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Supporting Information for An aza-Diels–Alder approach to chlorinated quinolines, benzoquinolines, and polybenzoquinolines

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I. General Information and Procedures.

A. Materials. The starting materials and standard solvents were purchased obtained from Sigma Aldrich, Acros Organics, and/or Combi-Blocks, as necessary. The deuterated solvents used for NMR spectroscopy were purchased from Cambridge Isotope Laboratories. The toluene, chloroform, and tetrahydrofuran (THF) solvents were dried with 3 Å molecular sieves (Davison or Macron) and typically stored under argon.

B. General Reaction Conditions. The glassware was washed, oven dried at 150 °C, and cooled under argon prior to use. The reactions were performed under an inert dry argon atmosphere, unless otherwise noted.

C. Small Molecule Chromatographic Purification. Flash chromatography was performed with a CombiFlash Rf_{200} purification system (Teledyne ISCO, Inc.) according to the manufacturer's recommended protocols. When required, the silica gel columns/cartridges were flushed with 1:9 triethylamine:hexanes to deactivate the silica gel and were then flushed again with hexanes to remove any residual triethylamine. This general procedure was followed when necessary, unless otherwise noted.

D. Reaction Product Characterization. The intermediates and products were all routinely characterized via ¹H and ¹³C nuclear magnetic resonance (NMR) spectroscopy, as well as high resolution mass spectrometry. The ¹H NMR and ¹³C NMR were obtained on either a Bruker AVANCE400 instrument, a Bruker DRX500 instrument, a Bruker DRX500 instrument outfitted with a CryoProbe (Bruker TCI 500 MHz, 5 mm diameter tubes), or an AVANCE600 instrument. The chemical shifts were reported in ppm for both ¹H and ¹³C NMR. The chemical shifts for the NMR data were referenced as follows: for samples in CDCl₃, the ¹H NMR was referenced to the CHCl₃ peak at 7.26 ppm or tetramethylsilane (TMS) at 0.00 ppm, and the ¹³C NMR was referenced to the CHCl₃ peak at 77.16 ppm; for samples in CD₂Cl₂, the ¹H NMR was referenced to the CH₂Cl₂ peak at 5.32 ppm, and the ¹³C NMR was referenced to the CH₂Cl₂ peak at 54.00 ppm. The data were labeled with the chemical shift, multiplicity (s = singlet, d = doublet, dd =doublet of doublets, dt = doublet of triplets, t = triplet, td = triplet of doublets, q = quartet, quint = quintet, m = multiplet, br s = broad singlet, br = broad peak), coupling constants in Hertz, and integration values. Accurate mass measurements were obtained via electrospray ionization (ESI) high resolution mass spectrometry (HRMS) at the University of California, Irvine Mass Spectrometry Facility on a Waters LCT Premier time-of-flight instrument. This combination of procedures facilitated confirmation of the identities of the synthesized intermediates and products.

E. Polymer Characterization. The crude and purified polymers were analyzed via size exclusion chromatography (SEC) with a refractive index detector (SEC-RI) by use of an Agilent Technologies 1260 Infinity Series separations module equipped with two Agilent ResiPore columns connected in series (7.5 mm x 300 mm, 3 µm particle size). The separations module was also connected to Agilent 1260 infinity dual angle light scattering, refractive index, and viscosity detectors in series. The typical analysis conditions were as follows: solvent, benzene; flow rate, ~ 1.0 mL/minute; injection volume, ~ 25 – 100 µL; sample concentration: ~ 1.0 - 2.5 mg/mL; temperature: 60 °C. The molecular weights of the synthesized polymers (M_n and M_w) were estimated via calibration against polystyrene standards (EasiVial PS-H, Agilent).

II. NMR Spectroscopy and Size Exclusion Chromatography Characterization Data.



Figure S1. The ¹H NMR spectrum obtained for 1a (recorded in CDCl₃).



Figure S2. The ¹³C NMR spectrum obtained for 1a (recorded in CDCl₃).



Figure S3. The ¹H NMR spectrum obtained for 1b (recorded in CDCl₃).



Figure S4. The ¹³C NMR spectrum obtained for 1b (recorded in CDCl₃).



Figure S5. The ¹H NMR spectrum obtained for 1c (recorded in CDCl₃).



Figure S6. The ¹³C NMR spectrum obtained for 1c (recorded in CDCl₃).



Figure S7. The ¹H NMR spectrum obtained for 1d (recorded in CDCl₃).



Figure S8. The ¹³C NMR spectrum obtained for 1d (recorded in CDCl₃).



Figure S9. The ¹H NMR spectrum obtained for 1e (recorded in CDCl₃).



Figure S10. The ¹³C NMR spectrum obtained for 1e (recorded in CDCl₃).



Figure S11. The ¹H NMR spectrum obtained for 1f (recorded in CDCl₃).



Figure S12. The ¹³C NMR spectrum obtained for 1f (recorded in CDCl₃).



Figure S13. The ¹H NMR spectrum obtained for 2a (recorded in CD₂Cl₂).



Figure S14. The ¹³C NMR spectrum obtained for 2a (recorded in CD₂Cl₂).



Figure S15. The ¹H NMR spectrum obtained for 2b (recorded in CD₂Cl₂).



Figure S16. The ¹³C NMR spectrum obtained for 2b (recorded in CD₂Cl₂).



Figure S17. The ¹H NMR spectrum obtained for 2c (recorded in CD₂Cl₂).



Figure S18. The ¹³C NMR spectrum obtained for 2c (recorded in CD₂Cl₂).



Figure S19. The ¹H NMR spectrum obtained for 2d (recorded in CD₂Cl₂).



Figure S20. The 13 C NMR spectrum obtained for 2d (recorded in CD₂Cl₂).



Figure S21. The ¹H NMR spectrum obtained for 2e (recorded in CDCl₃).



Figure S22. The ¹³C NMR spectrum obtained for 2e (recorded in CDCl₃).



Figure S23. The ¹H NMR spectrum obtained for 2f (recorded in CD₂Cl₂).



Figure S24. The ¹³C NMR spectrum obtained for 2f (recorded in CD₂Cl₂).



Figure S25. The ¹H NMR spectrum obtained for 3 (recorded in CDCl₃).



Figure S26. The ¹H NMR spectrum obtained for 4 (recorded in CDCl₃).



Figure S27. The ¹³C NMR spectrum obtained for 4 (recorded in CDCl₃).



Figure S28. The ¹H NMR spectrum obtained for 5 (recorded in CD₂Cl₂).



Figure S29. The ¹³C NMR spectrum obtained for 5 (recorded in CD₂Cl₂).



Figure S30. The ¹H NMR spectrum obtained for 6 (recorded in CDCl₃, TMS^{*} = trimethylsilyl).



Figure S31. The ¹³C NMR spectrum obtained for 6 (recorded in $CDCl_3$, TMS^* = trimethylsilyl).



Figure S32. The ¹H NMR spectrum obtained for 7 (recorded in CDCl₃).



Figure S33. The ¹³C NMR spectrum obtained for 7 (recorded in CDCl₃).



Figure S34. The ¹H NMR spectrum obtained for 8 (recorded in CD₂Cl₂).



Figure S35. The ¹³C NMR spectrum obtained for 8 (recorded in CD₂Cl₂).



Figure S36. The ¹H NMR spectrum obtained for 9 (recorded in CD₂Cl₂).



Figure S37. The ¹³C NMR spectrum obtained for 9 (recorded in CD₂Cl₂).



Figure S38. The ¹H NMR spectrum obtained for 10 (recorded in CD₂Cl₂).



Figure S39. The ¹³C NMR spectrum obtained for 10 (recorded in CD₂Cl₂).



Figure S40. The ¹H NMR spectrum obtained for 11 (recorded in CDCl₃, TMS^{*} = trimethylsilyl).



Figure S41. The ¹³C NMR spectrum obtained for 11 (recorded in CDCl₃, TMS^{*} = trimethylsilyl).



Figure S42. The ¹H NMR spectrum obtained for 12 (recorded in CDCl₃).



Figure S43. The ¹³C NMR spectrum obtained for 12 (recorded in CDCl₃).



Figure S44. The ¹H NMR spectrum obtained for P1 (recorded in CDCl₃).



Figure S45. The SEC-RI chromatograms obtained for crude P1 (black solid line) and purified P1 (red solid line).

III. Combined X-ray Data Collection, Structure Solution, and Refinement Protocols.

A. General Procedures. A crystal of 4 was prepared by slow evaporation of the solvent from a tetrahydrofuran solution of the compound. For analysis, a yellow crystal with approximate dimensions of 0.130 x 0.137 x 0.266 mm was mounted on a glass fiber and transferred to a Bruker SMART APEX II diffractometer. The APEX2^{1S} program package was used to determine the unit-cell parameters and to collect the data (25 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT^{2S} and SADABS^{3S} to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL^{4S} program. There were no systematic absences nor any diffraction symmetry other than the Friedel condition. The centrosymmetric triclinic space group P_1 was assigned and later determined to be correct.

The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors⁵⁸ for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model. There were two molecules of the formula unit present.

B. Definitions for the Crystallographic Analysis.

$$\begin{split} wR2 &= \left[\Sigma [w(F_o^2 - F_c^2)^2] \, / \, \Sigma [w(F_o^2)^2] \, \right]^{1/2} \\ R1 &= \Sigma ||F_o| - |F_c|| \, / \, \Sigma |F_o| \\ Goof &= S = \left[\Sigma [w(F_o^2 - F_c^2)^2] \, / \, (n-p) \right]^{1/2} \text{ where n is the number of reflections and p is the total number of parameters refined.} \end{split}$$

At convergence, wR2 = 0.0614 and Goof = 1.076 for 271 variables refined against 4701 data (0.74Å), and R1 = 0.0235 for those 4304 data with I > $2.0\sigma(I)$.



Figure S46. A snapshot from the crystal structure for compound 4. The carbon, hydrogen, iodine, chlorine, nitrogen, and oxygen atoms are indicated in yellow, white, purple, green, blue, and red.

Identification code	4	
Empirical formula	C ₁₀ H ₅ ClINO ₂	
Formula weight	333.50	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	рĪ	
Unit cell dimensions	a = 8.8632(5) Å	a= 102.9660(6)°.
	b = 9.5113(6) Å	b=90.5478(7)°.
	c = 13.0140(8) Å	$g = 109.4789(6)^{\circ}$.
Volume	$1003.66(11) \text{ Å}^3$	
Z	4	
Density (calculated)	2.207 Mg/m^3	
Absorption coefficient	3.432 mm ⁻¹	
F(000)	632	
Crystal color	yellow	
Crystal size	$0.266 \ge 0.137 \ge 0.130 \text{ mm}^3$	
Theta range for data collection	1.613 to 28.703°	
Index ranges	$-11 \le h \le 11, -12 \le k \le 12, -12$	$17 \le l \le 16$
Reflections collected	11841	
Independent reflections	4701 [R(int) = 0.0138]	
Completeness to theta = 25.500°	99.8 %	
Absorption correction	Numerical	
Max. and minutes. transmission	0.7747 and 0.5420	
Refinement method	Full-matrix least-squares on	\mathbf{F}^{2}
Data / restraints / parameters	4701 / 0 / 271	
Goodness-of-fit on F ²	1.076	
Final R indices [I>2sigma(I) = 4304 data]	R1 = 0.0235, wR2 = 0.0597	,
R indices (all data, 0.74Å)	R1 = 0.0264, wR2 = 0.0614	
Largest diff. peak and hole	$1.088 \text{ and } -0.597 \text{ e.Å}^{-3}$	

 Table S1. Crystal data and structure refinement for 4.

	х	У	Z	U(eq)
I(1)	2898(1)	5458(1)	4733(1)	21(1)
Cl(1)	5153(1)	5203(1)	2684(1)	22(1)
O(1)	5836(3)	9879(3)	1116(2)	28(1)
O(2)	6055(3)	11762(2)	2457(2)	29(1)
N(1)	5646(3)	10411(3)	2031(2)	16(1)
C(1)	4911(3)	9271(3)	2671(2)	16(1)
C(2)	5265(3)	7953(3)	2435(2)	17(1)
C(3)	4677(3)	6859(3)	3034(2)	17(1)
C(4)	3769(3)	7099(3)	3854(2)	16(1)
C(5)	3382(3)	8481(3)	4110(2)	14(1)
C(6)	2448(3)	8789(3)	4956(2)	18(1)
C(7)	2042(3)	10093(3)	5158(2)	21(1)
C(8)	2521(3)	11124(3)	4519(2)	20(1)
C(9)	3439(3)	10927(3)	3704(2)	18(1)
C(10)	3941(3)	9596(3)	3494(2)	14(1)
I(2)	-2248(1)	8121(1)	9530(1)	25(1)
Cl(2)	137(1)	8449(1)	7548(1)	25(1)
O(3)	977(3)	3304(2)	6197(2)	26(1)
O(4)	1143(3)	2407(3)	7558(2)	31(1)
N(2)	753(3)	3240(3)	7117(2)	18(1)
C(11)	-1(3)	4314(3)	7718(2)	16(1)
C(12)	309(3)	5662(3)	7418(2)	18(1)
C(13)	-330(3)	6757(3)	7950(2)	18(1)
C(14)	-1294(3)	6476(3)	8750(2)	17(1)
C(15)	-1649(3)	5060(3)	9073(2)	15(1)
C(16)	-2647(3)	4722(3)	9894(2)	20(1)
C(17)	-2935(3)	3379(3)	10202(2)	21(1)
C(18)	-2289(3)	2298(3)	9700(2)	20(1)
C(19)	-1335(3)	2537(3)	8882(2)	17(1)
C(20)	-974(3)	3940(3)	8553(2)	15(1)

Table S2. Atomic coordinates $(x \ 10^4)$ and equivalent isotropic displacement parameters $(\text{\AA}^2 x \ 10^3)$ for **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

I(1)-C(4)	2.087(2)	
Cl(1)-C(3)	1.729(3)	
O(1)-N(1)	1.222(3)	
O(2)-N(1)	1.206(3)	
N(1)-C(1)	1.496(3)	
C(1)-C(2)	1.362(4)	
C(1)-C(10)	1.425(3)	
C(2)-C(3)	1.404(4)	
C(3)-C(4)	1.367(4)	
C(4)-C(5)	1.436(3)	
C(5)-C(6)	1.420(3)	
C(5)-C(10)	1.432(3)	
C(6)-C(7)	1.375(4)	
C(7)-C(8)	1.389(4)	
C(8)-C(9)	1.361(4)	
C(9)-C(10)	1.449(4)	
I(2)-C(14)	2.093(3)	
Cl(2)-C(13)	1.724(3)	
O(3)-N(2)	1.227(3)	
O(4)-N(2)	1.209(3)	
N(2)-C(11)	1.485(3)	
C(11)-C(12)	1.365(4)	
C(11)-C(20)	1.429(3)	
C(12)-C(13)	1.400(4)	
C(13)-C(14)	1.369(4)	
C(14)-C(15)	1.437(4)	
C(15)-C(16)	1.418(4)	
C(15)-C(20)	1.435(4)	
C(16)-C(17)	1.368(4)	
C(17)-C(18)	1.381(4)	
C(18)-C(19)	1.378(4)	
C(19)-C(20)	1.428(4)	
O(2)-N(1)-O(1)	125.3(2)	
O(2)-N(1)-C(1)	118.5(2)	
O(1)-N(1)-C(1)	116.1(2)	

C(2)-C(1)-C(10)	123.1(2)
C(2)-C(1)-N(1)	116.1(2)
C(10)-C(1)-N(1)	120.8(2)
C(1)-C(2)-C(3)	119.3(2)
C(4)-C(3)-C(2)	121.2(2)
C(4)-C(3)-Cl(1)	121.8(2)
C(2)-C(3)-Cl(1)	117.0(2)
C(3)-C(4)-C(5)	120.1(2)
C(3)-C(4)-I(1)	120.71(19)
C(5)-C(4)-I(1)	119.18(18)
C(6)-C(5)-C(10)	118.1(2)
C(6)-C(5)-C(4)	122.3(2)
C(10)-C(5)-C(4)	119.5(2)
C(7)-C(6)-C(5)	121.1(2)
C(6)-C(7)-C(8)	120.1(2)
C(9)-C(8)-C(7)	122.4(3)
C(8)-C(9)-C(10)	118.9(2)
C(1)-C(10)-C(5)	116.7(2)
C(1)-C(10)-C(9)	124.1(2)
C(5)-C(10)-C(9)	119.1(2)
O(4)-N(2)-O(3)	124.5(2)
O(4)-N(2)-C(11)	119.3(2)
O(3)-N(2)-C(11)	116.3(2)
C(12)-C(11)-C(20)	123.1(2)
C(12)-C(11)-N(2)	115.5(2)
C(20)-C(11)-N(2)	121.4(2)
C(11)-C(12)-C(13)	119.6(2)
C(14)-C(13)-C(12)	120.8(2)
C(14)-C(13)-Cl(2)	121.9(2)
C(12)-C(13)-Cl(2)	117.3(2)
C(13)-C(14)-C(15)	120.6(2)
C(13)-C(14)-I(2)	120.2(2)
C(15)-C(14)-I(2)	119.14(19)
C(16)-C(15)-C(20)	118.3(2)
C(16)-C(15)-C(14)	122.4(2)
C(20)-C(15)-C(14)	119.3(2)

C(17)-C(16)-C(15)	121.1(3)
C(16)-C(17)-C(18)	120.7(3)
C(19)-C(18)-C(17)	121.4(3)
C(18)-C(19)-C(20)	119.7(3)
C(19)-C(20)-C(11)	124.7(2)
C(19)-C(20)-C(15)	118.8(2)
C(11)-C(20)-C(15)	116.5(2)

 Table S3. Bond lengths [Å] and angles [°] for 4.

	U^{11}	U^{22}	U ³³	U ²³	U^{13}	U^{12}	
I(1)	27(1)	17(1)	21(1)	10(1)	3(1)	7(1)	
Cl(1)	24(1)	17(1)	26(1)	4(1)	2(1)	11(1)	
O(1)	34(1)	33(1)	19(1)	10(1)	11(1)	9(1)	
O(2)	33(1)	22(1)	32(1)	12(1)	12(1)	6(1)	
N(1)	13(1)	24(1)	11(1)	5(1)	4(1)	4(1)	
C(1)	16(1)	18(1)	13(1)	6(1)	2(1)	2(1)	
C(2)	16(1)	20(1)	15(1)	3(1)	2(1)	6(1)	
C(3)	19(1)	14(1)	18(1)	2(1)	-2(1)	7(1)	
C(4)	17(1)	14(1)	16(1)	6(1)	-1(1)	4(1)	
C(5)	14(1)	15(1)	12(1)	2(1)	-1(1)	4(1)	
C(6)	18(1)	20(1)	16(1)	7(1)	3(1)	6(1)	
C(7)	21(1)	22(1)	18(1)	0(1)	5(1)	9(1)	
C(8)	22(1)	17(1)	23(1)	2(1)	3(1)	10(1)	
C(9)	18(1)	18(1)	15(1)	6(1)	2(1)	1(1)	
C(10)	13(1)	14(1)	12(1)	2(1)	0(1)	3(1)	
I(2)	27(1)	18(1)	29(1)	1(1)	5(1)	12(1)	
Cl(2)	32(1)	19(1)	29(1)	12(1)	5(1)	12(1)	
O(3)	30(1)	27(1)	20(1)	4(1)	10(1)	11(1)	
O(4)	33(1)	31(1)	39(1)	16(1)	16(1)	21(1)	
N(2)	12(1)	21(1)	18(1)	4(1)	5(1)	5(1)	
C(11)	14(1)	18(1)	16(1)	3(1)	3(1)	7(1)	
C(12)	17(1)	22(1)	15(1)	7(1)	3(1)	5(1)	
C(13)	20(1)	16(1)	19(1)	8(1)	0(1)	5(1)	
C(14)	17(1)	16(1)	19(1)	2(1)	-1(1)	7(1)	
C(15)	15(1)	16(1)	13(1)	3(1)	1(1)	5(1)	
C(16)	17(1)	23(1)	16(1)	2(1)	4(1)	6(1)	
C(17)	20(1)	25(1)	15(1)	7(1)	4(1)	1(1)	
C(18)	19(1)	19(1)	20(1)	10(1)	1(1)	2(1)	
C(19)	15(1)	19(1)	17(1)	6(1)	1(1)	5(1)	
C(20)	12(1)	16(1)	15(1)	4(1)	0(1)	2(1)	

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **4.** The anisotropic displacement factor exponent takes the form: $-2p^2[\text{ h}^2 a^{*2}U^{11} + ... + 2 \text{ h k } a^{*} \text{ b}^{*} U^{12}]$.

	Х	У	Z	U(eq)	
H(2A)	5902	7775	1871	21	
H(6A)	2097	8081	5389	21	
H(7A)	1434	10289	5735	25	
H(8A)	2196	12000	4656	24	
H(9A)	3746	11650	3278	22	
H(12A)	955	5857	6853	21	
H(16A)	-3125	5439	10236	23	
H(17A)	-3584	3187	10767	26	
H(18A)	-2508	1371	9924	23	
H(19A)	-919	1772	8538	20	

Table S5. Hydrogen coordinates $(x \ 10^4)$ and isotropic displacement parameters $(\text{\AA}^2 x \ 10^3)$ for 4.

O(2)-N(1)-C(1)-C(2)	-144.9(3)
O(1)-N(1)-C(1)-C(2)	32.4(3)
O(2)-N(1)-C(1)-C(10)	33.4(4)
O(1)-N(1)-C(1)-C(10)	-149.3(2)
C(10)-C(1)-C(2)-C(3)	-1.0(4)
N(1)-C(1)-C(2)-C(3)	177.2(2)
C(1)-C(2)-C(3)-C(4)	-0.6(4)
C(1)-C(2)-C(3)-Cl(1)	179.4(2)
C(2)-C(3)-C(4)-C(5)	0.8(4)
Cl(1)-C(3)-C(4)-C(5)	-179.14(19)
C(2)-C(3)-C(4)-I(1)	179.80(19)
Cl(1)-C(3)-C(4)-I(1)	-0.1(3)
C(3)-C(4)-C(5)-C(6)	-179.8(2)
I(1)-C(4)-C(5)-C(6)	1.2(3)
C(3)-C(4)-C(5)-C(10)	0.5(4)
I(1)-C(4)-C(5)-C(10)	-178.48(18)
C(10)-C(5)-C(6)-C(7)	2.2(4)
C(4)-C(5)-C(6)-C(7)	-177.5(2)
C(5)-C(6)-C(7)-C(8)	1.2(4)
C(6)-C(7)-C(8)-C(9)	-2.2(4)
C(7)-C(8)-C(9)-C(10)	-0.2(4)
C(2)-C(1)-C(10)-C(5)	2.3(4)
N(1)-C(1)-C(10)-C(5)	-175.8(2)
C(2)-C(1)-C(10)-C(9)	-174.7(2)
N(1)-C(1)-C(10)-C(9)	7.2(4)
C(6)-C(5)-C(10)-C(1)	178.3(2)
C(4)-C(5)-C(10)-C(1)	-2.0(3)
C(6)-C(5)-C(10)-C(9)	-4.5(3)
C(4)-C(5)-C(10)-C(9)	175.1(2)
C(8)-C(9)-C(10)-C(1)	-179.5(2)
C(8)-C(9)-C(10)-C(5)	3.6(4)
O(4)-N(2)-C(11)-C(12)	148.5(3)
O(3)-N(2)-C(11)-C(12)	-29.4(3)
O(4)-N(2)-C(11)-C(20)	-31.1(4)
O(3)-N(2)-C(11)-C(20)	150.9(2)

C(20)-C(11)-C(12)-C(13)	0.6(4)	
N(2)-C(11)-C(12)-C(13)	-179.0(2)	
C(11)-C(12)-C(13)-C(14)	-1.6(4)	
C(11)-C(12)-C(13)-Cl(2)	178.9(2)	
C(12)-C(13)-C(14)-C(15)	1.1(4)	
Cl(2)-C(13)-C(14)-C(15)	-179.4(2)	
C(12)-C(13)-C(14)-I(2)	-179.67(19)	
Cl(2)-C(13)-C(14)-I(2)	-0.2(3)	
C(13)-C(14)-C(15)-C(16)	-179.7(3)	
I(2)-C(14)-C(15)-C(16)	1.0(3)	
C(13)-C(14)-C(15)-C(20)	0.4(4)	
I(2)-C(14)-C(15)-C(20)	-178.92(18)	
C(20)-C(15)-C(16)-C(17)	1.5(4)	
C(14)-C(15)-C(16)-C(17)	-178.5(3)	
C(15)-C(16)-C(17)-C(18)	-1.7(4)	
C(16)-C(17)-C(18)-C(19)	0.3(4)	
C(17)-C(18)-C(19)-C(20)	1.2(4)	
C(18)-C(19)-C(20)-C(11)	180.0(2)	
C(18)-C(19)-C(20)-C(15)	-1.3(4)	
C(12)-C(11)-C(20)-C(19)	179.5(3)	
N(2)-C(11)-C(20)-C(19)	-0.9(4)	
C(12)-C(11)-C(20)-C(15)	0.8(4)	
N(2)-C(11)-C(20)-C(15)	-179.6(2)	
C(16)-C(15)-C(20)-C(19)	0.0(4)	
C(14)-C(15)-C(20)-C(19)	180.0(2)	
C(16)-C(15)-C(20)-C(11)	178.8(2)	
C(14)-C(15)-C(20)-C(11)	-1.2(4)	

 Table S6. Torsion angles [°] for 4.

IV. References.

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