

Figure S1. Crystal Structure of Compound 11.

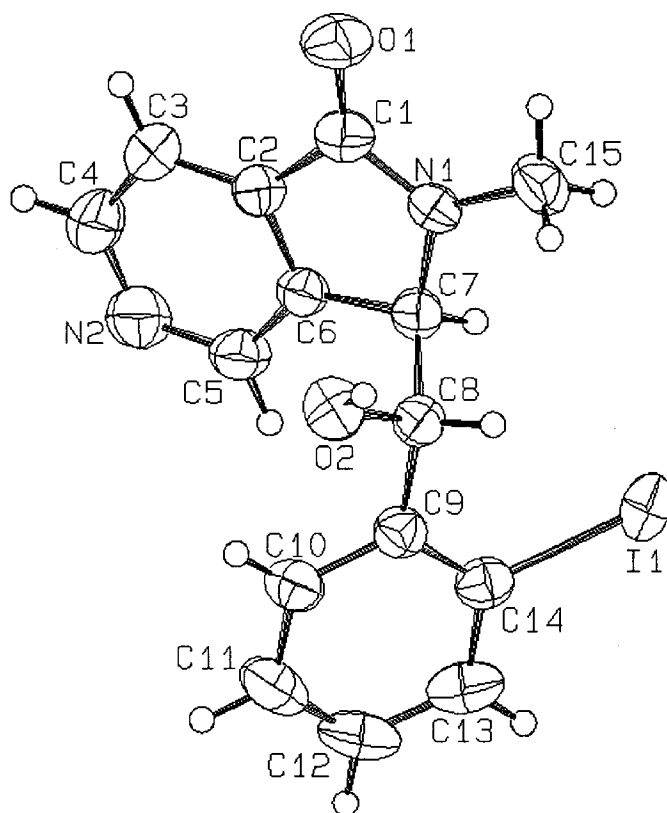


Table S1. Crystal data and structure refinement for compound **11**

Identification code	indol2	
Empirical formula	C15 H13 I N2 O2	
Formula weight	380.17	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2(1)/n	
Unit cell dimensions	a = 8.6048(12) Å	$\alpha = 90^\circ$.
	b = 15.925(2) Å	$\beta = 111.593(2)^\circ$.
	c = 11.2474(16) Å	$\gamma = 90^\circ$.
Volume	1433.1(3) Å ³	
Z	4	
Density (calculated)	1.762 Mg/m ³	
Absorption coefficient	2.237 mm ⁻¹	
F(000)	744	
Crystal size	.35 x .30 x .10 mm ³	
Theta range for data collection	2.33 to 30.04°	
Index ranges	-11 ≤ h ≤ 11, -22 ≤ k ≤ 22, -15 ≤ l ≤ 15	
Reflections collected	12841	
Independent reflections	3795 [R(int) = 0.0346]	
Completeness to theta = 30.04°	90.4 %	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3795 / 0 / 181	
Goodness-of-fit on F ²	0.841	
Final R indices [I > 2σ(I)]	R1 = 0.0319, wR2 = 0.0694	
R indices (all data)	R1 = 0.0599, wR2 = 0.0745	
Largest diff. peak and hole	0.945 and -0.616 e.Å ⁻³	

Table S2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for compound **11**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
O(1)	5548(3)	1094(1)	11388(2)	58(1)
C(1)	4281(4)	1225(2)	10431(3)	44(1)
C(2)	2619(4)	1479(2)	10403(3)	41(1)
C(3)	2061(4)	1647(2)	11388(3)	53(1)
C(4)	436(4)	1933(2)	11035(3)	62(1)
N(2)	-579(3)	2069(2)	9828(3)	61(1)
C(5)	-31(4)	1890(2)	8894(3)	48(1)
C(6)	1576(3)	1589(2)	9154(3)	38(1)
C(7)	2466(3)	1345(2)	8284(2)	39(1)
N(1)	4149(3)	1178(2)	9201(2)	43(1)
C(8)	1731(3)	553(2)	7466(3)	39(1)
O(2)	1700(2)	-115(1)	8279(2)	52(1)
C(9)	-21(3)	717(2)	6513(3)	38(1)
C(10)	-1385(4)	410(2)	6757(3)	49(1)
C(11)	-3005(4)	563(2)	5916(4)	63(1)
C(12)	-3270(4)	988(2)	4807(3)	65(1)
C(13)	-1963(4)	1287(2)	4517(3)	59(1)
C(14)	-332(4)	1165(2)	5393(3)	43(1)
I(1)	1600(1)	1732(1)	4941(1)	56(1)
C(15)	5529(4)	992(2)	8794(3)	54(1)

Table S3. Bond lengths [Å] and angles [°] for compound 11

O(1)-C(1)	1.236(3)
C(1)-N(1)	1.348(4)
C(1)-C(2)	1.476(4)
C(2)-C(6)	1.372(4)
C(2)-C(3)	1.386(4)
C(3)-C(4)	1.383(5)
C(4)-N(2)	1.334(4)
N(2)-C(5)	1.330(4)
C(5)-C(6)	1.390(4)
C(6)-C(7)	1.499(4)
C(7)-N(1)	1.461(3)
C(7)-C(8)	1.553(4)
N(1)-C(15)	1.451(4)
C(8)-O(2)	1.409(3)
C(8)-C(9)	1.517(4)
C(9)-C(14)	1.385(4)
C(9)-C(10)	1.388(4)
C(10)-C(11)	1.388(4)
C(11)-C(12)	1.362(5)
C(12)-C(13)	1.367(5)
C(13)-C(14)	1.400(4)
C(14)-I(1)	2.112(3)
O(1)-C(1)-N(1)	126.8(3)
O(1)-C(1)-C(2)	127.1(3)
N(1)-C(1)-C(2)	106.2(2)
C(6)-C(2)-C(3)	120.4(3)
C(6)-C(2)-C(1)	108.7(2)
C(3)-C(2)-C(1)	130.8(3)
C(4)-C(3)-C(2)	116.4(3)
N(2)-C(4)-C(3)	124.1(3)
C(5)-N(2)-C(4)	118.6(3)
N(2)-C(5)-C(6)	121.5(3)
C(2)-C(6)-C(5)	119.0(3)
C(2)-C(6)-C(7)	109.7(2)
C(5)-C(6)-C(7)	131.4(3)
N(1)-C(7)-C(6)	101.4(2)
N(1)-C(7)-C(8)	110.6(2)
C(6)-C(7)-C(8)	113.8(2)
C(1)-N(1)-C(15)	124.4(2)
C(1)-N(1)-C(7)	113.7(2)
C(15)-N(1)-C(7)	121.9(2)
O(2)-C(8)-C(9)	109.7(2)
O(2)-C(8)-C(7)	109.2(2)
C(9)-C(8)-C(7)	111.1(2)
C(14)-C(9)-C(10)	117.8(3)
C(14)-C(9)-C(8)	122.7(3)
C(10)-C(9)-C(8)	119.5(3)
C(9)-C(10)-C(11)	120.9(3)
C(12)-C(11)-C(10)	119.9(3)
C(11)-C(12)-C(13)	121.1(3)
C(12)-C(13)-C(14)	118.9(3)
C(9)-C(14)-C(13)	121.3(3)
C(9)-C(14)-I(1)	122.3(2)
C(13)-C(14)-I(1)	116.4(2)

4

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	42(1)	69(2)	48(1)	4(1)	-1(1)	9(1)
C(1)	39(2)	44(2)	44(2)	0(1)	8(1)	1(1)
C(2)	40(2)	43(2)	38(2)	-1(1)	13(1)	-3(1)
C(3)	54(2)	65(2)	39(2)	-2(1)	18(1)	-4(2)
C(4)	59(2)	82(3)	53(2)	-14(2)	29(2)	-1(2)
N(2)	47(2)	74(2)	64(2)	-17(2)	23(1)	2(1)
C(5)	38(2)	56(2)	46(2)	-9(1)	9(1)	1(1)
C(6)	32(1)	41(2)	38(1)	-3(1)	11(1)	-1(1)
C(7)	33(2)	47(2)	36(1)	4(1)	11(1)	1(1)
N(1)	25(1)	58(2)	42(1)	-1(1)	9(1)	-1(1)
C(8)	36(2)	42(2)	39(1)	1(1)	14(1)	3(1)
O(2)	49(1)	48(1)	57(1)	14(1)	17(1)	7(1)
C(9)	37(2)	38(2)	40(1)	-5(1)	14(1)	0(1)
C(10)	41(2)	54(2)	50(2)	-7(1)	14(1)	-8(1)
C(11)	38(2)	66(2)	81(3)	-17(2)	19(2)	-13(2)
C(12)	38(2)	61(2)	72(2)	-9(2)	-7(2)	1(2)
C(13)	62(2)	50(2)	46(2)	-3(2)	-3(2)	3(2)
C(14)	44(2)	41(2)	41(2)	-4(1)	12(1)	3(1)
I(1)	68(1)	63(1)	45(1)	5(1)	30(1)	0(1)
C(15)	35(2)	63(2)	65(2)	-2(2)	21(2)	-2(1)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for compound **11**

	x	y	z	U(eq)
H(3)	2742	1570	12241	63
H(4)	25	2037	11678	74
H(5)	-740	1969	8049	58
H(7)	2483	1818	7730	47
H(8)	2450	397	6998	47
HO2	2417	-460	8302	63
H(10)	-1210	97	7494	59
H(11)	-3908	376	6109	75
H(12)	-4359	1076	4238	77
H(13)	-2154	1567	3751	70
H(151)	5343	458	8368	64
H(152)	6552	974	9527	64
H(153)	5603	1421	8217	64