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Supporting information for article:

Structural and theoretical study of four novel norcantharidine derivatives: two new cases of conditional isomorphism

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Table S1 Crystallographic data of four analogical crystals.

Abbreviation (ref code)	**NCA-A (GOLKAU)**	**DNCA-AE (LAQWEH)**	**DNCA (OXHEPA02)**	**NCA (QIWJEM)**

Space group	*P* $2_1/c$ (14)	*P c* (7)	*P* $2_12_12_1$ (19)	*P* $na2_1$ (33)
a /Å	9.5914(4)	5.4619(12)	5.360(1)	10.448(3)
b /Å	8.4345(3)	6.8337(15)	6.976(1)	6.539(1)
c /Å	14.4101(6)	12.546(3)	18.844(4)	10.263(2)
α /°	90.00	90.00	90.00	90.00
β /°	93.468(3)	92.047(3)	90.00	90.00
γ /°	90.00	90.00	90.00	90.00
V /Å^3	1163.62(8)	467.97(18)	704.6(3)	701.1(3)
Z	4	2	4	4

Table S2 Selected π, π –interaction geometry for **DNCA-A** (the centroid-centroid distance (*d*), the dihedral angles (*α*), slipping angles between centroid–centroid distance and the normal to the plane I (*β*), slipping angles between centroid–centroid distance and the normal to the plane J (*γ*), the perpendicular distance of centroid I to plane J (*e*) and the perpendicular distance of centroid J to plane I (*f*)) (Å, °).

notation	π,π–interactions (I→J)	*d*	*α*	*β*	*γ*	*e*	*f*	role
a	Cg1→Cg1 #1	4.9844	53.24	6.94	60.00	2.492	4.948	1D chains parallel to the *b* axis
b	Cg1→Cg2 #1	4.3966	36.04	50.21	16.63	4.213	2.814	1D chains parallel to the *b* axis
b	Cg2→Cg1 #2	4.3966	36.04	16.63	50.21	2.814	4.213	
c	Cg2→Cg2 #3	5.0987	70.17	2.29	70.34	1.715	5.095	1D chains parallel to the *b* axis

Ring 1: N_1 C_7 C_2 C_3 C_8

Ring2: C_9 C_{10} C_{11} C_{12} C_{13} C_{14}

Symmetry codes : #1: -*x*, -1/2+*y*, 1/2-*z*; #2: -*x*, 1/2+*y*, 1/2-*z*; #3: 1-*x*, -1/2+*y*, 1/2-*z*.

Table S3 Selected C-H···π interaction geometry for **DNCA-A** (the H-centroid distance (H···Cg), the perpendicular distance of H to plane I (H-Perp), slipping angles between H···Cg and the normal to the plane I (*γ*), the C-H···Cg angles (C-H···Cg), the C-centroid distance (C···Cg), the angles between C-H bond line and plane I (C-H···π)) (Å, °).

notation	C-H···π (plane I)	H···Cg	H-Perp	*γ*	C-H···Cg	C···Cg	C-H···π	role
d	C2-H2···Cg2 #1	2.5750	2.573	2.13	163.87	3.5077	74.15	1D chains parallel to the *b* axis
e	C13-H13···Cg2 #2	3.2013	2.982	21.31	133.34	3.9345	64.48	1D chains parallel to the *b* axis

Ring2: C_9 C_{10} C_{11} C_{12} C_{13} C_{14}

Symmetry codes : #1: -*x*, -1/2+*y*, 1/2-*z*; #2: 1-*x*, 1/2+*y*, 1/2-*z*.

Table S4 Hydrogen bond geometry of **DNCA-NA** in crystal packing (Å, °).

notation	D—H···A	D—H	H···A	D···A	D—H···A	role

b	C10-H10···O3^{i}	0.94(7)	2.52(6)	3.143(7)	124(5)	1D chains parallel to the *c* axis
f	C2-H2···O4^{ii}	0.89(6)	2.54(5)	3.228(8)	135(4)	1D chains parallel to the *b* axis

Symmetry codes: (i) *x*, *y*, 1+*z*; (ii) 2−*x*, -1/2+*y*, 1−*z*.

Table S5 Selected π, π –interaction geometry for **DNCA-NA** (the centroid-centroid distance (*d*), the dihedral angles (*α*), slipping angles between centroid–centroid distance and the normal to the plane I (*β*), slipping angles between centroid–centroid distance and the normal to the plane J (*γ*), the perpendicular distance of centroid I to plane J (*e*) and the perpendicular distance of centroid J to plane I (*f*)) (Å, °).

notation	π,π–interactions (I→J)	*d*	*α*	*β*	*γ*	*e*	*f*	role
a	Cg2→Cg1 #1	5.966(5)	55.0(3)	24.4	72.4	1.801(2)	5.434(2)	1D chains parallel to [3 0 5] direction
c	Cg1→Cg1 #2	5.285(4)	0.0(3)	18.9	18.9	4.999(2)	4.999(2)	1D chains parallel to the *a* axis
c	Cg1→Cg1 #3	5.285(4)	0.0(3)	18.9	18.9	5.000(2)	5.000(2)	
d	Cg1→Cg2 #2	5.244(4)	55.0(3)	27.2	49.4	3.416(2)	4.664(2)	1D chains parallel to the *a* axis
d	Cg2→Cg1 #3	5.245(4)	55.0(3)	49.4	27.2	4.664(2)	3.417(2)	
e	Cg2→Cg2 #2	5.285(5)	0.0(3)	54.3	54.3	3.085(2)	3.084(2)	1D chains parallel to the *a* axis
e	Cg2→Cg2 #3	5.285(5)	0.0(3)	54.3	54.3	3.084(2)	3.085(2)	

Ring 1: N_1 C_7 C_2 C_3 C_8

Ring2: C_9 C_{10} C_{11} C_{12} C_{13} C_{14}

Symmetry codes : #1: 1+*x*, *y*, 1+*z*; #2: -1+*x*, *y*, *z*; #3: 1+*x*, *y*, *z*.

Table S6 Hydrogen bond geometry of **NCA-NA** in crystal packing (Å, °).

notation	D—H···A	D—H	H···A	D···A	D—H···A	role
a	C6-H6A···O3^{i}	0.87(7)	2.55(6)	3.180(6)	130(5)	1D chains parallel to [3 0 5] direction
b	C14-H14···O2^{iii}	0.96(4)	2.40(4)	3.128(5)	132(3)	1D chains parallel to the *c* axis
f	C6-H6B···O4^{ii}	1.00(6)	2.57(6)	3.503(7)	154(4)	1D chains parallel to the *b* axis
intra	C13-H13···O5	0.95(5)	2.32(5)	2.693(7)	103(4)	

Symmetry codes: (i) *-1+x,y,-1+z*; (ii) *2-x,-1/2+y,1-z*; (iii) *x,y,1+z*.

Table S7 Selected π, π –interaction geometry for **NCA-NA** (the centroid-centroid distance (*d*), the dihedral angles (*α*), slipping angles between centroid–centroid distance and the normal to the plane I (*β*), slipping angles between centroid–centroid distance and the normal to the plane J (*γ*), the perpendicular distance of centroid I to plane J (*e*) and the perpendicular distance of centroid J to plane I (*f*)) (Å, °).

notation	π,π–interactions (I→J)	*d*	*α*	*β*	*γ*	*e*	*f*	role
c	Cg1→Cg1 #1	5.366(2)	0.00(19)	18.8	18.8	5.0791(15)	5.0790(15)	1D chains parallel to the *a* axis
c	Cg1→Cg1 #2	5.366(2)	0.00(19)	18.8	18.8	5.0791(15)	5.0792(15)	
d	Cg1→Cg2 #1	5.177(2)	55.60(19)	27.1	49.4	3.3667(16)	4.6090(17)	1D chains parallel to the *a* axis
d	Cg2→Cg1 #2	5.177(2)	55.60(19)	49.4	27.1	4.6087(17)	3.3668(16)	

e	Cg2→Cg2 #1	5.366(2)	0.00(19)	55.4	55.4	3.0452(16)	3.0452(16)	1D chains parallel to the *a* axis
e	Cg2→Cg2 #2	5.366(2)	0.00(19)	55.4	55.4	3.0453(16)	3.0452(16)	

Ring 1: N_1 C_7 C_2 C_3 C_8

Ring2: C_9 C_{10} C_{11} C_{12} C_{13} C_{14}

Symmetry codes : #1: -1+*x*, *y*, *z*; #2: 1+*x*, *y*, *z*.

Table S8 Hydrogen bond geometry of **NCA-AE** in crystal packing (Å, °).

notation	D—H···A	D—H	H···A	D···A	D—H···A	role
a	O3-H7···O1^{i}	0.82	2.46	2.920(10)	116.7	1D chains parallel to the *b* axis
b	C1-H1A···O2^{ii}	0.95(6)	2.59(6)	3.511(6)	164(5)	2D layers parallel to the [0 1 0] plane.
intra	O3-H7···N1	0.82	2.55	2.924(8)	109.3	

Symmetry codes: (i) *x,* 1+*y, z*; (ii) 1/2-*x,*1-*y,*-1/2+*z*.

Table S9 Selected π, π –interaction geometry for **NCA-AE** (the centroid-centroid distance (*d*), the dihedral angles (*α*), slipping angles between centroid–centroid distance and the normal to the plane I (*β*), slipping angles between centroid–centroid distance and the normal to the plane J (*γ*), the perpendicular distance of centroid I to plane J (*e*) and the perpendicular distance of centroid J to plane I (*f*)) (Å, °).

notation	π,π–interactions (I→J)	*d*	*α*	*β*	*γ*	*e*	*f*	role
c	Cg1→Cg1 #1	5.594(3)	0.00(2)	15.5	15.5	5.3890(18)	5.3889(18)	1D chains parallel to the *b* axis
c	Cg1→Cg1 #2	5.594(3)	0.00(2)	15.5	15.5	5.3890(18)	5.3890(18)	1D chains parallel to the *b* axis
c	Cg1→Cg1 #3	5.594(3)	0.00(2)	15.5	15.5	5.3890(18)	5.3889(18)	1D chains parallel to the *b* axis
c	Cg1→Cg1 #4	5.594(3)	0.00(2)	15.5	15.5	5.3890(18)	5.3890(18)	1D chains parallel to the *b* axis

Ring 1: O_1 C_2 C_1 C_{1A} C_{2A}

Symmetry codes : #1: *x*, -1+*y*, *z*; #2: *x*, 1+*y*, *z*; #3: 1-*x*, -1+*y*, *z*; #4: 1-*x*, 1+*y*, *z*.

Table S10 Selected π, π –interaction geometry for **NCA-A(GOLKAU)** (the centroid-centroid distance (*d*), the dihedral angles (*α*), slipping angles between centroid–centroid distance and the normal to the plane I (*β*), slipping angles between centroid–centroid distance and the normal to the plane J (*γ*), the perpendicular distance of centroid I to plane J (*e*) and the perpendicular distance of centroid J to plane I (*f*)) (Å, °).

Notation	π, π –interactions (I→J)	*d*	*α*	*β*	*γ*	*e*	*f*	role
a	Cg1→Cg1 #1	5.0438(10)	56.27	5.31	61.38	2.416	5.022	1D chains parallel to the *b* axis
b	Cg1→Cg2 #1	4.5693(11)	33.25	49.23	18.82	4.325	2.984	1D chains parallel to the *b* axis
b	Cg2→Cg1 #2	4.5693(11)	33.25	18.82	49.23	2.984	4.325	
c	Cg2→Cg2 #3	5.1772(12)	63.65	4.88	67.18	2.008	5.158	1D chains parallel to the *b* axis

Ring 1: N_1 C_7 C_2 C_3 C_8

Ring2: C_9 C_{10} C_{11} C_{12} C_{13} C_{14}

Symmetry codes : #1: -*x*, 1/2+*y*, 3/2-*z*; #2: -*x*, -1/2+*y*, 3/2-*z*; #3: 1-*x*, 1/2+*y*, 3/2-*z*.

Table S11 Selected C-H···π interaction geometry for **NCA-A(GOLKAU)** (the H-centroid distance (H···Cg), the perpendicular distance of H to plane I (H-Perp), slipping angles between H···Cg and the normal to the plane I (*γ*), the C-H···Cg angles (C-H···Cg), the C-centroid distance (C···Cg), the angles between C-H bond line and plane I (C-H···π)) (Å, °).

Notation	C-H···π (plane I)	H···Cg	H-Perp	*γ*	C-H···Cg	C···Cg	C-H···π	role
d	C2-H2···Cg2 #1	2.7564	2.748	4.45	163.07	3.7051(18)	73.03	1D chains parallel to the *b* axis
e	C13-H13···Cg2 #2	3.3392	3.150	19.39	132.04	4.022(3)	60.48	1D chains parallel to the *b* axis

Ring2: C_9 C_{10} C_{11} C_{12} C_{13} C_{14}

Symmetry codes : #1: -*x*, 1/2+*y*, 3/2-*z*; #2: 1-*x*, -1/2+*y*, 3/2-*z*.

Table S12 Hydrogen bond geometry of **NCA-A(GOLKAU)** in crystal packing (Å, °).

Notation	D—H···A	D—H	H···A	D···A	D—H···A	role
f	C5—H5b···O3^{i}	0.97	2.59	3.502(3)	156	dimer

Symmetry code: (i) −*x*, 1-*y*, 1−*z*.

Table S13 Hydrogen bond geometry of **DNCA-AE(LAQWEH)** in crystal packing (Å, °).

Notation	D—H···A	D—H	H···A	D···A	D—H···A	role
a	O4-H11···O3^{i}	0.92(6)	1.99(5)	2.902(3)	170(5)	1D chains parallel to the *b* axis
b	C1-H1···O4^{ii}	0.98	2.44	3.217(3)	136	1D chains stretching along [3 0 -8] direction.
c	C2-H2···O3^{iii}	0.98	2.40	3.338(3)	160	1D chains parallel to the *c* axis
intra	C9-H8···O3	0.97	2.58	2.910(3)	100	

Symmetry codes: (i) x, 1+y, z ; (ii) 1+x, 2-y, -1/2+z; (iii) x, 1-y, -1/2+z.

Table S14 Selected π, π –interaction geometry for **DNCA-AE(LAQWEH)** (the centroid-centroid distance (*d*), the dihedral angles (*α*), slipping angles between centroid–centroid distance and the normal to the plane I (*β*), slipping angles between centroid–centroid distance and the normal to the plane J (*γ*), the perpendicular distance of centroid I to plane J (*e*) and the perpendicular distance of centroid J to plane I (*f*)) (Å, °).

Notation	π, π –interactions (I→J)	*d*	*α*	*β*	*γ*	*e*	*f*	role
d	Cg1→Cg1 #1	5.4619(18)	0.03(12)	21.1	21.1	5.0951(9)	5.0951(9)	1D chains parallel to the *a* axis
d	Cg1→Cg1 #2	5.4619(18)	0.03(12)	21.1	21.1	5.0951(9)	5.0951(9)	1D chains parallel to the *a* axis

Ring 1: N_1 C_7 C_2 C_3 C_8

Symmetry codes : #1: -1+*x*, *y*, *z*; #2: 1+*x*, *y*, *z*.

Table S15 Hydrogen bond geometry of **DNCA(OXHEPA02)** in crystal packing (Å, °).

Notation	D—H···A	D—H	H···A	D···A	D—H···A	role
a	C3-H2···O3^{i}	0.98	2.56	3.517(2)	166	1D chains parallel to the *b* axis
b	C6-H5···O1^{ii}	0.98	2.48	3.317(2)	143	1D chains parallel to the *b* axis
c	C6-H5···O2^{iii}	0.98	2.48	3.069(2)	119	1D chains parallel to the *a* axis

Symmetry codes: (i) 2-x ,-1/2+y, 3/2-z ; (ii) x, 1+y, z ;(iii) -1/2+x, 3/2-y, 2-z.

Table S16 Selected π, π –interaction geometry for **DNCA(OXHEPA02)** (the centroid-centroid distance (*d*), the dihedral angles (*α*), slipping angles between centroid–centroid distance and the normal to the plane I (*β*), slipping angles between centroid–centroid distance and the normal to the plane J (*γ*), the perpendicular distance of centroid I to plane J (*e*) and the perpendicular distance of centroid J to plane I (*f*)) (Å, °).

Notation	π, π –interactions (I→J)	*d*	*α*	*β*	*γ*	*e*	*f*	role
d	Cg1→Cg1 #1	4.2900(14)	52.29	15.84	65.71	1.765	4.127	1D chains parallel to the *a* axis

Ring 1: O_4 C_1 C_2 C_7 C_8

Symmetry code: #1: -1/2+*x*, 1/2-*y*, 2-*z*.

Table S17 Selected C-O···π interaction geometry for **DNCA(OXHEPA02)** (the O-centroid distance (O···Cg), the perpendicular distance of O to plane I (O-Perp), slipping angles between O···Cg and the normal to the plane I (*γ*), the C-O···Cg angles (C-O···Cg), the C-centroid distance (C···Cg), the angles between C-O bond line and plane I (C-O···π)) (Å, °).

Notation	C-O···π (plane I)	O···Cg	O-Perp	*γ*	C-O···Cg	C···Cg	C-O···π	role
e	C8-O2···Cg1 #1	3.6475(18)	3.310	24.86	90.33(12)	3.841(2)	22.06	1D chains parallel to the *a* axis

Ring1: O_4 C_1 C_2 C_7 C_8

Symmetry code : #1: 1/2+*x*, 1/2-*y*, 2-*z*.

Table S18 Hydrogen bond geometry of **NCA(QIWJEM)** in crystal packing (Å, °).

Notation	D—H···A	D—H	H···A	D···A	D—H···A	role
a	C2-H1···O2^{i}	0.98	2.45	3.123(3)	126	1D chains parallel to the *b* axis
b	C2-H1···O1^{ii}	0.98	2.54	3.244(3)	126	1D chains parallel to the *c* axis
c	C4-H3···O1^{ii}	0.97	2.53	3.255(3)	131	1D chains parallel to the *c* axis

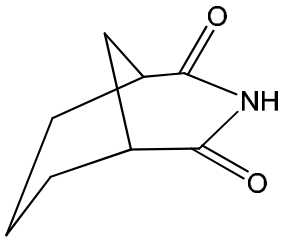
Symmetry codes: (i) x, 1+y, z ; (ii) -x, 1-y, 1/2+z.

Table S19 Selected π, π –interaction geometry for **NCA(QIWJEM)** (the centroid-centroid distance (*d*), the dihedral angles (*α*), slipping angles between centroid–centroid distance and the normal to the plane I (*β*), slipping angles between centroid–centroid distance and the normal to the plane J (*γ*), the perpendicular distance of centroid I to plane J (*e*) and the perpendicular distance of centroid J to plane I (*f*)) (Å, °).

Notation	π, π –interactions (I→J)	*d*	*α*	*β*	*γ*	*e*	*f*	role
d	Cg1→Cg1 #1	5.238(2)	17.94	12.00	17.14	5.005	5.123	1D chains parallel to the *a* axis
d	Cg1→Cg1 #2	5.238(2)	17.94	17.14	12.00	5.123	5.005	

Ring 1: O_4 C_1 C_2 C_7 C_8

Symmetry codes : #1: -1/2+*x*, 1/2-*y*, *z*; #2: 1/2+*x*, 1/2-*y*, *z*.



Scheme S1. A simple glutarimide derivative in the 2001 CCDC blind test.

Figure S1. ^{1}HNMR spectrum of **DNCA-A**.

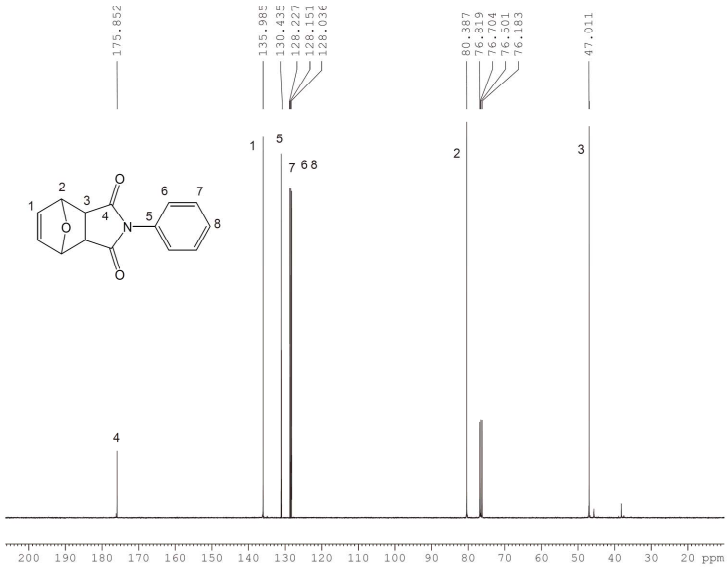


Figure S2. ^{13}CNMR spectrum of **DNCA-A**.

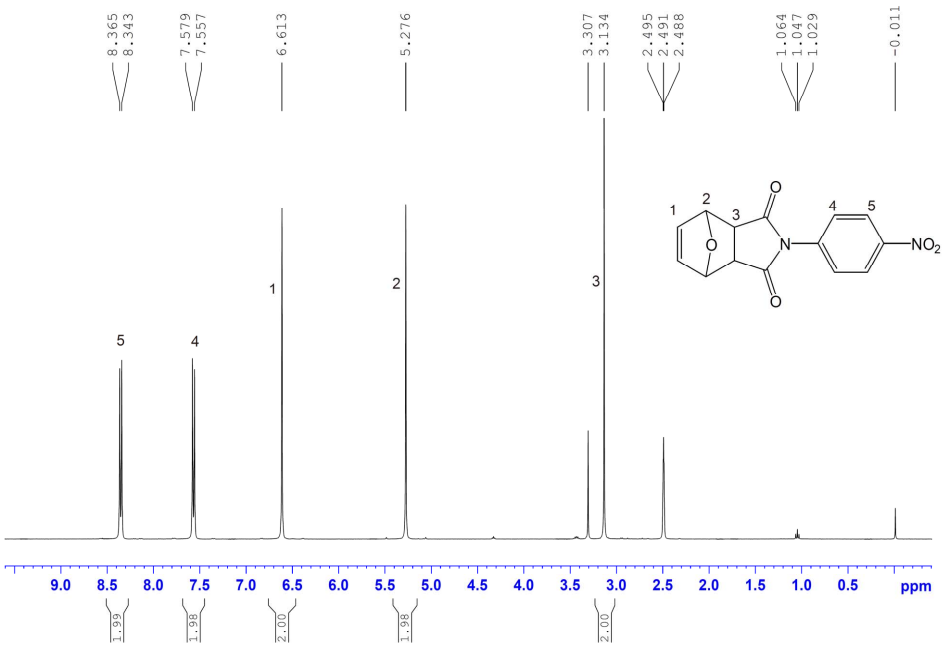


Figure S3. ^{1}HNMR spectrum of **DNCA-NA**.

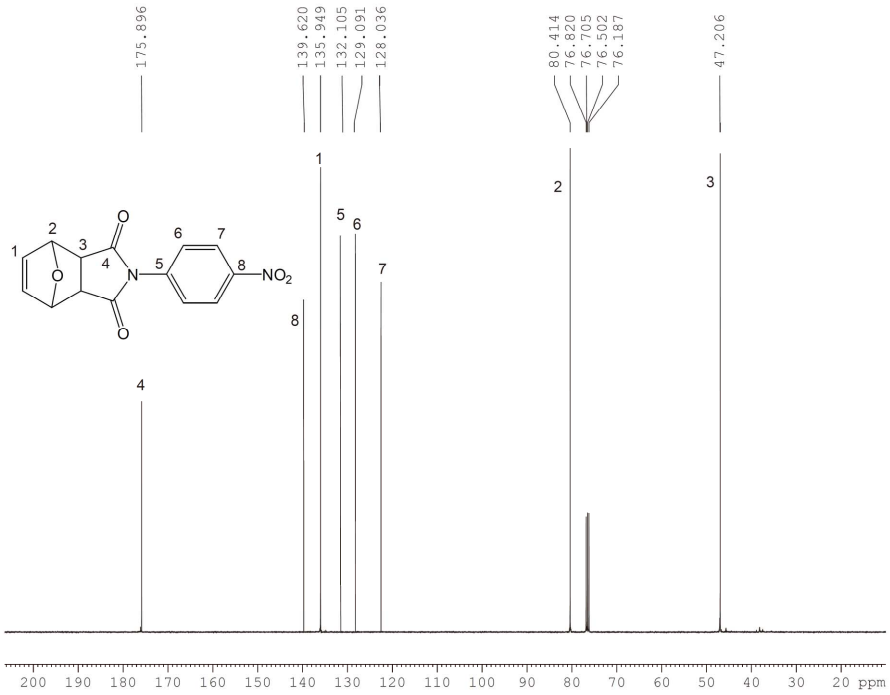


Figure S4. ^{13}CNMR spectrum of **DNCA-NA**.

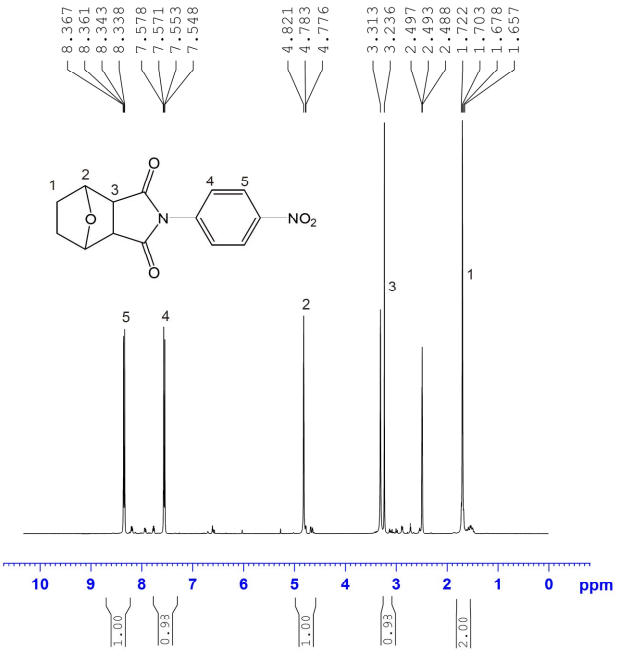


Figure S5. ^{1}HNMR spectrum of **NCA-NA.**

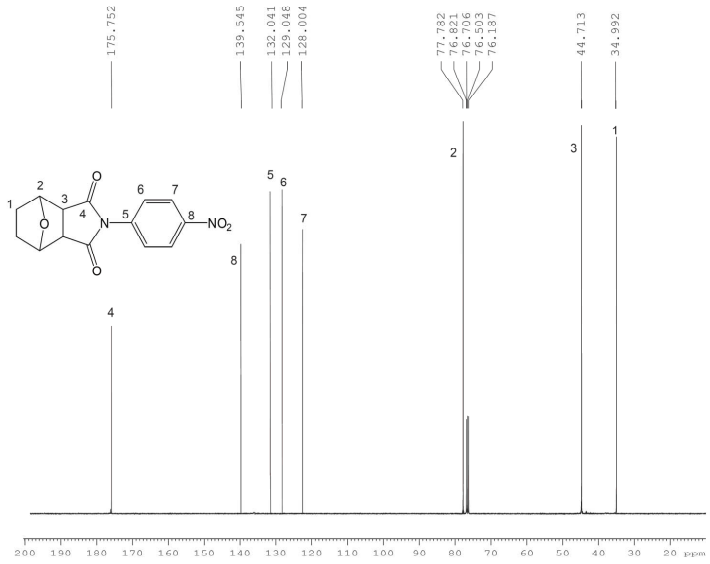


Figure S6. ^{13}CNMR spectrum of **NCA-NA**.

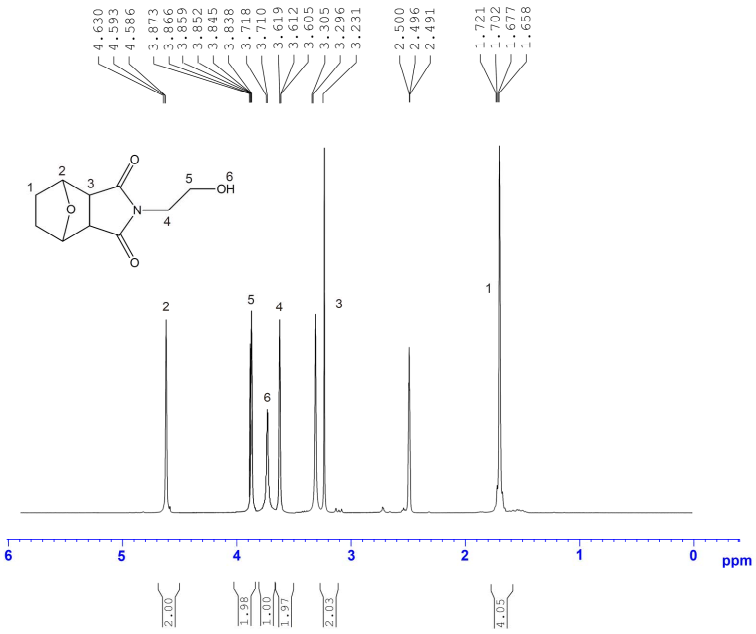


Figure S7. ^{1}HNMR spectrum of **NCA-AE.**

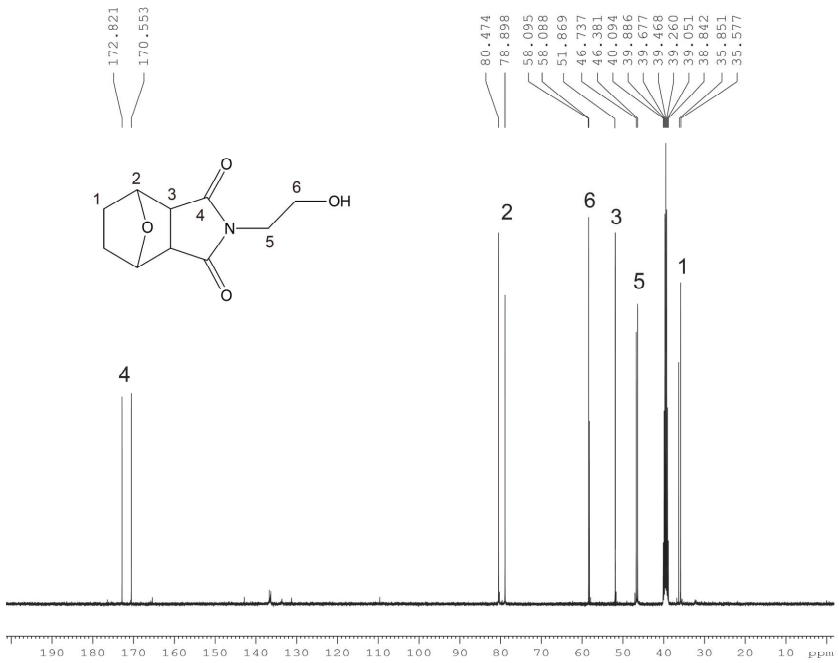


Figure S8. ^{13}CNMR spectrum of **NCA-AE**.

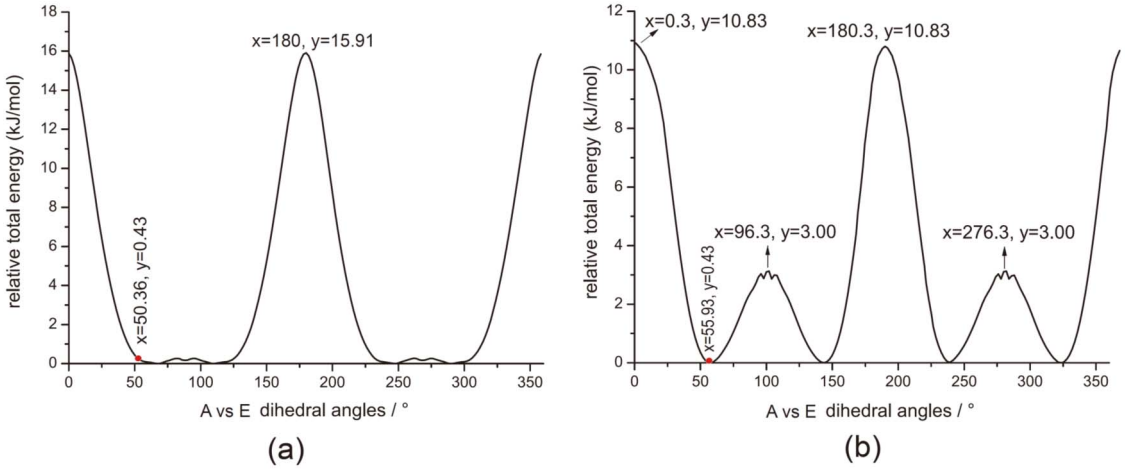


Figure S9. Molecular energy profiles scanned along the dihedral angles of planes A vs E in (a) **DNCA-A** and (b) **DNCA-NA** (both defined in Fig. 1) at the B3LYP\6-311+g(d,p) level. Two red points represent the dihedral angle values in crystal structures, i.e. 50.36° and 55.93°.

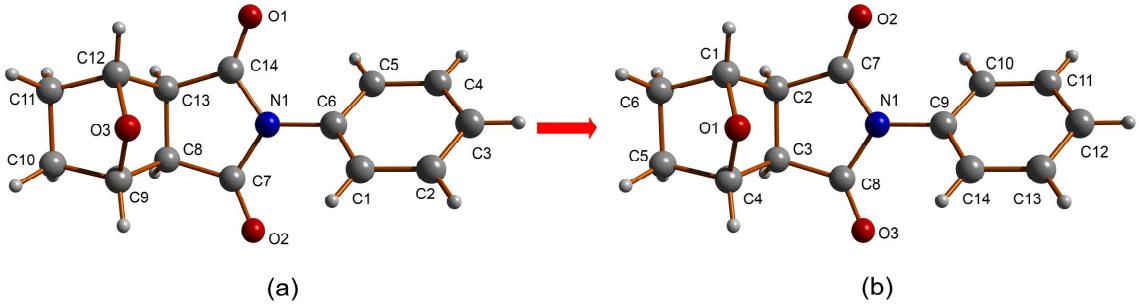


Figure S10. Changing information of atom numbers in **NCA-A(GOLKAU)**. (a) atom numbers reported in ref [1]; (b) atom numbers used in the following figures and tables, aiming for comparison with the title compound **DNCA-A**.

[1] W.-Z. Zhu, Q.-Y. Lin (2009), 8-Phenyl-10-oxa-8-azatricyclo-[4.3.0.1^{2,5}]decane-7,9-dione, *Acta Crystallogr.,Sect.E(Structure Rep.Online),***65,**'o287'