

**Synthesis, molecular structure and biological activity
of novel bis-1,3-tropolones based on 4-chloro-2,7-dimethyl-1,8-naphthyridine**

Evgeniy A. Gusakov, Yurii A. Sayapin, Elena V. Vetrova, Ekaterina A. Lukbanova,
Ekaterina V. Alilueva, Alexandra A. Kolodina, Valery V. Tkachev, Inna O. Tupaeva,
Anton V. Lisovin, Dmitry V. Steglenko, Tatyana A. Krasnikova, Mikhail V. Nikogosov,
Anna S. Goncharova, Anatoly V. Metelitsa, Sergey M. Aldoshin and Vladimir I. Minkin

Content	
Experimental	S3
Methods and materials	S3
Synthesis of 1,3-tropolones 3 , 5-7 (method i)	S3
Synthesis of 1,3-tropolones 5-7 (method ii)	S5
<i>NMR studies</i>	S6
Figure S1 The assignment of chemical shifts in the ^1H , ^{13}C , ^{15}N NMR spectra of compound 3 in CDCl_3	S6
Figure S2 Scheme of NOESY correlations of compound 6	S6
Figure S3 The assignment of chemical shifts signals in the ^1H , ^{13}C , and ^{15}N NMR spectra of compound 6 in CDCl_3	S7
Figure S4 Scheme of correlations of HMBC COSY compound 5	S7
Table S1 Coordinates of cross-peaks in the ^1H - ^{13}C HMQC and HMBC spectra of compound 5	S8
Figure S5 ^1H NMR spectrum of compound 3 in CDCl_3	S9
Figure S6 ^{13}C NMR spectrum of compound 3 in CDCl_3	S10
Figure S7 ^1H NMR spectrum of compound 5 in CDCl_3	S11
Figure S8 ^{13}C NMR spectrum of compound 5 in CDCl_3	S12
Figure S9 ^1H NMR spectrum of compound 6 in CDCl_3	S13
Figure S10 ^{13}C NMR spectrum of compound 6 in CDCl_3	S14
Figure S11 ^1H NMR spectrum of compound 7 in CDCl_3	S15
Figure S12 ^{13}C NMR spectrum of compound 7 in CDCl_3	S16
Figure S13 IR spectrum of compound 3	S17
Figure S14 IR spectrum of compound 5	S18
Figure S15 IR spectrum of compound 6	S19
Figure S16 IR spectrum of compound 7	S20
<i>X-ray diffraction analysis</i>	S21
Figure S17 Molecular structure of compound 5	S21
Table S2 Crystal data and structure refinement for 5	S21
Table S3 Bond lengths for compound 5	S22
Table S4 Bond angles for compound 5	S23
Table S5 Torsion angles for compound 5	S24
Figure S18 Molecular structure of 7	S26
Table S6 Crystal data and structure refinement for 7	S26
Table S7 Bond lengths for compound 7	S27
Table S8 Bond angles for compound 7	S28
Table S9 Torsion angles for compound 7	S30

<i>UV-vis and photoluminescence data</i>	S31
Table S10 UIV-Vis and photoluminescence data for compounds 5 and 7 in different solvent sand in solid state	S32
Figure S19 Absorption, emission and excitation spectra for 5 in heptane and toluene	S33
Figure S20 Absorption, emission and excitation spectra for 5 in chloroform and THF	S34
Figure S21 Absorption, emission and excitation spectra for 5 in acetonitrile and ethanol	S35
Figure S22 Absorption 5 in different solvents	S36
Figure S23 Absorption, emission and excitation spectra for 7 in heptane and toluene	S37
Figure S24 Absorption, emission and excitation spectra for 7 in THF and in acetonitrile	S38
Figure S25 Absorption, emission and excitation spectra for 7 in ethanol	S39
Figure S26 Absorption 7 in different solvents	S39
<i>Computational methods</i>	S40
Figure S27 Optimized structures of (NH) and (OH) isomers of tropolone 3	S40
Table S11 Optimized geometries of tropolone 3 isomers (gas)	S40
Table S12 Optimized geometries of tropolone 3 isomers (DMSO)	S41
Figure S28 Optimized structures of tropolone 5 isomers	S43
Table S13 Optimized geometries of tropolone 5 isomers (gas)	S43
Table S14 Optimized geometries of tropolone 5 isomers (DMSO)	S46
Figure S29 Optimized structures of tropolone 6 isomers	S50
Table S15 Optimized geometries of tropolone 6 isomers (gas)	S50
Table S16 Optimized geometries of tropolone 6 isomers (DMSO)	S53
Figure S30 Optimized structures of tropolone 7 isomers	S57
Table S17 Optimized geometries of tropolone 7 isomers (gas)	S57
Table S18 Optimized geometries of tropolone 7 isomers (DMSO)	S60
<i>Biologic studies</i>	S64
Table S19 Cytotoxic activity <i>in vitro</i> of bistropolone 7	S65
Figure S31 IC50 curves for the cell lines studied with bistropolone 7	S66
<i>References</i>	S67

Experimental

Methods and materials

The ^1H , ^{13}C , ^{15}N NMR spectra were recorded on a Bruker Avance 600 spectrometer. The chemical shifts are given with respect to the signal of SiMe_4 , using the solvent signal as an internal standard. Attenuated total internal reflectance IR (ATR-IR) spectra were measured on a Varian 3100 FT-IR Excalibur Series spectrometer. IR, NMR and electronic spectra were recorded using the equipment of the “Molecular Spectroscopy” Center for collective use of the Southern Federal University. HRMS were registered on a Bruker UHR-TOF MaxisTM Impact instrument. Chromatography was performed on columns packed with Al_2O_3 (Brockmann activity II—III). The melting point was measured on a Fisher—Johns apparatus. The reaction were provided in glacial acetic acid (99.4%), CAS 64-19-7 (Alfa Aesar). 4-Chloro-2,7-dimethyl-1,8-naphthyridine **1** and of 4,6-di-*tert*-butyl-3-nitro-1,2-benzoquinone **2** were obtained according to the described methods.^{S1,S2}

Synthesis of 5,7-di-*tert*-butyl-2-(4-chloro-7-methyl-1,8-naphthyridin-2-yl)-3-hydroxy-4-nitrotropone (3), 2,2'-(4-chloro-1,8-naphthyridin-2,7-diyl)bis(5,7-di-*tert*-butyl-3-hydroxytropone) (5), 5,7-di-*tert*-butyl-2-[5-chloro-7-(5,7-di-*tert*-butyl-3-hydroxy-cyclohepta-2,4,6-trienon-2-yl)-1,8-naphthyridin-2-yl]-3-hydroxy-4-nitrotropone (6) and 2,2'-(4-chloro-1,8-naphthyridin-2,7-diyl)bis(5,7-di-*tert*-butyl-3-hydroxy-4-nitrotropone) (7) (method i).

A solution of 4-chloro-2,7-dimethyl-1,8-naphthyridine **1** (1.93 g, 10 mmol) and of 4,6-di-*tert*-butyl-3-nitro-1,2-benzoquinone **2** (5.3 g, 20 mmol) in glacial acetic acid (30 ml) was heated at 80 °C for 25 h. After cooled to the room temperature, the reaction mixture was diluted with water and extracted with dichloromethane (100 ml + 2×50 ml). The combined organic layers were washed with water (2×100 ml) and then dried with anhydrous Na_2SO_4 and the solvent was removed *in vacuo*. The residue was purified by alumina column chromatography with petroleum/dichloromethane (1:2) collecting the first orange fraction, the second yellow fraction, the third and fourth orange fractions. The first fraction is compound **5** ($R_f \sim 0.9$), the second fraction is compound **3** ($R_f \sim 0.6$), the third fraction is compound **6** ($R_f \sim 0.3$), the fourth fraction is compound **7** ($R_f \sim 0.1$) (eluent – petroleum/dichloromethane (1:2)). After removal of the solvent *in vacuo*, the residues were recrystallized from propane-2-ol.

5,7-Di-*tert*-butyl-2-(4-chloro-7-methyl-1,8-naphthyridin-2-yl)-3-hydroxy-4-nitrotropone (3).

Yellow crystals. Yield (4%), mp 241 °C. IR (v): 3074, 2955, 2913, 2869, 1673, 1600, 1568, 1538, 1515, 1477, 1461, 1353, 1329, 1312, 1275, 1251, 1156, 1132, 1104, 1062, 1041, 964, 901, 884, 867, 817, 801, 781, 767, 732. 689, 668, 646, 600, 574, 535 cm^{-1} . ^1H NMR (600 MHz, CDCl_3) δ , ppm: 1.27 (s, 9H, $\text{Bu}^t(5)$), 1.27 (s, 9H, $\text{Bu}^t(7)$), 2.69 (s, 3H, Me), 6.31 (s, 1H, H(6)), 7.33 (d, 1H, H_{Ar} , $J = 3.6$ Hz), 8.22 (d, 1H, H_{Ar} , $J = 3.6$ Hz), 8.24 (s, 1H, H_{Ar}), 17.04 (s, 1H, OH(3)). ^{13}C NMR (151 MHz, CDCl_3) δ , ppm: 25.3, 29.4, 30.3, 37.2, 37.9, 114.0, 116.2, 118.8, 118.9, 122.8, 133.3,

142.8, 145.1, 146.8, 150.4, 152.3, 153.9, 165.5, 177.0, 194.5. HRMS (ESI) calcd. for $C_{38}H_{45}ClN_2O_4$ requires 455.9400 m/z ; found 478.1506 m/z $[M + Na]^+$. Calcd. for $C_{24}H_{26}ClN_3O_4$ (%): C 63,22; H 5,75; N 9,22 Found (%): C 63,08; H 5,62; N 9,06.

2,2'-(4-Chloro-1,8-naphthyridin-2,7-diyl)bis(5,7-di-*tert*-butyl-3-hydroxytropone) (5). Orange crystals. Yield (6%), mp. 304 °C. IR (ν): 3114, 3062, 2952, 2902, 2864, 1647, 1583, 1532, 1509, 1487, 1458, 1379, 1360, 1327, 1281, 1246, 1199, 1177, 1138, 1099, 1015, 1000, 980, 962, 932, 919, 875, 836, 818, 795727, 696, 631, 557 cm^{-1} . 1H NMR (600 MHz, $CDCl_3$) δ , ppm: 1.25 (s, 18H, $Bu^t(5,5')$), 1.38 (s, 9H, $Bu^t(7)$), 1.38 (s, 9H, $Bu^t(7')$), 6.64 (d, 1H, H(4), $J = 1.8$ Hz), 6.65 (d, 1H, H(4'), $J = 1.8$ Hz), 6.78 (d, 1H, H(6'), $J = 1.8$ Hz), 6.79 (d, 1H, H(6), $J = 1.8$ Hz), 8.11 (d, 1H, H_{Ar} , $J = 3.6$ Hz), 8.14 (s, 1H, H(3'')), 8.31 (d, 1H, H_{Ar} , $J = 3.6$ Hz), 17.51 (s, 1H, OH(3)), 17.57 (s, 1H, OH(3')). ^{13}C NMR (151 MHz, $CDCl_3$) δ , ppm: 28.7, 29.6, 29.7, 29.9, 31.1, 37.3, 38.3, 38.4, 106.9, 114.7, 115.2, 117.1, 120.2, 121.2, 123.4, 123.5, 123.6, 123.7, 133.50 143.0, 147.9, 155.5, 155.5, 155.6, 158.8, 160.0, 171.8, 171.8, 194.7, 194.9. HRMS (ESI) calcd. for $C_{38}H_{45}ClN_2O_4$ requires 629.2464 m/z ; found 651.2961 m/z $[M + Na]^+$. Calcd. for $C_{38}H_{45}ClN_2O_4$ (%): C 72,53; H 7,21; N 4,45. Found (%): C 72,42; H 7,10; N 4,34.

5,7-Di-*tert*-butyl-2-[5-chloro-7-(5,7-di-*tert*-butyl-3-hydroxy-cyclohepta-2,4,6-trienon-2-yl)-1,8-naphthyridin-2-yl]-3-hydroxy-4-nitrotropone (6). Orange crystals. Yield (7%), mp. 286 °C. IR (ν): 3125, 2957, 2905, 2869, 1656, 1603, 1579, 1540, 1497, 1461, 1359, 1314, 1270, 1238, 1199, 1182, 1148, 1100, 982, 958, 914, 870 ,849, 814, 730, 633, 601, 578 cm^{-1} . 1H NMR (600 MHz, $CDCl_3$) δ , ppm: 1.27 (s, 9H, $Bu^t(5)$), 1.29 (s, 9H, $Bu^t(7')$), 1.31 (s, 9H, $Bu^t(5')$), 1.39 (s, 9H, $Bu^t(7)$), 6.40 (s, 1H, H(6')), 6.67 (s, 1H, H(4)), 6.85 (s, 1H, H(6)), 8.14 (d, 1H, H(6''), $J = 3.6$ Hz), 8.15 (s, 1H, H(3'')), 8.31 (d, 1H, H_{Ar} , $J = 3.6$ Hz), 15.84 (s, 1H, OH(3)), 17.95 (s, 1H, OH(3')). ^{13}C NMR (151 MHz, $CDCl_3$) δ , ppm: 29.0, 29.9, 30.3, 31.1, 37.5, 37.93, 38.5, 114.8, 114.9, 116.4, 119.4, 120.2, 120.7, 122.8, 123.9, 134.7, 143.0, 143.8, 145.2, 149.5, 154.1, 154.2, 155.8, 156.7, 159.6, 169.6, 174.3, 194.3, 194.4. HRMS (ESI) calcd. for $C_{38}H_{44}ClN_3O_6$ requires 674.2439 m/z ; found 696.2823 m/z $[M + Na]^+$. Calcd. for $C_{38}H_{44}ClN_3O_6$ (%): C 67,69; H 6,58; N 6,23. Found (%): C 67,54; H 6,46; N 6,12.

2,2'-(4-Chloro-1,8-naphthyridin-2,7-diyl)bis(5,7-di-*tert*-butyl-3-hydroxy-4-nitrotropone) (7). Orange crystals. Yield (10%), mp. 306 °C. IR (ν): 3125, 2957, 2908, 2870, 1661, 1637, 1607, 1540, 1494, 1463, 1362, 1270, 1198, 1181, 1148, 1126, 1101, 1021, 989, 964, 886, 871, 834, 812, 792, 749, 730, 677, 648, 635, 600, 577, 540 cm^{-1} . 1H NMR (600 MHz, $CDCl_3$) δ , ppm: 1.28-1.30 (m, 36H, $Bu^t(5,5',7,7')$), 6.50 (s, 1H, H(6')), 6.50 (s, 1H, H(6)), 8.12 (d, 1H, H_{Ar} , $J = 3.6$ Hz), 8.16 (s, 1H, H(3'')), 8.34 (d, 1H, H_{Ar} , $J = 3.6$ Hz), 17.23 (s, 1H, OH(3)), 17.28 (s, 1H, OH(3')). ^{13}C NMR (151 MHz, $CDCl_3$) δ , ppm: 28.7, 29.1, 30.4, 37.8, 38.0, 38.1, 115.5, 116.0, 116.7, 119.8, 120.3, 120.3, 120.5, 120.6, 120.7, 120.9, 129.7, 134.5, 134.7, 144.3, 144.4, 144.7, 145.2, 147.9,

154.4, 154.5, 155.0, 156.1, 168.5, 193.7, 193.9. HRMS (ESI) calcd. for $C_{38}H_{43}ClN_4O_8$ requires 719.2414 m/z ; found 741.2652 m/z $[M + Na]^+$. Calcd. for $C_{38}H_{43}ClN_4O_8$ (%): C 63,46; H 6,03; N 7,79. Found (%): C 63,32; H 5,94; N 7,68.

Synthesis of 2,2'-(4-chloro-1,8-naphthyridin-2,7-diyl)bis(5,7-di-*tert*-butyl-3-hydroxytropone) (5), 5,7-di-*tert*-butyl-2-[5-chloro-7-(5,7-di-*tert*-butyl-3-hydroxy-cyclohepta-2,4,6-trienon-2-yl)-1,8-naphthyridin-2-yl]-3-hydroxy-4-nitrotropone (6) and 2,2'-(4-chloro-1,8-naphthyridin-2,7-diyl)bis(5,7-di-*tert*-butyl-3-hydroxy-4-nitrotropone) (7) (method ii).

A solution of 2,7-dimethyl-4-chloro-1,8-naphthyridine **1** (1.93 g, 10 mmol) and of 4,6-di-*tert*-butyl-3-nitro-1,2-benzoquinone **2** (10.6 g, 40 mmol) in glacial acetic acid (60 ml) was heated at 80 °C for 45 h. After cooled to the room temperature, the reaction mixture was diluted with water and extracted with dichloromethane (150 ml + 2×100 ml). The combined organic layers were washed with water (3×100 ml) and then dried with anhydrous Na_2SO_4 and the solvent was removed *in vacuo*. The residue was purified by alumina column chromatography with petroleum/dichloromethane (1:2) collecting the first orange fraction, the second and third orange fractions. The first fraction is compound **5** ($R_f \sim 0.9$), the second fraction is compound **6** ($R_f \sim 0.3$), the third fraction is compound **7** ($R_f \sim 0.1$). After removal of the solvent *in vacuo*, the residues were recrystallized from propane-2-ol.

2,2'-(4-Chloro-1,8-naphthyridin-2,7-diyl)bis(5,7-di-*tert*-butyl-3-hydroxytropone) (5). Orange crystals. Yield (15%), mp. 304 °C.

5,7-Di-*tert*-butyl-2-[5-chloro-7-(5,7-di-*tert*-butyl-3-hydroxy-cyclohepta-2,4,6-trienon-2-yl)-1,8-naphthyridin-2-yl]-3-hydroxy-4-nitrotropone (6). Orange crystals. Yield (18%), mp. 286 °C.

2,2'-(4-Chloro-1,8-naphthyridin-2,7-diyl)bis(5,7-di-*tert*-butyl-3-hydroxy-4-nitrotropone) (7). Orange crystals. Yield (25%), mp. 306 °C.

NMR studies

For establishing the structure of 5,7-di-*tert*-butyl-2-(4-chloro-7-methyl-1,8-naphthyridin-2-yl)-3-hydroxy-4-nitrotropone **3** (Figure S1), and also unsymmetrical 5,7-di-*tert*-butyl-2-[5-chloro-7-(3-hydroxy-5,7-di-*tert*-butyl-cyclohepta-2,4,6-trienon-2-yl)-1,8-naphthyridin-2-yl]-3-hydroxy-4-nitrotropone **6**, a complete assignment of the ^1H and ^{13}C NMR spectra signals was carried out based on the characteristic values of chemical shifts and analysis of cross-peaks in the two-dimensional ^1H - ^1H correlations spectra (COSY, NOESY) (Figure S2) and in two-dimensional heterocorrelation spectra ^1H - ^{13}C and ^1H - ^{15}N (Figure S3). The ^1H - ^{15}N HMBC spectrum of compound **3** contains cross peaks of the nitrogen atom N(8'') at 287.3 ppm. with protons of the methyl group δ_{H} 2.69 ppm. and H(6') δ_{H} 7.33 ppm.

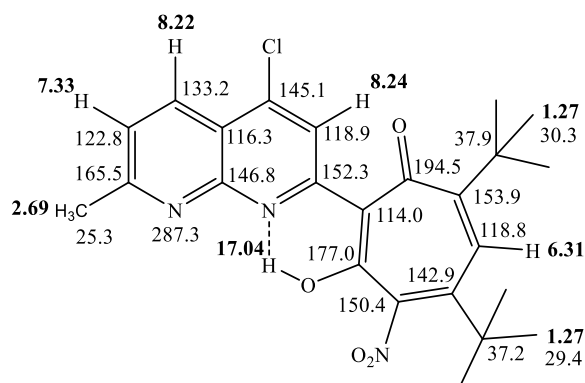


Figure S1 The assignment of chemical shifts in the ^1H , ^{13}C , ^{15}N NMR spectra of compound **3** in CDCl_3 .

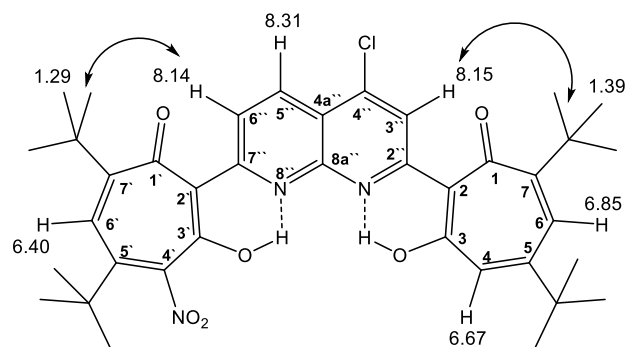


Figure S2 Scheme of NOESY correlations of compound **6**.

The 4-nitro-1,3-tropolone ring of compound **6** in solution exists in the $\text{C}=\text{O}\cdots\text{NH}$ -tautomeric form with localization of the proton on the pyridine nitrogen of naphthyridine, forming a six-membered chelate ring with a strong intramolecular hydrogen bond with the carbonyl of the tropolone ring, about which indicate: shift of the NH proton to an extremely weak field of 17.95 ppm in the ^1H NMR spectra and a shift of the carbonyl carbon of the tropolone ring by 20 ppm in a high field compared to free carbonyl in the ^{13}C NMR spectra. The ^1H - ^{15}N HMBC spectrum of compound **6** contains cross peaks of the nitrogen atom N(8'') at 173.4 ppm with the NH proton δ_{H} 17.95 ppm and H(6'') δ_{H} 8.14 ppm, and in the ^1H - ^{13}C HMBC spectrum there are cross peaks of the NH proton δ_{H} 17.95 ppm with atoms C(6''), C(4'a), C(2') at δ_{H} 120.2, 116.4, 114.9 ppm, respectively (Figure S3).

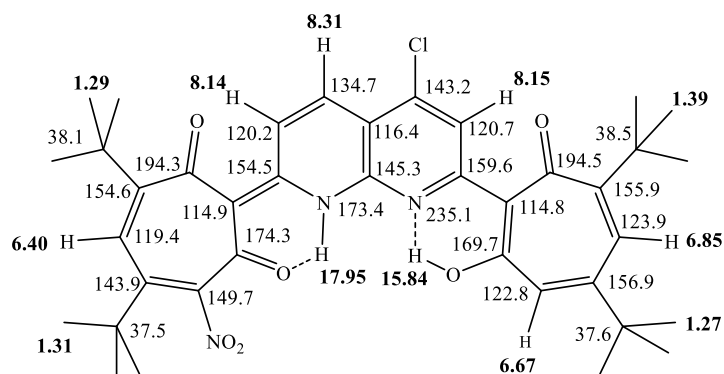


Figure S3 The assignment of chemical shifts signals in the ^1H , ^{13}C , and ^{15}N NMR spectra of compound **6** in CDCl_3 based on two-dimensional correlation spectroscopy data.

The cross-peak coordinates of the ^1H - ^{13}C heteronuclear correlation spectra HMQC and HMBC of compound **5** are given in Table S1. These data are the basis for the complete assignment of signals in the ^{13}C spectrum, as well as the final interpretation of the ^1H spectrum signals. The most important HMBC correlations for the analysis of structure **5** are schematically depicted in Figure S4.

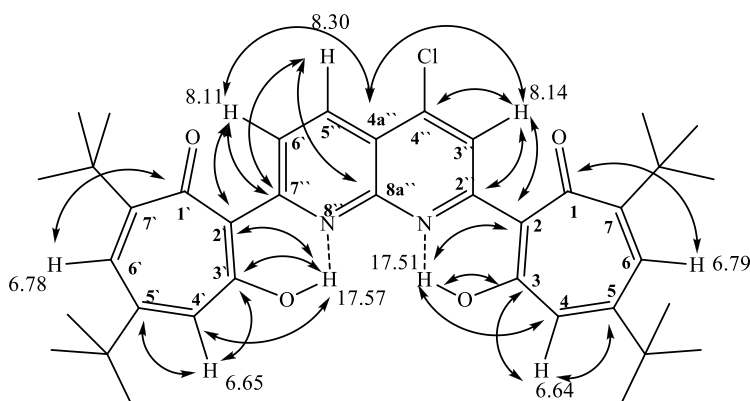


Figure S4 Scheme of correlations of HMBC COSY 2,2'-(4-chloro-1,8-naphthyridin-2,7-diyl)bis(5,7-di-*tert*-butyl-3-hydroxytropone) **5**.

Table S1 Coordinates of cross-peaks in the ^1H - ^{13}C HMQC and HMBC spectra of compound 5.

^1H signal, δ , ppm	Cross-peaks in the ^{13}C , δ , ppm	
	HMQC	HMBC
17.57 (O(3')H $\cdots$ N)	-	171.8 (C3'), 123.70 (C4'), 115.2 (C2')
17.51 (O(3)H $\cdots$ N)	-	171.7 (C3), 123.67 (C4), 114.8 (C2)
8.30 (H5'')	133.5	160.0 (C7''), 148.0 (C8''a), 143.0 (C4''), 121.2. (C6'')
8.14 (H3'')	120.2	158.8. (C2''), 143.0 (C4''), 117.1 (C4''a), 114.8. (C2)
8.11 (H6'')	121.2	160.0 (C7''), 133.5 (C5''), 117.1 (C4''a), 115.2 (C2')
6.79 (H6)	123.5	194.7 (C1), 155.7 (C7), 123.67 (C4), 38.4 (C7' <u>C</u> (CH ₃) ₃)
6.78 (H6')	123.4	194.9 (C1'), 155.7 (C7'), 123.70 (C4'), 38.4 (C7' <u>C</u> (CH ₃) ₃)
6.65 (H4')	123.7	171.8 (C3'), 155.49 (C5'), 123.4 (C6'), 37.3 (C5' <u>C</u> (CH ₃) ₃)
6.64 (H4)	123.7	171.7 (C3), 155.55 (C5), 123.5 (C6), 37.3 (C5' <u>C</u> (CH ₃) ₃)
1.38 (C7/7' <u>C</u> (CH ₃) ₃)	29.9	155.7 (C7/7'), 38.4 (C7/7' <u>C</u> (CH ₃) ₃)
1.25 (C5/5' <u>C</u> (CH ₃) ₃)	31.1	155.6 (C5/5'), 37.3 (C5/5' <u>C</u> (CH ₃) ₃)

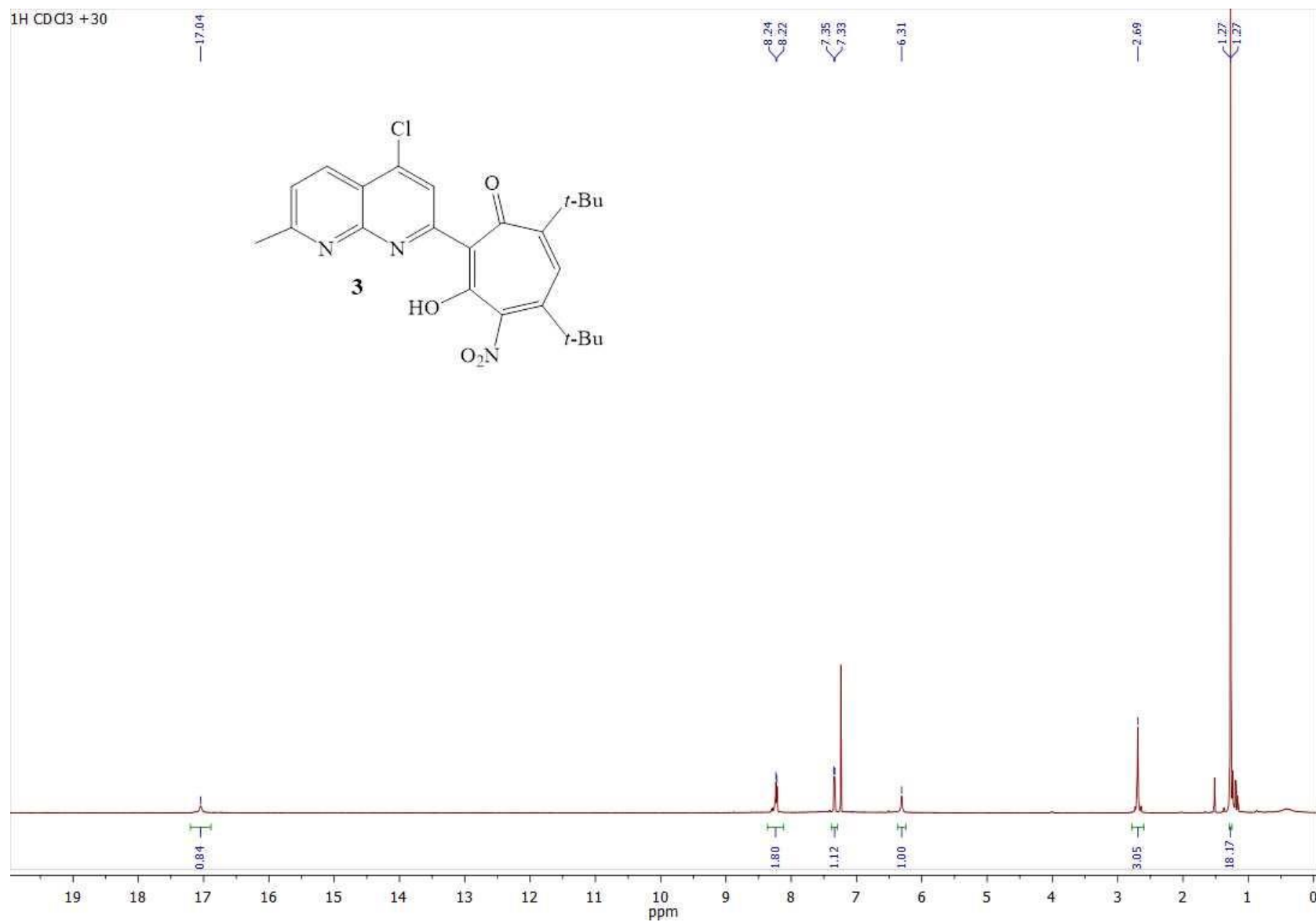


Figure S5 ¹H NMR spectrum of compound **3** in CDCl₃.

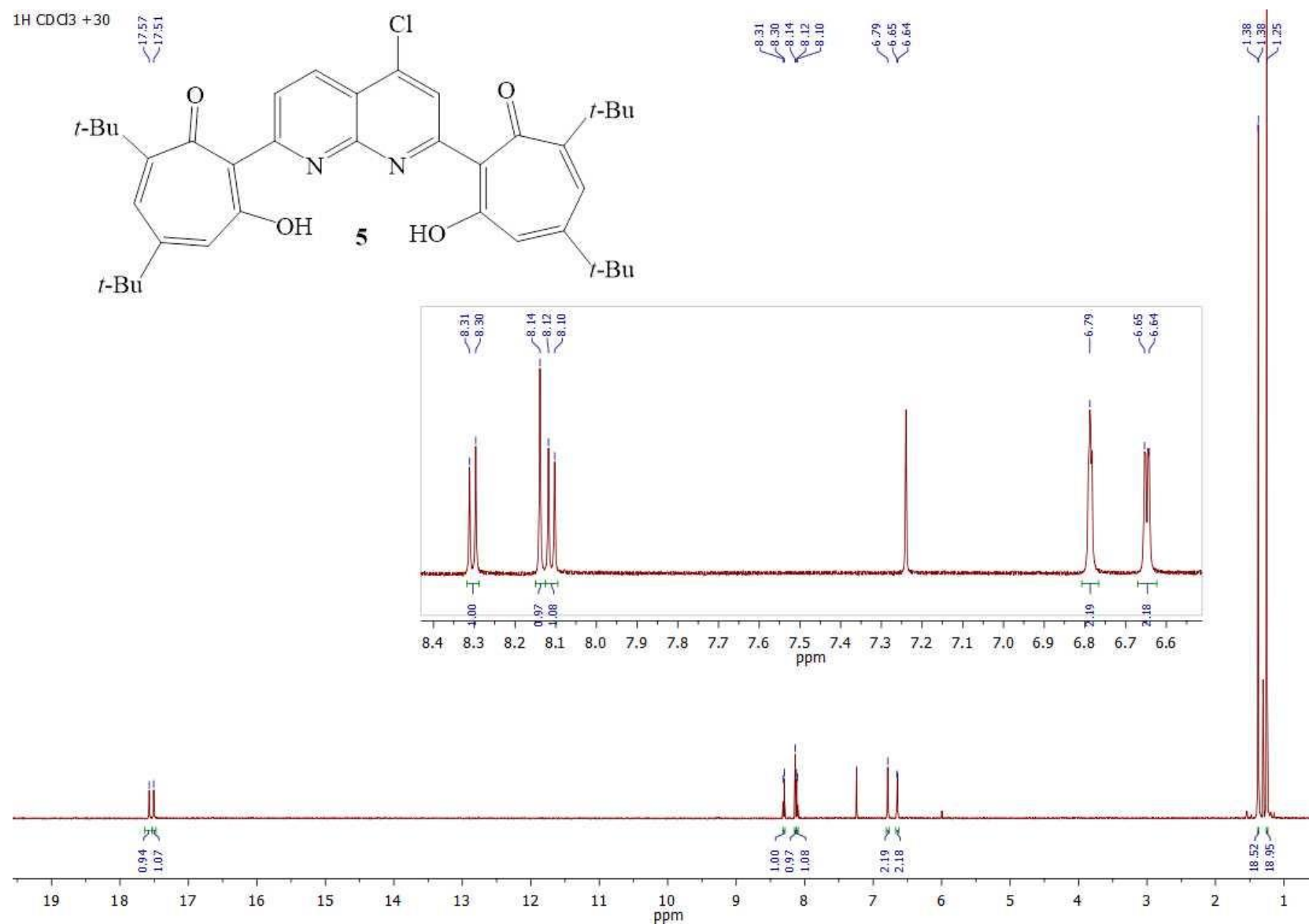


Figure S7 ¹H NMR spectrum of compound **5** in CDCl₃.

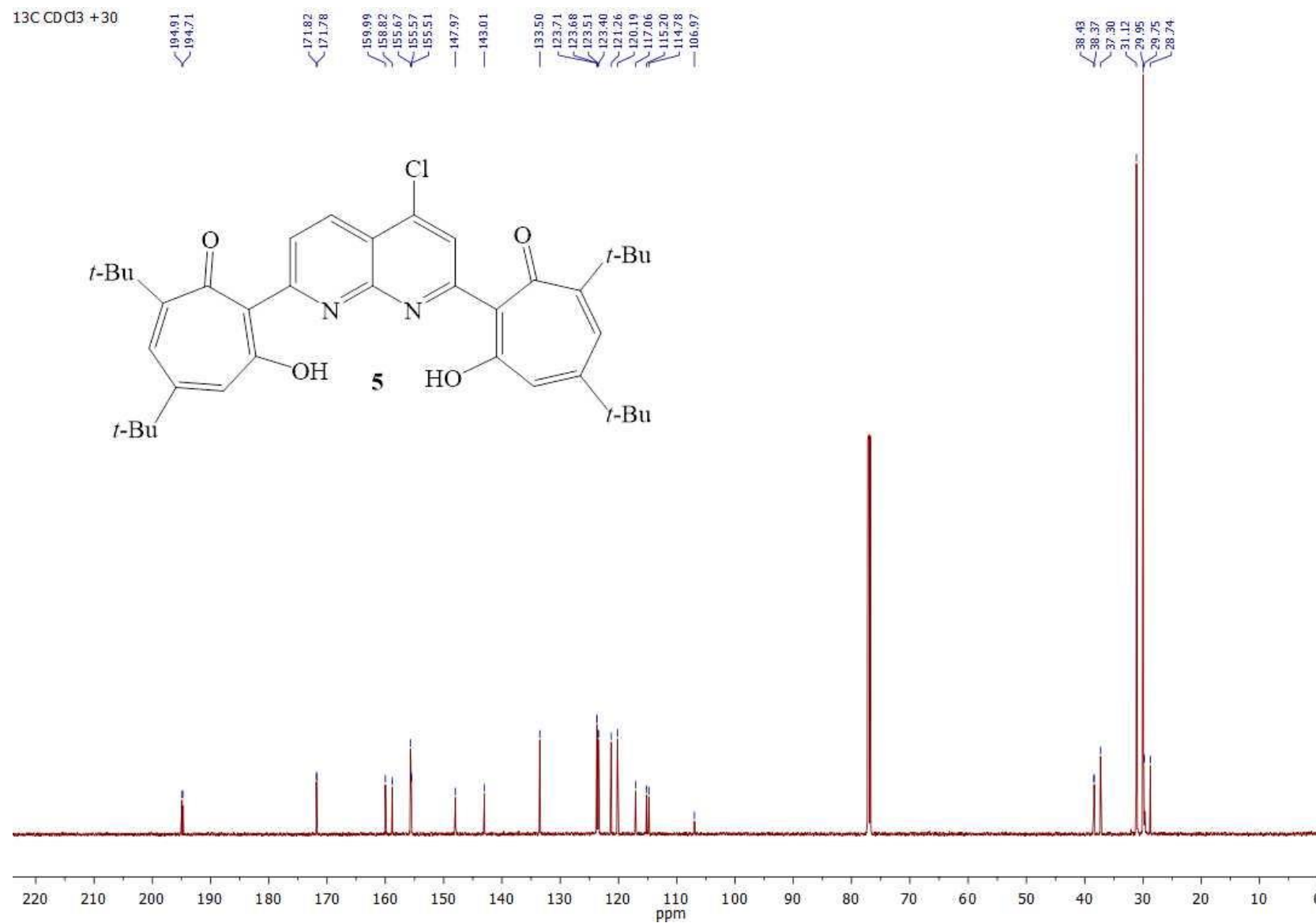


Figure S8 ¹³C NMR spectrum of compound **5** in CDCl₃.

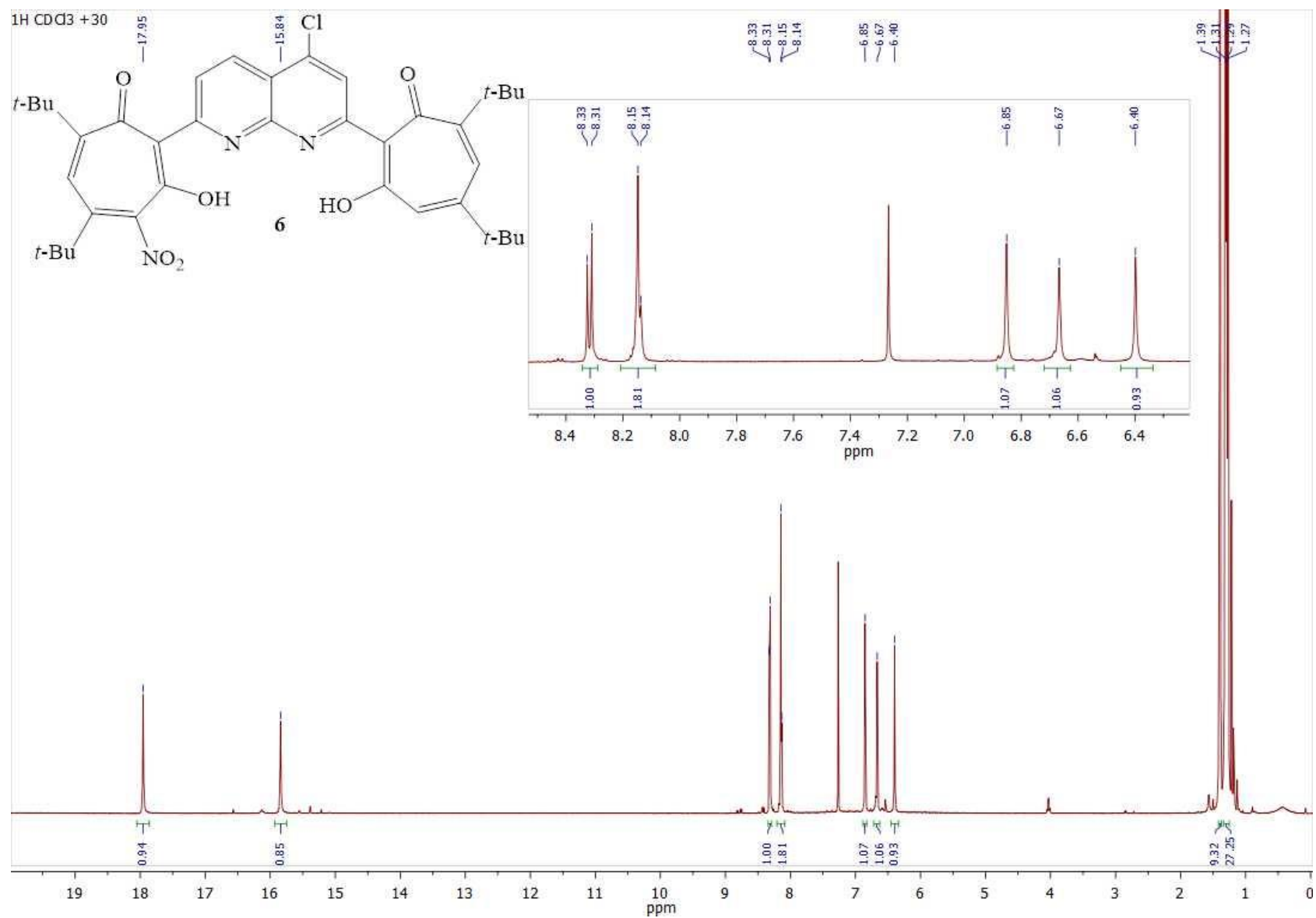


Figure S9 ¹H NMR spectrum of compound **6** in CDCl₃.

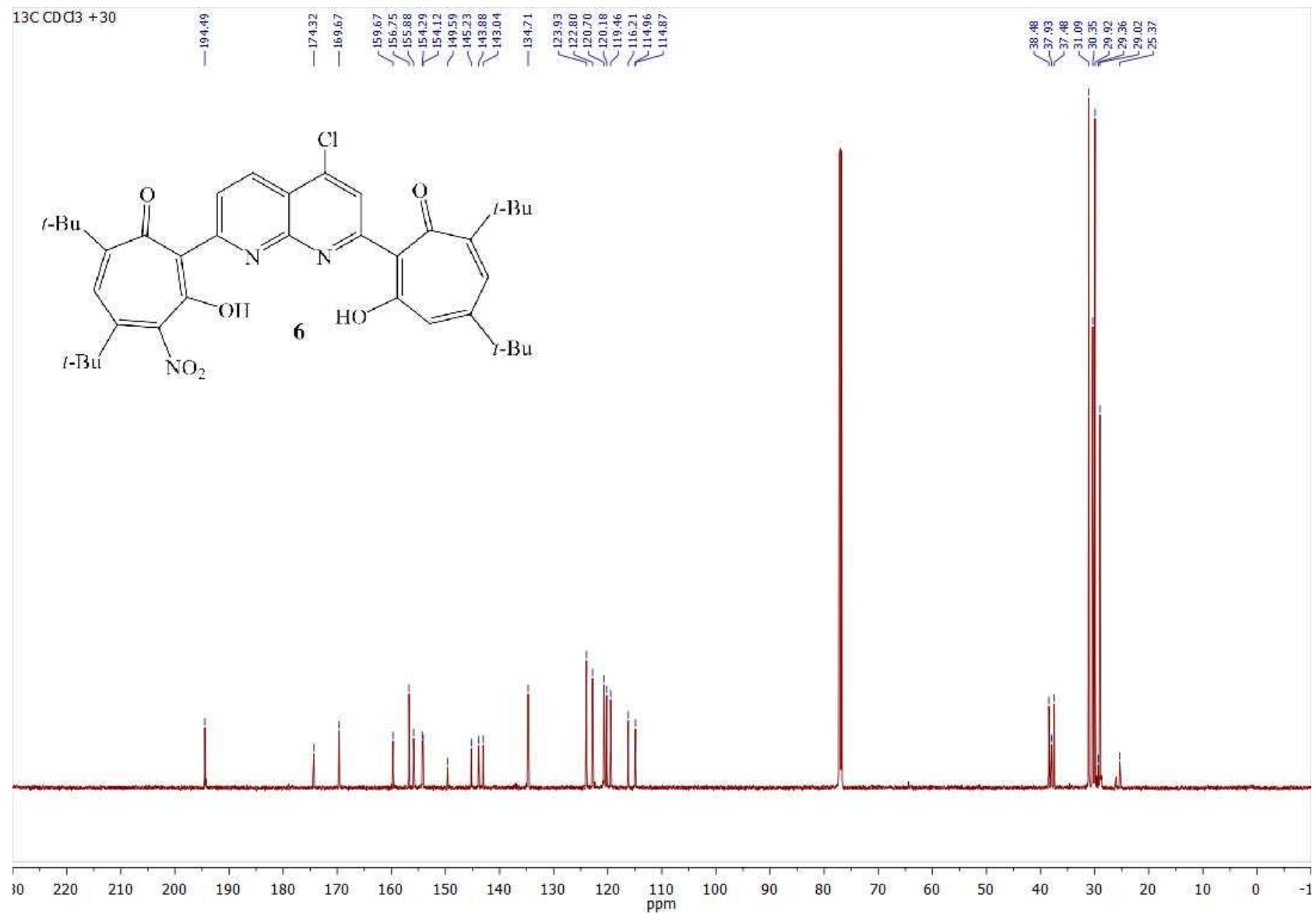


Figure S10 ¹³C NMR spectrum of compound **6** in CDCl₃.

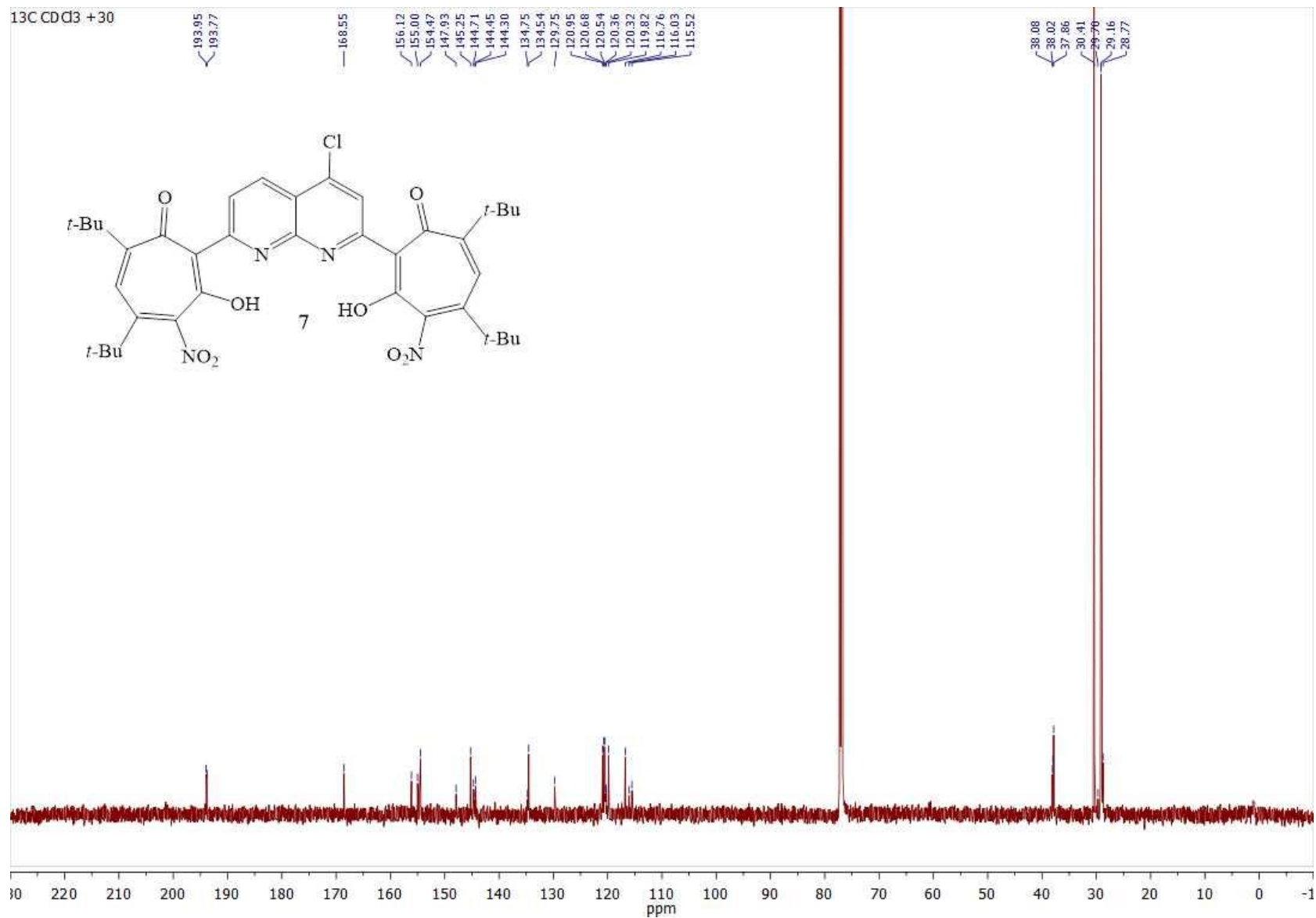


Figure S12 ¹³C NMR spectrum of compound 7 in CDCl₃.

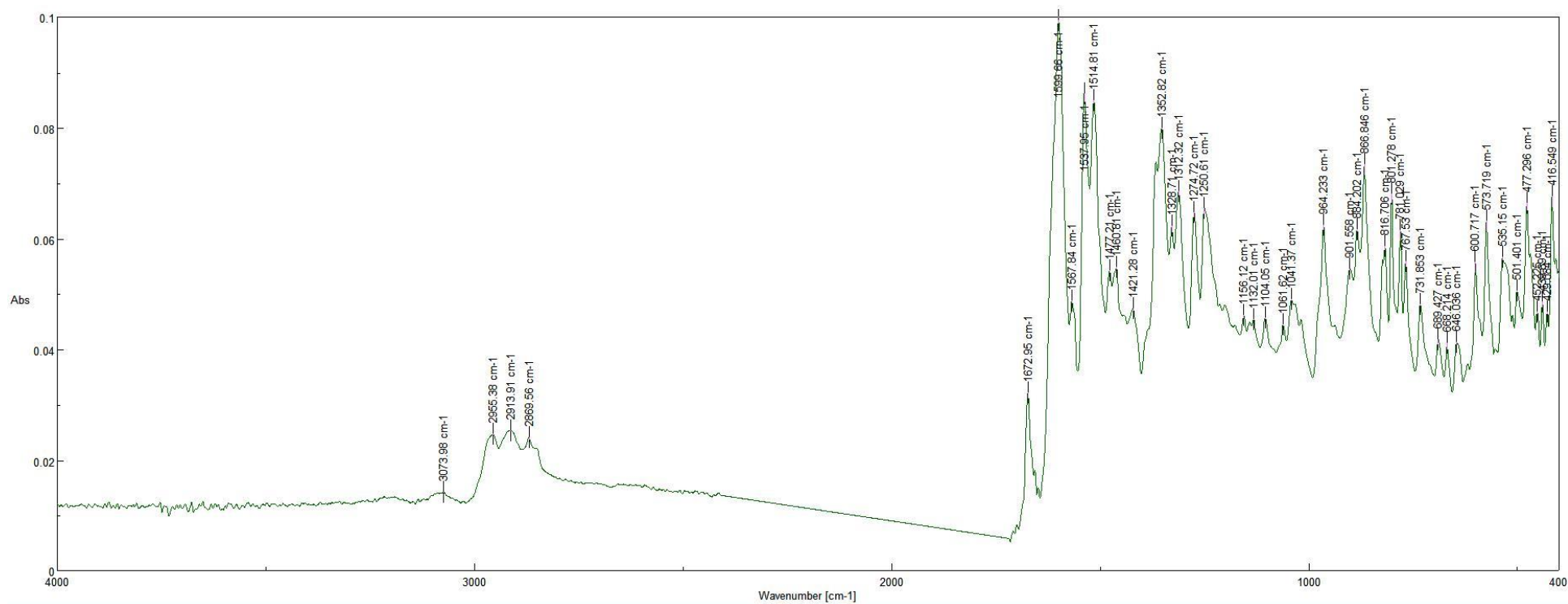


Figure S13 IR spectrum of compound 3.

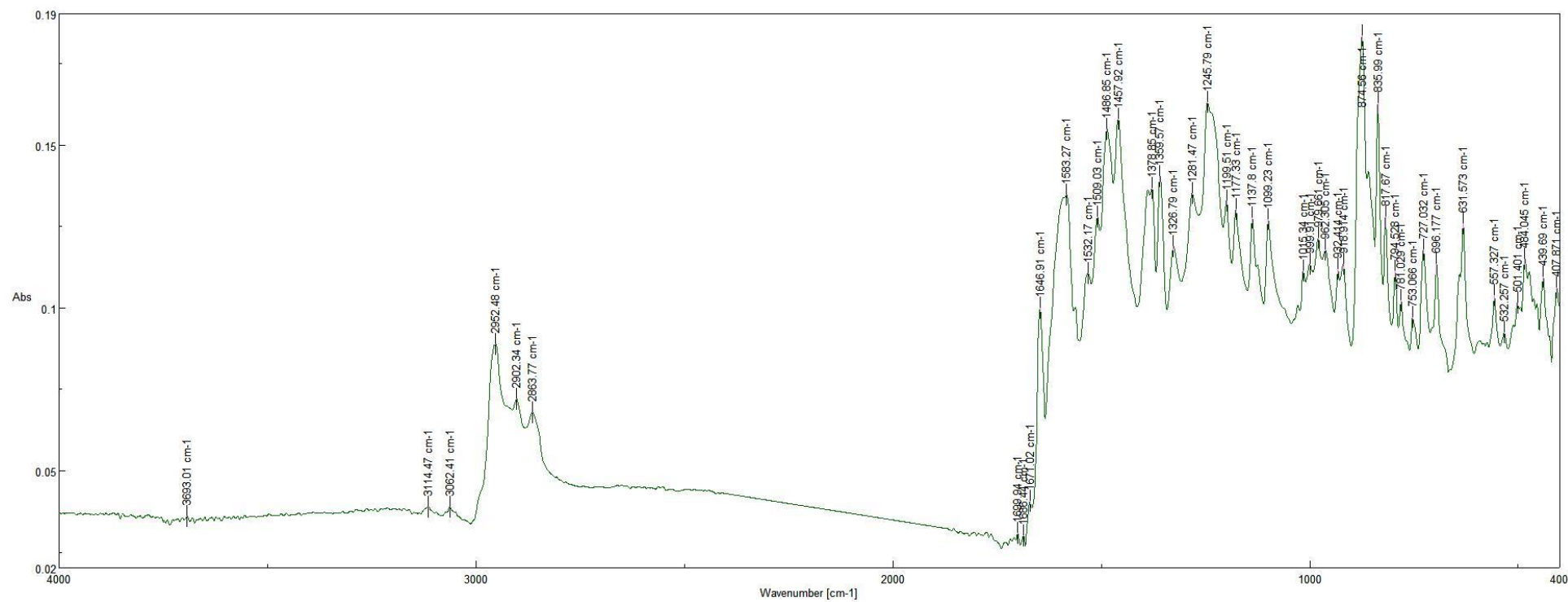


Figure S14 IR spectrum of compound **5**.

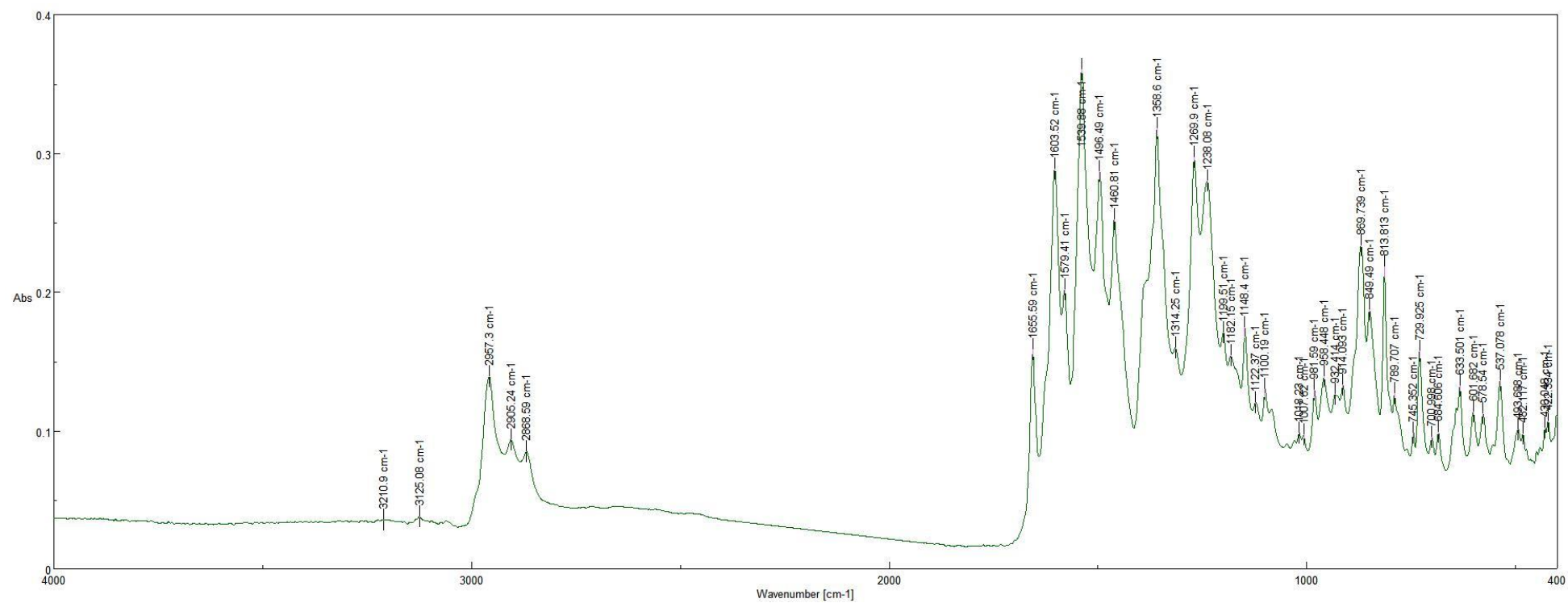


Figure S15 IR spectrum of compound 6.

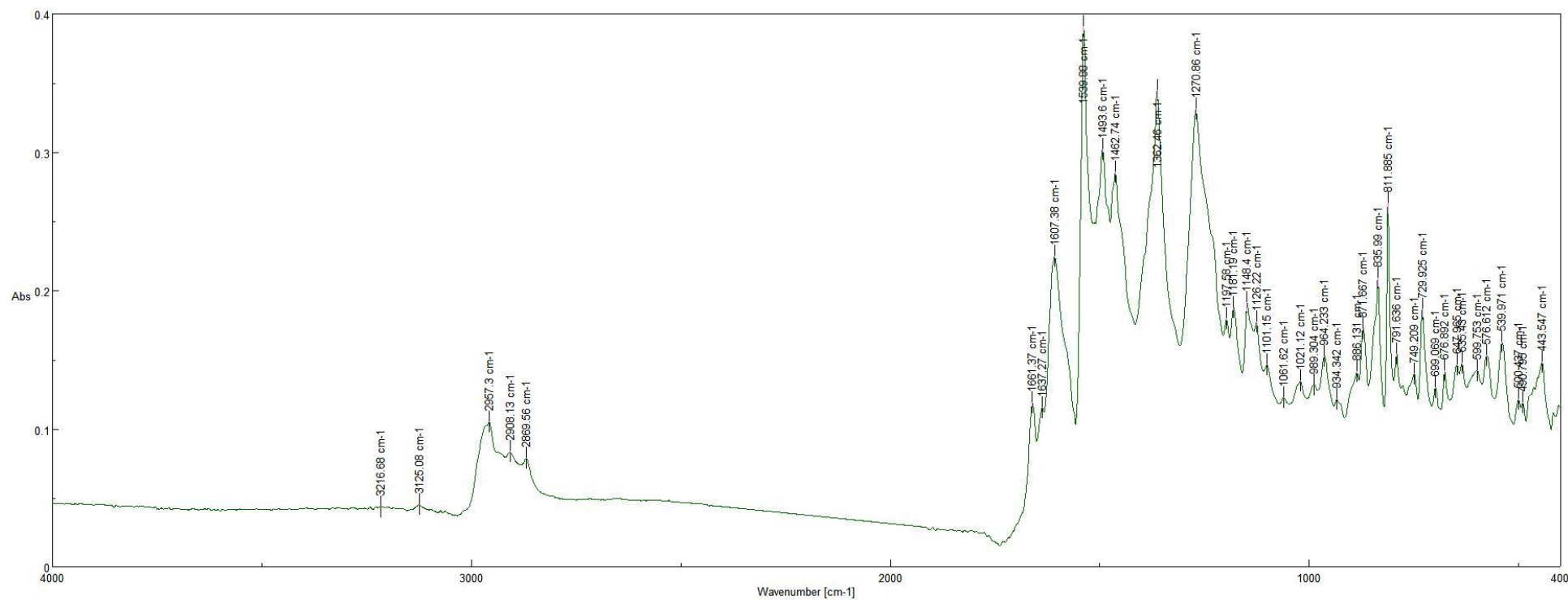


Figure S16 IR spectrum of compound 7.

X-ray diffraction analysis

The unit cell parameters of crystals **5** and **7** and three-dimensional sets of their intensities were obtained at a temperature of 100 K on an Agilent EOS CCD-type XCalibur automated diffractometer (MoK α radiation, graphite monochromator).

The intensities of reflections for **5** and **7** were measured in the angle range ($2\theta \leq 52.14$) using the ω -scanning method from single crystals with $0.53 \times 0.46 \times 0.35$ mm and $0.30 \times 0.23 \times 0.20$ mm dimensions. An empirical accounting of absorption was carried out using the Multiscan procedure. The structures were solved by the direct method and refined by the full-matrix least squares method (LSM) using F^2 using the SHELXTL^{S3} program in the anisotropic approximation for non-hydrogen atoms. Most of the H atoms in crystal structures **5** and **7** are localized in Fourier difference syntheses, then the coordinates and isotropic thermal parameters of all atoms H were calculated using the least squares procedure in the *rider* model.

Full information about the studied structures is contained in CIF files deposited with CCDC numbered 2041292 (**5**) and 2041318 (**7**), from where they can be obtained freely upon request at the following Internet site: www.ccdc.cam.ac.uk/data_request/cif.

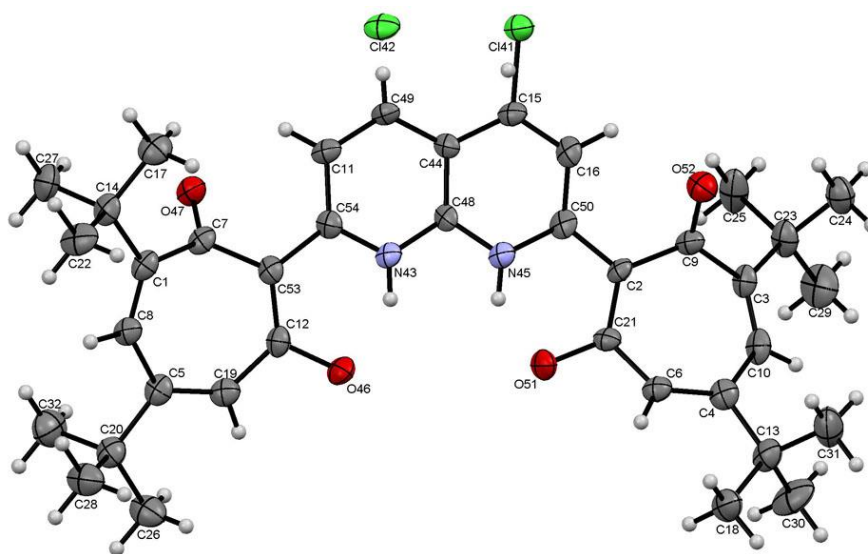


Figure S17 Molecular structure of compound **5**.

Table S2 Crystal data and structure refinement for **5**.

CCDC Number	2041292
Empirical formula	C ₃₈ H ₄₅ ClN ₂ O ₄
Formula weight	629.21
Temperature/K	293(2)
Crystal system	monoclinic
Space group	<i>P</i> -1
<i>a</i> /Å	9.6816(9)
<i>b</i> /Å	12.1524(12)

c/Å	15.9775(16)
$\alpha/^\circ$	107.492(9)
$\beta/^\circ$	104.677(8)
$\gamma/^\circ$	94.924(8)
Volume/Å ³	1707.4(3)
Z	2
ρ_{calc} g/cm ³	1.246
μ/mm^{-1}	0.154
F(000)	658
Crystal size/mm ³	0.53 × 0.46 × 0.35
Radiation	MoK α (λ = 0.71073)
Index ranges	-11 ≤ h ≤ 13, -16 ≤ k ≤ 16, -21 ≤ l ≤ 18
Reflections collected	14757
Independent reflections	9132[R _{int} = 0.0714, R _{sigma} = 0.1284]
Data/restraints/parameters	9132/0/11
Goodness-of-fit on F ²	1.374
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.1696, wR ₂ = 0.4387
Final R indexes [all data]	R ₁ = 0.2328, wR ₂ = 0.4849
Largest diff. peak/hole / e Å ⁻³	1.246/-0.504

Table S3 Bond lengths for compound 5.

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl41	C15	1.705(3)	C53	C54	1.4573	C6	C21	1.4505
Cl42	C49	1.7102	C53	C7	1.4755	C12	C19	1.4583
N43	C54	1.3459	C54	C11	1.4341	C13	C18	1.5440
N43	C48	1.3536	C1	C8	1.3333	C13	C31	1.5482
C44	C49	1.3892	C1	C7	1.5100	C13	C30	1.5569
C44	C48	1.4094	C1	C14	1.5414	C14	C27	1.5407
C44	C15	1.4333	C2	C21	1.4015	C14	C17	1.5492
N45	C50	1.3558	C2	C9	1.4733	C14	C22	1.5532
N45	C48	1.3659	C3	C10	1.3286	C15	C16	1.3731
O46	C12	1.3491	C3	C9	1.5058	C20	C26	1.5323
O47	C7	1.2372	C3	C23	1.5473	C20	C32	1.5468
C49	C11	1.3832	C4	C6	1.3492	C20	C28	1.5543
C50	C16	1.4240	C4	C10	1.4568	C23	C29	1.5459
C50	C2	1.4644	C4	C13	1.5282	C23	C24	1.5475
O51	C21	1.3358	C5	C19	1.3429	C23	C25	1.5592
O52	C9	1.2323	C5	C8	1.4617			
C53	C12	1.4006	C5	C20	1.5437			

Table S4 Bond angles for compound 5.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C54	N43	C48	120.5	O52	C9	C2	121.4
C49	C44	C48	117.3	O52	C9	C3	121.1
C49	C44	C15	127.1	C2	C9	C3	117.2
C48	C44	C15	115.5	C3	C10	C4	129.4
C50	N45	C48	120.2	C49	C11	C54	118.6
N43	C48	N45	114.4	O46	C12	C53	121.1
N43	C48	C44	122.3	O46	C12	C19	111.5
N45	C48	C44	123.3	C53	C12	C19	127.1
C11	C49	C44	121.1	C4	C13	C18	112.7
C11	C49	Cl42	118.3	C4	C13	C31	108.1
C44	C49	Cl42	120.6	C18	C13	C31	108.3
N45	C50	C16	119.8	C4	C13	C30	110.5
N45	C50	C2	115.0	C18	C13	C30	106.7
C16	C50	C2	125.2	C31	C13	C30	110.5
C12	C53	C54	121.8	C27	C14	C1	108.9
C12	C53	C7	119.0	C27	C14	C17	109.7
C54	C53	C7	119.1	C1	C14	C17	111.6
N43	C54	C11	120.1	C27	C14	C22	109.4
N43	C54	C53	115.2	C1	C14	C22	110.2
C11	C54	C53	124.7	C17	C14	C22	107.1
C8	C1	C7	120.7	C16	C15	C44	121.1
C8	C1	C14	123.3	C16	C15	Cl41	120.41(9)
C7	C1	C14	115.8	C44	C15	Cl41	118.53(9)
C21	C2	C50	120.4	C15	C16	C50	120.0
C21	C2	C9	120.9	C5	C19	C12	128.8
C50	C2	C9	118.7	C26	C20	C5	111.9
C10	C3	C9	122.3	C26	C20	C32	109.5
C10	C3	C23	122.4	C5	C20	C32	107.7
C9	C3	C23	115.3	C26	C20	C28	108.0
C6	C4	C10	123.0	C5	C20	C28	109.9
C6	C4	C13	121.5	C32	C20	C28	109.7
C10	C4	C13	115.3	O51	C21	C2	121.9
C19	C5	C8	123.4	O51	C21	C6	111.6
C19	C5	C20	120.9	C2	C21	C6	126.2
C8	C5	C20	115.5	C29	C23	C3	111.0
C4	C6	C21	129.0	C29	C23	C24	109.2
O47	C7	C53	121.6	C3	C23	C24	109.8
O47	C7	C1	119.3	C29	C23	C25	108.1
C53	C7	C1	118.6	C3	C23	C25	108.9
C1	C8	C5	129.6	C24	C23	C25	109.8

Table S5 Torsion Angles for compound 5.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C54	N43	C48	N45	177.7	C44	C49	C11	C54	-0.7
C54	N43	C48	C44	-1.4	Cl42	C49	C11	C54	178.6
C50	N45	C48	N43	176.9	N43	C54	C11	C49	0.5
C50	N45	C48	C44	-4.0	C53	C54	C11	C49	178.7
C49	C44	C48	N43	1.2	C54	C53	C12	O46	-2.6
C15	C44	C48	N43	-176.4	C7	C53	C12	O46	175.1
C49	C44	C48	N45	-177.9	C54	C53	C12	C19	-176.2
C15	C44	C48	N45	4.5	C7	C53	C12	C19	1.5
C48	C44	C49	C11	-0.1	C6	C4	C13	C18	-2.6
C15	C44	C49	C11	177.2	C10	C4	C13	C18	-177.5
C48	C44	C49	Cl42	-179.4	C6	C4	C13	C31	-122.3
C15	C44	C49	Cl42	-2.1	C10	C4	C13	C31	62.9
C48	N45	C50	C16	1.8	C6	C4	C13	C30	116.6
C48	N45	C50	C2	-177.6	C10	C4	C13	C30	-58.2
C48	N43	C54	C11	0.5	C8	C1	C14	C27	-87.7
C48	N43	C54	C53	-177.8	C7	C1	C14	C27	88.8
C12	C53	C54	N43	-10.8	C8	C1	C14	C17	151.1
C7	C53	C54	N43	171.5	C7	C1	C14	C17	-32.4
C12	C53	C54	C11	171.0	C8	C1	C14	C22	32.3
C7	C53	C54	C11	-6.7	C7	C1	C14	C22	-151.2
N45	C50	C2	C21	-9.5	C49	C44	C15	C16	179.4
C16	C50	C2	C21	171.1	C48	C44	C15	C16	-3.2
N45	C50	C2	C9	172.5	C49	C44	C15	Cl41	-1.55(10)
C16	C50	C2	C9	-6.9	C48	C44	C15	Cl41	175.78(10)
C10	C4	C6	C21	1.1	C44	C15	C16	C50	1.5
C13	C4	C6	C21	-173.3	Cl41	C15	C16	C50	-177.54(40)
C12	C53	C7	O47	-134.4	N45	C50	C16	C15	-0.7
C54	C53	C7	O47	43.4	C2	C50	C16	C15	178.7
C12	C53	C7	C1	53.7	C8	C5	C19	C12	1.1
C54	C53	C7	C1	-128.5	C20	C5	C19	C12	-174.3
C8	C1	C7	O47	129.4	O46	C12	C19	C5	153.8
C14	C1	C7	O47	-47.2	C53	C12	C19	C5	-32.1
C8	C1	C7	C53	-58.5	C19	C5	C20	C26	-4.1
C14	C1	C7	C53	124.9	C8	C5	C20	C26	-179.8
C7	C1	C8	C5	4.0	C19	C5	C20	C32	-124.6
C14	C1	C8	C5	-179.6	C8	C5	C20	C32	59.7

C19	C5	C8	C1	28.1	C19	C5	C20	C28	115.9
C20	C5	C8	C1	-156.3	C8	C5	C20	C28	-59.8
C21	C2	C9	O52	-134.9	C50	C2	C21	O51	-1.9
C50	C2	C9	O52	43.1	C9	C2	C21	O51	176.0
C21	C2	C9	C3	51.2	C50	C2	C21	C6	-174.8
C50	C2	C9	C3	-130.8	C9	C2	C21	C6	3.2
C10	C3	C9	O52	128.7	C4	C6	C21	O51	153.3
C23	C3	C9	O52	-49.7	C4	C6	C21	C2	-33.2
C10	C3	C9	C2	-57.3	C10	C3	C23	C29	22.2
C23	C3	C9	C2	124.2	C9	C3	C23	C29	-159.4
C9	C3	C10	C4	4.7	C10	C3	C23	C24	-98.6
C23	C3	C10	C4	-176.9	C9	C3	C23	C24	79.8
C6	C4	C10	C3	28.2	C10	C3	C23	C25	141.1
C13	C4	C10	C3	-157.1	C9	C3	C23	C25	-40.4

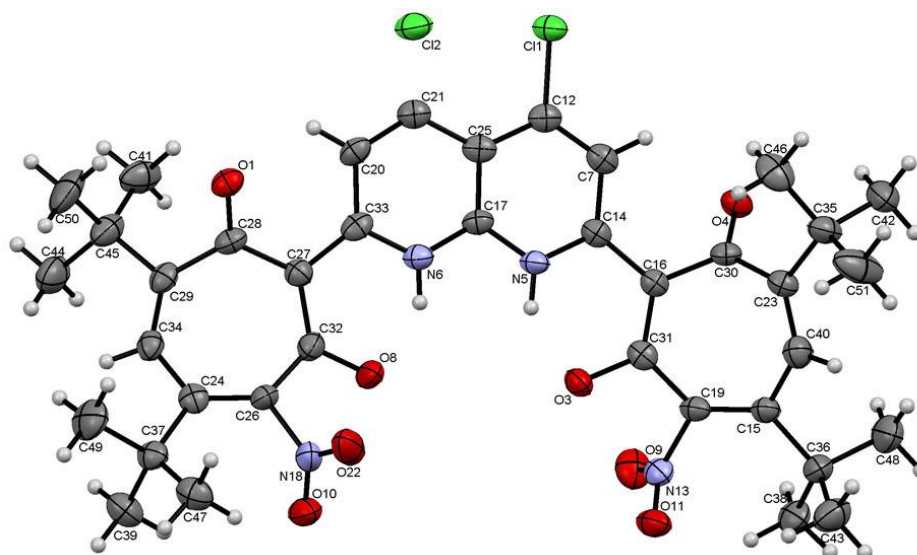


Figure S18 Molecular structure of **7**.

Table S6 Crystal data and structure refinement for **7**.

CCDC Number	2041318
Empirical formula	C ₃₈ H ₄₃ N ₄ O ₈ Cl
Formula weight	719.21
Temperature/K	293(2)
Crystal system	rhombic
Space group	<i>Pbca</i>
a/Å	19.5970(7)
b/Å	12.8733(6)
c/Å	29.2894(12)
$\alpha/^\circ$	90
$\beta/^\circ$	90
$\gamma/^\circ$	90
Volume/Å ³	7389.1(5)
Z	8
$\rho_{\text{calc}}/\text{cm}^3$	1.293
μ/mm^{-1}	0.160
F(000)	3040
Crystal size/mm ³	0.30 × 0.23 × 0.20
Radiation	MoK α (λ = 0.71073)
Index ranges	-13 ≤ h ≤ 24, -15 ≤ k ≤ 8, -22 ≤ l ≤ 36
Reflections collected	19714
Independent reflections	7300 [R _{int} = 0.0826, R _{sigma} = 0.1167]
Data/restraints/parameters	7300/0/470
Goodness-of-fit on F ²	0.964
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0739, wR ₂ = 0.1698
Final R indexes [all data]	R ₁ = 0.1352, wR ₂ = 0.2102
Largest diff. peak/hole / e Å ⁻³	0.551/-0.327

Table S7 Bond lengths for compound 7

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl1	C12	1.711(3)	C21	C25	1.431(5)	C41	H41 ^b	0.9600
Cl2	C21	1.673(4)	C23	C40	1.333(5)	C41	H41 ^c	0.9600
O1	C28	1.226(4)	C23	C30	1.496(4)	C42	H42 ^a	0.9600
O3	C31	1.327(4)	C23	C35	1.545(5)	C42	H42 ^b	0.9600
O4	C30	1.227(4)	C24	C26	1.352(5)	C42	H42 ^c	0.9600
N5	C14	1.332(4)	C24	C34	1.456(5)	C43	H43 ^a	0.9600
N5	C17	1.354(4)	C24	C37	1.544(5)	C43	H43 ^b	0.9600
N5	H5 ^a	0.8600	C26	C32	1.479(5)	C43	H43 ^c	0.9600
N6	C33	1.337(4)	C27	C32	1.420(5)	C44	C45	1.556(5)
N6	C17	1.352(4)	C27	C33	1.454(5)	C44	H44 ^a	0.9600
N6	H6 ^a	0.8600	C27	C28	1.469(5)	C44	H44 ^b	0.9600
C7	C12	1.367(5)	C28	C29	1.508(5)	C44	H44 ^c	0.9600
C7	C14	1.417(4)	C29	C34	1.338(5)	C45	C50	1.554(5)
C7	H7 ^a	0.9300	C29	C45	1.540(5)	C46	H46 ^a	0.9600
O8	C32	1.295(4)	C34	H34 ^a	0.9300	C46	H46 ^b	0.9600
O9	N13	1.234(4)	C35	C51	1.519(5)	C46	H46 ^c	0.9600
O10	N18	1.230(4)	C35	C46	1.532(5)	C47	H47 ^a	0.9600
O11	N13	1.223(4)	C35	C42	1.534(5)	C47	H47 ^b	0.9600
C12	C25	1.415(4)	C36	C43	1.537(5)	C47	H47 ^c	0.9600
N13	C19	1.476(4)	C36	C38	1.541(5)	C48	H48 ^a	0.9600
C14	C16	1.473(4)	C36	C48	1.546(5)	C48	H48 ^b	0.9600
C15	C19	1.355(5)	C37	C39	1.534(5)	C48	H48 ^c	0.9600
C15	C40	1.467(5)	C37	C47	1.542(5)	C49	H49 ^a	0.9600
C15	C36	1.543(5)	C37	C49	1.547(5)	C49	H49 ^b	0.9600
C16	C31	1.391(4)	C38	H38 ^a	0.9600	C49	H49 ^c	0.9600
C16	C30	1.479(4)	C38	H38 ^b	0.9600	C50	H50 ^a	0.9600
C17	C25	1.393(4)	C38	H38 ^c	0.9600	C50	H50 ^b	0.9600
N18	O22	1.230(4)	C39	H39 ^a	0.9600	C50	H50 ^c	0.9600
N18	C26	1.479(4)	C39	H39 ^b	0.9600	C51	H51 ^a	0.9600
C19	C31	1.468(4)	C39	H39 ^c	0.9600	C51	H51 ^b	0.9600
C20	C21	1.357(5)	C40	H40 ^a	0.9300	C51	H51 ^c	0.9600
C20	C33	1.427(4)	C41	C45	1.528(5)			
C20	H20 ^a	0.9300	C41	H41 ^a	0.9600			

Table S8 Bond angles for compound 7.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C14	N5	C17	120.8(3)	C39	C37	C47	109.1(3)
C14	N5	H5 ^a	119.6	C39	C37	C24	108.3(3)
C17	N5	H5 ^a	119.6	C47	C37	C24	115.7(3)
C33	N6	C17	124.9(3)	C39	C37	C49	109.8(3)
C33	N6	H6 ^a	117.6	C47	C37	C49	105.3(3)
C17	N6	H6 ^a	117.6	C24	C37	C49	108.6(3)
C12	C7	C14	119.6(3)	C36	C38	H38 ^a	109.5
C12	C7	H7 ^a	120.2	C36	C38	H38 ^b	109.5
C14	C7	H7 ^a	120.2	H38 ^a	C38	H38 ^b	109.5
C7	C12	C25	121.1(3)	C36	C38	H38 ^c	109.5
C7	C12	Cl1	120.6(3)	H38 ^a	C38	H38 ^c	109.5
C25	C12	Cl1	118.3(3)	H38 ^b	C38	H38 ^c	109.5
O11	N13	O9	124.2(3)	C37	C39	H39 ^a	109.5
O11	N13	C19	117.9(3)	C37	C39	H39 ^b	109.5
O9	N13	C19	117.8(3)	H39 ^a	C39	H39 ^b	109.5
N5	C14	C7	119.6(3)	C37	C39	H39 ^c	109.5
N5	C14	C16	115.3(3)	H39 ^a	C39	H39 ^c	109.5
C7	C14	C16	125.0(3)	H39 ^b	C39	H39 ^c	109.5
C19	C15	C40	119.0(3)	C23	C40	C15	130.4(3)
C19	C15	C36	127.1(3)	C23	C40	H40 ^a	114.8
C40	C15	C36	113.9(3)	C15	C40	H40 ^a	114.8
C31	C16	C14	120.8(3)	C45	C41	H41 ^a	109.5
C31	C16	C30	120.9(3)	C45	C41	H41 ^b	109.5
C14	C16	C30	118.2(3)	H41 ^a	C41	H41 ^b	109.5
N6	C17	N5	116.2(3)	C45	C41	H41 ^c	109.5
N6	C17	C25	120.7(3)	H41 ^a	C41	H41 ^c	109.5
N5	C17	C25	123.1(3)	H41 ^b	C41	H41 ^c	109.5
O10	N18	O22	125.2(3)	C35	C42	H42 ^a	109.5
O10	N18	C26	116.9(3)	C35	C42	H42 ^b	109.5
O22	N18	C26	117.9(3)	H42 ^a	C42	H42 ^b	109.5
C15	C19	C31	130.0(3)	C35	C42	H42 ^c	109.5
C15	C19	N13	120.4(3)	H42 ^a	C42	H42 ^c	109.5
C31	C19	N13	109.0(3)	H42 ^b	C42	H42 ^c	109.5
C21	C20	C33	120.7(3)	C36	C43	H43 ^a	109.5
C21	C20	H20 ^a	119.6	C36	C43	H43 ^b	109.5
C33	C20	H20 ^a	119.6	H43 ^a	C43	H43 ^b	109.5
C20	C21	C25	121.3(3)	C36	C43	H43 ^c	109.5
C20	C21	Cl2	122.4(3)	H43 ^a	C43	H43 ^c	109.5
C25	C21	Cl2	116.3(3)	H43 ^b	C43	H43 ^c	109.5
C40	C23	C30	120.9(3)	C45	C44	H44 ^a	109.5
C40	C23	C35	122.9(3)	C45	C44	H44 ^b	109.5
C30	C23	C35	116.1(3)	H44 ^a	C44	H44 ^b	109.5
C26	C24	C34	119.1(3)	C45	C44	H44 ^c	109.5
C26	C24	C37	125.1(3)	H44 ^a	C44	H44 ^c	109.5

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C34	C24	C37	115.6(3)	H44 ^b	C44	H44 ^c	109.5
C17	C25	C12	115.8(3)	C41	C45	C29	111.2(3)
C17	C25	C21	116.0(3)	C41	C45	C50	110.5(3)
C12	C25	C21	128.2(3)	C29	C45	C50	108.3(3)
C24	C26	N18	120.8(3)	C41	C45	C44	107.9(3)
C24	C26	C32	131.5(3)	C29	C45	C44	110.7(3)
N18	C26	C32	107.5(3)	C50	C45	C44	108.2(3)
C32	C27	C33	118.4(3)	C35	C46	H46 ^a	109.5
C32	C27	C28	122.9(3)	C35	C46	H46 ^b	109.5
C33	C27	C28	118.6(3)	H46 ^a	C46	H46 ^b	109.5
O1	C28	C27	121.7(3)	C35	C46	H46 ^c	109.5
O1	C28	C29	119.5(3)	H46 ^a	C46	H46 ^c	109.5
C27	C28	C29	118.4(3)	H46 ^b	C46	H46 ^c	109.5
C34	C29	C28	123.2(3)	C37	C47	H47 ^a	109.5
C34	C29	C45	121.1(3)	C37	C47	H47 ^b	109.5
C28	C29	C45	115.4(3)	H47 ^a	C47	H47 ^b	109.5
O4	C30	C16	122.6(3)	C37	C47	H47 ^c	109.5
O4	C30	C23	121.6(3)	H47 ^a	C47	H47 ^c	109.5
C16	C30	C23	115.3(3)	H47 ^b	C47	H47 ^c	109.5
O3	C31	C16	122.1(3)	C36	C48	H48 ^a	109.5
O3	C31	C19	112.4(3)	C36	C48	H48 ^b	109.5
C16	C31	C19	125.3(3)	H48 ^a	C48	H48 ^b	109.5
O8	C32	C27	122.7(3)	C36	C48	H48 ^c	109.5
O8	C32	C26	112.8(3)	H48 ^a	C48	H48 ^c	109.5
C27	C32	C26	123.8(3)	H48 ^b	C48	H48 ^c	109.5
N6	C33	C20	116.3(3)	C37	C49	H49 ^a	109.5
N6	C33	C27	117.0(3)	C37	C49	H49 ^b	109.5
C20	C33	C27	126.7(3)	H49 ^a	C49	H49 ^b	109.5
C29	C34	C24	130.5(3)	C37	C49	H49 ^c	109.5
C29	C34	H34a	114.7	H49 ^a	C49	H49 ^c	109.5
C24	C34	H34a	114.7	H49 ^b	C49	H49 ^c	109.5
C51	C35	C46	108.3(3)	C45	C50	H50 ^a	109.5
C51	C35	C42	109.2(4)	C45	C50	H50 ^b	109.5
C46	C35	C42	109.7(3)	H50 ^a	C50	H50 ^b	109.5
C51	C35	C23	110.1(3)	C45	C50	H50 ^c	109.5
C46	C35	C23	110.1(3)	H50 ^a	C50	H50 ^c	109.5
C42	C35	C23	109.4(3)	H50 ^b	C50	H50 ^c	109.5
C43	C36	C38	108.3(3)	C35	C51	H51 ^a	109.5
C43	C36	C15	108.7(3)	C35	C51	H51 ^b	109.5
C38	C36	C15	115.3(3)	H51 ^a	C51	H51 ^b	109.5
C43	C36	C48	110.6(3)	C35	C51	H51 ^c	109.5
C38	C36	C48	105.3(3)	H51 ^a	C51	H51 ^c	109.5
C15	C36	C48	108.6(3)	H51 ^b	C51	H51 ^c	109.5

Table S9 Torsion angles for compound 7.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C14	C7	C12	C25	0.2(5)	C40	C23	C30	C16	60.0(4)
C14	C7	C12	Cl1	-178.0(2)	C35	C23	C30	C16	-122.6(3)
C17	N5	C14	C7	-0.3(5)	C14	C16	C31	O3	0.5(5)
C17	N5	C14	C16	177.5(3)	C30	C16	C31	O3	-178.5(3)
C12	C7	C14	N5	-0.3(5)	C14	C16	C31	C19	174.8(3)
C12	C7	C14	C16	-177.9(3)	C30	C16	C31	C19	-4.3(5)
N5	C14	C16	C31	6.7(4)	C15	C19	C31	O3	-151.7(3)
C7	C14	C16	C31	-175.6(3)	N13	C19	C31	O3	20.3(4)
N5	C14	C16	C30	-174.2(3)	C15	C19	C31	C16	33.5(6)
C7	C14	C16	C30	3.5(5)	N13	C19	C31	C16	-154.5(3)
C33	N6	C17	N5	-179.6(3)	C33	C27	C32	O8	-7.4(5)
C33	N6	C17	C25	0.2(5)	C28	C27	C32	O8	176.7(3)
C14	N5	C17	N6	-179.2(3)	C33	C27	C32	C26	162.1(3)
C14	N5	C17	C25	1.0(5)	C28	C27	C32	C26	-13.9(5)
C40	C15	C19	C31	3.5(5)	C24	C26	C32	O8	-155.6(4)
C36	C15	C19	C31	180.0(3)	N18	C26	C32	O8	20.1(4)
C40	C15	C19	N13	-167.7(3)	C24	C26	C32	C27	34.0(6)
C36	C15	C19	N13	8.7(5)	N18	C26	C32	C27	-150.3(3)
O11	N13	C19	C15	68.6(4)	C17	N6	C33	C20	1.7(5)
O9	N13	C19	C15	-113.7(4)	C17	N6	C33	C27	-179.1(3)
O11	N13	C19	C31	-104.3(3)	C21	C20	C33	N6	-1.5(5)
O9	N13	C19	C31	73.4(4)	C21	C20	C33	C27	179.3(3)
C33	C20	C21	C25	-0.4(5)	C32	C27	C33	N6	2.6(5)
C33	C20	C21	Cl2	177.5(3)	C28	C27	C33	N6	178.7(3)
N6	C17	C25	C12	179.2(3)	C32	C27	C33	C20	-178.3(3)
N5	C17	C25	C12	-1.1(5)	C28	C27	C33	C20	-2.2(5)
N6	C17	C25	C21	-2.2(4)	C28	C29	C34	C24	-2.0(6)
N5	C17	C25	C21	177.6(3)	C45	C29	C34	C24	-175.6(3)
C7	C12	C25	C17	0.4(4)	C26	C24	C34	C29	-35.3(6)
Cl1	C12	C25	C17	178.7(2)	C37	C24	C34	C29	149.2(4)
C7	C12	C25	C21	-178.1(3)	C40	C23	C35	C51	-25.4(5)
Cl1	C12	C25	C21	0.2(5)	C30	C23	C35	C51	157.3(3)
C20	C21	C25	C17	2.2(5)	C40	C23	C35	C46	-144.7(4)
Cl2	C21	C25	C17	-175.8(3)	C30	C23	C35	C46	37.9(4)
C20	C21	C25	C12	-179.3(3)	C40	C23	C35	C42	94.6(4)
Cl2	C21	C25	C12	2.7(5)	C30	C23	C35	C42	-82.7(4)

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C34	C24	C26	N18	-168.8(3)	C19	C15	C36	C43	-99.2(4)
C37	C24	C26	N18	6.2(5)	C40	C15	C36	C43	77.5(4)
C34	C24	C26	C32	6.3(6)	C19	C15	C36	C38	22.6(5)
C37	C24	C26	C32	-178.7(3)	C40	C15	C36	C38	-160.8(3)
O10	N18	C26	C24	72.3(4)	C19	C15	C36	C48	140.4(4)
O22	N18	C26	C24	-110.1(4)	C40	C15	C36	C48	-42.9(4)
O10	N18	C26	C32	-103.9(3)	C26	C24	C37	C39	-96.2(4)
O22	N18	C26	C32	73.6(4)	C34	C24	C37	C39	78.9(4)
C32	C27	C28	O1	147.5(3)	C26	C24	C37	C47	26.5(5)
C33	C27	C28	O1	-28.4(5)	C34	C24	C37	C47	-158.3(3)
C32	C27	C28	C29	-39.9(5)	C26	C24	C37	C49	144.6(4)
C33	C27	C28	C29	144.2(3)	C34	C24	C37	C49	-40.3(4)
O1	C28	C29	C34	-133.7(4)	C30	C23	C40	C15	-1.1(6)
C27	C28	C29	C34	53.4(5)	C35	C23	C40	C15	-178.3(3)
O1	C28	C29	C45	40.2(4)	C19	C15	C40	C23	-36.2(6)
C27	C28	C29	C45	-132.6(3)	C36	C15	C40	C23	146.9(4)
C31	C16	C30	O4	134.6(3)	C34	C29	C45	C41	-144.8(3)
C14	C16	C30	O4	-44.5(5)	C28	C29	C45	C41	41.1(4)
C31	C16	C30	C23	-53.6(4)	C34	C29	C45	C50	93.6(4)
C14	C16	C30	C23	127.3(3)	C28	C29	C45	C50	-80.5(4)
C40	C23	C30	O4	-128.1(4)	C34	C29	C45	C44	-24.8(5)
C35	C23	C30	O4	49.3(4)	C28	C29	C45	C44	161.1(3)

UV-vis and photoluminescence data

UV-vis spectra of the compounds have been recorded for $2 \cdot 10^{-5}$ M solutions on a “Varian Cary 50” spectrophotometer. Fluorescence emission and fluorescence excitation spectra for $(1.0\text{--}3.0) \cdot 10^{-6}$ M solutions and for solid state (as powders) have been recorded on a “Cary Eclipse Fluorescence spectrophotometer”. Absorption and fluorescence spectra have been recorded using standard 1 cm quartz cells at room temperature. Stokes shifts have been estimated considering the lowest energetic absorption band. The fluorescence quantum yields have been measured with using Absolute PL quantum yields spectrometer C11347 “Quantaurs-QY”.

Table S10 UV-Vis and photoluminescence data for compounds **5** and **7** in different solvents and in solid state (as powder).

Solvent	Compd.	Absorption λ_{max} , nm ($\epsilon, 10^3 \text{ M}^{-1}\text{cm}^{-1}$)	Photoluminescence			
			Excitation λ_{max} , nm	Emission λ_{max} , nm	Stokes shift $\Delta\nu_{\text{St}}$ (cm^{-1})	Quantum yield ϕ_f^1
Heptane	5	453 (29.0), 509 ^{sh} (6.8), 434 ^{sh} , 364 (11.7), 349 (11.8), 310 ^{sh} (13.8), 288 (17.7), 262 (24.6)	509, 476, 446, 428 ^{sh} , 368 ^{sh} , 344	519, 556, 590 ^{sh}	378	-
	7	504 (26.2), 474 (30.0), 450 (26.3), 354 (20.0), 266 (28.6)	503, 474, 450 ^{sh} , 348, 266	547, 574 ^{sh} , 527 ^{sh}	1559	0.04
Toluene	5	456 (30.8), 505 ^{sh} (10.5), 364 (14.2), 351 (13.9)	505, 475, 446, 427 ^{sh} , 344	521, 555, 590 ^{sh}	608	-
	7	505 (31.4), 475 (30.9), 453 ^{sh} (20.2), 356 (19.2)	507, 476, 454 ^{sh} , 356	556, 595 ^{sh}	1816	0.06
CHCl ₃	5	455 (30.1), 502 ^{sh} (13.5), 362 (13.4), 351 (13.2), 288 ^{sh} (21.3), 265 (27.2)	502, 470, 450 ^{sh} , 345, 296, 272	520, 552, 590 ^{sh}	690	-
	7	504 (30.9), 475 (30.6), 454 ^{sh} (20.7), 355 (19.3), 272 (23.5)	506, 475, 454 ^{sh} , 360, 273	557, 593 ^{sh}	1823	0.02
THF	5	454 (30.5), 503 ^h (8.6), 363 (13.1), 351 (13.3), 283 ^{sh} (20.0), 262 (27.0)	503, 473, 449 ^{sh} , 344, 299	523, 554	760	-
	7	503 (30.0), 474 (30.5), 453 ^{sh} (21.2), 355 (19.6)	503, 475, 453 ^{sh} , 355,	555, 593 ^{sh}	1863	0.01
MeCN	5	452 (26.7), 496 ^{sh} (12.5), 357 (18.4), 283 (18.1), 263 (22.8)	496, 468, 345, 262	521, 541	967	-
	7	497 (29.0), 470 (27.0), 450 ^{sh} (18.0), 354 (16.6), 290 ^{sh} (17.8), 269 (20.3)	497, 470, 450 ^{sh} , 355, 290 ^{sh} , 270	551, 587 ^{sh}	1972	0.01
EtOH	5	452 (27.8), 492 ^{sh} (12.3), 360 (14.4), 283 ^{sh} (21.3), 262 (29.2)	492, 465, 445 ^{sh} , 344, 296, 275	523, 550,	1205	-
	7	501 (29.4), 400 (14.7), 380 (15.3), 269 (15.8), 262 (30.9)	500, 475 ^{sh} , 400, 380	557, 590	2047	0.004
Solid state	5		534	578	1426	-
	7		547	573	830	0.09

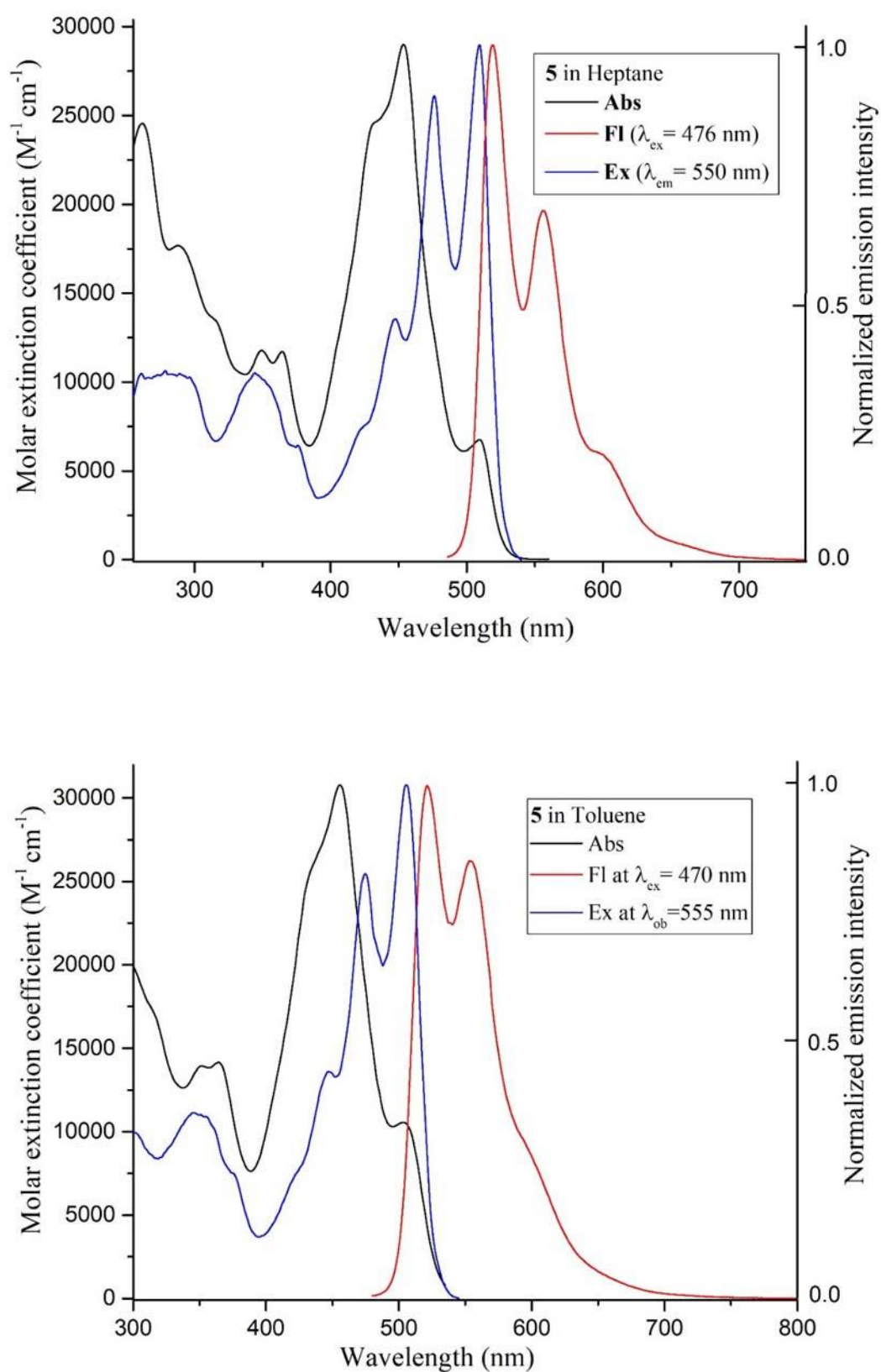


Figure S19 Absorption, emission, and excitation spectra for **5** in heptane and toluene.

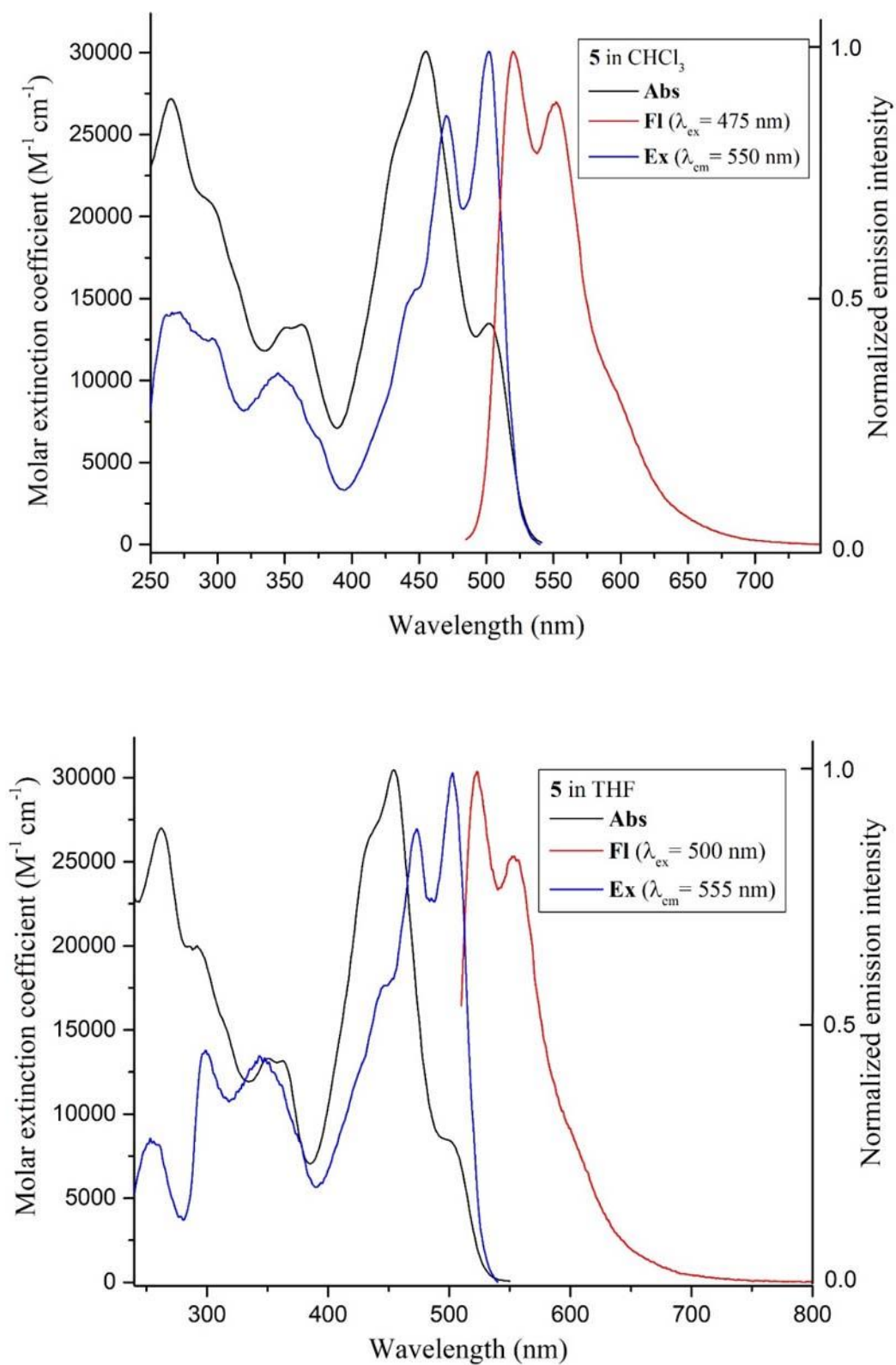


Figure S20 Absorption, emission, and excitation spectra for **5** in chloroform and THF.

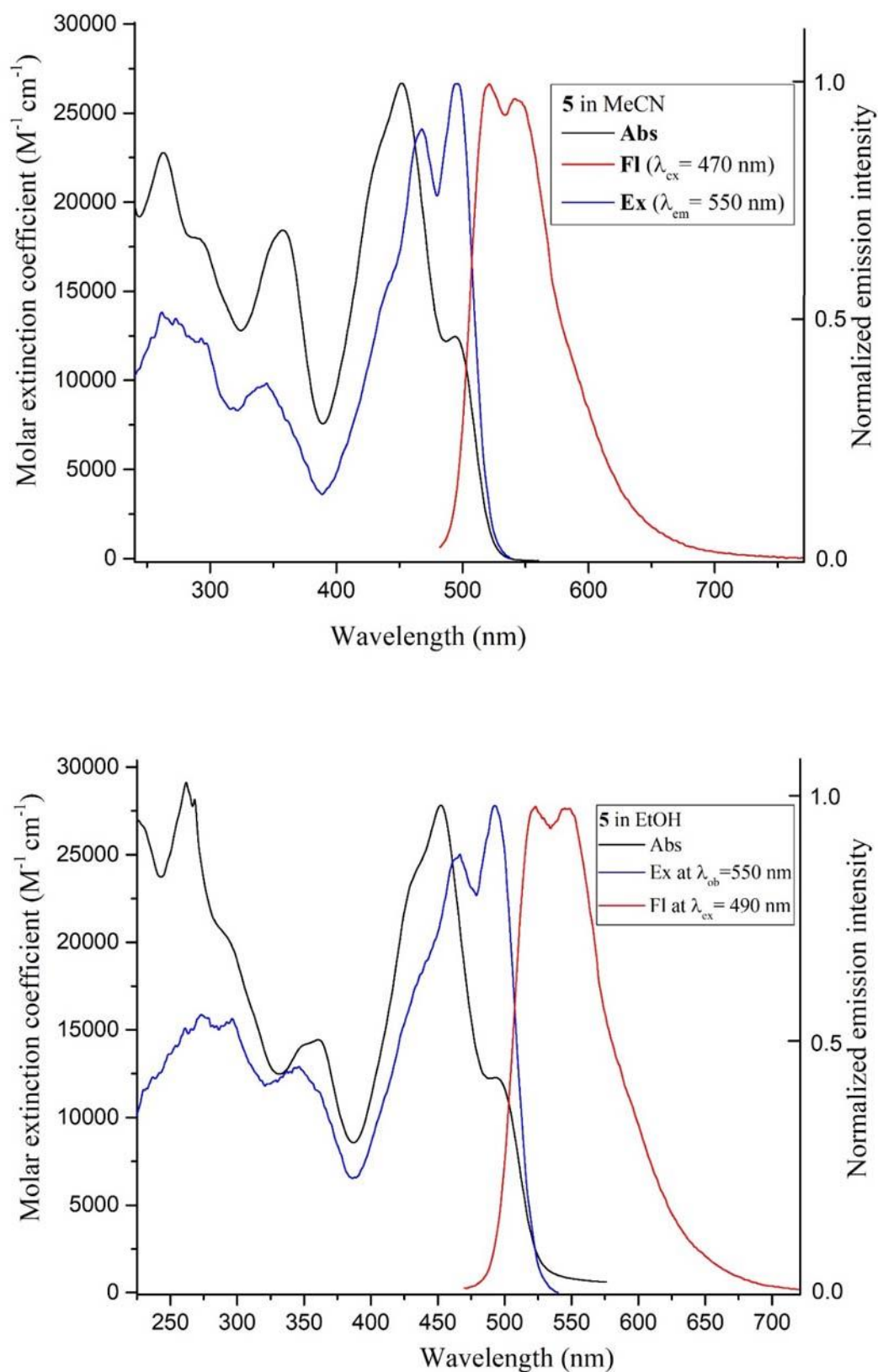


Figure S21 Absorption, emission, and excitation spectra for **5** in acetonitrile and ethanol.

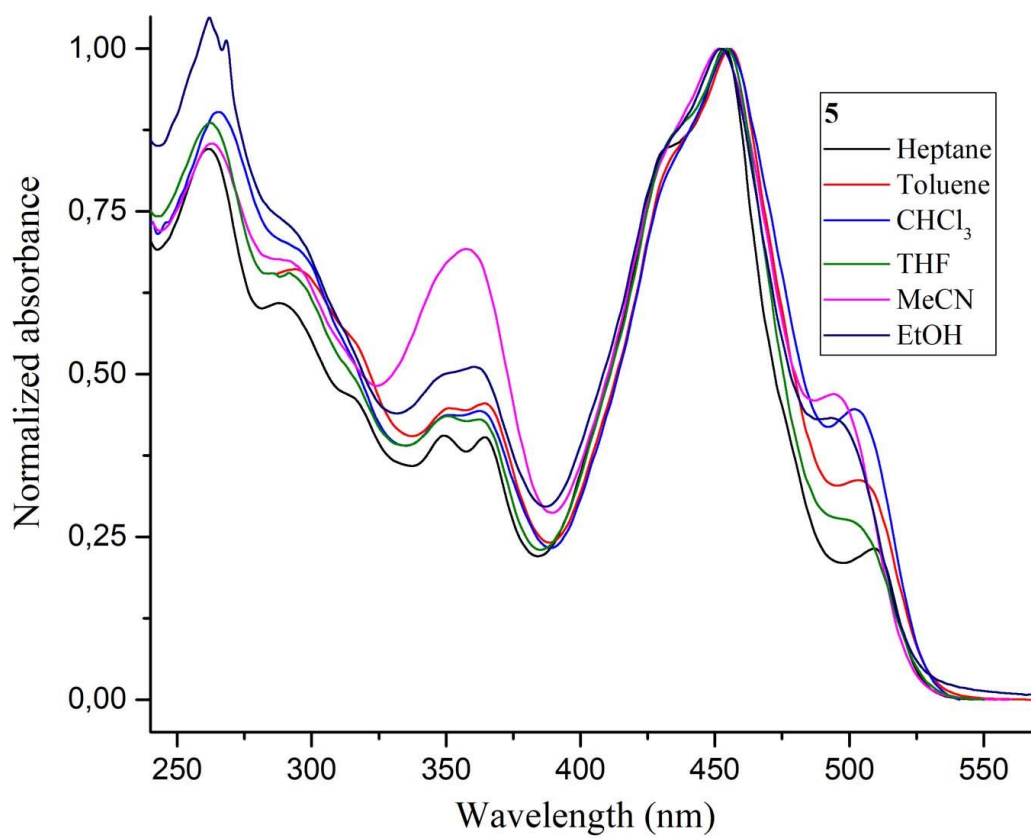


Figure S22 Absorption 5 in different solvents.

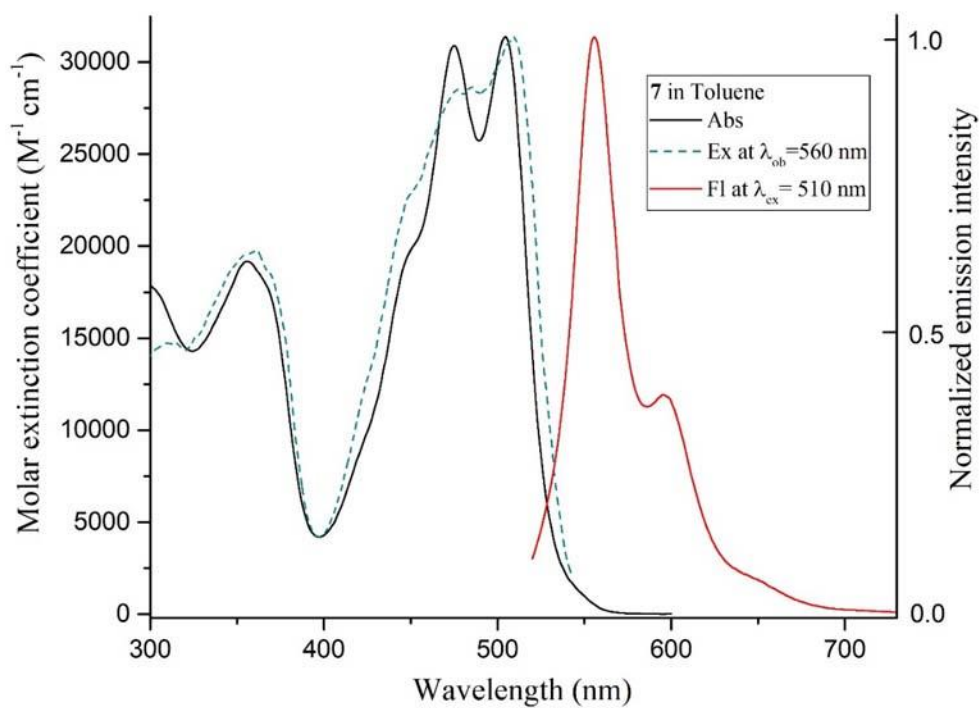
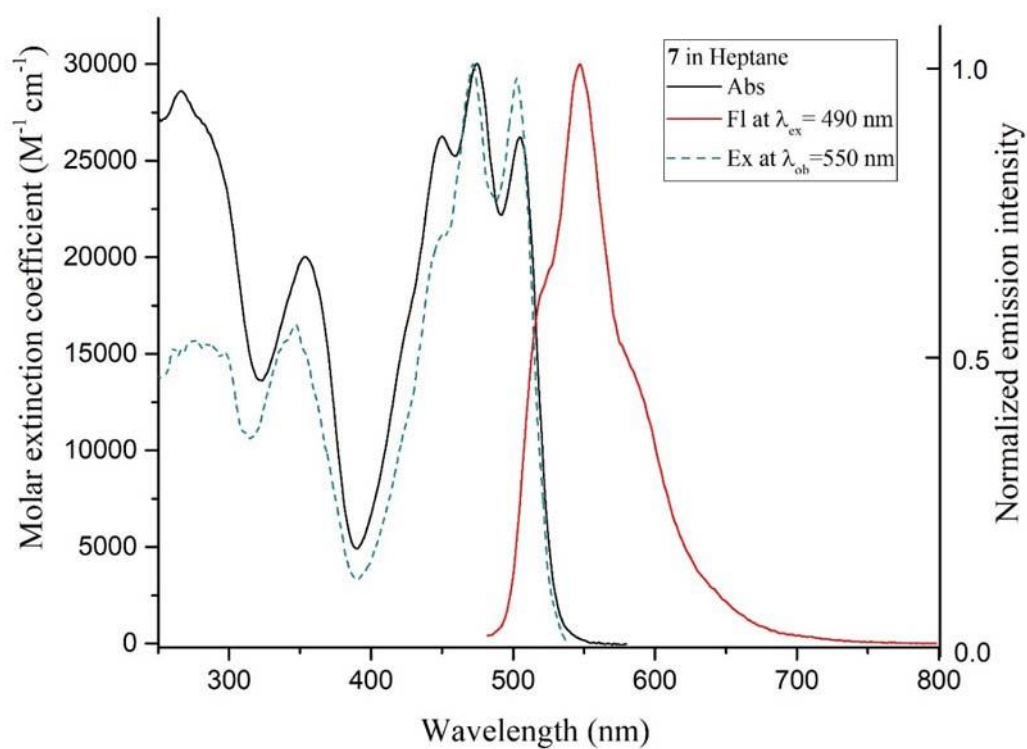


Figure S23 Absorption, emission, and excitation spectra for 7 in heptane and toluene.

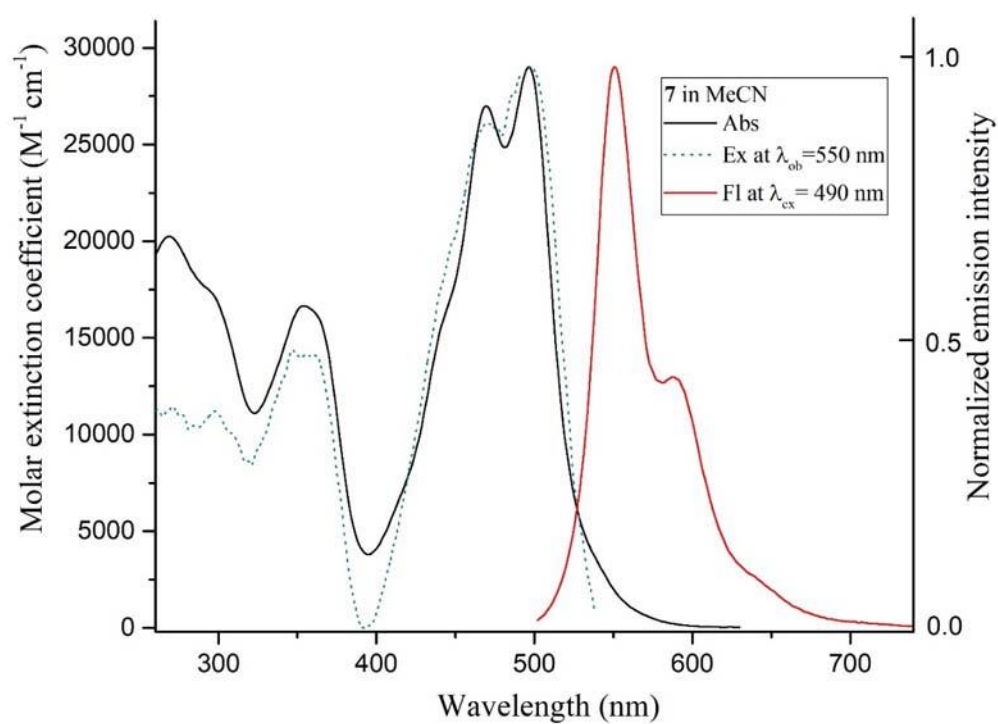
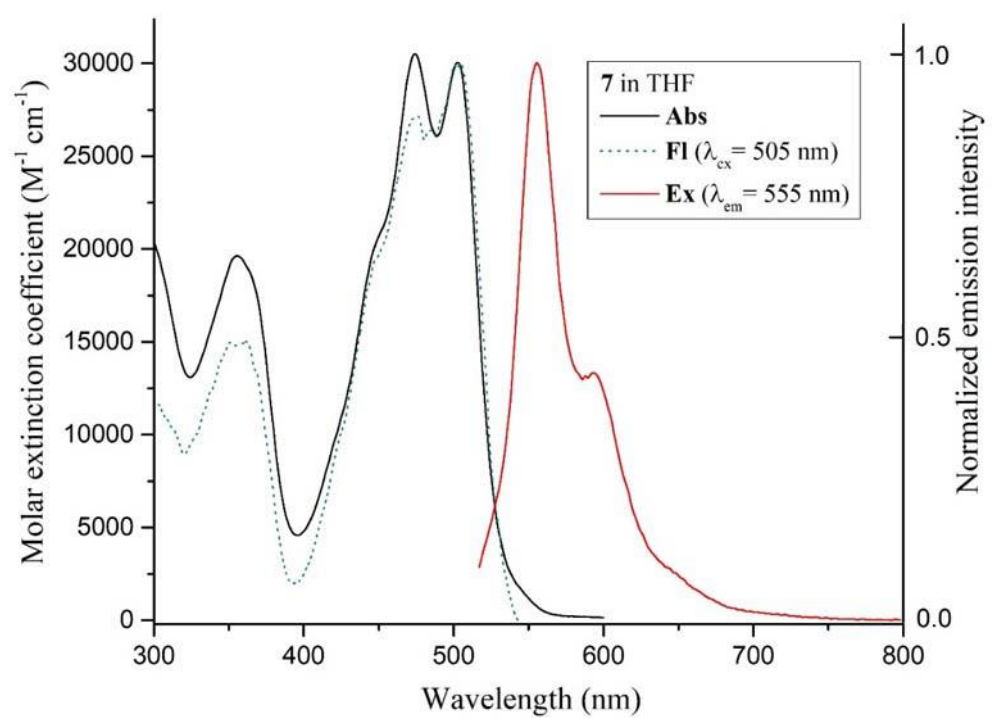


Figure S24 Absorption, emission, and excitation spectra for **7** in THF and in acetonitrile.

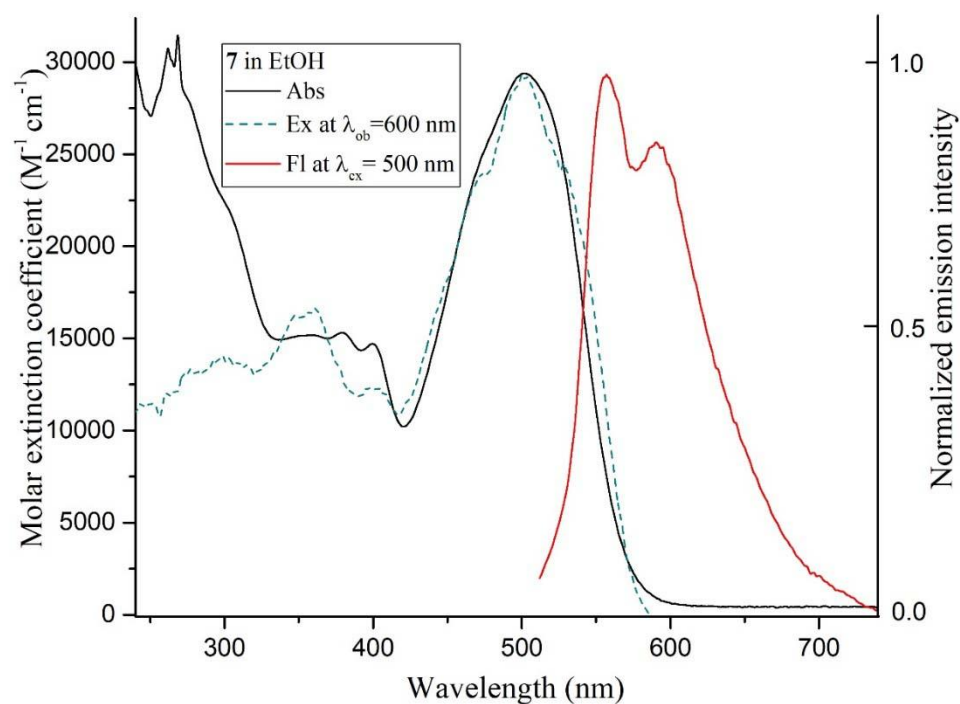


Figure S25 Absorption, emission, and excitation spectra for **7** in ethanol.

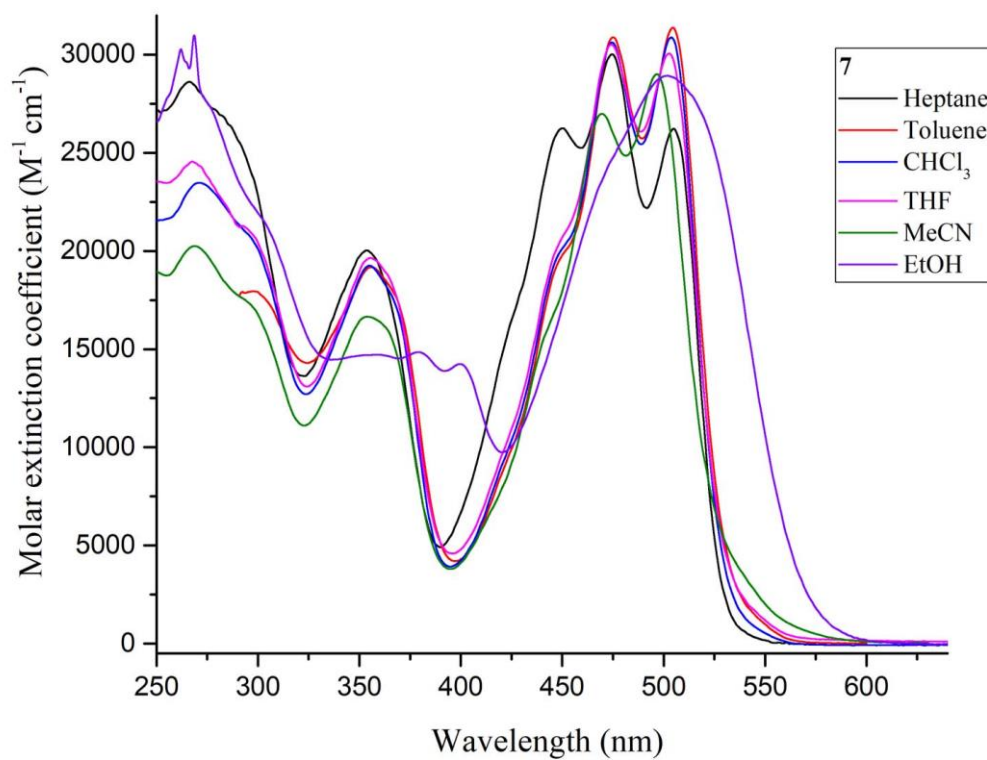


Figure S26 Absorption **7** in different solvents.

Computational methods

DFT calculations were performed using B3LYP^{S4-S6} together with the standard 6-311++G(d,p) basis set. Geometry optimization was carried out using Bemy's analytical gradient optimization method. The stationary points of the MEPs were characterized by frequency calculations. Solvent effects were considered in the context of a polarizable continuum model (PCM)^{S7}. All calculations were carried out using the Gaussian 16 suite of programs^{S8}.

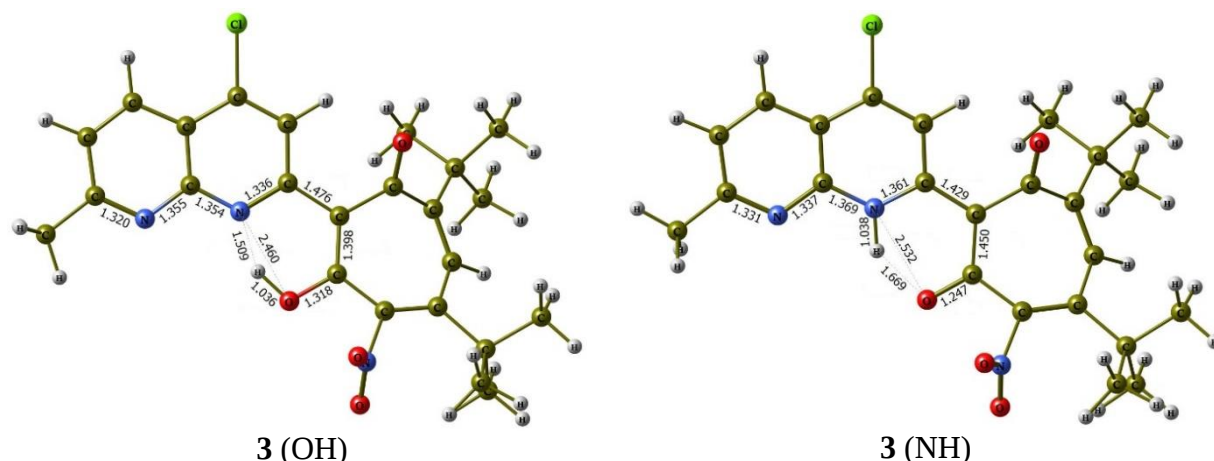


Figure S27 Optimized structures of (NH) and (OH) isomers of tropolone **3** according to B3LYP/6-311 ++G(d,p) calculations in the gas phase. Bond lengths are given in angstroms.

Table S11 Optimized geometries of tropolone **3** isomers. B3LYP/6-311++G(d,p) calculations in the gas phase. Coordinates in Angstroms.

3 (OH)				3 (NH)			
17	4.295435000	2.844510000	-1.153039000	17	4.217754000	2.790944000	-1.403362000
1	6.203781000	1.022674000	-0.379072000	1	6.183536000	1.023321000	-0.624797000
7	3.987882000	-2.002104000	0.657491000	7	4.045002000	-1.904697000	0.759201000
6	4.180929000	0.278762000	-0.178768000	6	4.185669000	0.298578000	-0.258430000
7	2.062546000	-0.849682000	0.165201000	7	2.100196000	-0.779968000	0.269822000
1	1.000853000	-1.900266000	0.381671000	1	1.567970000	-1.591966000	0.635700000
6	3.416017000	-0.856995000	0.213465000	6	3.468632000	-0.807169000	0.259362000
6	5.587442000	0.180985000	-0.089697000	6	5.586980000	0.206849000	-0.238511000
6	1.382023000	0.216881000	-0.263744000	6	1.331714000	0.238800000	-0.204313000
8	0.004400000	-2.182617000	0.356713000	8	-0.027158000	-2.076722000	0.718564000
8	-0.552488000	2.102129000	-1.463327000	8	-0.589821000	2.123546000	-1.352123000
6	5.303740000	-2.072453000	0.730651000	6	5.373755000	-1.974624000	0.769839000
6	-0.090426000	0.115787000	-0.251786000	6	-0.092211000	0.137072000	-0.136205000
6	-2.055777000	1.620184000	0.298469000	6	-2.114477000	1.586566000	0.371736000
6	-3.210063000	-0.628046000	-0.016231000	6	-3.215630000	-0.668465000	-0.044815000
6	-2.114381000	-1.418764000	-0.150236000	6	-2.109605000	-1.440181000	-0.093207000
6	-0.891586000	1.311429000	-0.592011000	6	-0.913620000	1.309588000	-0.492469000
6	-3.051016000	0.730353000	0.484229000	6	-3.100524000	0.685393000	0.508174000
1	-3.901510000	1.070346000	1.058872000	1	-3.968526000	0.983645000	1.081646000
6	6.145759000	-0.985889000	0.362537000	6	6.181073000	-0.927313000	0.274471000
1	7.221425000	-1.090784000	0.441795000	1	7.259424000	-1.020534000	0.300094000
6	-4.691307000	-1.062425000	-0.225625000	6	-4.666434000	-1.097154000	-0.402172000
6	3.443158000	1.402697000	-0.633936000	6	3.399970000	1.389386000	-0.748902000

6	2.078021000	1.387682000	-0.691597000	6	2.039899000	1.369749000	-0.735909000
1	1.531987000	2.229203000	-1.083568000	1	1.467777000	2.181272000	-1.153537000
6	-4.897755000	-2.221914000	-1.227923000	6	-4.762709000	-2.221017000	-1.459264000
1	-4.377532000	-2.040996000	-2.170719000	1	-4.154194000	-2.000897000	-2.339116000
1	-5.965192000	-2.292505000	-1.449450000	1	-5.802355000	-2.294492000	-1.787528000
1	-4.597021000	-3.192109000	-0.839257000	1	-4.486200000	-3.200767000	-1.076194000
6	-0.693651000	-1.113831000	0.028048000	6	-0.686434000	-1.127427000	0.249959000
6	-2.105223000	3.037691000	0.912650000	6	-2.180956000	2.984532000	1.027290000
6	-2.534831000	4.065105000	-0.163415000	6	-2.576782000	4.047989000	-0.026065000
1	-3.529043000	3.825894000	-0.551102000	1	-3.560016000	3.824019000	-0.449179000
1	-1.837444000	4.079209000	-0.999362000	1	-1.856709000	4.086206000	-0.841730000
1	-2.575774000	5.064830000	0.280945000	1	-2.628075000	5.033350000	0.448634000
6	-0.710691000	3.419147000	1.462588000	6	-0.802887000	3.345217000	1.630609000
1	-0.377532000	2.708716000	2.224787000	1	-0.494962000	2.611256000	2.381061000
1	-0.756695000	4.408823000	1.924872000	1	-0.859263000	4.321431000	2.119969000
1	0.040919000	3.461113000	0.673747000	1	-0.027687000	3.406409000	0.865418000
6	-3.104305000	3.113372000	2.083965000	6	-3.215204000	3.025099000	2.169258000
1	-4.140199000	2.986614000	1.758926000	1	-4.239463000	2.901090000	1.808253000
1	-3.036657000	4.101731000	2.545730000	1	-3.167581000	4.001224000	2.659072000
1	-2.887888000	2.368395000	2.854676000	1	-3.018753000	2.260367000	2.925807000
6	-5.282402000	-1.464218000	1.147079000	6	-5.379166000	-1.550506000	0.894397000
1	-4.759120000	-2.329336000	1.557848000	1	-4.889452000	-2.427756000	1.320338000
1	-6.338966000	-1.722248000	1.029206000	1	-6.418831000	-1.807584000	0.670577000
1	-5.219215000	-0.648514000	1.872577000	1	-5.388930000	-0.761040000	1.651132000
6	-5.494847000	0.132930000	-0.804069000	6	-5.419003000	0.116853000	-1.006907000
1	-5.073195000	0.468503000	-1.755259000	1	-4.917771000	0.484079000	-1.906440000
1	-5.542521000	0.991667000	-0.134266000	1	-5.520950000	0.952049000	-0.313467000
1	-6.522425000	-0.189638000	-0.987483000	1	-6.427394000	-0.196642000	-1.287868000
8	-1.965431000	-3.267964000	-1.548940000	8	-1.725796000	-3.245974000	-1.496818000
7	-2.263892000	-2.884350000	-0.431922000	7	-2.189327000	-2.894857000	-0.424156000
8	-2.659556000	-3.589535000	0.481865000	8	-2.687429000	-3.634453000	0.408920000
6	5.907230000	-3.359703000	1.224303000	6	5.976645000	-3.230240000	1.335497000
1	6.514654000	-3.185983000	2.118084000	1	7.066693000	-3.195692000	1.328539000
1	5.119507000	-4.072545000	1.462423000	1	5.631918000	-3.381729000	2.361545000
1	6.564921000	-3.795211000	0.465495000	1	5.646334000	-4.096635000	0.756266000

Table S12 Optimized geometries of tropolone **3** isomers. PCM/B3LYP/6-311++G(d,p) calculations (DMSO). Coordinates in Angstroms.

3 (OH)				3 (NH)			
17	4.280424000	2.911864000	-0.964295000	17	4.227386000	2.832356000	-1.229860000
1	6.202355000	1.057185000	-0.291822000	1	6.195557000	1.036656000	-0.494085000
7	3.995850000	-2.032323000	0.562033000	7	4.034469000	-1.972465000	0.673439000
6	4.179406000	0.292303000	-0.148541000	6	4.188065000	0.283348000	-0.223955000
7	2.066660000	-0.864889000	0.113871000	7	2.097543000	-0.830579000	0.189244000
1	1.030303000	-1.886413000	0.322016000	1	1.562844000	-1.658310000	0.504371000
6	3.420843000	-0.867204000	0.175198000	6	3.466730000	-0.851002000	0.216131000
6	5.586853000	0.199165000	-0.054603000	6	5.591220000	0.199800000	-0.169432000
6	1.381492000	0.219843000	-0.260522000	6	1.337984000	0.206014000	-0.244534000
8	0.025513000	-2.191729000	0.326763000	8	-0.042328000	-2.151827000	0.564496000
8	-0.564823000	2.040696000	-1.547031000	8	-0.602551000	2.028112000	-1.488083000
6	5.314582000	-2.097573000	0.642081000	6	5.364779000	-2.034014000	0.718350000
6	-0.091468000	0.106795000	-0.264746000	6	-0.095226000	0.095297000	-0.199093000
6	-2.054931000	1.622176000	0.249078000	6	-2.068564000	1.598589000	0.322588000
6	-3.209778000	-0.636666000	-0.001560000	6	-3.236988000	-0.632646000	-0.017038000
6	-2.111620000	-1.427478000	-0.134924000	6	-2.145913000	-1.426009000	-0.113433000
6	-0.897505000	1.289288000	-0.636058000	6	-0.908497000	1.267295000	-0.572275000
6	-3.046928000	0.732996000	0.461770000	6	-3.071892000	0.724369000	0.507719000
1	-3.897182000	1.089239000	1.026062000	1	-3.914462000	1.056060000	1.099168000
6	6.149532000	-0.986162000	0.337959000	6	6.176562000	-0.954757000	0.300598000

1	7.224589000	-1.088415000	0.419697000	1	7.253773000	-1.042707000	0.353138000
6	-4.694290000	-1.069937000	-0.184162000	6	-4.713440000	-1.030517000	-0.298678000
6	3.437131000	1.435661000	-0.541645000	6	3.409207000	1.391710000	-0.675548000
6	2.071249000	1.416096000	-0.608959000	6	2.046317000	1.363563000	-0.697218000
1	1.528084000	2.284284000	-0.940577000	1	1.488252000	2.202474000	-1.075180000
6	-4.919518000	-2.287004000	-1.109608000	6	-4.896999000	-2.198039000	-1.293918000
1	-4.414468000	-2.165917000	-2.070044000	1	-4.333115000	-2.036406000	-2.215191000
1	-5.990144000	-2.362280000	-1.310285000	1	-5.954332000	-2.251816000	-1.561904000
1	-4.623029000	-3.234309000	-0.663738000	1	-4.633635000	-3.168703000	-0.878266000
6	-0.690218000	-1.122298000	0.013893000	6	-0.700223000	-1.159561000	0.159673000
6	-2.111722000	3.054390000	0.829120000	6	-2.074867000	3.005466000	0.962462000
6	-2.570785000	4.048623000	-0.265715000	6	-2.457989000	4.071308000	-0.092979000
1	-3.564200000	3.783421000	-0.637528000	1	-3.451581000	3.869720000	-0.502674000
1	-1.879255000	4.060844000	-1.107169000	1	-1.744662000	4.092458000	-0.915675000
1	-2.624220000	5.055942000	0.158665000	1	-2.478537000	5.058664000	0.378769000
6	-0.715201000	3.467653000	1.349017000	6	-0.672521000	3.324760000	1.531646000
1	-0.357867000	2.776098000	2.117195000	1	-0.373364000	2.588380000	2.282782000
1	-0.773596000	4.463794000	1.794928000	1	-0.687547000	4.307194000	2.010781000
1	0.023942000	3.511081000	0.548428000	1	0.089778000	3.353166000	0.751304000
6	-3.096075000	3.144783000	2.011996000	6	-3.083831000	3.091414000	2.124111000
1	-4.134651000	3.000776000	1.704814000	1	-4.118331000	2.996361000	1.785208000
1	-3.029070000	4.143720000	2.449992000	1	-2.991415000	4.070752000	2.600486000
1	-2.859736000	2.418435000	2.794249000	1	-2.894996000	2.328897000	2.884528000
6	-5.290104000	-1.378504000	1.210886000	6	-5.388799000	-1.396545000	1.045113000
1	-4.779110000	-2.224103000	1.675820000	1	-4.915979000	-2.272391000	1.493993000
1	-6.348279000	-1.632166000	1.103432000	1	-6.443559000	-1.625887000	0.869713000
1	-5.220368000	-0.521832000	1.885407000	1	-5.342587000	-0.574764000	1.763835000
6	-5.480938000	0.098693000	-0.836617000	6	-5.446852000	0.181592000	-0.931660000
1	-5.058585000	0.360048000	-1.810457000	1	-4.971616000	0.481758000	-1.869380000
1	-5.508098000	0.999598000	-0.224457000	1	-5.487085000	1.051963000	-0.277027000
1	-6.514320000	-0.219349000	-0.991479000	1	-6.476697000	-0.108031000	-1.152943000
8	-1.987555000	-3.324882000	-1.483692000	8	-1.903991000	-3.272775000	-1.510897000
7	-2.258147000	-2.900891000	-0.371625000	7	-2.277371000	-2.883934000	-0.413922000
8	-2.607448000	-3.591483000	0.573358000	8	-2.710342000	-3.609487000	0.468872000
6	5.931584000	-3.399585000	1.070189000	6	5.968589000	-3.308991000	1.233940000
1	6.538376000	-3.259704000	1.969720000	1	7.056889000	-3.257628000	1.258083000
1	5.158618000	-4.139346000	1.273029000	1	5.601196000	-3.517701000	2.242123000
1	6.597120000	-3.782734000	0.290823000	1	5.669747000	-4.148229000	0.599806000

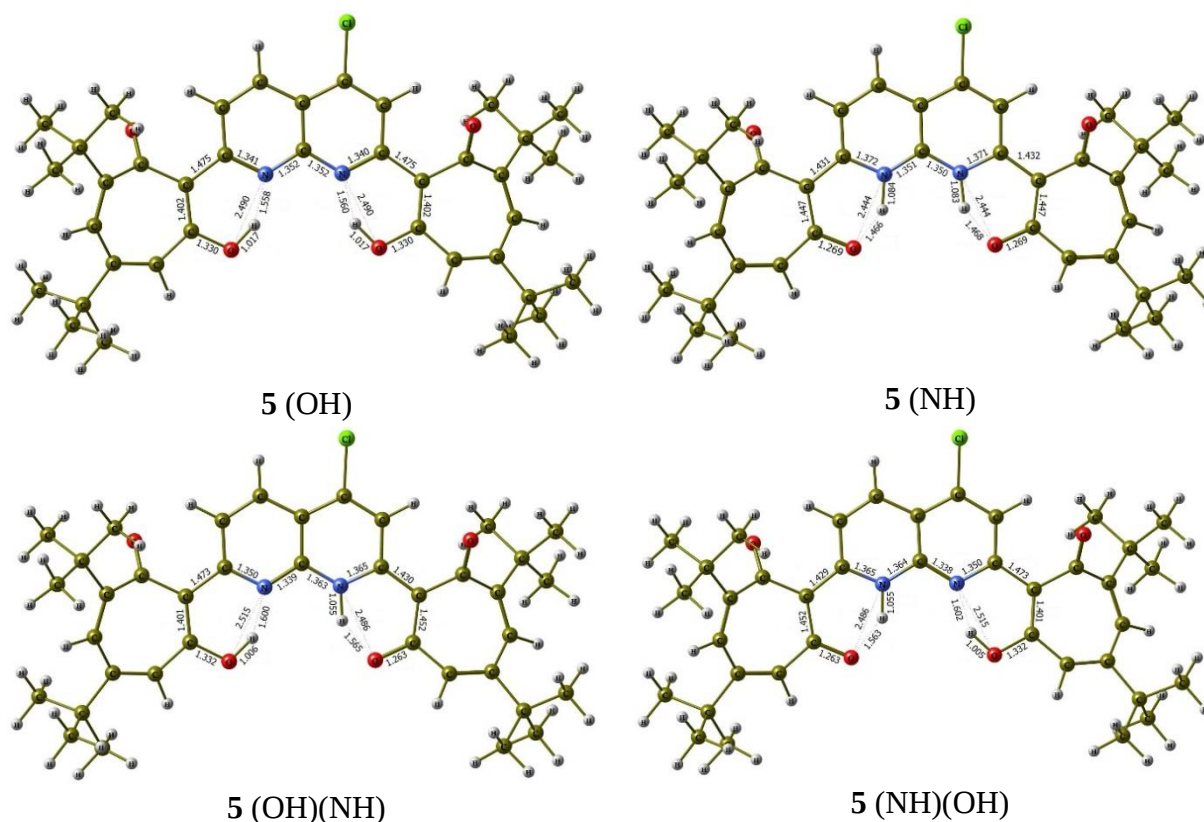


Figure S28 Optimized structures of tropolone 5 isomers according to B3LYP/6-311 ++G(d,p) calculations in the gas phase. Bond lengths are given in angstroms.

Table S13 Optimized geometries of tropolone 5 isomers. B3LYP/6-311++G(d,p) calculations in the gas phase. Coordinates in Angstroms.

5 (OH)				5 (NH)			
17	1.360689000	-4.941870000	-0.163142000	17	-1.361529000	-4.991673000	0.126517000
1	-1.304953000	-4.324327000	0.190832000	1	1.309063000	-4.377482000	-0.166269000
7	-1.198934000	-0.472936000	0.143404000	7	1.209379000	-0.563997000	-0.126475000
1	-1.567776000	1.036917000	0.253221000	1	1.313016000	0.514423000	-0.158170000
6	-0.033360000	-2.585501000	0.014459000	6	0.031612000	-2.643433000	-0.015071000
7	1.083484000	-0.434547000	-0.127571000	7	-1.095221000	-0.525024000	0.114092000
1	1.412958000	1.083475000	-0.266286000	1	-1.168567000	0.555084000	0.157197000
8	-2.269765000	1.763043000	0.372276000	8	2.222364000	1.649856000	-0.341271000
8	-5.013059000	-1.888967000	1.268386000	8	5.083889000	-1.982627000	-1.056680000
6	-0.045412000	-1.165631000	0.009392000	6	0.044885000	-1.238126000	-0.008349000
6	-1.274353000	-3.242127000	0.175746000	6	1.283816000	-3.295334000	-0.155023000
6	2.278411000	-1.022354000	-0.277673000	6	-2.337905000	-1.087575000	0.252243000
8	2.096353000	1.823758000	-0.402372000	8	-2.049486000	1.711823000	0.357462000
8	4.946032000	-1.774762000	-1.199912000	8	-5.013805000	-1.859034000	0.990441000
6	-3.577643000	-0.235238000	0.385591000	6	3.578497000	-0.298970000	-0.354559000
6	-2.379214000	-1.090119000	0.296502000	6	2.437224000	-1.158542000	-0.270552000
6	-6.073351000	-0.408861000	-0.223071000	6	6.062348000	-0.341419000	0.319797000
6	3.456793000	-0.139705000	-0.371931000	6	-3.458438000	-0.200013000	0.340480000
6	5.949051000	-0.230964000	0.265614000	6	-5.937314000	-0.159055000	-0.351120000
6	5.653906000	2.200513000	-0.394003000	6	-5.580613000	2.199245000	0.524269000
6	-5.836814000	2.045606000	0.373983000	6	5.766138000	2.043627000	-0.504575000
6	4.325425000	2.238569000	-0.667588000	6	-4.256075000	2.194449000	0.794476000
1	3.895030000	3.159575000	-1.036979000	1	-3.807832000	3.063084000	1.258321000

6	-4.894458000	-0.887891000	0.567945000	6	4.913889000	-0.924460000	-0.454647000
6	-6.462345000	0.886981000	-0.228843000	6	6.408177000	0.959072000	0.226699000
1	-7.400483000	1.099822000	-0.723344000	1	7.317231000	1.250951000	0.735438000
6	4.792414000	-0.760051000	-0.526051000	6	-4.810615000	-0.790414000	0.416936000
6	6.304164000	1.074297000	0.243156000	6	-6.248272000	1.148118000	-0.232281000
1	7.230921000	1.324160000	0.741837000	1	-7.145877000	1.475406000	-0.739779000
6	-2.426382000	-2.519072000	0.323476000	6	2.446294000	-2.588497000	-0.287953000
1	-3.365346000	-3.019316000	0.488655000	1	3.384309000	-3.095022000	-0.438491000
6	-3.454698000	1.160689000	0.422316000	6	3.378033000	1.132282000	-0.431657000
6	6.547185000	3.433300000	-0.659752000	6	-6.466020000	3.402336000	0.919512000
6	-6.918540000	-1.495537000	-0.933306000	6	6.907380000	-1.338454000	1.151038000
6	1.236317000	-3.192888000	-0.145921000	6	-1.249744000	-3.246817000	0.121846000
6	2.371831000	-2.447558000	-0.300269000	6	-2.394752000	-2.513977000	0.262202000
1	3.321195000	-2.925421000	-0.469275000	1	-3.345146000	-2.995992000	0.414339000
6	-5.993741000	-2.525851000	-1.622832000	6	5.979093000	-2.307766000	1.920583000
1	-5.387769000	-3.073410000	-0.901904000	1	5.388895000	-2.926312000	1.244811000
1	-5.328344000	-2.041114000	-2.343503000	1	5.298101000	-1.761977000	2.580622000
1	-6.599832000	-3.255555000	-2.166623000	1	6.580566000	-2.977395000	2.541599000
6	5.817464000	4.546119000	-1.433758000	6	-5.730964000	4.415290000	1.815587000
1	5.431146000	4.189501000	-2.392136000	1	-5.351725000	3.949496000	2.728838000
1	6.518215000	5.359006000	-1.640937000	1	-6.425699000	5.206292000	2.110013000
1	4.987356000	4.970690000	-0.863647000	1	-4.894265000	4.892467000	1.299487000
6	-4.508050000	2.125344000	0.637272000	6	4.441121000	2.080658000	-0.770378000
1	-4.100179000	3.066105000	0.981519000	1	4.015929000	2.970569000	-1.215137000
6	-6.760429000	3.261115000	0.615016000	6	6.682724000	3.230273000	-0.878325000
6	3.296515000	1.251537000	-0.435807000	6	-3.218387000	1.223981000	0.439304000
6	-7.819546000	-0.886314000	-2.027704000	6	7.775361000	-0.609939000	2.197669000
1	-8.610258000	-0.253371000	-1.617189000	1	8.562379000	-0.004333000	1.741231000
1	-8.313890000	-1.695293000	-2.571784000	1	8.272829000	-1.353203000	2.826211000
1	-7.244676000	-0.298873000	-2.749052000	1	7.176535000	0.033341000	2.848436000
6	6.811462000	-1.277909000	1.013708000	6	-6.802268000	-1.114574000	-1.210328000
6	7.744139000	-2.011444000	0.018413000	6	-7.768813000	-1.922951000	-0.310109000
1	8.411421000	-1.302256000	-0.479855000	1	-8.434668000	-1.251781000	0.240001000
1	7.171724000	-2.536625000	-0.744130000	1	-7.223454000	-2.529672000	0.410366000
1	8.362908000	-2.734918000	0.559594000	1	-8.387790000	-2.578972000	-0.931247000
6	5.902067000	-2.308302000	1.723576000	6	-5.893614000	-2.088027000	-1.998080000
1	5.219760000	-1.817843000	2.424309000	1	-5.195953000	-1.543552000	-2.641628000
1	6.518091000	-3.009338000	2.293262000	1	-6.507946000	-2.727534000	-2.637935000
1	5.314800000	-2.889517000	1.013585000	1	-5.322582000	-2.737334000	-1.334832000
6	-6.054773000	4.412781000	1.353756000	6	5.972483000	4.281568000	-1.749892000
1	-5.652610000	4.092084000	2.318292000	1	5.577590000	3.845711000	-2.671238000
1	-6.775176000	5.212362000	1.544703000	1	6.687520000	5.059460000	-2.030306000
1	-5.240040000	4.843459000	0.766316000	1	5.150858000	4.770240000	-1.220514000
6	-7.824852000	-2.220763000	0.092030000	6	7.847819000	-2.148604000	0.225189000
1	-7.233161000	-2.709210000	0.864307000	1	7.282774000	-2.721867000	-0.507471000
1	-8.431136000	-2.974440000	-0.421405000	1	8.452577000	-2.836384000	0.825681000
1	-8.504295000	-1.512920000	0.575522000	1	8.528168000	-1.481217000	-0.311590000
6	-7.265892000	3.807705000	-0.742717000	6	7.174098000	3.935037000	0.409911000
1	-6.428943000	4.126152000	-1.369824000	1	6.329988000	4.315235000	0.991298000
1	-7.913221000	4.673541000	-0.575368000	1	7.814255000	4.782351000	0.147043000
1	-7.845287000	3.070463000	-1.302677000	1	7.757470000	3.273894000	1.054526000
6	7.687628000	-0.617700000	2.098546000	6	-7.645255000	-0.339539000	-2.243907000
1	8.468080000	0.020997000	1.677325000	1	-8.419257000	0.275126000	-1.777377000
1	8.194348000	-1.399671000	2.669967000	1	-8.157758000	-1.054984000	-2.892320000
1	7.092755000	-0.023240000	2.797589000	1	-7.026495000	0.303269000	-2.876248000
6	7.027044000	4.028158000	0.686915000	6	-6.932781000	4.147058000	-0.355315000
1	6.176961000	4.340708000	1.299150000	1	-6.076297000	4.515852000	-0.925846000
1	7.652895000	4.906071000	0.501756000	1	-7.550431000	5.006040000	-0.076920000
1	7.620898000	3.321247000	1.270334000	1	-7.531635000	3.515781000	-1.015493000
6	7.770997000	2.996297000	-1.500656000	6	-7.698581000	2.885350000	1.699733000
1	7.455530000	2.583830000	-2.462902000	1	-7.392710000	2.367407000	2.612869000
1	8.372789000	2.238891000	-0.994172000	1	-8.301765000	2.192372000	1.109433000

1	8.415978000	3.857862000	-1.695943000	1	-8.339109000	3.725110000	1.984483000
6	-7.966020000	2.814584000	1.476979000	6	7.897936000	2.696648000	-1.674431000
1	-7.632631000	2.435975000	2.447066000	1	7.574692000	2.206602000	-2.596934000
1	-8.551426000	2.028647000	0.995362000	1	8.484336000	1.975281000	-1.101490000
1	-8.632036000	3.663814000	1.654946000	1	8.559971000	3.524579000	-1.944246000
5 (OH)(NH)				5 (NH)(OH)			
17	-1.350188000	-4.951320000	0.234112000	17	1.376385000	-4.950608000	-0.060921000
1	1.317092000	-4.332291000	-0.110144000	1	-1.305208000	-4.337822000	0.251259000
7	1.191336000	-0.482654000	-0.170356000	7	-1.212948000	-0.528135000	0.102476000
1	1.571216000	1.059474000	-0.363067000	1	-1.274448000	0.525085000	0.091043000
6	0.038822000	-2.600113000	0.011802000	6	-0.027282000	-2.604029000	0.040085000
7	-1.099087000	-0.486042000	0.088586000	7	1.075306000	-0.449222000	-0.160527000
1	-1.132789000	0.568332000	0.085511000	1	1.413719000	1.099030000	-0.391965000
8	2.277325000	1.759027000	-0.515111000	8	-2.275040000	1.714023000	0.262450000
8	5.044674000	-1.927693000	-1.179493000	8	-5.072058000	-1.943863000	1.117089000
6	0.063507000	-1.189073000	-0.025000000	6	-0.027230000	-1.192693000	-0.009298000
6	1.280076000	-3.250485000	-0.124039000	6	-1.280834000	-3.256170000	0.209986000
6	-2.334902000	-1.039839000	0.256126000	6	2.283615000	-1.037598000	-0.284368000
8	-2.104953000	1.780000000	0.271934000	8	2.101677000	1.811391000	-0.564726000
8	-5.000546000	-1.822907000	1.052087000	8	4.980628000	-1.816127000	-1.102647000
6	3.578136000	-0.245010000	-0.403354000	6	-3.584984000	-0.267160000	0.350854000
6	2.384564000	-1.101004000	-0.298181000	6	-2.434965000	-1.112096000	0.276227000
6	6.055873000	-0.385803000	0.283137000	6	-6.069273000	-0.359426000	-0.311598000
6	-3.465972000	-0.168307000	0.332904000	6	3.456436000	-0.153312000	-0.396198000
6	-5.946808000	-0.183077000	-0.347371000	6	5.926814000	-0.203191000	0.325569000
6	-5.638067000	2.191854000	0.491964000	6	5.655385000	2.184398000	-0.481841000
6	5.841262000	2.032183000	-0.448859000	6	-5.817990000	2.037696000	0.483000000
6	-4.313091000	2.216351000	0.754169000	6	4.335788000	2.204335000	-0.798037000
1	-3.880053000	3.096407000	1.211158000	1	3.917022000	3.102111000	-1.232256000
6	4.902947000	-0.901448000	-0.522891000	6	-4.911755000	-0.905485000	0.478769000
6	6.446880000	0.908211000	0.234860000	6	-6.440663000	0.934446000	-0.239464000
1	7.368699000	1.147424000	0.747720000	1	-7.351723000	1.204282000	-0.757107000
6	-4.809121000	-0.774256000	0.438792000	6	4.800383000	-0.774633000	-0.479970000
6	-6.285328000	1.118369000	-0.253208000	6	6.283427000	1.098878000	0.242624000
1	-7.186062000	1.421040000	-0.770746000	1	7.191275000	1.378922000	0.759759000
6	2.433925000	-2.523725000	-0.285979000	6	-2.438722000	-2.547783000	0.332139000
1	3.374160000	-3.026389000	-0.434487000	1	-3.375392000	-3.050346000	0.503280000
6	3.460582000	1.146957000	-0.510541000	6	-3.409089000	1.173623000	0.390617000
6	-6.548834000	3.377058000	0.883363000	6	6.557050000	3.399894000	-0.792782000
6	6.872669000	-1.436764000	1.074877000	6	-6.886877000	-1.387339000	-1.131959000
6	-1.243567000	-3.204725000	0.178184000	6	1.242074000	-3.205701000	-0.094754000
6	-2.384933000	-2.472430000	0.306367000	6	2.379262000	-2.456008000	-0.265046000
1	-3.333283000	-2.951497000	0.479358000	1	3.330281000	-2.936348000	-0.416355000
6	5.920481000	-2.427545000	1.784690000	6	-5.932421000	-2.347862000	-1.879967000
1	5.334575000	-3.008434000	1.073100000	1	-5.332970000	-2.942115000	-1.190422000
1	5.235099000	-1.904670000	2.458442000	1	-5.258901000	-1.797879000	-2.544084000
1	6.504495000	-3.131694000	2.383455000	1	-6.514387000	-3.041129000	-2.493687000
6	-5.832429000	4.412473000	1.768700000	6	5.852886000	4.462954000	-1.655210000
1	-5.438585000	3.961347000	2.683140000	1	5.496411000	4.048610000	-2.601859000
1	-6.542935000	5.190281000	2.060982000	1	6.560669000	5.262211000	-1.889394000
1	-5.008635000	4.903730000	1.245062000	1	5.005997000	4.920993000	-1.138160000
6	4.519961000	2.097718000	-0.751647000	6	-4.493249000	2.101192000	0.740169000
1	4.122781000	3.019080000	-1.155620000	1	-4.082178000	3.000250000	1.180087000
6	6.773066000	3.231905000	-0.731428000	6	-6.757644000	3.206194000	0.856354000
6	-3.252365000	1.266847000	0.391421000	6	3.300737000	1.231903000	-0.537782000
6	7.739628000	-0.773975000	2.165446000	6	-7.763791000	-0.694097000	-2.194843000
1	8.545596000	-0.164722000	1.748857000	1	-8.565173000	-0.097339000	-1.751961000
1	8.212940000	-1.554839000	2.766253000	1	-8.242711000	-1.457236000	-2.814056000
1	7.143820000	-0.149054000	2.836517000	1	-7.174485000	-0.048975000	-2.852409000
6	-6.784085000	-1.174056000	-1.193201000	6	6.756807000	-1.207205000	1.163114000
6	-7.737301000	-1.987627000	-0.283674000	6	7.723488000	-1.997474000	0.246944000
1	-8.423165000	-1.321856000	0.248099000	1	8.411699000	-1.318753000	-0.265001000

1	-7.182480000	-2.565515000	0.453171000	1	7.178956000	-2.564548000	-0.505962000
1	-8.335475000	-2.671395000	-0.895338000	1	8.318489000	-2.689803000	0.851629000
6	-5.848139000	-2.141218000	-1.956087000	6	5.816567000	-2.193771000	1.894687000
1	-5.158389000	-1.593509000	-2.605301000	1	5.112701000	-1.663115000	2.542835000
1	-6.442817000	-2.807636000	-2.587098000	1	6.407579000	-2.865286000	2.523302000
1	-5.266733000	-2.764135000	-1.276504000	1	5.251257000	-2.810739000	1.196895000
6	6.090755000	4.339600000	-1.554394000	6	-6.065277000	4.275652000	1.720088000
1	5.715333000	3.964533000	-2.510060000	1	-5.657337000	3.851631000	2.641283000
1	6.817943000	5.126480000	-1.770327000	1	-6.794555000	5.040361000	2.000456000
1	5.260894000	4.803916000	-1.015813000	1	-5.255837000	4.777985000	1.184719000
6	7.808775000	-2.215617000	0.118045000	6	-7.814881000	-2.203981000	-0.199444000
1	7.241099000	-2.741788000	-0.647458000	1	-7.241786000	-2.750908000	0.547057000
1	8.394901000	-2.943301000	0.689007000	1	-8.398918000	-2.916067000	-0.792197000
1	8.506308000	-1.534973000	-0.378458000	1	-8.514424000	-1.543797000	0.321341000
6	7.239827000	3.854023000	0.607581000	6	-7.270038000	3.895326000	-0.432049000
1	6.385772000	4.207439000	1.191346000	1	-6.436823000	4.291201000	-1.018720000
1	7.892959000	4.709031000	0.410252000	1	-7.927436000	4.729660000	-0.169857000
1	7.801942000	3.149688000	1.224612000	1	-7.841609000	3.218929000	-1.071426000
6	-7.637786000	-0.437991000	-2.246117000	6	7.593649000	-0.487323000	2.240829000
1	-8.427127000	0.168802000	-1.795236000	1	8.390622000	0.126349000	1.813437000
1	-8.131265000	-1.176619000	-2.883332000	1	8.076983000	-1.236066000	2.873666000
1	-7.029358000	0.205941000	-2.887248000	1	6.974814000	0.145688000	2.882860000
6	-7.038786000	4.102311000	-0.393883000	6	6.994613000	4.074877000	0.530369000
1	-6.193646000	4.486664000	-0.971076000	1	6.126095000	4.421637000	1.096510000
1	-7.675021000	4.948743000	-0.118593000	1	7.625418000	4.941514000	0.312263000
1	-7.625803000	3.452626000	-1.046830000	1	7.570837000	3.405505000	1.172785000
6	-7.765639000	2.837843000	1.672980000	6	7.806491000	2.913676000	-1.566381000
1	-7.443670000	2.333399000	2.588152000	1	7.521610000	2.444186000	-2.511875000
1	-8.354687000	2.126587000	1.090147000	1	8.390917000	2.188516000	-0.996286000
1	-8.424523000	3.664394000	1.954845000	1	8.458394000	3.762418000	-1.792159000
6	8.002246000	2.736617000	-1.531323000	6	-7.957715000	2.650735000	1.660221000
1	7.696498000	2.303757000	-2.487722000	1	-7.619914000	2.171573000	2.583243000
1	8.572389000	1.979347000	-0.989191000	1	-8.530424000	1.914132000	1.092797000
1	8.674468000	3.574355000	-1.737791000	1	-8.636535000	3.465279000	1.929457000

Table S14 Optimized geometries of tropolone 5 isomers. PCM/B3LYP/6-311++G(d,p) calculations (DMSO). Coordinates in Angstroms.

5 (OH)				5 (NH)			
17	1.360172000	-4.890853000	-0.174672000	17	1.361869000	-4.948022000	-0.137368000
1	-1.320287000	-4.272836000	0.102439000	1	-1.317501000	-4.336103000	0.152908000
7	-1.198297000	-0.420887000	0.123780000	7	-1.208923000	-0.525182000	0.138781000
1	-1.582309000	1.075437000	0.107587000	1	-1.291747000	0.537420000	0.152525000
6	-0.036700000	-2.534491000	-0.016755000	6	-0.033988000	-2.603118000	0.012028000
7	1.085620000	-0.384900000	-0.131709000	7	1.093699000	-0.486842000	-0.116684000
1	1.431100000	1.120322000	-0.142580000	1	1.147102000	0.576947000	-0.134634000
8	-2.288552000	1.811461000	0.142113000	8	-2.249914000	1.710459000	0.307821000
8	-4.920748000	-1.757669000	1.473456000	8	-5.062210000	-1.896390000	1.212271000
6	-0.045534000	-1.115507000	-0.008803000	6	-0.045957000	-1.199784000	0.010917000
6	-1.281680000	-3.191165000	0.113356000	6	-1.285719000	-3.254459000	0.152398000
6	2.280585000	-0.973007000	-0.272976000	6	2.333999000	-1.045718000	-0.263503000
8	2.118617000	1.872774000	-0.197006000	8	2.077488000	1.773239000	-0.305890000
8	4.876755000	-1.656325000	-1.403968000	8	4.989802000	-1.779679000	-1.142960000
6	-3.581274000	-0.184569000	0.343335000	6	-3.579989000	-0.256775000	0.371171000
6	-2.380275000	-1.037528000	0.258423000	6	-2.435382000	-1.116005000	0.285271000
6	-6.101994000	-0.456544000	-0.099472000	6	-6.060325000	-0.370984000	-0.286806000
6	3.463791000	-0.093880000	-0.347104000	6	3.458985000	-0.159540000	-0.351256000
6	5.976886000	-0.284261000	0.166582000	6	5.937517000	-0.190438000	0.320778000
6	5.691791000	2.208582000	-0.230131000	6	5.624630000	2.200499000	-0.468036000

6	-5.870632000	2.055392000	0.212291000	6	-5.809243000	2.044862000	0.447702000
6	4.353821000	2.292146000	-0.453724000	6	4.297987000	2.227448000	-0.735917000
1	3.932272000	3.254411000	-0.711248000	1	3.872343000	3.120347000	-1.175069000
6	-4.872572000	-0.834034000	0.660020000	6	-4.907384000	-0.887347000	0.522293000
6	-6.505721000	0.830684000	-0.223896000	6	-6.428928000	0.926496000	-0.250578000
1	-7.475358000	0.978282000	-0.678853000	1	-7.338049000	1.183422000	-0.777363000
6	4.779655000	-0.714108000	-0.616393000	6	4.803126000	-0.756606000	-0.480999000
6	6.346850000	1.015271000	0.260780000	6	6.272319000	1.114951000	0.256131000
1	7.299662000	1.201606000	0.736815000	1	7.172055000	1.407946000	0.780184000
6	-2.432645000	-2.464952000	0.255224000	6	-2.445553000	-2.543936000	0.293257000
1	-3.374930000	-2.971979000	0.372997000	1	-3.381292000	-3.058170000	0.427935000
6	-3.475864000	1.210563000	0.266286000	6	-3.402238000	1.176202000	0.410926000
6	6.594469000	3.451355000	-0.395926000	6	6.531842000	3.397384000	-0.828859000
6	-6.984592000	-1.614765000	-0.631989000	6	-6.873413000	-1.417934000	-1.088069000
6	1.234924000	-3.142735000	-0.160033000	6	1.246354000	-3.206225000	-0.131837000
6	2.373036000	-2.396891000	-0.293049000	6	2.389837000	-2.469903000	-0.274515000
1	3.324555000	-2.880912000	-0.426195000	1	3.338294000	-2.957630000	-0.416048000
6	-6.104537000	-2.736656000	-1.230182000	6	-5.915382000	-2.398492000	-1.804244000
1	-5.485598000	-3.216457000	-0.472849000	1	-5.323100000	-2.980711000	-1.097948000
1	-5.455315000	-2.351879000	-2.022181000	1	-5.234242000	-1.866254000	-2.474702000
1	-6.745530000	-3.506373000	-1.667756000	1	-6.495942000	-3.102538000	-2.406352000
6	5.856813000	4.649675000	-1.020113000	6	5.818996000	4.446010000	-1.701359000
1	5.431924000	4.403132000	-1.996795000	1	5.433956000	4.010506000	-2.627270000
1	6.565639000	5.468796000	-1.163964000	1	6.531444000	5.229053000	-1.972856000
1	5.055334000	5.022607000	-0.377368000	1	4.990947000	4.927384000	-1.175045000
6	-4.531522000	2.180218000	0.409262000	6	-4.484151000	2.113036000	0.716820000
1	-4.131591000	3.160682000	0.629658000	1	-4.084091000	3.026548000	1.137047000
6	-6.801347000	3.280849000	0.352878000	6	-6.747455000	3.226298000	0.779878000
6	3.321099000	1.299605000	-0.297142000	6	3.242291000	1.267888000	-0.407908000
6	-7.931388000	-1.131393000	-1.750898000	6	-7.740394000	-0.746439000	-2.172808000
1	-8.697164000	-0.442821000	-1.386819000	1	-8.541824000	-0.136313000	-1.749637000
1	-8.453827000	-1.995914000	-2.168139000	1	-8.215533000	-1.523927000	-2.776569000
1	-7.384629000	-0.644141000	-2.562868000	1	-7.142963000	-0.119705000	-2.840500000
6	6.866303000	-1.405074000	0.763565000	6	6.770547000	-1.196936000	1.152939000
6	7.773650000	-2.007778000	-0.337099000	6	7.727430000	-1.998090000	0.236455000
1	8.417897000	-1.238284000	-0.771579000	1	8.409236000	-1.325128000	-0.291266000
1	7.182245000	-2.455104000	-1.134923000	1	7.176207000	-2.578857000	-0.501448000
1	8.415045000	-2.779802000	0.099924000	1	8.328901000	-2.681449000	0.844559000
6	5.989681000	-2.521621000	1.376762000	6	5.829335000	-2.173568000	1.896640000
1	5.314952000	-2.121961000	2.139507000	1	5.139464000	-1.634338000	2.552397000
1	6.631802000	-3.265734000	1.855066000	1	6.421702000	-2.850841000	2.517721000
1	5.397123000	-3.036814000	0.621483000	1	5.246627000	-2.785119000	1.207266000
6	-6.082588000	4.518906000	0.918837000	6	-6.063223000	4.313046000	1.628369000
1	-5.633408000	4.318847000	1.895267000	1	-5.669552000	3.909644000	2.565132000
1	-6.809114000	5.325023000	1.046949000	1	-6.795875000	5.084050000	1.879761000
1	-5.303009000	4.887584000	0.247344000	1	-5.246277000	4.802490000	1.092257000
6	-7.847746000	-2.194311000	0.515754000	6	-7.812404000	-2.209425000	-0.145054000
1	-7.224184000	-2.600007000	1.311421000	1	-7.247956000	-2.754237000	0.610164000
1	-8.485080000	-2.994611000	0.126190000	1	-8.399683000	-2.924872000	-0.729693000
1	-8.495227000	-1.422254000	0.940748000	1	-8.507861000	-1.534565000	0.361978000
6	-7.375511000	3.657458000	-1.035447000	6	-7.237387000	3.884747000	-0.533476000
1	-6.572326000	3.913818000	-1.731599000	1	-6.393821000	4.266719000	-1.114841000
1	-8.029884000	4.528078000	-0.936318000	1	-7.896171000	4.725462000	-0.297996000
1	-7.965686000	2.852884000	-1.478915000	1	-7.800808000	3.194539000	-1.164819000
6	7.770743000	-0.863650000	1.890803000	6	7.621897000	-0.476851000	2.218605000
1	8.533173000	-0.172807000	1.523942000	1	8.411556000	0.136737000	1.778513000
1	8.297542000	-1.702282000	2.353062000	1	8.111493000	-1.226916000	2.845057000
1	7.191477000	-0.359515000	2.669218000	1	7.011085000	0.156801000	2.867389000
6	7.131092000	3.891207000	0.988751000	6	7.006661000	4.098518000	0.467797000
1	6.308116000	4.150770000	1.660139000	1	6.154492000	4.471531000	1.042380000
1	7.765072000	4.774515000	0.871134000	1	7.642715000	4.950554000	0.211449000
1	7.732632000	3.118206000	1.471367000	1	7.589265000	3.437944000	1.113295000

6	7.780700000	3.089654000	-1.322850000	6	7.758941000	2.877688000	-1.616558000
1	7.424132000	2.790598000	-2.312538000	1	7.447886000	2.390652000	-2.545155000
1	8.387374000	2.275081000	-0.922097000	1	8.347504000	2.160896000	-1.040175000
1	8.431200000	3.959988000	-1.445316000	1	8.413347000	3.714746000	-1.875336000
6	-7.959883000	2.924208000	1.316118000	6	-7.962390000	2.694586000	1.578331000
1	-7.576556000	2.670028000	2.308344000	1	-7.640625000	2.237725000	2.518542000
1	-8.554041000	2.081277000	0.957514000	1	-8.532012000	1.949745000	1.018764000
1	-8.629273000	3.782478000	1.420691000	1	-8.637964000	3.520862000	1.816581000
5 (OH)(NH)				5 (NH)(OH)			
17	1.338652000	-4.900954000	-0.367711000	17	-1.388310000	-4.899379000	-0.060183000
1	-1.339723000	-4.277490000	-0.059992000	1	1.305407000	-4.293494000	-0.327490000
7	-1.182891000	-0.431364000	0.121330000	7	1.220384000	-0.486697000	-0.147750000
1	-1.571500000	1.101082000	0.194442000	1	1.275742000	0.558961000	-0.108492000
6	-0.043208000	-2.550567000	-0.109050000	6	0.028497000	-2.558352000	-0.109503000
7	1.107469000	-0.442754000	-0.133310000	7	-1.066890000	-0.402957000	0.117393000
1	1.137039000	0.603534000	-0.091408000	1	-1.412098000	1.136194000	0.233815000
8	-2.276567000	1.818826000	0.272426000	8	2.314308000	1.766420000	-0.226340000
8	-4.937745000	-1.804916000	1.388639000	8	5.061393000	-1.851905000	-1.285704000
6	-0.059962000	-1.141903000	-0.038645000	6	0.032191000	-1.149058000	-0.043732000
6	-1.290657000	-3.197850000	-0.005095000	6	1.278815000	-3.212453000	-0.280310000
6	2.338290000	-0.997862000	-0.305770000	6	-2.275990000	-0.987163000	0.234345000
8	2.149253000	1.834575000	-0.213817000	8	-2.097248000	1.869742000	0.339835000
8	4.989781000	-1.734821000	-1.221300000	8	-4.886983000	-1.708912000	1.312483000
6	-3.570602000	-0.188839000	0.352232000	6	3.597451000	-0.228769000	-0.375904000
6	-2.378498000	-1.045131000	0.230322000	6	2.438360000	-1.071518000	-0.322044000
6	-6.085922000	-0.427028000	-0.142624000	6	6.071710000	-0.409070000	0.285035000
6	3.480609000	-0.130286000	-0.352741000	6	-3.447887000	-0.102877000	0.357282000
6	5.953736000	-0.238649000	0.327278000	6	-5.956810000	-0.246363000	-0.195916000
6	5.701735000	2.184437000	-0.372746000	6	-5.666706000	2.212610000	0.365010000
6	-5.856038000	2.059935000	0.320176000	6	5.875591000	2.029763000	-0.378586000
6	4.377878000	2.249211000	-0.644646000	6	-4.330929000	2.274332000	0.608777000
1	3.974288000	3.164486000	-1.058043000	1	-3.908114000	3.215629000	0.933009000
6	-4.871643000	-0.847015000	0.619115000	6	4.914677000	-0.872738000	-0.551539000
6	-6.486186000	0.865591000	-0.199883000	6	6.468507000	0.879985000	0.292796000
1	-7.446899000	1.042059000	-0.663504000	1	7.377215000	1.102795000	0.835742000
6	4.813687000	-0.744159000	-0.508212000	6	-4.773215000	-0.728150000	0.577814000
6	6.319825000	1.059406000	0.317510000	6	-6.320507000	1.057866000	-0.212570000
1	7.219948000	1.312213000	0.861734000	1	-7.264872000	1.279647000	-0.690209000
6	-2.438223000	-2.465779000	0.169033000	6	2.439115000	-2.503444000	-0.390456000
1	-3.382611000	-2.972062000	0.269388000	1	3.372620000	-3.015619000	-0.546697000
6	-3.464223000	1.207791000	0.353964000	6	3.448072000	1.210201000	-0.360398000
6	6.638359000	3.371059000	-0.689833000	6	-6.565179000	3.446589000	0.601526000
6	-6.957973000	-1.552407000	-0.755971000	6	6.852921000	-1.499084000	1.059999000
6	1.235548000	-3.157556000	-0.279541000	6	-1.245155000	-3.157788000	0.009621000
6	2.381891000	-2.426023000	-0.383422000	6	-2.377810000	-2.404244000	0.186022000
1	3.327477000	-2.913206000	-0.544224000	1	-3.331705000	-2.887423000	0.302696000
6	-6.067014000	-2.643199000	-1.393814000	6	5.866998000	-2.485110000	1.728990000
1	-5.466524000	-3.165843000	-0.650037000	1	5.273154000	-3.030351000	0.994956000
1	-5.399106000	-2.218866000	-2.149206000	1	5.187101000	-1.963587000	2.409025000
1	-6.699774000	-3.385954000	-1.886373000	1	6.425866000	-3.221218000	2.313085000
6	5.954955000	4.463030000	-1.532183000	6	-5.830216000	4.595774000	1.314880000
1	5.567017000	4.066296000	-2.474191000	1	-5.419947000	4.281513000	2.278290000
1	6.686121000	5.238749000	-1.773410000	1	-6.536909000	5.407428000	1.504169000
1	5.133616000	4.944857000	-0.995861000	1	-5.018311000	5.006662000	0.709492000
6	-4.519451000	2.169076000	0.542858000	6	4.553367000	2.130880000	-0.648078000
1	-4.120771000	3.133646000	0.826532000	1	4.172617000	3.061638000	-1.048237000
6	-6.786102000	3.276870000	0.521948000	6	6.840256000	3.198196000	-0.679380000
6	3.295475000	1.304893000	-0.345653000	6	-3.301254000	1.290030000	0.396343000
6	-7.878561000	-1.006007000	-1.867676000	6	7.717932000	-0.882545000	2.178468000
1	-8.650557000	-0.335366000	-1.483937000	1	8.536112000	-0.273457000	1.787016000
1	-8.393718000	-1.844899000	-2.342376000	1	8.170227000	-1.689437000	2.760912000
1	-7.312562000	-0.477725000	-2.639803000	1	7.123335000	-0.267797000	2.859684000

6	6.753205000	-1.297899000	1.126062000	6	-6.838751000	-1.324227000	-0.876234000
6	7.705911000	-2.078806000	0.188104000	6	-7.763057000	-1.994887000	0.169760000
1	8.410321000	-1.398540000	-0.299000000	1	-8.412581000	-1.253892000	0.644009000
1	7.152882000	-2.612646000	-0.583185000	1	-7.184564000	-2.494982000	0.945397000
1	8.282787000	-2.802744000	0.772702000	1	-8.398899000	-2.735190000	-0.326186000
6	5.782185000	-2.286202000	1.813655000	6	-5.954071000	-2.400780000	-1.546473000
1	5.093182000	-1.762006000	2.482361000	1	-5.265881000	-1.954475000	-2.270309000
1	6.351791000	-3.001572000	2.412941000	1	-6.589463000	-3.110347000	-2.082660000
1	5.197971000	-2.855629000	1.090215000	1	-5.375262000	-2.966364000	-0.816837000
6	-6.073544000	4.475218000	1.174615000	6	6.181661000	4.320518000	-1.501411000
1	-5.639859000	4.213495000	2.143446000	1	5.782313000	3.949522000	-2.449128000
1	-6.800377000	5.273883000	1.341541000	1	6.930902000	5.082307000	-1.731253000
1	-5.283043000	4.882814000	0.539409000	1	5.373290000	4.812787000	-0.954954000
6	-7.847032000	-2.190018000	0.340052000	6	7.788843000	-2.276210000	0.102155000
1	-7.242131000	-2.638199000	1.127360000	1	7.224097000	-2.781803000	-0.679727000
1	-8.475458000	-2.967778000	-0.105496000	1	8.353042000	-3.024349000	0.668391000
1	-8.503687000	-1.440405000	0.790319000	1	8.504984000	-1.598521000	-0.371182000
6	-7.337711000	3.739749000	-0.849371000	6	7.341860000	3.812744000	0.650695000
1	-6.523358000	4.034617000	-1.516654000	1	6.505697000	4.198849000	1.240022000
1	-7.990605000	4.605406000	-0.706909000	1	8.019954000	4.644132000	0.437775000
1	-7.923941000	2.966156000	-1.349528000	1	7.888207000	3.094428000	1.265578000
6	7.604061000	-0.642700000	2.233244000	6	-7.725506000	-0.708575000	-1.979032000
1	8.411860000	-0.027078000	1.830582000	1	-8.491857000	-0.040847000	-1.579033000
1	8.069702000	-1.429014000	2.833053000	1	-8.247090000	-1.514079000	-2.502049000
1	6.997003000	-0.024961000	2.900629000	1	-7.133990000	-0.156783000	-2.714686000
6	7.120470000	4.019368000	0.631333000	6	-7.079399000	3.980879000	-0.758290000
1	6.273232000	4.394653000	1.211753000	1	-6.245403000	4.278061000	-1.399764000
1	7.778971000	4.863355000	0.406786000	1	-7.709056000	4.859167000	-0.590802000
1	7.681903000	3.324575000	1.259480000	1	-7.679350000	3.245944000	-1.298870000
6	7.858625000	2.849435000	-1.486588000	6	-7.766561000	3.030336000	1.484977000
1	7.542788000	2.399658000	-2.432241000	1	-7.426188000	2.662277000	2.456925000
1	8.426718000	2.100992000	-0.930184000	1	-8.371767000	2.249090000	1.020778000
1	8.533746000	3.679073000	-1.714421000	1	-8.413814000	3.894626000	1.657065000
6	-7.960264000	2.864291000	1.442994000	6	8.045219000	2.660375000	-1.488610000
1	-7.593232000	2.546806000	2.423041000	1	7.715822000	2.234007000	-2.440453000
1	-8.550716000	2.047778000	1.022557000	1	8.596730000	1.889389000	-0.946502000
1	-8.628908000	3.716697000	1.590916000	1	8.739492000	3.477164000	-1.705079000

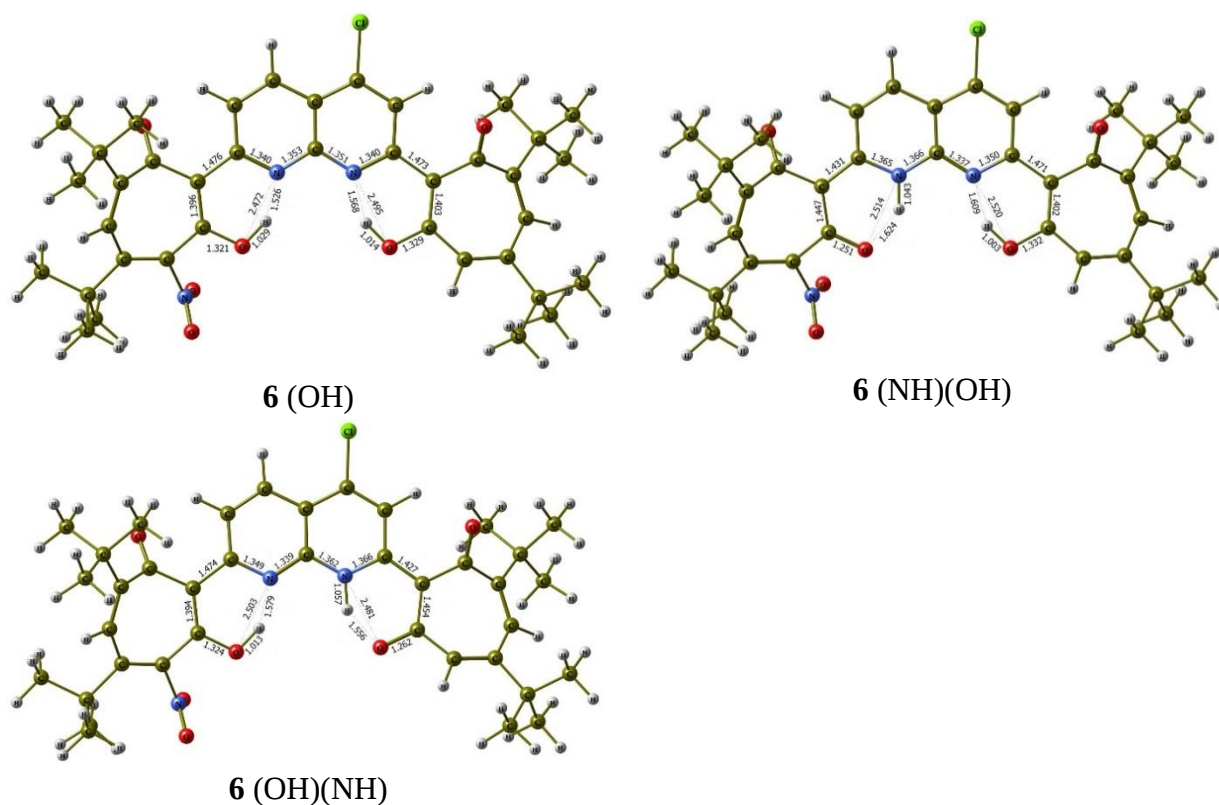


Figure S29 Optimized structures of tropolone **6** isomers according to B3LYP/6-311 ++G(d,p) calculations in the gas phase. Bond lengths are given in angstroms.

Table S15 Optimized geometries of tropolone **6** isomers. B3LYP/6-311++G(d,p) calculations in the gas phase. Coordinates in Angstroms.

6 (OH)				6 (NH)
17	-1.817339000	-5.090853000	-0.257119000	<i>not localized</i>
1	0.874330000	-4.569035000	-0.532168000	
7	0.950943000	-0.742465000	-0.094865000	
1	1.373777000	0.723626000	-0.114198000	
6	-0.312491000	-2.797691000	-0.186847000	
7	-1.330555000	-0.618911000	0.157068000	
1	-1.595366000	0.899707000	0.445926000	
8	2.107750000	1.439066000	-0.201368000	
8	4.806824000	-2.276633000	-1.119992000	
6	-0.237363000	-1.387029000	-0.040944000	
6	0.896099000	-3.494076000	-0.404464000	
6	-2.554007000	-1.160851000	0.235656000	
8	-2.248822000	1.648104000	0.647612000	
8	-5.263632000	-1.877827000	1.054346000	
6	3.336337000	-0.594449000	-0.318124000	
6	2.100507000	-1.400988000	-0.297405000	
6	5.717346000	-0.833660000	0.519702000	
6	-3.691790000	-0.240477000	0.403469000	
6	-6.174864000	-0.160042000	-0.271655000	
6	-5.784840000	2.182723000	0.620587000	
6	5.694840000	1.592269000	-0.252285000	
6	-4.461427000	2.135271000	0.917031000	
1	-3.998691000	2.997578000	1.377600000	

6	4.640182000	-1.289324000	-0.416804000
6	6.149515000	0.443011000	0.518221000
1	6.998376000	0.666611000	1.149640000
6	-5.056125000	-0.812542000	0.480862000
6	-6.471752000	1.152171000	-0.130342000
1	-7.377279000	1.490132000	-0.615726000
6	2.085474000	-2.817246000	-0.467947000
1	3.003821000	-3.339775000	-0.677971000
6	3.258867000	0.799522000	-0.303491000
6	-6.628135000	3.424404000	0.987742000
6	6.370663000	-1.915021000	1.409659000
6	-1.612718000	-3.357762000	-0.099529000
6	-2.712596000	-2.577204000	0.115930000
1	-3.685951000	-3.022971000	0.226441000
6	5.276492000	-2.819732000	2.023194000
1	4.716893000	-3.358010000	1.257593000
1	4.572499000	-2.238047000	2.625325000
1	5.739530000	-3.564451000	2.676081000
6	-5.865663000	4.425791000	1.874130000
1	-5.513751000	3.964238000	2.800445000
1	-6.534491000	5.246204000	2.146527000
1	-5.007356000	4.864507000	1.359247000
6	4.374383000	1.715033000	-0.544833000
6	6.806316000	2.641991000	-0.550618000
6	-3.472433000	1.130104000	0.606487000
6	7.164059000	-1.288595000	2.573180000
1	8.042460000	-0.735608000	2.230563000
1	7.527466000	-2.086377000	3.225972000
1	6.544724000	-0.618803000	3.176161000
6	-7.069856000	-1.091690000	-1.126234000
6	-8.051125000	-1.871398000	-0.216416000
1	-8.694528000	-1.182024000	0.337829000
1	-7.516240000	-2.491767000	0.500562000
1	-8.692128000	-2.511604000	-0.831462000
6	-6.195229000	-2.091845000	-1.918362000
1	-5.479617000	-1.569915000	-2.560718000
1	-6.832105000	-2.706914000	-2.559813000
1	-5.647406000	-2.764013000	-1.258859000
6	6.536225000	3.552159000	-1.771435000
1	6.258979000	2.974183000	-2.655354000
1	7.458930000	4.088293000	-2.005203000
1	5.775666000	4.308279000	-1.590898000
6	7.339786000	-2.777892000	0.564582000
1	6.819131000	-3.273436000	-0.253272000
1	7.803727000	-3.537734000	1.201722000
1	8.135923000	-2.160736000	0.138926000
6	6.999048000	3.521693000	0.708042000
1	6.091434000	4.084878000	0.931711000
1	7.813861000	4.231385000	0.537203000
1	7.257961000	2.924738000	1.586865000
6	-7.896832000	-0.293256000	-2.155287000
1	-8.654642000	0.339109000	-1.686003000
1	-8.428580000	-0.994403000	-2.803631000
1	-7.264089000	0.335181000	-2.788188000
6	-7.055034000	4.163200000	-0.304502000
1	-6.180518000	4.491409000	-0.872410000
1	-7.643830000	5.048319000	-0.046771000
1	-7.669463000	3.542257000	-0.960028000
6	-7.886075000	2.966355000	1.764789000
1	-7.608022000	2.452630000	2.689094000
1	-8.510549000	2.287506000	1.180310000
1	-8.496427000	3.834407000	2.029847000

6	8.132209000	1.901669000	-0.871365000				
1	8.015054000	1.236891000	-1.731314000				
1	8.515212000	1.311908000	-0.038420000				
1	8.896763000	2.641263000	-1.120408000				
7	3.838794000	2.990241000	-1.125277000				
8	3.762078000	3.952784000	-0.379431000				
8	3.504180000	2.968914000	-2.296478000				
6 (OH)(NH)				6 (NH)(OH)			
17	1.809311000	5.102256000	-0.235641000	17	1.815164000	5.082315000	-0.373291000
1	-0.883547000	4.576647000	-0.475600000	1	-0.895764000	4.554240000	-0.562265000
7	-0.939414000	0.741219000	-0.120029000	7	-0.955027000	0.784843000	0.002291000
1	-1.382691000	-0.771375000	-0.219308000	1	-1.034535000	-0.246980000	0.129993000
6	0.311064000	2.808189000	-0.180416000	6	0.314949000	2.801619000	-0.188168000
7	1.353197000	0.662277000	0.109839000	7	1.333533000	0.634510000	0.222786000
1	1.342536000	-0.388167000	0.225935000	1	1.618625000	-0.898958000	0.619636000
8	-2.121268000	-1.453879000	-0.337812000	8	-2.150011000	-1.425864000	0.068499000
8	-4.834920000	2.309616000	-1.000695000	8	-4.837224000	2.317910000	-0.916170000
6	0.223846000	1.403046000	-0.065239000	6	0.261594000	1.405812000	0.014079000
6	-0.898417000	3.499457000	-0.369422000	6	-0.913636000	3.483640000	-0.401485000
6	2.616369000	1.173091000	0.200832000	6	2.568460000	1.179173000	0.254909000
8	2.255750000	-1.608866000	0.537088000	8	2.283591000	-1.611856000	0.855138000
8	5.324463000	1.912526000	0.885862000	8	5.313827000	1.928036000	0.923301000
6	-3.335272000	0.596404000	-0.319994000	6	-3.346596000	0.606218000	-0.200180000
6	-2.101927000	1.403757000	-0.294438000	6	-2.155104000	1.398434000	-0.212352000
6	-5.682789000	0.801875000	0.614731000	6	-5.749826000	0.758285000	0.607774000
6	3.705918000	0.265807000	0.360823000	6	3.706561000	0.265346000	0.435263000
6	6.172796000	0.095122000	-0.349164000	6	6.154425000	0.136869000	-0.351203000
6	5.770695000	-2.163273000	0.738933000	6	5.815030000	-2.138691000	0.713934000
6	-5.705797000	-1.576843000	-0.286263000	6	-5.693862000	-1.602871000	-0.339989000
6	4.451495000	-2.099206000	1.023398000	6	4.506296000	-2.070396000	1.067308000
1	3.989100000	-2.906891000	1.575266000	1	4.067410000	-2.899833000	1.605104000
6	-4.642800000	1.296824000	-0.343580000	6	-4.654309000	1.285594000	-0.279031000
6	-6.122786000	-0.470816000	0.565041000	6	-6.174077000	-0.512738000	0.514893000
1	-6.946107000	-0.725244000	1.218337000	1	-7.018280000	-0.798146000	1.128841000
6	5.077792000	0.817039000	0.385747000	6	5.076192000	0.835919000	0.418290000
6	6.451352000	-1.204459000	-0.124250000	6	6.461597000	-1.163143000	-0.139599000
1	7.326856000	-1.602251000	-0.620108000	1	7.340773000	-1.534556000	-0.648518000
6	-2.090709000	2.816556000	-0.433383000	6	-2.103583000	2.816363000	-0.421361000
1	-3.011753000	3.341979000	-0.622632000	1	-3.025175000	3.333917000	-0.628466000
6	-3.269147000	-0.795262000	-0.376679000	6	-3.231111000	-0.834922000	-0.149450000
6	6.634268000	-3.344067000	1.236059000	6	6.677683000	-3.352015000	1.126379000
6	-6.287934000	1.840646000	1.585112000	6	-6.405893000	1.774712000	1.569496000
6	1.624351000	3.367732000	-0.098753000	6	1.612467000	3.359971000	-0.146854000
6	2.731761000	2.600311000	0.091743000	6	2.720156000	2.583686000	0.078927000
1	3.704326000	3.049865000	0.197132000	1	3.694097000	3.035072000	0.155800000
6	-5.159425000	2.701978000	2.198815000	6	-5.312473000	2.624017000	2.259448000
1	-4.623381000	3.272473000	1.439432000	1	-4.740854000	3.212148000	1.540185000
1	-4.439636000	2.083464000	2.742738000	1	-4.618973000	1.993969000	2.824037000
1	-5.587052000	3.417841000	2.905824000	1	-5.776904000	3.322718000	2.960718000
6	5.890564000	-4.246563000	2.236902000	6	5.960693000	-4.287824000	2.116355000
1	5.538431000	-3.684946000	3.106082000	1	5.652077000	-3.762080000	3.023727000
1	6.570833000	-5.023172000	2.596308000	1	6.643853000	-5.087437000	2.413638000
1	5.033812000	-4.749528000	1.781862000	1	5.080253000	-4.761489000	1.675061000
6	-4.397455000	-1.689859000	-0.632541000	6	-4.366678000	-1.714747000	-0.561616000
6	-6.835043000	-2.600660000	-0.605550000	6	-6.799812000	-2.595807000	-0.796889000
6	3.428304000	-1.144302000	0.580115000	6	3.502224000	-1.089601000	0.732004000
6	-7.040303000	1.160420000	2.745484000	6	-7.213894000	1.067757000	2.675278000
1	-7.936716000	0.632588000	2.409964000	1	-8.087223000	0.541320000	2.281654000
1	-7.369966000	1.925675000	3.452804000	1	-7.585989000	1.816676000	3.379309000
1	-6.403910000	0.455570000	3.287623000	1	-6.602486000	0.355215000	3.235837000
6	7.039518000	0.952236000	-1.304205000	6	6.996760000	1.011497000	-1.312249000
6	8.042742000	1.811771000	-0.496410000	6	8.021447000	1.851707000	-0.510690000

1	8.706690000	1.174591000	0.094794000	1	8.698079000	1.201860000	0.051562000
1	7.526798000	2.489160000	0.181584000	1	7.523456000	2.517196000	0.192275000
1	8.660944000	2.399093000	-1.183592000	1	8.624155000	2.451165000	-1.200824000
6	6.135170000	1.876246000	-2.153884000	6	6.073919000	1.954882000	-2.119093000
1	5.410767000	1.296096000	-2.733387000	1	5.329263000	1.389759000	-2.687622000
1	6.748602000	2.444160000	-2.858815000	1	6.671263000	2.529904000	-2.831670000
1	5.594065000	2.594097000	-1.537385000	1	5.556502000	2.666392000	-1.476205000
6	-6.617606000	-3.432568000	-1.891020000	6	-6.467786000	-3.382372000	-2.085736000
1	-6.368648000	-2.800769000	-2.746107000	1	-6.133027000	-2.720941000	-2.887775000
1	-7.552527000	-3.947401000	-2.123875000	1	-7.378867000	-3.879548000	-2.427420000
1	-5.857074000	-4.203043000	-1.787701000	1	-5.723457000	-4.161639000	-1.938247000
6	-7.280787000	2.755106000	0.826225000	6	-7.363531000	2.705287000	0.785777000
1	-6.789005000	3.288739000	0.014425000	1	-6.834435000	3.257079000	0.010592000
1	-7.709972000	3.484489000	1.520612000	1	-7.828219000	3.418107000	1.474876000
1	-8.100195000	2.168226000	0.402035000	1	-8.159632000	2.126242000	0.309481000
6	-6.985008000	-3.556280000	0.602606000	6	-7.072314000	-3.592315000	0.355214000
1	-6.073765000	-4.136863000	0.755437000	1	-6.184508000	-4.189317000	0.570208000
1	-7.811061000	-4.249734000	0.419774000	1	-7.884680000	-4.267903000	0.071124000
1	-7.205623000	-3.013872000	1.526127000	1	-7.373097000	-3.080799000	1.273802000
6	7.841983000	0.070888000	-2.283172000	6	7.770623000	0.147324000	-2.329240000
1	8.610803000	-0.520600000	-1.779630000	1	8.555994000	-0.450871000	-1.860464000
1	8.357351000	0.714734000	-3.000725000	1	8.262764000	0.804131000	-3.051050000
1	7.195202000	-0.608258000	-2.845545000	1	7.107831000	-0.523079000	-2.883358000
6	7.060723000	-4.219935000	0.032466000	6	7.043795000	-4.179861000	-0.130089000
1	6.185838000	-4.620919000	-0.486007000	1	6.143980000	-4.547018000	-0.630596000
1	7.663375000	-5.062938000	0.383216000	1	7.646821000	-5.044822000	0.160743000
1	7.661990000	-3.670401000	-0.695195000	1	7.624299000	-3.607059000	-0.856503000
6	7.892152000	-2.785573000	1.943702000	6	7.970025000	-2.840894000	1.807970000
1	7.614749000	-2.174124000	2.806759000	1	7.735307000	-2.262713000	2.705834000
1	8.501146000	-2.168431000	1.279790000	1	8.564243000	-2.205981000	1.147557000
1	8.517480000	-3.609807000	2.298900000	1	8.594353000	-3.688539000	2.104332000
6	-8.167360000	-1.835794000	-0.826776000	6	-8.095444000	-1.802358000	-1.110120000
1	-8.079619000	-1.118376000	-1.646991000	1	-7.925260000	-1.063518000	-1.897760000
1	-8.513887000	-1.298785000	0.056344000	1	-8.505460000	-1.282718000	-0.243793000
1	-8.945752000	-2.555056000	-1.091745000	1	-8.859963000	-2.499220000	-1.462192000
7	-3.892186000	-2.931051000	-1.306864000	7	-3.789317000	-2.924074000	-1.223271000
8	-3.802322000	-3.938602000	-0.625248000	8	-3.785463000	-3.964871000	-0.586275000
8	-3.593339000	-2.838079000	-2.484325000	8	-3.338533000	-2.779556000	-2.347659000

Table S16 Optimized geometries of tropolone **6** isomers. PCM/B3LYP/6-311++G(d,p) calculations (DMSO). Coordinates in Angstroms.

6 (OH)				6 (NH)			
17	-1.827598000	-5.051299000	-0.302094000	17	-1.803443000	-5.084663000	-0.258082000
1	0.878363000	-4.547456000	-0.520415000	1	0.896720000	-4.555619000	-0.468226000
7	0.958147000	-0.716306000	-0.131867000	7	0.945649000	-0.766604000	-0.069391000
1	1.380170000	0.719166000	-0.097301000	1	1.044046000	0.273283000	0.020109000
6	-0.310043000	-2.767340000	-0.211649000	6	-0.314708000	-2.794704000	-0.161567000
7	-1.322681000	-0.583655000	0.116990000	7	-1.358610000	-0.655945000	0.162367000
1	-1.592958000	0.933592000	0.279891000	1	-1.377481000	0.406448000	0.284266000
8	2.115791000	1.451833000	-0.142350000	8	2.128965000	1.443084000	-0.051295000
8	4.788002000	-2.190178000	-1.298122000	8	4.820901000	-2.241980000	-1.106978000
6	-0.231669000	-1.356841000	-0.075775000	6	-0.249035000	-1.400142000	-0.022009000
6	0.897679000	-3.470885000	-0.410282000	6	0.908679000	-3.479404000	-0.356419000
6	-2.546951000	-1.120746000	0.196182000	6	-2.622727000	-1.175886000	0.236626000
8	-2.243499000	1.706873000	0.408954000	8	-2.251321000	1.608762000	0.550789000
8	-5.173337000	-1.786620000	1.259987000	8	-5.318103000	-1.876532000	1.016040000
6	3.343401000	-0.574612000	-0.338874000	6	3.336913000	-0.586497000	-0.269828000
6	2.106594000	-1.380316000	-0.320942000	6	2.147566000	-1.391904000	-0.262978000
6	5.733316000	-0.882209000	0.440254000	6	5.728590000	-0.804499000	0.544299000

6	-3.684060000	-0.196956000	0.360889000	6	-3.711577000	-0.258063000	0.391046000
6	-6.203804000	-0.211143000	-0.160031000	6	-6.176229000	-0.132329000	-0.322221000
6	-5.795150000	2.212972000	0.481283000	6	-5.781300000	2.172713000	0.665399000
6	5.716714000	1.589649000	-0.177710000	6	5.707517000	1.601937000	-0.280191000
6	-4.455149000	2.207883000	0.708417000	6	-4.461566000	2.122169000	0.963194000
1	-3.987092000	3.117923000	1.058519000	1	-4.010971000	2.958798000	1.480959000
6	4.642068000	-1.265238000	-0.507350000	6	4.643238000	-1.264525000	-0.385136000
6	6.171368000	0.391448000	0.511931000	6	6.163776000	0.466973000	0.523790000
1	7.033224000	0.569116000	1.139714000	1	7.003514000	0.710588000	1.160318000
6	-5.029881000	-0.776046000	0.570739000	6	-5.081273000	-0.809864000	0.446505000
6	-6.507869000	1.108160000	-0.123292000	6	-6.456800000	1.176916000	-0.155881000
1	-7.449462000	1.387881000	-0.575098000	1	-7.333305000	1.549199000	-0.668464000
6	2.089259000	-2.796755000	-0.470522000	6	2.100219000	-2.807261000	-0.414650000
1	3.005382000	-3.333717000	-0.649942000	1	3.015850000	-3.342975000	-0.596833000
6	3.273022000	0.815681000	-0.267177000	6	3.228124000	0.844597000	-0.216062000
6	-6.634791000	3.477047000	0.770943000	6	-6.646642000	3.375848000	1.100552000
6	6.395000000	-2.016941000	1.255170000	6	6.355385000	-1.872933000	1.468519000
6	-1.613961000	-3.321316000	-0.135701000	6	-1.621635000	-3.358082000	-0.091138000
6	-2.711499000	-2.534122000	0.069284000	6	-2.735057000	-2.592560000	0.109313000
1	-3.687941000	-2.978791000	0.148183000	1	-3.704651000	-3.051798000	0.190727000
6	5.309093000	-2.964203000	1.815968000	6	5.237393000	-2.728805000	2.108750000
1	4.753361000	-3.465766000	1.022834000	1	4.663164000	-3.278441000	1.361279000
1	4.600894000	-2.423709000	2.450220000	1	4.548533000	-2.109349000	2.689867000
1	5.781874000	-3.739052000	2.424702000	1	5.682079000	-3.463120000	2.785475000
6	-5.839712000	4.569231000	1.508976000	6	-5.909947000	4.325819000	2.061795000
1	-5.430536000	4.206415000	2.455636000	1	-5.562657000	3.807379000	2.959468000
1	-6.507105000	5.404561000	1.734461000	1	-6.595513000	5.115914000	2.378176000
1	-5.018837000	4.963391000	0.904543000	1	-5.052161000	4.809597000	1.587878000
6	4.393133000	1.734822000	-0.454042000	6	4.384990000	1.727208000	-0.538890000
6	6.837078000	2.643380000	-0.419406000	6	6.832694000	2.609977000	-0.648959000
6	-3.472514000	1.186291000	0.451962000	6	-3.438992000	1.148955000	0.580459000
6	7.193259000	-1.460462000	2.450691000	6	7.163317000	-1.226152000	2.610373000
1	8.068506000	-0.885251000	2.139455000	1	8.049256000	-0.699073000	2.248010000
1	7.559010000	-2.297892000	3.049964000	1	7.511845000	-2.011988000	3.285252000
1	6.573780000	-0.831246000	3.095410000	1	6.556620000	-0.527821000	3.193124000
6	-7.149282000	-1.220272000	-0.860855000	6	-7.038157000	-1.030360000	-1.244286000
6	-8.089674000	-1.878484000	0.178650000	6	-8.048850000	-1.852515000	-0.407579000
1	-8.695886000	-1.122468000	0.685445000	1	-8.710149000	-1.190109000	0.158143000
1	-7.524519000	-2.429324000	0.929314000	1	-7.539622000	-2.512425000	0.293059000
1	-8.767586000	-2.571934000	-0.329200000	1	-8.668112000	-2.459445000	-1.075879000
6	-6.331658000	-2.316824000	-1.582192000	6	-6.130237000	-1.991220000	-2.047475000
1	-5.630888000	-1.881246000	-2.300488000	1	-5.401535000	-1.437410000	-2.646601000
1	-7.010795000	-2.972501000	-2.133249000	1	-6.742245000	-2.586509000	-2.730321000
1	-5.773775000	-2.937181000	-0.881519000	1	-5.592633000	-2.683888000	-1.399540000
6	6.550671000	3.668966000	-1.539467000	6	6.530798000	3.512252000	-1.866442000
1	6.248043000	3.181608000	-2.468513000	1	6.203719000	2.930013000	-2.730579000
1	7.475983000	4.212213000	-1.741697000	1	7.454604000	4.023006000	-2.146317000
1	5.808491000	4.416613000	-1.266796000	1	5.798195000	4.289989000	-1.659781000
6	7.362633000	-2.819397000	0.350959000	6	7.305432000	-2.787800000	0.657790000
1	6.837263000	-3.277391000	-0.486264000	1	6.773290000	-3.313745000	-0.133706000
1	7.838138000	-3.609400000	0.940345000	1	7.757210000	-3.526279000	1.327347000
1	8.148776000	-2.171557000	-0.046121000	1	8.110333000	-2.203467000	0.203546000
6	7.091664000	3.400080000	0.906876000	6	7.118479000	3.500330000	0.584575000
1	6.206878000	3.962710000	1.211655000	1	6.243266000	4.098959000	0.845005000
1	7.916860000	4.103953000	0.768470000	1	7.945114000	4.179029000	0.356993000
1	7.364550000	2.722897000	1.719710000	1	7.404236000	2.910427000	1.458799000
6	-8.021360000	-0.524435000	-1.927267000	6	-7.833830000	-0.189696000	-2.263859000
1	-8.747435000	0.166333000	-1.492708000	1	-8.603565000	0.424344000	-1.790351000
1	-8.590358000	-1.285083000	-2.467627000	1	-8.344137000	-0.864857000	-2.955559000
1	-7.414467000	0.022223000	-2.654204000	1	-7.181399000	0.462940000	-2.850322000
6	-7.143722000	4.077651000	-0.562914000	6	-7.066566000	4.191548000	-0.147302000
1	-6.306355000	4.358176000	-1.207504000	1	-6.188610000	4.568367000	-0.678964000

1	-7.730795000	4.977193000	-0.357733000	1	-7.669980000	5.049421000	0.162705000
1	-7.783747000	3.388193000	-1.117242000	1	-7.665154000	3.607584000	-0.849538000
6	-7.840963000	3.085917000	1.659327000	6	-7.909086000	2.849670000	1.825630000
1	-7.503642000	2.671119000	2.613360000	1	-7.636421000	2.281798000	2.719706000
1	-8.487649000	2.348363000	1.179846000	1	-8.514313000	2.203377000	1.186602000
1	-8.446006000	3.972098000	1.869576000	1	-8.534324000	3.691404000	2.136084000
6	8.132814000	1.906351000	-0.853384000	6	8.112840000	1.815796000	-1.021389000
1	7.970686000	1.338550000	-1.773367000	1	7.931113000	1.156611000	-1.874417000
1	8.520222000	1.224691000	-0.096794000	1	8.500612000	1.211707000	-0.201477000
1	8.908918000	2.649834000	-1.048021000	1	8.895248000	2.524161000	-1.303158000
7	3.855452000	3.047947000	-0.938825000	7	3.833501000	2.980065000	-1.140202000
8	3.759404000	3.953108000	-0.124378000	8	3.773550000	3.971775000	-0.428998000
8	3.514999000	3.122283000	-2.108586000	8	3.436597000	2.928088000	-2.294685000
6 (OH)(NH)				6 (NH)(OH)			
17	-1.801347000	-5.077199000	-0.100953000	17	-1.842511000	-5.013862000	-0.466046000
1	0.897405000	-4.555974000	-0.363584000	1	0.879233000	-4.508088000	-0.625397000
7	0.938048000	-0.712503000	-0.106396000	7	0.958036000	-0.737484000	-0.080655000
1	1.375841000	0.773040000	-0.131422000	1	1.036334000	0.288602000	0.055558000
6	-0.305574000	-2.782508000	-0.109431000	6	-0.323303000	-2.746974000	-0.259362000
7	-1.352601000	-0.634090000	0.140678000	7	-1.327841000	-0.574288000	0.153812000
1	-1.333552000	0.411670000	0.214552000	1	-1.612590000	0.969806000	0.384584000
8	2.110098000	1.478218000	-0.203918000	8	2.188957000	1.473491000	0.022392000
8	4.782773000	-2.199287000	-1.240747000	8	4.820160000	-2.220564000	-1.159131000
6	-0.221741000	-1.376230000	-0.027139000	6	-0.261546000	-1.352263000	-0.060084000
6	0.904789000	-3.476407000	-0.290229000	6	0.898228000	-3.436706000	-0.472702000
6	-2.610617000	-1.144208000	0.248977000	6	-2.563356000	-1.110958000	0.194948000
8	-2.284028000	1.666093000	0.467187000	8	-2.270581000	1.718539000	0.532288000
8	-5.303269000	-1.843191000	1.074530000	8	-5.201665000	-1.811792000	1.203906000
6	3.330042000	-0.563007000	-0.326777000	6	3.353817000	-0.573386000	-0.270702000
6	2.099711000	-1.374546000	-0.278077000	6	2.150113000	-1.358734000	-0.292751000
6	5.718230000	-0.848516000	0.470363000	6	5.740561000	-0.848384000	0.539287000
6	-3.708884000	-0.234664000	0.384050000	6	-3.698524000	-0.193272000	0.381009000
6	-6.175411000	-0.154071000	-0.324004000	6	-6.209297000	-0.198605000	-0.189934000
6	-5.817490000	2.170206000	0.624172000	6	-5.823405000	2.202328000	0.543127000
6	5.709156000	1.599259000	-0.232359000	6	5.765255000	1.574244000	-0.229893000
6	-4.496483000	2.143251000	0.915771000	6	-4.489011000	2.192931000	0.802167000
1	-4.056538000	2.991044000	1.424804000	1	-4.033139000	3.091452000	1.195300000
6	4.632514000	-1.257695000	-0.472485000	6	4.650090000	-1.264840000	-0.406105000
6	6.158004000	0.425915000	0.502331000	6	6.200534000	0.414090000	0.550293000
1	7.016571000	0.623660000	1.128605000	1	7.041593000	0.628394000	1.195746000
6	-5.072455000	-0.796678000	0.465683000	6	-5.048845000	-0.782462000	0.547134000
6	-6.477881000	1.152687000	-0.184399000	6	-6.518245000	1.117837000	-0.116512000
1	-7.356276000	1.503916000	-0.708774000	1	-7.450438000	1.410410000	-0.579445000
6	2.092176000	-2.789547000	-0.381184000	6	2.091946000	-2.772973000	-0.496535000
1	3.010478000	-3.325740000	-0.549852000	1	3.005644000	-3.307767000	-0.690985000
6	3.265292000	0.827580000	-0.305050000	6	3.270539000	0.858322000	-0.170887000
6	-6.702294000	3.362243000	1.050461000	6	-6.673470000	3.453406000	0.856537000
6	6.372650000	-1.958142000	1.324257000	6	6.340028000	-1.950452000	1.441701000
6	-1.615139000	-3.342540000	-0.004561000	6	-1.626077000	-3.297472000	-0.221322000
6	-2.723194000	-2.570476000	0.174497000	6	-2.725766000	-2.512460000	0.007680000
1	-3.692583000	-3.024727000	0.281840000	1	-3.702737000	-2.959775000	0.057665000
6	5.281161000	-2.882288000	1.911862000	6	5.200409000	-2.793826000	2.060055000
1	4.726628000	-3.408177000	1.133703000	1	4.615237000	-3.312705000	1.299070000
1	4.572563000	-2.318821000	2.525293000	1	4.524601000	-2.171371000	2.653140000
1	5.748821000	-3.638444000	2.547420000	1	5.625515000	-3.553596000	2.721128000
6	-5.979686000	4.332710000	2.001795000	6	-5.900932000	4.519103000	1.654673000
1	-5.622146000	3.827718000	2.903127000	1	-5.515566000	4.122433000	2.597734000
1	-6.677275000	5.114477000	2.312762000	1	-6.576413000	5.344215000	1.893146000
1	-5.130622000	4.825912000	1.521923000	1	-5.065881000	4.936884000	1.086663000
6	4.387021000	1.737138000	-0.520157000	6	4.445197000	1.726738000	-0.483193000
6	6.833354000	2.640252000	-0.507849000	6	6.907893000	2.568832000	-0.580431000
6	-3.455879000	1.183787000	0.531220000	6	-3.496996000	1.185878000	0.529837000

6	7.169055000	-1.364948000	2.503072000	6	7.159008000	-1.347245000	2.599428000
1	8.046255000	-0.802091000	2.175289000	1	8.057535000	-0.832517000	2.250449000
1	7.531225000	-2.183289000	3.130188000	1	7.487853000	-2.155196000	3.257931000
1	6.549346000	-0.713731000	3.125299000	1	6.566621000	-0.648109000	3.195768000
6	-7.012315000	-1.085309000	-1.235727000	6	-7.138136000	-1.187581000	-0.939817000
6	-8.006443000	-1.920712000	-0.392444000	6	-8.101405000	-1.872194000	0.061058000
1	-8.685572000	-1.267194000	0.162430000	1	-8.718810000	-1.129375000	0.573720000
1	-7.484564000	-2.559178000	0.318698000	1	-7.553176000	-2.442879000	0.809575000
1	-8.608331000	-2.550754000	-1.055237000	1	-8.767588000	-2.551984000	-0.479679000
6	-6.077326000	-2.035151000	-2.020611000	6	-6.305729000	-2.265475000	-1.671964000
1	-5.360647000	-1.472630000	-2.626011000	1	-5.585170000	-1.812227000	-2.359073000
1	-6.670906000	-2.657592000	-2.695583000	1	-6.972745000	-2.901821000	-2.259154000
1	-5.524283000	-2.703178000	-1.359624000	1	-5.768668000	-2.908883000	-0.975840000
6	6.553877000	3.626807000	-1.664151000	6	6.621173000	3.498534000	-1.780810000
1	6.253147000	3.108270000	-2.576780000	1	6.283021000	2.937949000	-2.654992000
1	7.481661000	4.159743000	-1.881794000	1	7.553523000	3.998091000	-2.052608000
1	5.813273000	4.385879000	-1.420371000	1	5.902275000	4.284877000	-1.559076000
6	7.339857000	-2.793339000	0.449705000	6	7.271592000	-2.869778000	0.614844000
1	6.815555000	-3.277142000	-0.373600000	1	6.730465000	-3.366587000	-0.189285000
1	7.810676000	-3.565064000	1.066368000	1	7.704032000	-3.632366000	1.270032000
1	8.129396000	-2.161750000	0.033738000	1	8.091227000	-2.294656000	0.175403000
6	7.086256000	3.442454000	0.791847000	6	7.209587000	3.430882000	0.669202000
1	6.202152000	4.017794000	1.073996000	1	6.345118000	4.040088000	0.940780000
1	7.913634000	4.138832000	0.630698000	1	8.048409000	4.098811000	0.454572000
1	7.355363000	2.793948000	1.628952000	1	7.484213000	2.819556000	1.532228000
6	-7.823754000	-0.278831000	-2.270134000	6	-7.985545000	-0.461376000	-2.005859000
1	-8.607480000	0.325717000	-1.807403000	1	-8.720630000	0.218203000	-1.568898000
1	-8.317664000	-0.975813000	-2.952093000	1	-8.542958000	-1.206097000	-2.579395000
1	-7.184532000	0.378743000	-2.865540000	1	-7.361949000	0.104029000	-2.703721000
6	-7.138375000	4.159641000	-0.203544000	6	-7.147857000	4.100660000	-0.468270000
1	-6.267953000	4.547727000	-0.739517000	1	-6.294297000	4.405852000	-1.079508000
1	-7.757198000	5.009085000	0.099412000	1	-7.742806000	4.991024000	-0.246606000
1	-7.726700000	3.558540000	-0.900026000	1	-7.770731000	3.430329000	-1.064001000
6	-7.954566000	2.821685000	1.782315000	6	-7.902104000	3.028372000	1.697428000
1	-7.671096000	2.266138000	2.680806000	1	-7.589521000	2.579556000	2.644436000
1	-8.549419000	2.159585000	1.149701000	1	-8.534444000	2.308236000	1.174345000
1	-8.593740000	3.655249000	2.086536000	1	-8.514122000	3.905804000	1.923397000
6	8.127673000	1.883702000	-0.911513000	6	8.173754000	1.759466000	-0.968090000
1	7.966206000	1.284184000	-1.811261000	1	7.980496000	1.119970000	-1.833507000
1	8.510507000	1.228088000	-0.129978000	1	8.549945000	1.132837000	-0.159752000
1	8.906840000	2.617193000	-1.130155000	1	8.968946000	2.458867000	-1.236297000
7	3.855123000	3.033497000	-1.054863000	7	3.913722000	2.998412000	-1.061300000
8	3.759222000	3.967892000	-0.274330000	8	3.874009000	3.979875000	-0.334452000
8	3.519278000	3.065546000	-2.227794000	8	3.509968000	2.972158000	-2.214564000

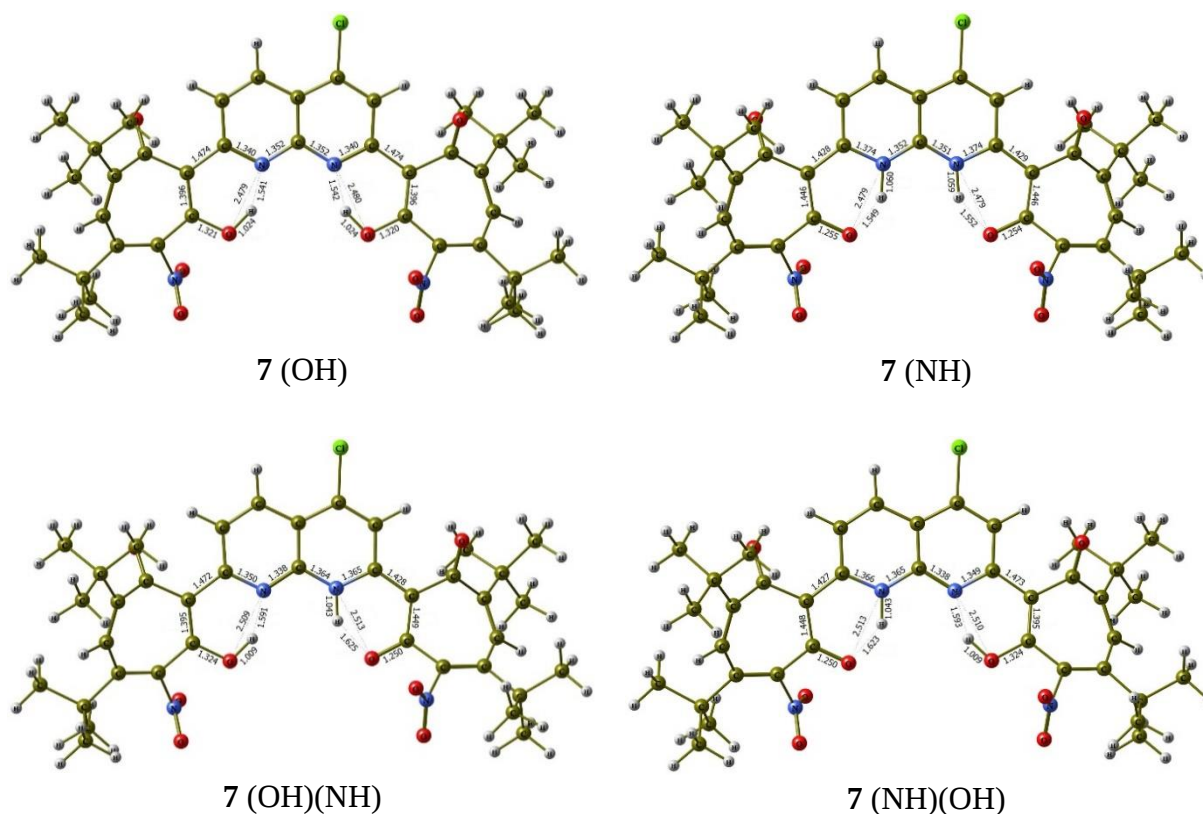


Figure S30 Optimized structures of tropolone 7 isomers according to B3LYP/6-311 ++G(d,p) calculations in the gas phase. Bond lengths are given in angstroms.

Table S17 Optimized geometries of tropolone 7 isomers. B3LYP/6-311++G(d,p) calculations in the gas phase. Coordinates in Angstroms.

7 (OH)				7 (NH)			
17	-1.384792000	5.378337000	-0.109025000	17	-1.384809000	5.372677000	-0.047652000
1	1.287107000	4.767292000	0.157160000	1	1.298124000	4.764619000	0.066647000
7	1.189890000	0.914112000	0.109451000	7	1.202975000	0.952338000	0.058824000
1	1.554556000	-0.568603000	0.315336000	1	1.278151000	-0.103609000	0.102584000
6	0.016409000	3.024433000	0.019850000	6	0.016537000	3.028159000	0.008522000
7	-1.100033000	0.871177000	-0.088448000	7	-1.113855000	0.909655000	-0.045048000
1	-1.422872000	-0.619699000	-0.316859000	1	-1.156572000	-0.147456000	-0.090483000
8	2.260756000	-1.289646000	0.488660000	8	2.280006000	-1.265194000	0.319568000
8	5.144105000	2.388042000	0.830862000	8	5.184074000	2.434843000	0.541937000
6	0.031262000	1.604060000	0.013029000	6	0.031510000	1.624867000	0.007001000
6	1.259979000	3.685142000	0.138209000	6	1.274403000	3.682488000	0.062749000
6	-2.297843000	1.461936000	-0.193206000	6	-2.365562000	1.471083000	-0.113191000
8	-2.109077000	-1.356288000	-0.501954000	8	-2.128449000	-1.336648000	-0.313513000
8	-5.097926000	2.245497000	-0.770946000	8	-5.134896000	2.286906000	-0.496651000
6	3.571577000	0.687619000	0.303928000	6	3.589686000	0.706789000	0.185735000
6	2.370866000	1.538343000	0.218849000	6	2.438665000	1.549691000	0.127234000
6	5.923058000	0.705511000	-0.640504000	6	5.946768000	0.608410000	-0.754313000
6	-3.475834000	0.579967000	-0.285214000	6	-3.494260000	0.597007000	-0.171791000
6	-5.822034000	0.513698000	0.670228000	6	-5.846910000	0.419902000	0.768697000
6	-5.673922000	-1.758808000	-0.465609000	6	-5.669869000	-1.744384000	-0.562891000
6	5.835865000	-1.590025000	0.454799000	6	5.832865000	-1.574648000	0.552958000
6	-4.363415000	-1.739606000	-0.820620000	6	-4.353488000	-1.711703000	-0.864191000
6	4.906879000	1.328607000	0.267274000	6	4.928690000	1.324682000	0.089052000
6	6.302539000	-0.577978000	-0.483528000	6	6.311642000	-0.656205000	-0.484787000
1	7.112063000	-0.924117000	-1.111346000	1	7.104990000	-1.078976000	-1.087012000

6	-4.828406000	1.181705000	-0.230102000	6	-4.849080000	1.175562000	-0.063873000
6	-6.165729000	-0.777011000	0.491827000	6	-6.176050000	-0.851137000	0.483684000
1	-6.962396000	-1.157050000	1.116518000	1	-6.958139000	-1.302790000	1.079654000
6	2.419686000	2.965563000	0.241322000	6	2.444660000	2.978774000	0.124421000
1	3.365778000	3.463633000	0.374207000	1	3.391733000	3.484674000	0.210534000
6	3.438241000	-0.691929000	0.474562000	6	3.405830000	-0.714236000	0.377201000
6	-6.725684000	-2.828001000	-0.884757000	6	-6.725454000	-2.738038000	-1.124322000
6	6.576728000	1.628933000	-1.692755000	6	6.597872000	1.426847000	-1.892084000
6	-1.258665000	3.632741000	-0.094135000	6	-1.272130000	3.631419000	-0.046320000
6	-2.398513000	2.884842000	-0.206099000	6	-2.422773000	2.896199000	-0.111723000
1	-3.357566000	3.356557000	-0.339559000	1	-3.384112000	3.373486000	-0.202933000
6	5.490978000	2.490281000	-2.379630000	6	5.509848000	2.217449000	-2.656425000
1	4.986591000	3.150070000	-1.672664000	1	5.005496000	2.940095000	-2.013376000
1	4.739668000	1.864429000	-2.869889000	1	4.759215000	1.546189000	-3.083820000
1	5.952227000	3.120458000	-3.144674000	1	5.968321000	2.773151000	-3.478833000
6	-6.456893000	-3.507817000	-2.247656000	6	-6.416590000	-3.272961000	-2.541587000
1	-6.263635000	-2.776262000	-3.034968000	1	-6.180591000	-2.464149000	-3.236549000
1	-7.352127000	-4.066341000	-2.530433000	1	-7.308513000	-3.779963000	-2.917275000
1	-5.639426000	-4.224645000	-2.223089000	1	-5.610644000	-4.002984000	-2.563574000
6	4.524515000	-1.613853000	0.806561000	6	4.516926000	-1.582086000	0.858353000
6	6.916096000	-2.636923000	0.857883000	6	6.917215000	-2.544713000	1.100906000
6	-3.302862000	-0.792455000	-0.476367000	6	-3.268725000	-0.817041000	-0.371488000
6	7.292894000	0.818276000	-2.790657000	6	7.311877000	0.514293000	-2.908214000
1	8.163483000	0.277691000	-2.410448000	1	8.179937000	0.009091000	-2.476962000
1	7.657749000	1.504750000	-3.558914000	1	7.679946000	1.124003000	-3.737386000
1	6.622037000	0.102168000	-3.273174000	1	6.639320000	-0.242258000	-3.321711000
6	-6.494613000	1.399404000	1.742839000	6	-6.520784000	1.205549000	1.916564000
6	-7.558398000	2.311417000	1.083774000	6	-7.586403000	2.172495000	1.344826000
1	-8.335624000	1.712599000	0.600861000	1	-8.362076000	1.618451000	0.808882000
1	-7.113739000	2.962070000	0.332480000	1	-7.143743000	2.890349000	0.656368000
1	-8.034740000	2.930313000	1.850859000	1	-8.064568000	2.717164000	2.165367000
6	-5.427559000	2.273977000	2.442448000	6	-5.454394000	2.013461000	2.693371000
1	-4.658945000	1.657440000	2.917496000	1	-4.687095000	1.355877000	3.112435000
1	-5.901068000	2.877264000	3.221509000	1	-5.928064000	2.545345000	3.522867000
1	-4.942842000	2.960463000	1.747213000	1	-4.968414000	2.758291000	2.061612000
6	6.664304000	-3.346274000	2.208958000	6	6.627910000	-3.102523000	2.513510000
1	6.450323000	-2.633350000	3.007917000	1	6.372199000	-2.307715000	3.217592000
1	7.573998000	-3.884995000	2.483911000	1	7.534670000	-3.588731000	2.881068000
1	5.866597000	-4.084453000	2.171255000	1	5.842383000	-3.854583000	2.530478000
6	7.614390000	2.553978000	-1.010597000	6	7.638117000	2.413375000	-1.307263000
1	7.150344000	3.176545000	-0.247249000	1	7.177395000	3.107924000	-0.606756000
1	8.077260000	3.201192000	-1.762446000	1	8.099728000	2.983609000	-2.119893000
1	8.405159000	1.965281000	-0.537367000	1	8.429548000	1.872386000	-0.781150000
6	7.013046000	-3.696532000	-0.266063000	6	7.070762000	-3.720581000	0.106351000
1	6.074037000	-4.242889000	-0.368548000	1	6.144548000	-4.293047000	0.034919000
1	7.805696000	-4.411516000	-0.026903000	1	7.866027000	-4.388529000	0.450128000
1	7.254476000	-3.244497000	-1.232064000	1	7.339136000	-3.374706000	-0.895768000
6	-7.185197000	0.549187000	2.827055000	6	-7.211432000	0.260390000	2.918975000
1	-8.043169000	-0.006086000	2.439344000	1	-8.065390000	-0.261566000	2.479527000
1	-7.564440000	1.210973000	3.609853000	1	-7.596347000	0.848746000	3.755861000
1	-6.494247000	-0.158641000	3.293185000	1	-6.519576000	-0.483742000	3.323091000
6	-6.792269000	-3.908327000	0.221522000	6	-6.849910000	-3.927979000	-0.142566000
1	-5.838479000	-4.430259000	0.314408000	1	-5.908567000	-4.475566000	-0.073891000
1	-7.565128000	-4.640805000	-0.029136000	1	-7.625408000	-4.613858000	-0.496055000
1	-7.045187000	-3.479329000	1.195045000	1	-7.130918000	-3.600210000	0.862164000
6	-8.113809000	-2.148362000	-1.026365000	6	-8.093424000	-2.014925000	-1.235432000
1	-8.087721000	-1.347196000	-1.769750000	1	-8.028542000	-1.145522000	-1.895115000
1	-8.492525000	-1.731264000	-0.093109000	1	-8.486953000	-1.681057000	-0.275039000
1	-8.837699000	-2.894459000	-1.362146000	1	-8.823951000	-2.706480000	-1.661870000
6	8.285307000	-1.922740000	1.012913000	6	8.265495000	-1.786003000	1.215500000
1	8.236729000	-1.134447000	1.768830000	1	8.179115000	-0.925212000	1.883956000
1	8.654289000	-1.480962000	0.087138000	1	8.647185000	-1.432245000	0.257453000

1	9.028394000	-2.654459000	1.338223000	1	9.015624000	-2.461756000	1.633145000
7	3.962616000	-2.768744000	1.581243000	7	3.926258000	-2.642803000	1.730823000
8	3.823699000	-3.824537000	0.986850000	8	3.837650000	-3.766760000	1.266263000
8	3.670821000	-2.562804000	2.746285000	8	3.552263000	-2.300401000	2.840552000
8	-3.487372000	-2.630903000	-2.777676000	8	-3.361686000	-2.381062000	-2.850133000
7	-3.770983000	-2.864890000	-1.615916000	7	-3.730376000	-2.745950000	-1.745763000
8	-3.601481000	-3.926367000	-1.039915000	8	-3.612475000	-3.872095000	-1.293214000
7 (OH)(NH)				7 (NH)(OH)			
17	1.402529000	5.352079000	0.127392000	17	-1.373096000	5.364931000	-0.024647000
1	-1.280042000	4.755371000	-0.073684000	1	1.315439000	4.742722000	0.146846000
7	-1.187107000	0.903463000	-0.156946000	7	1.202597000	0.932398000	0.010696000
1	-1.585292000	-0.609930000	-0.443048000	1	1.237566000	-0.110388000	0.007280000
6	-0.012647000	3.012261000	-0.022270000	6	0.022061000	3.012997000	0.005443000
7	1.113218000	0.889634000	-0.006909000	7	-1.096154000	0.862243000	-0.143024000
1	1.117071000	-0.153324000	-0.004264000	1	-1.451776000	-0.659333000	-0.450467000
8	-2.304627000	-1.291707000	-0.634154000	8	2.304354000	-1.317857000	0.202472000
8	-5.167943000	2.419092000	-0.697997000	8	5.173814000	2.393837000	0.639254000
6	-0.049449000	1.601695000	-0.061969000	6	0.014315000	1.601860000	-0.043450000
6	-1.253163000	3.673388000	-0.090539000	6	1.285177000	3.661217000	0.107599000
6	2.359101000	1.436554000	0.104026000	6	-2.304146000	1.460403000	-0.201600000
8	2.152714000	-1.388580000	0.202691000	8	-2.152626000	-1.356840000	-0.652075000
8	5.124945000	2.251634000	0.580976000	8	-5.120493000	2.275055000	-0.644287000
6	-3.582268000	0.692595000	-0.302888000	6	3.588599000	0.677583000	0.181337000
6	-2.378080000	1.535454000	-0.217405000	6	2.433305000	1.513848000	0.125439000
6	-5.893168000	0.682368000	0.738093000	6	5.964819000	0.619776000	-0.710680000
6	3.492876000	0.570039000	0.162529000	6	-3.485850000	0.585887000	-0.291091000
6	5.864162000	0.430713000	-0.734043000	6	-5.789321000	0.492840000	0.762151000
6	5.686115000	-1.760675000	0.547565000	6	-5.715016000	-1.721495000	-0.486517000
6	-5.876658000	-1.552671000	-0.475345000	6	5.847821000	-1.594849000	0.537270000
6	4.364154000	-1.745356000	0.820712000	6	-4.421205000	-1.695344000	-0.898412000
6	-4.913499000	1.338907000	-0.185905000	6	4.926409000	1.302530000	0.137852000
6	-6.291571000	-0.588632000	0.535312000	6	6.338274000	-0.647486000	-0.469714000
1	-7.075038000	-0.961034000	1.180957000	1	7.143898000	-1.048923000	-1.070533000
6	4.846679000	1.156482000	0.103500000	6	-4.833672000	1.192105000	-0.155079000
6	6.202536000	-0.842504000	-0.473286000	6	-6.152620000	-0.785552000	0.540775000
1	6.996303000	-1.275390000	-1.068019000	1	-6.922136000	-1.190190000	1.183831000
6	-2.420779000	2.955896000	-0.191318000	6	2.445440000	2.949088000	0.169412000
1	-3.366972000	3.461847000	-0.286999000	1	3.394182000	3.444960000	0.289747000
6	-3.473384000	-0.676420000	-0.546410000	6	3.414020000	-0.753828000	0.317270000
6	6.740950000	-2.751807000	1.114292000	6	-6.795903000	-2.757953000	-0.912807000
6	-6.487370000	1.559402000	1.862307000	6	6.622330000	1.476048000	-1.816209000
6	1.281258000	3.609601000	0.076017000	6	-1.249100000	3.622661000	-0.062506000
6	2.422063000	2.867904000	0.143306000	6	-2.397483000	2.876295000	-0.170983000
1	3.384576000	3.335986000	0.265471000	1	-3.356584000	3.356155000	-0.269802000
6	-5.360437000	2.372964000	2.540952000	6	5.536695000	2.278007000	-2.571989000
1	-4.877529000	3.060164000	1.844926000	1	5.017556000	2.977691000	-1.915312000
1	-4.597738000	1.714982000	2.967361000	1	4.797365000	1.612513000	-3.027077000
1	-5.778666000	2.971234000	3.354700000	1	6.000115000	2.860903000	-3.372595000
6	6.409568000	-3.310788000	2.517060000	6	-6.596391000	-3.365206000	-2.321132000
1	6.152306000	-2.514385000	3.218836000	1	-6.430550000	-2.593814000	-3.076039000
1	7.298470000	-3.815466000	2.903128000	1	-7.509757000	-3.899420000	-2.592477000
1	5.609732000	-4.047854000	2.512082000	1	-5.787072000	-4.089797000	-2.372369000
6	-4.581289000	-1.569267000	-0.882921000	6	4.526165000	-1.620466000	0.811525000
6	-6.984776000	-2.565240000	-0.889188000	6	6.930365000	-2.564473000	1.089014000
6	3.277191000	-0.854415000	0.313278000	6	-3.337883000	-0.776146000	-0.552628000
6	-7.165468000	0.702748000	2.949198000	6	7.358243000	0.599408000	-2.848164000
1	-8.058154000	0.190706000	2.580957000	1	8.224523000	0.089156000	-2.419278000
1	-7.488466000	1.353933000	3.765369000	1	7.732296000	1.235661000	-3.654496000
1	-6.483466000	-0.043185000	3.366431000	1	6.697943000	-0.150665000	-3.292098000
6	6.542815000	1.250318000	-1.854758000	6	-6.400663000	1.334547000	1.904140000
6	7.590697000	2.215058000	-1.247811000	6	-7.483337000	2.285676000	1.337598000
1	8.367452000	1.656864000	-0.717769000	1	-8.288250000	1.716825000	0.864005000

1	7.132111000	2.909403000	-0.545738000	1	-7.067275000	2.967239000	0.597355000
1	8.070489000	2.786330000	-2.049170000	1	-7.917302000	2.872210000	2.153599000
6	5.477015000	2.065424000	-2.624746000	6	-5.291577000	2.165799000	2.590980000
1	4.721371000	1.410311000	-3.068020000	1	-4.509681000	1.520747000	3.002174000
1	5.954455000	2.622231000	-3.435602000	1	-5.720865000	2.738747000	3.417067000
1	4.975710000	2.789720000	-1.981042000	1	-4.830787000	2.877797000	1.904947000
6	-6.798205000	-3.199899000	-2.287176000	6	6.616177000	-3.152975000	2.483650000
1	-6.609231000	-2.445362000	-3.053594000	1	6.337791000	-2.374407000	3.197272000
1	-7.725140000	-3.713152000	-2.552916000	1	7.519185000	-3.638427000	2.861548000
1	-6.008933000	-3.947089000	-2.324494000	1	5.837092000	-3.911800000	2.468472000
6	-7.541251000	2.528792000	1.272933000	6	7.644892000	2.455751000	-1.190399000
1	-7.103266000	3.184287000	0.521809000	1	7.168265000	3.123541000	-0.474617000
1	-7.962680000	3.142358000	2.075545000	1	8.109338000	3.055215000	-1.980145000
1	-8.359297000	1.973270000	0.806116000	1	8.436126000	1.907788000	-0.671251000
6	-7.046224000	-3.684801000	0.177807000	6	7.118155000	-3.718680000	0.075382000
1	-6.110009000	-4.244355000	0.210266000	1	6.199809000	-4.299070000	-0.027165000
1	-7.856044000	-4.378235000	-0.066963000	1	7.913271000	-4.385119000	0.422628000
1	-7.242391000	-3.285283000	1.176642000	1	7.403815000	-3.349809000	-0.913690000
6	7.255489000	0.336654000	-2.870773000	6	-7.049645000	0.441470000	2.979406000
1	8.108686000	-0.187734000	-2.432746000	1	-7.930779000	-0.087372000	2.607048000
1	7.645245000	0.948662000	-3.688336000	1	-7.384817000	1.069759000	3.808480000
1	6.576086000	-0.404157000	-3.301253000	1	-6.345886000	-0.293312000	3.379980000
6	6.897050000	-3.925419000	0.117709000	6	-6.822969000	-3.895322000	0.136607000
1	5.962954000	-4.481434000	0.022689000	1	-5.871517000	-4.429119000	0.157758000
1	7.673094000	-4.608653000	0.475314000	1	-7.613988000	-4.607040000	-0.116965000
1	7.193384000	-3.579069000	-0.876363000	1	-7.027129000	-3.517154000	1.142117000
6	8.098835000	-2.016834000	1.262793000	6	-8.181830000	-2.060503000	-0.953321000
1	8.012046000	-1.158021000	1.933736000	1	-8.182239000	-1.221578000	-1.654294000
1	8.506531000	-1.664289000	0.315045000	1	-8.512515000	-1.690427000	0.017309000
1	8.828582000	-2.707104000	1.692816000	1	-8.928114000	-2.782166000	-1.293285000
6	-8.350849000	-1.830691000	-0.945164000	6	8.267522000	-1.794376000	1.247668000
1	-8.325982000	-1.002912000	-1.658826000	1	8.157551000	-0.948215000	1.931182000
1	-8.674294000	-1.436922000	0.018556000	1	8.664605000	-1.416777000	0.305078000
1	-9.115661000	-2.536686000	-1.276749000	1	9.016441000	-2.470409000	1.667221000
7	-4.065139000	-2.684338000	-1.743512000	7	3.925014000	-2.702825000	1.648256000
8	-3.917169000	-3.773681000	-1.216330000	8	3.862361000	-3.819892000	1.162354000
8	-3.816259000	-2.413891000	-2.905398000	8	3.514846000	-2.385088000	2.752721000
8	3.330155000	-2.451859000	2.771867000	8	-3.639047000	-2.487107000	-2.935683000
7	3.731919000	-2.797641000	1.672699000	7	-3.876704000	-2.782222000	-1.777459000
8	3.637720000	-3.919583000	1.203471000	8	-3.696811000	-3.874952000	-1.267543000

Table S18 Optimized geometries of tropolone **7** isomers. PCM/B3LYP/6-311++G(d,p) calculations (DMSO). Coordinates in Angstroms.

7 (OH)				7 (NH)			
17	-1.379227000	5.352652000	-0.161756000	17	-1.382458000	5.341547000	-0.096529000
1	1.294939000	4.740821000	0.141030000	1	1.303004000	4.734707000	0.102163000
7	1.187007000	0.889194000	0.110426000	7	1.200308000	0.924279000	0.094379000
1	1.546288000	-0.569764000	0.177491000	1	1.260291000	-0.123771000	0.112938000
6	0.018837000	2.999416000	-0.001983000	6	0.018288000	2.999836000	0.008842000
7	-1.099991000	0.848991000	-0.113330000	7	-1.112012000	0.883431000	-0.074172000
1	-1.420983000	-0.620785000	-0.209441000	1	-1.140733000	-0.165154000	-0.094109000
8	2.249490000	-1.324874000	0.268421000	8	2.295878000	-1.317210000	0.283638000
8	5.065170000	2.269840000	1.192938000	8	5.152594000	2.343768000	0.888769000
6	0.031091000	1.580300000	-0.002381000	6	0.031780000	1.597763000	0.009397000
6	1.261292000	3.659138000	0.132834000	6	1.272806000	3.653172000	0.101708000
6	-2.294965000	1.439626000	-0.237863000	6	-2.356645000	1.442963000	-0.174552000
8	-2.104810000	-1.390133000	-0.317088000	8	-2.147437000	-1.386063000	-0.278974000
8	-5.037651000	2.149188000	-1.111722000	8	-5.106980000	2.210262000	-0.821464000
6	3.564720000	0.655036000	0.326618000	6	3.586022000	0.672737000	0.259639000

6	2.366565000	1.511037000	0.238491000	6	2.429838000	1.518207000	0.194048000
6	5.975954000	0.807843000	-0.438307000	6	5.962738000	0.708621000	-0.624614000
6	-3.473083000	0.555203000	-0.320796000	6	-3.491923000	0.568118000	-0.239611000
6	-5.868103000	0.621350000	0.501219000	6	-5.863943000	0.518639000	0.655658000
6	-5.686078000	-1.778270000	-0.336335000	6	-5.709845000	-1.763175000	-0.458578000
6	5.840659000	-1.617823000	0.332732000	6	5.869275000	-1.597738000	0.445618000
6	-4.359587000	-1.803673000	-0.635335000	6	-4.390610000	-1.765444000	-0.759706000
6	4.890856000	1.299759000	0.464656000	6	4.920712000	1.306021000	0.275457000
6	6.354944000	-0.486751000	-0.424701000	6	6.346154000	-0.571833000	-0.483673000
1	7.214671000	-0.741534000	-1.028119000	1	7.157471000	-0.914968000	-1.111153000
6	-4.819032000	1.165334000	-0.414131000	6	-4.842985000	1.163640000	-0.235537000
6	-6.214404000	-0.681627000	0.461174000	6	-6.213386000	-0.768521000	0.490347000
1	-7.053124000	-0.975429000	1.076518000	1	-7.012923000	-1.145963000	1.113259000
6	2.416939000	2.936042000	0.259098000	6	2.438411000	2.944204000	0.198137000
1	3.358157000	3.442584000	0.390121000	1	3.378464000	3.458778000	0.299587000
6	3.433317000	-0.732771000	0.353515000	6	3.421206000	-0.751705000	0.360252000
6	-6.731095000	-2.885861000	-0.660388000	6	-6.776066000	-2.794395000	-0.924213000
6	6.703625000	1.857680000	-1.309150000	6	6.610747000	1.650831000	-1.664113000
6	-1.253642000	3.608935000	-0.139430000	6	-1.266482000	3.604037000	-0.087792000
6	-2.392530000	2.860436000	-0.263395000	6	-2.413895000	2.864776000	-0.183989000
1	-3.346632000	3.340015000	-0.399260000	1	-3.368472000	3.349833000	-0.292494000
6	5.674049000	2.818570000	-1.947540000	6	5.516597000	2.495365000	-2.358134000
1	5.134533000	3.397587000	-1.197283000	1	4.992412000	3.144784000	-1.655247000
1	4.947816000	2.273879000	-2.557349000	1	4.781478000	1.857741000	-2.857176000
1	6.193321000	3.527967000	-2.596762000	1	5.975817000	3.135678000	-3.115708000
6	-6.392674000	-3.777663000	-1.876535000	6	-6.457275000	-3.504133000	-2.259271000
1	-6.146772000	-3.184023000	-2.759424000	1	-6.202400000	-2.790446000	-3.045701000
1	-7.278884000	-4.368672000	-2.116225000	1	-7.353175000	-4.039616000	-2.580476000
1	-5.591531000	-4.489007000	-1.686428000	1	-5.665871000	-4.246721000	-2.178794000
6	4.510262000	-1.685957000	0.607188000	6	4.550885000	-1.641956000	0.748152000
6	6.908975000	-2.706333000	0.646793000	6	6.964255000	-2.607973000	0.890924000
6	-3.304378000	-0.827805000	-0.375431000	6	-3.286731000	-0.850373000	-0.354065000
6	7.493993000	1.191508000	-2.452585000	6	7.355044000	0.857990000	-2.756076000
1	8.335919000	0.597533000	-2.089269000	1	8.226602000	0.327412000	-2.365195000
1	7.908601000	1.972248000	-3.095005000	1	7.719028000	1.556989000	-3.513294000
1	6.856467000	0.552403000	-3.069350000	1	6.700894000	0.135980000	-3.252144000
6	-6.595117000	1.628817000	1.421080000	6	-6.529095000	1.421204000	1.719404000
6	-7.621151000	2.447852000	0.599886000	6	-7.567264000	2.355920000	1.052134000
1	-8.365569000	1.790058000	0.143226000	1	-8.346460000	1.773889000	0.552419000
1	-7.134405000	3.018669000	-0.189897000	1	-7.100785000	3.009744000	0.316607000
1	-8.143452000	3.143558000	1.263755000	1	-8.043734000	2.974560000	1.818897000
6	-5.567227000	2.587609000	2.065864000	6	-5.449826000	2.271860000	2.429521000
1	-4.819918000	2.037062000	2.644089000	1	-4.699901000	1.637915000	2.910908000
1	-6.083474000	3.269376000	2.746334000	1	-5.919190000	2.884610000	3.203513000
1	-5.052328000	3.197098000	1.322305000	1	-4.941643000	2.948408000	1.740475000
6	6.572896000	-3.639930000	1.831871000	6	6.665004000	-3.356943000	2.208901000
1	6.295343000	-3.077562000	2.725739000	1	6.388835000	-2.669245000	3.011107000
1	7.470321000	-4.213608000	2.071940000	1	7.575889000	-3.873279000	2.519073000
1	5.794809000	-4.366799000	1.607769000	1	5.895714000	-4.120262000	2.110110000
6	7.693985000	2.668149000	-0.437065000	6	7.625439000	2.590984000	-0.968730000
1	7.177631000	3.201541000	0.360112000	1	7.141889000	3.214474000	-0.217934000
1	8.216631000	3.396590000	-1.064585000	1	8.090198000	3.240320000	-1.717087000
1	8.441231000	2.009784000	0.014083000	1	8.415974000	2.013698000	-0.481498000
6	7.124584000	-3.560369000	-0.626327000	6	7.171969000	-3.638797000	-0.245094000
1	6.213663000	-4.099432000	-0.894252000	1	6.265600000	-4.224201000	-0.411936000
1	7.916040000	-4.291556000	-0.440630000	1	7.978751000	-4.323360000	0.030982000
1	7.427487000	-2.951736000	-1.481700000	1	7.450218000	-3.159861000	-1.186965000
6	-7.344683000	0.911242000	2.560740000	6	-7.251016000	0.586005000	2.794649000
1	-8.182166000	0.310816000	2.197819000	1	-8.111890000	0.045255000	2.394049000
1	-7.760264000	1.662821000	3.236449000	1	-7.627785000	1.258438000	3.569460000
1	-6.679983000	0.267177000	3.142674000	1	-6.578942000	-0.132561000	3.271383000
6	-6.900652000	-3.779126000	0.592561000	6	-6.951386000	-3.856008000	0.188696000

1	-5.971935000	-4.302771000	0.827870000	1	-6.028392000	-4.419153000	0.340157000
1	-7.678007000	-4.524071000	0.402084000	1	-7.739416000	-4.556634000	-0.100920000
1	-7.200694000	-3.201399000	1.470068000	1	-7.240171000	-3.406454000	1.141864000
6	-8.087286000	-2.212583000	-1.003777000	6	-8.122108000	-2.056231000	-1.150695000
1	-7.987141000	-1.544779000	-1.863449000	1	-8.019761000	-1.277585000	-1.911207000
1	-8.512178000	-1.643337000	-0.177527000	1	-8.521402000	-1.597948000	-0.246200000
1	-8.807273000	-2.991606000	-1.263868000	1	-8.861972000	-2.777952000	-1.504173000
6	8.240562000	-2.008043000	1.033837000	6	8.288056000	-1.836367000	1.136807000
1	8.107205000	-1.366637000	1.908963000	1	8.162203000	-1.079114000	1.915188000
1	8.665578000	-1.405764000	0.231500000	1	8.674814000	-1.345628000	0.244012000
1	8.975837000	-2.775051000	1.286746000	1	9.048265000	-2.544339000	1.474601000
7	3.912233000	-2.940445000	1.170733000	7	3.968759000	-2.800516000	1.492802000
8	3.776973000	-3.889601000	0.414169000	8	3.851361000	-3.858877000	0.893856000
8	3.566652000	-2.925321000	2.341157000	8	3.606064000	-2.609142000	2.643807000
8	-3.409817000	-2.971405000	-2.414810000	8	-3.413892000	-2.668429000	-2.670555000
7	-3.737925000	-3.026806000	-1.240560000	7	-3.775428000	-2.892819000	-1.525112000
8	-3.567594000	-3.991903000	-0.511827000	8	-3.632198000	-3.959775000	-0.947415000
7 (OH)(NH)				7 (NH)(OH)			
17	1.381091000	5.328501000	0.209609000	17	-1.388439000	5.340798000	-0.026649000
1	-1.305173000	4.729052000	-0.041569000	1	1.302924000	4.722101000	0.195713000
7	-1.191217000	0.878294000	-0.138836000	7	1.192943000	0.913457000	0.064082000
1	-1.573732000	-0.622449000	-0.301906000	1	1.221254000	-0.124345000	0.041344000
6	-0.027621000	2.989392000	0.022108000	6	0.011017000	2.992020000	0.033586000
7	1.105032000	0.870932000	0.051582000	7	-1.101622000	0.841045000	-0.129821000
1	1.104139000	-0.166801000	0.030436000	1	-1.442569000	-0.667890000	-0.326677000
8	-2.283356000	-1.341097000	-0.429717000	8	2.314745000	-1.350688000	0.194223000
8	-5.118509000	2.310238000	-1.041047000	8	5.132827000	2.313932000	0.955751000
6	-0.058529000	1.580107000	-0.022889000	6	0.005515000	1.582156000	-0.012860000
6	-1.269328000	3.647966000	-0.067751000	6	1.268812000	3.640957000	0.161039000
6	2.342621000	1.419715000	0.182890000	6	-2.307317000	1.435742000	-0.214153000
8	2.168604000	-1.420731000	0.194068000	8	-2.133266000	-1.400607000	-0.473740000
8	5.087244000	2.184613000	0.890148000	8	-5.083519000	2.185666000	-0.956423000
6	-3.579836000	0.654227000	-0.323744000	6	3.579070000	0.656565000	0.254745000
6	-2.381186000	1.505105000	-0.223949000	6	2.416204000	1.495067000	0.198346000
6	-5.953789000	0.765478000	0.554616000	6	5.966474000	0.728295000	-0.596322000
6	3.486071000	0.553161000	0.236182000	6	-3.484715000	0.555135000	-0.313649000
6	5.867920000	0.545785000	-0.632568000	6	-5.844300000	0.571368000	0.606587000
6	5.729289000	-1.760487000	0.427529000	6	-5.712374000	-1.761640000	-0.402724000
6	-5.873346000	-1.598923000	-0.387002000	6	5.884226000	-1.597127000	0.427518000
6	4.407146000	-1.781900000	0.711980000	6	-4.398518000	-1.770935000	-0.753962000
6	-4.911704000	1.306948000	-0.370740000	6	4.909393000	1.294980000	0.307748000
6	-6.343896000	-0.522702000	0.472638000	6	6.362957000	-0.550013000	-0.477689000
1	-7.175284000	-0.815549000	1.098452000	1	7.182987000	-0.873837000	-1.104281000
6	4.832373000	1.156631000	0.267257000	6	-4.835396000	1.168835000	-0.320872000
6	6.231578000	-0.740386000	-0.495428000	6	-6.199585000	-0.724568000	0.494892000
1	7.039420000	-1.095504000	-1.120936000	1	-7.010639000	-1.058880000	1.126655000
6	-2.429788000	2.924537000	-0.195341000	6	2.427814000	2.926132000	0.246975000
1	-3.372214000	3.436013000	-0.293578000	1	3.368980000	3.433021000	0.373885000
6	-3.463114000	-0.728577000	-0.440802000	6	3.426520000	-0.773115000	0.312050000
6	6.802064000	-2.787900000	0.886386000	6	-6.776853000	-2.836018000	-0.770481000
6	-6.623900000	1.760295000	1.528901000	6	6.610125000	1.698954000	-1.611904000
6	1.260267000	3.589226000	0.149611000	6	-1.260389000	3.601100000	-0.061107000
6	2.401831000	2.846570000	0.234721000	6	-2.403556000	2.850822000	-0.189317000
1	3.356834000	3.325137000	0.365711000	1	-3.359304000	3.334792000	-0.293915000
6	-5.551111000	2.667225000	2.174862000	6	5.509751000	2.540005000	-2.300268000
1	-5.039942000	3.286986000	1.437197000	1	4.968834000	3.167342000	-1.589883000
1	-4.803960000	2.076864000	2.712598000	1	4.789200000	1.901156000	-2.818559000
1	-6.027989000	3.339781000	2.892220000	1	5.965986000	3.202225000	-3.040686000
6	6.475819000	-3.525637000	2.204320000	6	-6.494569000	-3.622548000	-2.070824000
1	6.203668000	-2.829210000	3.000442000	1	-6.277188000	-2.956516000	-2.908394000
1	7.373699000	-4.057199000	2.526640000	1	-7.394971000	-4.185128000	-2.325389000
1	5.693455000	-4.274934000	2.100797000	1	-5.693470000	-4.352485000	-1.974034000

6	-4.555897000	-1.655511000	-0.720141000	6	4.562267000	-1.658301000	0.707758000
6	-6.965726000	-2.650876000	-0.737721000	6	6.983128000	-2.602264000	0.874376000
6	3.294799000	-0.871581000	0.306055000	6	-3.329122000	-0.820978000	-0.461152000
6	-7.362079000	1.024611000	2.664432000	6	7.376222000	0.937550000	-2.711074000
1	-8.226751000	0.461356000	2.305680000	1	8.250985000	0.411533000	-2.321128000
1	-7.736129000	1.763372000	3.377498000	1	7.737965000	1.655686000	-3.451309000
1	-6.700257000	0.341908000	3.204036000	1	6.737175000	0.216066000	-3.227194000
6	6.529304000	1.482246000	-1.668953000	6	-6.520708000	1.519489000	1.622232000
6	7.553586000	2.410306000	-0.971647000	6	-7.579899000	2.391236000	0.903961000
1	8.336295000	1.823674000	-0.482897000	1	-8.348475000	1.765324000	0.442614000
1	7.076039000	3.039279000	-0.221626000	1	-7.128401000	3.010090000	0.129477000
1	8.027520000	3.054196000	-1.718993000	1	-8.066274000	3.044792000	1.634499000
6	5.445749000	2.339938000	-2.363753000	6	-5.457985000	2.432815000	2.276282000
1	4.705234000	1.711206000	-2.866070000	1	-4.688333000	1.844920000	2.784123000
1	5.913390000	2.977468000	-3.118567000	1	-5.937885000	3.072827000	3.020870000
1	4.926296000	2.993089000	-1.660623000	1	-4.973917000	3.085970000	1.549027000
6	-6.683224000	-3.505040000	-1.994264000	6	6.672122000	-3.372255000	2.177435000
1	-6.427747000	-2.886342000	-2.856927000	1	6.377355000	-2.698218000	2.984667000
1	-7.596638000	-4.049578000	-2.241703000	1	7.583256000	-3.884198000	2.494253000
1	-5.908835000	-4.255051000	-1.846553000	1	5.911562000	-4.141188000	2.056862000
6	-7.647488000	2.635133000	0.764137000	6	7.604123000	2.641508000	-0.890450000
1	-7.166553000	3.216285000	-0.021817000	1	7.104531000	3.243952000	-0.132983000
1	-8.128978000	3.324700000	1.464214000	1	8.065899000	3.311208000	-1.622579000
1	-8.424263000	2.014447000	0.309502000	1	8.398784000	2.067414000	-0.406132000
6	-7.151048000	-3.587729000	0.480697000	6	7.218376000	-3.614866000	-0.272419000
1	-6.238898000	-4.153338000	0.681296000	1	6.320515000	-4.206615000	-0.461393000
1	-7.957019000	-4.296268000	0.271235000	1	8.027792000	-4.295441000	0.005958000
1	-7.419162000	-3.036422000	1.385036000	1	7.506001000	-3.119497000	-1.202920000
6	7.266303000	0.682402000	-2.760777000	6	-7.218884000	0.731520000	2.747922000
1	8.130195000	0.140297000	-2.368644000	1	-8.075820000	0.157523000	2.387633000
1	7.640710000	1.378177000	-3.515925000	1	-7.597767000	1.438845000	3.489745000
1	6.604499000	-0.030670000	-3.259608000	1	-6.530346000	0.049985000	3.254573000
6	7.002883000	-3.826409000	-0.243709000	6	-6.896793000	-3.830047000	0.410269000
1	6.088190000	-4.396737000	-0.417088000	1	-5.961013000	-4.371438000	0.562364000
1	7.795316000	-4.523731000	0.041986000	1	-7.684089000	-4.556543000	0.191386000
1	7.297920000	-3.355372000	-1.184523000	1	-7.158043000	-3.326772000	1.344227000
6	8.136791000	-2.038939000	1.142049000	6	-8.143099000	-2.134641000	-0.997426000
1	8.017137000	-1.276536000	1.916398000	1	-8.078067000	-1.400542000	-1.804768000
1	8.539857000	-1.558304000	0.250898000	1	-8.527582000	-1.632310000	-0.110322000
1	8.881558000	-2.758656000	1.489410000	1	-8.878140000	-2.889138000	-1.286017000
6	-8.298522000	-1.910034000	-1.029959000	6	8.295185000	-1.820915000	1.149881000
1	-8.185818000	-1.216563000	-1.867471000	1	8.150534000	-1.075856000	1.936752000
1	-8.683217000	-1.353260000	-0.176053000	1	8.688810000	-1.313771000	0.269281000
1	-9.055378000	-2.648624000	-1.303014000	1	9.058136000	-2.525565000	1.488577000
7	-3.991639000	-2.869348000	-1.396641000	7	3.979472000	-2.832270000	1.426128000
8	-3.840295000	-3.873444000	-0.718366000	8	3.885700000	-3.884704000	0.812443000
8	-3.686952000	-2.768556000	-2.574196000	8	3.591101000	-2.659625000	2.571989000
8	3.412755000	-2.726757000	2.593044000	8	-3.517831000	-2.799431000	-2.650267000
7	3.794686000	-2.928303000	1.449711000	7	-3.809004000	-2.946976000	-1.474187000
8	3.672309000	-3.987764000	0.853435000	8	-3.625715000	-3.968679000	-0.830976000

Biologic studies

Cell lines

The cell lines of human non-small cell lung cancer A549 and H1299, human colon cancer HT29, mouse colon cancer CT26 and mouse melanoma B16F10 were employed in the work. Cells were cultured in RPMI1640 medium supplemented with 10% FBS and 100 µg/ml streptomycin in 5% CO₂ at 37 °C.

MTT test

The metabolic activity of cells was estimated by a modified Mosman method based on the reduction of tetrazolium salt by living cells to form the blue formazan product^{S9}.

The cell lines under study were transferred into plate wells of 2×10⁵ cells/ml and incubated at 37 °C. After a 24-hour incubation period, studied bistropolone dissolved in DMSO was added to each well at final concentrations of 16, 32, and 64 µg/mL. After a 48-hour incubation period, 20 µL of 5 mg/mL MTT solution was added. The plate was further incubated at 37°C for 4 hours. At the end of the incubation, the wells were washed with PBS, allowed to dry for 2 hours, and 200 µl of DMSO was added. After dissolution of the formazan crystals, metabolic activity was assessed spectrophotometrically at 492 nm using a microplate reader. Experimental wells of the plate were compared with control wells in which tumor cells were not exposed. The growth inhibition percentage was calculated by the following formula:

$$\% \text{ cellular inhibition} = 100 - [(A_t - A_b) / (A_c - A_b)] \times 100,$$

where A_t = absorbance value of test compound, A_b = absorbance value of blank and A_c = absorbance value of control.^{S10}

The percentage of viable cells was calculated by the formula:

$$\% \text{ Viable Cells} = 100 - \% \text{ Cellular Inhibition.}$$

During the experiment, the MTT test was performed in triplicate for each cell line, so the results represent the average of the experiments performed. Statistical analysis was performed using GraphPad Prism 10 software, p-value less than 0.05 was considered to be statistically significant.

Table S19 Cytotoxic activity *in vitro* of bistropolone 7.

Concentration, μg/ml	Absorbance, M±m	Inhibition, %
A549		
Control	0.981±0.001	-
16	0.678±0.007	31.1
32	0.460±0.002	53.6
64	0.170±0.007	83.3
H1299		
Control	0.964±0.002	-
16	0.775±0.008	19.1
32	0.383±0.003	61.4
64	0.111±0.005	90.2
HT29		
Control	0.954±0.004	-
16	0.593±0.001	38.4
32	0.386±0.007	60.5
64	0.144±0.002	86.3
CT26		
Control	0.937±0.002	-
16	0.788±0.001	15.9
32	0.424±0.001	54.9
64	0.200±0.001	79.0
B16F10		
Control	0.931±0.001	-
16	0.885±0.001	5.0
32	0.459±0.005	51.8
64	0.098±0.002	91.4

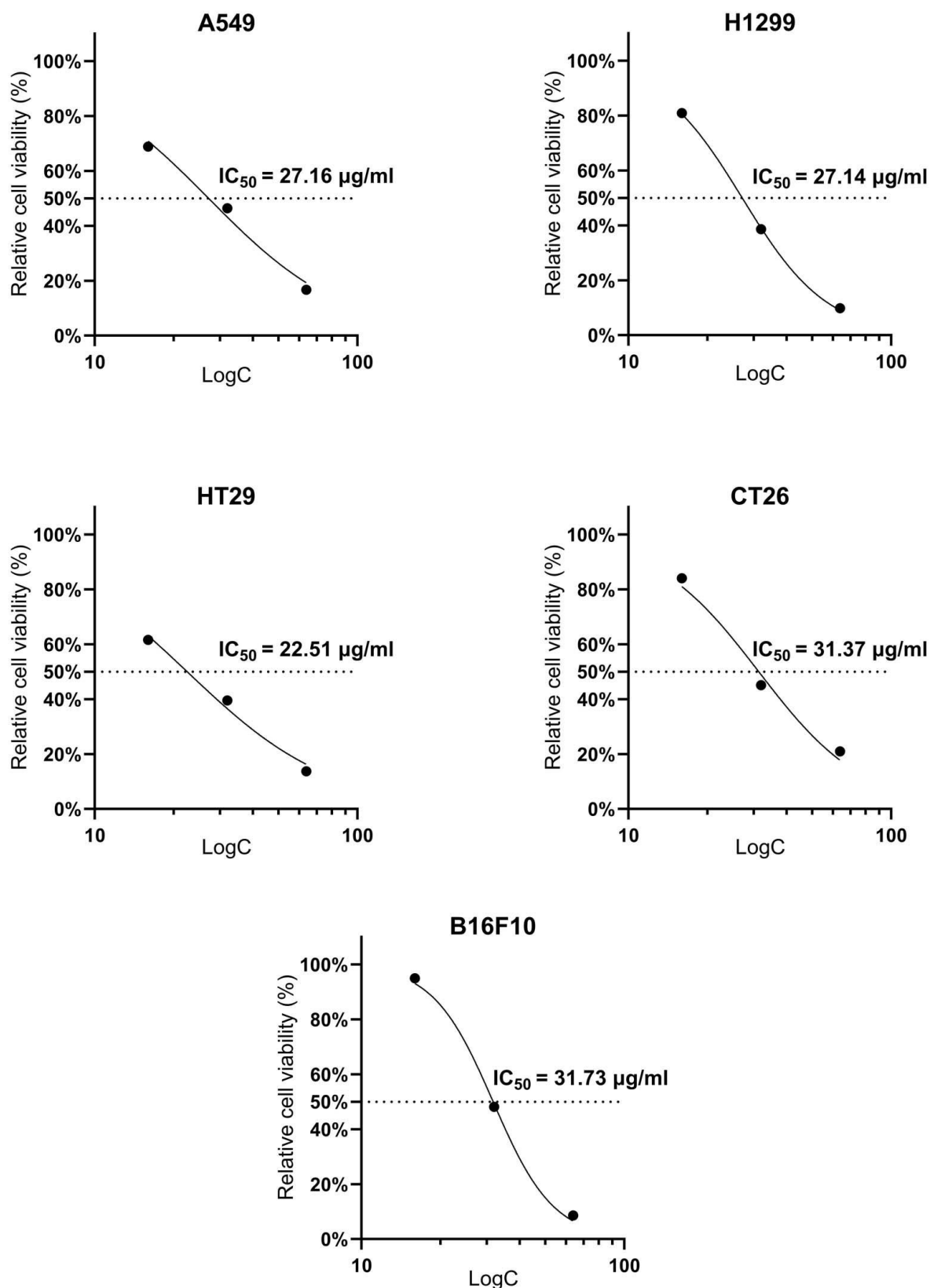


Figure S31 IC₅₀ curves for the cell lines studied with bistropolone 7.

References:

- S1. C. J. Chandler, L. W. Deady, J. A. Reiss and V. Tzimos, *J. Heterocycl. Chem.*, 1982, **19**, 1017.
- S2. K. Ley and E. Müller, *Chem. Ber.*, 1956, **89**, 1402.
- S3. G. M. Sheldrick, *SHELXTL*, v. 6.14, Structure Determination Software Suite, Bruker AXS, Madison, WI, 2000.
- S4. A. D. Becke, *Phys. Rev. A*, 1988, **38**, 3098.
- S5. A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648.
- S6. C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785.
- S7. V. Barone, M. Cossi and J. Tomasi, *J. Chem. Phys.*, 1997, **107**, 3210.
- S8. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, *Gaussian 16, Revision C.01*, Gaussian, Inc., Wallingford CT, 2016.
- S9. T. Mosmann, *J. Immunol. Methods*, 1983, **65**, 55.
- S10. F. Nemati, A. A. Dehpouri, B. Eslami, V. Mahdavi and S. Mirzanejad, *Iran Red Crescent Med. J.*, 2013, **15**, e8871.