Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

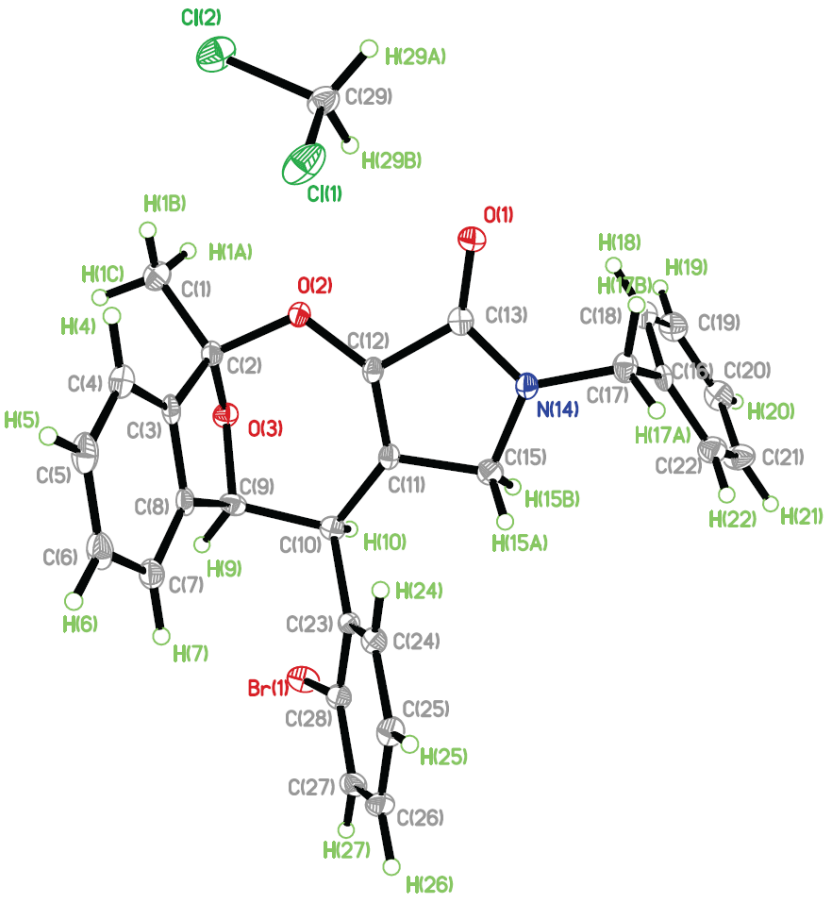


Figure S1. The ORTEP drawing of **4ai** (30% propability)

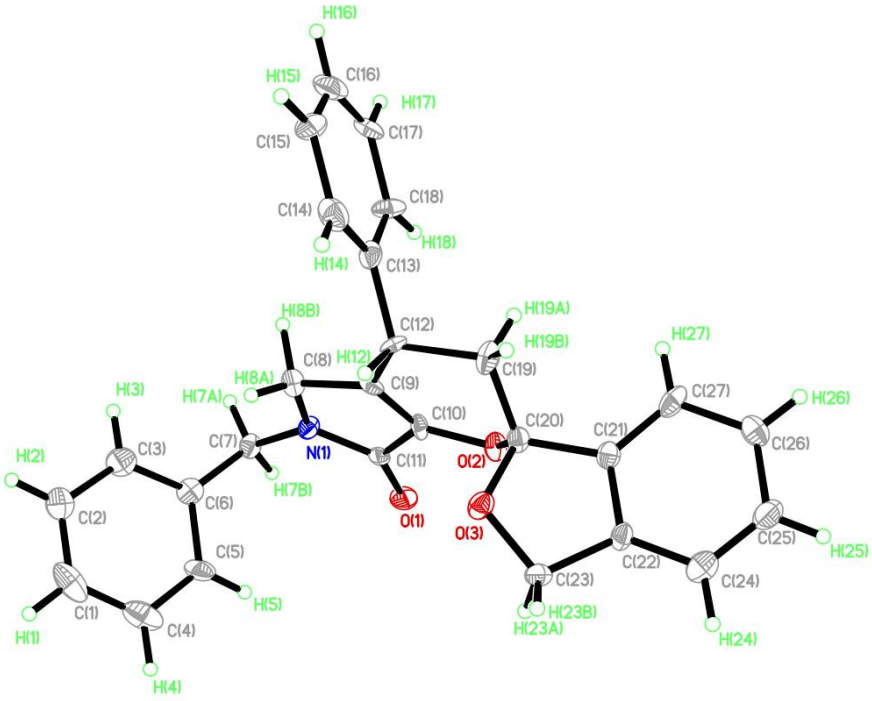
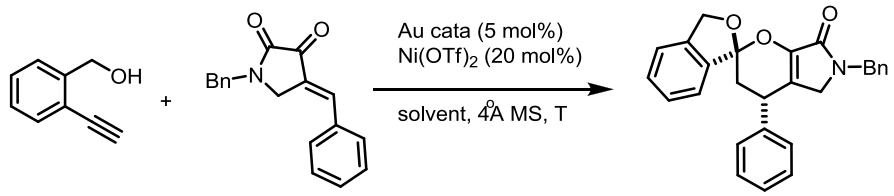


Figure S2. The ORTEP drawing of **3aa** (30% propability)

Table S1. Reaction condition screenings on the reaction of 1a and 2a for the construction of 3aa.



1a **2a** **3aa**

Entry	Au catal	Solvent	T(^{o}C)	Yield(%)[b]
1	Ph_3PAuCl	toluene	30	66
2	Ph_3PAuCl	toluene	50	88
3	Ph_3PAuCl	toluene	80	72
4	Ph_3PAuCl	CH_3CN	50	83
5	Ph_3PAuCl	Dioxane	50	62
6	Ph_3PAuCl	THF	50	56
7	Ph_3PAuCl	DCE	50	19
8	Ph_3PAuCl	DCM	50	<10
9	IPrAuCl	toluene	50	82
10	Me_2SAuCl	toluene	50	42
11	$Ph_3PAuCl/AgNTf_2$	toluene	50	64

[a]Reaction conditions: **1a** (40 mg, 0.3 mmol, 1.5 equiv.), **2a** (55 mg, 0.2 mmol), Au catal (5 mol%), $Ni(OTf)_2$ (13 mg, 0.04 mmol, 0.2 equiv.), 4Å MS (40 mg), solvent (2 mL) at given temperature under N_2. [b]Isolated yield.

Table S2. Crystal data and structure refinement for shelxl 4ai.

Identification code	shelxl
Empirical formula	$C_{27}H_{22}BrNO_3$
Formula weight	573.29
Temperature	120 K
Wavelength	λ = 0.71073 Å
Crystal system, space group	Triclinic, *P-1(2)*
Unit cell dimensions	*a* = 10.1230 (9) Å alpha = 112.093 (11) °
	b = 11.6920 (12) Å beta = 106.874 (10) °
	c = 12.5199 (16) Å gamma = 97.913 (8) °
Volume	4337.5 (15) $Å^3$
Z, Calculated density	2, 1.509 Mg m^{-3}
Absorption coefficient	1.87 mm^{-1}
F(000)	584
Theta range for data collection	3.3–24.4 °
Limiting indices	*h* = −12→9, *k* = −13→13, *l* = −13→14
Reflections collected / unique	7421/ 4434 [R(int) = 0.037]
Completeness to theta	25
Absorption correction	multi-scan *CrystalClear*
Max. and min. transmission	1.000 and 0.815
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4434 / 0 / 317
Goodness-of-fit on F^2	1.00
Final R indices [I> 2sigma(I)]	R1 = 0.0453, wR2 = 0.0860
R indices (all data)	R1 = 0.0722, wR2 = 0.0762
Absolute structure parameter	0.001
Largest diff. peak and hole	0.40 and −0.45 e.A^-3

Table S3. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	1.15997 (4)	0.38786 (4)	0.77174 (4)	0.03119 (13)
Cl2	0.46102 (11)	0.28116 (11)	−0.06124 (9)	0.0433 (3)
Cl1	0.30121 (11)	0.29401 (10)	0.09948 (9)	0.0492 (3)
O3	0.8969 (2)	0.3013 (2)	0.3722 (2)	0.0229 (6)
O1	0.5869 (2)	0.5846 (2)	0.3304 (2)	0.0280 (6)

O2	0.7015 (2)	0.3736 (2)	0.2944 (2)	0.0229 (6)
N14	0.6855 (3)	0.6378 (3)	0.5392 (3)	0.0230 (7)
C11	0.7865 (3)	0.4672 (3)	0.5256 (3)	0.0182 (8)
C23	0.8610 (4)	0.3761 (3)	0.6817 (3)	0.0203 (8)
C10	0.8836 (3)	0.3977 (3)	0.5747 (3)	0.0204 (8)
H10	0.9816	0.4538	0.6088	0.025*
C12	0.7181 (3)	0.4548 (3)	0.4113 (3)	0.0193 (8)
C3	0.6696 (4)	0.1634 (3)	0.2930 (3)	0.0232 (9)
C8	0.7385 (4)	0.1692 (3)	0.4079 (3)	0.0214 (8)
C15	0.7719 (4)	0.5892 (3)	0.6166 (3)	0.0252 (9)
H15A	0.7246	0.5711	0.6680	0.030*
H15B	0.8653	0.6505	0.6699	0.030*
C13	0.6532 (4)	0.5640 (3)	0.4164 (3)	0.0221 (8)
C25	0.7004 (4)	0.3365 (3)	0.7829 (3)	0.0263 (9)
H25	0.6086	0.3250	0.7849	0.032*
C9	0.8795 (4)	0.2726 (3)	0.4709 (3)	0.0239 (8)
H9	0.9577	0.2390	0.5028	0.029*
C27	0.9493 (4)	0.3498 (3)	0.8711 (3)	0.0260 (9)
H27	1.0253	0.3469	0.9324	0.031*
C24	0.7246 (4)	0.3567 (3)	0.6875 (3)	0.0221 (8)
H24	0.6478	0.3573	0.6253	0.026*
C16	0.7939 (4)	0.8711 (3)	0.6590 (3)	0.0219 (8)
C28	0.9712 (4)	0.3703 (3)	0.7750 (3)	0.0240 (8)
C19	0.9971 (4)	1.0009 (3)	0.6560 (4)	0.0337 (10)
H19	1.0461	1.0233	0.6112	0.040*
C26	0.8126 (4)	0.3334 (3)	0.8754 (3)	0.0283 (9)
H26	0.7967	0.3205	0.9400	0.034*
C2	0.7609 (4)	0.2638 (3)	0.2773 (3)	0.0232 (8)

C20	1.0547 (4)	1.0618 (3)	0.7835 (4)	0.0336 (10)
H20	1.1420	1.1252	0.8252	0.040*
C21	0.9813 (4)	1.0276 (4)	0.8491 (4)	0.0353 (10)
H21	1.0190	1.0686	0.9355	0.042*
C4	0.5387 (4)	0.0738 (3)	0.2116 (3)	0.0304 (9)
H4	0.4930	0.0706	0.1341	0.036*
C18	0.8673 (4)	0.9069 (3)	0.5937 (3)	0.0307 (9)
H18	0.8288	0.8674	0.5073	0.037*
C17	0.6564 (4)	0.7621 (3)	0.5895 (3)	0.0271 (9)
H17A	0.6067	0.7629	0.6453	0.032*
H17B	0.5940	0.7747	0.5221	0.032*
C7	0.6789 (4)	0.0847 (3)	0.4463 (4)	0.0291 (9)
H7	0.7250	0.0884	0.5240	0.035*
C22	0.8527 (4)	0.9331 (3)	0.7875 (3)	0.0315 (9)
H22	0.8045	0.9106	0.8327	0.038*
C5	0.4778 (4)	−0.0109 (3)	0.2488 (4)	0.0341 (10)
H5	0.3898	−0.0714	0.1959	0.041*
C6	0.5473 (4)	−0.0059 (3)	0.3642 (4)	0.0355 (10)
H6	0.5055	−0.0640	0.3874	0.043*
C1	0.7784 (4)	0.2251 (4)	0.1535 (3)	0.0342 (10)
H1A	0.8423	0.2958	0.1563	0.051*
H1B	0.6864	0.2021	0.0891	0.051*
H1C	0.8174	0.1528	0.1367	0.051*

Table S4. Geometric parameters (Å, º)

Br1—C28	1.908 (3)	C27—C28	1.383 (5)
C27—C26	1.390 (4)	C24—H24	0.9300
O3—C9	1.446 (4)	C16—C18	1.387 (5)
O3—C2	1.411 (4)	C16—C17	1.514 (4)
O1—C13	1.219 (4)	C16—C22	1.384 (5)
O2—C12	1.356 (4)	C19—H19	0.9300
O2—C2	1.462 (4)	C19—C20	1.374 (5)
N14—C15	1.445 (4)	C19—C18	1.380 (5)
N14—C13	1.359 (4)	C26—H26	0.9300
N14—C17	1.461 (4)	C2—C1	1.513 (4)
C11—C10	1.499 (4)	C20—H20	0.9300
C11—C12	1.337 (4)	C20—C21	1.381 (5)
C11—C15	1.513 (4)	C21—H21	0.9300
C23—C10	1.526 (4)	C21—C22	1.374 (5)
C23—C24	1.394 (4)	C4—H4	0.9300
C23—C28	1.392 (5)	C4—C5	1.387 (5)
C10—H10	0.9800	C18—H18	0.9300
C10—C9	1.534 (4)	C17—H17A	0.9700
C12—C13	1.504 (4)	C17—H17B	0.9700
C3—C8	1.376 (5)	C7—H7	0.9300
C3—C2	1.500 (5)	C7—C6	1.397 (5)
C3—C4	1.387 (5)	C22—H22	0.9300
C8—C9	1.509 (5)	C5—H5	0.9300
C8—C7	1.390 (5)	C5—C6	1.386 (5)
C15—H15A	0.9700	C15—H15B	0.9700
C25—H25	0.9300	C6—H6	0.9300
C25—C24	1.382 (5)	C1—H1A	0.9600

C25—C26	1.382 (5)	C1—H1B	0.9600
C9—H9	0.9800	C1—H1C	0.9600
C27—H27	0.9300		
C2—O3—C9	109.1 (2)	C27—C28—C23	122.4 (3)
C12—O2—C2	118.4 (3)	C20—C19—H19	119.7
C15—N14—C17	122.8 (3)	C20—C19—C18	120.6 (4)
C13—N14—C15	112.2 (3)	C18—C19—H19	119.7
C13—N14—C17	124.4 (3)	C25—C26—C27	119.6 (3)
C10—C11—C15	118.8 (3)	C25—C26—H26	120.2
C12—C11—C10	133.2 (3)	C27—C26—H26	120.2
C12—C11—C15	107.4 (3)	O3—C2—O2	110.0 (3)
C24—C23—C10	120.4 (3)	O3—C2—C3	104.8 (3)
C28—C23—C10	122.8 (3)	O3—C2—C1	109.3 (3)
C28—C23—C24	116.7 (3)	O2—C2—C3	110.0 (3)
C11—C10—C23	114.2 (3)	O2—C2—C1	105.3 (3)
C11—C10—H10	106.1	C3—C2—C1	117.3 (3)
C11—C10—C9	112.0 (3)	C19—C20—H20	120.4
C23—C10—H10	106.1	C19—C20—C21	119.2 (4)
C23—C10—C9	111.7 (3)	C21—C20—H20	120.4
C9—C10—H10	106.1	C20—C21—H21	119.8
O2—C12—C13	113.1 (3)	C22—C21—C20	120.3 (4)
C11—C12—O2	135.7 (3)	C22—C21—H21	119.8
C11—C12—C13	111.0 (3)	C3—C4—H4	120.9
C8—C3—C2	108.6 (3)	C5—C4—C3	118.3 (4)
C8—C3—C4	121.5 (3)	C5—C4—H4	120.9
C4—C3—C2	130.0 (4)	C16—C18—H18	119.8
C3—C8—C9	108.3 (3)	C19—C18—C16	120.5 (4)

C3—C8—C7	120.9 (3)	C19—C18—H18	119.8
C7—C8—C9	130.8 (3)	N14—C17—C16	111.3 (3)
N14—C15—C11	104.4 (3)	N14—C17—H17A	109.4
N14—C15—H15A	110.9	N14—C17—H17B	109.4
N14—C15—H15B	110.9	C16—C17—H17A	109.4
C11—C15—H15A	110.9	C16—C17—H17B	109.4
C11—C15—H15B	110.9	H17A—C17—H17B	108.0
H15A—C15—H15B	108.9	C8—C7—H7	121.1
O1—C13—N14	126.5 (3)	C8—C7—C6	117.7 (4)
O1—C13—C12	128.4 (3)	C6—C7—H7	121.1
N14—C13—C12	105.1 (3)	C16—C22—H22	119.5
C24—C25—H25	120.0	C21—C22—C16	120.9 (4)
C26—C25—H25	120.0	C21—C22—H22	119.5
C26—C25—C24	120.0 (3)	C4—C5—H5	119.8
O3—C9—C10	107.9 (3)	C6—C5—C4	120.4 (4)
O3—C9—C8	103.8 (3)	C6—C5—H5	119.8
O3—C9—H9	109.9	C8—C9—H9	109.9
C10—C9—H9	109.9	C28—C27—H27	120.3
C8—C9—C10	115.2 (3)	C28—C27—C26	119.4 (3)
C26—C27—H27	120.3	C7—C6—H6	119.4
C23—C24—H24	119.1	C5—C6—C7	121.2 (4)
C25—C24—C23	121.9 (3)	C5—C6—H6	119.4
C25—C24—H24	119.1	C2—C1—H1A	109.5
C18—C16—C17	119.8 (3)	C2—C1—H1B	109.5
C22—C16—C18	118.4 (3)	C2—C1—H1C	109.5
C22—C16—C17	121.7 (3)	H1A—C1—H1B	109.5
C23—C28—Br1	120.1 (3)	H1A—C1—H1C	109.5

C27—C28—Br1	117.5 (3)	H1B—C1—H1C	109.5

Table S5. Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0214 (2)	0.0398 (3)	0.0370 (3)	0.00633 (17)	0.00971 (18)	0.0232 (2)
O3	0.0236 (14)	0.0252 (14)	0.0235 (14)	0.0065 (11)	0.0132 (12)	0.0113 (12)
O1	0.0315 (16)	0.0275 (15)	0.0236 (15)	0.0106 (12)	0.0063 (12)	0.0120 (13)
O2	0.0301 (15)	0.0193 (14)	0.0206 (14)	0.0082 (11)	0.0118 (11)	0.0079 (12)
N14	0.0254 (18)	0.0212 (17)	0.0228 (18)	0.0099 (14)	0.0102 (14)	0.0080 (15)
C11	0.018 (2)	0.0166 (19)	0.022 (2)	0.0036 (15)	0.0119 (16)	0.0066 (17)
C23	0.026 (2)	0.0153 (19)	0.020 (2)	0.0034 (15)	0.0096 (17)	0.0076 (16)
C10	0.017 (2)	0.021 (2)	0.024 (2)	0.0016 (15)	0.0088 (16)	0.0112 (17)
C12	0.019 (2)	0.0168 (19)	0.022 (2)	0.0051 (15)	0.0108 (16)	0.0062 (17)
C3	0.029 (2)	0.0136 (19)	0.030 (2)	0.0085 (16)	0.0184 (18)	0.0066 (18)
C8	0.028 (2)	0.0148 (19)	0.026 (2)	0.0097 (16)	0.0174 (18)	0.0073 (17)
C15	0.028 (2)	0.022 (2)	0.026 (2)	0.0027 (16)	0.0112 (18)	0.0115 (18)
C13	0.016 (2)	0.021 (2)	0.027 (2)	0.0023 (15)	0.0080 (17)	0.0088 (18)
C25	0.025 (2)	0.024 (2)	0.030 (2)	0.0013 (16)	0.0157 (18)	0.0097 (18)
C9	0.025 (2)	0.029 (2)	0.028 (2)	0.0111 (17)	0.0140 (17)	0.0187 (19)
C27	0.029 (2)	0.022 (2)	0.026 (2)	0.0025 (16)	0.0083 (18)	0.0121 (18)
C24	0.020 (2)	0.019 (2)	0.024 (2)	0.0013 (15)	0.0081 (17)	0.0088 (17)
C16	0.024 (2)	0.0138 (19)	0.026 (2)	0.0071 (15)	0.0092 (17)	0.0063 (17)
C28	0.026 (2)	0.022 (2)	0.027 (2)	0.0038 (16)	0.0130 (18)	0.0114 (18)
C19	0.038 (3)	0.030 (2)	0.042 (3)	0.0073 (19)	0.022 (2)	0.020 (2)
C26	0.038 (3)	0.027 (2)	0.027 (2)	0.0058 (18)	0.018 (2)	0.0152 (19)
C2	0.031 (2)	0.018 (2)	0.024 (2)	0.0098 (17)	0.0145 (18)	0.0090 (18)
C20	0.029 (2)	0.027 (2)	0.039 (3)	−0.0007 (17)	0.009 (2)	0.013 (2)

C21	0.040 (3)	0.030 (2)	0.025 (2)	−0.0015 (19)	0.0037 (19)	0.011 (2)
C4	0.033 (2)	0.024 (2)	0.029 (2)	0.0080 (18)	0.0119 (19)	0.0062 (19)
C18	0.039 (3)	0.025 (2)	0.028 (2)	0.0116 (19)	0.0138 (19)	0.0107 (19)
C17	0.022 (2)	0.026 (2)	0.029 (2)	0.0078 (17)	0.0085 (17)	0.0083 (19)
C7	0.037 (2)	0.023 (2)	0.033 (2)	0.0106 (18)	0.020 (2)	0.0117 (19)
C22	0.037 (3)	0.030 (2)	0.031 (2)	0.0071 (19)	0.015 (2)	0.016 (2)
C5	0.031 (2)	0.021 (2)	0.045 (3)	0.0012 (18)	0.022 (2)	0.006 (2)
C6	0.047 (3)	0.021 (2)	0.047 (3)	0.0064 (19)	0.032 (2)	0.013 (2)
C1	0.044 (3)	0.035 (2)	0.029 (2)	0.015 (2)	0.019 (2)	0.013 (2)

Table S6. Crystal data and structure refinement for shelxl 3aa.

Identification code	shelxl	
Empirical formula	$C_{27}H_{23}NO_3$	
Formula weight	408.45	
Temperature	120 K	
Wavelength	λ = 0.71073 Å	
Crystal system, space group	Orthorhombic, *Pna*2_1	
Unit cell dimensions	*a* = 16.242 (3) Å	alpha = 90 °
	b = 11.4667 (17) Å	beta = 90 °
	c = 22.485 (4) Å	gamma = 90 °
Volume	4187.6 (11) $Å^3$	
Z, Calculated density	8, 1.296 Mg m^{-3}	
Absorption coefficient	0.08 mm^{-1}	
F(000)	1720	
Theta range for data collection	3.1–20 °	
Limiting indices	*h* = −10→19, *k* = −8→13, *l* = −19→26	
Reflections collected / unique	9885/ 5974 [R(int) = 0.110]	
Completeness to theta	25	
Absorption correction	multi-scan *CrystalClear*	
Max. and min. transmission	1.000 and 0.834	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5974 / 1 / 571	
Goodness-of-fit on F^2	0.93	
Final R indices [I> 2sigma(I)]	R1 = 0.0887, wR2 = 0.2807	
R indices (all data)	R1 = 0.2131, wR2 = 0.1846	

Absolute structure parameter	0.001
Largest diff. peak and hole	0.30 and −0.32 e.A^-3

Table S7. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O3	0.5820 (5)	0.2898 (8)	0.5171 (4)	0.032 (3)
O2	0.7181 (5)	0.2346 (7)	0.5354 (5)	0.033 (2)
O1	0.8426 (6)	0.2411 (8)	0.4393 (5)	0.038 (3)
N1	0.8384 (7)	0.4408 (9)	0.4573 (5)	0.026 (3)
C8	0.7922 (8)	0.5221 (12)	0.4932 (7)	0.028 (3)
H8A	0.7683	0.5783	0.4746	0.033*
C11	0.8171 (8)	0.3282 (12)	0.4666 (6)	0.028 (3)
C12	0.6767 (8)	0.4786 (10)	0.5754 (6)	0.024 (3)
H12	0.6299	0.5161	0.5556	0.029*
C22	0.5487 (8)	0.1043 (11)	0.5507 (6)	0.029 (3)
C21	0.6064 (8)	0.1507 (11)	0.5892 (7)	0.029 (4)
C9	0.7386 (8)	0.4422 (11)	0.5294 (6)	0.026 (3)
C10	0.7541 (7)	0.3338 (11)	0.5151 (6)	0.024 (3)
C13	0.7127 (9)	0.5617 (11)	0.6206 (6)	0.034 (4)
C23	0.5412 (8)	0.1843 (11)	0.4988 (6)	0.034 (4)
H23A	0.5676	0.1512	0.4640	0.040*
H23B	0.4838	0.1993	0.4897	0.040*
C20	0.6384 (7)	0.2611 (11)	0.5626 (7)	0.027 (3)
C7	0.8946 (8)	0.4797 (12)	0.4095 (6)	0.029 (3)
H7A	0.9375	0.5285	0.4262	0.035*
H7B	0.9205	0.4125	0.3911	0.035*
C6	0.8485 (8)	0.5456 (12)	0.3644 (7)	0.030 (3)

C16	0.7769 (11)	0.7137 (15)	0.7055 (7)	0.048 (4)
H16	0.7989	0.7643	0.7336	0.058*
C27	0.6228 (8)	0.1011 (12)	0.6445 (8)	0.040 (4)
H27	0.6607	0.1346	0.6703	0.047*
C26	0.5800 (9)	−0.0015 (12)	0.6602 (7)	0.042 (4)
H26	0.5879	−0.0364	0.6971	0.051*
C3	0.8487 (9)	0.6643 (14)	0.3616 (8)	0.045 (4)
H3	0.8819	0.7044	0.3884	0.054*
C18	0.7877 (8)	0.5407 (12)	0.6475 (6)	0.036 (4)
H18	0.8169	0.4738	0.6374	0.043*
C24	0.5102 (9)	0.0024 (13)	0.5652 (8)	0.040 (4)
H24	0.4735	−0.0316	0.5387	0.048*
C4	0.7524 (9)	0.5487 (17)	0.2810 (8)	0.056 (5)
H4	0.7198	0.5091	0.2537	0.067*
C25	0.5254 (9)	−0.0495 (13)	0.6187 (8)	0.045 (4)
H25	0.4987	−0.1190	0.6279	0.054*
C5	0.7991 (9)	0.4872 (13)	0.3215 (6)	0.041 (4)
H5	0.7984	0.4061	0.3207	0.049*
C2	0.8029 (11)	0.7298 (15)	0.3213 (9)	0.055 (5)
H2	0.8051	0.8109	0.3217	0.066*
C15	0.7042 (12)	0.7360 (12)	0.6819 (8)	0.050 (5)
H15	0.6758	0.8030	0.6930	0.060*
C14	0.6688 (10)	0.6580 (13)	0.6394 (7)	0.045 (4)
H14	0.6163	0.6721	0.6245	0.055*
C19	0.6474 (9)	0.3637 (11)	0.6045 (7)	0.033 (4)
H19A	0.6863	0.3426	0.6355	0.039*
H19B	0.5947	0.3777	0.6235	0.039*
C17	0.8206 (10)	0.6162 (14)	0.6889 (6)	0.044 (4)

H17	0.8720	0.6013	0.7054	0.053*
C1	0.7541 (10)	0.6714 (17)	0.2811 (8)	0.058 (5)
H1	0.7223	0.7130	0.2540	0.069*
H8B	0.835 (8)	0.565 (11)	0.522 (6)	0.05 (4)*

Table S8. Geometric parameters (Å, º)

O3—C23	1.439 (14)	C6—C3	1.36 (2)
O3—C20	1.411 (17)	C6—C5	1.423 (19)
C27—C26	1.412 (18)	C16—H16	0.9300
O2—C10	1.358 (14)	C16—C15	1.32 (2)
O2—C20	1.463 (15)	C16—C17	1.38 (2)
O1—C11	1.244 (15)	C27—H27	0.9300
C26—H26	0.9300	C26—C25	1.40 (2)
N1—C8	1.445 (17)	C3—H3	0.9300
N1—C11	1.352 (16)	C3—C2	1.39 (2)
N1—C7	1.478 (16)	C18—H18	0.9300
C18—C17	1.378 (19)	C24—H24	0.9300
C8—H8A	0.8600	C24—C25	1.36 (2)
C8—H8B	1.07 (14)	C8—C9	1.504 (18)
C12—H12	0.9800	C11—C10	1.496 (18)
C12—C9	1.502 (18)	C4—H4	0.9300
C12—C13	1.511 (18)	C4—C5	1.38 (2)
C12—C19	1.546 (17)	C4—C1	1.41 (2)
C5—H5	0.9300	C25—H25	0.9300
C14—H14	0.9300	C2—H2	0.9300
C22—C21	1.383 (19)	C2—C1	1.38 (2)
C22—C23	1.489 (18)	C22—C24	1.364 (19)

C21—C20	1.494 (18)	C21—C27	1.39 (2)
C15—C14	1.43 (2)	C15—H15	0.9300
C9—C10	1.308 (17)	C19—H19A	0.9700
C13—C18	1.382 (18)	C19—H19B	0.9700
C13—C14	1.381 (18)	C7—H7B	0.9700
C23—H23A	0.9700	C17—H17	0.9300
C23—H23B	0.9700	C20—C19	1.515 (19)
C7—H7A	0.9700	C1—H1	0.9300
C7—C6	1.468 (19)	C44—H44	0.9300
C20—O3—C23	108.1 (10)	C3—C6—C5	116.1 (15)
C10—O2—C20	110.3 (9)	C5—C6—C7	120.9 (13)
C8—N1—C7	122.2 (10)	C17—C16—H16	119.7
C11—N1—C8	113.3 (11)	C15—C16—H16	119.7
C11—N1—C7	124.0 (12)	C15—C16—C17	120.7 (16)
C21—C27—C26	118.0 (14)	C21—C27—H27	121.0
N1—C8—H8A	116.4	C26—C27—H27	121.0
N1—C8—C9	102.1 (10)	C27—C26—H26	120.9
N1—C8—H8B	108 (7)	C25—C26—C27	118.2 (15)
H8A—C8—H8B	104.0	C25—C26—H26	120.9
C9—C8—H8A	117.3	C6—C3—H3	117.7
C9—C8—H8B	109 (7)	C6—C3—C2	124.7 (16)
O1—C11—N1	127.1 (13)	C2—C3—H3	117.7
O1—C11—C10	128.5 (12)	C13—C18—H18	119.1
N1—C11—C10	104.3 (12)	C17—C18—C13	121.8 (14)
C22—C24—H24	119.9	C17—C18—H18	119.1
C25—C24—H24	119.9	C22—C24—C25	120.1 (15)
C9—C12—H12	109.1	C9—C12—C13	112.4 (11)

C9—C12—C19	105.1 (10)	C13—C12—H12	109.1
C13—C12—C19	111.8 (12)	C19—C12—H12	109.1
C5—C4—C1	120.0 (16)	C5—C4—H4	120.0
C26—C25—H25	119.0	C1—C4—H4	120.0
N2—C34—C31	112.4 (11)	C24—C25—C26	122.0 (14)
C3—C6—C7	123.1 (14)	C24—C25—H25	119.0
C4—C5—C6	121.2 (15)	C6—C5—H5	119.4
C21—C22—C23	108.0 (11)	C4—C5—H5	119.4
C24—C22—C21	119.3 (14)	C24—C22—C23	132.7 (14)
C22—C21—C20	108.1 (12)	C22—C21—C27	122.1 (13)
C27—C21—C20	129.6 (13)	C1—C2—H2	120.9
C1—C2—C3	118.2 (16)	C3—C2—H2	120.9
C12—C9—C8	126.2 (11)	C14—C15—H15	119.8
C10—C9—C8	109.5 (12)	C16—C15—H15	119.8
C10—C9—C12	124.3 (12)	C16—C15—C14	120.5 (15)
C9—C10—O2	129.0 (12)	C13—C14—C15	119.8 (15)
C9—C10—C11	110.6 (12)	C13—C14—H14	120.1
C12—C19—H19A	108.5	C15—C14—H14	120.1
C20—C19—C12	115.3 (12)	C12—C19—H19B	108.5
C20—C19—H19B	108.5	C20—C19—H19A	108.5
C18—C13—C12	121.7 (12)	H19A—C19—H19B	107.5
C14—C13—C12	120.7 (14)	C14—C13—C18	117.4 (14)
O3—C23—C22	104.9 (11)	O3—C23—H23A	110.8
O3—C23—H23B	110.8	C22—C23—H23A	110.8
C22—C23—H23B	110.8	C16—C17—C18	119.6 (16)
H23A—C23—H23B	108.8	C16—C17—H17	120.2
O3—C20—O2	108.7 (12)	C18—C17—H17	120.2
O3—C20—C21	105.2 (10)	O3—C20—C19	109.5 (11)

O2—C20—C21	107.4 (10)	N1—C7—H7B	109.7
O2—C20—C19	109.6 (10)	C4—C1—H1	120.0
C21—C20—C19	116.2 (13)	C2—C1—C4	119.9 (17)
N1—C7—H7A	109.7	C2—C1—H1	120.0
H7A—C7—H7B	108.2	C6—C7—N1	110.0 (11)
C6—C7—H7A	109.7	C6—C7—H7B	109.7

Table S9. Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.025 (5)	0.029 (5)	0.043 (7)	−0.004 (4)	−0.004 (5)	0.002 (5)
O2	0.033 (5)	0.028 (5)	0.037 (7)	0.003 (5)	0.002 (5)	0.007 (5)
O1	0.051 (6)	0.033 (6)	0.028 (7)	0.005 (5)	0.003 (5)	−0.011 (5)
N1	0.028 (6)	0.023 (6)	0.027 (7)	−0.004 (5)	0.007 (5)	−0.003 (5)
C8	0.015 (6)	0.033 (8)	0.035 (9)	0.004 (6)	0.005 (6)	0.007 (7)
C11	0.024 (7)	0.035 (8)	0.023 (8)	−0.011 (7)	−0.013 (6)	0.007 (7)
C12	0.023 (7)	0.020 (7)	0.029 (8)	−0.006 (6)	−0.002 (6)	−0.012 (6)
C22	0.031 (8)	0.021 (7)	0.037 (10)	−0.001 (6)	−0.002 (7)	0.006 (7)
C21	0.029 (8)	0.025 (7)	0.033 (10)	0.002 (7)	0.002 (7)	0.001 (7)
C9	0.030 (7)	0.033 (8)	0.015 (8)	0.006 (7)	−0.008 (6)	0.000 (7)
C10	0.018 (7)	0.028 (8)	0.026 (9)	−0.002 (6)	0.003 (6)	0.011 (7)
C13	0.050 (9)	0.021 (7)	0.031 (9)	0.003 (7)	0.013 (8)	−0.001 (7)
C23	0.041 (8)	0.030 (8)	0.029 (9)	−0.003 (7)	−0.010 (8)	−0.002 (7)
C20	0.020 (6)	0.028 (8)	0.031 (9)	−0.002 (7)	−0.001 (6)	0.005 (7)
C7	0.030 (8)	0.027 (8)	0.029 (9)	0.000 (6)	0.010 (7)	0.000 (7)
C6	0.022 (7)	0.036 (9)	0.032 (9)	0.005 (7)	0.013 (6)	−0.006 (7)
C16	0.060 (11)	0.064 (11)	0.021 (10)	−0.002 (10)	0.004 (8)	−0.005 (9)

C27	0.027 (8)	0.034 (8)	0.058 (12)	−0.013 (7)	0.008 (8)	−0.005 (9)
C26	0.048 (10)	0.044 (10)	0.035 (10)	0.005 (8)	−0.006 (8)	0.011 (8)
C3	0.032 (8)	0.052 (10)	0.051 (12)	−0.006 (8)	−0.003 (8)	0.001 (9)
C18	0.031 (8)	0.047 (9)	0.030 (9)	−0.003 (7)	0.004 (7)	−0.021 (8)
C24	0.026 (8)	0.040 (9)	0.054 (12)	0.000 (7)	0.001 (8)	−0.005 (9)
C4	0.024 (8)	0.103 (15)	0.040 (11)	−0.001 (10)	−0.003 (8)	0.002 (11)
C5	0.052 (10)	0.049 (9)	0.022 (9)	0.006 (8)	−0.004 (8)	−0.011 (8)
C2	0.067 (12)	0.043 (10)	0.055 (13)	0.004 (10)	−0.010 (10)	0.005 (9)
C15	0.084 (13)	0.026 (8)	0.040 (11)	0.007 (9)	−0.001 (10)	−0.013 (8)
C14	0.056 (10)	0.043 (9)	0.037 (11)	0.016 (8)	0.000 (8)	0.007 (8)
C19	0.031 (8)	0.015 (7)	0.052 (12)	0.012 (6)	0.007 (8)	0.004 (8)
C17	0.063 (11)	0.055 (10)	0.016 (8)	−0.007 (9)	−0.009 (8)	0.001 (8)
C1	0.042 (10)	0.098 (15)	0.033 (11)	0.012 (10)	0.020 (8)	0.025 (11)