Supplementary Information

Double helix quinine-based supergelator

Kinga Roszak,[a] Monika Piasecka,[a] Andrzej Katrusiak[a] and Karol Kacprzak[a]*

[a] Faculty of Chemistry, Adam Mickiewicz University, Umultowska 89b, 61-614 Poznań, Poland, phone +48 829 15 63, fax +48 61 829 1555
* E-mail: karol.kacprzak@gmail.com

Content:

General procedure for gel preparation

In small screw-caped vial 7.5 mg of finely powderized **DDQn** (prepared according to the procedure reported by K. M. Kacprzak[1]) was placed and dissolved in 0.25 mL of AcOEt (or other solvent) on heating. After dissolution of the gelator, resultant solution was cooled down to almost room temperature followed by the quick addition of 1 mL of hydrocarbon (hexane, pentane or heptane) or other solvent. Such prepared gels were found to be stable in closed vials for months.

For larger scale preparation 150 mg of **DDQn**, 5 mL of AcOEt and 20 mL hydrocarbon solvent were routinely used for the gelation with the same efficiency.

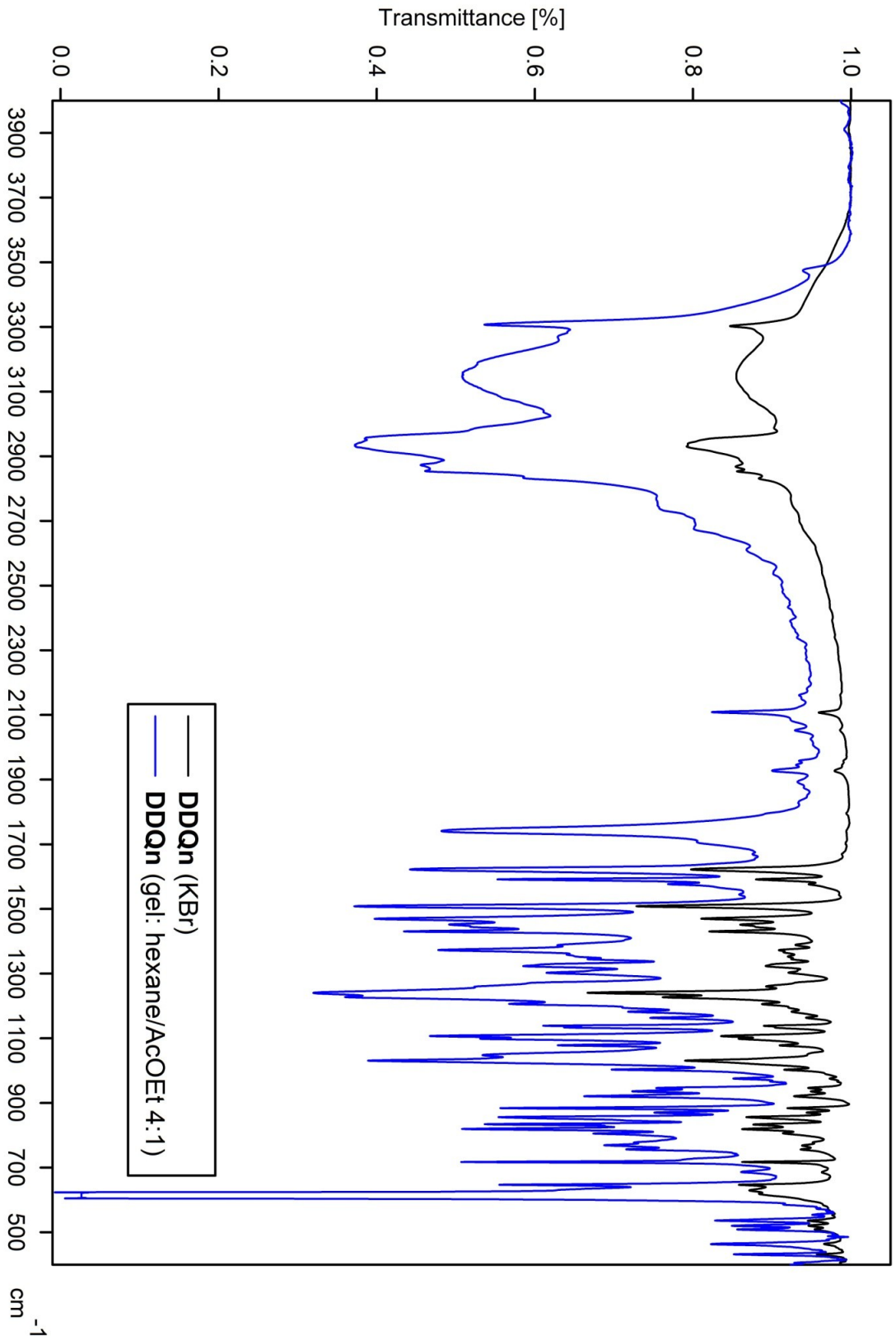

Figure S1. FT-IR spectra of **DDQn (**KBr disc) and **DDQn** in gel (AcOEt:He 1:4 v/v, film in KBr plates).

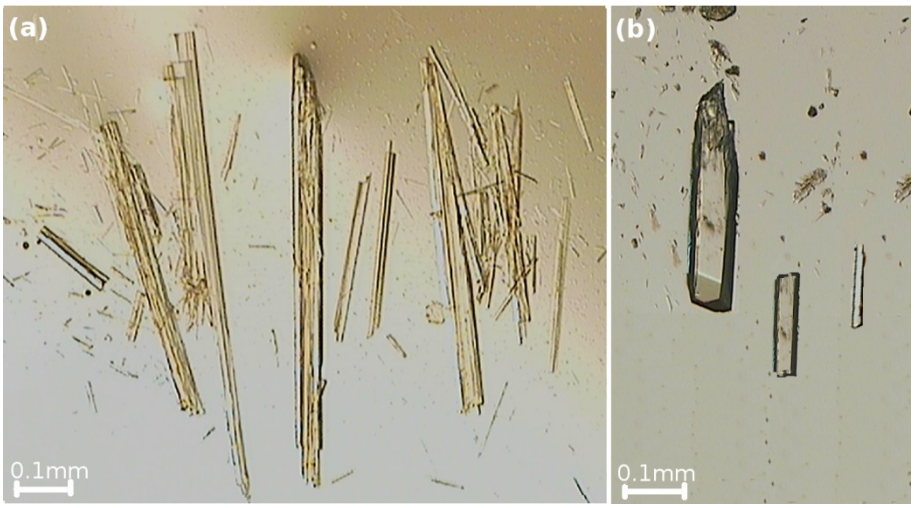

Figure S2. The crystals of (a) **DDQn** and (b) **DDQd** immersed in silicon oil.

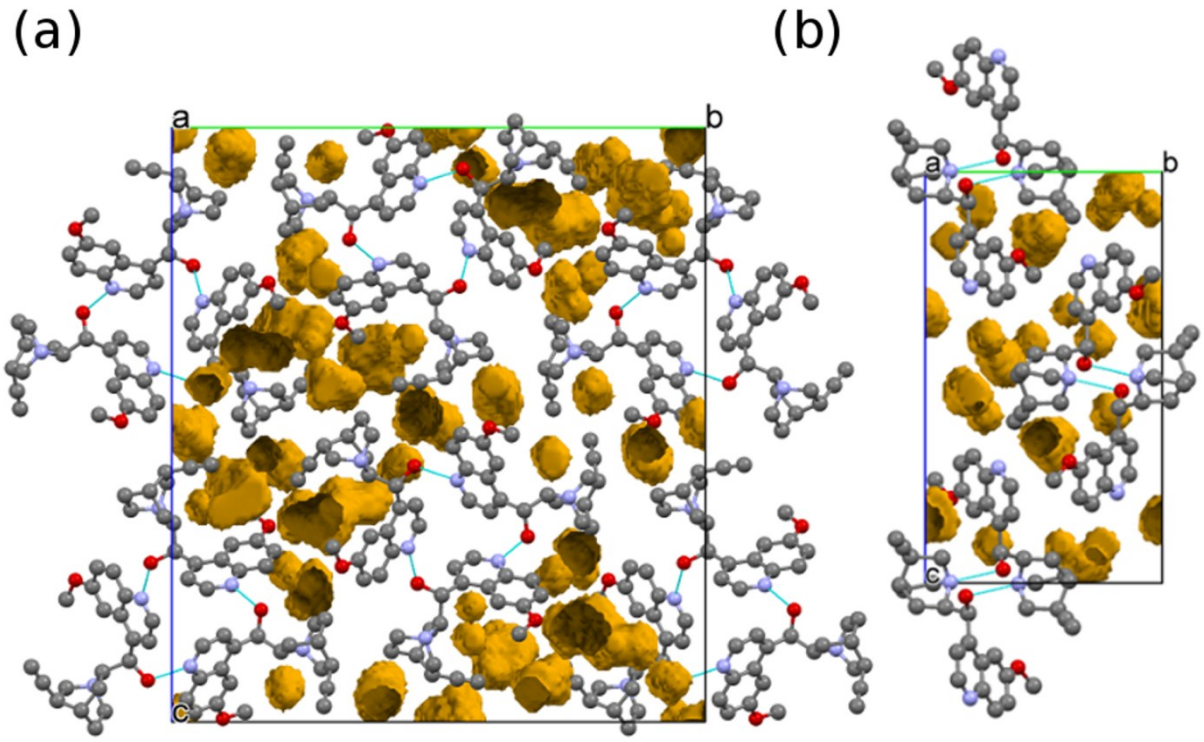

Figure S3. Voids in the crystal structure of (a) **DDQn** and (b) **DDQd**, as calculated by program Mercury[2] assuming the probing sphere of 0.8 Å and 0.2 Å step.

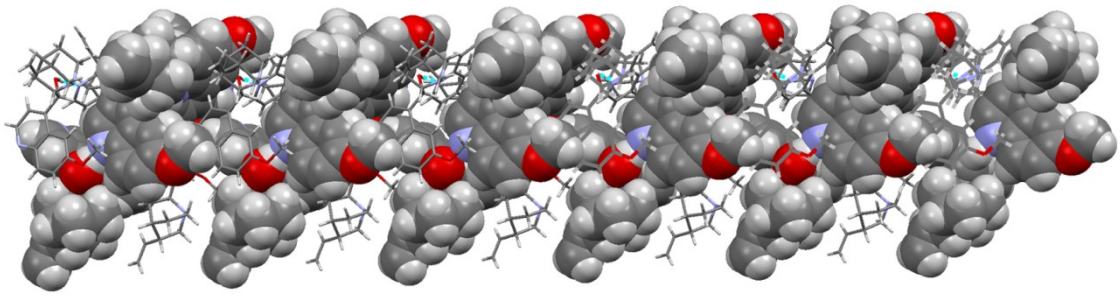

Figure S4. Projection of the OH···N bonded double helix of **Qn**: the molecular of one helix are represented as the space-filling models, and the other are the caped sticks.

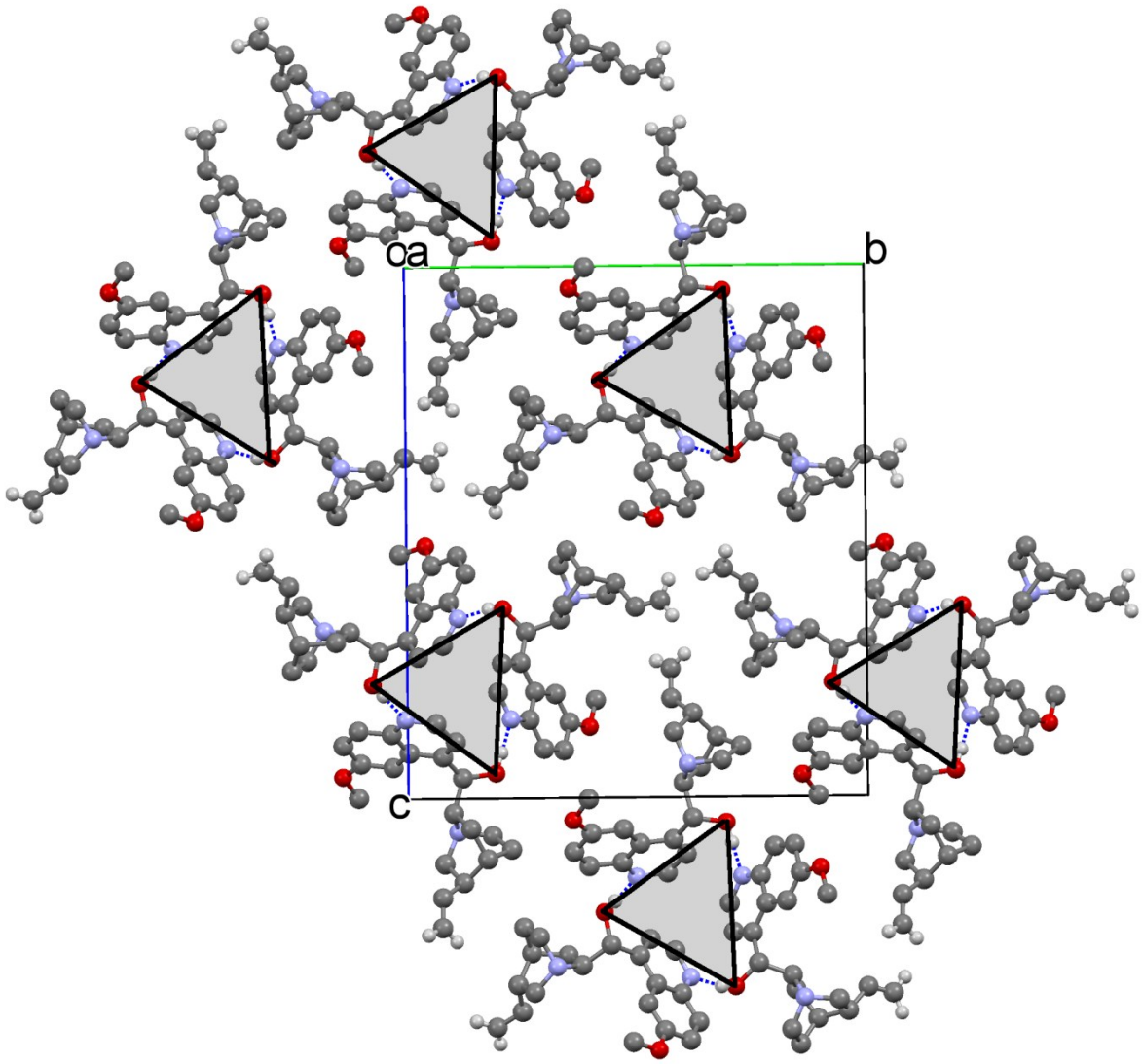

Figure S5. The crystal structure of quinine projected along the OH···N bonded chains down the crystal [x] axis. The H-atoms have been omitted for clarity.

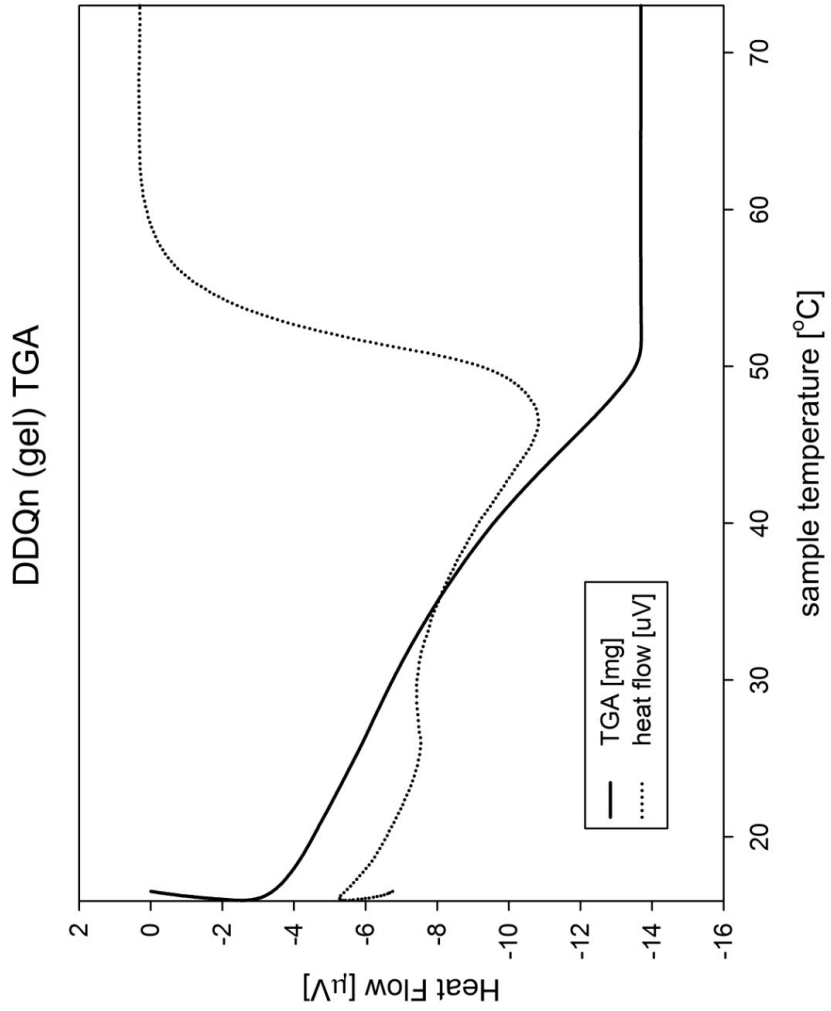

Figure S6. TGA analysis of **DDQn** gel. Sample (gel) 23 mg, heat gradient 10 ºC/min (Instrument Setsys 1200 Setaram).

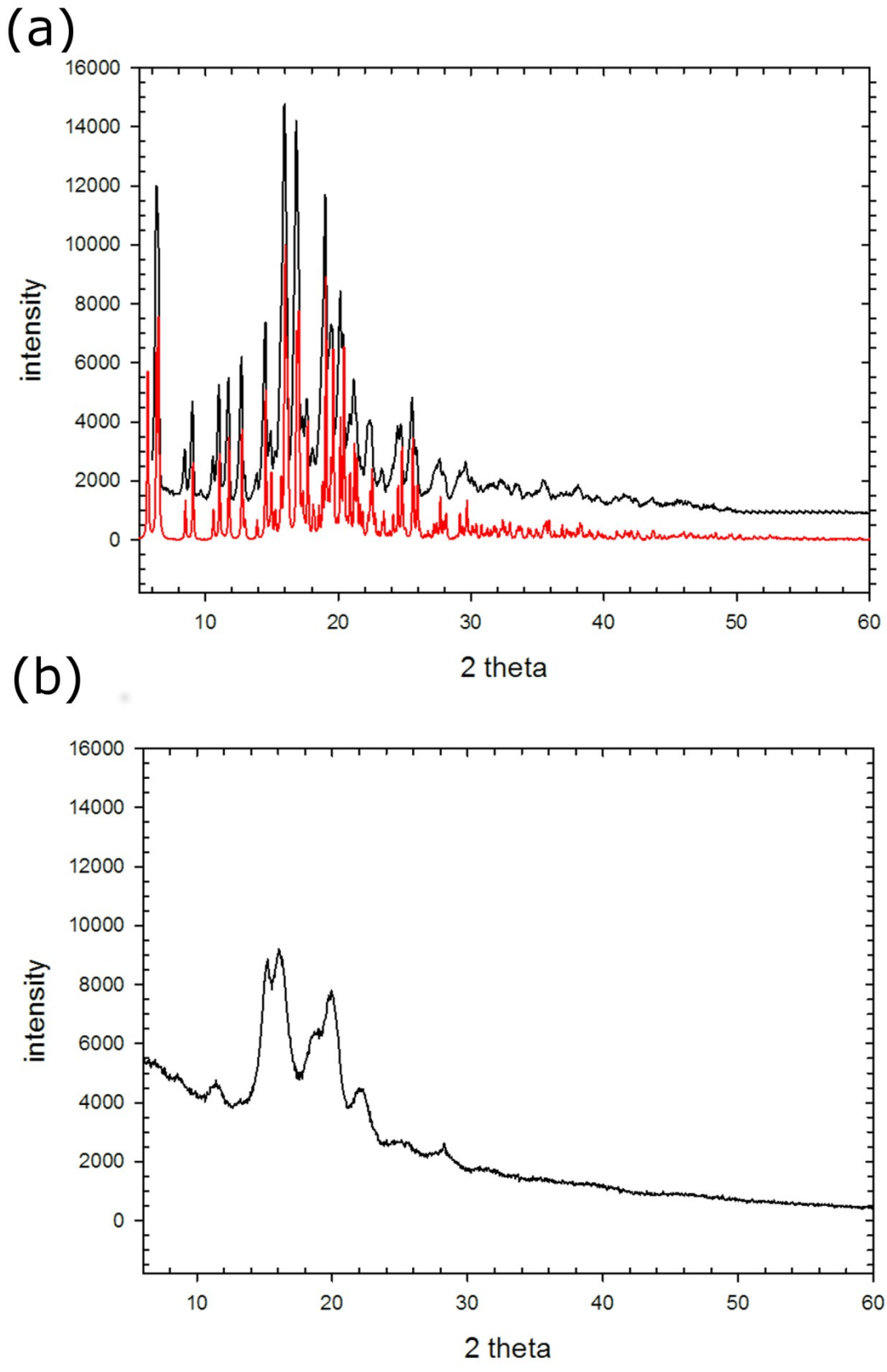

Figure S7. The XRPD pattern of **DDQn** shown in Figures S8 (a) and S9 (b) shown in their full 2θ range.

Table S1. Crystal data and structure refinement for 10,11-didehydroquinine and 10,11-didehydroquinidine.

	10,11-didehydroquinine	10,11-didehydroquinine	10,11-didehydroquinidine
Empirical formula	$C_{20}H_{22}N_2O_2$	$C_{20}H_{22}N_2O_2$	$C_{20}H_{22}N_2O_2$
Formula weight	322.40	322.40	322.40
Temperature	120(2) K	296(2) K	296(2) K
Wavelength	1.54184 Å	1.54184 Å	1.54184 Å
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic
Space group	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
Unit cell dimensions: a b c	5.98370(10) Å 27.8283(6) Å 30.8628(5) Å	6.0461(4) Å 27.8882(19) Å 31.178(2) Å	7.13240(10) Å 11.67130(10) Å 20.2977(2) Å
Volume	5139.16(16) $Å^3$	5257.0(6) $Å^3$	1689.67(3) $Å^3$
Z	12	12	4
Calculated density	1.250 gcm^{-3}	1.222 gcm^{-3}	1.267 gcm^{-3}
Absorption coefficient	0.646 mm^{-1}	0.631 mm^{-1}	0.655 mm^{-1}
F(000)	2064	2064	688
Crystal size	0.25 x 0.15 x 0.10 mm	0.15 x 0.10 x 0.08 mm	0.20 x 0.20 x 0.05 mm
Theta range for data collection	2.14 to 73.76°	2.12 to 71.10°	4.36 to 75.59°
Limiting indices h,k,l	-6/7, -34/33, -36/38	-7/7, -34/34, -37/37	-8/6, -13/14, -25/25
Reflections collected / unique	39117/10270 R_{int}=0.0550	82985/10026 R_{int}=0.0896	9289/3212 R_{int}= 0.0187
Completeness	to θ = 73.76 99.1 %	to θ = 71.10 98.7 %	to θ = 75.59 97.5 %
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/restraints/parameters	10270/3/659	10026/3/659	3212/0/222
Goodness-of-fit on F^2	1.122	1.040	1.050
Final *R* indices [I>2sigma(I)]	R_1 = 0.0743 wR_2 = 0.2239	R_1 = 0.0573 wR_2 = 0.1169	R_1 = 0.0292 wR_2 = 0.0774
R indices (all data)	R_1 = 0.0777 wR_2 = 0.2251	R_1 = 0.0994 wR_2 = 0.1386	R_1 = 0.0307 wR_2 = 0.0789
Largest diff. peak and hole	0.433 and -0.291 $e.A^{-3}$	0.154 and -0.144 $e.A^{-3}$	0.132 and -0.102 $e.A^{-3}$

Table S2. Bond lengths [Å] for 10,11-didehydroquinine in 296 K.

O(1) – C(9)	1.421(4)	O(1B) – C(9B)	1.426(4)	O(1C) – C(9C)	1.418(3)
N(2) – C(20)	1.369(4)	C(20B) – N(2B)	1.370(4)	C(20C) – N(2C)	1.370(4)
C(20) – C(19)	1.412(4)	C(19B) – C(20B)	1.418(5)	C(20C) – C(19C)	1.414(4)
C(20) – C(18)	1.415(4)	C(20B) – C(18B)	1.418(5)	C(20C) – C(18C)	1.421(4)
N(2) – C(12)	1.317(4)	N(2B) – C(12B)	1.307(4)	N(2C) – C(12C)	1.297(4)
O(2) – C(16)	1.376(4)	O(2B) – C(16B)	1.375(4)	O(2C) – C(16C)	1.364(4)
O(2) – C(21)	1.419(4)	O(2B) – C(21B)	1.427(5)	O(2C) – C(21C)	1.401(5)
C(13) – C(14)	1.360(5)	C(13B) – C(14B)	1.374(5)	C(13C) – C(14C)	1.370(4)
C(13) – C(12)	1.394(5)	C(13B) – C(12B)	1.394(5)	C(13C) – C(12C)	1.392(5)
C(15) – C(16)	1.362(4)	C(15B) – C(16B)	1.370(5)	C(15C) – C(16C)	1.365(5)
C(15) – C(19)	1.415(4)	C(15B) – C(19B)	1.420(4)	C(15C) – C(19C)	1.413(4)
C(17) – C(18)	1.342(5)	C(17B) – C(18B)	1.355(5)	C(17C) – C(18C)	1.342(5)
N(1) – C(8)	1.479(4)	C(8B) – N(1B)	1.473(4)	N(1C) – C(8C)	1.478(4)
C(7) – C(8)	1.549(4)	C(7B) – C(8B)	1.532(4)	C(7C) – C(8C)	1.525(4)
C(8) – C(9)	1.532(4)	C(8B) – C(9B)	1.533(4)	C(8C) – C(9C)	1.536(4)
C(14) – C(19)	1.430(4)	C(14B) – C(19B)	1.419(4)	C(14C) – C(19C)	1.422(4)
C(14) – C(9)	1.516(4)	C(14B) – C(9B)	1.519(5)	C(14C) – C(9C)	1.514(4)
C(4) – C(7)	1.521(4)	C(4B) – C(7B)	1.522(5)	C(4C) – C(7C)	1.525(5)
C(16) – C(17)	1.411(5)	C(16B) – C(17B)	1.393(5)	C(16C) – C(17C)	1.404(5)
N(1) – C(2)	1.459(4)	N(1B) – C(21B)	1.451(5)	N(1C) – C(2C)	1.464(5)
N(1) – C(6)	1.476(4)	N(1B) – C(6B)	1.492(6)	N(1C) – C(6C)	1.470(5)
C(4) – C(5)	1.512(5)	C(4B) – C(5B)	1.515(6)	C(4C) – C(5C)	1.531(6)
C(4) – C(3)	1.533(5)	C(4B) – C(3B)	1.535(6)	C(3C) – C(4C)	1.528(5)
C(10) – C(3)	1.473(6)	C(10B) – C(3B)	1.447(7)	C(10C) – C(3C)	1.445(7)
C(2) – C(3)	1.552(5)	C(2B) – C(3B)	1.534(6)	C(2C) – C(3C)	1.560(5)
C(6) – C(5)	1.530(5)	C(6B) – C(5B)	1.527(7)	C(6C) – C(5C)	1.536(6)
C(10) – C(11)	1.163(6)	C(10B) – C(11B)	1.161(7)	C(10C) – C(11C)	1.188(7)

Table S3. Bond lengths [Å] for 10,11-didehydroquinine in 120 K.

O(1) – C(9)	1.417(5)	O(1B) – C(9B)	1.418(5)	O(1C) – C(9C)	1.414(5)
N(2) – C(20)	1.367(6)	C(20B) – N(2B)	1.362(6)	C(20C) – N(2C)	1.366(6)
C(20) – C(19)	1.413(6)	C(19B) – C(20B)	1.434(6)	C(20C) – C(19C)	1.418(6)
C(20) – C(18)	1.420(6)	C(20B) – C(18B)	1.411(6)	C(20C) – C(18C)	1.423(6)
N(2) – C(12)	1.319(6)	N(2B) – C(12B)	1.325(6)	N(2C) – C(12C)	1.317(6)
O(2) – C(16)	1.370(6)	O(2B) – C(16B)	1.373(6)	O(2C) – C(16C)	1.351(5)
O(2) – C(21)	1.428(6)	O(2B) – C(21B)	1.427(7)	O(2C) – C(21C)	1.428(7)
C(13) – C(14)	1.382(7)	C(13B) – C(14B)	1.372(6)	C(13C) – C(14C)	1.370(6)
C(13) – C(12)	1.401(7)	C(13B) – C(12B)	1.404(7)	C(13C) – C(12C)	1.405(6)
C(15) – C(16)	1.373(6)	C(15B) – C(16B)	1.371(6)	C(15C) – C(16C)	1.373(6)
C(15) – C(19)	1.433(6)	C(15B) – C(19B)	1.418(6)	C(15C) – C(19C)	1.415(6)
C(17) – C(18)	1.359(7)	C(17B) – C(18B)	1.375(8)	C(17C) – C(18C)	1.360(7)
N(1) – C(8)	1.489(6)	C(8B) – N(1B)	1.477(6)	N(1C) – C(8C)	1.476(5)
C(7) – C(8)	1.555(6)	C(7B) – C(8B)	1.541(6)	C(7C) – C(8C)	1.543(6)
C(8) – C(9)	1.533(6)	C(8B) – C(9B)	1.534(6)	C(8C) – C(9C)	1.540(6)
C(14) – C(19)	1.436(6)	C(14B) – C(19B)	1.425(6)	C(14C) – C(19C)	1.431(5)
C(14) – C(9)	1.513(6)	C(14B) – C(9B)	1.522(6)	C(14C) – C(9C)	1.514(6)
C(4) – C(7)	1.537(6)	C(4B) – C(7B)	1.534(6)	C(4C) – C(7C)	1.531(6)
C(16) – C(17)	1.408(7)	C(16B) – C(17B)	1.412(7)	C(16C) – C(17C)	1.414(7)
N(1) – C(2)	1.458(6)	N(1B) – C(2B)	1.472(7)	N(1C) – C(2C)	1.465(6)
N(1) – C(6)	1.485(6)	N(1B) – C(6B)	1.485(7)	N(1C) – C(6C)	1.476(6)
C(4) – C(5)	1.513(6)	C(4B) – C(5B)	1.522(7)	C(4C) – C(5C)	1.537(7)
C(4) – C(3)	1.536(6)	C(4B) – C(3B)	1.537(7)	C(3C) – C(4C)	1.545(7)
C(10) – C(3)	1.471(7)	C(10B) – C(3B)	1.455(8)	C(10C) – C(3C)	1.463(8)
C(2) – C(3)	1.573(6)	C(2B) – C(3B)	1.569(7)	C(2C) – C(3C)	1.564(7)
C(6) – C(5)	1.549(6)	C(6B) – C(5B)	1.545(8)	C(6C) – C(5C)	1.539(7)
C(10) – C(11)	1.184(8)	C(10B) – C(11B)	1.162(9)	C(10C) – C(11C)	1.180(8)

Table S4. Bond lengths [Å] 10,11-didehydroquinidine.

O(1) – C(9)	1.4177(15)
N(2) – C(20)	1.3708(18)
C(20) – C(19)	1.4236(18)
C(20) – C(18)	1.405(2)
N(2) – C(12)	1.305(2)
O(2) – C(16)	1.3630(18)
O(2) – C(21)	1.4061(18)
C(13) – C(14)	1.363(2)
C(13) – C(12)	1.405(2)
C(15) – C(16)	1.3723(18)
C(15) – C(19)	1.4104(19)
C(17) – C(18)	1.364(2)
N(1) – C(8)	1.4869(16)
C(7) – C(8)	1.5423(17)
C(8) – C(9)	1.5392(18)
C(14) – C(19)	1.4303(18)
C(14) – C(9)	1.5207(18)
C(4) – C(7)	1.534(2)
C(16) – C(17)	1.4031(19)
N(1) – C(2)	1.4754(16)
N(1) – C(6)	1.4797(17)
C(4) – C(5)	1.521(2)
C(4) – C(3)	1.5397(19)
C(10) – C(3)	1.467(2)
C(2) – C(3)	1.5569(18)
C(6) – C(5)	1.541(2)
C(10) – C(11)	1.170(2)

Table S5.Angles [º] for 10,11-didehydroquinine in 296 K.

N(2) – C(20) – C(18)	117.6(3)	N(2B) – C(20B) – C(18B)	117.6(3)	N(2C) – C(20C) – C(18C)	117.5(3)
C(19) – C(20) – C(18)	119.2(3)	C(19B) – C(20B) – C(18B)	119.6(3)	C(19C) – C(20C) – C(18C)	119.4(3)
C(12) – N(2) – C(20)	116.9(3)	C(12B) – N(2B) – C(20B)	117.1(3)	C(12C) – N(2C) – C(20C)	116.7(3)
C(16) – O(2) – C(21)	117.6(3)	C(16B) – O(2B) – C(21B)	117.5(3)	C(16C) – O(2C) – C(21C)	117.4(3)
C(14) – C(13) – C(12)	120.8(3)	C(14B) – C(13B) – C(12B)	120.2(3)	C(14C) – C(13C) – C(12C)	120.0(3)
C(16) – C(15) – C(19)	119.9(3)	C(16B) – C(15B) – C(19B)	119.5(3)	C(16C) – C(15C) – C(19C)	119.7(3)
C(17) – C(18) – C(20)	121.3(3)	C(17B) – C(18B) – C(20B)	119.9(4)	C(17C) – C(18C) – C(20C)	119.9(3)
N(1) – C(8) – C(7)	111.1(2)	N(1B) – C(8B) – C(7B)	110.2(3)	N(1C) – C(8C) – C(7C)	111.1(2)
N(1) – C(8) – C(9)	112.6(3)	N(1B) – C(8B) – C(9B)	112.8(3)	N(1C) – C(8C) – C(9C)	111.5(3)
C(7) – C(8) – C(9)	113.4(3)	C(7B) – C(8B) – C(9B)	114.8(3)	C(7C) – C(8C) – C(9C)	114.2(3)
C(13) – C(14) – C(19)	117.7(3)	C(13B) – C(14B) – C(19B)	117.6(3)	C(13C) – C(14C) – C(19C)	117.5(3)
C(13) – C(14) – C(9)	120.8(3)	C(13B) – C(14B) – C(9B)	120.9(3)	C(13C) – C(14C) – C(9C)	120.7(3)
C(19) – C(14) – C(9)	121.4(3)	C(19B) – C(14B) – C(9B)	121.5(3)	C(19C) – C(14C) – C(9C)	121.7(3)
O(1) – C(9) – C(14)	110.8(3)	O(1B) – C(9B) – C(14B)	110.0(3)	O(1C) – C(9C) – C(14C)	112.1(3)
O(1) – C(9) – C(8)	109.8(2)	O(1B) – C(9B) – C(8B)	109.3(3)	O(1C) – C(9C) – C(8C)	109.3(2)
C(14) – C(9) – C(8)	109.4(2)	C(14B) – C(9B) – C(8B)	109.6(2)	C(14C) – C(9C) – C(8C)	110.3(2)
C(20) – C(19) – C(14)	117.4(3)	C(20B) – C(19B) – C(14B)	118.0(3)	C(20C) – C(19C) – C(14C)	117.7(3)
C(20) – C(19) – C(15)	118.7(3)	C(20B) – C(19B) – C(15B)	118.8(3)	C(20C) – C(19C) – C(15C)	119.0(3)
C(15) – C(19) – C(14)	123.9(3)	C(15B) – C(19B) – C(14B)	123.2(3)	C(15C) – C(19C) – C(14C)	123.3(3)
C(4) – C(7) – C(8)	108.3(3)	C(4B) – C(7B) – C(8B)	107.8(3)	C(4C) – C(7C) – C(8C)	108.2(3)
N(2) – C(12) – C(13)	123.8(3)	N(2B) – C(12B) – C(13B)	124.4(4)	N(2C) – C(12C) – C(13C)	125.1(3)
C(15) – C(16) – O(2)	125.4(3)	C(15B) – C(16B) – O(2B)	124.7(4)	C(15C) – C(16C) – O(2C)	124.7(4)
C(15) – C(16) – C(17)	121.3(3)	C(15B) – C(16B) – C(17B)	121.3(4)	C(15C) – C(16C) – C(17C)	120.9(3)
O(2) – C(16) – C(17)	113.3(3)	O(2B) – C(16B) – C(17B)	114.0(4)	O(2C) – C(16C) – C(17C)	114.4(3)
C(2) – N(1) – C(8)	108.0(3)	C(2B) – N(1B) – C(8B)	107.1(3)	C(2C) – N(1C) – C(8C)	107.6(3)
C(2) – N(1) – C(6)	107.9(3)	C(2B) – N(1B) – C(6B)	108.6(3)	C(2C) – N(1C) – C(6C)	108.2(3)
C(8) – N(1) – C(6)	111.3(3)	C(8B) – N(1B) – C(6B)	110.2(3)	C(8C) – N(1C) – C(6C)	111.2(3)
C(5) – C(4) – C(7)	108.6(3)	C(5B) – C(4B) – C(7B)	108.2(3)	C(5C) – C(4C) – C(7C)	107.6(3)
C(5) – C(4) – C(3)	108.1(3)	C(5B) – C(4B) – C(3B)	107.1(4)	C(5C) – C(4C) – C(3C)	107.1(3)
C(7) – C(4) – C(3)	110.1(3)	C(7B) – C(4B) – C(3B)	109.5(3)	C(7C) – C(4C) – C(3C)	110.6(3)
C(10) – C(3) – C(2)	112.9(3)	C(10B) – C(3B) – C(2B)	113.2(4)	C(10C) – C(3C) – C(2C)	110.0(4)
C(10) – C(3) – C(4)	112.0(3)	C(10B) – C(3B) – C(4B)	111.8(4)	C(10C) – C(3C) – C(4C)	113.5(3)
C(4) – C(3) – C(2)	107.3(3)	C(4B) – C(3B) – C(2B)	108.0(3)	C(4C) – C(3C) – C(2C)	107.4(3)
C(4) – C(5) – C(6)	109.2(3)	C(4B) – C(5B) – C(6B)	107.8(4)	C(4C) – C(5C) – C(6C)	108.7(3)
N(1) – C(2) – C(3)	112.2(3)	N(1B) – C(2B) – C(3B)	111.3(4)	N(1C) – C(2C) – C(3C)	111.4(3)
C(11) – C(10) – C(3)	179.0(5)	C(11B) – C(10B) – C(3B)	176.0(7)	C(11C) – C(10C) – C(3C)	177.5(5)
N(1) – C(6) – C(5)	111.3(3)	N(1B) – C(6B) – C(5B)	111.1(4)	N(1C) – C(6C) – C(5C)	110.8(3)
C(18) – C(17) – C(16)	119.5(3)	C(18B) – C(17B) – C(16B)	120.9(4)	C(18C) – C(17C) – C(16C)	121.1(3)
N(2) – C(20) – C(19)	123.3(3)	N(2B) – C(20B) – C(19B)	122.8(3)	N(2C) – C(20C) – C(19C)	123.0(3)

Table S6.Angles [º] for 10,11-didehydroquinine in 120 K.

N(2) – C(20) – C(18)	117.6(4)	N(2B) – C(20B) – C(18B)	118.2(4)	N(2C) – C(20C) – C(18C)	117.1(4)
C (19) – C(20) – C(18)	119.1(4)	C(19B) – C(20B) – C(18B)	119.3(4)	C(19C) – C(20C) – C(18C)	119.3(4)
C(12) – N(2) – C(20)	117.1(4)	C(12B) – N(2B) – C(20B)	117.9(4)	C(12C) – N(2C) – C(20C)	117.2(4)
C(16) – O(2) – C(21)	117.6(4)	C(16B) – O(2B) – C(21B)	117.1(4)	C(16C) – O(2C) – C(21C)	117.7(4)
C(14) – C(13) – C(12)	120.1(4)	C(14B) – C(13B) – C(12B)	120.7(4)	C(14C) – C(13C) – C(12C)	120.3(4)
C(16) – C(15) – C(19)	119.4(4)	C(16B) – C(15B) – C(19B)	120.6(5)	C(16C) – C(15C) – C(19C)	120.0(4)
C(17) – C(18) – C(20)	120.8(4)	C(17B) – C(18B) – C(20B)	120.7(5)	C(17C) – C(18C) – C(20C)	120.0(4)
N(1) – C(8) – C(7)	111.5(3)	N(1B) – C(8B) – C(7B)	110.3(4)	N(1C) – C(8C) – C(7C)	111.6(3)
N(1) – C(8) – C(9)	112.4(4)	N(1B) – C(8B) – C(9B)	112.9(4)	N(1C) – C(8C) – C(9C)	111.5(3)
C(7) – C(8) – C(9)	112.6(4)	C(7B) – C(8B) – C(9B)	113.8(4)	C(7C) – C(8C) – C(9C)	113.8(4)
C(13) – C(14) – C(19)	117.3(4)	C(13B) – C(14B) – C(19B)	117.8(4)	C(13C) – C(14C) – C(19C)	118.0(4)
C(13) – C(14) – C(9)	120.1(4)	C(13B) – C(14B) – C(9B)	119.7(4)	C(13C) – C(14C) – C(9C)	120.6(4)
C(19) – C(14) – C(9)	122.5(4)	C(19B) – C(14B) – C(9B)	122.4(4)	C(19C) – C(14C) – C(9C)	121.5(4)
O(1) – C(9) – C(14)	111.5(4)	O(1B) – C(9B) – C(14B)	110.5(4)	O(1C) – C(9C) – C(14C)	111.6(4)
O(1) – C(9) – C(8)	109.8(3)	O(1B) – C(9B) – C(8B)	110.0(3)	O(1C) – C(9C) – C(8C)	109.4(3)
C(14) – C(9) – C(8)	108.8(3)	C(14B) – C(9B) – C(8B)	109.2(3)	C(14C) – C(9C) – C(8C)	110.7(3)
C(20) – C(19) – C(14)	117.9(4)	C(20B) – C(19B) – C(14B)	117.8(4)	C(20C) – C(19C) – C(14C)	117.2(4)
C(20) – C(19) – C(15)	119.2(4)	C(20B) – C(19B) – C(15B)	118.5(4)	C(20C) – C(19C) – C(15C)	119.3(4)
C(15) – C(19) – C(14)	122.8(4)	C(15B) – C(19B) – C(14B)	123.7(4)	C(15C) – C(19C) – C(14C)	123.5(4)
C(4) – C(7) – C(8)	107.8(4)	C(4B) – C(7B) – C(8B)	107.6(4)	C(4C) – C(7C) – C(8C)	107.8(4)
N(2) – C(12) – C(13)	124.3(4)	N(2B) – C(12B) – C(13B)	123.3(4)	N(2C) – C(12C) – C(13C)	123.8(4)
C(15) – C(16) – O(2)	124.6(4)	C(15B) – C(16B) – O(2B)	125.1(5)	C(15C) – C(16C) – O(2C)	125.3(4)
C(15) – C(16) – C(17)	121.1(4)	C(15B) – C(16B) – C(17B)	120.9(5)	C(15C) – C(16C) – C(17C)	120.5(4)
O(2) – C(16) – C(17)	114.3(4)	O(2B) – C(16B) – C(17B)	114.0(4)	O(2C) – C(16C) – C(17C)	114.2(4)
C(2) – N(1) – C(8)	107.9(3)	C(2B) – N(1B) – C(8B)	106.8(4)	C(2C) – N(1C) – C(8C)	107.6(4)
C(2) – N(1) – C(6)	107.9(3)	C(2B) – N(1B) – C(6B)	107.4(4)	C(2C) – N(1C) – C(6C)	107.7(4)
C(8) – N(1) – C(6)	111.1(3)	C(8B) – N(1B) – C(6B)	111.6(4)	C(8C) – N(1C) – C(6C)	111.2(4)
C(5) – C(4) – C(7)	109.1(4)	C(5B) – C(4B) – C(7B)	107.9(4)	C(5C) – C(4C) – C(7C)	107.9(4)
C(5) – C(4) – C(3)	109.0(4)	C(5B) – C(4B) – C(3B)	107.7(5)	C(5C) – C(4C) – C(3C)	107.2(4)
C(7) – C(4) – C(3)	109.7(4)	C(7B) – C(4B) – C(3B)	110.2(4)	C(7C) – C(4C) – C(3C)	109.7(4)
C(10) – C(3) – C(2)	112.9(4)	C(10B) – C(3B) – C(2B)	113.0(5)	C(10C) – C(3C) – C(2C)	110.9(4)
C(10) – C(3) – C(4)	112.7(4)	C(10B) – C(3B) – C(4B)	111.9(4)	C(10C) – C(3C) – C(4C)	112.5(4)
C(4) – C(3) – C(2)	106.9(4)	C(4B) – C(3B) – C(2B)	106.9(4)	C(4C) – C(3C) – C(2C)	107.9(4)
C(4) – C(5) – C(6)	108.5(4)	C(4B) – C(5B) – C(6B)	107.7(4)	C(4C) – C(5C) – C(6C)	108.5(4)
N(1) – C(2) – C(3)	112.3(4)	N(1B) – C(2B) – C(3B)	111.2(4)	N(1C) – C(2C) – C(3C)	111.4(4)
C(11) – C(10) – C(3)	178.7(6)	C(11B) – C(10B) – C(3B)	178.4(7)	C(11C) – C(10C) – C(3C)	176.5(6)
N(1) – C(6) – C(5)	111.6(4)	N(1B) – C(6B) – C(5B)	111.4(4)	N(1C) – C(6C) – C(5C)	111.8(4)
C(18) – C(17) – C(16)	120.3(4)	C(18B) – C(17B) – C(16B)	119.9(5)	C(18C) – C(17C) – C(16C)	120.9(4)
N(2) – C(20) – C(19)	123.3(4)	N(2B) – C(20B) – C(19B)	122.5(4)	N(2C) – C(20C) – C(19C)	123.6(4)

Table S7.Angles[º] for 10,11-didehydroquinine.

N(2) – C(20) – C(18)	117.90(12)
C(19) – C(20) – C(18)	119.11(13)
C(12) – N(2) – C(20)	116.66(13)
C(16) – O(2) – C(21)	119.38(13)
C(14) – C(13) – C(12)	120.16 (14)
C(16) – C(15) – C(19)	121.02(12)
C(17) – C(18) – C(20)	121.31(13)
N(1) – C(8) – C(7)	109.86(10)
N(1) – C(8) – C(9)	111.76(9)
C(7) – C(8) – C(9)	114.54(11)
C(13) – C(14) – C(19)	117.54(13)
C(13) – C(14) – C(9)	121.30(12)
C(19) – C(14) – C(9)	121.16(11)
O(1) – C(9) – C(14)	111.13(11)
O(1) – C(9) – C(8)	110.44(10)
C(14) – C(9) – C(8)	110.98(10)
C(20) – C(19) – C(14)	117.76(12)
C(20) – C(19) – C(15)	118.31(12)
C(15) – C(19) – C(14)	123.92(12)
C(4) – C(7) – C(8)	107.73(11)
N(2) – C(12) – C(13)	124.87(15)
C(15) – C(16) – O(2)	116.20(12)
C(15) – C(16) – C(17)	120.32(13)
O(2) – C(16) – C(17)	123.48(13)
C(2) – N(1) – C(8)	110.76(10)
C(2) – N(1) – C(6)	107.96(10)
C(8) – N(1) – C(6)	107.83(10)
C(5) – C(4) – C(7)	109.76(12)
C(5) – C(4) – C(3)	107.39(13)
C(7) – C(4) – C(3)	108.65(11)
C(10) – C(3) – C(2)	112.27(13)
C(10) – C(3) – C(4)	113.69(13)
C(4) – C(3) – C(2)	106.46(11)
C(4) – C(5) – C(6)	108.34(11)
N(1) – C(2) – C(3)	111.40(11)
C(11) – C(10) – C(3)	178.04(17)
N(1) – C(6) – C(5)	110.46(11)
C(18) – C(17) – C(16)	119.91(13)
N(2) – C(20) – C(19)	122.99(13)

Table S8. Torsion angles [°] for 10,11-didehydroquinine and 10,11-didehydroquinidine.

10,11-ddQn	Mol A	Mol B	Mol C	Mol A	Mol B	Mol C
Temperature	296 K			120 K		
C(12) – C(13) –C(14) – C(19)	1.2(5)	0.9(5)	0.2(4)	1.0(6)	1.2(6)	-0.2(6)
C(13) – C(14) – C(19) – C1(5)	-179.1(3)	-180.0(3)	-179.6(3)	-179.2(4)	179.9(4)	-179.7(4)
C(14) – C(19) – C(15) – C(16)	-178.9(3)	177.2(3)	178.5(3)	-178.5(4)	177.7(4)	179.6(4)
C(19) – C(15) – C(16) – C(17)	-0.2(5)	0.7(5)	1.4(5)	0.5(6)	-0.3(7)	0.5(7)
C(20) – C(19) – C(14) – C(13)	0.6(4)	-1.2(4)	0.0(4)	1.0(6)	-1.7(6)	0.3(6)
C(19) – C(20) – C(18) – C(17)	0.8(5)	0.4(5)	0.6(5)	0.4(6)	0.9(7)	1.3(7)
C(15) – C(16) –C(17) – C(18)	-0.8(5)	0.8(6)	-0.8(6)	-1.9(7)	1.7(8)	0.4(7)
C(16) – C(17) – C(18) – C(20)	0.5(5)	-1.3(6)	-0.2(6)	1.4(7)	-2.0(8)	-1.2(7)
C(17) – C(18) – C(20) – N(2)	-178.9(3)	-178.4(3)	-178.8(3)	-179.2(4)	-178.7(5)	-179.0(4)
C(14) – C(19) – C(20) – N(2)	-1.7(4)	1.0(5)	-0.2(4)	-2.3(6)	1.5(6)	-0.1(6)
C(15) – C(19) – C(20) – N(2)	178.0(3)	179.8(3)	179.4(3)	177.9(4)	-180.0(4)	179.9(4)
N(2) – C(12) – C(13) –C(14)	-2.1(5)	-0.5(6)	-0.2(5)	-2.1(7)	-0.5(7)	0.0(7)
C(14) – C(19) – C(20) – C(18)	178.5(3)	-177.8(3)	-179.5(3)	178.1(4)	-178.1(4)	179.6(4)
C(15) – C(19) – C(20) – C(18)	-1.8(4)	1.0(5)	0.1(4)	-1.7(6)	0.4(6)	-0.4(6)
C(19) – C(20) – N(2) – C(12)	0.9(4)	-0.4(5)	0.3(4)	1.4(6)	-0.8(6)	-0.1(6)
C(20) – N(2) – C(12) – C(13)	1.0(5)	0.2(5)	-0.1(5)	0.9(6)	0.3(7)	0.2(6)
C(18) – C(20) – N(2) – C(12)	-179.3(3)	178.4(3)	179.5(3)	-179.0(4)	178.8(4)	-179.8(4)
C(20) – C(19) – C(15) – C(16)	1.5(4)	-1.5(5)	-1.1(4)	1.2(6)	-0.7(6)	-0.4(6)
C(20) – C(19) – C(14) – C(9)	178.6(3)	175.8(3)	179.6(3)	178.2(4)	174.2(4)	179.1(4)
C(21) – O(2) – C(16) – C(15)	0.6(5)	5.8(6)	10.2(6)	0.7(6)	6.5(7)	9.3(7)
C(21) – O(2) – C(16) – C(17)	-179.4(3)	-173.6(4)	-169.7(4)	-179.7(4)	-172.7(5)	-169.5(5)
C(12) – C(13) – C(14) – C(9)	-176.9(3)	-176.1(3)	-179.4(3)	-176.2(4)	-174.8(4)	-179.1(4)
C(13) – C(14) – C(9) – O(1)	-23.2(4)	-15.9(4)	-13.6(4)	-23.3(5)	-16.8(5)	-13.1(5)
C(19) – C(14) – C(9) – O(1)	158.8(3)	167.2(3)	166.8(3)	159.7(4)	167.3(4)	168.0(4)
C(15) – C(19) – C(14) – C(9)	-1.0(4)	-3.0(5)	0.0(4)	-2.0(6)	-4.2(6)	-0.9(6)
C(19) – C(15) – C(16) –O(2)	179.8(3)	-178.7(3)	-178.5(3)	-179.8(4)	-179.5(4)	-178.2(4)
O(2) – C(16) – C(17) – C(18)	179.2(3)	-179.8(4)	179.1(3)	178.4(4)	-179.1(5)	179.2(4)
C(13) – C(14) – C(9) – C(8)	97.9(3)	104.3(3)	108.3(3)	98.0(5)	104.3(5)	109.0(4)
C(19) – C(14) – C(9) – C(8)	-80.0(3)	-72.6(4)	-71.3(4)	-79.1(5)	-71.6(5)	-69.9(5)
C(2) – N(1) – C(8) – C(7)	64.0(3)	73.1(4)	70.1(4)	64.3(4)	73.6(5)	70.0(5)
C(6) – N(1) – C(8) – C(7)	-54.3(4)	-44.9(4)	-48.3(4)	-53.9(5)	-43.6(5)	-47.7(5)
C(2) –N(1) – C(8) – C(9)	-167.6(3)	-157.2(3)	-161.3(3)	-168.2(3)	-157.9(4)	-161.5(4)
C(6) – N(1) – C(8) – C(9)	74.2(3)	84.8(4)	80.3(3)	73.7(4)	85.0(5)	80.8(4)
C(4) – C(7) – C(8) – N(1)	-6.0(4)	-20.6(4)	-16.3(4)	-6.2(5)	-21.7(5)	-15.8(5)
C(9) – C(8) – C(7) – C(4)	-134.0(3)	-149.2(3)	-143.5(3)	-133.6(4)	-149.7(4)	-143.0(4)
C(14) – C(9) – C(8) – N(1)	158.3(3)	167.4(3)	156.8(3)	158.2(3)	169.5(4)	156.0(3)
O(1) – C(9) – C(8) –N(1)	-79.9(3)	-72.0(4)	-79.6(3)	-79.5(4)	-69.1(5)	-80.5(4)
C(7) – C(8) – C(9) – C(14)	-74.5(3)	-65.2(4)	-76.2(3)	-74.9(4)	-63.9(5)	-76.6(4)
O(1) – C(9) – C(8) – C(7)	47.3(3)	55.4(4)	47.3(4)	47.4(5)	57.5(5)	46.8(5)
C(8) – C(7) – C(4) – C(5)	62.7(4)	71.1(4)	68.1(4)	63.3(5)	71.7(5)	67.6(5)
C(8) – C(7) – C(4) – C(3)	-55.5(3)	-45.3(4)	-48.6(4)	-56.0(5)	-45.7(5)	-48.8(5)
C(11) – C(10) – C(3) – C(4)	-91(25)	98(8)	96(15)	14(27)	46(28)	97(11)
C(11) – C(10) – C(3) – C(2)	148(10)	-24(9)	-24(15)	-108(27)	-75(28)	-24(11)
C(5) – C(4) – C(3) – C(10)	176.9(3)	-177.6(4)	-176.1(3)	177.1(4)	-176.7(4)	-176.2(4)
C(7) – C(4) – C(3) – C(10)	-64.7(4)	-60.5(4)	-59.1(4)	-63.5(5)	-59.2(6)	-59.3(5)
C(5) – C(4) – C(3) – C(2)	-58.7(3)	-52.4(4)	-54.2(4)	-58.3(4)	-52.4(5)	-53.5(5)
C(7) – C(4) – C(3) – C(2)	59.7(3)	64.6(4)	62.8(4)	61.1(4)	65.1(5)	63.4(5)
C(6) – N(1) – C(2) – C(3)	60.9(3)	66.8(5)	66.3(4)	61.4(4)	68.0(6)	66.3(5)
C(8) – N(1) – C(2) – C(3)	-59.5(3)	-52.2(5)	-54.0(4)	-58.7(4)	-51.8(6)	-53.7(5)

C(10) – C(3) – C(2) – N(1)	122.4(4)	110.9(4)	114.5(4)	121.7(4)	109.7(5)	113.5(5)
C(4) – C(3) – C(2) – N(1)	-1.5(4)	-13.4(5)	-9.5(4)	-2.8(5)	-13.9(6)	-10.1(5)
C(2) – N(1) – C(6) – C(5)	-59.9(4)	-50.0(5)	-54.4(4)	-59.5(5)	-51.6(6)	-55.1(5)
C(8) – N(1) – C(6) – C(5)	58.5(4)	67.1(5)	63.6(4)	58.6(5)	65.1(6)	62.5(5)
C(7) – C(4) – C(5) – C(6)	-59.1(4)	-49.5(5)	-53.0(4)	-59.1(5)	-50.6(6)	-53.5(5)
C(3) – C(4) – C(5) – C(6)	60.3(4)	68.4(5)	66.0(4)	60.6(5)	68.3(5)	64.6(5)
N(1) – C(6) – C(5) – C(4)	-0.7(5)	-16.0(6)	-10.2(5)	-1.2(6)	-14.2(7)	-9.4(6)

Table S9.Torsion angles[º] for 10,11-didehydroquinidine.

C(12) – C(13) –C(14) – C(19)	-0.2(2)	C(19) – C(14) – C(9) – C(8)	82.21(14)
C(13) – C(14) – C(19) – C1(5)	179.21(13)	C(2) – N(1) – C(8) – C(7)	45.97(13)
C(14) – C(19) – C(15) – C(16)	179.31(13)	C(6) – N(1) – C(8) – C(7)	-71.98(12)
C(19) – C(15) – C(16) – C(17)	-0.7(2)	C(2) –N(1) – C(8) – C(9)	-82.32 (12)
C(20) – C(19) – C(14) – C(13)	-1.12(18)	C(6) – N(1) – C(8) – C(9)	159.73(10)
C(19) – C(20) – C(18) – C(17)	-1.3(2)	C(4) – C(7) – C(8) – N(1)	20.13 (14)
C(15) – C(16) –C(17) – C(18)	0.8(2)	C(9) – C(8) – C(7) – C(4)	146.87(11)
C(16) – C(17) – C(18) – C(20)	0.3(2)	C(14) – C(9) – C(8) – N(1)	-157.62(10)
C(17) – C(18) – C(20) – N(2)	178.64(14)	O(1) – C(9) – C(8) –N(1)	78.68(13)
C(14) – C(19) – C(20) – N(2)	1.70(19)	C(7) – C(8) – C(9) – C(14)	76.63(13)
C(15) – C(19) – C(20) – N(2)	-178.60(12)	O(1) – C(9) – C(8) – C(7)	-47.08(14)
N(2) – C(12) – C(13) –C(14)	1.0(3)	C(8) – C(7) – C(4) – C(5)	46.19 (14)
C(14) – C(19) – C(20) – C(18)	-178.36(12)	C(8) – C(7) – C(4) – C(3)	-70.97(14)
C(15) – C(19) – C(20) – C(18)	1.33(19)	C(11) – C(10) – C(3) – C(4)	-105(6)
C(19) – C(20) – N(2) – C(12)	-0.9(2)	C(11) – C(10) – C(3) – C(2)	134(6)
C(20) – N(2) – C(12) – C(13)	-0.6(3)	C(5) – C(4) – C(3) – C(10)	166.98(12)
C(18) – C(20) – N(2) – C(12)	179.20(15)	C(7) – C(4) – C(3) – C(10)	-74.36 (14)
C(20) – C(19) – C(15) – C(16)	-0.36(19)	C(5) – C(4) – C(3) – C(2)	-68.88(14)
C(20) – C(19) – C(14) – C(9)	178.59(11)	C(7) – C(4) – C(3) – C(2)	49.77(15)
C(21) – O(2) – C(16) – C(15)	172.83(15)	C(6) – N(1) – C(2) – C(3)	50.07(15)
C(21) – O(2) – C(16) – C(17)	-7.7(2)	C(8) – N(1) – C(2) – C(3)	-67.78(14)
C(12) – C(13) – C(14) – C(9)	-179.82(14)	C(10) – C(3) – C(2) – N(1)	141.03(12)
C(13) – C(14) – C(9) – O(1)	25.22(17)	C(4) – C(3) – C(2) – N(1)	16.02(16)
C(19) – C(14) – C(9) – O(1)	-154.48(11)	C(2) – N(1) – C(6) – C(5)	-68.76(15)
C(15) – C(19) – C(14) – C(9)	-1.09(19)	C(8) – N(1) – C(6) – C(5)	50.97(15)
C(19) – C(15) – C(16) –O(2)	178.76(12)	C(7) – C(4) – C(5) – C(6)	-66.27(15)
O(2) – C(16) – C(17) – C(18)	-178.65(14)	C(3) – C(4) – C(5) – C(6)	51.68(15)
C(13) – C(14) – C(9) – C(8)	-98.09(15)	N(1) – C(6) – C(5) – C(4)	15.07(17)

Table S10. Hydrogen bonds for 10,11-didehydroquinine in 120 K [Å and °].

D-H···A	H···A	D···A	D-H···A
O(1) – H(1)···N(2B)	1.978	2.786(5)	168.05
O(1B) – H(1B)···N(2C)^{i}	1.939	2.758(5)	177.03
O(1C) – H(1C)···N(2)^{i}	1.956	2.775(5)	173.31

Symmetry codes: (i)=-1+x,y,z; (ii)= -x,1/2+y,1.5-z

References

1 K. M. Kacprzak, W. Linder, N. M. Maier, *Chirality*, 2008, **20**, 441-445
2 C. F. Macrae, P. R. Edgington, P. McCabe, E. Pidcock, G. P. Shields, R. Taylor, M. Towler, J. van de Streek, *J. Appl. Crystallogr.* 2006, **39**, 453–457.