Synthesis and biological activity of imidazole based 1,4-naphthoquinones

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Supplementary

Figure Legends

Table Legends

Table S1	FT-IR Frequencies (in cm^{-1}) for **B-2**, **B-3**, **A-1** to **A-4** and **I-1** to **I-4**
Table S2a	^{13}C chemical Shift (δ (ppm)) of **B-3**, **A-1** to **A-4**, **I-1** to **I-4** in $CDCl_3$
Table S2b	^{1}H NMR chemical shifts in **B-3**, **A-1** to **A-4** and **I-1** to **I-4** derivatives
Table S3	Hydrogen bond geometries for **B-3**, **A-1** to **A-3** and **I-2** to **I-4**
Table S4	Crystal data and structure refinement for **B-3**
Table S5	Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **B-3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor
Table S6	Bond lengths [Å] and angles [°] for **B-3**
Table S7	Anisotropic displacement parameters (Å^{2}x 10^3) for **B-3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$
Table S8	Crystal data and structure refinement for **A-1**
Table S9	Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3)for **A-1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor
Table S10	Bond lengths [Å] and angles [°] for **A-1**
Table S11	Anisotropic displacement parameters (Å^{2}x 10^3) for **A-1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$
Table S12	Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3)for **A-1**
Table S13	Torsion angles [°] for **A-1**
Table S14	Crystal data and structure refinement for **A-2**
Table S15	Bond lengths [Å] and angles [°] for **A-2**
Table S16	Torsion Angles **A-2**
Table S17	Crystal data and structure refinement for **A-3**
Table S18	Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **A-3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.
Table S19	Bond lengths [Å] and angles [°] for **A-3**
Table S20	Anisotropic displacement parameters (Å^{2}x 10^3) for **A-3**. The anisotropicdisplacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$
Table S21	Torsion angles [°] for **A-3**
Table S22	Crystal data and structure refinement for **I-2**

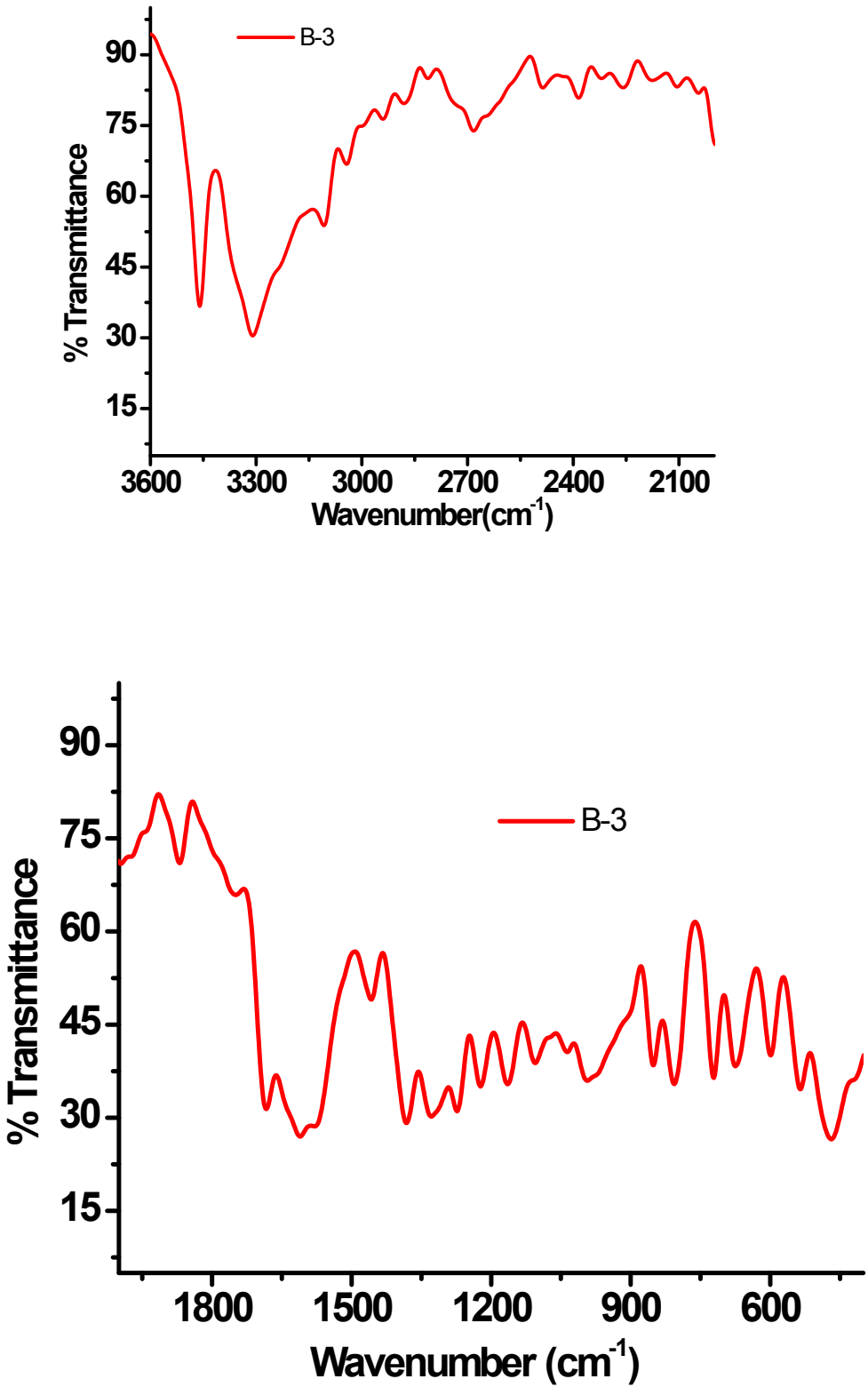


Fig.S1 FT-IR spectra of **B-3**

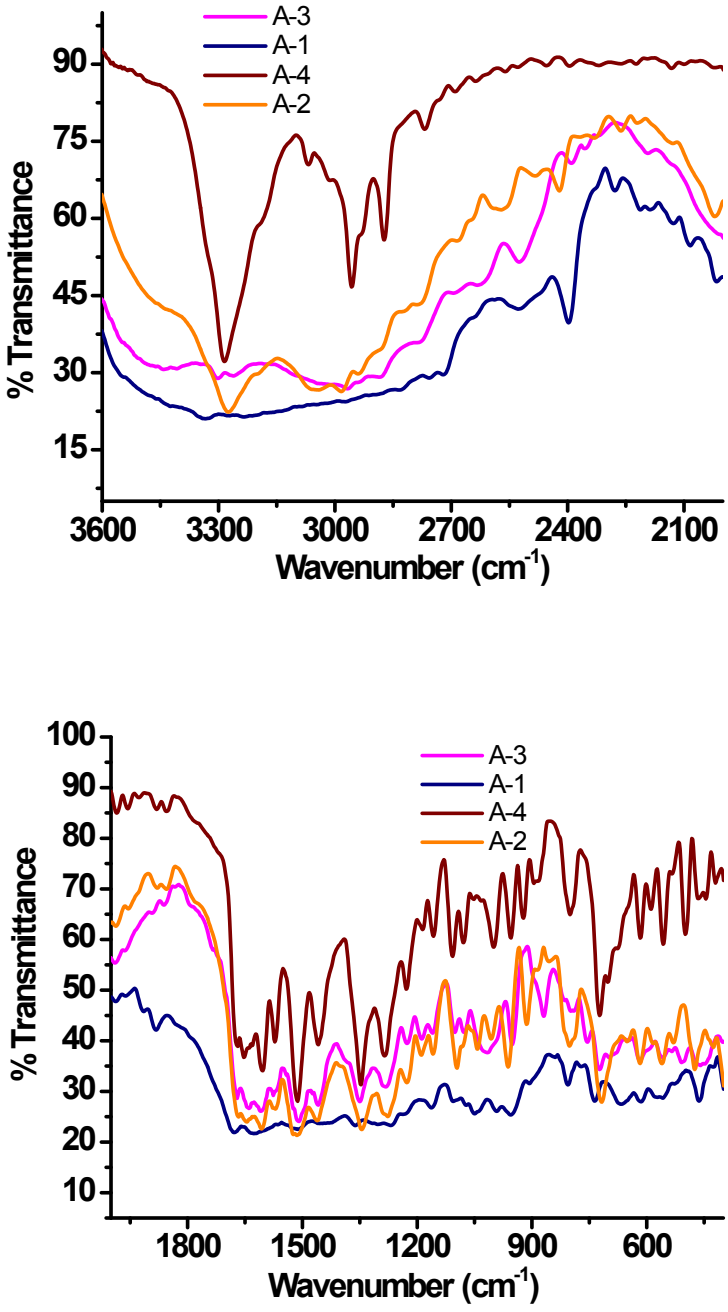


Fig.S2 FT-IR spectra of **A-1**, **A-2**, **A-3** and **A-4**

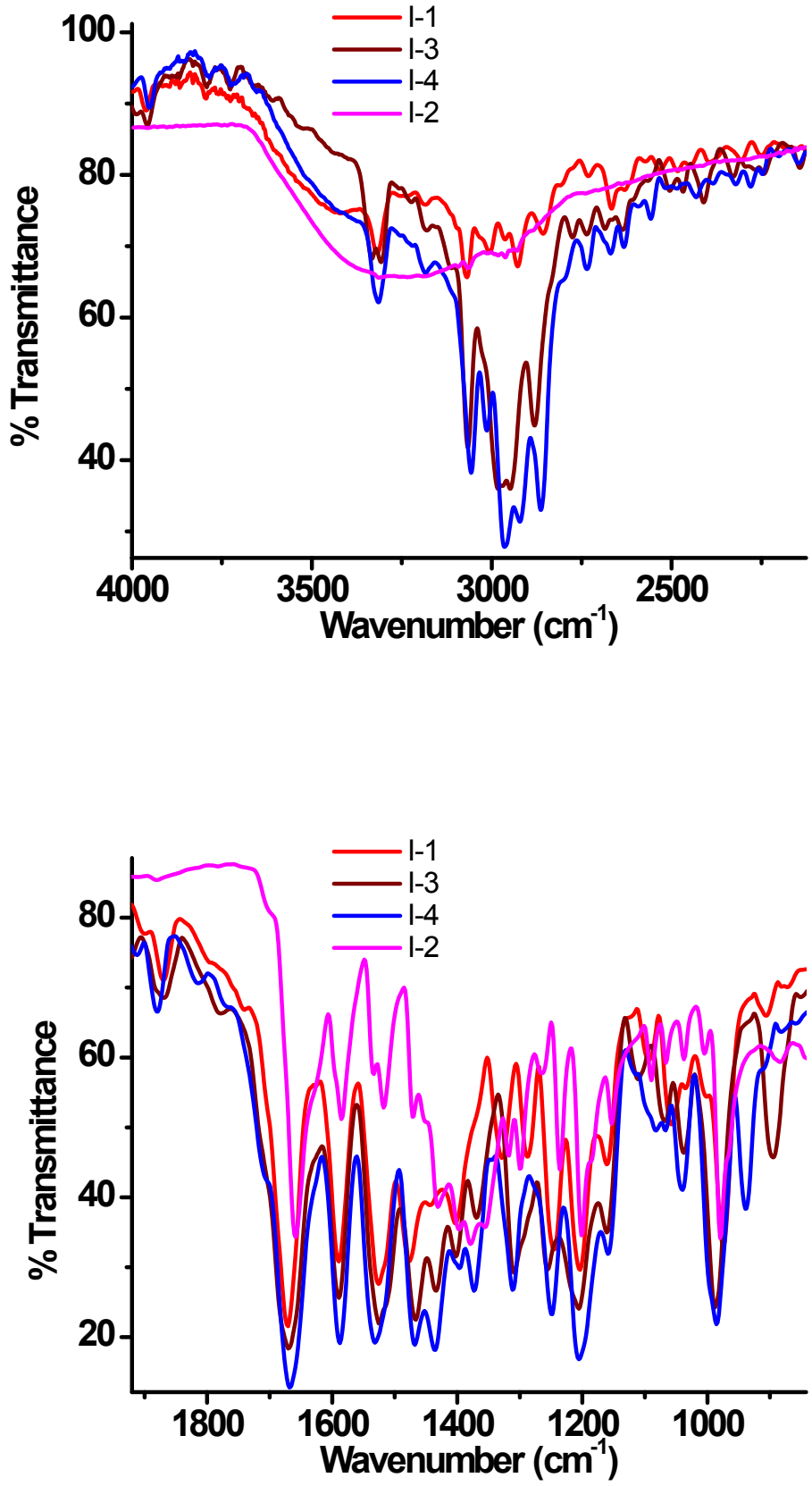


Fig.S3 FT-IR spectra of **I-1**, **I-2**, **I-3** and **I-4**

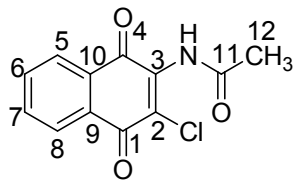
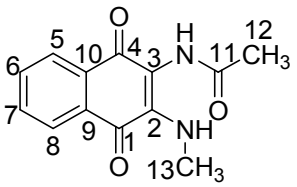
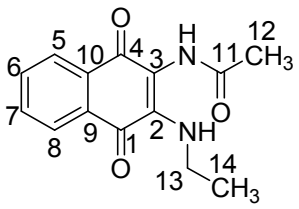
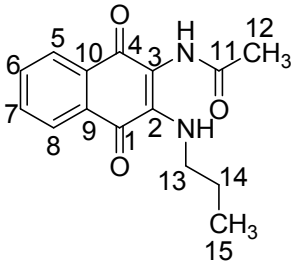
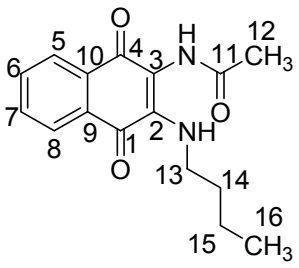
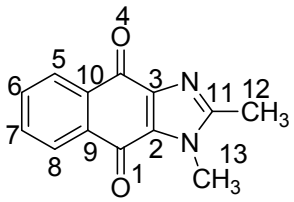
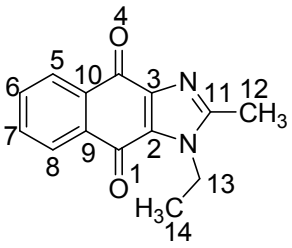
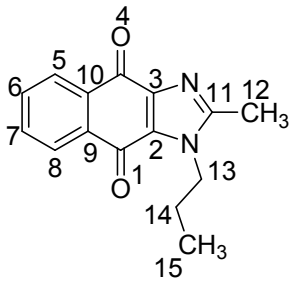
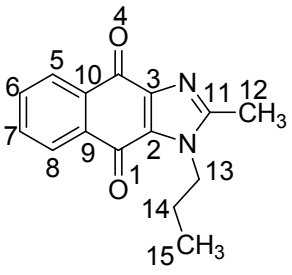
Structure	
 **B-3**	 **A-1**
 **A-2**	 **A-3**
 **A-4**	 **I-1**
 **I-2**	 **I-3**
 **I-4**	

Fig.S4 Atom numbering scheme of 1,4-naphthoquinone compounds

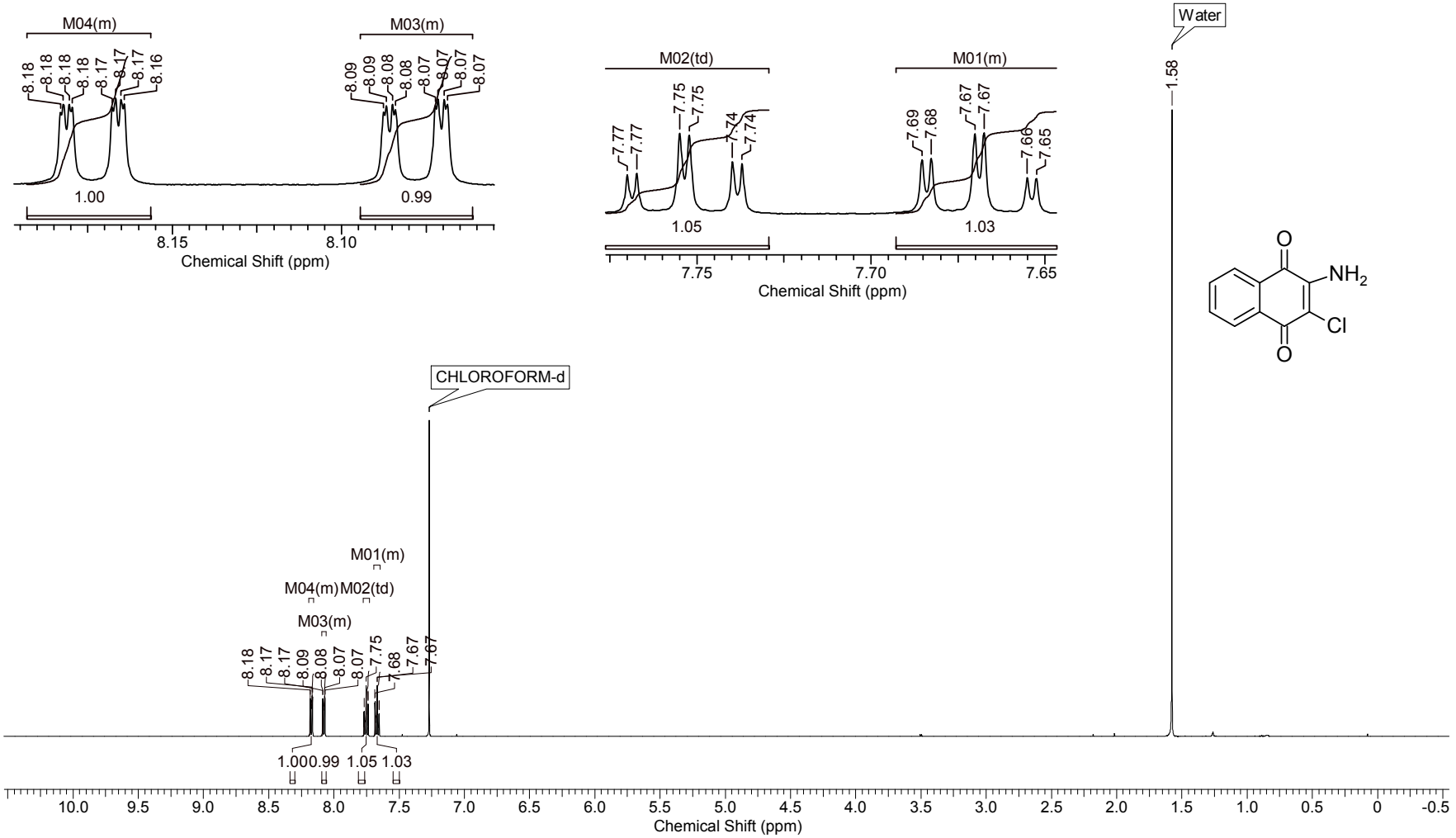


Fig.S5 ^{1}H NMR of **B-2** in $CDCl_3$ at 293K

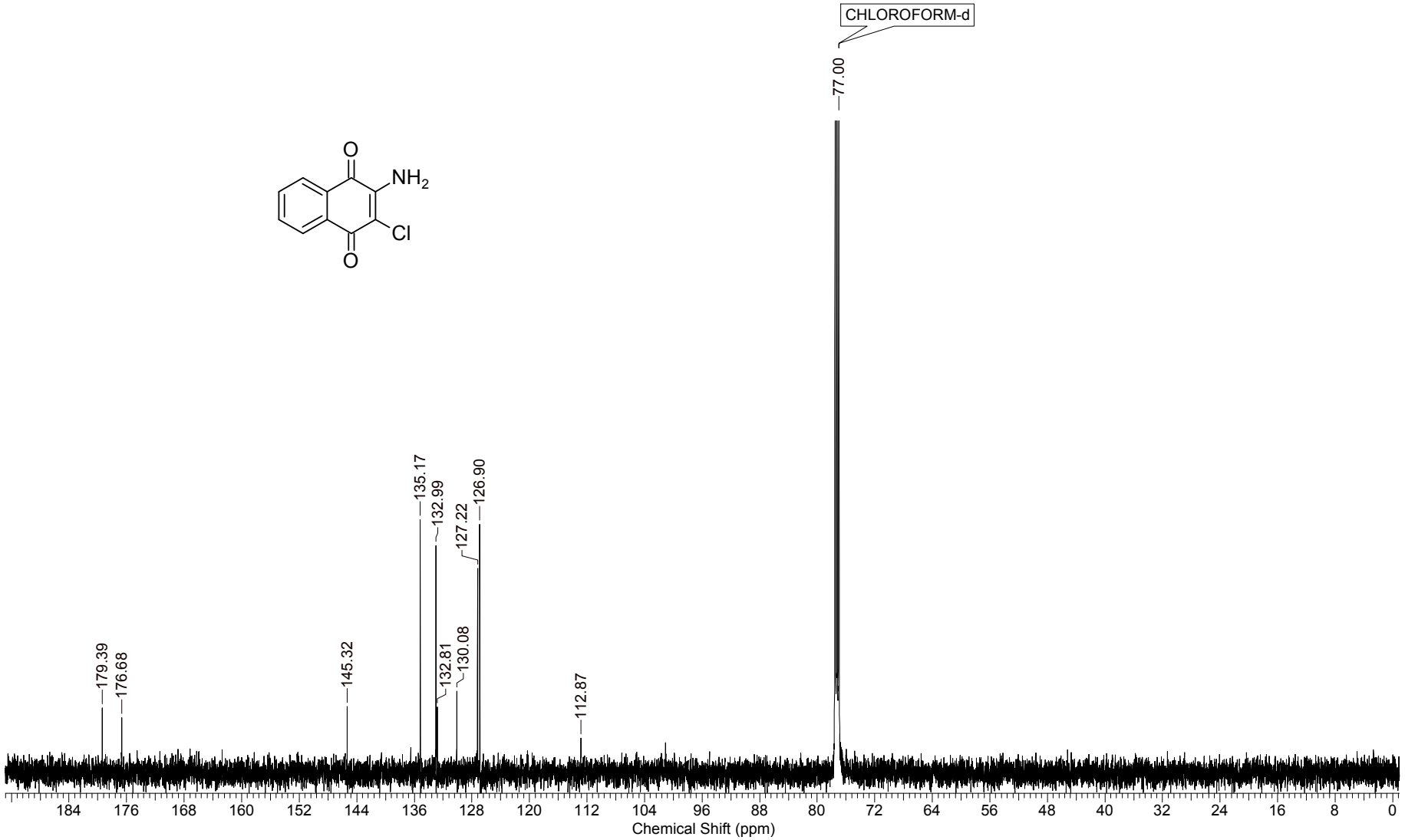


Fig.S6 ^{13}C NMR of **B-2** in $CDCl_3$ at 293K

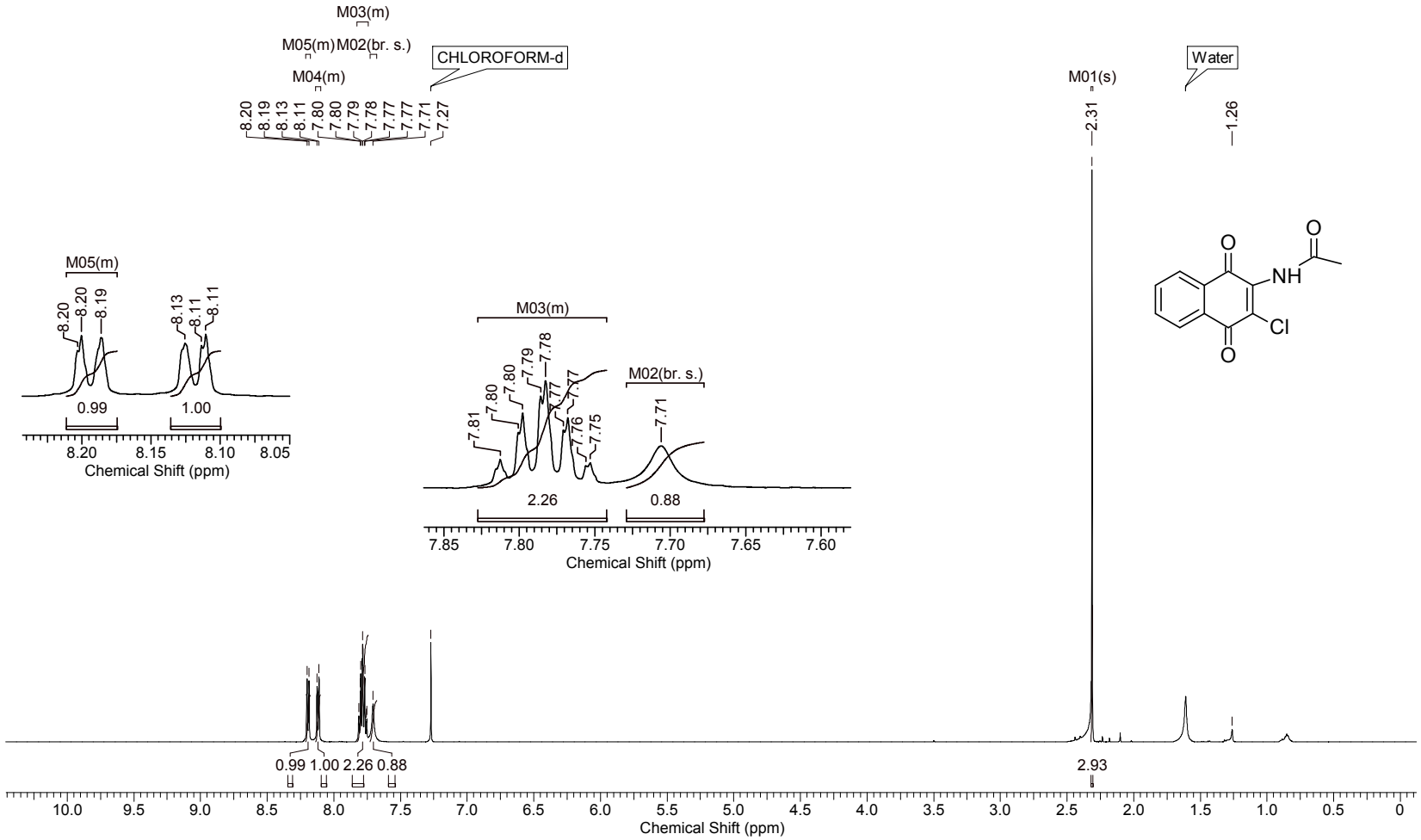


Fig.S7 ^{1}H NMR of **B-3** in $CDCl_3$ at 293K

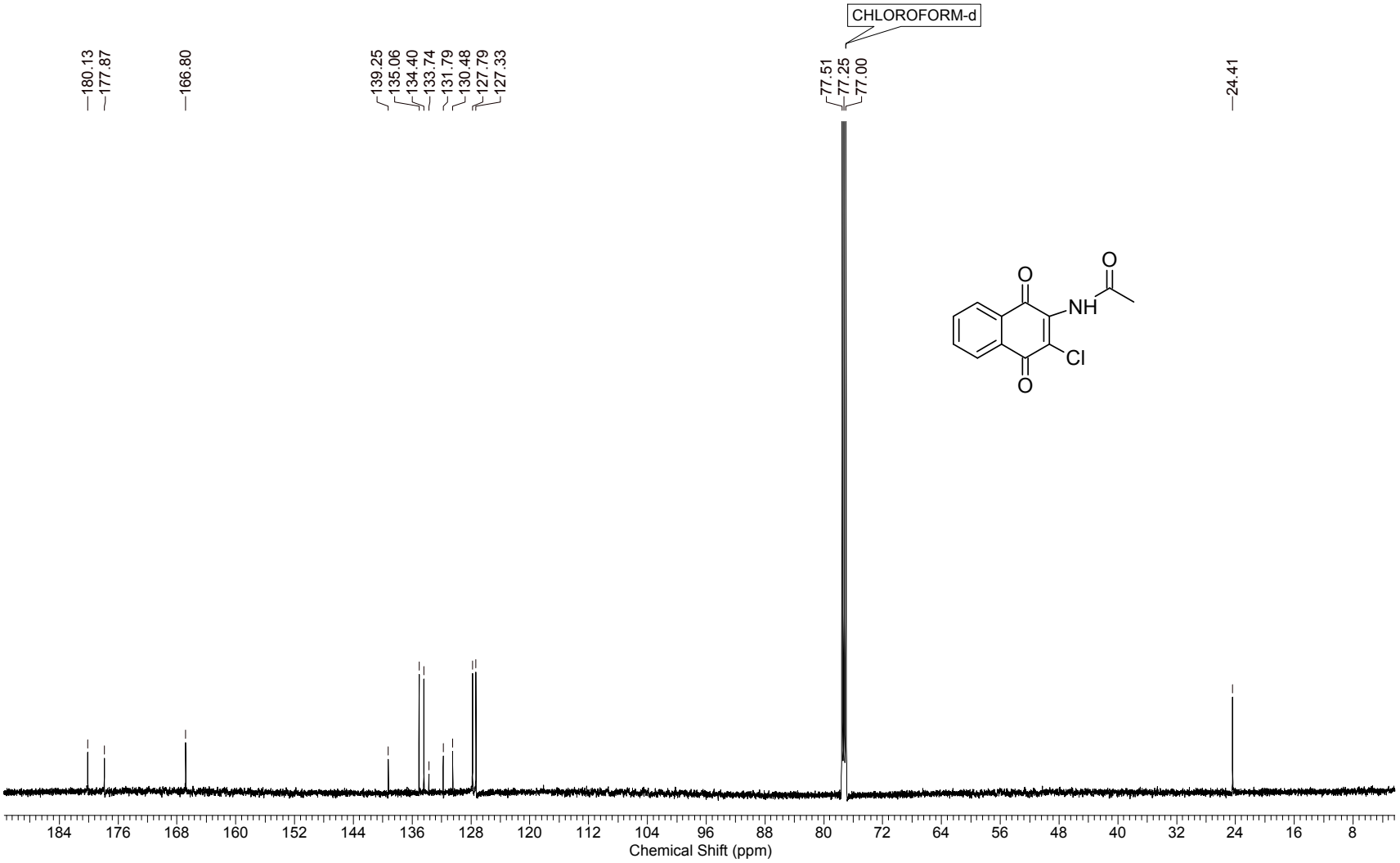


Fig.S8 ^{13}C NMR of **B-3** in $CDCl_3$ at 293K

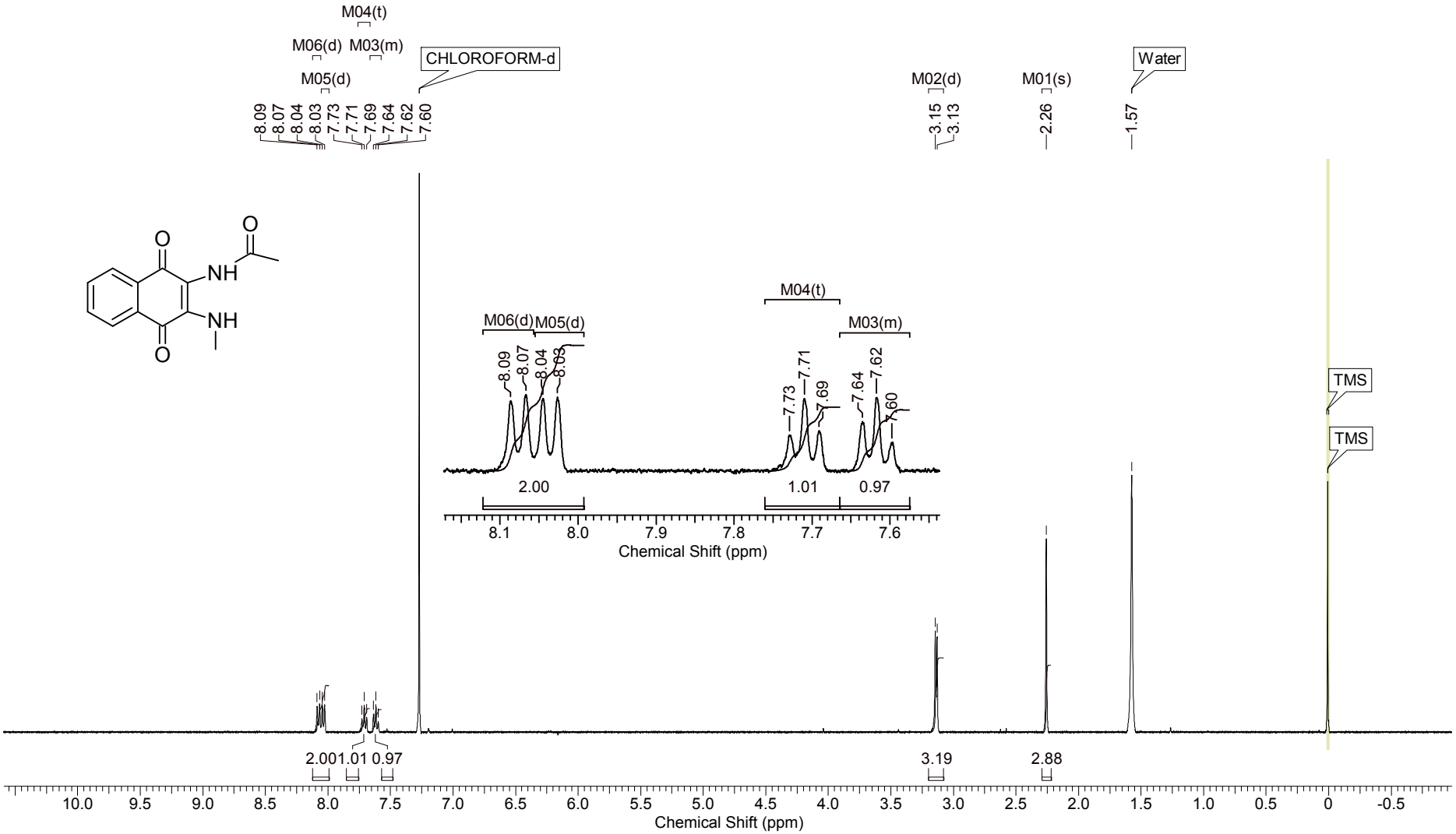


Fig.S9 ^{1}H NMR of **A-1** in $CDCl_3$ at 293K

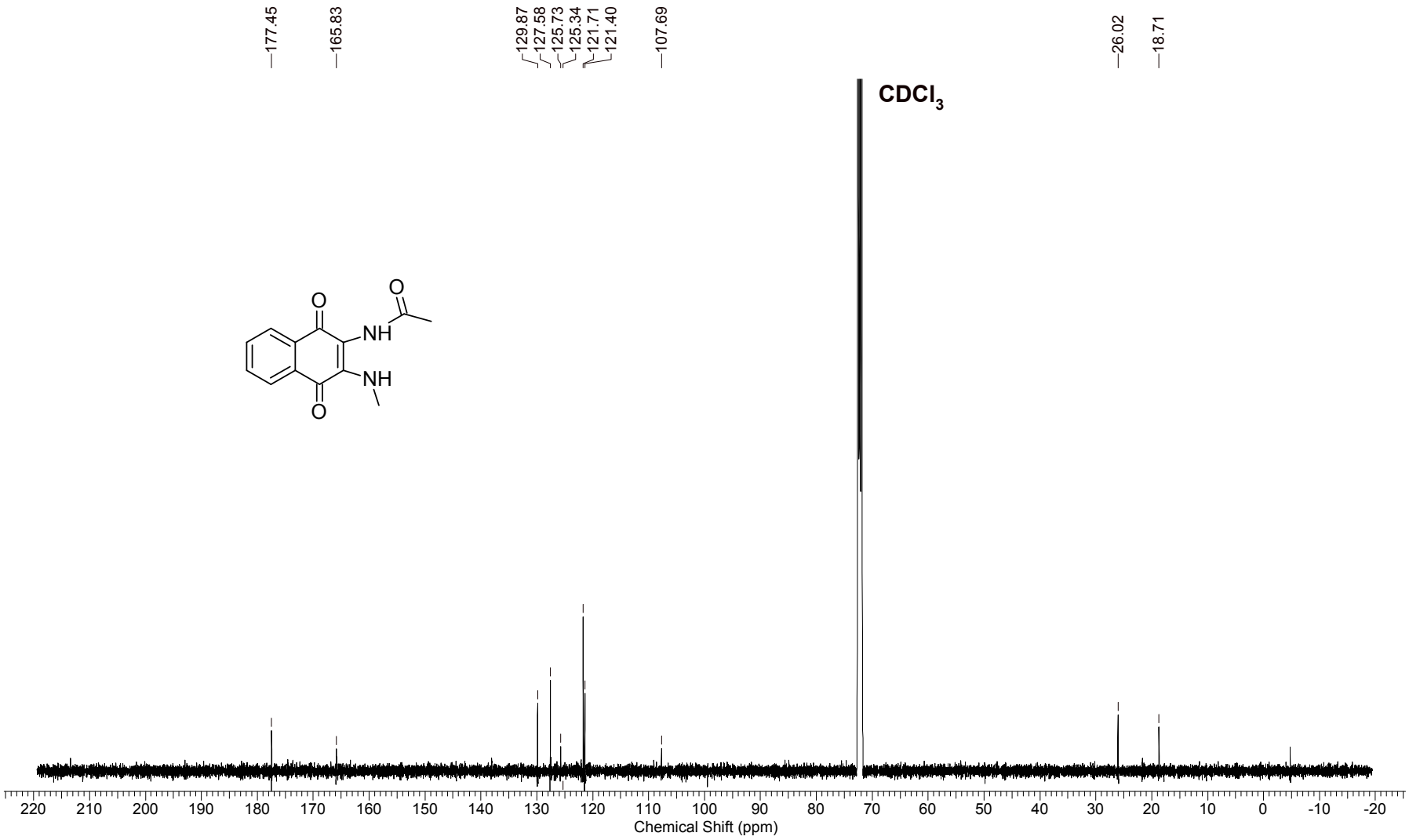


Fig.S10 ^{13}C NMR of **A-1** in $CDCl_3$ at 293K

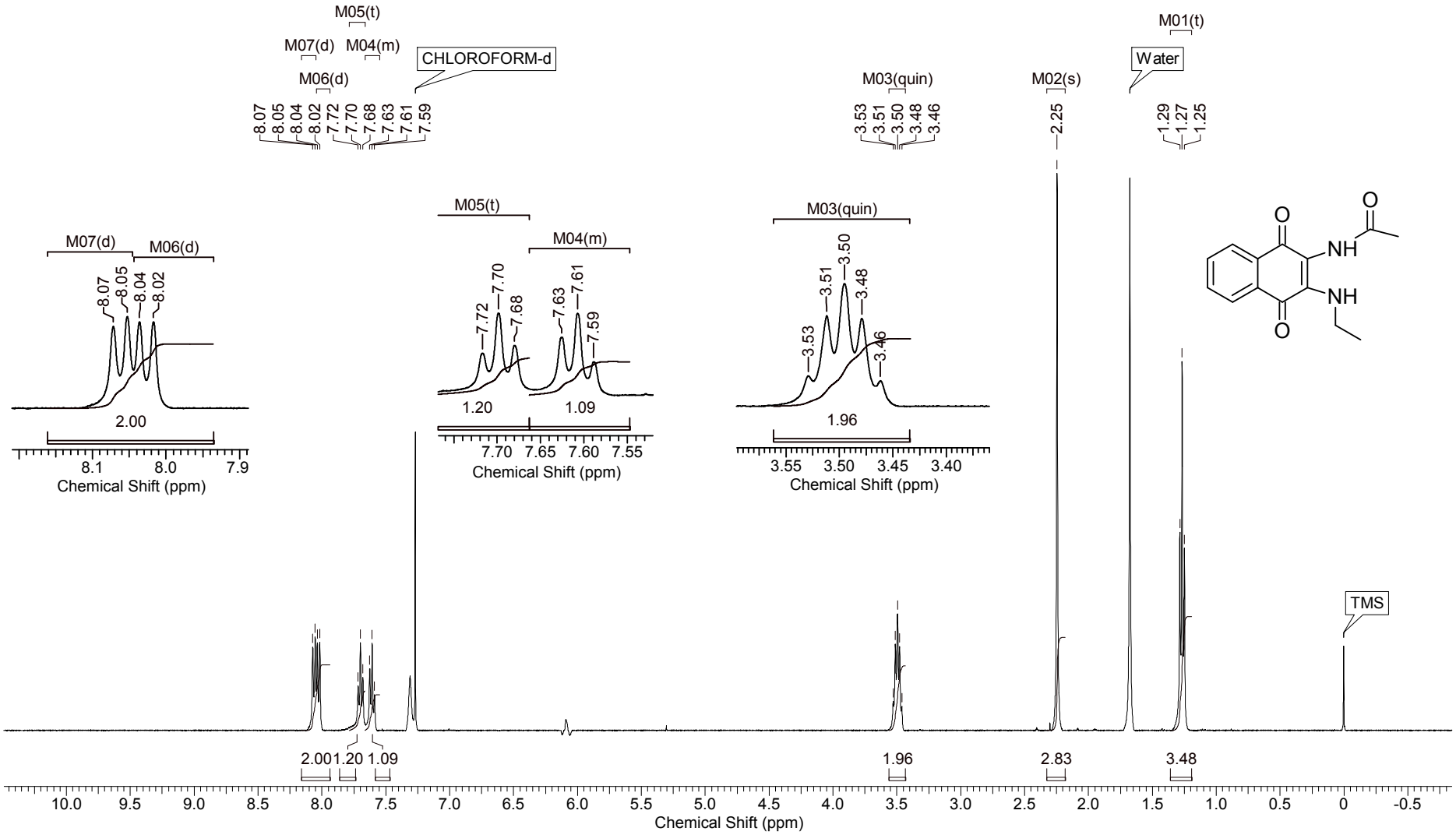


Fig.S11 ^{1}H NMR of **A-2** in $CDCl_3$ at 293K

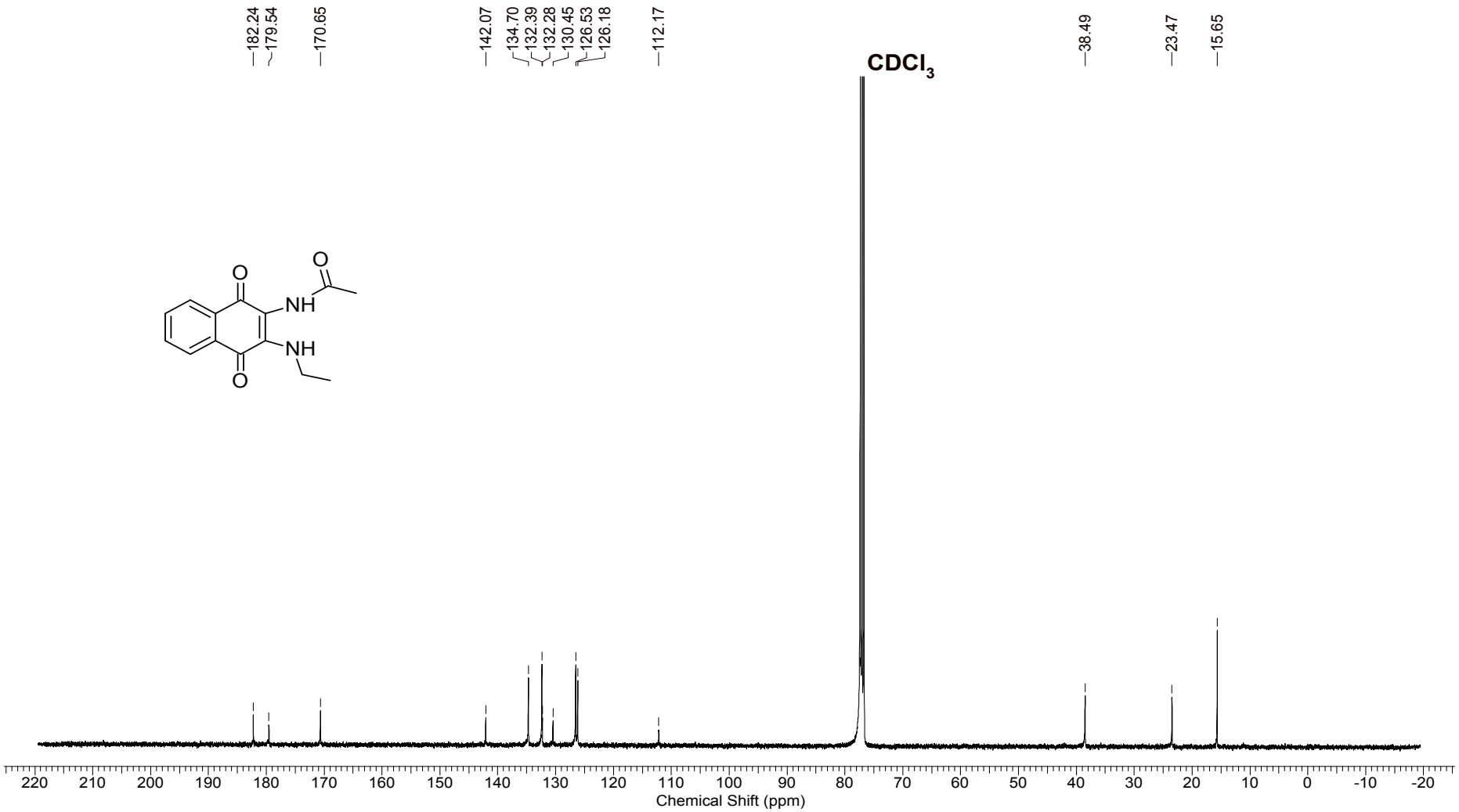


Fig.S12 ^{13}C NMR of **A-2** in $CDCl_3$ at 293K

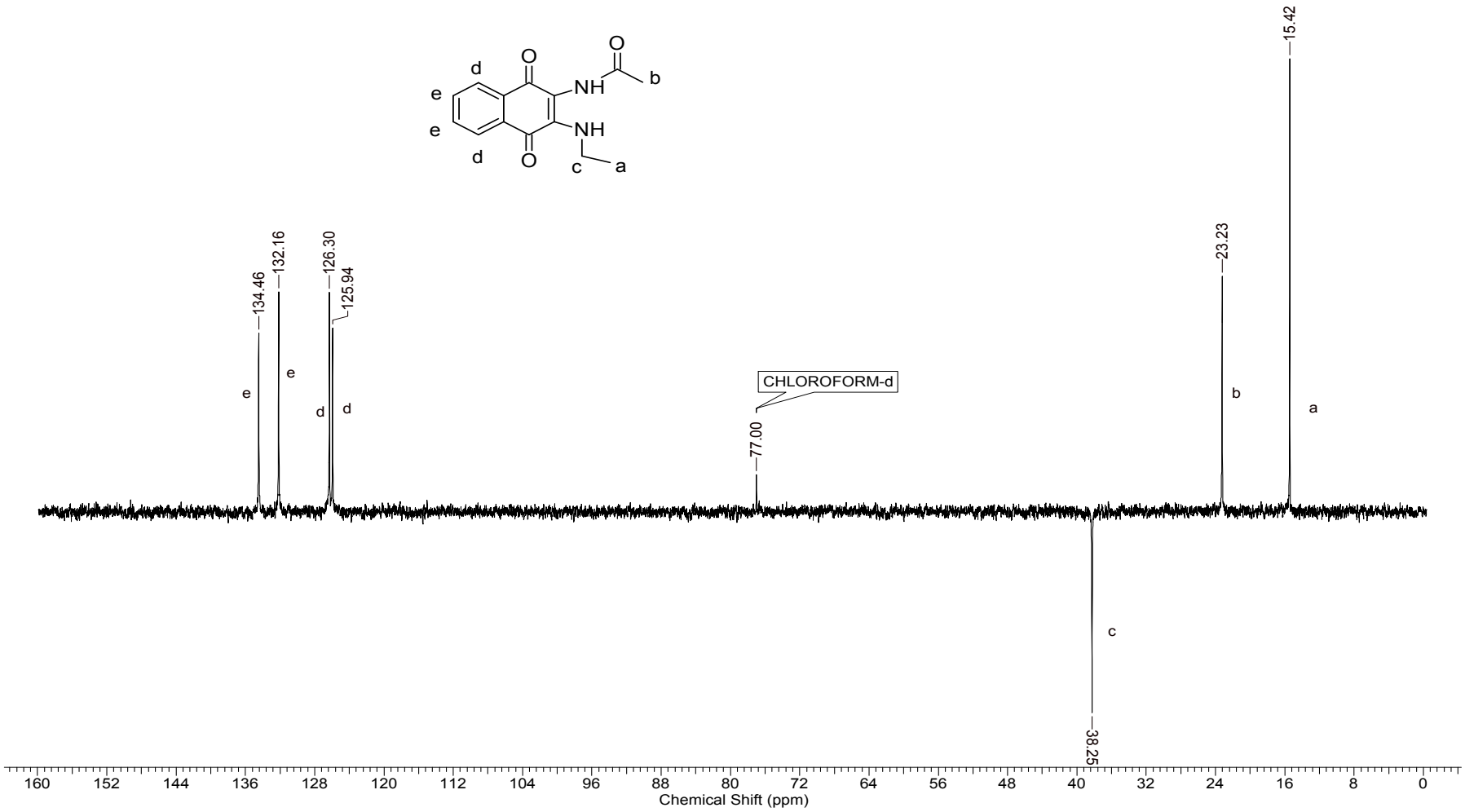


Fig.S13 DEPT NMR of **A-2** in $CDCl_3$ at 293K

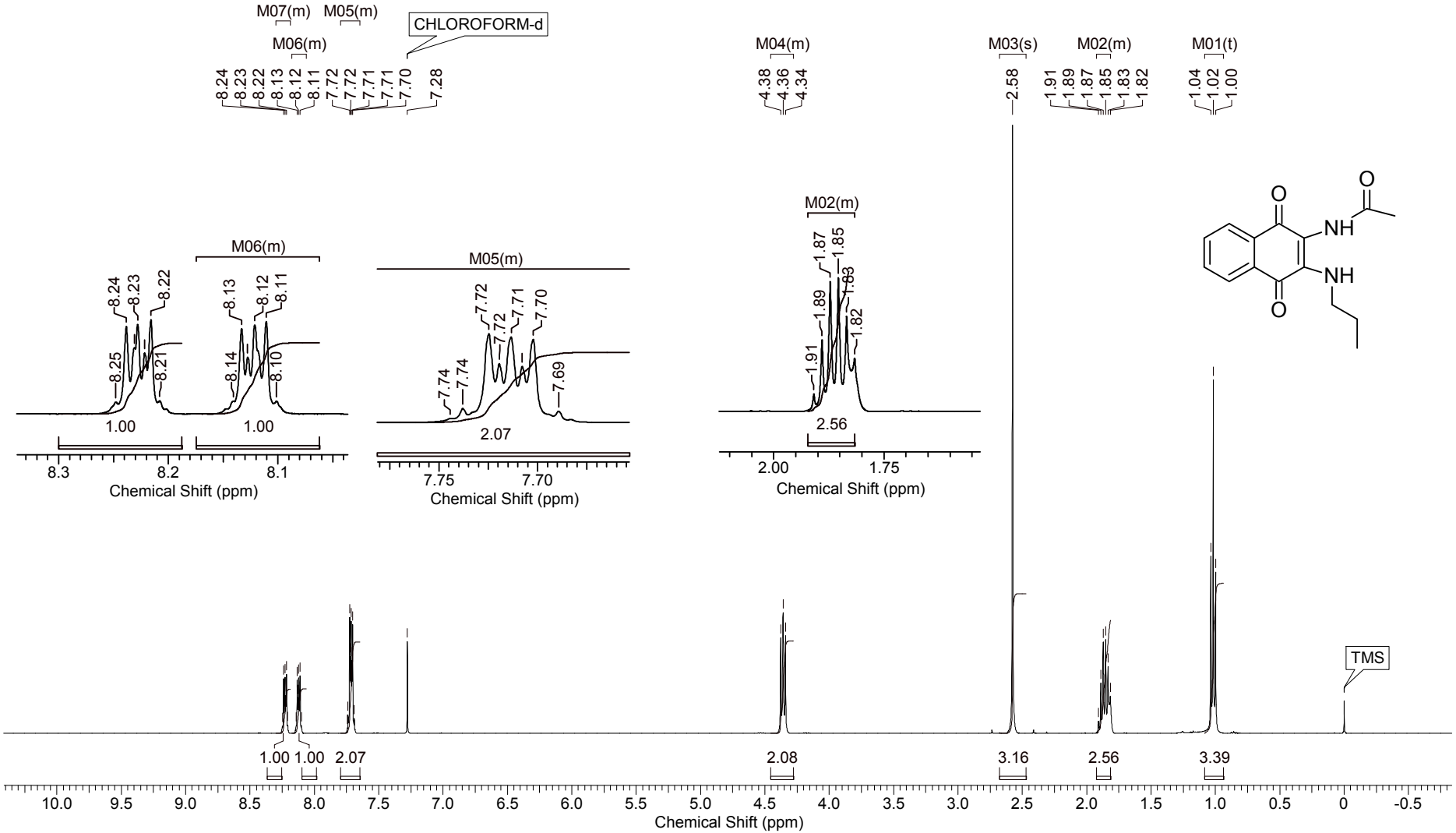


Fig.S14 ^{1}H NMR of **A-3** in $CDCl_3$ at 293K

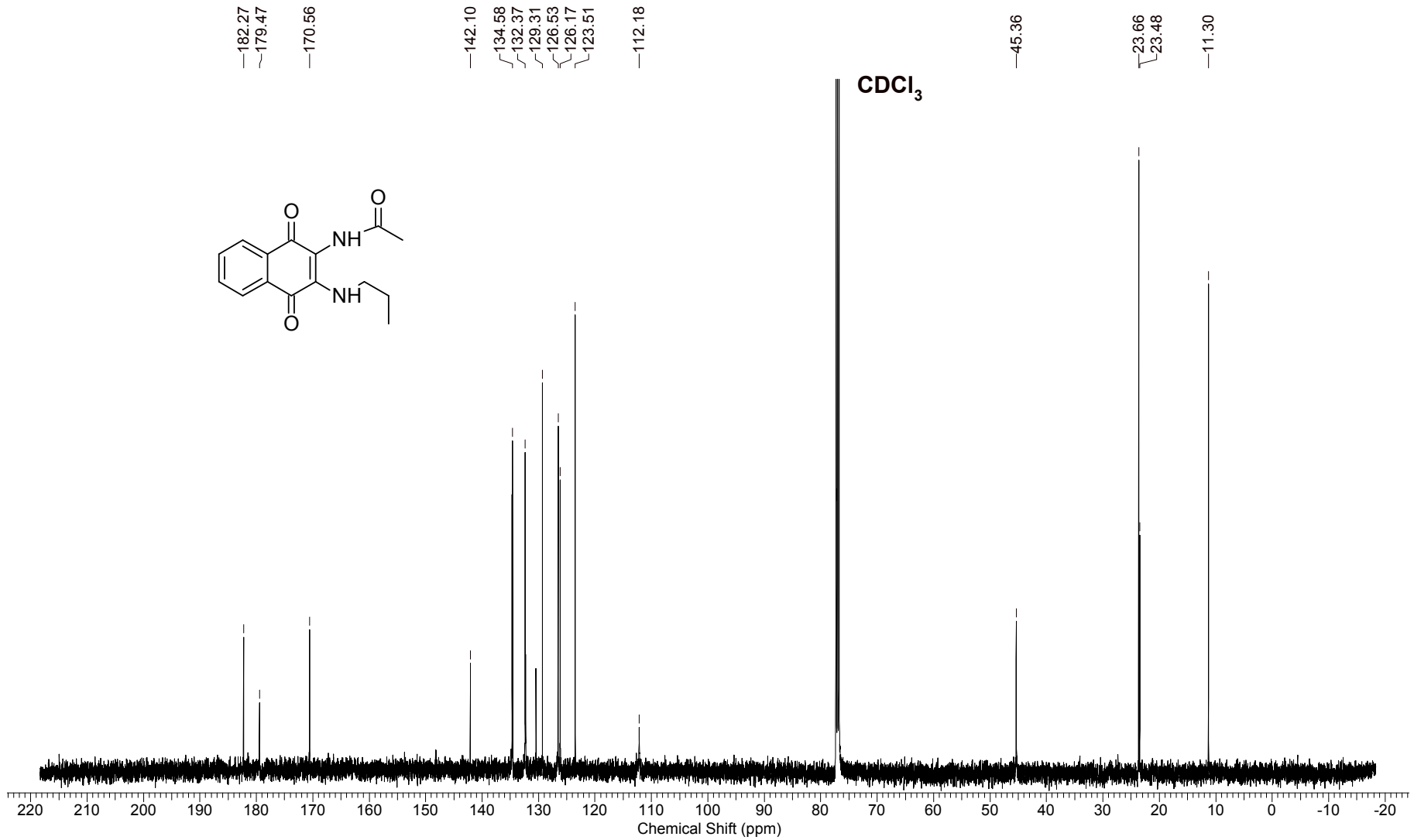


Fig.S15 ^{13}C NMR of **A-3** in $CDCl_3$ at 293K

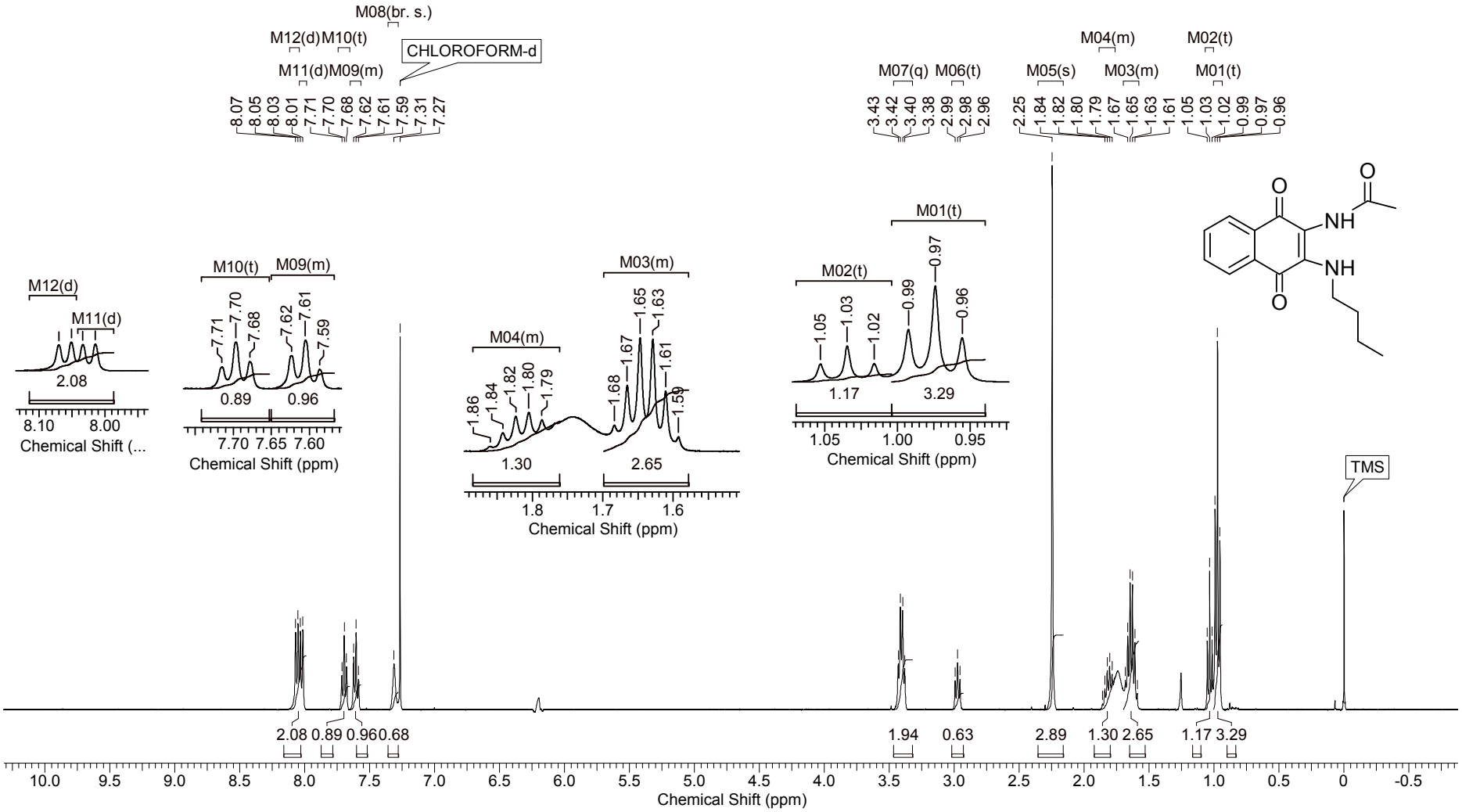


Fig.S16 ^{1}H NMR of **A-4** in $CDCl_3$ at 293K

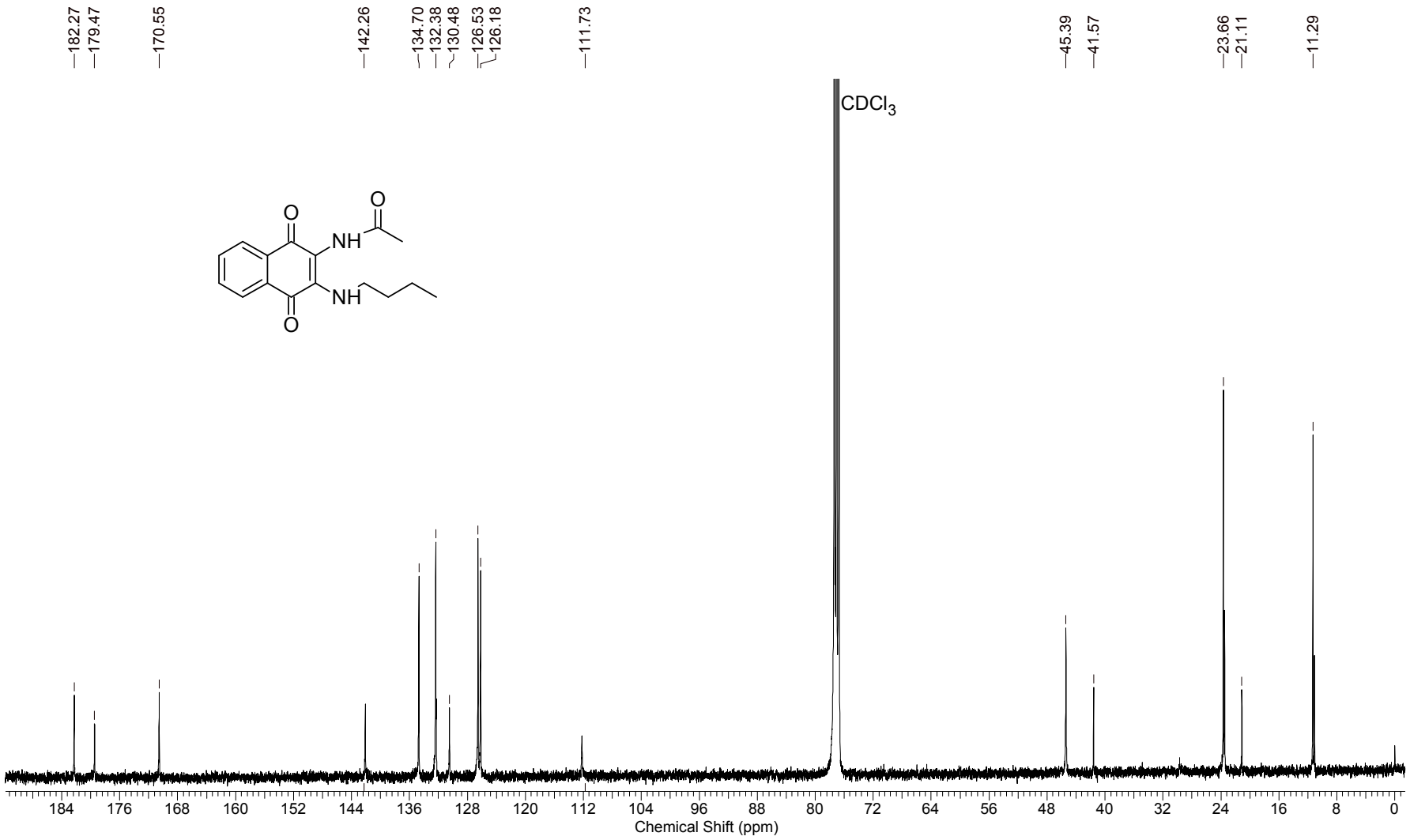


Fig.S17 ^{13}C NMR of **A-4** in $CDCl_3$ at 293K

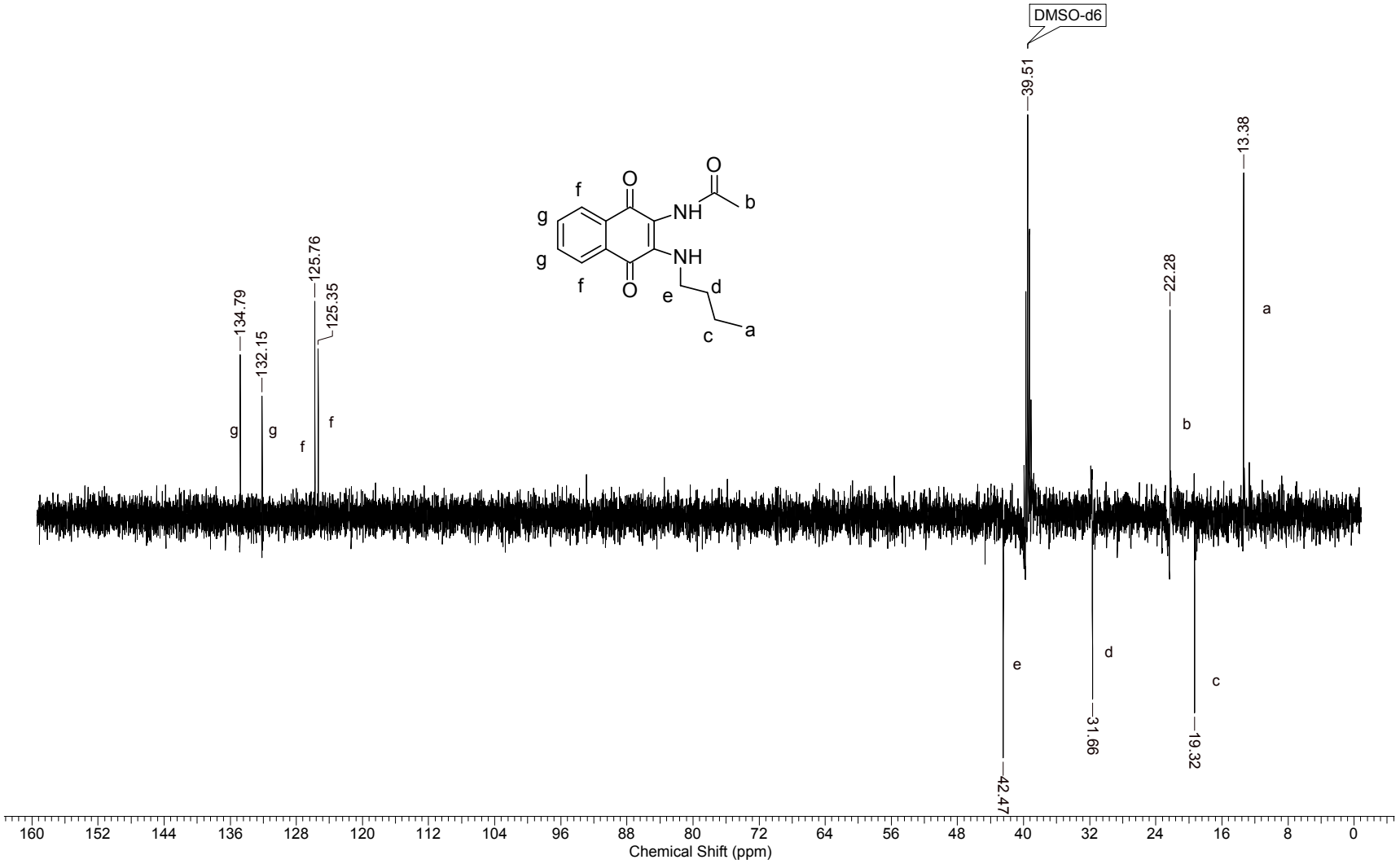


Fig.S18 DEPT NMR of **A-4** in DMSO-d_6 at 293K

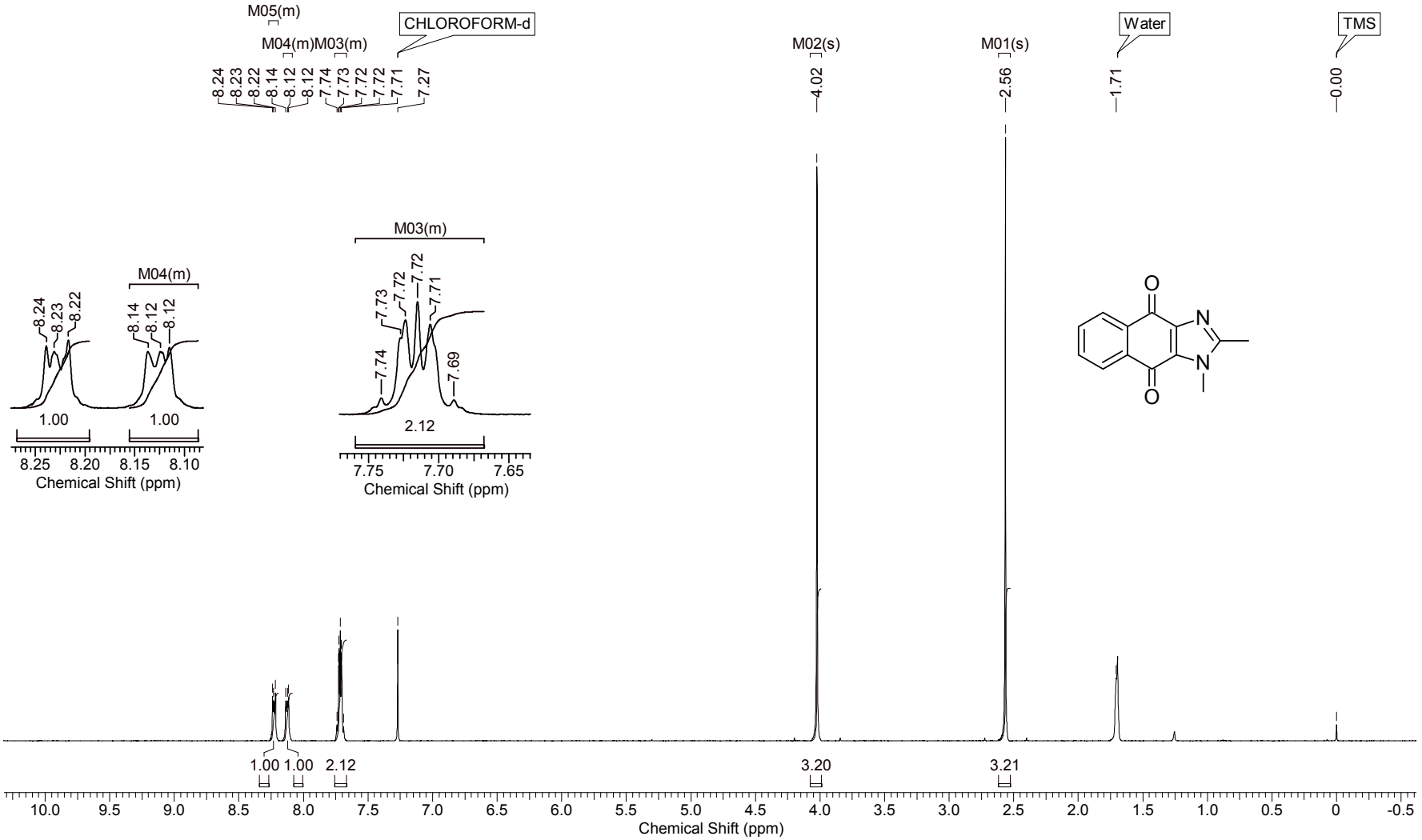


Fig.S19 ^{1}H NMR of **I-1** in $CDCl_3$ at 293 K

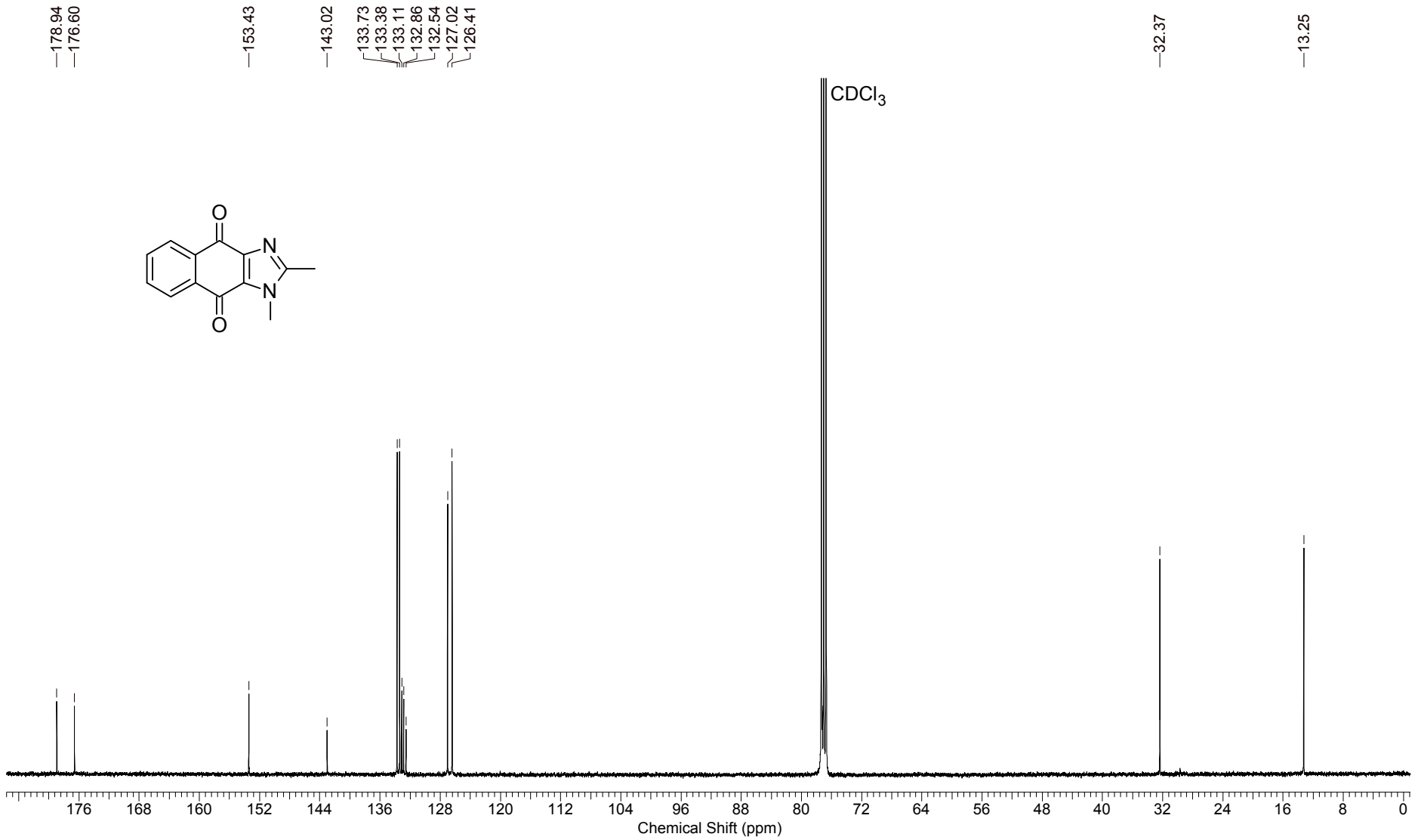


Fig.S20 ^{13}C NMR of **I-1** in *$CDCl_3$* at 293 K

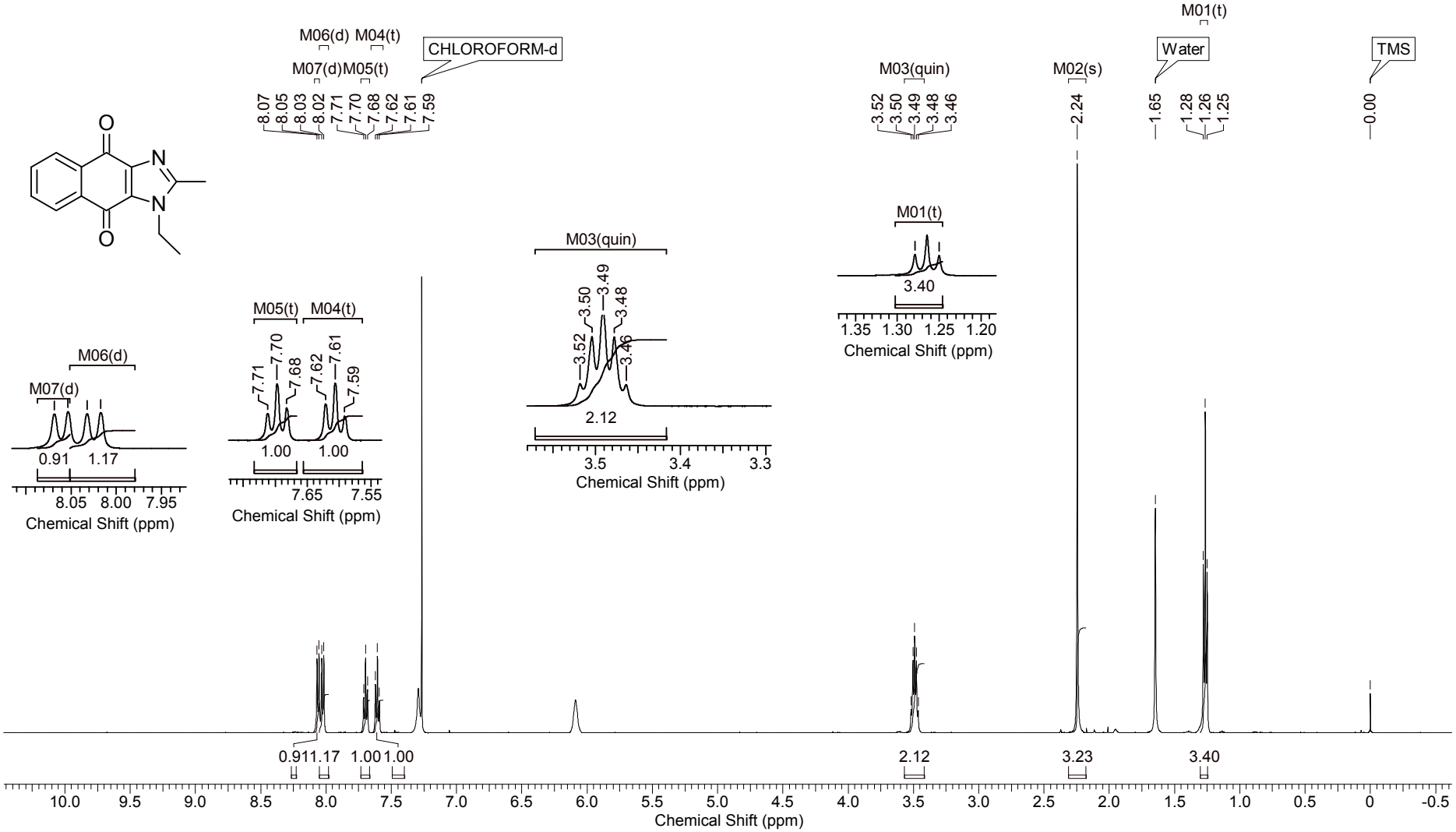


Fig.S21 ^{1}H NMR of **I-2** in $CDCl_3$ at 293 K

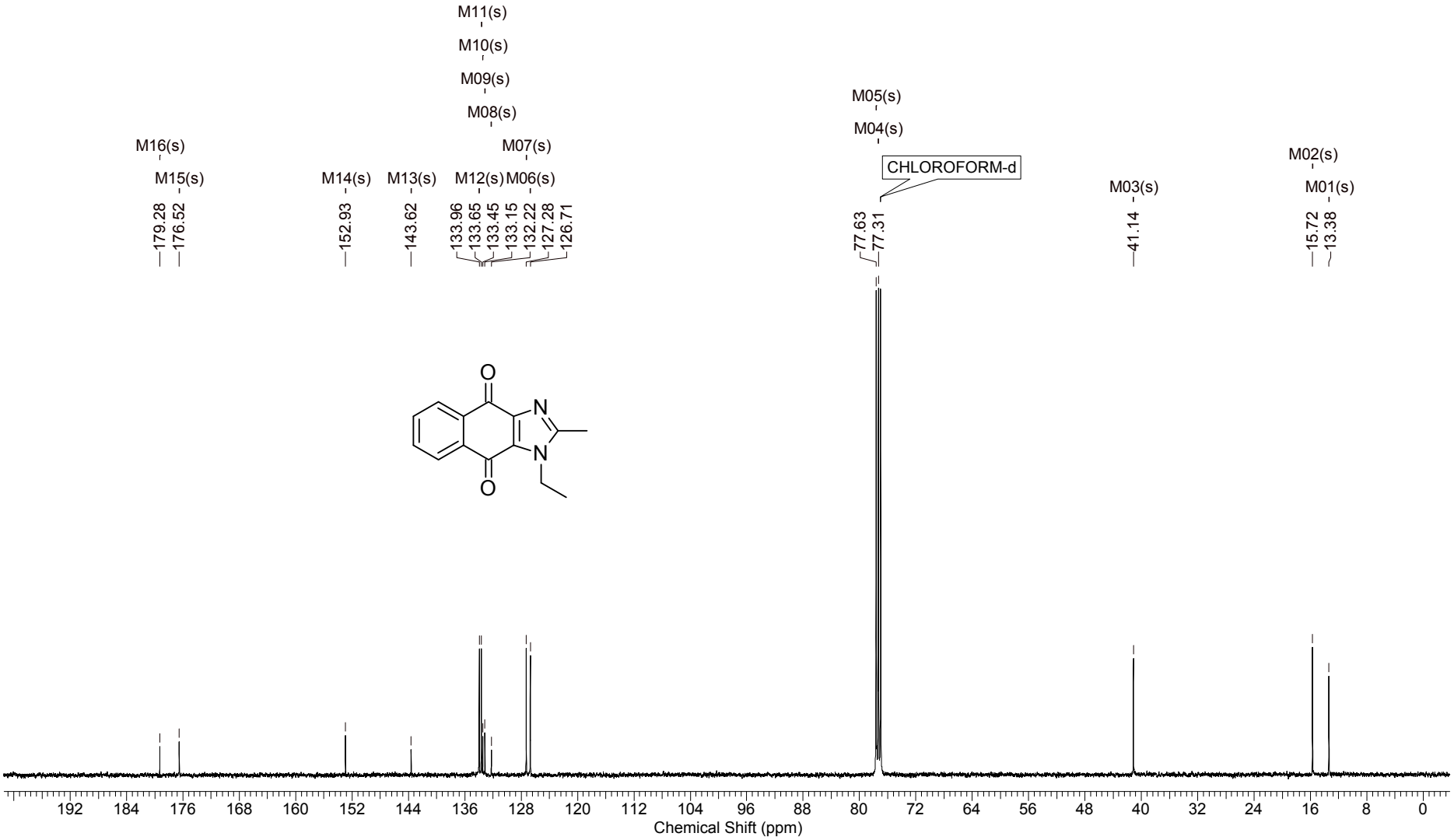


Fig.S22 ^{13}C NMR of **I-2** in $CDCl_3$ at 293 K

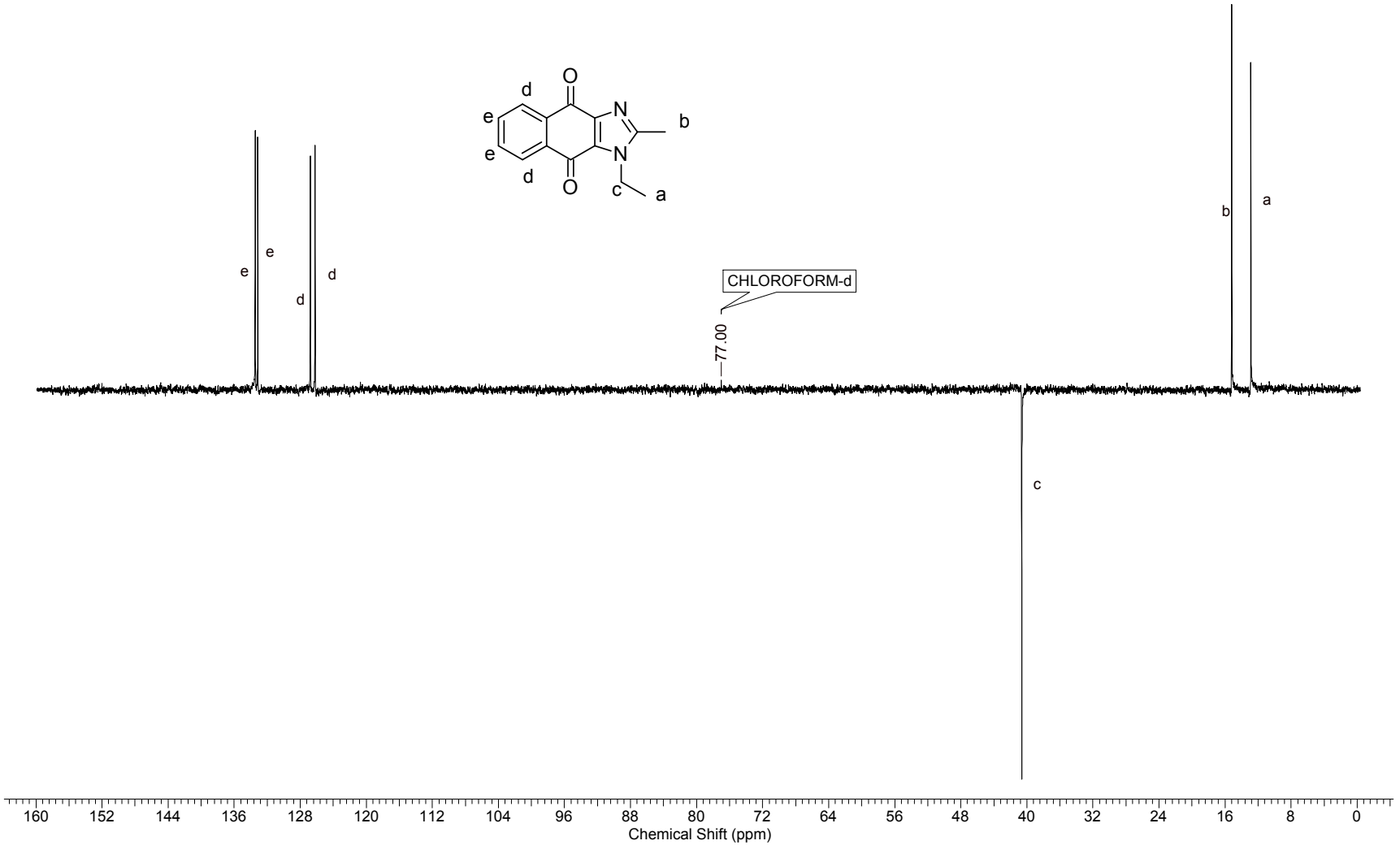


Fig.S23 DEPT NMR of **I-2** in $CDCl_3$ at 293 K

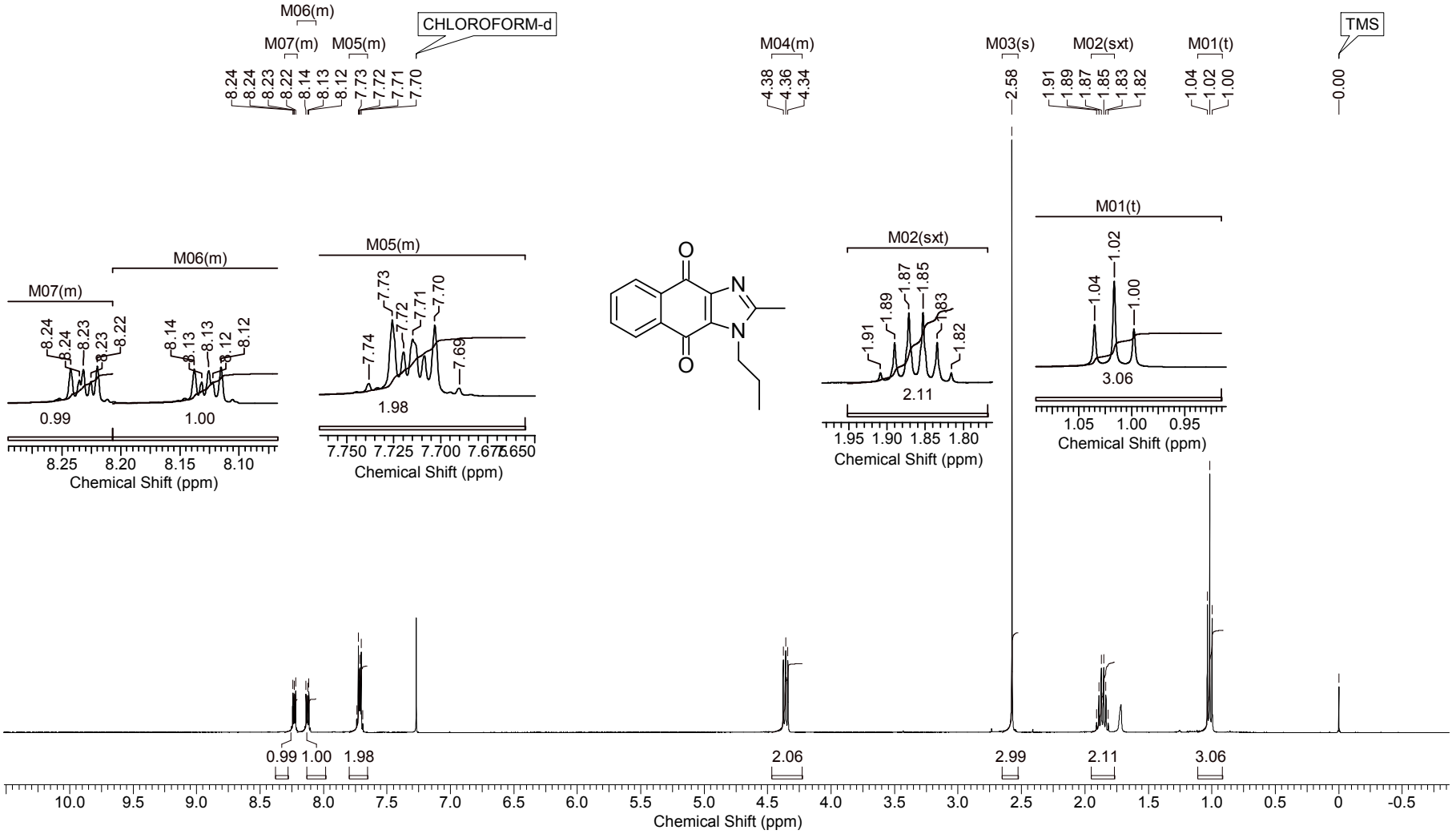


Fig.S24 ^{1}H NMR of **I-3** in $CDCl_3$ at 293 K

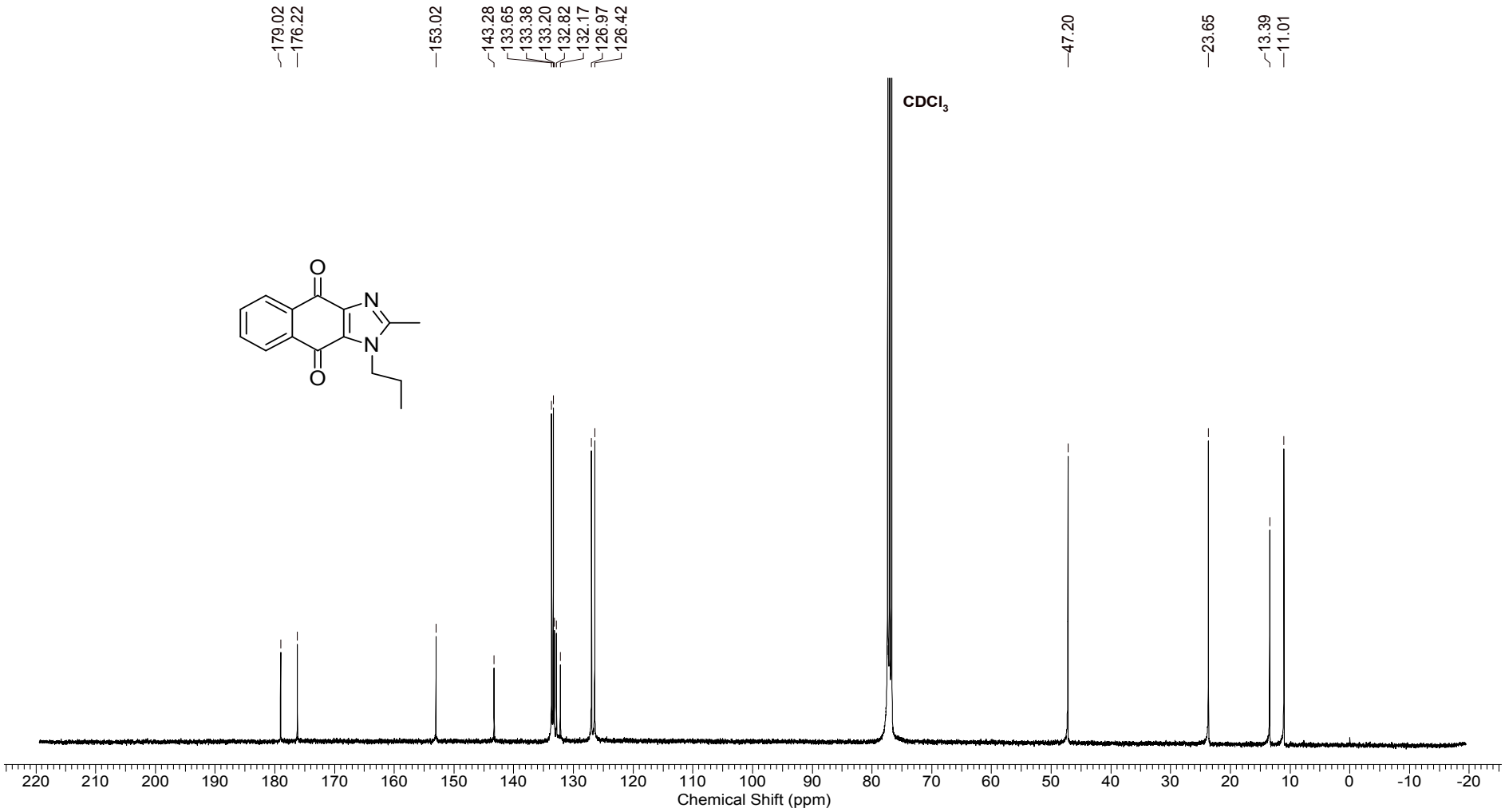


Fig.S25 ^{13}C NMR of **I-3** in *$CDCl_3$* at 293 K

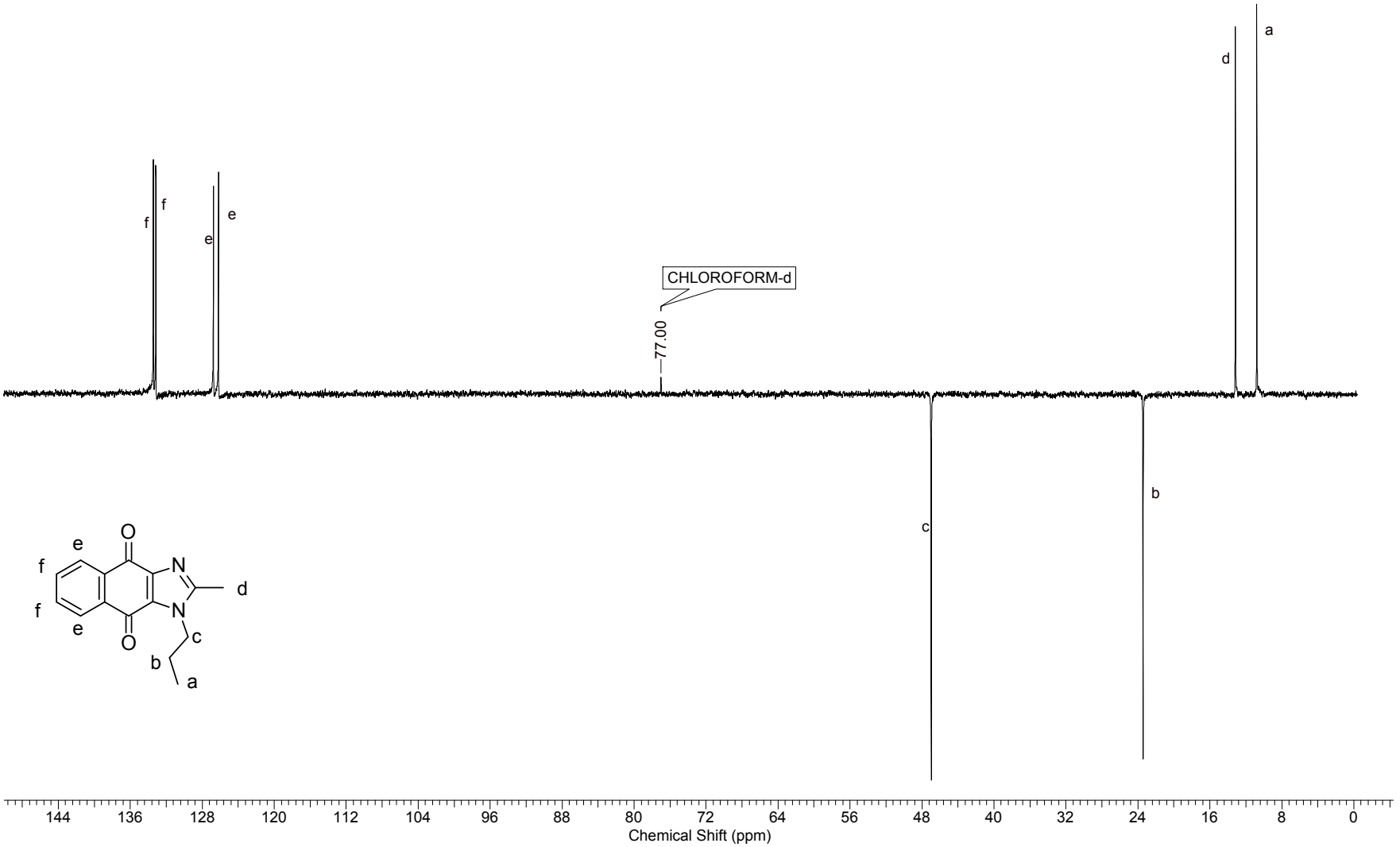


Fig.S26 DEPT NMR of **I-3** in $CDCl_3$ at 293 K

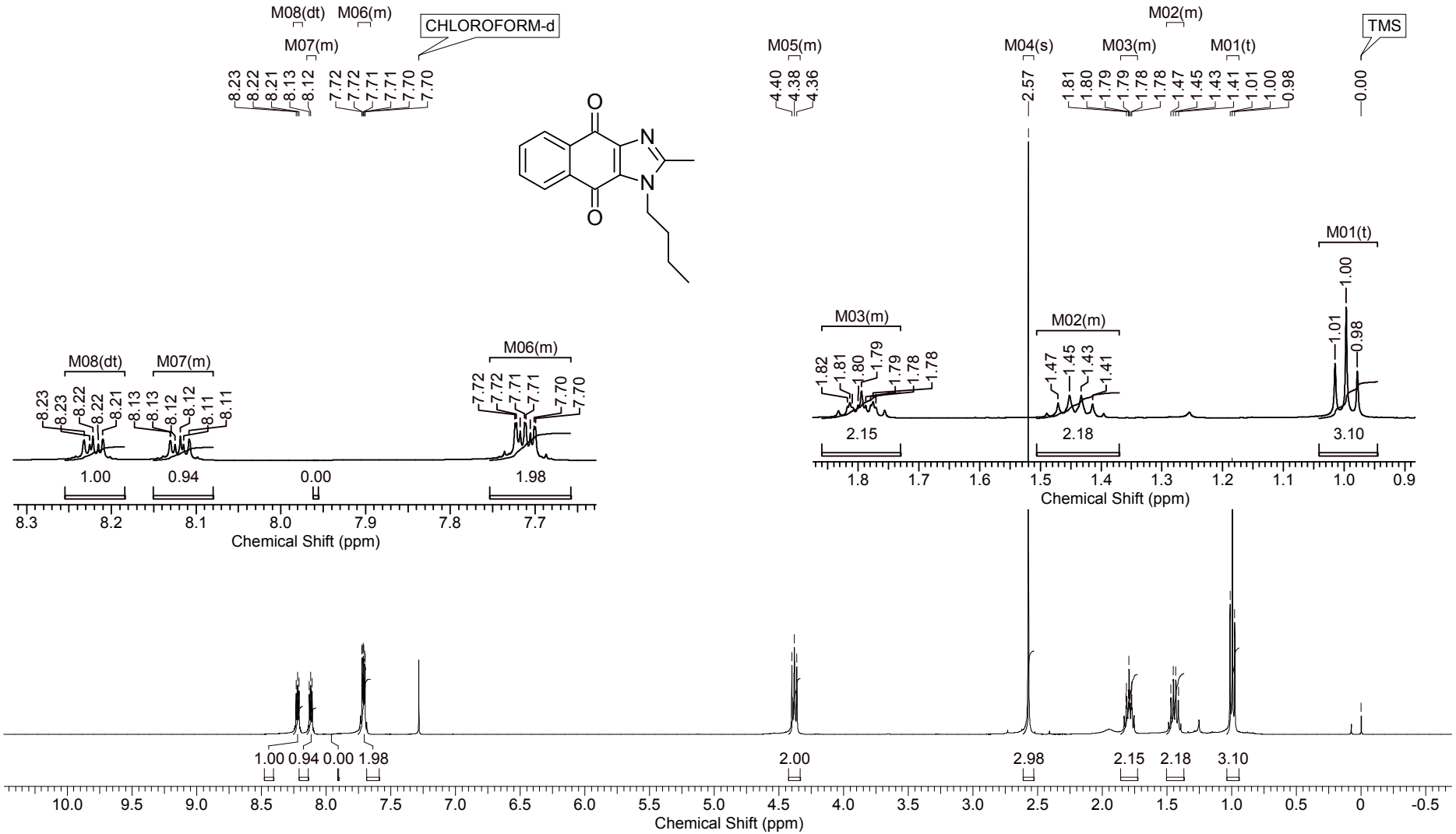


Fig.S27 ^{1}H NMR of **I-4** in $CDCl_3$ at 293 K

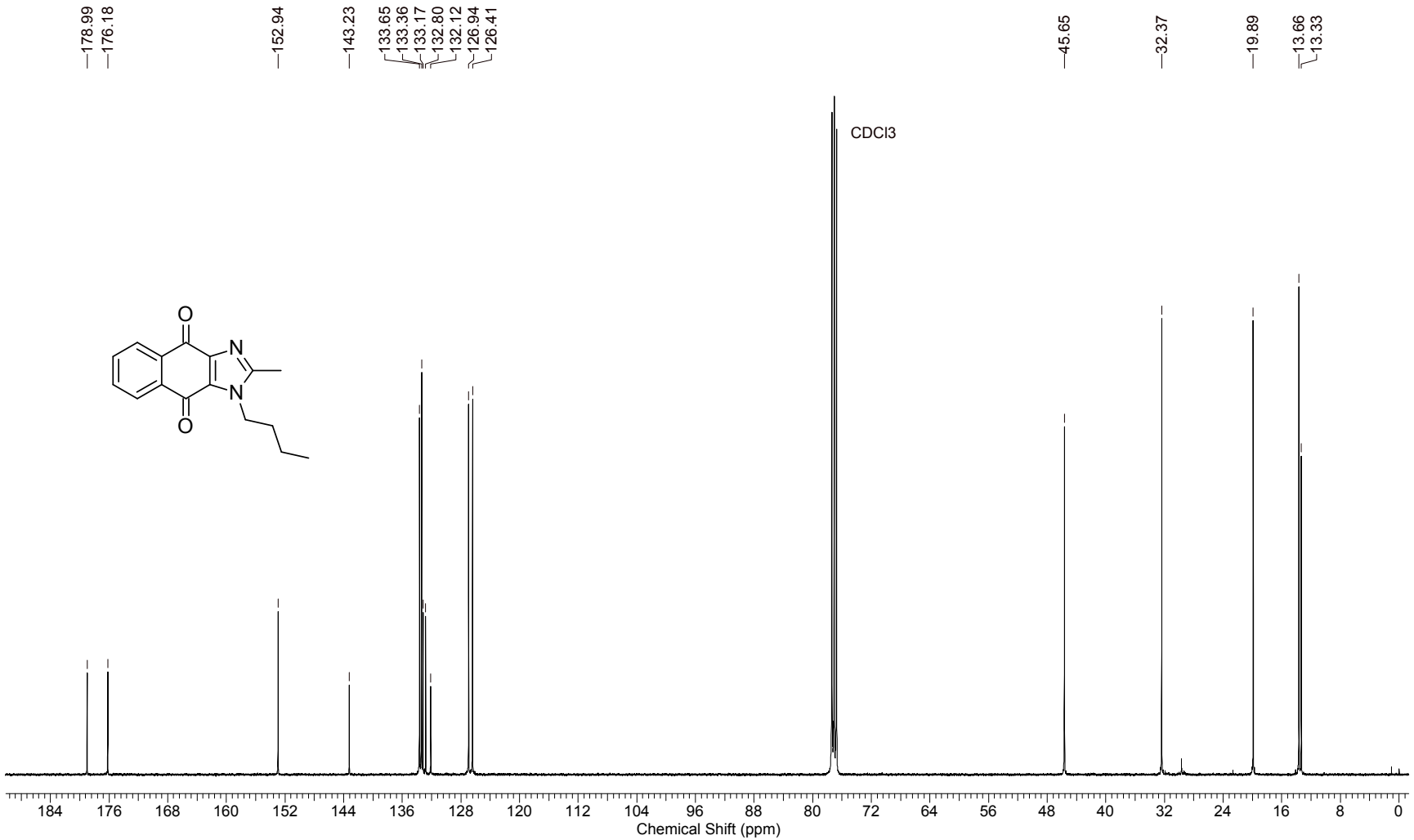


Fig.S28 ^{13}C NMR of **I-4** in $CDCl_3$ at 293 K

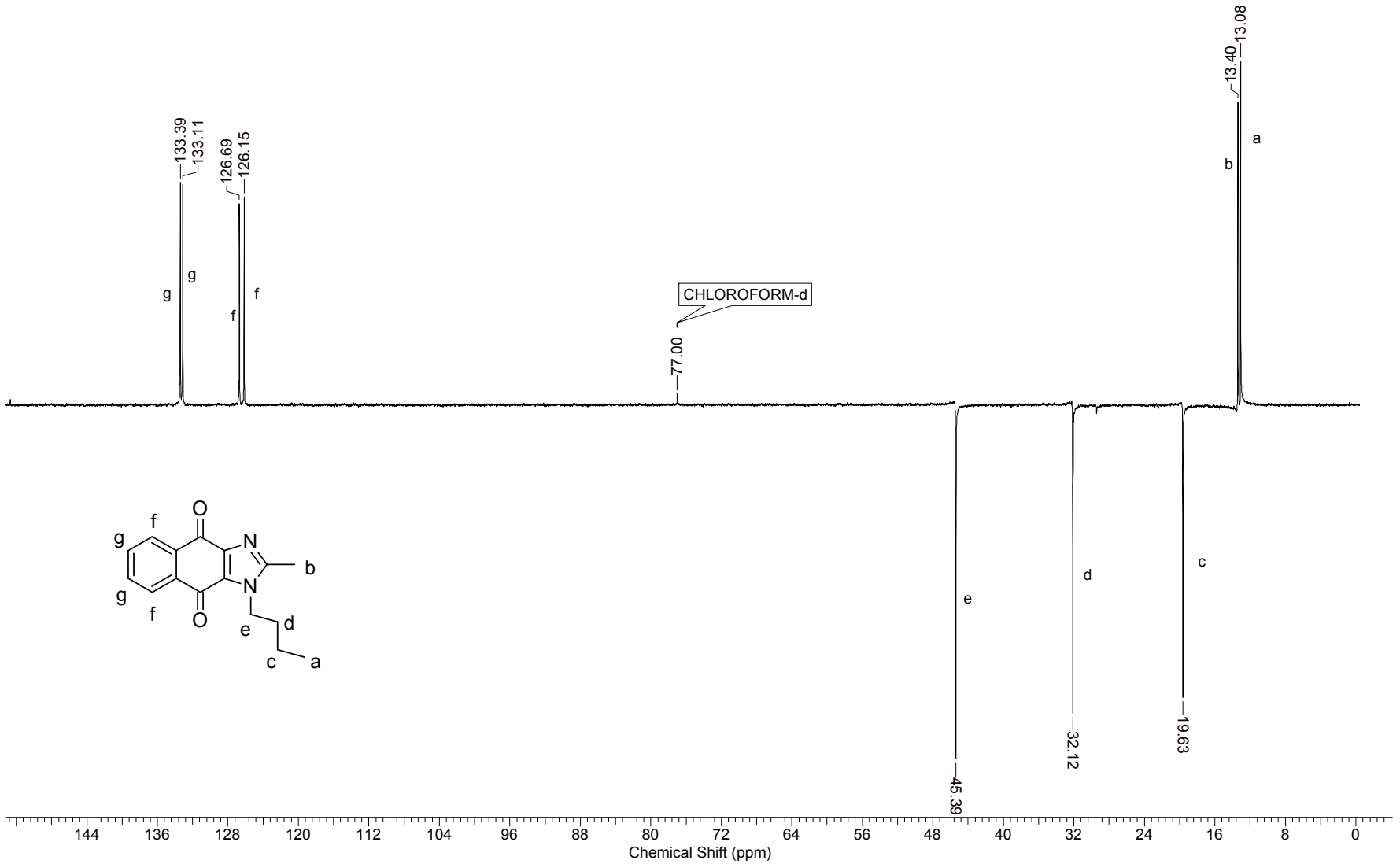


Fig.S29 DEPT NMR of **I-4** in $CDCl_3$ at 293 K

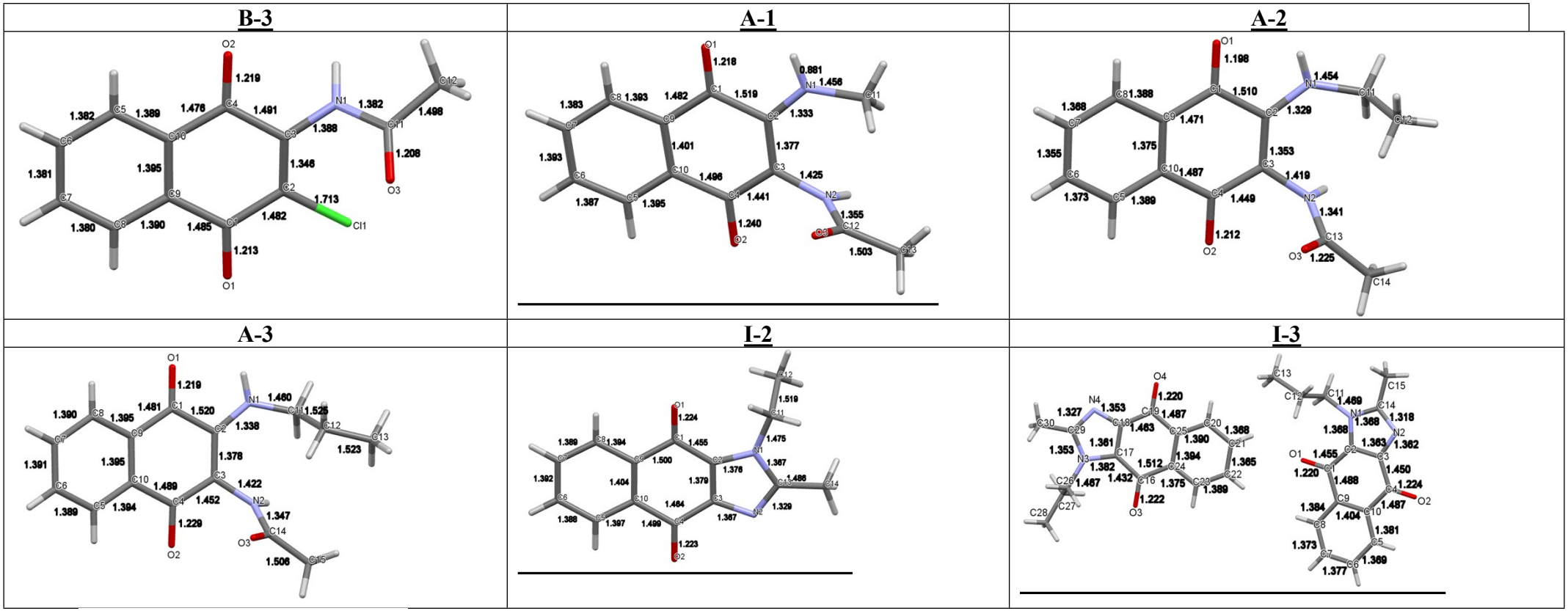


Fig.S30 Bond distances (Å) of **B-3**, **A-1** to **A-3** and **I-2** to **I-4**

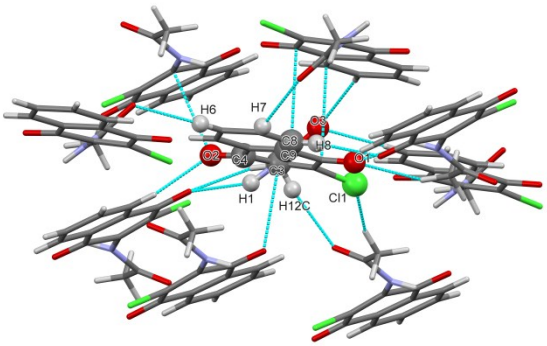


Fig.S31 Molecular association of **B-3** molecules via hydrogen bonding

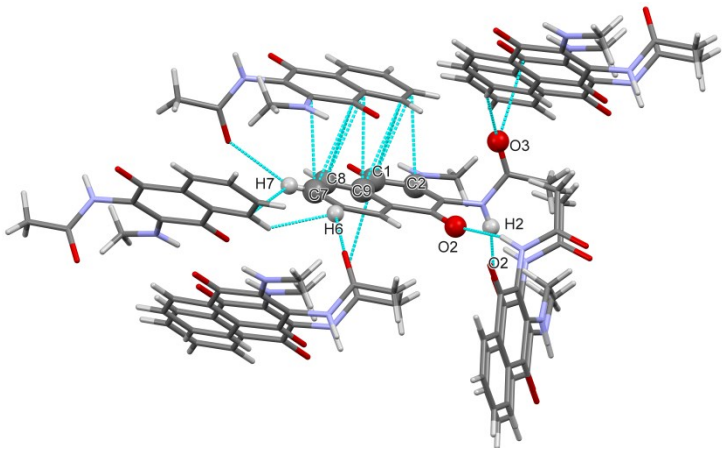


Fig.S32 Molecular association of **A-1** molecules via hydrogen bonding

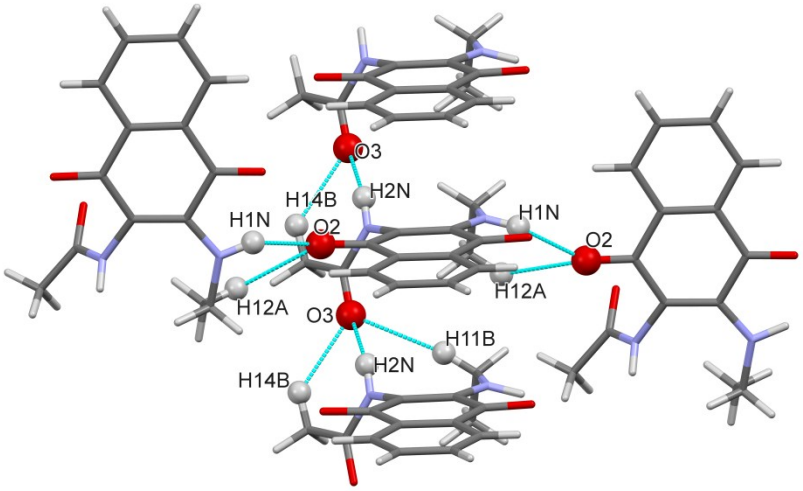


Fig.S33 Association of four similar neighboring molecules of **A-2** through C-H···O and N-H···O interaction

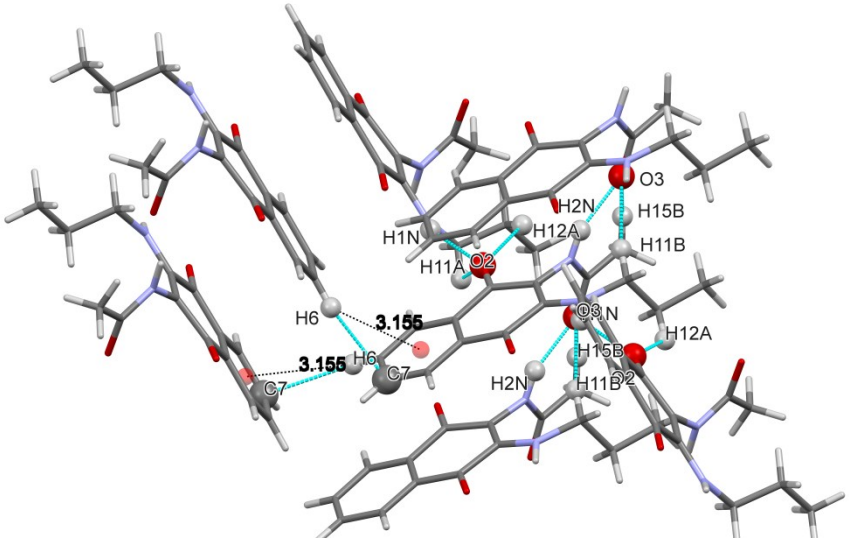


Fig.S34 Molecular association of six neighboring molecules to **A-3**

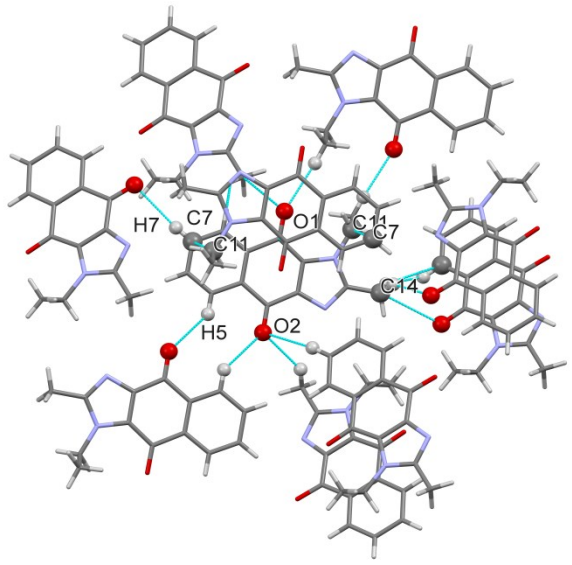


Fig.S35 Molecular association of **I-2** molecule to nine similar molecules via C-H···O and π-π packing interactions

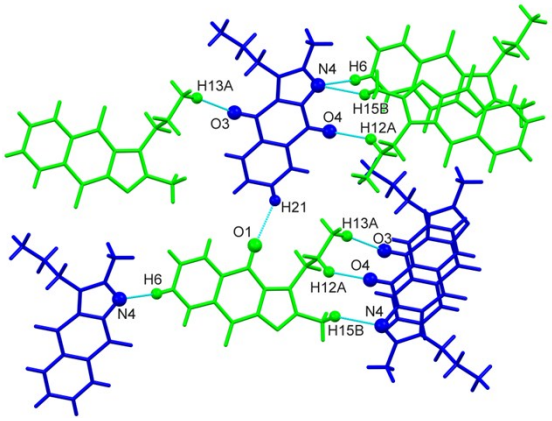


Fig.S36 Molecular association of each molecule of asymmetric unit of **I-3**

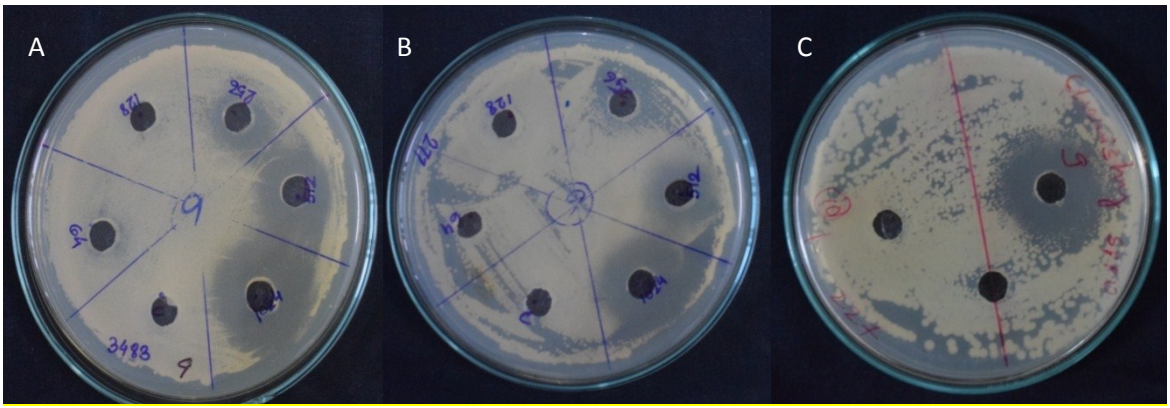


Fig.S37 Antifungal activity **B-2** against A: *Candida albicans* NCIM strains 3483; B and C: *Candida albicans* ATCC 10231

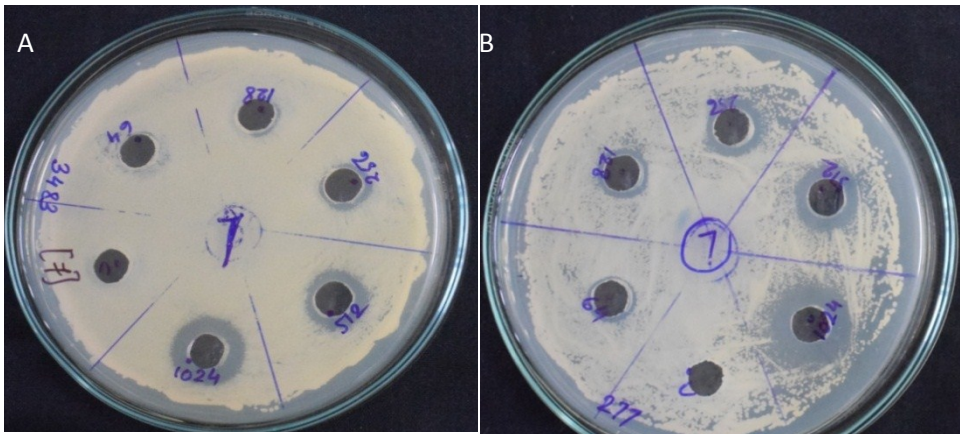


Fig.S38 Antifungal activity **B-3** against *Candida* strains viz. A: *C. albicans* NCIM 3483 and B: *C. albicans* ATCC 10231

Table S1 FT-IR Frequencies (in cm^{-1}) for **B-2**, **B-3**, **A-1** to **A-4** and **I-1** to **I-4**.

Sr. No.	Compounds	ν_{NH2} cm^{-1}	ν_{NH}  cm^{-1}	ν_{C-H}  cm^{-1}	$\nu_{(C-N)}$ cm^{-1}	$\nu_{(C=O)}$ cm^{-1}	$\nu_{(NH-C=O)}$  cm^{-1}	ν_{P-NQ} cm^{-1}
1	**B-2**	3272			1678	1684		1260
2	**B-3**		3469		1714	1720	1573	1256
3	**A-1**		3205	2965	1601	1651	1560	1261
4	**A-2**		3304	2964	1604	1654	1570	1260
5	**A-3**		3273	2983	1623	1673	1596	1262
6	**A-4**		3285	2953	1613	1668	1651	1258
7	**I-1**				1590	1665		1253
8	**I-2**				1593	1665		1257
9	**I-3**				1586	1667		1255
10	**I-4**				1587	1665		1256

Table S2a ^{13}C chemical Shift (δ (ppm)) of **B-3**, **A-1** to **A-4**, **I-1** to **I-4** in $CDCl_3$

	B-3	**A-1**	**A-2**	**A-3**	**A-4**	**I-1**	**I-2**	**I-3**	**I-4**
C_1	177	177	179	179	179	177	179	176	176
C_2	134	138	142	142	142	143	176	143	143
C_3	132	108	112	112	112	134	153	134	134
C_4	180	177	182	182	182	179	143	179	179
C_5	134	126	126	124	130	133	134	133	133
C_6	139	130	135	135	135	134	133	133	133
C_7	135	128	133	132	132	133	133	133	133
C_8	130	125	130	129	132	132	133	132	132
C_9	128	122	127	127	127	127	132	127	127
C_{10}	127	121	126	126	126	126	126	126	126
C_{11}	166	166	171	171	171	153	41	153	153
C_{12}	24	19	16	11	11	13	15	13	13
C_{13}		26	39	45	46	32	13	47	46
C_{14}			23	24	42			24	32
C_{15}				23	24			11	20
C_{16}					21				14

Table S2b ^{1}H NMR chemical shifts in **B-3**, **A-1** to **A-4** and **I-1** to **I-4** derivatives.

	B-3	**A-1**	**A-2**	**A-3**	**A-4**	**I-1**	**I-2**	**I-3**	**I-4**
H1	8.5	6.3	6.2	6.3	6.3				
H2		8.0	8.2	7.8	7.8				
H5	10	10.1	9.7	9.9	9.8	9.8	9.6	10	10.7
H6	9.8	10	9.4	9.6	9.2	9.5	9.6	9.5	9.6
H7	9.8	9.7	9.7	9.4	9.4	9.6	9.8	9.4	9.4
H8	10	9.9	4.2	9.9	10.1	10.4	10.2	10.3	9.8
H11		3.1	2.2	4.3	4.1	4.8	5.2	5.1	5.2
H12	3.1		3.2	2.6	2.6		2.4	2.7	2.7
H13		3.9		1.9	2.3	3.5		2.1	2.5
H14							3.6		2.3
H15				3.1				3.4	
H16					3				3.5

Table S3 Hydrogen bond geometries for **B-3**, **A-1** to **A-3** and **I-2** to **I-4**

Compound	D–H···A	D···H(Å)	H···A(Å)	D···A(Å)	D–H···A(º)	Symmetry
B-3	N(1)-H(1)···O(1)	0.860	2.400	3.172(2)	149.6	x,1/2-y,-1/2+z
	C(6)-H(6)···O(3)	0.929	2.511	3.417(3)	165	-1+x,y,z
	C(12)-H(12C)···O(3)	0.959	2.633	3.572(3)	166.2	1-x,-1/2+y,1.5-z
	C(7)-H(7)···O(3)	0.930	2.573	3.345(3)	140.7	-x,1-y,2-z
	C(8)-H(8)···O(2)	0.931	2.470	3.394(3)	172.1	x,1/2-y,-1/2+z
	C(12)-H(12B)···O(1)	0.960	2.517	3.378(3)	149.3	x,1/2-y,-1/2+z
	C(12)-H(12A)···Cl(1)	0.960	2.9447	3.767(2)	144.4	1-x,-1/2+y,1.5-z
	N(1)-H(1)···O(2)	0.860	2.501	2.661(2)	115	*Intra*
A-1						
	C(7)-H(7)···O(3)	0.950	2.690	3.450(2)	137.4	-x,-y,-z
	C(7)-H(7)···C(8)	0.950	2.669	3.572(3)	129.8	-1/2+x,-1/2-y,-z
	C(6)-H(6)···O(3)	0.950	2.467	3.324(3)	150.0	--1/2-x,-1/2+y,z
	N(2)-H(2)···O(2)	0.880	2.039	2.879(2)	159.3	-1/2+x,y,1/2-z
	C(1)···O(3)			3.183(2)		1/2-x,-1/2+y,z
	C(2)···C(7)			3.290(3)		-x,-y,-z
	C(1)···C(7)			3.311(3)		-x,-y,-z
	C(1)···C(8)			3.248(3)		-x,-y,-z
	C(8)···C(9)			3.365(3)		-x,-y,-z
	C(9)···C(9)			3.392(3)		-x,-y,-z
	N(1)-H(1)···O(1)	0.861	2.180	2.661(2)	110.5	*Intra*
A-2	N(1)-H(1N)···O(2)	0.91(4)	2.08(4)	2.831(8)	140(3)	x,1-y,-1/2+z
	C(12)-H(12A)···O(2)	0.960	2.716	3.404(8)	129.1	x,1-y,-1/2+z
	N(2)-H(2N)···O(3)	0.84(4)	2.15(4)	2.908(8)	151.(3)	x,-1+y,z
	C(14)-H(14B)···O(3)	0.961	2.371	3.106(6)	132.9	x,-1+y,z
	C(11)-H(11B)···O(3)	0.971	2.645	3.586(9)	163.4	x,-1+y,z
	N(1)-H(1N)···O(1)	0.91(4)	2.11(4)	2.611(5)	114(3)	*Intra*
A-3	N(2)-H(2N)···O(3)	0.89(2)	1.96(2)	2.805(1)	160.(2)	x,-1+y,z
	N(1)-H(1N)···O(2)	0.89(2)	2.12(2)	2.817(2)	134(2)	x,1.5-y,-1/2+z
	C(15)-H(15B)···O(3)	0.980	2.296	3.127(2)	141.93	x,-1+y,z

	C(11)-H(11B)···O(3)	0.990	2.611	3.582(2)	167.09	x,-1+y,z
	C(6)-H(6)···C(7)	0.950	2.748	3.651(2)	159.05	1-x,-1/2+y,1.5-z
	C(12)-H(12A)···O(2)	0.990	2.707	3.334(2)	121.61	x,1.5-y,-1/2+z
	C(11)-H(11B)···O(3)	0.971	2.645	3.586(9)	167.09	x,-1+y,z
	N(1)-H(1N)···O(1)	0.89(2)	2.17(2)	2.616(2)	110.0(2)	*Intra*
I-2	C(12)-H(12B)···O(1)	0.980	2.5350	3.500(1)	168.09	-x,1-y,-z
	C(14)-H(14A)···O(2)	0.980	2.641	3.496(2)	145.96	-1/2+x,1.5-y, 1/2+z
	C(14)-H(14B)···C(8)	0.980	2.875	3.674(2)	139.28	1/2-x,-1/2+y,1/2-z
	C(7)-H(7)···O(2)	0.950	2.659	3.601(2)	171.32	1/2-x,-1/2+y,1/2-z
	C(5)-H(5)···O(2)	0.945	2.5898	3.374(1)	140.13	1-x,1-y,2-z
	C(14)···O(1)			3.182(2)		1/2-x,-1/2+y,1/2-z
I-3	C(6)-H(6)···N(4)	0.930	2.509	3.386(6)	157.5	x,y,1+z
	C(15)-H(15B)···N(4)	0.959	2.741	3.582(4)	146.8	1-x,-y,1-z
	C(12)-H(12A)···O(4)	0.970	2.502	3.321(4)	142.1	x,y,z
	C(21)-H(21)···O(1)	0.930	2.570	3.280(5)	133.5	x,y,z
	C(13)-H(13A)···O(3)	0.960	2.467	3.410(5)	167.2	x,-1+y,z
I-4						
	C(8)-H(8)···N(2)	0.930	2.723	3.569(3)	151.8	-1/2+x,1/2+y,z
	C(7)-H(7)···O(3)	0.931	2.646	3.525(4)	157.8	-1/2+x,1/2+y,z
	C(16)-H(16C)···O(2)	0.961	2.515	3.464(4)	169.9	-1/2+x,1/2+y,z

Table S4 Crystal data and structure refinement for **B-3**

Empirical formula	C_{12} H_8 Cl N O_3
Formula weight	249.64
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 21/c
Unit cell dimensions	a = 10.1825(5) Å
	b = 6.9858(3) Å β= 95.202(2)°
	c = 15.3143(7) Å
Volume	1084.86(9) $Å^3$
Z	4
Density (calculated)	1.528 Mg/m^3
Absorption coefficient	0.346 mm^{-1}
F(000)	512
Crystal size	0.47 x 0.44 x 0.13 mm^3
Theta range for data collection	3.194 to 28.440°
Index ranges	-13<=h<=13, -9<=k<=9, -20<=l<=20
Reflections collected	31340
Independent reflections	2734 [R(int) = 0.0470]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2734 / 0 / 155
Goodness-of-fit on F^2	0.985
Final R indices [I>2sigma(I)]	R1 = 0.0481, wR2 = 0.1031
R indices (all data)	R1 = 0.0739, wR2 = 0.1156
Extinction coefficient	n/a
Largest diff. peak and hole	0.291 and -0.262 $e.Å^{-3}$

Table S5 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) For **B-3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Cl(1)	3289(1)	1714(1)	9278(1)	51(1)
O(1)	1238(2)	1977(3)	10451(1)	47(1)
O(2)	-486(2)	3779(3)	7168(1)	56(1)
O(3)	3708(2)	5108(3)	8180(1)	52(1)
N(1)	2101(2)	3264(3)	7491(1)	36(1)
C(1)	826(2)	2419(3)	9711(1)	31(1)
C(2)	1713(2)	2498(3)	8996(1)	32(1)
C(3)	1309(2)	3078(3)	8178(1)	30(1)
C(4)	-122(2)	3426(3)	7931(1)	34(1)
C(5)	-2370(2)	3772(3)	8411(2)	40(1)
C(6)	-3227(2)	3761(3)	9061(2)	45(1)
C(7)	-2772(2)	3301(3)	9912(2)	45(1)
C(8)	-1462(2)	2853(3)	10124(1)	38(1)
C(9)	-585(2)	2887(3)	9479(1)	29(1)
C(10)	-1046(2)	3344(3)	8619(1)	31(1)
C(11)	3294(2)	4220(3)	7536(1)	36(1)
C(12)	4027(2)	4022(4)	6736(2)	49(1)

Table S6 Bond lengths [Å] and angles [°] for **B-3**

Cl(1)-C(2)	1.713(2)
O(1)-C(1)	1.213(2)
O(2)-C(4)	1.219(2)
O(3)-C(11)	1.208(3)
N(1)-C(11)	1.382(3)
N(1)-C(3)	1.388(2)
C(1)-C(9)	1.485(3)
C(1)-C(2)	1.482(3)
C(2)-C(3)	1.346(3)
C(3)-C(4)	1.491(3)
C(4)-C(10)	1.476(3)
C(5)-C(6)	1.381(3)
C(5)-C(10)	1.390(3)
C(6)-C(7)	1.381(3)
C(7)-C(8)	1.380(3)
C(8)-C(9)	1.390(3)
C(9)-C(10)	1.395(3)
C(11)-C(12)	1.497(3)
C(11)-N(1)-C(3)	125.15(17)
O(1)-C(1)-C(9)	121.64(18)
O(1)-C(1)-C(2)	121.16(18)
C(9)-C(1)-C(2)	117.20(16)
C(3)-C(2)-C(1)	122.93(18)
C(3)-C(2)-Cl(1)	122.08(15)
C(1)-C(2)-Cl(1)	114.95(14)
C(2)-C(3)-N(1)	125.75(18)
C(2)-C(3)-C(4)	119.60(17)
N(1)-C(3)-C(4)	114.47(16)
O(2)-C(4)-C(10)	122.24(19)
O(2)-C(4)-C(3)	118.77(18)
C(10)-C(4)-C(3)	118.99(16)
C(6)-C(5)-C(10)	119.8(2)
C(5)-C(6)-C(7)	120.1(2)

C(8)-C(7)-C(6)	120.6(2)
C(7)-C(8)-C(9)	119.8(2)
C(8)-C(9)-C(10)	119.50(18)
C(8)-C(9)-C(1)	119.75(18)
C(10)-C(9)-C(1)	120.75(17)
C(5)-C(10)-C(9)	120.13(18)
C(5)-C(10)-C(4)	119.78(18)
C(9)-C(10)-C(4)	120.07(17)
O(3)-C(11)-N(1)	121.94(19)
O(3)-C(11)-C(12)	123.5(2)
N(1)-C(11)-C(12)	114.55(19)

Symmetry transformations used to generate equivalent atoms:

Table S7 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **B-3**. 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}
Cl(1)	35(1)	73(1)	48(1)	17(1)	9(1)	17(1)
O(1)	44(1)	68(1)	30(1)	13(1)	4(1)	8(1)
O(2)	44(1)	95(2)	28(1)	5(1)	0(1)	8(1)
O(3)	50(1)	64(1)	41(1)	-7(1)	4(1)	-17(1)
N(1)	35(1)	49(1)	25(1)	-6(1)	6(1)	-5(1)
C(1)	34(1)	30(1)	28(1)	1(1)	3(1)	1(1)
C(2)	29(1)	35(1)	33(1)	2(1)	4(1)	3(1)
C(3)	31(1)	33(1)	28(1)	-3(1)	5(1)	-1(1)
C(4)	34(1)	40(1)	26(1)	-2(1)	2(1)	0(1)
C(5)	33(1)	44(1)	40(1)	-2(1)	-2(1)	-3(1)
C(6)	28(1)	50(1)	58(1)	-5(1)	5(1)	-2(1)
C(7)	36(1)	50(1)	50(1)	-7(1)	17(1)	-5(1)
C(8)	41(1)	40(1)	33(1)	-1(1)	9(1)	-4(1)
C(9)	31(1)	27(1)	31(1)	-2(1)	5(1)	-2(1)
C(10)	30(1)	31(1)	31(1)	-4(1)	3(1)	-2(1)
C(11)	34(1)	42(1)	33(1)	5(1)	4(1)	-1(1)
C(12)	42(1)	63(2)	44(1)	5(1)	15(1)	-3(1)

Table S8 Crystal data and structure refinement for **A-1**

Empirical formula	C13 H12 N2 O3
Formula weight	244.25
Temperature	273(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	*Pbca*
Unit cell dimensions	a = 7.8552(6) Å
	b = 13.266 (1) Å
	c = 21.197(2) Å
Volume	2208.9(3) $Å^3$
Z	8
Density (calculated)	1.469 g/cc
Absorption coefficient	0.106 mm^{-1}
F(000)	1024
Crystal size	0.36 x 0.11 x 0.05 mm^3
Theta range for data collection	3.07 to 25.00°
Index ranges	-9<=h<=9, -15<=k<=15, -25<=l<=25
Reflections collected	53103
Independent reflections	1949 [R(int) = 0.0786]
Completeness to theta = 25.00°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9944 and 0.9624
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1949 / 0 / 165
Goodness-of-fit on F^2	1.161
Final R indices [I>2sigma(I)]	R1 = 0.0481, wR2 = 0.0981
R indices (all data)	R1 = 0.0604, wR2 = 0.1026
Largest diff. peak and hole	0.247 and -0.237 $e.Å^{-3}$

Table S9 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **A-1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	3147(2)	-641(1)	120(1)	11(1)
O(2)	-914(2)	455(1)	2031(1)	14(1)
O(3)	1477(2)	2725(1)	1347(1)	17(1)
N(1)	4382(2)	661(1)	929(1)	10(1)
N(2)	2194(2)	1394(1)	1965(1)	9(1)
C(1)	2197(3)	-401(1)	548(1)	8(1)
C(2)	2793(3)	356(1)	1039(1)	8(1)
C(3)	1711(3)	646(1)	1516(1)	8(1)
C(4)	34(3)	221(1)	1587(1)	8(1)
C(5)	-2254(3)	-887(1)	1139(1)	9(1)
C(6)	-2864(3)	-1532(1)	676(1)	10(1)
C(7)	-1832(3)	-1805(2)	170(1)	9(1)
C(8)	-185(3)	-1441(1)	132(1)	9(1)
C(9)	443(2)	-805(1)	600(1)	7(1)
C(10)	-595(2)	-515(1)	1106(1)	8(1)
C(11)	5436(3)	1345(2)	1297(1)	12(1)
C(12)	2047(2)	2393(2)	1844(1)	10(1)
C(13)	2703(3)	3070(2)	2358(1)	15(1)

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Table S10 Bond lengths [Å] and angles [°] for **A-1**

O(1)-C(1)	1.218(2)
O(2)-C(4)	1.240(2)
O(3)-C(12)	1.227(2)
N(1)-C(2)	1.333(3)
N(1)-C(11)	1.456(3)
N(1)-H(1)	0.8800
N(2)-C(12)	1.355(3)
N(2)-C(3)	1.425(3)
N(2)-H(2)	0.8800
C(1)-C(9)	1.482(3)
C(1)-C(2)	1.519(3)
C(2)-C(3)	1.377(3)
C(3)-C(4)	1.441(3)
C(4)-C(10)	1.496(3)
C(5)-C(6)	1.387(3)
C(5)-C(10)	1.395(3)
C(5)-H(5)	0.9500
C(6)-C(7)	1.393(3)
C(6)-H(6)	0.9500
C(7)-C(8)	1.383(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.393(3)
C(8)-H(8)	0.9500
C(9)-C(10)	1.401(3)
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-C(13)	1.503(3)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(2)-N(1)-C(11)	128.94(17)
C(2)-N(1)-H(1)	115.5

C(11)-N(1)-H(1)	115.5
C(12)-N(2)-C(3)	122.18(17)
C(12)-N(2)-H(2)	118.9
C(3)-N(2)-H(2)	118.9
O(1)-C(1)-C(9)	122.00(18)
O(1)-C(1)-C(2)	119.62(18)
C(9)-C(1)-C(2)	118.36(17)
N(1)-C(2)-C(3)	128.44(19)
N(1)-C(2)-C(1)	111.73(17)
C(3)-C(2)-C(1)	119.83(17)
C(2)-C(3)-N(2)	121.35(18)
C(2)-C(3)-C(4)	122.11(18)
N(2)-C(3)-C(4)	116.54(17)
O(2)-C(4)-C(3)	122.00(18)
O(2)-C(4)-C(10)	118.91(18)
C(3)-C(4)-C(10)	119.09(17)
C(6)-C(5)-C(10)	120.36(19)
C(6)-C(5)-H(5)	119.8
C(10)-C(5)-H(5)	119.8
C(5)-C(6)-C(7)	120.27(19)
C(5)-C(6)-H(6)	119.9
C(7)-C(6)-H(6)	119.9
C(8)-C(7)-C(6)	119.91(19)
C(8)-C(7)-H(7)	120.0
C(6)-C(7)-H(7)	120.0
C(7)-C(8)-C(9)	120.08(19)
C(7)-C(8)-H(8)	120.0
C(9)-C(8)-H(8)	120.0
C(8)-C(9)-C(10)	120.35(18)
C(8)-C(9)-C(1)	119.73(18)
C(10)-C(9)-C(1)	119.88(18)
C(5)-C(10)-C(9)	119.01(18)
C(5)-C(10)-C(4)	120.32(18)
C(9)-C(10)-C(4)	120.61(18)
N(1)-C(11)-H(11A)	109.5
N(1)-C(11)-H(11B)	109.5

H(11A)-C(11)-H(11B)	109.5
N(1)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
O(3)-C(12)-N(2)	122.97(18)
O(3)-C(12)-C(13)	122.27(18)
N(2)-C(12)-C(13)	114.71(17)
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5

Table S11 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **A-1**. 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)	10(1)	12(1)	11(1)	-2(1)	6(1)	0(1)
O(2)	13(1)	19(1)	12(1)	-6(1)	5(1)	-1(1)
O(3)	23(1)	13(1)	15(1)	1(1)	-7(1)	4(1)
N(1)	7(1)	13(1)	9(1)	-3(1)	1(1)	-1(1)
N(2)	9(1)	11(1)	5(1)	0(1)	-2(1)	2(1)
C(1)	10(1)	6(1)	9(1)	3(1)	-1(1)	3(1)
C(2)	8(1)	7(1)	10(1)	4(1)	0(1)	2(1)
C(3)	12(1)	5(1)	8(1)	1(1)	-3(1)	2(1)
C(4)	10(1)	9(1)	7(1)	2(1)	2(1)	4(1)
C(5)	9(1)	8(1)	10(1)	3(1)	2(1)	3(1)
C(6)	7(1)	8(1)	15(1)	4(1)	-1(1)	0(1)
C(7)	12(1)	6(1)	10(1)	1(1)	-3(1)	0(1)
C(8)	12(1)	7(1)	9(1)	2(1)	2(1)	4(1)
C(9)	8(1)	5(1)	9(1)	3(1)	1(1)	2(1)
C(10)	11(1)	5(1)	9(1)	3(1)	-1(1)	2(1)
C(11)	7(1)	14(1)	16(1)	-3(1)	0(1)	-3(1)
C(12)	5(1)	12(1)	12(1)	0(1)	1(1)	2(1)
C(13)	20(1)	12(1)	14(1)	-3(1)	-1(1)	-1(1)

Table S12 Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **A-1**

	x	y	z	U(eq)
H(1)	4860	415	586	12
H(2)	2602	1200	2332	10
H(5)	-2969	-699	1480	10
H(6)	-3991	-1788	704	12
H(7)	-2259	-2240	-149	11
H(8)	519	-1626	-214	11
H(11A)	4981	2031	1265	18
H(11B)	6604	1333	1135	18
H(11C)	5434	1133	1740	18
H(13A)	3838	3316	2245	23
H(13B)	2768	2691	2755	23
H(13C)	1928	3643	2411	23

Table S13 Torsion angles [°] for **A-1**

C(11)-N(1)-C(2)-C(3)	3.2(3)
C(11)-N(1)-C(2)-C(1)	-177.39(18)
O(1)-C(1)-C(2)-N(1)	-0.9(3)
C(9)-C(1)-C(2)-N(1)	-179.21(16)
O(1)-C(1)-C(2)-C(3)	178.61(18)
C(9)-C(1)-C(2)-C(3)	0.3(3)
N(1)-C(2)-C(3)-N(2)	2.8(3)
C(1)-C(2)-C(3)-N(2)	-176.62(16)
N(1)-C(2)-C(3)-C(4)	-177.79(19)
C(1)-C(2)-C(3)-C(4)	2.8(3)
C(12)-N(2)-C(3)-C(2)	82.9(2)
C(12)-N(2)-C(3)-C(4)	-96.6(2)
C(2)-C(3)-C(4)-O(2)	177.24(19)
N(2)-C(3)-C(4)-O(2)	-3.3(3)
C(2)-C(3)-C(4)-C(10)	-3.7(3)
N(2)-C(3)-C(4)-C(10)	175.78(16)
C(10)-C(5)-C(6)-C(7)	-0.7(3)
C(5)-C(6)-C(7)-C(8)	0.7(3)
C(6)-C(7)-C(8)-C(9)	0.1(3)
C(7)-C(8)-C(9)-C(10)	-1.0(3)
C(7)-C(8)-C(9)-C(1)	-178.70(17)
O(1)-C(1)-C(9)-C(8)	-3.1(3)
C(2)-C(1)-C(9)-C(8)	175.24(17)
O(1)-C(1)-C(9)-C(10)	179.24(18)
C(2)-C(1)-C(9)-C(10)	-2.5(3)
C(6)-C(5)-C(10)-C(9)	-0.2(3)
C(6)-C(5)-C(10)-C(4)	176.91(17)
C(8)-C(9)-C(10)-C(5)	1.0(3)
C(1)-C(9)-C(10)-C(5)	178.74(17)
C(8)-C(9)-C(10)-C(4)	-176.06(17)
C(1)-C(9)-C(10)-C(4)	1.6(3)
O(2)-C(4)-C(10)-C(5)	3.4(3)
C(3)-C(4)-C(10)-C(5)	-175.70(17)
O(2)-C(4)-C(10)-C(9)	-179.53(18)

C(3)-C(4)-C(10)-C(9)	1.4(3)
C(3)-N(2)-C(12)-O(3)	0.7(3)
C(3)-N(2)-C(12)-C(13)	-177.01(17)

Table S14 Crystal data and structure refinement for **A-2**

Identification code	**A-2**
Empirical formula	$C_{14}H_{14}N_2O_3$
Formula weight	258.27
Temperature	293(2) K
Wavelength	1.54184 Å
Crystal system	Monoclinic
Space group	*C 2/c*
Unit cell dimensions	a = 37.44(5) Å, b = 4.665(13) Å, c = 14.44(4) Å, β = 98.0(2)°
Volume	2496(11) $Å^3$
Z	8
Density (calculated)	1.374 Mg/m^3
Absorption coefficient	0.809 mm^{-1}
F(000)	1088
Crystal size	0.300 x 0.210 x 0.140 mm^3
Theta range for data collection	4.771 to 66.728°.
Index ranges	-43<=h<=44, -5<=k<=5, -16<=l<=17
Reflections collected	10094
Independent Reflections	2137 [R(int) = 0.0986]
Completeness to theta = 25.242°	96.2 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2137 / 0 / 183
Goodness-of-fit on F^2	1.012
Final R indices [I>2sigma(I)]	R1 = 0.0652, wR2 = 0.1768
R indices (all data)	R1 = 0.1084, wR2 = 0.2066
Extinction coefficient	n/a
Largest diff. peak and hole	0.245 and -0.229 $e.Å^{-3}$

Table S15 Bond lengths [Å] and angles [°] for **A-2**

Bond		Length
O1-	C1	1.220(4)
O2-	C4	1.224(4)
N1-	C2	1.368(5)
N1-	C11	1.469(4)
N1-	C14	1.368(5)
N2-	C3	1.362(5)
N2-	C14	1.318(5)
C1-	C2	1.455(5)
C1-	C9	1.488(5)
C2-	C3	1.363(4)
C3-	C4	1.450(5)
C4-	C10	1.487(5)
C5-	H5	0.93
C5-	C6	1.369(6)
C5-	C10	1.381(5)
C6-	H6	0.93
C6-	C7	1.377(6)
C7-	H7	0.93
C7-	C8	1.373(7)
C8-	H8	0.929
C8-	C9	1.384(5)
C9-	C10	1.404(4)
C11-	H11A	0.97
C11--	H11B	0.971
C11-	C12	1.501(5)
C12-	H12A	0.97
C12-	H12B	0.97
C12-	C13	1.515(5)
C13-	H13A	0.96
C13-	H13B	0.96
C13-	H13C	0.96
C14-	C15	1.488(5)
C15-	H15A	0.96
C15-	H15B	0.959
C15-	H15C	0.96
O3-	C16	1.222(4)
O4-	C19	1.220(4)
N3-	C17	1.382(4)
N3-	C26	1.467(4)

N3-	C29	1.353(4)
N4-	C18	1.353(4)
N4-	C29	1.327(5)
C16-	C17	1.432(4)
C16-	C24	1.512(5)
C17-	C18	1.361(5)
C18-	C19	1.463(5)
C19-	C25	1.487(4)
C20-	H20	0.93
C20-	C21	1.368(5)
C20-	C25	1.390(5)
C21-	H21	0.93
C21-	C22	1.365(7)
C22-	H22	0.93
C22-	C23	1.389(6)
C23-	H23	0.93
C23-	C24	1.375(4)
C24-	C25	1.394(5)
C26-	H26A	0.97
C26-	H26B	0.97
C26-	C27	1.490(4)
C27-	H27A	0.969
C27-	H27B	0.971
C27-	C28	1.512(5)
C28-	H28A	0.959
C28-	H28B	0.96
C28-	H28C	0.96
C29-	C30	1.483(5)
C30-	H30A	0.959
C30-	H30B	0.96
C30-	H30C	0.96

Atom1	Atom2	Atom3	Angle
C2	N1	C11	131.1(3)
C2	N1	H1N	109(3)
C11	N1	H1N	119(3)
C3	N2	C13	119.9(3)
C3	N2	H2N	118(2)
C13	N2	H2N	122(2)
O1	C1	C2	119.2(3)
O1	C1	C9	120.6(3)
C2	C1	C9	120.2(3)

N1	C2	C1	112.6(3)
N1	C2	C3	128.6(3)
C1	C2	C3	118.8(3)
N2	C3	C2	122.9(3)
N2	C3	C4	115.4(3)
C2	C3	C4	121.5(3)
O2	C4	C3	120.5(3)
O2	C4	C10	119.4(3)
C3	C4	C10	120.1(3)
H5	C5	C6	119.7
H5	C5	C10	119.8
C6	C5	C10	120.5(3)
C5	C6	H6	119.8
C5	C6	C7	120.5(4)
H6	C6	C7	119.7
C6	C7	H7	120.2
C6	C7	C8	119.6(4)
H7	C7	C8	120.2
C7	C8	H8	119.5
C7	C8	C9	121.2(3)
H8	C8	C9	119.3
C1	C9	C8	121.7(3)
C1	C9	C10	119.2(3)
C8	C9	C10	119.1(3)
C4	C10	C5	120.8(3)
C4	C10	C9	120.1(3)
C5	C10	C9	119.1(3)
N1	C11	H11A	109
N1	C11	H11B	109
N1	C11	C12	113.0(3)
H11A	C11	H11B	107.7
H11A	C11	C12	109
H11B	C11	C12	108.9
C11	C12	H12A	109.4
C11	C12	H12B	109.5
C11	C12	H12C	109.5
H12A	C12	H12B	109.6
H12A	C12	H12C	109.5
H12B	C12	H12C	109.3
O3	C13	N2	121.2(3)
O3	C13	C14	121.3(3)
N2	C13	C14	117.5(3)
C13	C14	H14A	109.5

C13	C14	H14B	109.4
C13	C14	H14C	109.4
H14A	C14	H14B	109.6
H14A	C14	H14C	109.5
H14B	C14	H14C	109.4

Table S16 Torsion Angles for **A-2**

Atom1	Atom2	Atom3	Atom4	Torsion
C11	N1	C2	C1	180.0(3)
C11	N1	C2	C3	-0.7(6)
H1N	N1	C2	C1	13(3)
H1N	N1	C2	C3	-168(3)
C2	N1	C11	H11A	152.1
C2	N1	C11	H11B	34.8
C2	N1	C11	C12	-86.5(5)
H1N	N1	C11	H11A	-42
H1N	N1	C11	H11B	-159
H1N	N1	C11	C12	80(3)
C13	N2	C3	C2	108.9(3)
C13	N2	C3	C4	-65.9(4)
H2N	N2	C3	C2	-76(3)
H2N	N2	C3	C4	110(3)
C3	N2	C13	O3	-9.2(4)
C3	N2	C13	C14	171.9(3)
H2N	N2	C13	O3	175(3)
H2N	N2	C13	C14	-3(3)
O1	C1	C2	N1	1.2(4)
O1	C1	C2	C3	-178.2(3)
C9	C1	C2	N1	-177.5(3)
C9	C1	C2	C3	3.0(4)
O1	C1	C9	C8	-2.2(5)
O1	C1	C9	C10	177.6(3)
C2	C1	C9	C8	176.5(3)
C2	C1	C9	C10	-3.7(4)
N1	C2	C3	N2	6.9(5)
N1	C2	C3	C4	-178.6(3)
C1	C2	C3	N2	-173.8(3)
C1	C2	C3	C4	0.7(4)
N2	C3	C4	O2	-7.8(4)
N2	C3	C4	C10	171.1(3)
C2	C3	C4	O2	177.3(3)
C2	C3	C4	C10	-3.7(4)
O2	C4	C10	C5	3.1(5)
O2	C4	C10	C9	-178.0(3)
C3	C4	C10	C5	-175.9(3)

C3	C4	C10	C9	3.0(4)
H5	C5	C6	H6	-0.1
H5	C5	C6	C7	180
C10	C5	C6	H6	179.9
C10	C5	C6	C7	-0.1(6)
H5	C5	C10	C4	-0.6
H5	C5	C10	C9	-179.5
C6	C5	C10	C4	179.5(3)
C6	C5	C10	C9	0.5(5)
C5	C6	C7	H7	179.7
C5	C6	C7	C8	-0.3(6)
H6	C6	C7	H7	-0.3
H6	C6	C7	C8	179.8
C6	C7	C8	H8	-179.8
C6	C7	C8	C9	0.2(6)
H7	C7	C8	H8	0.3
H7	C7	C8	C9	-179.8
C7	C8	C9	C1	-180.0(3)
C7	C8	C9	C10	0.2(5)
H8	C8	C9	C1	0
H8	C8	C9	C10	-179.8
C1	C9	C10	C4	0.7(4)
C1	C9	C10	C5	179.6(3)
C8	C9	C10	C4	-179.5(3)
C8	C9	C10	C5	-0.6(5)
N1	C11	C12	H12A	-59
N1	C11	C12	H12B	-179.2
N1	C11	C12	H12C	61
H11A	C11	C12	H12A	62.4
H11A	C11	C12	H12B	-57.8
H11A	C11	C12	H12C	-177.6
H11B	C11	C12	H12A	179.7
H11B	C11	C12	H12B	59.5
H11B	C11	C12	H12C	-60.3
O3	C13	C14	H14A	-75.4
O3	C13	C14	H14B	164.4
O3	C13	C14	H14C	44.6
N2	C13	C14	H14A	103.4
N2	C13	C14	H14B	-16.7
N2	C13	C14	H14C	-136.5

Table S17 Crystal data and structure refinement for **A-3**

Identification code	**A-3**
Empirical formula	$C_{15}\ H_{16}\ N_2\ O_3$
Formula weight	272.30
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	*P 21/c*
Unit cell dimensions	a = 20.7144(13) Å
	b = 4.6497(3) Å β= 108.849(3)°
	c = 14.7226(10) Å
Volume	1341.97(15) $Å^3$
Z	4
Density (calculated)	1.348 Mg/m^3
Absorption coefficient	0.095 mm^{-1}
F(000)	576
Crystal size	0.200 x 0.120 x 0.090 mm^3
Theta range for data collection	2.769 to 28.788°
Index ranges	-27<=h<=28, -6<=k<=6, -19<=l<=19
Reflections collected	25638
Independent reflections	3472 [R(int) = 0.0333]
Completeness to theta = 25.242°	99.1 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.991 and 0.981
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3472 / 0 / 191
Goodness-of-fit on F^2	1.136
Final R indices [I>2sigma(I)]	R1 = 0.0494, wR2 = 0.1188
R indices (all data)	R1 = 0.0539, wR2 = 0.1215
Extinction coefficient	n/a
Largest diff. peak and hole	0.467 and -0.330 $e.Å^{-3}$

Table S18 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **A-3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	3801(1)	6315(2)	3889(1)	21(1)
O(2)	2661(1)	6111(2)	6658(1)	20(1)
O(3)	1433(1)	4489(2)	4883(1)	23(1)
N(1)	2673(1)	9255(3)	3573(1)	15(1)
N(2)	1936(1)	8849(2)	5026(1)	12(1)
C(1)	3533(1)	6126(3)	4511(1)	13(1)
C(2)	2878(1)	7775(3)	4397(1)	12(1)
C(3)	2579(1)	7597(3)	5106(1)	12(1)
C(4)	2894(1)	6018(3)	5990(1)	13(1)
C(5)	3756(1)	2387(3)	6863(1)	16(1)
C(6)	4318(1)	658(3)	6941(1)	18(1)
C(7)	4634(1)	754(3)	6239(1)	19(1)
C(8)	4382(1)	2544(3)	5447(1)	16(1)
C(9)	3812(1)	4250(3)	5361(1)	13(1)
C(10)	3501(1)	4191(3)	6072(1)	13(1)
C(11)	2050(1)	10931(3)	3168(1)	16(1)
C(12)	1433(1)	9067(3)	2665(1)	19(1)
C(13)	789(1)	10887(4)	2292(1)	32(1)
C(14)	1402(1)	7118(3)	4962(1)	14(1)
C(15)	746(1)	8540(3)	4952(1)	17(1)

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Table S19 Bond lengths [Å] and angles [°] for **A-3**

O(1)-C(1)	1.2194(16)
O(2)-C(4)	1.2293(16)
O(3)-C(14)	1.2313(17)
N(1)-C(2)	1.3381(16)
N(1)-C(11)	1.4601(17)
N(1)-H(1N)	0.89(2)
N(2)-C(14)	1.3474(17)
N(2)-C(3)	1.4219(16)
N(2)-H(2N)	0.89(2)
C(1)-C(9)	1.4809(18)
C(1)-C(2)	1.5196(17)
C(2)-C(3)	1.3781(17)
C(3)-C(4)	1.4523(17)
C(4)-C(10)	1.4890(18)
C(5)-C(6)	1.3885(19)
C(5)-C(10)	1.3939(18)
C(5)-H(5)	0.9500
C(6)-C(7)	1.391(2)
C(6)-H(6)	0.9500
C(7)-C(8)	1.390(2)
C(7)-H(7)	0.9500
C(8)-C(9)	1.3946(18)
C(8)-H(8)	0.9500
C(9)-C(10)	1.3950(18)
C(11)-C(12)	1.524(2)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.523(2)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-C(15)	1.5056(18)

C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800

C(2)-N(1)-C(11)	128.62(11)
C(2)-N(1)-H(1N)	115.1(13)
C(11)-N(1)-H(1N)	115.3(12)
C(14)-N(2)-C(3)	119.17(11)
C(14)-N(2)-H(2N)	117.3(12)
C(3)-N(2)-H(2N)	123.1(12)
O(1)-C(1)-C(9)	121.90(12)
O(1)-C(1)-C(2)	119.24(12)
C(9)-C(1)-C(2)	118.82(11)
N(1)-C(2)-C(3)	129.01(12)
N(1)-C(2)-C(1)	111.69(11)
C(3)-C(2)-C(1)	119.30(11)
C(2)-C(3)-N(2)	123.36(11)
C(2)-C(3)-C(4)	121.78(11)
N(2)-C(3)-C(4)	114.83(11)
O(2)-C(4)-C(3)	121.27(12)
O(2)-C(4)-C(10)	119.70(12)
C(3)-C(4)-C(10)	119.01(11)
C(6)-C(5)-C(10)	119.91(13)
C(6)-C(5)-H(5)	120.0
C(10)-C(5)-H(5)	120.0
C(5)-C(6)-C(7)	120.24(13)
C(5)-C(6)-H(6)	119.9
C(7)-C(6)-H(6)	119.9
C(8)-C(7)-C(6)	120.18(13)
C(8)-C(7)-H(7)	119.9
C(6)-C(7)-H(7)	119.9
C(7)-C(8)-C(9)	119.63(13)
C(7)-C(8)-H(8)	120.2
C(9)-C(8)-H(8)	120.2
C(8)-C(9)-C(10)	120.23(12)
C(8)-C(9)-C(1)	120.02(12)

C(10)-C(9)-C(1)	119.74(11)
C(5)-C(10)-C(9)	119.78(12)
C(5)-C(10)-C(4)	119.54(11)
C(9)-C(10)-C(4)	120.67(11)
N(1)-C(11)-C(12)	112.80(11)
N(1)-C(11)-H(11A)	109.0
C(12)-C(11)-H(11A)	109.0
N(1)-C(11)-H(11B)	109.0
C(12)-C(11)-H(11B)	109.0
H(11A)-C(11)-H(11B)	107.8
C(13)-C(12)-C(11)	111.00(13)
C(13)-C(12)-H(12A)	109.4
C(11)-C(12)-H(12A)	109.4
C(13)-C(12)-H(12B)	109.4
C(11)-C(12)-H(12B)	109.4
H(12A)-C(12)-H(12B)	108.0
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
O(3)-C(14)-N(2)	122.18(12)
O(3)-C(14)-C(15)	120.63(12)
N(2)-C(14)-C(15)	117.15(12)
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S20 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **A-3**. 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)	20(1)	29(1)	17(1)	3(1)	11(1)	4(1)
O(2)	22(1)	28(1)	13(1)	5(1)	10(1)	6(1)
O(3)	20(1)	11(1)	39(1)	0(1)	13(1)	1(1)
N(1)	17(1)	19(1)	11(1)	2(1)	7(1)	2(1)
N(2)	14(1)	10(1)	13(1)	0(1)	7(1)	2(1)
C(1)	13(1)	16(1)	12(1)	-2(1)	5(1)	-1(1)
C(2)	13(1)	11(1)	11(1)	-1(1)	4(1)	-1(1)
C(3)	13(1)	11(1)	12(1)	-1(1)	5(1)	0(1)
C(4)	14(1)	13(1)	12(1)	0(1)	5(1)	-1(1)
C(5)	16(1)	17(1)	13(1)	1(1)	3(1)	-1(1)
C(6)	18(1)	15(1)	17(1)	0(1)	0(1)	0(1)
C(7)	14(1)	18(1)	20(1)	-3(1)	1(1)	4(1)
C(8)	14(1)	18(1)	17(1)	-4(1)	6(1)	1(1)
C(9)	12(1)	14(1)	13(1)	-2(1)	3(1)	-1(1)
C(10)	12(1)	13(1)	12(1)	-2(1)	3(1)	-1(1)
C(11)	19(1)	16(1)	13(1)	4(1)	6(1)	4(1)
C(12)	19(1)	23(1)	14(1)	1(1)	5(1)	1(1)
C(13)	20(1)	39(1)	34(1)	9(1)	4(1)	5(1)
C(14)	15(1)	13(1)	14(1)	0(1)	6(1)	2(1)
C(15)	14(1)	14(1)	25(1)	1(1)	9(1)	1(1)

Table S21 Torsion angles [°] for **A-3**

C(11)-N(1)-C(2)-C(3)	-4.8(2)
C(11)-N(1)-C(2)-C(1)	175.28(12)
O(1)-C(1)-C(2)-N(1)	0.89(18)
C(9)-C(1)-C(2)-N(1)	-176.88(11)
O(1)-C(1)-C(2)-C(3)	-179.06(12)
C(9)-C(1)-C(2)-C(3)	3.17(18)
N(1)-C(2)-C(3)-N(2)	5.9(2)
C(1)-C(2)-C(3)-N(2)	-174.21(11)
N(1)-C(2)-C(3)-C(4)	-176.08(13)
C(1)-C(2)-C(3)-C(4)	3.86(19)
C(14)-N(2)-C(3)-C(2)	112.19(14)
C(14)-N(2)-C(3)-C(4)	-66.00(15)
C(2)-C(3)-C(4)-O(2)	172.51(13)
N(2)-C(3)-C(4)-O(2)	-9.26(18)
C(2)-C(3)-C(4)-C(10)	-9.19(19)
N(2)-C(3)-C(4)-C(10)	169.03(11)
C(10)-C(5)-C(6)-C(7)	1.0(2)
C(5)-C(6)-C(7)-C(8)	-1.1(2)
C(6)-C(7)-C(8)-C(9)	0.2(2)
C(7)-C(8)-C(9)-C(10)	0.9(2)
C(7)-C(8)-C(9)-C(1)	-178.95(12)
O(1)-C(1)-C(9)-C(8)	-2.6(2)
C(2)-C(1)-C(9)-C(8)	175.10(12)
O(1)-C(1)-C(9)-C(10)	177.54(13)
C(2)-C(1)-C(9)-C(10)	-4.75(18)
C(6)-C(5)-C(10)-C(9)	0.0(2)
C(6)-C(5)-C(10)-C(4)	179.44(12)
C(8)-C(9)-C(10)-C(5)	-0.99(19)
C(1)-C(9)-C(10)-C(5)	178.86(12)
C(8)-C(9)-C(10)-C(4)	179.60(12)
C(1)-C(9)-C(10)-C(4)	-0.55(18)
O(2)-C(4)-C(10)-C(5)	6.38(19)
C(3)-C(4)-C(10)-C(5)	-171.94(12)
O(2)-C(4)-C(10)-C(9)	-174.21(12)

C(3)-C(4)-C(10)-C(9)	7.47(18)
C(2)-N(1)-C(11)-C(12)	-80.10(17)
N(1)-C(11)-C(12)-C(13)	177.51(12)
C(3)-N(2)-C(14)-O(3)	-6.80(19)
C(3)-N(2)-C(14)-C(15)	175.64(11)

Symmetry transformations used to generate equivalent atoms:

Table S22 Crystal data and structure refinement for **I-2**

Identification code	**I-2**
Empirical formula	$C_{14}\ H_{12}\ N_2\ O_2$
Formula weight	240.26
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 8.1220(3) Å
	b = 15.5877(5) Å β= 104.5190(10)°
	c = 9.2916(3) Å
Volume	1138.78(7) $Å^3$
Z	4
Density (calculated)	1.401 Mg/m^3
Absorption coefficient	0.096 mm^{-1}
F(000)	504
Crystal size	0.240 x 0.160 x 0.080 mm^3
Theta range for data collection	2.902 to 27.996°
Index ranges	-10<=h<=10, -20<=k<=18, -12<=l<=12
Reflections collected	17799
Independent reflections	2731 [R(int) = 0.0310]
Completeness to theta = 25.242°	99.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.992 and 0.977
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2731 / 0 / 165
Goodness-of-fit on F^2	1.006
Final R indices [I>2sigma(I)]	R1 = 0.0419, wR2 = 0.1026
R indices (all data)	R1 = 0.0449, wR2 = 0.1053
Extinction coefficient	n/a
Largest diff. peak and hole	0.385 and -0.317 $e.Å^{-3}$

Table S23 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **I-2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	560(1)	4403(1)	3150(1)	22(1)
O(2)	4814(1)	5816(1)	8037(1)	24(1)
N(1)	2042(1)	6181(1)	3172(1)	15(1)
N(2)	3832(1)	6743(1)	5190(1)	17(1)
C(12)	1818(2)	5770(1)	542(1)	24(1)
C(11)	913(2)	6124(1)	1661(1)	17(1)
C(2)	2326(1)	5559(1)	4255(1)	14(1)
C(1)	1594(2)	4705(1)	4221(1)	15(1)
C(9)	2189(2)	4217(1)	5649(1)	15(1)
C(8)	1601(2)	3381(1)	5711(1)	19(1)
C(7)	2104(2)	2902(1)	7008(2)	22(1)
C(6)	3170(2)	3269(1)	8267(2)	21(1)
C(3)	3419(2)	5922(1)	5481(1)	15(1)
C(13)	2983(2)	6877(1)	3787(1)	16(1)
C(14)	3015(2)	7696(1)	2973(1)	22(1)
C(4)	3934(2)	5481(1)	6915(1)	16(1)
C(10)	3277(2)	4582(1)	6917(1)	15(1)
C(5)	3740(2)	4106(1)	8230(1)	18(1)

Table S24 Bond lengths [Å] and angles [°] for **I-2**

O(1)-C(1)	1.2241(15)
O(2)-C(4)	1.2232(15)
N(1)-C(13)	1.3671(15)
N(1)-C(2)	1.3755(14)
N(1)-C(11)	1.4747(14)
N(2)-C(13)	1.3294(15)
N(2)-C(3)	1.3674(15)
C(12)-C(11)	1.5186(17)
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(2)-C(3)	1.3786(16)
C(2)-C(1)	1.4548(16)
C(1)-C(9)	1.5004(16)
C(9)-C(8)	1.3942(17)
C(9)-C(10)	1.4041(16)
C(8)-C(7)	1.3894(18)
C(8)-H(8)	0.9500
C(7)-C(6)	1.3916(19)
C(7)-H(7)	0.9500
C(6)-C(5)	1.3876(17)
C(6)-H(6)	0.9500
C(3)-C(4)	1.4643(16)
C(13)-C(14)	1.4858(16)
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(4)-C(10)	1.4988(16)
C(10)-C(5)	1.3966(16)
C(5)-H(5)	0.9500
C(13)-N(1)-C(2)	106.30(9)

C(13)-N(1)-C(11)	126.51(10)
C(2)-N(1)-C(11)	127.17(10)
C(13)-N(2)-C(3)	104.41(10)
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
N(1)-C(11)-C(12)	112.43(10)
N(1)-C(11)-H(11A)	109.1
C(12)-C(11)-H(11A)	109.1
N(1)-C(11)-H(11B)	109.1
C(12)-C(11)-H(11B)	109.1
H(11A)-C(11)-H(11B)	107.8
C(3)-C(2)-N(1)	105.65(10)
C(3)-C(2)-C(1)	124.67(10)
N(1)-C(2)-C(1)	129.59(10)
O(1)-C(1)-C(2)	124.21(11)
O(1)-C(1)-C(9)	121.86(11)
C(2)-C(1)-C(9)	113.92(10)
C(8)-C(9)-C(10)	119.64(11)
C(8)-C(9)-C(1)	118.21(11)
C(10)-C(9)-C(1)	122.13(10)
C(7)-C(8)-C(9)	120.61(12)
C(7)-C(8)-H(8)	119.7
C(9)-C(8)-H(8)	119.7
C(8)-C(7)-C(6)	119.55(12)
C(8)-C(7)-H(7)	120.2
C(6)-C(7)-H(7)	120.2
C(5)-C(6)-C(7)	120.49(11)
C(5)-C(6)-H(6)	119.8
C(7)-C(6)-H(6)	119.8
N(2)-C(3)-C(2)	111.10(10)
N(2)-C(3)-C(4)	126.29(10)
C(2)-C(3)-C(4)	122.47(11)

N(2)-C(13)-N(1)	112.53(10)
N(2)-C(13)-C(14)	124.27(11)
N(1)-C(13)-C(14)	123.19(11)
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
O(2)-C(4)-C(3)	123.18(11)
O(2)-C(4)-C(10)	122.01(11)
C(3)-C(4)-C(10)	114.81(10)
C(5)-C(10)-C(9)	119.47(11)
C(5)-C(10)-C(4)	118.69(11)
C(9)-C(10)-C(4)	121.83(10)
C(6)-C(5)-C(10)	120.20(12)
C(6)-C(5)-H(5)	119.9
C(10)-C(5)-H(5)	119.9

Symmetry transformations used to generate equivalent atoms:

Table S25 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **I-2**. 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)	18(1)	-4(1)	0(1)	-3(1)
O(2)	30(1)	21(1)	16(1)	1(1)	-3(1)	-5(1)
N(1)	17(1)	15(1)	13(1)	1(1)	3(1)	2(1)
N(2)	21(1)	14(1)	15(1)	1(1)	3(1)	0(1)
C(12)	22(1)	36(1)	15(1)	-4(1)	2(1)	4(1)
C(11)	16(1)	21(1)	13(1)	1(1)	0(1)	2(1)
C(2)	16(1)	15(1)	12(1)	0(1)	3(1)	2(1)
C(1)	17(1)	14(1)	15(1)	-2(1)	4(1)	1(1)
C(9)	18(1)	14(1)	16(1)	-1(1)	6(1)	2(1)
C(8)	24(1)	15(1)	20(1)	-4(1)	9(1)	-2(1)
C(7)	28(1)	14(1)	26(1)	1(1)	13(1)	0(1)
C(6)	22(1)	19(1)	23(1)	7(1)	9(1)	5(1)
C(3)	16(1)	13(1)	15(1)	-1(1)	3(1)	1(1)
C(13)	18(1)	15(1)	15(1)	0(1)	5(1)	1(1)
C(14)	29(1)	17(1)	20(1)	5(1)	6(1)	0(1)
C(4)	17(1)	15(1)	15(1)	0(1)	2(1)	1(1)
C(10)	15(1)	14(1)	16(1)	1(1)	4(1)	2(1)
C(5)	17(1)	20(1)	17(1)	3(1)	3(1)	3(1)

Table S26 Torsion angles [°] for **I-2**

C(13)-N(1)-C(11)-C(12)	92.45(14)
C(2)-N(1)-C(11)-C(12)	-89.44(14)
C(13)-N(1)-C(2)-C(3)	0.66(12)
C(11)-N(1)-C(2)-C(3)	-177.76(10)
C(13)-N(1)-C(2)-C(1)	177.28(12)
C(11)-N(1)-C(2)-C(1)	-1.14(19)
C(3)-C(2)-C(1)-O(1)	176.25(12)
N(1)-C(2)-C(1)-O(1)	0.2(2)
C(3)-C(2)-C(1)-C(9)	-2.35(17)
N(1)-C(2)-C(1)-C(9)	-178.40(11)
O(1)-C(1)-C(9)-C(8)	3.38(17)
C(2)-C(1)-C(9)-C(8)	-177.98(10)
O(1)-C(1)-C(9)-C(10)	-175.18(11)
C(2)-C(1)-C(9)-C(10)	3.46(16)
C(10)-C(9)-C(8)-C(7)	-1.05(18)
C(1)-C(9)-C(8)-C(7)	-179.65(11)
C(9)-C(8)-C(7)-C(6)	1.65(18)
C(8)-C(7)-C(6)-C(5)	-0.44(18)
C(13)-N(2)-C(3)-C(2)	0.20(13)
C(13)-N(2)-C(3)-C(4)	-175.53(11)
N(1)-C(2)-C(3)-N(2)	-0.55(13)
C(1)-C(2)-C(3)-N(2)	-177.38(10)
N(1)-C(2)-C(3)-C(4)	175.37(10)
C(1)-C(2)-C(3)-C(4)	-1.47(18)
C(3)-N(2)-C(13)-N(1)	0.24(13)
C(3)-N(2)-C(13)-C(14)	179.14(11)
C(2)-N(1)-C(13)-N(2)	-0.58(13)
C(11)-N(1)-C(13)-N(2)	177.85(10)
C(2)-N(1)-C(13)-C(14)	-179.49(11)
C(11)-N(1)-C(13)-C(14)	-1.06(18)
N(2)-C(3)-C(4)-O(2)	0.1(2)
C(2)-C(3)-C(4)-O(2)	-175.14(12)
N(2)-C(3)-C(4)-C(10)	179.33(11)
C(2)-C(3)-C(4)-C(10)	4.06(16)

C(8)-C(9)-C(10)-C(5)	-0.76(17)
C(1)-C(9)-C(10)-C(5)	177.78(11)
C(8)-C(9)-C(10)-C(4)	-179.42(11)
C(1)-C(9)-C(10)-C(4)	-0.88(17)
O(2)-C(4)-C(10)-C(5)	-2.33(18)
C(3)-C(4)-C(10)-C(5)	178.47(10)
O(2)-C(4)-C(10)-C(9)	176.34(11)
C(3)-C(4)-C(10)-C(9)	-2.86(16)
C(7)-C(6)-C(5)-C(10)	-1.38(18)
C(9)-C(10)-C(5)-C(6)	1.97(18)
C(4)-C(10)-C(5)-C(6)	-179.33(11)

Symmetry transformations used to generate equivalent atoms:

Table S27 Crystal data and structure refinement for **I-3**

Identification code	**I-3**
CCDC Number	1814959
Empirical formula	$C_{30}H_{28}N_4O_4$
Formula weight	508.56
Temperature	293(2) K
Wavelength	1.54184 Å
Crystal system	Triclinic
Space group	*P -1*
Unit cell dimensions	a = 7.650(3) Å, α = 89.143(17)° b = 11.624(5) Å , β = 79.65(2)° c = 15.228(9) Å , γ = 72.548(16)°
Volume	1269.6(10) $Å^3$
Z	2
Density (calculated)	1.330 Mg/m^3
Absorption coefficient	0.728 mm^{-1}
F(000)	536
Crystal size	0.210 x 0.160 x 0.100 mm^3
Theta range for data collection	2.952 to 65.802°.
Index ranges	-9<=h<=8, -13<=k<=13, -17<=l<=16
Reflections collected	21637
Independent reflections	4319 [R(int) = 0.0897]
Completeness to theta = 25.242°	98.2 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4319 / 0 / 348
Goodness-of-fit on F^2	1.019
Final R indices [I>2sigma(I)]	R1 = 0.0598, wR2 = 0.1293
R indices (all data)	R1 = 0.1361, wR2 = 0.1666
Extinction coefficient	0.0042(5)
Largest diff. peak and hole	0.219 and -0.171 $e.Å^{-3}$

Table S28 Bond length and bond angles of **I-3**

Atom1	Atom2	Length
O1	C1	1.220(4)
O2	C4	1.224(4)
N1	C2	1.368(5)
N1	C11	1.469(4)
N1	C14	1.368(5)
N2	C3	1.362(5)
N2	C14	1.318(5)
C1	C2	1.455(5)
C1	C9	1.488(5)
C2	C3	1.363(4)
C3	C4	1.450(5)
C4	C10	1.487(5)
C5	H5	0.93
C5	C6	1.369(6)
C5	C10	1.381(5)
C6	H6	0.93
C6	C7	1.377(6)
C7	H7	0.93
C7	C8	1.373(7)
C8	H8	0.929
C8	C9	1.384(5)
C9	C10	1.404(4)
C11	H11A	0.97
C11	H11B	0.971
C11	C12	1.501(5)
C12	H12A	0.97
C12	H12B	0.97
C12	C13	1.515(5)
C13	H13A	0.96
C13	H13B	0.96
C13	H13C	0.96
C14	C15	1.488(5)
C15	H15A	0.96
C15	H15B	0.959
C15	H15C	0.96
O3	C16	1.222(4)
O4	C19	1.220(4)
N3	C17	1.382(4)
N3	C26	1.467(4)
N3	C29	1.353(4)

N4	C18	1.353(4)
N4	C29	1.327(5)
C16	C17	1.432(4)
C16	C24	1.512(5)
C17	C18	1.361(5)
C18	C19	1.463(5)
C19	C25	1.487(4)
C20	H20	0.93
C20	C21	1.368(5)
C20	C25	1.390(5)
C21	H21	0.93
C21	C22	1.365(7)
C22	H22	0.93
C22	C23	1.389(6)
C23	H23	0.93
C23	C24	1.375(4)
C24	C25	1.394(5)
C26	H26A	0.97
C26	H26B	0.97
C26	C27	1.490(4)
C27	H27A	0.969
C27	H27B	0.971
C27	C28	1.512(5)
C28	H28A	0.959

C28	H28B	0.96
C28	H28C	0.96
C29	C30	1.483(5)
C30	H30A	0.959
C30	H30B	0.96
C30	H30C	0.96

Atom1	Atom2	Atom3	Angle
C2	N1	C11	126.7(3)
C2	N1	C14	106.0(3)
C11	N1	C14	127.2(3)
C3	N2	C14	104.6(3)
O1	C1	C2	123.9(3)
O1	C1	C9	122.1(3)
C2	C1	C9	114.0(3)
N1	C2	C1	129.3(3)
N1	C2	C3	106.0(3)
C1	C2	C3	124.7(3)
N2	C3	C2	111.1(3)
N2	C3	C4	126.6(3)
C2	C3	C4	122.3(3)
O2	C4	C3	123.2(3)
O2	C4	C10	121.1(3)
C3	C4	C10	115.7(3)
H5	C5	C6	119.3
H5	C5	C10	119.5
C6	C5	C10	121.2(3)
C5	C6	H6	120.2
C5	C6	C7	119.7(4)
H6	C6	C7	120.1
C6	C7	H7	119.8
C6	C7	C8	120.3(4)
H7	C7	C8	119.9
C7	C8	H8	119.6
C7	C8	C9	120.8(4)
H8	C8	C9	119.6
C1	C9	C8	119.0(3)
C1	C9	C10	122.1(3)
C8	C9	C10	118.9(3)
C4	C10	C5	119.5(3)
C4	C10	C9	121.3(3)
C5	C10	C9	119.2(3)
N1	C11	H11A	109.4
N1	C11	H11B	109.3
N1	C11	C12	111.6(3)
H11A	C11	H11B	107.9
H11A	C11	C12	109.3
H11B	C11	C12	109.3
C11	C12	H12A	109.3
C11	C12	H12B	109.3

C11	C12	C13	111.8(3)
H12A	C12	H12B	107.9
H12A	C12	C13	109.3
H12B	C12	C13	109.3
C12	C13	H13A	109.4
C12	C13	H13B	109.4
C12	C13	H13C	109.5
H13A	C13	H13B	109.6
H13A	C13	H13C	109.5
H13B	C13	H13C	109.4
N1	C14	N2	112.2(3)
N1	C14	C15	123.3(3)
N2	C14	C15	124.5(3)
C14	C15	H15A	109.5
C14	C15	H15B	109.4
C14	C15	H15C	109.5
H15A	C15	H15B	109.5
H15A	C15	H15C	109.5
H15B	C15	H15C	109.5
C17	N3	C26	126.9(3)
C17	N3	C29	106.5(3)
C26	N3	C29	126.4(3)
C18	N4	C29	104.5(3)
O3	C16	C17	124.8(3)
O3	C16	C24	120.8(3)
C17	C16	C24	114.3(3)
N3	C17	C16	129.6(3)
N3	C17	C18	105.0(3)
C16	C17	C18	125.4(3)
N4	C18	C17	111.8(3)
N4	C18	C19	126.3(3)
C17	C18	C19	121.8(3)
O4	C19	C18	122.8(3)
O4	C19	C25	121.9(3)
C18	C19	C25	115.3(3)
H20	C20	C21	119.7
H20	C20	C25	119.6
C21	C20	C25	120.7(3)
C20	C21	H21	119.7
C20	C21	C22	120.6(4)
H21	C21	C22	119.7
C21	C22	H22	120.1
C21	C22	C23	119.8(4)

H22	C22	C23	120.1
C22	C23	H23	120
C22	C23	C24	120.1(3)
H23	C23	C24	119.9
C16	C24	C23	118.9(3)
C16	C24	C25	121.1(3)
C23	C24	C25	120.1(3)
C19	C25	C20	119.2(3)
C19	C25	C24	122.0(3)
C20	C25	C24	118.7(3)
N3	C26	H26A	109.2
N3	C26	H26B	109.1
N3	C26	C27	112.2(3)
H26A	C26	H26B	107.9
H26A	C26	C27	109.2
H26B	C26	C27	109.2
C26	C27	H27A	109.2
C26	C27	H27B	109.2
C26	C27	C28	112.1(3)
H27A	C27	H27B	107.9
H27A	C27	C28	109.2
H27B	C27	C28	109.1
C27	C28	H28A	109.4
C27	C28	H28B	109.4
C27	C28	H28C	109.4
H28A	C28	H28B	109.6
H28A	C28	H28C	109.5
H28B	C28	H28C	109.4
N3	C29	N4	112.2(3)
N3	C29	C30	124.0(3)
N4	C29	C30	123.9(3)
C29	C30	H30A	109.5
C29	C30	H30B	109.4
C29	C30	H30C	109.4
H30A	C30	H30B	109.5
H30A	C30	H30C	109.6
H30B	C30	H30C	109.5

Table S29 Torsion Angles **I-3**

Atom1	Atom2	Atom3	Atom4	Torsion
C11	N1	C2	C1	2.2(6)
C11	N1	C2	C3	-177.6(3)
C14	N1	C2	C1	178.9(3)
C14	N1	C2	C3	-0.9(4)
C2	N1	C11	H11A	-39.3
C2	N1	C11	H11B	-157.2
C2	N1	C11	C12	81.7(4)
C14	N1	C11	H11A	144.6
C14	N1	C11	H11B	26.7
C14	N1	C11	C12	-94.3(4)
C2	N1	C14	N2	1.2(4)
C2	N1	C14	C15	-178.6(3)
C11	N1	C14	N2	177.9(3)
C11	N1	C14	C15	-1.9(6)
C14	N2	C3	C2	0.3(4)
C14	N2	C3	C4	-179.5(3)
C3	N2	C14	N1	-0.9(4)
C3	N2	C14	C15	178.9(3)
O1	C1	C2	N1	0.1(6)
O1	C1	C2	C3	179.9(3)
C9	C1	C2	N1	-179.8(3)
C9	C1	C2	C3	-0.0(5)
O1	C1	C9	C8	-1.2(5)
O1	C1	C9	C10	179.2(3)
C2	C1	C9	C8	178.8(3)
C2	C1	C9	C10	-0.8(5)
N1	C2	C3	N2	0.4(4)
N1	C2	C3	C4	-179.8(3)
C1	C2	C3	N2	-179.4(3)
C1	C2	C3	C4	0.3(5)
N2	C3	C4	O2	-0.3(6)
N2	C3	C4	C10	179.9(3)
C2	C3	C4	O2	180.0(3)
C2	C3	C4	C10	0.2(5)
O2	C4	C10	C5	-0.2(5)
O2	C4	C10	C9	179.2(3)
C3	C4	C10	C5	179.6(3)
C3	C4	C10	C9	-1.0(5)

H5	C5	C6	H6	0.6
H5	C5	C6	C7	-179.4
C10	C5	C6	H6	-179.3
C10	C5	C6	C7	0.7(6)
H5	C5	C10	C4	-2.2
H5	C5	C10	C9	178.5
C6	C5	C10	C4	177.7(3)
C6	C5	C10	C9	-1.6(5)
C5	C6	C7	H7	-179.3
C5	C6	C7	C8	0.7(7)
H6	C6	C7	H7	0.7
H6	C6	C7	C8	-179.3
C6	C7	C8	H8	178.7
C6	C7	C8	C9	-1.2(6)
H7	C7	C8	H8	-1.3
H7	C7	C8	C9	178.8
C7	C8	C9	C1	-179.4(4)
C7	C8	C9	C10	0.3(6)
H8	C8	C9	C1	0.7
H8	C8	C9	C10	-179.7
C1	C9	C10	C4	1.4(5)
C1	C9	C10	C5	-179.3(3)
C8	C9	C10	C4	-178.2(3)
C8	C9	C10	C5	1.1(5)
N1	C11	C12	H12A	63.4
N1	C11	C12	H12B	-54.5
N1	C11	C12	C13	-175.6(3)
H11A	C11	C12	H12A	-175.6
H11A	C11	C12	H12B	66.6
H11A	C11	C12	C13	-54.5
H11B	C11	C12	H12A	-57.7
H11B	C11	C12	H12B	-175.6
H11B	C11	C12	C13	63.4
C11	C12	C13	H13A	-61.2
C11	C12	C13	H13B	178.8
C11	C12	C13	H13C	58.9
H12A	C12	C13	H13A	59.9
H12A	C12	C13	H13B	-60.1
H12A	C12	C13	H13C	179.9
H12B	C12	C13	H13A	177.8
H12B	C12	C13	H13B	57.7
H12B	C12	C13	H13C	-62.2
N1	C14	C15	H15A	-178.7

N1	C14	C15	H15B	61.3
N1	C14	C15	H15C	-58.7
N2	C14	C15	H15A	1.5
N2	C14	C15	H15B	-118.5
N2	C14	C15	H15C	121.5
C26	N3	C17	C16	-3.6(5)
C26	N3	C17	C18	176.9(3)
C29	N3	C17	C16	-179.8(3)
C29	N3	C17	C18	0.7(3)
C17	N3	C26	H26A	155.5
C17	N3	C26	H26B	37.8
C17	N3	C26	C27	-83.3(4)
C29	N3	C26	H26A	-29
C29	N3	C26	H26B	-146.7
C29	N3	C26	C27	92.2(4)
C17	N3	C29	N4	-0.7(4)
C17	N3	C29	C30	178.8(3)
C26	N3	C29	N4	-177.0(3)
C26	N3	C29	C30	2.5(5)
C29	N4	C18	C17	0.0(4)
C29	N4	C18	C19	177.7(3)
C18	N4	C29	N3	0.4(4)
C18	N4	C29	C30	-179.1(3)
O3	C16	C17	N3	-0.1(6)
O3	C16	C17	C18	179.2(3)
C24	C16	C17	N3	179.6(3)
C24	C16	C17	C18	-1.0(5)
O3	C16	C24	C23	0.0(5)
O3	C16	C24	C25	-179.8(3)
C17	C16	C24	C23	-179.7(3)
C17	C16	C24	C25	0.5(4)
N3	C17	C18	N4	-0.5(4)
N3	C17	C18	C19	-178.2(3)
C16	C17	C18	N4	-180.0(3)
C16	C17	C18	C19	2.2(5)
N4	C18	C19	O4	-1.1(5)
N4	C18	C19	C25	179.9(3)
C17	C18	C19	O4	176.3(3)
C17	C18	C19	C25	-2.7(5)
O4	C19	C25	C20	1.6(5)
O4	C19	C25	C24	-176.9(3)
C18	C19	C25	C20	-179.4(3)
C18	C19	C25	C24	2.2(5)

H20	C20	C21	H21	0.6
H20	C20	C21	C22	-179.4
C25	C20	C21	H21	-179.4
C25	C20	C21	C22	0.6(6)
H20	C20	C25	C19	0.4
H20	C20	C25	C24	178.9
C21	C20	C25	C19	-179.5(3)
C21	C20	C25	C24	-1.1(5)
C20	C21	C22	H22	-179.6
C20	C21	C22	C23	0.5(6)
H21	C21	C22	H22	0.4
H21	C21	C22	C23	-179.6
C21	C22	C23	H23	179.1
C21	C22	C23	C24	-0.9(6)
H22	C22	C23	H23	-0.9
H22	C22	C23	C24	179.1
C22	C23	C24	C16	-179.5(3)
C22	C23	C24	C25	0.4(5)
H23	C23	C24	C16	0.5
H23	C23	C24	C25	-179.6
C16	C24	C25	C19	-1.1(5)
C16	C24	C25	C20	-179.6(3)
C23	C24	C25	C19	179.0(3)
C23	C24	C25	C20	0.6(5)
N3	C26	C27	H27A	57.8
N3	C26	C27	H27B	-60
N3	C26	C27	C28	179.0(3)
H26A	C26	C27	H27A	179
H26A	C26	C27	H27B	61.2
H26A	C26	C27	C28	-59.8
H26B	C26	C27	H27A	-63.3
H26B	C26	C27	H27B	178.9
H26B	C26	C27	C28	57.9
C26	C27	C28	H28A	-58.6
C26	C27	C28	H28B	-178.7
C26	C27	C28	H28C	61.4
H27A	C27	C28	H28A	62.6
H27A	C27	C28	H28B	-57.5
H27A	C27	C28	H28C	-177.4
H27B	C27	C28	H28A	-179.7
H27B	C27	C28	H28B	60.2
H27B	C27	C28	H28C	-59.7
N3	C29	C30	H30A	167.6

N3	C29	C30	H30B	47.7
N3	C29	C30	H30C	-72.3
N4	C29	C30	H30A	-12.9
N4	C29	C30	H30B	-132.9
N4	C29	C30	H30C	107.2

Table S30 Crystal data and structure refinement for **I-4**

Identification code	**I-4**
Empirical formula	C16 H17 N2 O2
Formula weight	269.32
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C 2/c
Unit cell dimensions	a = 14.6578(15) Å
	b = 8.7453(11) Å β = 106.460(7)°
	c = 22.209(4) Å
Volume	2730.2(7) $Å^3$
Z	8
Density (calculated)	1.310 Mg/m^3
Absorption coefficient	0.088 mm^{-1}
F(000)	1144
Crystal size	0.285 x 0.152 x 0.087 mm^3
Theta range for data collection	2.743 to 24.989°
Index ranges	-17<=h<=17, -10<=k<=10, -26<=l<=26
Reflections collected	38016
Independent reflections	2409 [R(int) = 0.0895]
Completeness to theta = 25.242°	97.2 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2409 / 0 / 183
Goodness-of-fit on F^2	1.043
Final R indices [I>2sigma(I)]	R1 = 0.0668, wR2 = 0.1420
R indices (all data)	R1 = 0.1060, wR2 = 0.1601
Extinction coefficient	n/a
Largest diff. peak and hole	0.172 and -0.442 $e.Å^{-3}$

Table S31Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **I-4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(2)	1316(2)	779(3)	555(1)	69(1)
O(3)	-1270(2)	4445(3)	-1170(1)	67(1)
N(1)	-374(2)	2278(2)	764(1)	38(1)
N(2)	-1414(2)	3812(3)	64(1)	46(1)
C(1)	755(2)	1645(3)	172(1)	41(1)
C(2)	-67(2)	2388(3)	264(1)	36(1)
C(3)	-720(2)	3334(3)	-163(1)	38(1)
C(4)	-672(2)	3657(3)	-775(1)	42(1)
C(5)	275(2)	3168(3)	-1462(1)	55(1)
C(6)	1048(2)	2517(4)	-1580(2)	64(1)
C(7)	1727(2)	1637(4)	-1134(2)	61(1)
C(8)	1637(2)	1371(3)	-567(1)	50(1)
C(9)	852(2)	2002(3)	-440(1)	40(1)
C(10)	169(2)	2927(3)	-890(1)	40(1)
C(11)	-1187(2)	3167(3)	618(1)	39(1)
C(12)	80(2)	1367(3)	1337(1)	42(1)
C(13)	909(2)	2185(3)	1832(1)	53(1)
C(14)	1442(2)	1145(4)	2385(1)	59(1)
C(15)	2031(3)	-87(5)	2241(2)	82(1)
C(16)	-1759(2)	3332(4)	1032(1)	57(1)

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Table S32 Bond lengths [Å] and angles [°] for **I-4**

O(2)-C(1)	1.256(3)
O(3)-C(4)	1.255(3)
N(1)-C(2)	1.317(3)
N(1)-C(11)	1.383(3)
N(1)-C(12)	1.488(3)
N(2)-C(11)	1.308(3)
N(2)-C(3)	1.324(3)
N(2)-H(2)	0.8600
C(1)-C(2)	1.433(4)
C(1)-C(9)	1.439(4)
C(2)-C(3)	1.408(3)
C(3)-C(4)	1.411(4)
C(4)-C(10)	1.473(4)
C(5)-C(10)	1.340(4)
C(5)-C(6)	1.360(4)
C(5)-H(5)	0.9300
C(6)-C(7)	1.416(5)
C(6)-H(6)	0.9300
C(7)-C(8)	1.325(4)
C(7)-H(7)	0.9300
C(8)-C(9)	1.376(4)
C(8)-H(8)	0.9300
C(9)-C(10)	1.445(4)
C(11)-C(16)	1.417(4)
C(12)-C(13)	1.563(4)
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(13)-C(14)	1.549(4)
C(13)-H(13A)	0.9700
C(13)-H(13B)	0.9700
C(14)-C(15)	1.470(5)
C(14)-H(14A)	0.9700
C(14)-H(14B)	0.9700
C(15)-H(15A)	0.9600

C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600

C(2)-N(1)-C(11)	103.8(2)
C(2)-N(1)-C(12)	125.7(2)
C(11)-N(1)-C(12)	130.5(2)
C(11)-N(2)-C(3)	101.7(2)
C(11)-N(2)-H(2)	129.2
C(3)-N(2)-H(2)	129.2
O(2)-C(1)-C(2)	126.3(3)
O(2)-C(1)-C(9)	123.4(2)
C(2)-C(1)-C(9)	110.3(2)
N(1)-C(2)-C(3)	106.3(2)
N(1)-C(2)-C(1)	126.1(2)
C(3)-C(2)-C(1)	127.6(2)
N(2)-C(3)-C(2)	112.4(2)
N(2)-C(3)-C(4)	123.8(2)
C(2)-C(3)-C(4)	123.8(2)
O(3)-C(4)-C(3)	124.6(3)
O(3)-C(4)-C(10)	124.8(2)
C(3)-C(4)-C(10)	110.6(2)
C(10)-C(5)-C(6)	116.4(3)
C(10)-C(5)-H(5)	121.8
C(6)-C(5)-H(5)	121.8
C(5)-C(6)-C(7)	123.5(3)
C(5)-C(6)-H(6)	118.3
C(7)-C(6)-H(6)	118.3
C(8)-C(7)-C(6)	121.4(3)
C(8)-C(7)-H(7)	119.3
C(6)-C(7)-H(7)	119.3
C(7)-C(8)-C(9)	116.1(3)
C(7)-C(8)-H(8)	122.0
C(9)-C(8)-H(8)	122.0

C(8)-C(9)-C(1)	114.7(3)
C(8)-C(9)-C(10)	122.6(3)
C(1)-C(9)-C(10)	122.7(2)
C(5)-C(10)-C(9)	120.1(3)
C(5)-C(10)-C(4)	115.0(3)
C(9)-C(10)-C(4)	124.9(2)
N(2)-C(11)-N(1)	115.9(2)
N(2)-C(11)-C(16)	121.8(3)
N(1)-C(11)-C(16)	122.3(2)
N(1)-C(12)-C(13)	115.2(2)
N(1)-C(12)-H(12A)	108.5
C(13)-C(12)-H(12A)	108.5
N(1)-C(12)-H(12B)	108.5
C(13)-C(12)-H(12B)	108.5
H(12A)-C(12)-H(12B)	107.5
C(14)-C(13)-C(12)	113.9(2)
C(14)-C(13)-H(13A)	108.8
C(12)-C(13)-H(13A)	108.8
C(14)-C(13)-H(13B)	108.8
C(12)-C(13)-H(13B)	108.8
H(13A)-C(13)-H(13B)	107.7
C(15)-C(14)-C(13)	117.0(3)
C(15)-C(14)-H(14A)	108.0
C(13)-C(14)-H(14A)	108.0
C(15)-C(14)-H(14B)	108.0
C(13)-C(14)-H(14B)	108.0
H(14A)-C(14)-H(14B)	107.3
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(11)-C(16)-H(16A)	109.5
C(11)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5

C(11)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S33 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **I-4**. 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)	67(1)	86(2)	56(1)	18(1)	21(1)	36(1)
O(3)	81(2)	74(2)	50(1)	24(1)	25(1)	30(1)
N(1)	39(1)	38(1)	35(1)	3(1)	10(1)	3(1)
N(2)	44(1)	45(1)	47(2)	7(1)	12(1)	16(1)
C(1)	38(2)	39(2)	44(2)	-4(1)	7(1)	5(1)
C(2)	40(2)	32(2)	36(2)	-2(1)	10(1)	-3(1)
C(3)	39(2)	32(2)	40(2)	1(1)	9(1)	1(1)
C(4)	51(2)	34(2)	39(2)	5(1)	10(1)	3(1)
C(5)	72(2)	48(2)	49(2)	2(2)	24(2)	-4(2)
C(6)	76(2)	67(2)	62(2)	-2(2)	41(2)	-8(2)
C(7)	59(2)	67(2)	68(2)	-14(2)	36(2)	-9(2)
C(8)	42(2)	52(2)	56(2)	-11(2)	15(2)	-4(2)
C(9)	41(2)	38(2)	41(2)	-9(1)	9(1)	-10(1)
C(10)	47(2)	34(2)	39(2)	-3(1)	12(1)	-7(1)
C(11)	39(2)	41(2)	37(2)	1(1)	9(1)	2(1)
C(12)	47(2)	40(2)	40(2)	5(1)	14(1)	-2(1)
C(13)	66(2)	46(2)	42(2)	-1(1)	6(2)	-2(2)
C(14)	67(2)	71(2)	37(2)	4(2)	11(2)	1(2)
C(15)	76(3)	99(3)	68(2)	16(2)	16(2)	28(2)
C(16)	56(2)	69(2)	50(2)	5(2)	22(2)	9(2)

Table S34 Torsion angles [°] for **I-4**

C(11)-N(1)-C(2)-C(3)	-0.5(3)
C(12)-N(1)-C(2)-C(3)	178.8(2)
C(11)-N(1)-C(2)-C(1)	-178.7(2)
C(12)-N(1)-C(2)-C(1)	0.6(4)
O(2)-C(1)-C(2)-N(1)	-0.5(5)
C(9)-C(1)-C(2)-N(1)	178.3(2)
O(2)-C(1)-C(2)-C(3)	-178.3(3)
C(9)-C(1)-C(2)-C(3)	0.5(4)
C(11)-N(2)-C(3)-C(2)	0.0(3)
C(11)-N(2)-C(3)-C(4)	176.3(3)
N(1)-C(2)-C(3)-N(2)	0.4(3)
C(1)-C(2)-C(3)-N(2)	178.6(2)
N(1)-C(2)-C(3)-C(4)	-176.0(2)
C(1)-C(2)-C(3)-C(4)	2.2(4)
N(2)-C(3)-C(4)-O(3)	1.0(4)
C(2)-C(3)-C(4)-O(3)	176.9(3)
N(2)-C(3)-C(4)-C(10)	-178.3(2)
C(2)-C(3)-C(4)-C(10)	-2.4(4)
C(10)-C(5)-C(6)-C(7)	-0.5(5)
C(5)-C(6)-C(7)-C(8)	1.0(5)
C(6)-C(7)-C(8)-C(9)	-0.1(5)
C(7)-C(8)-C(9)-C(1)	177.8(3)
C(7)-C(8)-C(9)-C(10)	-1.2(4)
O(2)-C(1)-C(9)-C(8)	-2.8(4)
C(2)-C(1)-C(9)-C(8)	178.4(2)
O(2)-C(1)-C(9)-C(10)	176.2(3)
C(2)-C(1)-C(9)-C(10)	-2.6(4)
C(6)-C(5)-C(10)-C(9)	-0.7(4)
C(6)-C(5)-C(10)-C(4)	179.5(3)
C(8)-C(9)-C(10)-C(5)	1.7(4)
C(1)-C(9)-C(10)-C(5)	-177.2(3)
C(8)-C(9)-C(10)-C(4)	-178.6(3)
C(1)-C(9)-C(10)-C(4)	2.5(4)
O(3)-C(4)-C(10)-C(5)	0.6(4)

C(3)-C(4)-C(10)-C(5)	179.9(2)
O(3)-C(4)-C(10)-C(9)	-179.1(3)
C(3)-C(4)-C(10)-C(9)	0.2(4)
C(3)-N(2)-C(11)-N(1)	-0.3(3)
C(3)-N(2)-C(11)-C(16)	-178.3(3)
C(2)-N(1)-C(11)-N(2)	0.6(3)
C(12)-N(1)-C(11)-N(2)	-178.7(2)
C(2)-N(1)-C(11)-C(16)	178.5(3)
C(12)-N(1)-C(11)-C(16)	-0.8(4)
C(2)-N(1)-C(12)-C(13)	84.4(3)
C(11)-N(1)-C(12)-C(13)	-96.4(3)
N(1)-C(12)-C(13)-C(14)	-173.3(2)
C(12)-C(13)-C(14)-C(15)	69.5(4)

Symmetry transformations used to generate equivalent atoms: