1)	3414(1)	1186(1)	20(1)
C(8A)	4220(1)	4360(1)	3617(1)	22(1)
C(8B)	4585(1)	858(1)	3320(1)	21(1)
C(8C)	5758(1)	2730(1)	1616(1)	20(1)

Table S16 Bond lengths [Å] and angles [°] for CCDC 2288838.

O(1A)-N(1A)	1.2465(13)
O(1B)-N(1B)	1.2485(13)
O(1C)-N(1C)	1.2483(13)
O(2A)-N(3A)	1.3765(14)
O(2A)-N(4A)	1.4630(12)
O(2B)-N(3B)	1.3817(13)
O(2B)-N(4B)	1.4602(12)
O(2C)-N(3C)	1.3794(13)
O(2C)-N(4C)	1.4652(13)
O(3A)-N(4A)	1.2349(14)
O(3B)-N(4B)	1.2352(13)
O(3C)-N(4C)	1.2323(13)
N(1A)-N(2A)	1.3035(14)
N(1A)-C(1A)	1.4663(14)
N(1B)-N(2B)	1.3005(13)
N(1B)-C(1B)	1.4626(14)
N(1C)-N(2C)	1.3000(14)
N(1C)-C(1C)	1.4601(14)
N(2A)-C(8A)	1.3730(16)
N(2B)-C(8B)	1.3719(15)
N(2C)-C(8C)	1.3726(15)
N(3A)-C(8A)	1.3158(16)
N(3B)-C(8B)	1.3159(15)
N(3C)-C(8C)	1.3162(15)

N(4A)-C(7A)	1.3140(15)
N(4B)-C(7B)	1.3157(15)
N(4C)-C(7C)	1.3170(15)
C(1A)-C(2A)	1.3881(16)
C(1A)-C(6A)	1.4015(16)
C(1B)-C(2B)	1.3879(15)
C(1B)-C(6B)	1.4016(16)
C(1C)-C(2C)	1.3887(16)
C(1C)-C(6C)	1.4041(16)
C(2A)-H(2A)	0.9500
C(2A)-C(3A)	1.3863(17)
C(2B)-H(2B)	0.9500
C(2B)-C(3B)	1.3880(16)
C(2C)-H(2C)	0.9500
C(2C)-C(3C)	1.3856(17)
C(3A)-H(3A)	0.9500
C(3A)-C(4A)	1.3978(18)
C(3B)-H(3B)	0.9500
C(3B)-C(4B)	1.3955(17)
C(3C)-H(3C)	0.9500
C(3C)-C(4C)	1.3965(19)
C(4A)-H(4A)	0.9500
C(4A)-C(5A)	1.3846(16)
C(4B)-H(4B)	0.9500
C(4B)-C(5B)	1.3837(16)
C(4C)-H(4C)	0.9500
C(4C)-C(5C)	1.3864(17)
C(5A)-H(5A)	0.9500
C(5A)-C(6A)	1.3971(16)
C(5B)-H(5B)	0.9500
C(5B)-C(6B)	1.3957(15)
C(5C)-H(5C)	0.9500
C(5C)-C(6C)	1.3947(16)
C(6A)-C(7A)	1.4310(15)
C(6B)-C(7B)	1.4287(15)
C(6C)-C(7C)	1.4309(15)
C(7A)-C(8A)	1.4051(16)
C(7B)-C(8B)	1.4047(16)
C(7C)-C(8C)	1.4042(16)

N(3A)-O(2A)-N(4A)	108.39(8)
N(3B)-O(2B)-N(4B)	108.47(8)
N(3C)-O(2C)-N(4C)	108.46(8)
O(1A)-N(1A)-N(2A)	118.35(10)
O(1A)-N(1A)-C(1A)	116.82(10)
N(2A)-N(1A)-C(1A)	124.83(10)
O(1B)-N(1B)-N(2B)	118.15(9)
O(1B)-N(1B)-C(1B)	116.85(9)
N(2B)-N(1B)-C(1B)	125.00(9)
O(1C)-N(1C)-N(2C)	118.13(9)
O(1C)-N(1C)-C(1C)	116.62(9)
N(2C)-N(1C)-C(1C)	125.25(9)
N(1A)-N(2A)-C(8A)	114.68(10)
N(1B)-N(2B)-C(8B)	114.73(9)
N(1C)-N(2C)-C(8C)	114.73(9)
C(8A)-N(3A)-O(2A)	105.53(9)
C(8B)-N(3B)-O(2B)	105.33(9)
C(8C)-N(3C)-O(2C)	105.31(9)
O(3A)-N(4A)-O(2A)	118.07(9)
O(3A)-N(4A)-C(7A)	135.82(10)
C(7A)-N(4A)-O(2A)	106.10(9)
O(3B)-N(4B)-O(2B)	118.18(9)
O(3B)-N(4B)-C(7B)	135.72(10)
C(7B)-N(4B)-O(2B)	106.10(9)
O(3C)-N(4C)-O(2C)	117.91(9)
O(3C)-N(4C)-C(7C)	136.06(11)
C(7C)-N(4C)-O(2C)	106.03(9)
C(2A)-C(1A)-N(1A)	118.24(10)
C(2A)-C(1A)-C(6A)	121.21(11)
C(6A)-C(1A)-N(1A)	120.55(10)
C(2B)-C(1B)-N(1B)	118.39(10)
C(2B)-C(1B)-C(6B)	121.18(10)
C(6B)-C(1B)-N(1B)	120.43(10)
C(2C)-C(1C)-N(1C)	118.49(10)
C(2C)-C(1C)-C(6C)	121.18(10)
C(6C)-C(1C)-N(1C)	120.31(10)
C(1A)-C(2A)-H(2A)	120.7
C(3A)-C(2A)-C(1A)	118.55(11)
C(3A)-C(2A)-H(2A)	120.7
C(1B)-C(2B)-H(2B)	120.9

C(1B)-C(2B)-C(3B)	118.25(11)
C(3B)-C(2B)-H(2B)	120.9
C(1C)-C(2C)-H(2C)	120.7
C(3C)-C(2C)-C(1C)	118.55(11)
C(3C)-C(2C)-H(2C)	120.7
C(2A)-C(3A)-H(3A)	119.6
C(2A)-C(3A)-C(4A)	120.81(11)
C(4A)-C(3A)-H(3A)	119.6
C(2B)-C(3B)-H(3B)	119.5
C(2B)-C(3B)-C(4B)	121.07(11)
C(4B)-C(3B)-H(3B)	119.5
C(2C)-C(3C)-H(3C)	119.6
C(2C)-C(3C)-C(4C)	120.77(11)
C(4C)-C(3C)-H(3C)	119.6
C(3A)-C(4A)-H(4A)	119.7
C(5A)-C(4A)-C(3A)	120.57(11)
C(5A)-C(4A)-H(4A)	119.7
C(3B)-C(4B)-H(4B)	119.7
C(5B)-C(4B)-C(3B)	120.59(11)
C(5B)-C(4B)-H(4B)	119.7
C(3C)-C(4C)-H(4C)	119.6
C(5C)-C(4C)-C(3C)	120.73(11)
C(5C)-C(4C)-H(4C)	119.6
C(4A)-C(5A)-H(5A)	120.4
C(4A)-C(5A)-C(6A)	119.19(11)
C(6A)-C(5A)-H(5A)	120.4
C(4B)-C(5B)-H(5B)	120.5
C(4B)-C(5B)-C(6B)	119.00(11)
C(6B)-C(5B)-H(5B)	120.5
C(4C)-C(5C)-H(5C)	120.5
C(4C)-C(5C)-C(6C)	119.08(11)
C(6C)-C(5C)-H(5C)	120.5
C(1A)-C(6A)-C(7A)	114.12(10)
C(5A)-C(6A)-C(1A)	119.65(10)
C(5A)-C(6A)-C(7A)	126.23(11)
C(1B)-C(6B)-C(7B)	114.06(10)
C(5B)-C(6B)-C(1B)	119.90(10)
C(5B)-C(6B)-C(7B)	126.03(11)
C(1C)-C(6C)-C(7C)	113.97(10)
C(5C)-C(6C)-C(1C)	119.67(11)

C(5C)-C(6C)-C(7C)	126.36(11)
N(4A)-C(7A)-C(6A)	132.11(11)
N(4A)-C(7A)-C(8A)	107.53(10)
C(8A)-C(7A)-C(6A)	120.36(11)
N(4B)-C(7B)-C(6B)	131.92(11)
N(4B)-C(7B)-C(8B)	107.55(10)
C(8B)-C(7B)-C(6B)	120.51(10)
N(4C)-C(7C)-C(6C)	131.96(11)
N(4C)-C(7C)-C(8C)	107.43(10)
C(8C)-C(7C)-C(6C)	120.59(10)
N(2A)-C(8A)-C(7A)	125.43(11)
N(3A)-C(8A)-N(2A)	122.13(11)
N(3A)-C(8A)-C(7A)	112.44(11)
N(2B)-C(8B)-C(7B)	125.18(10)
N(3B)-C(8B)-N(2B)	122.28(10)
N(3B)-C(8B)-C(7B)	112.55(11)
N(2C)-C(8C)-C(7C)	125.07(10)
N(3C)-C(8C)-N(2C)	122.15(10)
N(3C)-C(8C)-C(7C)	112.77(10)

Table S17 Anisotropic displacement parameters ($Å^2$ x10^3) for CCDC 2288838. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1A)	33(1)	26(1)	30(1)	-4(1)	4(1)	5(1)
O(1B)	26(1)	24(1)	24(1)	-4(1)	4(1)	1(1)
O(1C)	27(1)	26(1)	25(1)	5(1)	4(1)	-2(1)
O(2A)	23(1)	27(1)	31(1)	2(1)	0(1)	-6(1)
O(2B)	20(1)	28(1)	28(1)	-1(1)	2(1)	-7(1)
O(2C)	22(1)	30(1)	27(1)	0(1)	3(1)	3(1)
O(3A)	31(1)	29(1)	27(1)	-4(1)	4(1)	1(1)
O(3B)	27(1)	30(1)	23(1)	-3(1)	4(1)	-1(1)
O(3C)	36(1)	29(1)	24(1)	5(1)	5(1)	-3(1)
N(1A)	25(1)	19(1)	22(1)	0(1)	-2(1)	2(1)
N(1B)	21(1)	18(1)	20(1)	1(1)	-2(1)	1(1)
N(1C)	21(1)	18(1)	19(1)	-1(1)	-1(1)	-1(1)
N(2A)	26(1)	19(1)	27(1)	0(1)	-4(1)	-2(1)
N(2B)	21(1)	18(1)	23(1)	0(1)	-2(1)	-2(1)

N(2C)	22(1)	19(1)	22(1)	0(1)	-2(1)	3(1)
N(3A)	27(1)	22(1)	30(1)	2(1)	-3(1)	-4(1)
N(3B)	24(1)	24(1)	26(1)	-1(1)	-1(1)	-5(1)
N(3C)	24(1)	25(1)	24(1)	0(1)	1(1)	4(1)
N(4A)	22(1)	23(1)	24(1)	3(1)	-2(1)	-4(1)
N(4B)	20(1)	22(1)	22(1)	1(1)	-1(1)	-3(1)
N(4C)	23(1)	22(1)	21(1)	-1(1)	0(1)	0(1)
C(1A)	22(1)	19(1)	21(1)	2(1)	-4(1)	-1(1)
C(1B)	20(1)	16(1)	20(1)	1(1)	-3(1)	-1(1)
C(1C)	21(1)	18(1)	20(1)	-2(1)	-3(1)	1(1)
C(2A)	22(1)	26(1)	23(1)	3(1)	0(1)	0(1)
C(2B)	20(1)	22(1)	23(1)	2(1)	1(1)	0(1)
C(2C)	21(1)	25(1)	25(1)	-3(1)	0(1)	1(1)
C(3A)	21(1)	28(1)	27(1)	5(1)	-3(1)	-6(1)
C(3B)	19(1)	24(1)	26(1)	2(1)	-1(1)	-5(1)
C(3C)	23(1)	26(1)	30(1)	-6(1)	-4(1)	7(1)
C(4A)	27(1)	22(1)	22(1)	2(1)	-6(1)	-5(1)
C(4B)	25(1)	22(1)	22(1)	0(1)	-4(1)	-5(1)
C(4C)	31(1)	21(1)	25(1)	-3(1)	-9(1)	6(1)
C(5A)	25(1)	21(1)	19(1)	1(1)	-3(1)	-1(1)
C(5B)	24(1)	21(1)	18(1)	0(1)	0(1)	-1(1)
C(5C)	30(1)	20(1)	20(1)	-1(1)	-3(1)	1(1)
C(6A)	20(1)	19(1)	19(1)	3(1)	-3(1)	-1(1)
C(6B)	19(1)	19(1)	18(1)	3(1)	-2(1)	-1(1)
C(6C)	22(1)	18(1)	18(1)	-2(1)	-3(1)	1(1)
C(7A)	21(1)	19(1)	21(1)	3(1)	-3(1)	-1(1)
C(7B)	19(1)	20(1)	19(1)	2(1)	-1(1)	-1(1)
C(7C)	21(1)	20(1)	18(1)	-2(1)	-1(1)	-1(1)
C(8A)	23(1)	18(1)	23(1)	3(1)	-4(1)	-2(1)
C(8B)	20(1)	19(1)	22(1)	2(1)	-3(1)	-2(1)
C(8C)	21(1)	19(1)	19(1)	-3(1)	-2(1)	1(1)

Table S18 Hydrogen coordinates ($x10^4$) and isotropic displacement parameters ($Å^2$ $x10^3$) for CCDC 2288838

	x	y	z	U(eq)
H(2A)	9408	5159	3047	29

H(2B)	9826	1689	2847	26
H(2C)	592	3431	2283	29
H(3A)	10311	6395	3640	31
H(3B)	10833	2776	3611	28
H(3C)	-603	4541	1596	32
H(4A)	8653	7064	4426	29
H(4B)	9197	3343	4455	28
H(4C)	785	5140	682	32
H(5A)	6049	6522	4618	26
H(5B)	6546	2812	4571	25
H(5C)	3427	4671	462	28

Table S19 Torsion angles [°] for CCDC 2288838

O(1A)-N(1A)-N(2A)-C(8A)	-178.52(9)
O(1A)-N(1A)-C(1A)-C(2A)	-0.29(15)
O(1A)-N(1A)-C(1A)-C(6A)	179.29(10)
O(1B)-N(1B)-N(2B)-C(8B)	-178.46(9)
O(1B)-N(1B)-C(1B)-C(2B)	-2.89(14)
O(1B)-N(1B)-C(1B)-C(6B)	176.95(10)
O(1C)-N(1C)-N(2C)-C(8C)	-179.39(9)
O(1C)-N(1C)-C(1C)-C(2C)	0.20(15)
O(1C)-N(1C)-C(1C)-C(6C)	-178.53(10)
O(2A)-N(3A)-C(8A)-N(2A)	-179.33(10)
O(2A)-N(3A)-C(8A)-C(7A)	0.35(13)
O(2A)-N(4A)-C(7A)-C(6A)	179.89(11)
O(2A)-N(4A)-C(7A)-C(8A)	-0.09(12)
O(2B)-N(3B)-C(8B)-N(2B)	-179.20(9)
O(2B)-N(3B)-C(8B)-C(7B)	0.60(13)
O(2B)-N(4B)-C(7B)-C(6B)	-177.80(11)
O(2B)-N(4B)-C(7B)-C(8B)	0.61(12)
O(2C)-N(3C)-C(8C)-N(2C)	179.37(9)
O(2C)-N(3C)-C(8C)-C(7C)	0.65(13)
O(2C)-N(4C)-C(7C)-C(6C)	-178.06(11)
O(2C)-N(4C)-C(7C)-C(8C)	0.28(12)
O(3A)-N(4A)-C(7A)-C(6A)	-1.0(2)
O(3A)-N(4A)-C(7A)-C(8A)	179.06(12)
O(3B)-N(4B)-C(7B)-C(6B)	1.5(2)
O(3B)-N(4B)-C(7B)-C(8B)	179.93(12)

O(3C)-N(4C)-C(7C)-C(6C)	1.3(2)
O(3C)-N(4C)-C(7C)-C(8C)	179.67(12)
N(1A)-N(2A)-C(8A)-N(3A)	178.48(10)
N(1A)-N(2A)-C(8A)-C(7A)	-1.16(17)
N(1A)-C(1A)-C(2A)-C(3A)	-179.87(10)
N(1A)-C(1A)-C(6A)-C(5A)	179.38(10)
N(1A)-C(1A)-C(6A)-C(7A)	-0.54(15)
N(1B)-N(2B)-C(8B)-N(3B)	-179.26(10)
N(1B)-N(2B)-C(8B)-C(7B)	0.97(16)
N(1B)-C(1B)-C(2B)-C(3B)	179.47(10)
N(1B)-C(1B)-C(6B)-C(5B)	-178.88(10)
N(1B)-C(1B)-C(6B)-C(7B)	1.76(14)
N(1C)-N(2C)-C(8C)-N(3C)	179.95(10)
N(1C)-N(2C)-C(8C)-C(7C)	-1.49(16)
N(1C)-C(1C)-C(2C)-C(3C)	-177.88(10)
N(1C)-C(1C)-C(6C)-C(5C)	176.97(10)
N(1C)-C(1C)-C(6C)-C(7C)	-2.60(15)
N(2A)-N(1A)-C(1A)-C(2A)	179.22(10)
N(2A)-N(1A)-C(1A)-C(6A)	-1.19(16)
N(2B)-N(1B)-C(1B)-C(2B)	176.76(10)
N(2B)-N(1B)-C(1B)-C(6B)	-3.39(16)
N(2C)-N(1C)-C(1C)-C(2C)	179.24(10)
N(2C)-N(1C)-C(1C)-C(6C)	0.50(16)
N(3A)-O(2A)-N(4A)-O(3A)	-179.02(9)
N(3A)-O(2A)-N(4A)-C(7A)	0.31(11)
N(3B)-O(2B)-N(4B)-O(3B)	-179.74(9)
N(3B)-O(2B)-N(4B)-C(7B)	-0.28(11)
N(3C)-O(2C)-N(4C)-O(3C)	-179.42(9)
N(3C)-O(2C)-N(4C)-C(7C)	0.10(11)
N(4A)-O(2A)-N(3A)-C(8A)	-0.40(11)
N(4A)-C(7A)-C(8A)-N(2A)	179.51(11)
N(4A)-C(7A)-C(8A)-N(3A)	-0.16(14)
N(4B)-O(2B)-N(3B)-C(8B)	-0.20(12)
N(4B)-C(7B)-C(8B)-N(2B)	178.99(10)
N(4B)-C(7B)-C(8B)-N(3B)	-0.80(14)
N(4C)-O(2C)-N(3C)-C(8C)	-0.45(11)
N(4C)-C(7C)-C(8C)-N(2C)	-179.29(10)
N(4C)-C(7C)-C(8C)-N(3C)	-0.61(13)
C(1A)-N(1A)-N(2A)-C(8A)	1.97(16)
C(1A)-C(2A)-C(3A)-C(4A)	0.28(17)

C(1A)-C(6A)-C(7A)-N(4A)	-178.71(11)
C(1A)-C(6A)-C(7A)-C(8A)	1.27(15)
C(1B)-N(1B)-N(2B)-C(8B)	1.89(15)
C(1B)-C(2B)-C(3B)-C(4B)	-0.55(17)
C(1B)-C(6B)-C(7B)-N(4B)	179.04(11)
C(1B)-C(6B)-C(7B)-C(8B)	0.80(15)
C(1C)-N(1C)-N(2C)-C(8C)	1.59(15)
C(1C)-C(2C)-C(3C)-C(4C)	0.61(18)
C(1C)-C(6C)-C(7C)-N(4C)	-179.15(11)
C(1C)-C(6C)-C(7C)-C(8C)	2.70(15)
C(2A)-C(1A)-C(6A)-C(5A)	-1.05(17)
C(2A)-C(1A)-C(6A)-C(7A)	179.04(10)
C(2A)-C(3A)-C(4A)-C(5A)	-0.60(18)
C(2B)-C(1B)-C(6B)-C(5B)	0.96(16)
C(2B)-C(1B)-C(6B)-C(7B)	-178.40(10)
C(2B)-C(3B)-C(4B)-C(5B)	0.88(18)
C(2C)-C(1C)-C(6C)-C(5C)	-1.73(16)
C(2C)-C(1C)-C(6C)-C(7C)	178.70(10)
C(2C)-C(3C)-C(4C)-C(5C)	-1.21(18)
C(3A)-C(4A)-C(5A)-C(6A)	0.09(17)
C(3B)-C(4B)-C(5B)-C(6B)	-0.28(17)
C(3C)-C(4C)-C(5C)-C(6C)	0.31(18)
C(4A)-C(5A)-C(6A)-C(1A)	0.71(16)
C(4A)-C(5A)-C(6A)-C(7A)	-179.39(10)
C(4B)-C(5B)-C(6B)-C(1B)	-0.62(16)
C(4B)-C(5B)-C(6B)-C(7B)	178.66(10)
C(4C)-C(5C)-C(6C)-C(1C)	1.13(17)
C(4C)-C(5C)-C(6C)-C(7C)	-179.36(11)
C(5A)-C(6A)-C(7A)-N(4A)	1.4(2)
C(5A)-C(6A)-C(7A)-C(8A)	-178.64(11)
C(5B)-C(6B)-C(7B)-N(4B)	-0.3(2)
C(5B)-C(6B)-C(7B)-C(8B)	-178.51(11)
C(5C)-C(6C)-C(7C)-N(4C)	1.3(2)
C(5C)-C(6C)-C(7C)-C(8C)	-176.84(11)
C(6A)-C(1A)-C(2A)-C(3A)	0.55(17)
C(6A)-C(7A)-C(8A)-N(2A)	-0.48(17)
C(6A)-C(7A)-C(8A)-N(3A)	179.85(10)
C(6B)-C(1B)-C(2B)-C(3B)	-0.37(17)
C(6B)-C(7B)-C(8B)-N(2B)	-2.38(17)
C(6B)-C(7B)-C(8B)-N(3B)	177.83(10)

C(6C)-C(1C)-C(2C)-C(3C)	0.85(17)
C(6C)-C(7C)-C(8C)-N(2C)	-0.72(17)
C(6C)-C(7C)-C(8C)-N(3C)	177.95(10)

X-ray experiment details for compound 6

Table S20 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for CCDC 2288837. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
O(1)	1800(1)	3519(1)	3693(3)	22(1)
N(1)	4257(1)	5504(2)	8283(3)	18(1)
C(1)	3810(1)	5833(2)	6232(3)	17(1)
O(2)	1757(1)	4646(1)	723(3)	22(1)
N(2)	4935(1)	6144(2)	9163(3)	21(1)
C(2)	3115(1)	5024(2)	5477(4)	17(1)
N(3)	5968(1)	7849(2)	8552(4)	26(1)
O(3)	3954(1)	4542(1)	9270(3)	22(1)
C(3)	2719(1)	5333(2)	3508(4)	16(1)
O(4)	6072(1)	8758(1)	6952(3)	27(1)
N(4)	5341(1)	8572(2)	5299(3)	21(1)
C(4)	2947(1)	6424(2)	2311(4)	18(1)
N(5)	2039(1)	4438(2)	2572(3)	17(1)
O(5)	5334(1)	9282(2)	3721(3)	29(1)
C(5)	3642(1)	7214(2)	3087(3)	18(1)
C(6)	4090(1)	6909(2)	5040(4)	17(1)
C(7)	4852(1)	7582(2)	5986(4)	19(1)
C(8)	5244(1)	7171(2)	7958(4)	20(1)

Table S21 Bond lengths [Å] and angles [°] for CCDC 2288837

O(1)-N(5)	1.231(2)
N(1)-C(1)	1.455(3)
N(1)-N(2)	1.302(3)
N(1)-O(3)	1.253(2)
C(1)-C(2)	1.391(3)
C(1)-C(6)	1.401(3)

O(2)-N(5)	1.224(3)
N(2)-C(8)	1.378(3)
C(2)-H(2)	0.9500
C(2)-C(3)	1.375(3)
N(3)-O(4)	1.375(3)
N(3)-C(8)	1.313(3)
C(3)-C(4)	1.397(3)
C(3)-N(5)	1.472(2)
O(4)-N(4)	1.475(2)
N(4)-O(5)	1.221(3)
N(4)-C(7)	1.322(3)
C(4)-H(4)	0.9500
C(4)-C(5)	1.383(3)
C(5)-H(5)	0.9500
C(5)-C(6)	1.399(3)
C(6)-C(7)	1.427(3)
C(7)-C(8)	1.403(3)

N(2)-N(1)-C(1)	124.65(17)
O(3)-N(1)-C(1)	117.07(16)
O(3)-N(1)-N(2)	118.28(18)
C(2)-C(1)-N(1)	117.53(17)
C(2)-C(1)-C(6)	121.45(18)
C(6)-C(1)-N(1)	121.00(17)
N(1)-N(2)-C(8)	114.89(18)
C(1)-C(2)-H(2)	121.7
C(3)-C(2)-C(1)	116.64(18)
C(3)-C(2)-H(2)	121.7
C(8)-N(3)-O(4)	105.20(19)
C(2)-C(3)-C(4)	123.84(18)
C(2)-C(3)-N(5)	118.01(16)
C(4)-C(3)-N(5)	118.12(18)
N(3)-O(4)-N(4)	108.80(14)
O(5)-N(4)-O(4)	118.18(16)
O(5)-N(4)-C(7)	136.48(19)
C(7)-N(4)-O(4)	105.32(17)
C(3)-C(4)-H(4)	120.7
C(5)-C(4)-C(3)	118.6(2)
C(5)-C(4)-H(4)	120.7
O(1)-N(5)-C(3)	117.64(17)

O(2)-N(5)-O(1)	124.37(17)
O(2)-N(5)-C(3)	117.98(17)
C(4)-C(5)-H(5)	120.3
C(4)-C(5)-C(6)	119.50(18)
C(6)-C(5)-H(5)	120.3
C(1)-C(6)-C(7)	113.87(18)
C(5)-C(6)-C(1)	119.92(18)
C(5)-C(6)-C(7)	126.19(18)
N(4)-C(7)-C(6)	131.8(2)
N(4)-C(7)-C(8)	107.52(18)
C(8)-C(7)-C(6)	120.59(18)
N(2)-C(8)-C(7)	124.89(18)
N(3)-C(8)-N(2)	121.9(2)
N(3)-C(8)-C(7)	113.2(2)

Table S22 Anisotropic displacement parameters ($Å^2$ x 10^3) for CCDC 2288837. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	24(1)	19(1)	23(1)	4(1)	-2(1)	-4(1)
N(1)	18(1)	19(1)	17(1)	1(1)	0(1)	4(1)
C(1)	17(1)	18(1)	15(1)	0(1)	0(1)	5(1)
O(2)	25(1)	23(1)	19(1)	2(1)	-6(1)	-1(1)
N(2)	19(1)	25(1)	20(1)	-2(1)	-4(1)	5(1)
C(2)	17(1)	17(1)	17(1)	1(1)	2(1)	2(1)
N(3)	22(1)	29(1)	28(1)	-3(1)	-4(1)	1(1)
O(3)	25(1)	22(1)	20(1)	5(1)	-1(1)	3(1)
C(3)	16(1)	16(1)	17(1)	-1(1)	1(1)	1(1)
O(4)	21(1)	30(1)	29(1)	-4(1)	-5(1)	-6(1)
N(4)	18(1)	24(1)	23(1)	-3(1)	0(1)	-2(1)
C(4)	21(1)	18(1)	17(1)	1(1)	1(1)	1(1)
N(5)	16(1)	16(1)	19(1)	1(1)	-1(1)	2(1)
O(5)	29(1)	30(1)	28(1)	4(1)	3(1)	-10(1)
C(5)	21(1)	16(1)	18(1)	1(1)	1(1)	1(1)
C(6)	16(1)	18(1)	17(1)	-1(1)	3(1)	2(1)
C(7)	17(1)	18(1)	21(1)	-3(1)	2(1)	1(1)
C(8)	17(1)	21(1)	21(1)	-4(1)	0(1)	3(1)

Table S23 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for CCDC 2288837

	x	y	z	U(eq)
H(2)	2923	4295	6282	20
H(4)	2631	6619	994	22
H(5)	3814	7959	2299	22

Table S24 Torsion angles [°] for CCDC 2288837

N(1)-C(1)-C(2)-C(3)	-178.30(16)
N(1)-C(1)-C(6)-C(5)	-179.18(16)
N(1)-C(1)-C(6)-C(7)	2.3(2)
N(1)-N(2)-C(8)-N(3)	-174.78(18)
N(1)-N(2)-C(8)-C(7)	3.4(3)
C(1)-N(1)-N(2)-C(8)	-2.2(3)
C(1)-C(2)-C(3)-C(4)	-3.0(3)
C(1)-C(2)-C(3)-N(5)	174.83(16)
C(1)-C(6)-C(7)-N(4)	175.2(2)
C(1)-C(6)-C(7)-C(8)	-1.3(2)
N(2)-N(1)-C(1)-C(2)	177.86(17)
N(2)-N(1)-C(1)-C(6)	-0.6(3)
C(2)-C(1)-C(6)-C(5)	2.5(3)
C(2)-C(1)-C(6)-C(7)	-176.08(17)
C(2)-C(3)-C(4)-C(5)	3.3(3)
C(2)-C(3)-N(5)-O(1)	6.3(2)
C(2)-C(3)-N(5)-O(2)	-172.77(16)
N(3)-O(4)-N(4)-O(5)	-178.67(18)
N(3)-O(4)-N(4)-C(7)	-0.1(2)
O(3)-N(1)-C(1)-C(2)	-3.0(2)
O(3)-N(1)-C(1)-C(6)	178.63(16)
O(3)-N(1)-N(2)-C(8)	178.58(16)
C(3)-C(4)-C(5)-C(6)	-0.5(3)
O(4)-N(3)-C(8)-N(2)	178.87(17)
O(4)-N(3)-C(8)-C(7)	0.5(2)
O(4)-N(4)-C(7)-C(6)	-176.43(18)
O(4)-N(4)-C(7)-C(8)	0.4(2)

N(4)-C(7)-C(8)-N(2)	-178.90(18)
N(4)-C(7)-C(8)-N(3)	-0.6(2)
C(4)-C(3)-N(5)-O(1)	-175.73(17)
C(4)-C(3)-N(5)-O(2)	5.2(3)
C(4)-C(5)-C(6)-C(1)	-2.2(3)
C(4)-C(5)-C(6)-C(7)	176.12(18)
N(5)-C(3)-C(4)-C(5)	-174.59(16)
O(5)-N(4)-C(7)-C(6)	1.7(4)
O(5)-N(4)-C(7)-C(8)	178.6(2)
C(5)-C(6)-C(7)-N(4)	-3.2(3)
C(5)-C(6)-C(7)-C(8)	-179.69(18)
C(6)-C(1)-C(2)-C(3)	0.1(3)
C(6)-C(7)-C(8)-N(2)	-1.6(3)
C(6)-C(7)-C(8)-N(3)	176.64(18)
C(8)-N(3)-O(4)-N(4)	-0.3(2)

X-ray experiment details for compound 3

Table S25 Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2x10^3$) for CCDC 2288835. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
O(2)	6128(1)	8833(2)	6833(3)	35(1)
O(6)	3895(1)	4574(1)	9105(2)	25(1)
O(15)	1696(1)	3646(1)	3766(3)	26(1)
O(16)	1718(1)	4782(1)	886(3)	32(1)
N(1)	5459(1)	8676(2)	5252(3)	29(1)
N(3)	6025(1)	7911(2)	8420(3)	32(1)
N(5)	4949(1)	6165(2)	9012(3)	25(1)
N(6)	4246(1)	5546(2)	8153(3)	21(1)
N(14)	1988(1)	4560(1)	2653(3)	21(1)
C(4)	5295(1)	7205(2)	7831(3)	24(1)
C(7)	3830(1)	5903(2)	6146(3)	18(1)
C(8)	3101(1)	5103(2)	5430(3)	19(1)
C(9)	2728(1)	5435(2)	3514(3)	19(1)
C(10)	3014(1)	6524(2)	2327(3)	22(1)
C(11)	3741(1)	7305(2)	3072(3)	22(1)
C(12)	4164(1)	6986(2)	4980(3)	20(1)
C(13)	4953(1)	7669(2)	5902(3)	22(1)

Table S26 Bond lengths [Å] and angles [°] for CCDC 2288835

O(2)-N(1)	1.399(2)
O(2)-N(3)	1.378(3)
O(6)-N(6)	1.251(2)
O(15)-N(14)	1.230(2)
O(16)-N(14)	1.213(2)
N(1)-C(13)	1.307(2)
N(3)-C(4)	1.314(2)
N(5)-N(6)	1.301(2)
N(5)-C(4)	1.377(3)
N(6)-C(7)	1.457(2)
N(14)-C(9)	1.478(2)
C(4)-C(13)	1.404(3)
C(7)-C(8)	1.390(2)
C(7)-C(12)	1.398(3)
C(8)-H(8)	0.9500
C(8)-C(9)	1.376(3)
C(9)-C(10)	1.389(3)
C(10)-H(10)	0.9500
C(10)-C(11)	1.383(3)
C(11)-H(11)	0.9500
C(11)-C(12)	1.397(3)
C(12)-C(13)	1.444(2)
N(3)-O(2)-N(1)	112.52(13)
C(13)-N(1)-O(2)	103.56(17)
C(4)-N(3)-O(2)	103.50(17)
N(6)-N(5)-C(4)	113.92(17)
O(6)-N(6)-N(5)	118.31(16)
O(6)-N(6)-C(7)	117.01(15)
N(5)-N(6)-C(7)	124.68(16)
O(15)-N(14)-C(9)	117.80(15)
O(16)-N(14)-O(15)	124.52(16)
O(16)-N(14)-C(9)	117.68(15)
N(3)-C(4)-N(5)	122.25(19)
N(3)-C(4)-C(13)	110.47(18)
N(5)-C(4)-C(13)	127.28(17)
C(8)-C(7)-N(6)	116.98(16)
C(8)-C(7)-C(12)	121.72(17)
C(12)-C(7)-N(6)	121.29(16)

C(7)-C(8)-H(8)	121.8
C(9)-C(8)-C(7)	116.39(16)
C(9)-C(8)-H(8)	121.8
C(8)-C(9)-N(14)	117.75(15)
C(8)-C(9)-C(10)	124.07(17)
C(10)-C(9)-N(14)	118.17(16)
C(9)-C(10)-H(10)	120.8
C(11)-C(10)-C(9)	118.41(18)
C(11)-C(10)-H(10)	120.8
C(10)-C(11)-H(11)	120.1
C(10)-C(11)-C(12)	119.74(17)
C(12)-C(11)-H(11)	120.1
C(7)-C(12)-C(13)	114.55(17)
C(11)-C(12)-C(7)	119.61(16)
C(11)-C(12)-C(13)	125.83(17)
N(1)-C(13)-C(4)	109.94(17)
N(1)-C(13)-C(12)	131.81(19)
C(4)-C(13)-C(12)	118.24(16)

Table S27 Anisotropic displacement parameters ($Å^2x10^3$) for CCDC 2288835. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(2)	25(1)	41(1)	38(1)	-6(1)	-3(1)	-12(1)
O(6)	29(1)	24(1)	24(1)	6(1)	-3(1)	-1(1)
O(15)	28(1)	22(1)	26(1)	5(1)	-3(1)	-6(1)
O(16)	41(1)	30(1)	25(1)	7(1)	-12(1)	-10(1)
N(1)	26(1)	31(1)	31(1)	-5(1)	2(1)	-7(1)
N(3)	25(1)	35(1)	37(1)	-5(1)	-4(1)	-5(1)
N(5)	21(1)	27(1)	27(1)	-2(1)	-6(1)	3(1)
N(6)	20(1)	23(1)	21(1)	0(1)	-2(1)	3(1)
N(14)	21(1)	19(1)	24(1)	0(1)	-3(1)	-1(1)
C(4)	18(1)	26(1)	29(1)	-5(1)	0(1)	2(1)
C(7)	18(1)	19(1)	17(1)	-1(1)	1(1)	4(1)
C(8)	18(1)	18(1)	21(1)	2(1)	2(1)	1(1)
C(9)	18(1)	18(1)	21(1)	-2(1)	1(1)	0(1)
C(10)	26(1)	20(1)	21(1)	1(1)	-2(1)	1(1)
C(11)	28(1)	20(1)	20(1)	1(1)	3(1)	-2(1)
C(12)	19(1)	19(1)	23(1)	-2(1)	3(1)	1(1)
C(13)	20(1)	21(1)	24(1)	-4(1)	5(1)	0(1)

Table S28 Hydrogen coordinates ($x10^4$) and isotropic displacement parameters ($Å^2x10^3$) for CCDC 2288835

	x	y	z	U(eq)
H(8)	2874	4367	6222	23
H(10)	2719	6729	1033	27
H(11)	3952	8055	2290	27

Table S29 Torsion angles [°] for CCDC 2288835

O(2)-N(1)-C(13)-C(4)	-0.05(19)
O(2)-N(1)-C(13)-C(12)	-178.56(18)
O(2)-N(3)-C(4)-N(5)	-179.61(17)

O(2)-N(3)-C(4)-C(13)	0.6(2)
O(6)-N(6)-C(7)-C(8)	-2.2(2)
O(6)-N(6)-C(7)-C(12)	178.94(15)
O(15)-N(14)-C(9)-C(8)	5.6(2)
O(15)-N(14)-C(9)-C(10)	-175.60(17)
O(16)-N(14)-C(9)-C(8)	-173.56(17)
O(16)-N(14)-C(9)-C(10)	5.3(2)
N(1)-O(2)-N(3)-C(4)	-0.6(2)
N(3)-O(2)-N(1)-C(13)	0.4(2)
N(3)-C(4)-C(13)-N(1)	-0.3(2)
N(3)-C(4)-C(13)-C(12)	178.40(16)
N(5)-N(6)-C(7)-C(8)	177.92(16)
N(5)-N(6)-C(7)-C(12)	-0.9(3)
N(5)-C(4)-C(13)-N(1)	179.84(17)
N(5)-C(4)-C(13)-C(12)	-1.4(3)
N(6)-N(5)-C(4)-N(3)	-177.55(17)
N(6)-N(5)-C(4)-C(13)	2.3(3)
N(6)-C(7)-C(8)-C(9)	-178.74(15)
N(6)-C(7)-C(12)-C(11)	-179.37(15)
N(6)-C(7)-C(12)-C(13)	1.7(2)
N(14)-C(9)-C(10)-C(11)	-176.56(16)
C(4)-N(5)-N(6)-O(6)	179.12(15)
C(4)-N(5)-N(6)-C(7)	-1.1(2)
C(7)-C(8)-C(9)-N(14)	176.62(15)
C(7)-C(8)-C(9)-C(10)	-2.2(3)
C(7)-C(12)-C(13)-N(1)	177.76(18)
C(7)-C(12)-C(13)-C(4)	-0.6(2)
C(8)-C(7)-C(12)-C(11)	1.9(3)
C(8)-C(7)-C(12)-C(13)	-177.06(16)
C(8)-C(9)-C(10)-C(11)	2.2(3)
C(9)-C(10)-C(11)-C(12)	-0.1(3)
C(10)-C(11)-C(12)-C(7)	-1.8(3)
C(10)-C(11)-C(12)-C(13)	176.97(17)
C(11)-C(12)-C(13)-N(1)	-1.1(3)
C(11)-C(12)-C(13)-C(4)	-179.50(16)
C(12)-C(7)-C(8)-C(9)	0.1(2)

X-ray experiment details for compound 5

Table S30 Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2 x\ 10^3$) for CCDC 2288836. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
O(1)	4328(1)	2111(1)	6870(1)	20(1)
O(2)	8914(1)	5120(1)	6669(1)	20(1)
O(3)	4971(1)	2045(1)	4278(1)	20(1)
O(4)	3581(1)	3318(1)	3753(1)	21(1)
N(1)	4453(2)	2399(1)	6013(1)	18(1)
N(2)	5368(2)	2641(1)	7383(1)	20(1)
N(3)	7253(1)	3937(1)	7113(1)	18(1)
N(4)	7847(1)	4497(1)	6495(1)	15(1)
N(5)	4705(1)	2978(1)	4142(1)	15(1)
C(1)	6114(2)	3257(1)	6850(1)	16(1)
C(2)	7358(2)	4450(1)	5595(1)	14(1)
C(3)	8050(2)	5150(1)	5023(1)	16(1)
C(4)	7614(2)	5136(1)	4171(1)	16(1)
C(5)	6491(2)	4429(1)	3876(1)	16(1)
C(6)	5839(2)	3742(1)	4457(1)	14(1)
C(7)	6231(2)	3728(1)	5329(1)	14(1)
C(8)	5558(2)	3100(1)	6005(1)	15(1)

Table S31 Bond lengths [Å] and angles [°] for CCDC 2288836

O(1)-N(1)	1.3880(16)
O(1)-N(2)	1.3796(17)

O(2)-N(4)	1.2461(16)
O(3)-N(5)	1.2256(17)
O(4)-N(5)	1.2251(17)
N(1)-C(8)	1.307(2)
N(2)-C(1)	1.312(2)
N(3)-N(4)	1.3029(18)
N(3)-C(1)	1.373(2)
N(4)-C(2)	1.4654(17)
N(5)-C(6)	1.4664(18)
C(1)-C(8)	1.415(2)
C(2)-C(3)	1.394(2)
C(2)-C(7)	1.402(2)
C(3)-H(3)	0.95(2)
C(3)-C(4)	1.380(2)
C(4)-H(4)	0.99(2)
C(4)-C(5)	1.400(2)
C(5)-H(5)	0.96(2)
C(5)-C(6)	1.378(2)
C(6)-C(7)	1.4002(19)
C(7)-C(8)	1.4433(19)

N(2)-O(1)-N(1)	112.18(10)
C(8)-N(1)-O(1)	104.24(11)
C(1)-N(2)-O(1)	104.23(12)
N(4)-N(3)-C(1)	114.00(12)
O(2)-N(4)-N(3)	118.60(12)
O(2)-N(4)-C(2)	116.66(12)
N(3)-N(4)-C(2)	124.74(12)

O(3)-N(5)-C(6)	117.18(12)
O(4)-N(5)-O(3)	125.15(12)
O(4)-N(5)-C(6)	117.66(12)
N(2)-C(1)-N(3)	122.68(13)
N(2)-C(1)-C(8)	109.69(13)
N(3)-C(1)-C(8)	127.62(13)
C(3)-C(2)-N(4)	117.43(13)
C(3)-C(2)-C(7)	121.88(13)
C(7)-C(2)-N(4)	120.69(13)
C(2)-C(3)-H(3)	119.8(14)
C(4)-C(3)-C(2)	119.24(13)
C(4)-C(3)-H(3)	121.0(14)
C(3)-C(4)-H(4)	122.1(13)
C(3)-C(4)-C(5)	120.91(14)
C(5)-C(4)-H(4)	116.9(13)
C(4)-C(5)-H(5)	119.8(13)
C(6)-C(5)-C(4)	118.36(13)
C(6)-C(5)-H(5)	121.8(13)
C(5)-C(6)-N(5)	118.33(13)
C(5)-C(6)-C(7)	123.10(13)
C(7)-C(6)-N(5)	118.55(12)
C(2)-C(7)-C(8)	115.30(13)
C(6)-C(7)-C(2)	116.49(13)
C(6)-C(7)-C(8)	128.11(13)
N(1)-C(8)-C(1)	109.65(13)
N(1)-C(8)-C(7)	132.77(13)
C(1)-C(8)-C(7)	117.55(13)

Table S32 Anisotropic displacement parameters ($Å^2x10^3$) for CCDC 2288836. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	26(1)	19(1)	16(1)	2(1)	3(1)	-4(1)
O(2)	18(1)	21(1)	21(1)	-4(1)	-4(1)	-4(1)
O(3)	29(1)	11(1)	20(1)	1(1)	-2(1)	-3(1)
O(4)	15(1)	22(1)	24(1)	-7(1)	-4(1)	4(1)
N(1)	22(1)	16(1)	15(1)	2(1)	3(1)	-1(1)
N(2)	23(1)	20(1)	16(1)	0(1)	2(1)	0(1)
N(3)	21(1)	19(1)	14(1)	-1(1)	0(1)	1(1)
N(4)	15(1)	15(1)	16(1)	-3(1)	0(1)	1(1)
N(5)	15(1)	15(1)	14(1)	-2(1)	2(1)	-1(1)
C(1)	18(1)	15(1)	16(1)	-1(1)	2(1)	3(1)
C(2)	13(1)	14(1)	15(1)	-2(1)	0(1)	3(1)
C(3)	14(1)	13(1)	21(1)	-1(1)	2(1)	1(1)
C(4)	16(1)	14(1)	19(1)	1(1)	2(1)	0(1)
C(5)	18(1)	14(1)	15(1)	1(1)	1(1)	2(1)
C(6)	14(1)	12(1)	16(1)	-2(1)	-1(1)	1(1)
C(7)	14(1)	12(1)	16(1)	0(1)	1(1)	3(1)
C(8)	16(1)	13(1)	16(1)	0(1)	1(1)	2(1)

Table S33 Hydrogen coordinates ($x10^4$) and isotropic displacement parameters ($Å^2x10^3$) for CCDC 2288836

	x	y	z	U(eq)
H(3)	8800(30)	5634(19)	5225(15)	29(5)
H(4)	8060(20)	5627(18)	3741(15)	25(5)
H(5)	6220(20)	4417(17)	3278(14)	23(5)

Table S34 Torsion angles [°] for CCDC 2288836

O(1)-N(1)-C(8)-C(1)	-0.45(15)
O(1)-N(1)-C(8)-C(7)	-178.17(15)
O(1)-N(2)-C(1)-N(3)	179.09(12)
O(1)-N(2)-C(1)-C(8)	-0.89(15)
O(2)-N(4)-C(2)-C(3)	-4.18(18)
O(2)-N(4)-C(2)-C(7)	176.15(12)
O(3)-N(5)-C(6)-C(5)	123.47(14)
O(3)-N(5)-C(6)-C(7)	-55.33(17)
O(4)-N(5)-C(6)-C(5)	-55.41(17)
O(4)-N(5)-C(6)-C(7)	125.79(14)
N(1)-O(1)-N(2)-C(1)	0.63(15)
N(2)-O(1)-N(1)-C(8)	-0.10(15)
N(2)-C(1)-C(8)-N(1)	0.89(17)
N(2)-C(1)-C(8)-C(7)	179.01(12)
N(3)-N(4)-C(2)-C(3)	176.15(13)

N(3)-N(4)-C(2)-C(7)	-3.5(2)
N(3)-C(1)-C(8)-N(1)	-179.08(14)
N(3)-C(1)-C(8)-C(7)	-1.0(2)
N(4)-N(3)-C(1)-N(2)	-178.98(13)
N(4)-N(3)-C(1)-C(8)	1.0(2)
N(4)-C(2)-C(3)-C(4)	-179.54(12)
N(4)-C(2)-C(7)-C(6)	179.93(11)
N(4)-C(2)-C(7)-C(8)	3.27(19)
N(5)-C(6)-C(7)-C(2)	177.94(11)
N(5)-C(6)-C(7)-C(8)	-5.9(2)
C(1)-N(3)-N(4)-O(2)	-178.43(12)
C(1)-N(3)-N(4)-C(2)	1.24(19)
C(2)-C(3)-C(4)-C(5)	0.0(2)
C(2)-C(7)-C(8)-N(1)	176.32(15)
C(2)-C(7)-C(8)-C(1)	-1.26(19)
C(3)-C(2)-C(7)-C(6)	0.3(2)
C(3)-C(2)-C(7)-C(8)	-176.39(12)
C(3)-C(4)-C(5)-C(6)	-0.4(2)
C(4)-C(5)-C(6)-N(5)	-177.85(12)
C(4)-C(5)-C(6)-C(7)	0.9(2)
C(5)-C(6)-C(7)-C(2)	-0.8(2)
C(5)-C(6)-C(7)-C(8)	175.37(13)
C(6)-C(7)-C(8)-N(1)	0.1(3)
C(6)-C(7)-C(8)-C(1)	-177.47(13)
C(7)-C(2)-C(3)-C(4)	0.1(2)

X-ray experiment details for compound 8

Table S35 Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2x10^3$) for CCDC 2295832. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
O(1)	3826(2)	4257(2)	7343(2)	27(1)
O(5)	7160(2)	8181(2)	5790(3)	38(1)
O(15)	8355(2)	4227(2)	4247(3)	44(1)
O(16)	7881(2)	2542(3)	2640(3)	44(1)
O(18)	5233(2)	-1339(2)	3752(2)	33(1)
O(19)	3954(2)	-718(2)	5177(3)	38(1)
N(1)	4674(2)	4782(3)	6834(2)	24(1)
N(2)	4994(2)	6210(3)	7180(3)	30(1)
N(4)	6292(2)	8147(3)	6691(3)	36(1)
N(6)	7303(2)	6744(3)	5104(3)	34(1)
N(14)	7720(2)	3286(3)	3709(3)	30(1)
N(17)	4787(2)	-418(3)	4565(3)	28(1)
C(3)	5905(2)	6693(3)	6515(3)	29(1)
C(7)	6534(2)	5808(3)	5550(3)	27(1)
C(8)	6209(2)	4166(3)	5251(3)	23(1)
C(9)	6703(2)	2986(3)	4421(3)	25(1)
C(10)	6257(2)	1494(3)	4189(3)	25(1)
C(11)	5296(2)	1151(3)	4827(3)	23(1)
C(12)	4774(2)	2218(3)	5681(3)	23(1)
C(13)	5243(2)	3710(3)	5883(3)	22(1)

Table S36 Bond lengths [Å] and angles [°] for CCDC 2295832

O(1)-N(1)	1.248(3)
O(5)-N(4)	1.392(4)
O(5)-N(6)	1.375(3)
O(15)-N(14)	1.229(4)
O(16)-N(14)	1.216(4)
O(18)-N(17)	1.228(3)
O(19)-N(17)	1.225(3)
N(1)-N(2)	1.296(3)
N(1)-C(13)	1.462(3)

N(2)-C(3)	1.368(4)
N(4)-C(3)	1.313(4)
N(6)-C(7)	1.310(4)
N(14)-C(9)	1.468(3)
N(17)-C(11)	1.473(3)
C(3)-C(7)	1.422(4)
C(7)-C(8)	1.452(3)
C(8)-C(9)	1.407(4)
C(8)-C(13)	1.406(3)
C(9)-C(10)	1.378(4)
C(10)-H(10)	0.9500
C(10)-C(11)	1.382(4)
C(11)-C(12)	1.374(4)
C(12)-H(12)	0.9500
C(12)-C(13)	1.386(3)

N(6)-O(5)-N(4)	112.5(2)
O(1)-N(1)-N(2)	118.9(2)
O(1)-N(1)-C(13)	116.6(2)
N(2)-N(1)-C(13)	124.5(2)
N(1)-N(2)-C(3)	114.0(2)
C(3)-N(4)-O(5)	103.1(2)
C(7)-N(6)-O(5)	105.2(2)
O(15)-N(14)-C(9)	118.2(3)
O(16)-N(14)-O(15)	124.9(2)
O(16)-N(14)-C(9)	116.9(2)
O(18)-N(17)-C(11)	117.6(2)
O(19)-N(17)-O(18)	124.6(2)
O(19)-N(17)-C(11)	117.9(2)
N(2)-C(3)-C(7)	128.0(2)
N(4)-C(3)-N(2)	121.1(3)
N(4)-C(3)-C(7)	110.8(3)
N(6)-C(7)-C(3)	108.3(2)
N(6)-C(7)-C(8)	134.4(3)
C(3)-C(7)-C(8)	117.3(2)
C(9)-C(8)-C(7)	130.0(2)
C(13)-C(8)-C(7)	114.2(2)
C(13)-C(8)-C(9)	115.9(2)
C(8)-C(9)-N(14)	121.9(2)
C(10)-C(9)-N(14)	115.4(2)

C(10)-C(9)-C(8)	122.7(2)
C(9)-C(10)-H(10)	121.1
C(9)-C(10)-C(11)	117.9(2)
C(11)-C(10)-H(10)	121.1
C(10)-C(11)-N(17)	119.0(2)
C(12)-C(11)-N(17)	117.9(2)
C(12)-C(11)-C(10)	123.2(2)
C(11)-C(12)-H(12)	121.3
C(11)-C(12)-C(13)	117.3(2)
C(13)-C(12)-H(12)	121.3
C(8)-C(13)-N(1)	121.8(2)
C(12)-C(13)-N(1)	115.1(2)
C(12)-C(13)-C(8)	123.1(2)

Table S37 Anisotropic displacement parameters ($Å^2x10^3$) for CCDC 2295832. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	27(1)	28(1)	26(1)	-1(1)	6(1)	-1(1)
O(5)	32(1)	24(1)	59(2)	2(1)	-6(1)	-6(1)
O(15)	29(1)	32(1)	71(2)	3(1)	10(1)	-3(1)
O(16)	37(1)	72(2)	25(1)	3(1)	11(1)	3(1)
O(18)	40(1)	28(1)	30(1)	-10(1)	3(1)	4(1)
O(19)	34(1)	31(1)	48(2)	-10(1)	10(1)	-8(1)
N(1)	28(1)	23(1)	21(1)	-1(1)	0(1)	2(1)
N(2)	35(1)	25(1)	31(1)	-4(1)	-2(1)	-2(1)
N(4)	35(1)	28(1)	45(2)	-1(1)	-4(1)	-2(1)
N(6)	30(1)	27(1)	44(2)	7(1)	-4(1)	-3(1)
N(14)	28(1)	32(1)	31(1)	11(1)	6(1)	4(1)
N(17)	28(1)	25(1)	30(1)	-4(1)	1(1)	1(1)
C(3)	33(1)	23(1)	30(2)	2(1)	-4(1)	0(1)
C(7)	27(1)	24(1)	30(2)	6(1)	-6(1)	-1(1)
C(8)	26(1)	23(1)	22(1)	5(1)	-1(1)	2(1)
C(9)	23(1)	28(1)	22(1)	7(1)	1(1)	1(1)
C(10)	29(1)	26(1)	21(1)	2(1)	1(1)	5(1)
C(11)	29(1)	22(1)	19(1)	1(1)	-2(1)	0(1)
C(12)	26(1)	22(1)	21(1)	4(1)	0(1)	2(1)
C(13)	25(1)	22(1)	19(1)	2(1)	-3(1)	2(1)

Table S38 Hydrogen coordinates ($x10^4$) and isotropic displacement parameters ($Å^2x10^3$) for CCDC 2295832

	x	y	z	U(eq)
H(10)	6600	726	3610	30
H(12)	4118	1944	6115	27

Table S39 Torsion angles [°] for CCDC 2295832

O(1)-N(1)-N(2)-C(3)	–177.2(2)
O(1)-N(1)-C(13)-C(8)	–179.7(2)
O(1)-N(1)-C(13)-C(12)	–1.0(3)
O(5)-N(4)-C(3)-N(2)	-176.6(3)
O(5)-N(4)-C(3)-C(7)	1.6(3)
O(5)-N(6)-C(7)-C(3)	0.5(3)
O(5)-N(6)-C(7)-C(8)	179.2(3)
O(15)-N(14)-C(9)-C(8)	30.1(4)
O(15)-N(14)-C(9)-C(10)	–151.6(3)
O(16)-N(14)-C(9)-C(8)	–151.7(3)
O(16)-N(14)-C(9)-C(10)	26.6(4)
O(18)-N(17)-C(11)-C(10)	–2.0(4)
O(18)-N(17)-C(11)-C(12)	176.8(2)
O(19)-N(17)-C(11)-C(10)	177.6(3)
O(19)-N(17)-C(11)-C(12)	–3.6(4)
N(1)-N(2)-C(3)-N(4)	175.8(3)
N(1)-N(2)-C(3)-C(7)	–2.0(4)
N(2)-N(1)-C(13)-C(8)	–0.2(4)
N(2)-N(1)-C(13)-C(12)	178.5(3)
N(2)-C(3)-C(7)-N(6)	176.6(3)
N(2)-C(3)-C(7)-C(8)	–2.4(4)
N(4)-O(5)-N(6)-C(7)	0.5(3)
N(4)-C(3)-C(7)-N(6)	–1.4(3)
N(4)-C(3)-C(7)-C(8)	179.6(2)
N(6)-O(5)-N(4)-C(3)	–1.3(3)
N(6)-C(7)-C(8)-C(9)	5.7(5)
N(6)-C(7)-C(8)-C(13)	–173.4(3)
N(14)-C(9)-C(10)-C(11)	–179.6(2)
N(17)-C(11)-C(12)-C(13)	–178.0(2)

C(3)-C(7)-C(8)-C(9)	–175.7(3)
C(3)-C(7)-C(8)-C(13)	5.2(3)
C(7)-C(8)-C(9)-N(14)	1.5(4)
C(7)-C(8)-C(9)-C(10)	–176.7(3)
C(7)-C(8)-C(13)-N(1)	–4.2(3)
C(7)-C(8)-C(13)-C(12)	177.2(2)
C(8)-C(9)-C(10)-C(11)	–1.3(4)
C(9)-C(8)-C(13)-N(1)	176.5(2)
C(9)-C(8)-C(13)-C(12)	–2.1(4)
C(9)-C(10)-C(11)-N(17)	178.3(2)
C(9)-C(10)-C(11)-C(12)	–0.4(4)
C(10)-C(11)-C(12)-C(13)	0.8(4)
C(11)-C(12)-C(13)-N(1)	–178.2(2)
C(11)-C(12)-C(13)-C(8)	0.5(4)
C(13)-N(1)-N(2)-C(3)	3.3(4)
C(13)-C(8)-C(9)-N(14)	–179.4(2)
C(13)-C(8)-C(9)-C(10)	2.4(4)

Table S40 Unit cell volume (V), van der Waals volume (V_{vdW}), Kitaigorodskii packin index (KPI), volume enclosed by the 0.001 a.u. isosurface of the electron density (V_{001}), the biggest spherical void volume (V_{void}) and crystal density at 100 K.

Compound	V, Å^3	Z	V_{vdW}, Å^3	KPI	V_{001}, Å^3	V_{void}, Å^3	d, g cm^{-3}
1	769.42(2)	4	138.31	71.82%	193.8	5.58	1.624
3	912.06(2)	4	162.40	71.02%	222.2	4.19	1.698
5	1713.28(7)	8	162.77	75.76%	221.3	2.14	1.808
6	924.783(13)	4	171.04	73.69%	232.0	3.05	1.790
7	2400.54(4)	12	146.87	73.37%	203.6	5.58	1.695
8	1000.81(3)	4	186.13	74.13%	250.1	3.05	1.846

The molecular volume enclosed by the isosurface of the electron density ($\rho(\mathbf{r})$=0.001 a.u.) is calculated using B3LYP/6-31G(d,p) wave function of the optimized molecule. Kitaigorodskii packing indices[8] are calculated with Olex2 program[4].

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