Electronic supplementary information

Strategy to Enhance Solid-State Fluorescence and Aggregation-Induced Emission Enhancement Effect in Pyrimidine Boron Complexes

Yasuhiro Kubota,* Kouhei Kasatani, Hiroki Takai, Kazumasa Funabiki and Masaki Matsui*

Department of Chemistry and Biomolecular Science, Faculty of Engineering, Gifu University, 1-1 Yanagido, Gifu 501-1193, Japan

kubota@gifu-u.ac.jp (Y. Kubota), matsuim@gifu-u.ac.jp (M. Matsui)

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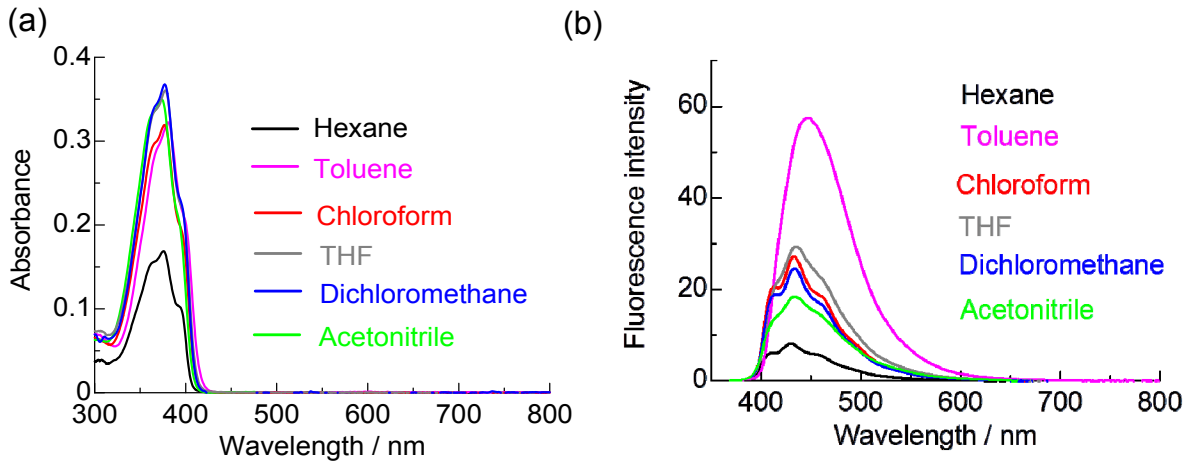


Figure S1. (a) UV-vis absorption and (b) fluorescence spectra of **8** in various solvents (1.0×10^{-5} M). The solubility of **8** in *n*-hexane was poor.

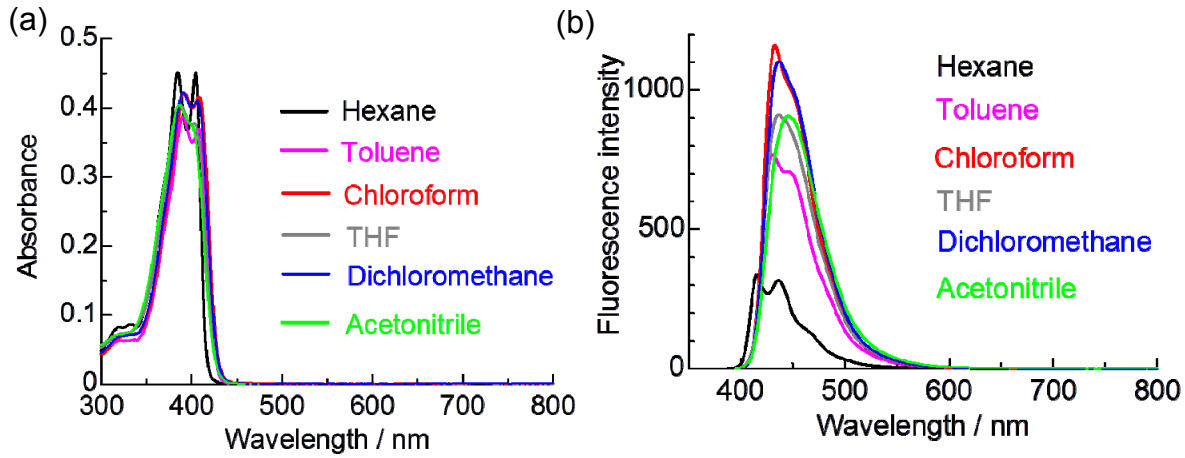


Figure S2. (a) UV-vis absorption and (b) fluorescence spectra of **9** in various solvents (1.0×10^{-5} M).

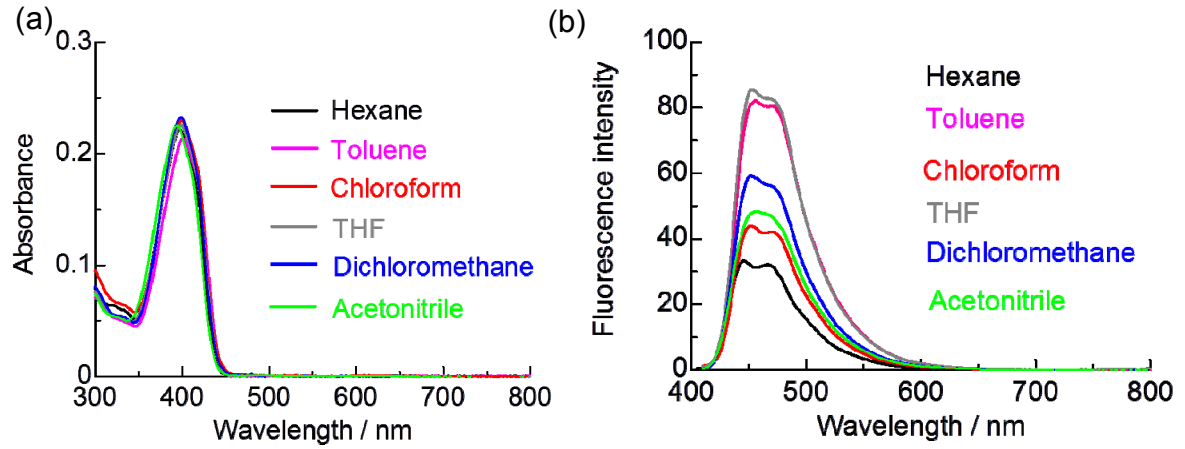


Figure S3. (a) UV-vis absorption and (b) fluorescence spectra of **11** in various solvents (1.0×10^{-5} M).

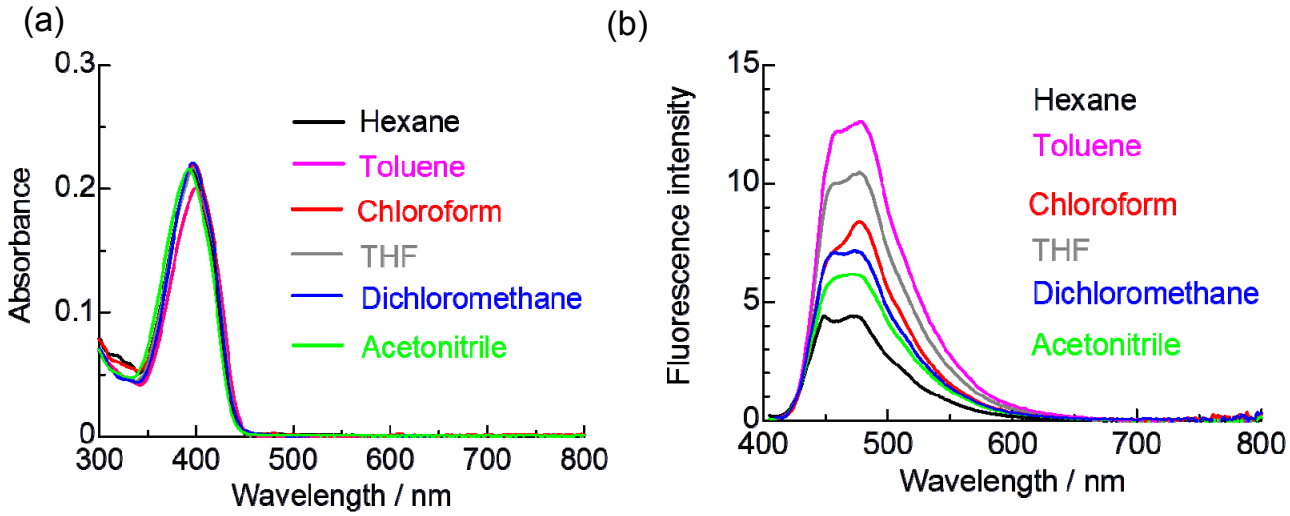


Figure S4. (a) UV-vis absorption and (b) fluorescence spectra of **12** in various solvents (1.0×10^{-5} M).

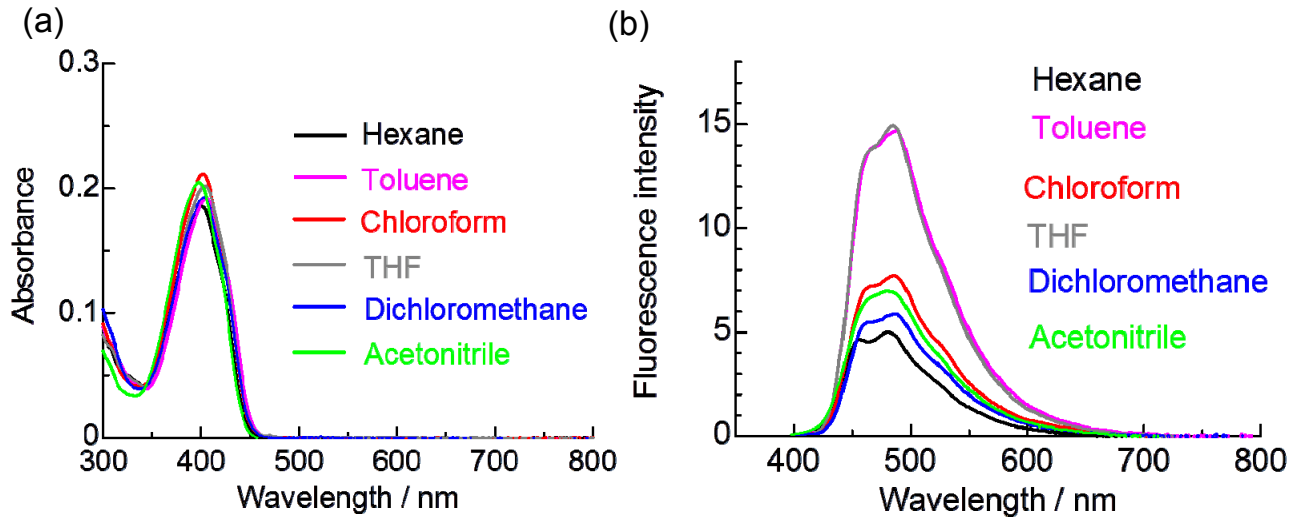


Figure S5. (a) UV-vis absorption and (b) fluorescence spectra of **13** in various solvents (1.0×10^{-5} M).

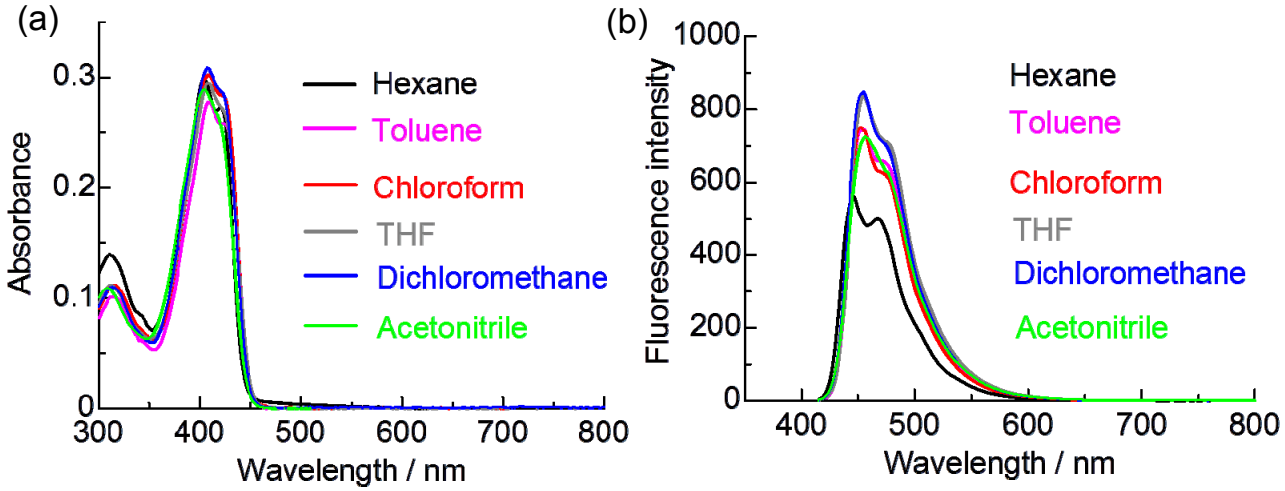


Figure S6. (a) UV-vis absorption and (b) fluorescence spectra of **14** in various solvents (1.0×10^{-5} M).

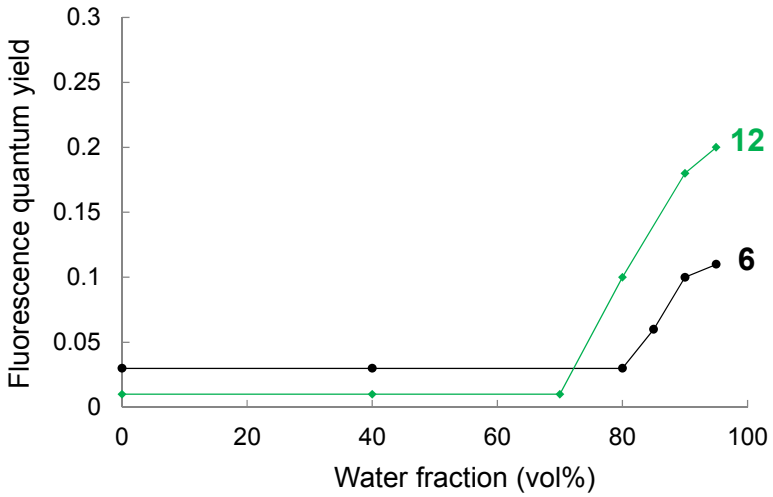


Figure S7. Fluorescence quantum yields of **6** and **12** in THF–water mixtures with different volume fractions of water (10^{-4} M).

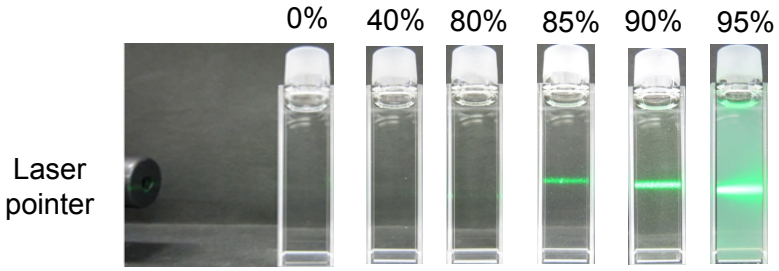


Figure S8. Check of Tyndall phenomenon of **6**.

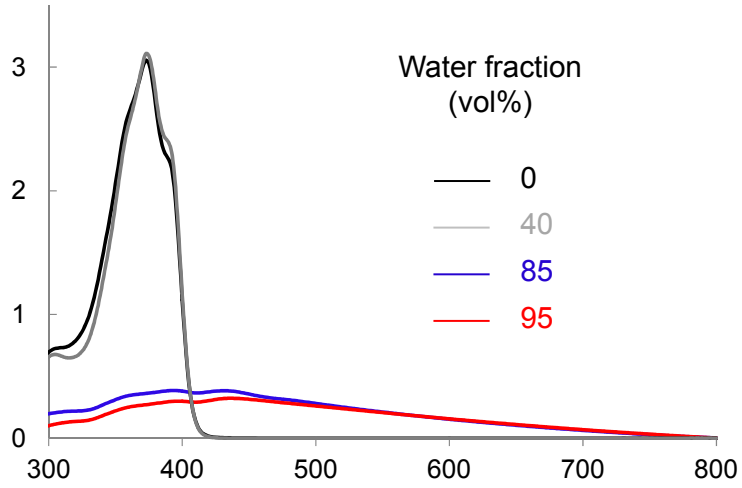


Figure S9. UV-vis absorption spectra of **6** in THF–water mixtures with different volume fractions of water (10^{-4} M).

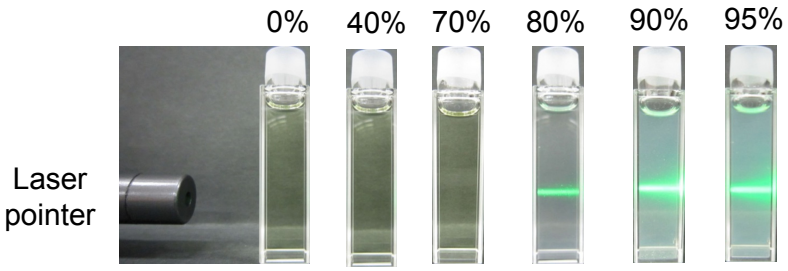


Figure S10. Check of Tyndall phenomenon of **12**.

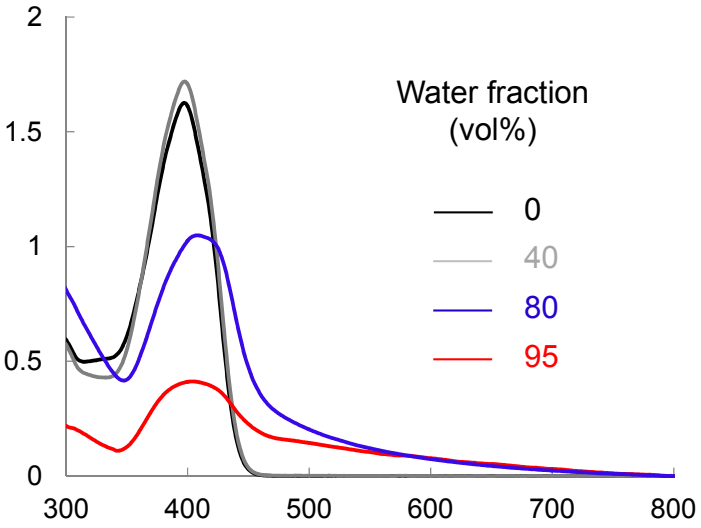


Figure S11. UV-vis absorption spectra of **12** in THF–water mixtures with different volume fractions of water (10^{-4} M).

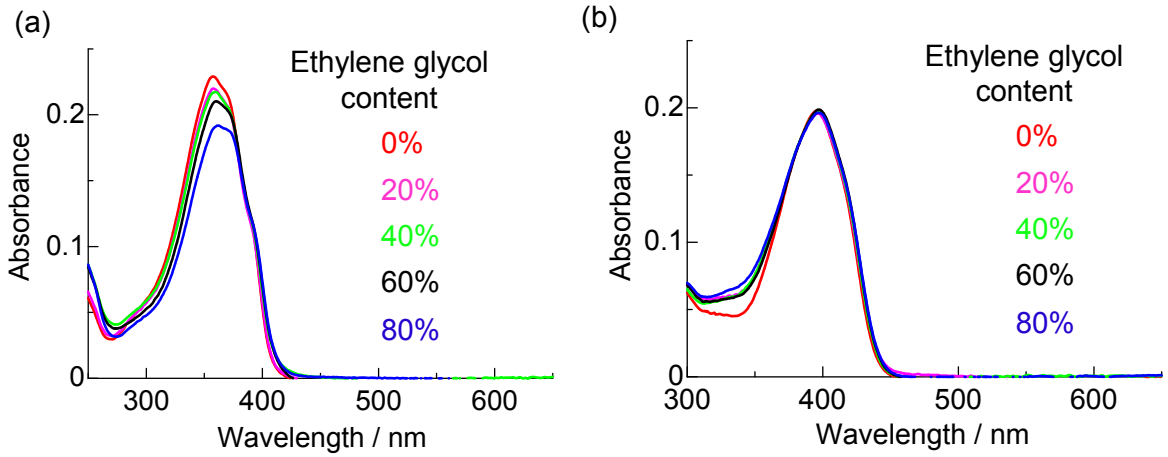
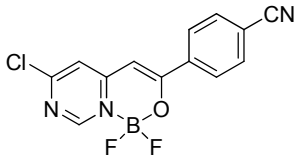


Figure S12. UV-vis absorption spectra of (a) **6** and (b) **12** in methanol–ethylene glycol mixtures with different volume fractions of ethylene glycol.

Table S1. Absorption and fluorescence properties of **8** in various solvents[a]

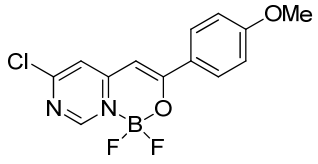


8

solvent	λ_{max} (ε) (nm)	F_{max}[b] (nm)	Stokes shift (cm^{-1})	ϕ_f[c]	τ_s[d] (ns)	k_f[e] (10^9 s^{-1})	k_{nr}[f] (10^9 s^{-1})
Hexane	376, 392[g]	411, 430	3,340	< 0.01	—[h]	—	—
Toluene	381 (32,200) 398 (21,100)	446	3,830	0.01	—[h]	—	—
$CHCl_3$	378 (31,900) 395 (20,100)	413, 433	3,360	0.01	—[h]	—	—
THF	378 (36,000) 395 (22,400)	435	3,470	0.01	—[h]	—	—
CH_2Cl_2	377 (36,800) 393 (23,300)	414, 433	3,430	0.01	—[h]	—	—
MeCN	374 (35,000) 391 (21,300)	434	3,700	0.01	—[h]	—	—

[a]Measured at a concentration of 1.0 x 10^{-5} mol dm^{-3}. [b] The excitation wavelengths (λ_{ex}) were as follows: hexane (371 nm), toluene (381 nm), chloroform (378 nm), THF (378 nm), dichloromethane (378 nm) and acetonitrile (354 nm). [c]Measured using an integrating sphere method. [d]Measured using a single-photon-counting method. [e]Radiative rate constant ($k_f = \Phi_f/\tau_s$). [f]Non-radiative rate constant ($k_{nr} = (1 - \Phi_f)/\tau_s$). [g]Poor solubility. [h]Too short to be measured ($\tau_s < 0.1$ ns).

Table S2. Absorption and fluorescence properties of **9** in various solvents[a]

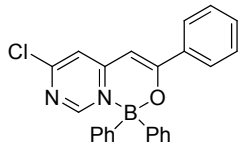


9

solvent	λ_{max} (ε) (nm)	F_{max}[b] (nm)	Stokes shift (cm^{-1})	ϕ_f[c]	τ_s[d] (ns)	k_f[e] (10^9 s^{-1})	k_{nr}[f] (10^9 s^{-1})
Hexane	385 (45,200) 405 (45,100)	415, 436	1,880	0.14	0.38	0.37	2.26
Toluene	390 (38,700) 408 (37,000)	431, 445	2,440	0.44	1.16	0.38	0.48
$CHCl_3$	392 (42,200) 408 (41,600)	433	2,420	0.53	1.38	0.38	0.34
THF	388 (40,400) 403 (37,700)	436	2,840	0.43	1.32	0.33	0.43
CH_2Cl_2	391 (42,200) 407 (41,000)	437	2,690	0.52	1.37	0.38	0.35
MeCN	386 (40,300) 399 (37,800)	445	3,440	0.44	1.34	0.33	0.42

[a]Measured at a concentration of 1.0 x 10^{-5} mol dm^{-3}. [b] The excitation wavelengths (λ_{ex}) were as follows: hexane (390 nm), toluene (390 nm), chloroform (390 nm), THF (390 nm), dichloromethane (390 nm) and acetonitrile (390 nm). [c]Measured using an integrating sphere method. [d]Measured using a single-photon-counting method. [e]Radiative rate constant ($k_f = \Phi_f/\tau_s$). [f]Non-radiative rate constant ($k_{nr} = (1 - \Phi_f)/\tau_s$).

Table S3. Absorption and fluorescence properties of **11** in various solvents[a]

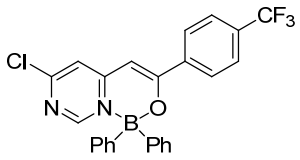


11

solvent	λ_{max} (ε) (nm)	F_{max}[b] (nm)	Stokes shift (cm^{-1})	ϕ_f[c]	τ_s[d] (ns)	k_f[e] (10^9 s^{-1})	k_{nr}[f] (10^9 s^{-1})
Hexane	397 (22,200)	445, 466	2,720	0.03	0.41	0.07	2.37
Toluene	401 (21,400)	456, 470	3,010	0.10	1.03	0.10	0.87
$CHCl_3$	399 (23,000)	451, 470	2,890	0.05	0.65	0.08	1.46
THF	399 (22,600)	452, 467	2,940	0.08	0.91	0.09	1.01
CH_2Cl_2	398 (23,300)	452, 469	3,000	0.05	0.67	0.07	1.42
MeCN	395 (22,500)	456	3,390	0.04	0.62	0.06	1.55

[a]Measured at a concentration of 1.0 x 10^{-5} mol dm^{-3}. [b] The excitation wavelengths (λ_{ex}) were as follows: hexane (397 nm), toluene (401 nm), toluene (399 nm), chloroform (400 nm), THF (399 nm), dichloromethane (400 nm) and acetonitrile (396 nm). [c]Measured using an integrating sphere method. [d]Measured using a single-photon-counting method. [e]Radiative rate constant ($k_f = \Phi_f/\tau_s$). [f]Non-radiative rate constant ($k_{nr} = (1 - \Phi_f)/\tau_s$).

Table S4. Absorption and fluorescence properties of **12** in various solvents[a]

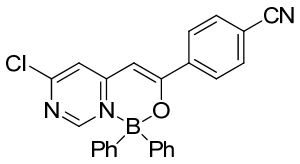


12

solvent	λ_{max} (ε) (nm)	F_{max}[b] (nm)	Stokes shift (cm^{-1})	ϕ_f[c]	τ_s[d] (ns)	k_f[e] (10^9 s^{-1})	k_{nr}[f] (10^9 s^{-1})
Hexane	396 (21,500)	449, 474	4,160	<0.01	___[g]	___[g]	___[g]
Toluene	400 (20,000)	459, 477	4,040	0.02	0.40	0.05	2.45
$CHCl_3$	397 (21,900)	455, 477	4,230	0.01	0.37	0.03	2.68
THF	397 (21,600)	459, 477	4,230	0.01	0.33	0.03	3.00
CH_2Cl_2	397 (22,100)	457, 473	4,230	0.01	0.30	0.03	3.30
MeCN	393 (21,600)	469	4,120	0.01	0.30	0.03	3.30

[a]Measured at a concentration of 1.0 x 10^{-5} mol dm^{-3}. [b] The excitation wavelengths (λ_{ex}) were as follows: hexane (397 nm), toluene (401 nm), chloroform (406 nm), THF (399 nm), dichloromethane (399 nm) and acetonitrile (396 nm). [c]Measured using an integrating sphere method. [d]Measured using a single-photon-counting method. [e]Radiative rate constant ($k_f = \Phi_f/\tau_s$). [f]Non-radiative rate constant ($k_{nr} = (1 - \Phi_f)/\tau_s$). [g]Too short to be measured ($\tau_s < 0.1$ ns).

Table S5. Absorption and fluorescence properties of **13** in various solvents[a]

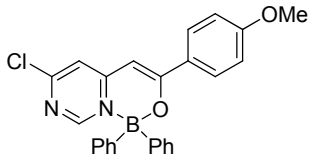


13

solvent	λ_{max} (ε) (nm)	F_{max}[b] (nm)	Stokes shift (cm^{-1})	ϕ_f[c]	τ_s[d] (ns)	k_f[e] (10^9 s^{-1})	k_{nr}[f] (10^9 s^{-1})
Hexane	401 (18,600)	456, 480	4,100	<0.01	—[h]	—	—
Toluene	405 (19,200)	489	4,240	0.01	—[h]	—	—
$CHCl_3$	404 (20,200)	486	4,180	<0.01	—[h]	—	—
THF	404 (19,300)	485	4,130	0.01	—[h]	—	—
CH_2Cl_2	403 (20,000)	466, 486	4,240	<0.01	—[h]	—	—
MeCN	398 (20,500)	480	4,290	<0.01	—[h]	—	—

[a]Measured at a concentration of 1.0 x 10^{-5} mol dm^{-3}. [b] The excitation wavelengths (λ_{ex}) were as follows: hexane (401 nm), toluene (405 nm), chloroform (400 nm), THF (404 nm), dichloromethane (404 nm) and acetonitrile (381 nm). [c]Measured using an integrating sphere method. [d]Measured using a single-photon-counting method. [e]Radiative rate constant ($k_f = \Phi_f/\tau_s$). [f]Non-radiative rate constant ($k_{nr} = (1 - \Phi_f)/\tau_s$).

Table S6. Absorption and fluorescence properties of **14** in various solvents[a]



14

solvent	λ_{max} (ε) (nm)	F_{max}[b] (nm)	Stokes shift (cm^{-1})	ϕ_f[c]	τ_s[d] (ns)	k_f[e] (10^9 s^{-1})	k_{nr}[f] (10^9 s^{-1})
Hexane	404 (29,800) 421 (27,300)	445, 468	2,280	0.35	1.89	0.19	0.34
Toluene	409 (27,800) 425 (25,800)	456, 469	2,520	0.58	2.70	0.22	0.16
$CHCl_3$	408 (30,300) 422 (28,400)	453, 469	2,440	0.48	2.30	0.21	0.23
THF	409(29,400)	455	2,470	0.53	2.76	0.19	0.17
CH_2Cl_2	408 (30,900)	455, 474	2,530	0.53	2.49	0.21	0.19
MeCN	404 (28,900)	457	2,870	0.46	2.51	0.18	0.22

[a]Measured at a concentration of 1.0 x 10^{-5} mol dm^{-3}. [b] The excitation wavelengths (λ_{ex}) were as follows: hexane (409 nm), toluene (409 nm), 1,4-dioxane (409 nm), chloroform (409 nm), THF (409 nm), dichloromethane (409 nm) and acetonitrile (409 nm). [c]Measured using an integrating sphere method. [d]Measured using a single-photon-counting method. [e]Radiative rate constant ($k_f = \Phi_f/\tau_s$). [f]Non-radiative rate constant ($k_{nr} = (1 - \Phi_f)/\tau_s$).

Table S7. Crystal data and structure refinement for **11**.

Identification code	11	
Empirical formula	C24 H18 B Cl N2 O	
Formula weight	396.66	
Temperature	293(2) K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 9.467(3) Å	α= 90°.
	b = 20.563(7) Å	β= 96.812(10)°.
	c = 10.445(3) Å	γ = 90°.
Volume	2019.0(11) $Å^3$	
Z	4	
Density (calculated)	1.305 Mg/m^3	

Absorption coefficient	0.207 mm^{-1}
F(000)	824
Crystal size	0.20 x 0.20 x 0.20 mm^3
Theta range for data collection	2.17 to 27.58°.
Index ranges	-12<=h<=12, -26<=k<=26, -13<=l<=13
Reflections collected	19713
Independent reflections	4594 [R(int) = 0.0825]
Completeness to theta = 27.58°	98.1 %
Absorption correction	Integration
Max. and min. transmission	0.9598 and 0.9598
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4594 / 0 / 262
Goodness-of-fit on F^2	1.026
Final R indices [I>2sigma(I)]	R1 = 0.0501, wR2 = 0.1300
R indices (all data)	R1 = 0.0618, wR2 = 0.1408
Largest diff. peak and hole	0.192 and -0.237 e.$Å^{-3}$

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **11**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4892(2)	-640(1)	7645(2)	43(1)
C(2)	4466(2)	-165(1)	6767(2)	48(1)
C(3)	3309(2)	-263(1)	5803(2)	42(1)
C(4)	2655(2)	240(1)	5040(2)	50(1)
C(5)	1637(2)	-965(1)	4737(2)	49(1)
C(6)	5972(2)	-556(1)	8768(2)	48(1)
C(7)	6380(2)	-1090(1)	9533(2)	70(1)
C(8)	7412(3)	-1033(1)	10569(3)	92(1)
C(9)	8057(3)	-443(1)	10871(2)	86(1)
C(10)	7660(3)	80(1)	10133(3)	90(1)
C(11)	6623(3)	37(1)	9086(2)	73(1)
C(12)	1552(2)	79(1)	4144(2)	49(1)
C(13)	4856(2)	-1677(1)	5380(2)	44(1)
C(14)	6230(2)	-1850(1)	5909(2)	50(1)
C(15)	7262(2)	-2044(1)	5145(2)	60(1)

C(16)	6950(2)	-2067(1)	3829(2)	65(1)
C(17)	5613(2)	-1901(1)	3272(2)	65(1)
C(18)	4586(2)	-1708(1)	4039(2)	55(1)
C(19)	2558(2)	-2051(1)	6591(2)	44(1)
C(20)	2460(2)	-2645(1)	5955(2)	59(1)
C(21)	1478(3)	-3116(1)	6261(2)	74(1)
C(22)	599(2)	-3001(1)	7183(2)	69(1)
C(23)	677(2)	-2423(1)	7833(2)	65(1)
C(24)	1646(2)	-1956(1)	7530(2)	53(1)
B(1)	3651(2)	-1482(1)	6293(2)	41(1)
N(1)	2768(1)	-878(1)	5606(1)	41(1)
N(2)	995(2)	-518(1)	3979(1)	53(1)
O(1)	4306(1)	-1225(1)	7560(1)	46(1)
Cl(1)	754(1)	671(1)	3133(1)	69(1)

Table S9. Bond lengths [Å] and angles [°] for **11**.

C(1)-O(1)	1.3244(18)
C(1)-C(2)	1.366(2)
C(1)-C(6)	1.472(2)
C(2)-C(3)	1.412(2)
C(3)-N(1)	1.3705(19)
C(3)-C(4)	1.404(2)
C(4)-C(12)	1.358(2)
C(5)-N(2)	1.315(2)
C(5)-N(1)	1.331(2)
C(6)-C(7)	1.385(3)
C(6)-C(11)	1.388(2)
C(7)-C(8)	1.374(3)
C(8)-C(9)	1.378(4)
C(9)-C(10)	1.350(4)
C(10)-C(11)	1.383(3)
C(12)-N(2)	1.339(2)
C(12)-Cl(1)	1.7247(17)
C(13)-C(18)	1.395(2)
C(13)-C(14)	1.397(2)
C(13)-B(1)	1.622(2)
C(14)-C(15)	1.391(3)

C(15)-C(16)	1.372(3)
C(16)-C(17)	1.372(3)
C(17)-C(18)	1.389(3)
C(19)-C(20)	1.388(2)
C(19)-C(24)	1.395(2)
C(19)-B(1)	1.616(2)
C(20)-C(21)	1.405(3)
C(21)-C(22)	1.367(3)
C(22)-C(23)	1.368(3)
C(23)-C(24)	1.390(2)
B(1)-O(1)	1.490(2)
B(1)-N(1)	1.616(2)

O(1)-C(1)-C(2)	121.11(14)
O(1)-C(1)-C(6)	113.89(13)
C(2)-C(1)-C(6)	124.97(14)
C(1)-C(2)-C(3)	121.25(14)
N(1)-C(3)-C(4)	117.55(14)
N(1)-C(3)-C(2)	118.92(13)
C(4)-C(3)-C(2)	123.52(14)
C(12)-C(4)-C(3)	117.58(15)
N(2)-C(5)-N(1)	126.40(15)
C(7)-C(6)-C(11)	118.18(18)
C(7)-C(6)-C(1)	119.14(15)
C(11)-C(6)-C(1)	122.67(16)
C(8)-C(7)-C(6)	120.7(2)
C(7)-C(8)-C(9)	120.6(2)
C(10)-C(9)-C(8)	119.0(2)
C(9)-C(10)-C(11)	121.6(2)
C(10)-C(11)-C(6)	119.9(2)
N(2)-C(12)-C(4)	124.82(15)
N(2)-C(12)-Cl(1)	115.49(13)
C(4)-C(12)-Cl(1)	119.68(13)
C(18)-C(13)-C(14)	115.90(15)
C(18)-C(13)-B(1)	122.95(14)
C(14)-C(13)-B(1)	121.11(15)
C(15)-C(14)-C(13)	122.01(17)
C(16)-C(15)-C(14)	120.12(17)
C(17)-C(16)-C(15)	119.62(17)
C(16)-C(17)-C(18)	120.03(19)

C(17)-C(18)-C(13)	122.30(17)
C(20)-C(19)-C(24)	116.57(15)
C(20)-C(19)-B(1)	123.59(16)
C(24)-C(19)-B(1)	119.84(14)
C(19)-C(20)-C(21)	120.4(2)
C(22)-C(21)-C(20)	121.08(19)
C(21)-C(22)-C(23)	119.88(18)
C(22)-C(23)-C(24)	119.1(2)
C(23)-C(24)-C(19)	122.96(18)
O(1)-B(1)-C(19)	107.11(13)
O(1)-B(1)-N(1)	105.16(11)
C(19)-B(1)-N(1)	109.42(12)
O(1)-B(1)-C(13)	111.25(13)
C(19)-B(1)-C(13)	116.37(13)
N(1)-B(1)-C(13)	106.97(12)
C(5)-N(1)-C(3)	118.88(13)
C(5)-N(1)-B(1)	122.07(12)
C(3)-N(1)-B(1)	118.52(12)
C(5)-N(2)-C(12)	114.63(15)
C(1)-O(1)-B(1)	120.54(12)

Symmetry transformations used to generate equivalent atoms:

Table S10. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **11**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	40(1)	41(1)	48(1)	-5(1)	6(1)	-3(1)
C(2)	45(1)	40(1)	59(1)	-2(1)	4(1)	-6(1)
C(3)	39(1)	38(1)	51(1)	1(1)	11(1)	2(1)
C(4)	47(1)	40(1)	63(1)	7(1)	7(1)	4(1)
C(5)	46(1)	44(1)	56(1)	1(1)	1(1)	2(1)
C(6)	44(1)	51(1)	49(1)	-6(1)	4(1)	-4(1)
C(7)	68(1)	62(1)	75(1)	8(1)	-19(1)	-11(1)
C(8)	90(2)	86(2)	87(2)	15(1)	-36(1)	-12(1)
C(9)	82(2)	96(2)	72(1)	-5(1)	-26(1)	-21(1)
C(10)	97(2)	77(2)	86(2)	-12(1)	-24(1)	-31(1)
C(11)	87(2)	57(1)	70(1)	-5(1)	-12(1)	-17(1)

C(12)	44(1)	49(1)	55(1)	7(1)	11(1)	9(1)
C(13)	41(1)	37(1)	53(1)	0(1)	3(1)	0(1)
C(14)	46(1)	44(1)	59(1)	6(1)	-2(1)	4(1)
C(15)	40(1)	54(1)	85(1)	2(1)	3(1)	9(1)
C(16)	50(1)	68(1)	80(1)	-15(1)	17(1)	7(1)
C(17)	57(1)	81(1)	58(1)	-16(1)	8(1)	5(1)
C(18)	42(1)	66(1)	56(1)	-9(1)	1(1)	6(1)
C(19)	41(1)	40(1)	49(1)	5(1)	-7(1)	-2(1)
C(20)	64(1)	45(1)	66(1)	-4(1)	0(1)	-9(1)
C(21)	85(2)	45(1)	88(2)	-4(1)	-12(1)	-18(1)
C(22)	57(1)	68(1)	75(1)	20(1)	-14(1)	-22(1)
C(23)	48(1)	77(1)	69(1)	14(1)	2(1)	-13(1)
C(24)	45(1)	53(1)	60(1)	5(1)	3(1)	-5(1)
B(1)	40(1)	38(1)	45(1)	1(1)	-2(1)	1(1)
N(1)	37(1)	39(1)	47(1)	0(1)	5(1)	2(1)
N(2)	47(1)	52(1)	57(1)	4(1)	-3(1)	5(1)
O(1)	49(1)	42(1)	47(1)	1(1)	-1(1)	-7(1)
Cl(1)	67(1)	61(1)	76(1)	20(1)	-4(1)	13(1)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **11**.

	x	y	z	U(eq)
H(2)	4948	230	6805	57
H(4)	2966	668	5144	60
H(7)	5950	-1490	9344	84
H(8)	7677	-1396	11071	110
H(9)	8755	-406	11573	103
H(10)	8095	479	10333	108
H(11)	6363	404	8595	87
H(14)	6461	-1834	6799	60
H(15)	8165	-2158	5527	72
H(16)	7641	-2194	3317	78
H(17)	5394	-1917	2381	78
H(18)	3687	-1594	3644	66
H(20)	3047	-2731	5322	71

H(21)	1426	-3512	5828	89
H(22)	-52	-3316	7369	82
H(23)	90	-2342	8469	78
H(23A)	1263	-1384	4659	78
H(24)	1689	-1563	7974	63

Table S12. Torsion angles [°] for **11**.

O(1)-C(1)-C(2)-C(3)	5.4(2)
C(6)-C(1)-C(2)-C(3)	-172.58(15)
C(1)-C(2)-C(3)-N(1)	-11.5(2)
C(1)-C(2)-C(3)-C(4)	167.35(15)
N(1)-C(3)-C(4)-C(12)	-1.3(2)
C(2)-C(3)-C(4)-C(12)	179.88(16)
O(1)-C(1)-C(6)-C(7)	6.5(2)
C(2)-C(1)-C(6)-C(7)	-175.41(18)
O(1)-C(1)-C(6)-C(11)	-174.62(18)
C(2)-C(1)-C(6)-C(11)	3.5(3)
C(11)-C(6)-C(7)-C(8)	-0.7(3)
C(1)-C(6)-C(7)-C(8)	178.3(2)
C(6)-C(7)-C(8)-C(9)	0.3(4)
C(7)-C(8)-C(9)-C(10)	0.0(5)
C(8)-C(9)-C(10)-C(11)	0.1(5)
C(9)-C(10)-C(11)-C(6)	-0.5(4)
C(7)-C(6)-C(11)-C(10)	0.7(3)
C(1)-C(6)-C(11)-C(10)	-178.2(2)
C(3)-C(4)-C(12)-N(2)	3.6(3)
C(3)-C(4)-C(12)-Cl(1)	-177.34(12)
C(18)-C(13)-C(14)-C(15)	-0.5(2)
B(1)-C(13)-C(14)-C(15)	177.41(15)
C(13)-C(14)-C(15)-C(16)	0.4(3)
C(14)-C(15)-C(16)-C(17)	-0.4(3)
C(15)-C(16)-C(17)-C(18)	0.3(3)
C(16)-C(17)-C(18)-C(13)	-0.4(3)
C(14)-C(13)-C(18)-C(17)	0.4(3)
B(1)-C(13)-C(18)-C(17)	-177.40(17)
C(24)-C(19)-C(20)-C(21)	0.2(3)
B(1)-C(19)-C(20)-C(21)	-179.69(16)

C(19)-C(20)-C(21)-C(22)	0.2(3)
C(20)-C(21)-C(22)-C(23)	-0.6(3)
C(21)-C(22)-C(23)-C(24)	0.7(3)
C(22)-C(23)-C(24)-C(19)	-0.3(3)
C(20)-C(19)-C(24)-C(23)	-0.1(2)
B(1)-C(19)-C(24)-C(23)	179.75(16)
C(20)-C(19)-B(1)-O(1)	-135.83(15)
C(24)-C(19)-B(1)-O(1)	44.31(18)
C(20)-C(19)-B(1)-N(1)	110.67(17)
C(24)-C(19)-B(1)-N(1)	-69.19(18)
C(20)-C(19)-B(1)-C(13)	-10.7(2)
C(24)-C(19)-B(1)-C(13)	169.47(14)
C(18)-C(13)-B(1)-O(1)	-156.59(14)
C(14)-C(13)-B(1)-O(1)	25.68(19)
C(18)-C(13)-B(1)-C(19)	80.37(19)
C(14)-C(13)-B(1)-C(19)	-97.35(17)
C(18)-C(13)-B(1)-N(1)	-42.26(19)
C(14)-C(13)-B(1)-N(1)	140.01(14)
N(2)-C(5)-N(1)-C(3)	3.4(3)
N(2)-C(5)-N(1)-B(1)	-168.11(16)
C(4)-C(3)-N(1)-C(5)	-1.9(2)
C(2)-C(3)-N(1)-C(5)	177.01(14)
C(4)-C(3)-N(1)-B(1)	169.93(13)
C(2)-C(3)-N(1)-B(1)	-11.2(2)
O(1)-B(1)-N(1)-C(5)	-153.34(14)
C(19)-B(1)-N(1)-C(5)	-38.58(19)
C(13)-B(1)-N(1)-C(5)	88.28(17)
O(1)-B(1)-N(1)-C(3)	35.11(17)
C(19)-B(1)-N(1)-C(3)	149.87(13)
C(13)-B(1)-N(1)-C(3)	-83.26(16)
N(1)-C(5)-N(2)-C(12)	-1.3(3)
C(4)-C(12)-N(2)-C(5)	-2.3(3)
Cl(1)-C(12)-N(2)-C(5)	178.55(13)
C(2)-C(1)-O(1)-B(1)	25.7(2)
C(6)-C(1)-O(1)-B(1)	-156.15(13)
C(19)-B(1)-O(1)-C(1)	-158.99(13)
N(1)-B(1)-O(1)-C(1)	-42.64(17)
C(13)-B(1)-O(1)-C(1)	72.81(16)

Symmetry transformations used to generate equivalent atoms:

Table S13. Crystal data and structure refinement for **12**.

Identification code	12	
Empirical formula	C25 H17 B Cl F3 N2 O	
Formula weight	464.67	
Temperature	293(2) K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 10.343(3) Å	α= 90°.
	b = 20.367(8) Å	β= 92.628(11)°.
	c = 10.514(2) Å	γ = 90°.
Volume	2212.5(12) $Å^3$	
Z	4	
Density (calculated)	1.395 Mg/m^3	
Absorption coefficient	0.219 mm^{-1}	
F(000)	952	
Crystal size	0.20 x 0.20 x 0.20 mm^3	
Theta range for data collection	1.97 to 27.92°.	
Index ranges	-13<=h<=13, -26<=k<=26, -13<=l<=13	
Reflections collected	22535	
Independent reflections	5121 [R(int) = 0.0351]	
Completeness to theta = 27.92°	96.7 %	
Absorption correction	Integration	
Max. and min. transmission	0.9576 and 0.9576	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5121 / 0 / 298	
Goodness-of-fit on F^2	1.104	
Final R indices [I>2sigma(I)]	R1 = 0.0511, wR2 = 0.1350	
R indices (all data)	R1 = 0.0699, wR2 = 0.1559	
Largest diff. peak and hole	0.168 and -0.217 $e.Å^{-3}$	

Table S14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **12**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)

C(1)	5481(2)	10635(1)	12313(2)	42(1)
C(2)	5793(2)	10154(1)	11479(2)	45(1)
C(3)	6822(2)	10238(1)	10635(2)	42(1)
C(4)	7349(2)	9722(1)	9947(2)	48(1)
C(5)	8355(2)	10919(1)	9740(2)	53(1)
C(6)	4517(2)	10558(1)	13307(2)	41(1)
C(7)	4167(2)	11104(1)	14021(2)	53(1)
C(8)	3244(2)	11052(1)	14928(2)	56(1)
C(9)	2661(2)	10453(1)	15153(2)	47(1)
C(10)	3005(2)	9906(1)	14461(2)	54(1)
C(11)	3929(2)	9957(1)	13546(2)	50(1)
C(12)	8340(2)	9861(1)	9166(2)	51(1)
C(13)	5482(2)	11690(1)	10092(2)	48(1)
C(14)	4241(2)	11848(1)	10477(2)	54(1)
C(15)	3261(2)	12051(1)	9613(3)	66(1)
C(16)	3501(3)	12102(1)	8338(3)	73(1)
C(17)	4712(3)	11956(1)	7925(3)	72(1)
C(18)	5680(2)	11753(1)	8786(2)	62(1)
C(19)	7670(2)	12026(1)	11527(2)	48(1)
C(20)	7758(2)	12631(1)	10923(3)	69(1)
C(21)	8689(3)	13089(1)	11313(3)	85(1)
C(22)	9542(3)	12960(1)	12312(3)	78(1)
C(23)	9485(3)	12366(1)	12928(3)	78(1)
C(24)	8558(2)	11909(1)	12535(2)	64(1)
C(25)	1640(2)	10408(1)	16113(2)	57(1)
O(1)	6053(1)	11217(1)	12310(1)	46(1)
N(1)	7349(2)	10848(1)	10499(2)	43(1)
N(2)	8877(2)	10452(1)	9051(2)	57(1)
F(1)	1464(2)	9802(1)	16542(2)	82(1)
F(2)	493(1)	10620(1)	15656(2)	85(1)
F(3)	1919(2)	10780(1)	17152(1)	79(1)
Cl(1)	8975(1)	9242(1)	8259(1)	69(1)
B(1)	6615(2)	11474(1)	11117(2)	45(1)

Table S15. Bond lengths [Å] and angles [°] for **12**.

C(1)-O(1)	1.325(2)

C(1)-C(2)	1.363(3)
C(1)-C(6)	1.485(3)
C(2)-C(3)	1.428(3)
C(3)-N(1)	1.367(2)
C(3)-C(4)	1.400(3)
C(4)-C(12)	1.372(3)
C(5)-N(2)	1.327(3)
C(5)-N(1)	1.348(3)
C(6)-C(11)	1.395(3)
C(6)-C(7)	1.399(3)
C(7)-C(8)	1.384(3)
C(8)-C(9)	1.387(3)
C(9)-C(10)	1.386(3)
C(9)-C(25)	1.497(3)
C(10)-C(11)	1.391(3)
C(12)-N(2)	1.334(3)
C(12)-Cl(1)	1.729(2)
C(13)-C(14)	1.401(3)
C(13)-C(18)	1.404(3)
C(13)-B(1)	1.616(3)
C(14)-C(15)	1.392(3)
C(15)-C(16)	1.379(4)
C(16)-C(17)	1.376(4)
C(17)-C(18)	1.382(3)
C(19)-C(24)	1.391(3)
C(19)-C(20)	1.391(3)
C(19)-B(1)	1.612(3)
C(20)-C(21)	1.390(3)
C(21)-C(22)	1.365(4)
C(22)-C(23)	1.375(4)
C(23)-C(24)	1.386(3)
C(25)-F(1)	1.329(3)
C(25)-F(2)	1.331(3)
C(25)-F(3)	1.350(3)
O(1)-B(1)	1.500(3)
N(1)-B(1)	1.633(3)

O(1)-C(1)-C(2)	121.51(17)
O(1)-C(1)-C(6)	114.27(16)
C(2)-C(1)-C(6)	124.21(16)

C(1)-C(2)-C(3)	121.29(17)
N(1)-C(3)-C(4)	117.58(18)
N(1)-C(3)-C(2)	119.04(16)
C(4)-C(3)-C(2)	123.36(17)
C(12)-C(4)-C(3)	118.21(18)
N(2)-C(5)-N(1)	126.26(19)
C(11)-C(6)-C(7)	118.35(18)
C(11)-C(6)-C(1)	122.18(16)
C(7)-C(6)-C(1)	119.46(16)
C(8)-C(7)-C(6)	120.91(18)
C(7)-C(8)-C(9)	120.21(18)
C(10)-C(9)-C(8)	119.60(19)
C(10)-C(9)-C(25)	120.76(18)
C(8)-C(9)-C(25)	119.62(18)
C(9)-C(10)-C(11)	120.33(18)
C(10)-C(11)-C(6)	120.60(18)
N(2)-C(12)-C(4)	124.51(18)
N(2)-C(12)-Cl(1)	115.96(16)
C(4)-C(12)-Cl(1)	119.53(16)
C(14)-C(13)-C(18)	116.0(2)
C(14)-C(13)-B(1)	121.03(19)
C(18)-C(13)-B(1)	122.90(19)
C(15)-C(14)-C(13)	121.9(2)
C(16)-C(15)-C(14)	120.0(2)
C(17)-C(16)-C(15)	119.8(2)
C(16)-C(17)-C(18)	120.0(3)
C(17)-C(18)-C(13)	122.3(2)
C(24)-C(19)-C(20)	116.4(2)
C(24)-C(19)-B(1)	119.99(18)
C(20)-C(19)-B(1)	123.6(2)
C(21)-C(20)-C(19)	121.3(2)
C(22)-C(21)-C(20)	120.8(2)
C(21)-C(22)-C(23)	119.5(2)
C(22)-C(23)-C(24)	119.6(3)
C(23)-C(24)-C(19)	122.4(2)
F(1)-C(25)-F(2)	106.9(2)
F(1)-C(25)-F(3)	105.94(19)
F(2)-C(25)-F(3)	105.30(18)
F(1)-C(25)-C(9)	113.39(17)
F(2)-C(25)-C(9)	112.42(19)

F(3)-C(25)-C(9)	112.34(19)
C(1)-O(1)-B(1)	120.24(15)
C(5)-N(1)-C(3)	118.76(16)
C(5)-N(1)-B(1)	122.51(15)
C(3)-N(1)-B(1)	118.24(15)
C(5)-N(2)-C(12)	114.60(19)
O(1)-B(1)-C(19)	107.63(16)
O(1)-B(1)-C(13)	110.81(16)
C(19)-B(1)-C(13)	116.74(16)
O(1)-B(1)-N(1)	105.42(14)
C(19)-B(1)-N(1)	109.20(16)
C(13)-B(1)-N(1)	106.47(15)

Symmetry transformations used to generate equivalent atoms:

Table S16. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **12**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	44(1)	35(1)	46(1)	2(1)	-1(1)	-3(1)
C(2)	48(1)	38(1)	50(1)	-3(1)	7(1)	-7(1)
C(3)	44(1)	39(1)	43(1)	-2(1)	-1(1)	-2(1)
C(4)	53(1)	41(1)	51(1)	-6(1)	3(1)	-1(1)
C(5)	52(1)	49(1)	59(1)	0(1)	10(1)	-5(1)
C(6)	43(1)	38(1)	43(1)	1(1)	2(1)	0(1)
C(7)	64(1)	38(1)	57(1)	-1(1)	13(1)	-5(1)
C(8)	67(1)	42(1)	58(1)	-4(1)	14(1)	4(1)
C(9)	45(1)	49(1)	49(1)	4(1)	5(1)	4(1)
C(10)	56(1)	43(1)	64(1)	-1(1)	12(1)	-8(1)
C(11)	56(1)	38(1)	58(1)	-3(1)	9(1)	-4(1)
C(12)	48(1)	54(1)	51(1)	-7(1)	1(1)	6(1)
C(13)	55(1)	33(1)	56(1)	0(1)	2(1)	-5(1)
C(14)	55(1)	40(1)	66(1)	-1(1)	3(1)	-3(1)
C(15)	56(1)	44(1)	99(2)	4(1)	-6(1)	0(1)
C(16)	76(2)	56(1)	83(2)	9(1)	-23(1)	-1(1)
C(17)	88(2)	69(2)	59(1)	10(1)	-7(1)	4(1)
C(18)	68(1)	61(1)	57(1)	5(1)	4(1)	6(1)
C(19)	50(1)	38(1)	56(1)	-5(1)	10(1)	-5(1)

C(20)	67(1)	47(1)	92(2)	10(1)	-1(1)	-13(1)
C(21)	79(2)	45(1)	130(3)	9(1)	4(2)	-22(1)
C(22)	70(2)	61(1)	104(2)	-18(1)	13(2)	-28(1)
C(23)	72(2)	81(2)	81(2)	-9(1)	-9(1)	-23(1)
C(24)	70(1)	53(1)	69(1)	-2(1)	-4(1)	-16(1)
C(25)	52(1)	60(1)	61(1)	1(1)	10(1)	7(1)
O(1)	53(1)	38(1)	49(1)	-4(1)	9(1)	-9(1)
N(1)	44(1)	38(1)	47(1)	1(1)	3(1)	-2(1)
N(2)	53(1)	60(1)	60(1)	-5(1)	11(1)	-3(1)
F(1)	85(1)	68(1)	96(1)	16(1)	40(1)	-4(1)
F(2)	52(1)	106(1)	96(1)	-1(1)	9(1)	19(1)
F(3)	83(1)	93(1)	61(1)	-11(1)	22(1)	-4(1)
Cl(1)	67(1)	72(1)	71(1)	-21(1)	15(1)	9(1)
B(1)	48(1)	36(1)	50(1)	-1(1)	6(1)	-4(1)

Table S17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **12**.

	x	y	z	U(eq)
H(2)	5326	9764	11460	54
H(4)	7035	9296	10018	58
H(5)	8717	11336	9694	63
H(7)	4560	11507	13885	63
H(8)	3013	11421	15387	67
H(10)	2616	9503	14609	64
H(11)	4157	9586	13089	60
H(14)	4066	11816	11335	65
H(15)	2446	12151	9896	80
H(16)	2847	12234	7758	87
H(17)	4878	11993	7066	87
H(18)	6492	11656	8490	74
H(20)	7183	12730	10245	82
H(21)	8732	13489	10889	102
H(22)	10156	13271	12573	94
H(23)	10066	12271	13605	94
H(24)	8527	11509	12962	77

Table S18. Torsion angles [°] for **12**.

O(1)-C(1)-C(2)-C(3)	5.1(3)
C(6)-C(1)-C(2)-C(3)	-173.42(17)
C(1)-C(2)-C(3)-N(1)	-11.8(3)
C(1)-C(2)-C(3)-C(4)	166.90(19)
N(1)-C(3)-C(4)-C(12)	-1.1(3)
C(2)-C(3)-C(4)-C(12)	-179.79(18)
O(1)-C(1)-C(6)-C(11)	-172.60(17)
C(2)-C(1)-C(6)-C(11)	6.0(3)
O(1)-C(1)-C(6)-C(7)	8.3(3)
C(2)-C(1)-C(6)-C(7)	-173.09(19)
C(11)-C(6)-C(7)-C(8)	-1.1(3)
C(1)-C(6)-C(7)-C(8)	178.03(19)
C(6)-C(7)-C(8)-C(9)	0.9(3)
C(7)-C(8)-C(9)-C(10)	-0.3(3)
C(7)-C(8)-C(9)-C(25)	-178.5(2)
C(8)-C(9)-C(10)-C(11)	0.1(3)
C(25)-C(9)-C(10)-C(11)	178.2(2)
C(9)-C(10)-C(11)-C(6)	-0.4(3)
C(7)-C(6)-C(11)-C(10)	0.8(3)
C(1)-C(6)-C(11)-C(10)	-178.26(18)
C(3)-C(4)-C(12)-N(2)	2.8(3)
C(3)-C(4)-C(12)-Cl(1)	-177.67(14)
C(18)-C(13)-C(14)-C(15)	0.5(3)
B(1)-C(13)-C(14)-C(15)	178.38(18)
C(13)-C(14)-C(15)-C(16)	-0.1(3)
C(14)-C(15)-C(16)-C(17)	-0.4(3)
C(15)-C(16)-C(17)-C(18)	0.5(4)
C(16)-C(17)-C(18)-C(13)	-0.1(4)
C(14)-C(13)-C(18)-C(17)	-0.4(3)
B(1)-C(13)-C(18)-C(17)	-178.2(2)
C(24)-C(19)-C(20)-C(21)	0.2(4)
B(1)-C(19)-C(20)-C(21)	-179.9(2)
C(19)-C(20)-C(21)-C(22)	-0.5(5)
C(20)-C(21)-C(22)-C(23)	0.7(5)
C(21)-C(22)-C(23)-C(24)	-0.6(4)

C(22)-C(23)-C(24)-C(19)	0.2(4)
C(20)-C(19)-C(24)-C(23)	0.0(4)
B(1)-C(19)-C(24)-C(23)	-180.0(2)
C(10)-C(9)-C(25)-F(1)	22.5(3)
C(8)-C(9)-C(25)-F(1)	-159.4(2)
C(10)-C(9)-C(25)-F(2)	-98.8(2)
C(8)-C(9)-C(25)-F(2)	79.3(3)
C(10)-C(9)-C(25)-F(3)	142.6(2)
C(8)-C(9)-C(25)-F(3)	-39.3(3)
C(2)-C(1)-O(1)-B(1)	25.9(3)
C(6)-C(1)-O(1)-B(1)	-155.49(16)
N(2)-C(5)-N(1)-C(3)	2.7(3)
N(2)-C(5)-N(1)-B(1)	-169.2(2)
C(4)-C(3)-N(1)-C(5)	-1.4(3)
C(2)-C(3)-N(1)-C(5)	177.38(17)
C(4)-C(3)-N(1)-B(1)	170.88(17)
C(2)-C(3)-N(1)-B(1)	-10.4(2)
N(1)-C(5)-N(2)-C(12)	-1.2(3)
C(4)-C(12)-N(2)-C(5)	-1.6(3)
Cl(1)-C(12)-N(2)-C(5)	178.80(16)
C(1)-O(1)-B(1)-C(19)	-158.84(16)
C(1)-O(1)-B(1)-C(13)	72.4(2)
C(1)-O(1)-B(1)-N(1)	-42.4(2)
C(24)-C(19)-B(1)-O(1)	45.3(3)
C(20)-C(19)-B(1)-O(1)	-134.7(2)
C(24)-C(19)-B(1)-C(13)	170.5(2)
C(20)-C(19)-B(1)-C(13)	-9.4(3)
C(24)-C(19)-B(1)-N(1)	-68.7(2)
C(20)-C(19)-B(1)-N(1)	111.4(2)
C(14)-C(13)-B(1)-O(1)	22.5(2)
C(18)-C(13)-B(1)-O(1)	-159.84(18)
C(14)-C(13)-B(1)-C(19)	-101.2(2)
C(18)-C(13)-B(1)-C(19)	76.5(2)
C(14)-C(13)-B(1)-N(1)	136.60(17)
C(18)-C(13)-B(1)-N(1)	-45.7(2)
C(5)-N(1)-B(1)-O(1)	-153.71(17)
C(3)-N(1)-B(1)-O(1)	34.4(2)
C(5)-N(1)-B(1)-C(19)	-38.3(2)
C(3)-N(1)-B(1)-C(19)	149.76(16)
C(5)-N(1)-B(1)-C(13)	88.5(2)

C(3)-N(1)-B(1)-C(13)	-83.39(19)

Symmetry transformations used to generate equivalent atoms:

Table S19. Crystal data and structure refinement for **13**.

Identification code	13	
Empirical formula	C25 H17 B Cl N3 O	
Formula weight	421.68	
Temperature	293(2) K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	P21/a	
Unit cell dimensions	a = 10.425(4) Å	α= 90°.
	b = 21.350(6) Å	β= 117.211(8)°.
	c = 10.573(3) Å	γ = 90°.
Volume	2092.8(12) $Å^3$	
Z	4	
Density (calculated)	1.338 Mg/m^3	
Absorption coefficient	0.205 mm^{-1}	
F(000)	872	
Crystal size	0.20 x 0.20 x 0.20 mm^3	
Theta range for data collection	1.91 to 27.48°.	
Index ranges	-13<=h<=13, -27<=k<=27, -13<=l<=13	
Reflections collected	20973	
Independent reflections	4786 [R(int) = 0.0497]	
Completeness to theta = 27.48°	99.7 %	
Absorption correction	Integration	
Max. and min. transmission	0.9601 and 0.9601	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4786 / 0 / 280	
Goodness-of-fit on F^2	1.062	
Final R indices [I>2sigma(I)]	R1 = 0.0549, wR2 = 0.1432	
R indices (all data)	R1 = 0.0782, wR2 = 0.1665	
Largest diff. peak and hole	0.186 and -0.395 $e.Å^{-3}$	

Table S20. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **13**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	7371(2)	9131(1)	5258(2)	46(1)
C(2)	7826(2)	9624(1)	4764(2)	51(1)
C(3)	8223(2)	9551(1)	3653(2)	45(1)
C(4)	8459(2)	10048(1)	2932(2)	54(1)
C(5)	8658(2)	8880(1)	2171(2)	53(1)
C(6)	6816(2)	9180(1)	6313(2)	48(1)
C(7)	6671(2)	8638(1)	6958(2)	54(1)
C(8)	6216(2)	8663(1)	7983(2)	59(1)
C(9)	5862(2)	9235(1)	8360(2)	52(1)
C(10)	5966(3)	9777(1)	7709(2)	61(1)
C(11)	6449(3)	9751(1)	6696(2)	60(1)
C(12)	8817(2)	9904(1)	1879(2)	54(1)
N(1)	8354(2)	8956(1)	3253(2)	44(1)
N(2)	8906(2)	9325(1)	1459(2)	55(1)
N(3)	5044(3)	9240(1)	10312(2)	78(1)
O(1)	7364(2)	8553(1)	4811(1)	49(1)
B(1)	8358(2)	8364(1)	4217(2)	44(1)
C(13)	9983(2)	8281(1)	5453(2)	46(1)
C(14)	10280(2)	8162(1)	6855(2)	52(1)
C(15)	11664(3)	8060(1)	7914(2)	60(1)
C(16)	12800(3)	8064(1)	7607(2)	66(1)
C(17)	12558(3)	8175(1)	6236(3)	69(1)
C(18)	11175(2)	8280(1)	5190(2)	59(1)
C(19)	7669(2)	7770(1)	3202(2)	50(1)
C(20)	8436(3)	7223(1)	3305(3)	71(1)
C(21)	7764(5)	6720(1)	2404(5)	107(1)
C(22)	6340(5)	6752(2)	1409(4)	114(2)
C(23)	5577(4)	7287(2)	1280(3)	94(1)
C(24)	6228(3)	7788(1)	2166(2)	66(1)
C(25)	5389(3)	9246(1)	9447(2)	60(1)
Cl(1)	9197(1)	10487(1)	991(1)	91(1)

Table S21. Bond lengths [Å] and angles [°] for **13**.

C(1)-O(1)	1.320(2)
C(1)-C(2)	1.354(3)
C(1)-C(6)	1.477(3)
C(2)-C(3)	1.422(3)
C(3)-N(1)	1.366(2)
C(3)-C(4)	1.392(3)
C(4)-C(12)	1.362(3)
C(5)-N(2)	1.309(3)
C(5)-N(1)	1.329(2)
C(6)-C(7)	1.386(3)
C(6)-C(11)	1.394(3)
C(7)-C(8)	1.369(3)
C(8)-C(9)	1.386(3)
C(9)-C(10)	1.377(3)
C(9)-C(25)	1.442(3)
C(10)-C(11)	1.377(3)
C(12)-N(2)	1.331(3)
C(12)-Cl(1)	1.711(2)
N(1)-B(1)	1.621(3)
N(3)-C(25)	1.127(3)
O(1)-B(1)	1.492(2)
B(1)-C(19)	1.604(3)
B(1)-C(13)	1.608(3)
C(13)-C(18)	1.392(3)
C(13)-C(14)	1.393(3)
C(14)-C(15)	1.381(3)
C(15)-C(16)	1.364(3)
C(16)-C(17)	1.373(3)
C(17)-C(18)	1.376(3)
C(19)-C(20)	1.390(3)
C(19)-C(24)	1.398(3)
C(20)-C(21)	1.394(4)
C(21)-C(22)	1.373(6)
C(22)-C(23)	1.364(5)
C(23)-C(24)	1.378(3)

O(1)-C(1)-C(2)	122.30(17)
O(1)-C(1)-C(6)	113.38(17)
C(2)-C(1)-C(6)	124.31(17)

C(1)-C(2)-C(3)	121.29(17)
N(1)-C(3)-C(4)	118.18(17)
N(1)-C(3)-C(2)	117.73(16)
C(4)-C(3)-C(2)	124.08(17)
C(12)-C(4)-C(3)	117.34(18)
N(2)-C(5)-N(1)	126.47(18)
C(7)-C(6)-C(11)	118.80(18)
C(7)-C(6)-C(1)	118.75(16)
C(11)-C(6)-C(1)	122.45(19)
C(8)-C(7)-C(6)	120.80(18)
C(7)-C(8)-C(9)	119.8(2)
C(10)-C(9)-C(8)	120.35(19)
C(10)-C(9)-C(25)	121.23(18)
C(8)-C(9)-C(25)	118.4(2)
C(9)-C(10)-C(11)	119.69(19)
C(10)-C(11)-C(6)	120.5(2)
N(2)-C(12)-C(4)	124.66(19)
N(2)-C(12)-Cl(1)	115.11(16)
C(4)-C(12)-Cl(1)	120.23(16)
C(5)-N(1)-C(3)	118.43(16)
C(5)-N(1)-B(1)	120.86(15)
C(3)-N(1)-B(1)	120.18(15)
C(5)-N(2)-C(12)	114.84(18)
C(1)-O(1)-B(1)	120.79(15)
O(1)-B(1)-C(19)	108.08(16)
O(1)-B(1)-C(13)	111.36(15)
C(19)-B(1)-C(13)	116.07(16)
O(1)-B(1)-N(1)	104.56(14)
C(19)-B(1)-N(1)	108.93(15)
C(13)-B(1)-N(1)	107.21(15)
C(18)-C(13)-C(14)	115.39(19)
C(18)-C(13)-B(1)	122.89(17)
C(14)-C(13)-B(1)	121.59(17)
C(15)-C(14)-C(13)	122.2(2)
C(16)-C(15)-C(14)	120.4(2)
C(15)-C(16)-C(17)	119.5(2)
C(16)-C(17)-C(18)	119.7(2)
C(17)-C(18)-C(13)	122.9(2)
C(20)-C(19)-C(24)	117.3(2)
C(20)-C(19)-B(1)	123.1(2)

C(24)-C(19)-B(1)	119.58(19)
C(19)-C(20)-C(21)	120.2(3)
C(22)-C(21)-C(20)	121.0(3)
C(23)-C(22)-C(21)	119.6(3)
C(22)-C(23)-C(24)	120.0(3)
C(23)-C(24)-C(19)	121.9(3)
N(3)-C(25)-C(9)	178.0(3)

Symmetry transformations used to generate equivalent atoms:

Table S22. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **13**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	48(1)	45(1)	48(1)	-8(1)	24(1)	3(1)
C(2)	64(1)	42(1)	54(1)	-10(1)	32(1)	0(1)
C(3)	49(1)	39(1)	48(1)	-6(1)	23(1)	-1(1)
C(4)	71(1)	38(1)	59(1)	-5(1)	35(1)	-2(1)
C(5)	72(1)	42(1)	56(1)	-4(1)	40(1)	-1(1)
C(6)	47(1)	51(1)	49(1)	-8(1)	26(1)	4(1)
C(7)	64(1)	45(1)	70(1)	-11(1)	45(1)	-1(1)
C(8)	71(1)	53(1)	71(1)	-5(1)	49(1)	-1(1)
C(9)	55(1)	59(1)	51(1)	-9(1)	31(1)	3(1)
C(10)	83(2)	53(1)	62(1)	-4(1)	45(1)	13(1)
C(11)	83(2)	51(1)	62(1)	1(1)	47(1)	14(1)
C(12)	68(1)	44(1)	54(1)	1(1)	32(1)	-4(1)
N(1)	53(1)	38(1)	48(1)	-4(1)	29(1)	-2(1)
N(2)	74(1)	45(1)	57(1)	-1(1)	40(1)	-1(1)
N(3)	111(2)	69(1)	83(1)	-2(1)	70(1)	10(1)
O(1)	60(1)	43(1)	58(1)	-9(1)	39(1)	-3(1)
B(1)	57(1)	37(1)	49(1)	-5(1)	34(1)	0(1)
C(13)	57(1)	39(1)	50(1)	-7(1)	32(1)	-2(1)
C(14)	62(1)	50(1)	53(1)	-2(1)	35(1)	0(1)
C(15)	73(1)	61(1)	50(1)	1(1)	31(1)	4(1)
C(16)	61(1)	73(2)	59(1)	-2(1)	24(1)	2(1)
C(17)	57(1)	89(2)	68(1)	-3(1)	36(1)	1(1)
C(18)	60(1)	72(1)	55(1)	-2(1)	36(1)	1(1)
C(19)	71(1)	42(1)	52(1)	-7(1)	42(1)	-11(1)

C(20)	100(2)	45(1)	96(2)	-15(1)	70(2)	-7(1)
C(21)	167(3)	55(2)	166(3)	-44(2)	135(3)	-33(2)
C(22)	179(4)	103(3)	114(3)	-69(2)	113(3)	-89(3)
C(23)	129(3)	102(2)	57(1)	-24(1)	50(2)	-65(2)
C(24)	81(2)	65(1)	55(1)	-4(1)	34(1)	-23(1)
C(25)	76(1)	55(1)	60(1)	-7(1)	42(1)	4(1)
Cl(1)	160(1)	51(1)	94(1)	5(1)	86(1)	-13(1)

Table S23. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **13**.

	x	y	z	U(eq)
H(2)	7880	10018	5160	61
H(4)	8376	10461	3161	65
H(5)	8697	8470	1892	63
H(7)	6886	8252	6691	65
H(8)	6144	8297	8425	71
H(10)	5710	10160	7951	73
H(11)	6531	10118	6265	72
H(14)	9520	8151	7086	62
H(15)	11823	7987	8841	72
H(16)	13732	7993	8320	79
H(17)	13325	8179	6015	82
H(18)	11031	8354	4267	71
H(20)	9399	7193	3978	85
H(21)	8288	6357	2477	128
H(22)	5899	6410	826	137
H(23)	4619	7315	595	112
H(24)	5692	8149	2071	79

Table S24. Torsion angles [°] for **13**.

O(1)-C(1)-C(2)-C(3)	4.7(3)
C(6)-C(1)-C(2)-C(3)	-174.09(19)

C(1)-C(2)-C(3)-N(1)	-10.3(3)
C(1)-C(2)-C(3)-C(4)	168.5(2)
N(1)-C(3)-C(4)-C(12)	-0.4(3)
C(2)-C(3)-C(4)-C(12)	-179.2(2)
O(1)-C(1)-C(6)-C(7)	14.6(3)
C(2)-C(1)-C(6)-C(7)	-166.5(2)
O(1)-C(1)-C(6)-C(11)	-166.26(19)
C(2)-C(1)-C(6)-C(11)	12.7(3)
C(11)-C(6)-C(7)-C(8)	-1.8(3)
C(1)-C(6)-C(7)-C(8)	177.4(2)
C(6)-C(7)-C(8)-C(9)	1.5(3)
C(7)-C(8)-C(9)-C(10)	0.0(4)
C(7)-C(8)-C(9)-C(25)	-179.8(2)
C(8)-C(9)-C(10)-C(11)	-1.2(4)
C(25)-C(9)-C(10)-C(11)	178.7(2)
C(9)-C(10)-C(11)-C(6)	0.8(4)
C(7)-C(6)-C(11)-C(10)	0.7(3)
C(1)-C(6)-C(11)-C(10)	-178.5(2)
C(3)-C(4)-C(12)-N(2)	2.5(3)
C(3)-C(4)-C(12)-Cl(1)	-177.34(16)
N(2)-C(5)-N(1)-C(3)	2.9(3)
N(2)-C(5)-N(1)-B(1)	-168.7(2)
C(4)-C(3)-N(1)-C(5)	-2.0(3)
C(2)-C(3)-N(1)-C(5)	176.87(18)
C(4)-C(3)-N(1)-B(1)	169.68(18)
C(2)-C(3)-N(1)-B(1)	-11.4(3)
N(1)-C(5)-N(2)-C(12)	-1.0(3)
C(4)-C(12)-N(2)-C(5)	-1.8(3)
Cl(1)-C(12)-N(2)-C(5)	178.02(17)
C(2)-C(1)-O(1)-B(1)	24.8(3)
C(6)-C(1)-O(1)-B(1)	-156.24(17)
C(1)-O(1)-B(1)-C(19)	-156.29(16)
C(1)-O(1)-B(1)-C(13)	75.1(2)
C(1)-O(1)-B(1)-N(1)	-40.4(2)
C(5)-N(1)-B(1)-O(1)	-154.64(17)
C(3)-N(1)-B(1)-O(1)	33.9(2)
C(5)-N(1)-B(1)-C(19)	-39.3(2)
C(3)-N(1)-B(1)-C(19)	149.20(17)
C(5)-N(1)-B(1)-C(13)	87.0(2)
C(3)-N(1)-B(1)-C(13)	-84.46(19)

O(1)-B(1)-C(13)-C(18)	-161.59(18)
C(19)-B(1)-C(13)-C(18)	74.2(2)
N(1)-B(1)-C(13)-C(18)	-47.8(2)
O(1)-B(1)-C(13)-C(14)	22.8(2)
C(19)-B(1)-C(13)-C(14)	-101.4(2)
N(1)-B(1)-C(13)-C(14)	136.65(17)
C(18)-C(13)-C(14)-C(15)	0.9(3)
B(1)-C(13)-C(14)-C(15)	176.79(19)
C(13)-C(14)-C(15)-C(16)	-0.8(3)
C(14)-C(15)-C(16)-C(17)	0.3(4)
C(15)-C(16)-C(17)-C(18)	0.1(4)
C(16)-C(17)-C(18)-C(13)	0.0(4)
C(14)-C(13)-C(18)-C(17)	-0.5(3)
B(1)-C(13)-C(18)-C(17)	-176.3(2)
O(1)-B(1)-C(19)-C(20)	-129.8(2)
C(13)-B(1)-C(19)-C(20)	-3.9(3)
N(1)-B(1)-C(19)-C(20)	117.2(2)
O(1)-B(1)-C(19)-C(24)	49.6(2)
C(13)-B(1)-C(19)-C(24)	175.50(17)
N(1)-B(1)-C(19)-C(24)	-63.4(2)
C(24)-C(19)-C(20)-C(21)	-0.4(3)
B(1)-C(19)-C(20)-C(21)	179.0(2)
C(19)-C(20)-C(21)-C(22)	-0.4(4)
C(20)-C(21)-C(22)-C(23)	1.3(5)
C(21)-C(22)-C(23)-C(24)	-1.3(4)
C(22)-C(23)-C(24)-C(19)	0.5(4)
C(20)-C(19)-C(24)-C(23)	0.3(3)
B(1)-C(19)-C(24)-C(23)	-179.07(19)
C(10)-C(9)-C(25)-N(3)	-150(8)
C(8)-C(9)-C(25)-N(3)	30(9)

Symmetry transformations used to generate equivalent atoms:

Table S25. Crystal data and structure refinement for **14**.

Identification code	14
Empirical formula	C25 H20 B Cl N2 O2
Formula weight	426.69
Temperature	293(2) K

Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 10.102(2) Å	α= 90°.
	b = 20.037(4) Å	β= 92.7166(10)°.
	c = 10.665(2) Å	γ = 90°.
Volume	2156.3(7) $Å^3$	
Z	4	
Density (calculated)	1.314 Mg/m^3	
Absorption coefficient	0.202 mm^{-1}	
F(000)	888	
Crystal size	0.20 x 0.20 x 0.20 mm^3	
Theta range for data collection	2.79 to 27.66°.	
Index ranges	-13<=h<=13, -26<=k<=26, -13<=l<=13	
Reflections collected	21280	
Independent reflections	4931 [R(int) = 0.0728]	
Completeness to theta = 27.66°	98.2 %	
Absorption correction	Integration	
Max. and min. transmission	0.9607 and 0.9607	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4931 / 0 / 281	
Goodness-of-fit on F^2	1.024	
Final R indices [I>2sigma(I)]	R1 = 0.0572, wR2 = 0.1527	
R indices (all data)	R1 = 0.0701, wR2 = 0.1682	
Largest diff. peak and hole	0.527 and -0.274 $e.Å^{-3}$	

Table S26. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **14**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	487(2)	10703(1)	7218(2)	41(1)
C(2)	811(2)	10193(1)	6443(2)	47(1)
C(3)	1844(2)	10256(1)	5595(2)	42(1)
C(4)	2366(2)	9709(1)	4959(2)	49(1)
C(5)	3392(2)	10916(1)	4615(2)	48(1)
C(6)	-477(2)	10648(1)	8210(2)	46(1)
C(7)	-885(2)	11219(1)	8835(2)	57(1)

C(8)	-1828(3)	11187(1)	9732(2)	67(1)
C(9)	-2368(2)	10583(1)	10051(2)	63(1)
C(10)	-1958(2)	10009(1)	9473(2)	65(1)
C(11)	-1021(2)	10042(1)	8546(2)	57(1)
C(12)	3356(2)	9826(1)	4170(2)	49(1)
C(13)	466(2)	11706(1)	4899(2)	43(1)
C(14)	-807(2)	11869(1)	5259(2)	49(1)
C(15)	-1817(2)	12023(1)	4382(3)	63(1)
C(16)	-1573(3)	12020(1)	3123(3)	70(1)
C(17)	-326(3)	11874(1)	2733(2)	69(1)
C(18)	670(2)	11718(1)	3613(2)	57(1)
C(19)	2700(2)	12098(1)	6266(2)	44(1)
C(20)	2805(3)	12682(1)	5587(3)	66(1)
C(21)	3770(3)	13158(1)	5911(3)	83(1)
C(22)	4625(3)	13064(1)	6919(3)	77(1)
C(23)	4533(3)	12492(1)	7621(3)	72(1)
C(24)	3581(2)	12017(1)	7289(2)	57(1)
C(25)	-3809(3)	10015(2)	11416(3)	82(1)
N(1)	2381(1)	10870(1)	5388(1)	40(1)
N(2)	3911(2)	10424(1)	3976(2)	53(1)
O(1)	1053(1)	11296(1)	7128(1)	44(1)
O(2)	-3293(2)	10612(1)	10955(2)	88(1)
Cl(1)	3987(1)	9164(1)	3344(1)	67(1)
B(1)	1630(2)	11519(1)	5934(2)	40(1)

Table S27. Bond lengths [Å] and angles [°] for **14**.

C(1)-O(1)	1.325(2)
C(1)-C(2)	1.364(3)
C(1)-C(6)	1.476(3)
C(2)-C(3)	1.419(3)
C(3)-N(1)	1.366(2)
C(3)-C(4)	1.405(3)
C(4)-C(12)	1.358(3)
C(5)-N(2)	1.320(2)
C(5)-N(1)	1.346(2)
C(6)-C(11)	1.386(3)
C(6)-C(7)	1.396(3)

C(7)-C(8)	1.383(3)
C(8)-C(9)	1.376(4)
C(9)-O(2)	1.375(3)
C(9)-C(10)	1.378(4)
C(10)-C(11)	1.402(3)
C(12)-N(2)	1.344(3)
C(12)-Cl(1)	1.7293(19)
C(13)-C(18)	1.397(3)
C(13)-C(14)	1.398(3)
C(13)-B(1)	1.618(3)
C(14)-C(15)	1.386(3)
C(15)-C(16)	1.376(4)
C(16)-C(17)	1.377(4)
C(17)-C(18)	1.378(3)
C(19)-C(20)	1.384(3)
C(19)-C(24)	1.385(3)
C(19)-B(1)	1.613(3)
C(20)-C(21)	1.395(3)
C(21)-C(22)	1.360(4)
C(22)-C(23)	1.374(4)
C(23)-C(24)	1.386(3)
C(25)-O(2)	1.402(3)
N(1)-B(1)	1.627(2)
O(1)-B(1)	1.494(2)

O(1)-C(1)-C(2)	120.82(16)
O(1)-C(1)-C(6)	114.84(16)
C(2)-C(1)-C(6)	124.34(16)
C(1)-C(2)-C(3)	121.57(16)
N(1)-C(3)-C(4)	117.61(17)
N(1)-C(3)-C(2)	119.60(16)
C(4)-C(3)-C(2)	122.79(17)
C(12)-C(4)-C(3)	117.98(17)
N(2)-C(5)-N(1)	126.63(18)
C(11)-C(6)-C(7)	117.64(18)
C(11)-C(6)-C(1)	122.27(18)
C(7)-C(6)-C(1)	120.09(17)
C(8)-C(7)-C(6)	121.4(2)
C(9)-C(8)-C(7)	120.4(2)
O(2)-C(9)-C(8)	115.3(2)

O(2)-C(9)-C(10)	125.3(2)
C(8)-C(9)-C(10)	119.4(2)
C(9)-C(10)-C(11)	120.3(2)
C(6)-C(11)-C(10)	120.8(2)
N(2)-C(12)-C(4)	125.02(17)
N(2)-C(12)-Cl(1)	116.04(15)
C(4)-C(12)-Cl(1)	118.93(15)
C(18)-C(13)-C(14)	116.49(18)
C(18)-C(13)-B(1)	122.54(17)
C(14)-C(13)-B(1)	120.97(17)
C(15)-C(14)-C(13)	121.6(2)
C(16)-C(15)-C(14)	119.8(2)
C(15)-C(16)-C(17)	120.3(2)
C(16)-C(17)-C(18)	119.4(2)
C(17)-C(18)-C(13)	122.4(2)
C(20)-C(19)-C(24)	116.64(19)
C(20)-C(19)-B(1)	124.07(18)
C(24)-C(19)-B(1)	119.29(17)
C(19)-C(20)-C(21)	121.2(2)
C(22)-C(21)-C(20)	120.8(3)
C(21)-C(22)-C(23)	119.3(2)
C(22)-C(23)-C(24)	119.8(3)
C(19)-C(24)-C(23)	122.2(2)
C(5)-N(1)-C(3)	118.62(15)
C(5)-N(1)-B(1)	123.01(14)
C(3)-N(1)-B(1)	117.79(14)
C(5)-N(2)-C(12)	114.06(17)
C(1)-O(1)-B(1)	121.09(14)
C(9)-O(2)-C(25)	119.1(2)
O(1)-B(1)-C(19)	108.14(15)
O(1)-B(1)-C(13)	110.54(15)
C(19)-B(1)-C(13)	116.16(15)
O(1)-B(1)-N(1)	105.87(13)
C(19)-B(1)-N(1)	109.52(14)
C(13)-B(1)-N(1)	106.12(14)

Symmetry transformations used to generate equivalent atoms:

Table S28. Anisotropic displacement parameters ($Å^2$x 10^3) for **14**. The anisotropic

displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	38(1)	43(1)	43(1)	5(1)	-1(1)	-4(1)
C(2)	44(1)	41(1)	57(1)	1(1)	5(1)	-7(1)
C(3)	37(1)	38(1)	49(1)	-2(1)	-1(1)	-1(1)
C(4)	46(1)	41(1)	61(1)	-7(1)	3(1)	-2(1)
C(5)	45(1)	45(1)	56(1)	0(1)	7(1)	-1(1)
C(6)	42(1)	54(1)	42(1)	6(1)	2(1)	-5(1)
C(7)	63(1)	58(1)	51(1)	-1(1)	14(1)	-7(1)
C(8)	77(2)	67(1)	59(1)	-7(1)	24(1)	-5(1)
C(9)	66(1)	73(1)	51(1)	4(1)	17(1)	-5(1)
C(10)	61(1)	63(1)	72(1)	19(1)	12(1)	-13(1)
C(11)	58(1)	55(1)	58(1)	7(1)	10(1)	-5(1)
C(12)	42(1)	49(1)	54(1)	-9(1)	-3(1)	7(1)
C(13)	43(1)	34(1)	52(1)	0(1)	1(1)	-2(1)
C(14)	46(1)	41(1)	62(1)	-1(1)	2(1)	-2(1)
C(15)	44(1)	51(1)	94(2)	10(1)	-6(1)	3(1)
C(16)	64(1)	65(1)	79(2)	14(1)	-22(1)	1(1)
C(17)	76(2)	73(2)	56(1)	9(1)	-9(1)	5(1)
C(18)	56(1)	61(1)	54(1)	4(1)	1(1)	7(1)
C(19)	41(1)	39(1)	53(1)	-7(1)	8(1)	-2(1)
C(20)	69(1)	50(1)	79(2)	8(1)	-2(1)	-13(1)
C(21)	85(2)	48(1)	116(2)	8(1)	6(2)	-23(1)
C(22)	62(1)	62(1)	106(2)	-21(1)	5(1)	-22(1)
C(23)	59(1)	75(2)	82(2)	-15(1)	-9(1)	-14(1)
C(24)	54(1)	53(1)	64(1)	-4(1)	-4(1)	-9(1)
C(25)	75(2)	103(2)	69(2)	13(1)	26(1)	-12(2)
N(1)	37(1)	37(1)	45(1)	0(1)	1(1)	-1(1)
N(2)	46(1)	53(1)	59(1)	-6(1)	10(1)	2(1)
O(1)	46(1)	42(1)	46(1)	-2(1)	7(1)	-6(1)
O(2)	97(1)	81(1)	90(1)	1(1)	49(1)	-4(1)
Cl(1)	64(1)	60(1)	77(1)	-21(1)	12(1)	9(1)
B(1)	38(1)	37(1)	45(1)	1(1)	4(1)	-2(1)

Table S29. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **14**.

	x	y	z	U(eq)
H(2)	344	9793	6472	57
H(4)	2044	9280	5076	59
H(5)	3763	11337	4521	58
H(7)	-515	11629	8645	69
H(8)	-2099	11575	10122	80
H(10)	-2304	9599	9697	78
H(11)	-761	9653	8152	68
H(14)	-980	11874	6108	59
H(15)	-2657	12128	4644	76
H(16)	-2254	12117	2534	84
H(17)	-158	11879	1883	82
H(18)	1507	11618	3340	68
H(20)	2221	12760	4902	79
H(21)	3830	13544	5432	100
H(22)	5265	13384	7132	92
H(23)	5108	12424	8316	87
H(24)	3534	11632	7770	69
H(25)	-4410	9823	10792	123
H(25A)	-4272	10106	12163	123
H(25B)	-3097	9709	11607	123

Table S30. Torsion angles [°] for **14**.

O(1)-C(1)-C(2)-C(3)	5.8(3)
C(6)-C(1)-C(2)-C(3)	-173.36(17)
C(1)-C(2)-C(3)-N(1)	-11.2(3)
C(1)-C(2)-C(3)-C(4)	167.81(18)
N(1)-C(3)-C(4)-C(12)	-0.9(3)
C(2)-C(3)-C(4)-C(12)	-179.89(18)
O(1)-C(1)-C(6)-C(11)	-170.94(17)
C(2)-C(1)-C(6)-C(11)	8.2(3)
O(1)-C(1)-C(6)-C(7)	9.9(3)
C(2)-C(1)-C(6)-C(7)	-170.89(19)
C(11)-C(6)-C(7)-C(8)	-1.9(3)

C(1)-C(6)-C(7)-C(8)	177.2(2)
C(6)-C(7)-C(8)-C(9)	1.5(4)
C(7)-C(8)-C(9)-O(2)	179.8(2)
C(7)-C(8)-C(9)-C(10)	0.2(4)
O(2)-C(9)-C(10)-C(11)	179.0(2)
C(8)-C(9)-C(10)-C(11)	-1.5(4)
C(7)-C(6)-C(11)-C(10)	0.7(3)
C(1)-C(6)-C(11)-C(10)	-178.47(19)
C(9)-C(10)-C(11)-C(6)	1.0(4)
C(3)-C(4)-C(12)-N(2)	2.3(3)
C(3)-C(4)-C(12)-Cl(1)	-178.32(14)
C(18)-C(13)-C(14)-C(15)	1.0(3)
B(1)-C(13)-C(14)-C(15)	-179.25(17)
C(13)-C(14)-C(15)-C(16)	-0.2(3)
C(14)-C(15)-C(16)-C(17)	-0.9(4)
C(15)-C(16)-C(17)-C(18)	1.2(4)
C(16)-C(17)-C(18)-C(13)	-0.3(4)
C(14)-C(13)-C(18)-C(17)	-0.7(3)
B(1)-C(13)-C(18)-C(17)	179.5(2)
C(24)-C(19)-C(20)-C(21)	1.2(4)
B(1)-C(19)-C(20)-C(21)	-178.8(2)
C(19)-C(20)-C(21)-C(22)	-1.0(5)
C(20)-C(21)-C(22)-C(23)	0.2(5)
C(21)-C(22)-C(23)-C(24)	0.5(4)
C(20)-C(19)-C(24)-C(23)	-0.5(3)
B(1)-C(19)-C(24)-C(23)	179.4(2)
C(22)-C(23)-C(24)-C(19)	-0.3(4)
N(2)-C(5)-N(1)-C(3)	2.7(3)
N(2)-C(5)-N(1)-B(1)	-168.34(18)
C(4)-C(3)-N(1)-C(5)	-1.4(3)
C(2)-C(3)-N(1)-C(5)	177.64(17)
C(4)-C(3)-N(1)-B(1)	170.13(16)
C(2)-C(3)-N(1)-B(1)	-10.8(2)
N(1)-C(5)-N(2)-C(12)	-1.4(3)
C(4)-C(12)-N(2)-C(5)	-1.2(3)
Cl(1)-C(12)-N(2)-C(5)	179.40(14)
C(2)-C(1)-O(1)-B(1)	24.0(2)
C(6)-C(1)-O(1)-B(1)	-156.79(15)
C(8)-C(9)-O(2)-C(25)	-174.5(2)
C(10)-C(9)-O(2)-C(25)	5.1(4)

C(1)-O(1)-B(1)-C(19)	-158.17(15)
C(1)-O(1)-B(1)-C(13)	73.64(19)
C(1)-O(1)-B(1)-N(1)	-40.9(2)
C(20)-C(19)-B(1)-O(1)	-136.1(2)
C(24)-C(19)-B(1)-O(1)	44.0(2)
C(20)-C(19)-B(1)-C(13)	-11.2(3)
C(24)-C(19)-B(1)-C(13)	168.87(18)
C(20)-C(19)-B(1)-N(1)	109.0(2)
C(24)-C(19)-B(1)-N(1)	-71.0(2)
C(18)-C(13)-B(1)-O(1)	-158.65(17)
C(14)-C(13)-B(1)-O(1)	21.6(2)
C(18)-C(13)-B(1)-C(19)	77.7(2)
C(14)-C(13)-B(1)-C(19)	-102.04(19)
C(18)-C(13)-B(1)-N(1)	-44.3(2)
C(14)-C(13)-B(1)-N(1)	135.99(16)
C(5)-N(1)-B(1)-O(1)	-155.15(16)
C(3)-N(1)-B(1)-O(1)	33.7(2)
C(5)-N(1)-B(1)-C(19)	-38.8(2)
C(3)-N(1)-B(1)-C(19)	150.08(15)
C(5)-N(1)-B(1)-C(13)	87.34(19)
C(3)-N(1)-B(1)-C(13)	-83.81(18)

Symmetry transformations used to generate equivalent atoms:

Table S31. Crystal data and structure refinement for **15**.

Identification code	15	
Empirical formula	C26 H23 B Cl N3 O	
Formula weight	439.73	
Temperature	293(2) K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	P21/n	
Unit cell dimensions	a = 8.885(8) Å	α= 90°.
	b = 12.288(11) Å	β= 97.033(12)°.
	c = 20.917(19) Å	γ = 90°.
Volume	2267(4) $Å^3$	
Z	4	
Density (calculated)	1.289 Mg/m^3	

Absorption coefficient	0.192 mm^{-1}
F(000)	920
Crystal size	0.20 x 0.20 x 0.20 mm^3
Theta range for data collection	2.62 to 27.48°.
Index ranges	-11<=h<=11, -15<=k<=15, -27<=l<=26
Reflections collected	21423
Independent reflections	5132 [R(int) = 0.0409]
Completeness to theta = 27.48°	98.8 %
Absorption correction	Integration
Max. and min. transmission	0.9626 and 0.9626
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5132 / 0 / 291
Goodness-of-fit on F^2	1.074
Final R indices [I>2sigma(I)]	R1 = 0.0534, wR2 = 0.1247
R indices (all data)	R1 = 0.0752, wR2 = 0.1370
Largest diff. peak and hole	0.153 and -0.187 e.$Å^{-3}$

Table S32. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **15**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	9588(2)	11730(1)	10831(1)	47(1)
C(2)	9054(2)	11114(2)	10307(1)	49(1)
C(3)	8035(2)	10251(1)	10349(1)	45(1)
C(4)	7238(2)	9742(2)	9809(1)	49(1)
C(5)	6759(2)	9088(2)	10982(1)	57(1)
C(6)	10534(2)	12694(1)	10790(1)	48(1)
C(7)	11356(2)	13141(2)	11338(1)	55(1)
C(8)	12299(2)	14018(2)	11307(1)	59(1)
C(9)	12445(2)	14533(2)	10721(1)	54(1)
C(10)	11618(3)	14086(2)	10168(1)	65(1)
C(11)	10703(2)	13196(2)	10205(1)	60(1)
C(12)	6267(2)	8924(2)	9914(1)	51(1)
C(19)	8021(2)	10279(2)	12194(1)	52(1)
C(24)	7219(3)	11162(2)	12372(1)	70(1)
C(23)	6405(3)	11125(2)	12904(1)	88(1)
C(22)	6354(3)	10192(2)	13253(1)	80(1)

C(21)	7130(3)	9304(2)	13091(1)	79(1)
C(20)	7963(3)	9352(2)	12568(1)	69(1)
C(13)	10444(2)	9608(2)	11619(1)	48(1)
C(14)	11811(2)	10063(2)	11894(1)	60(1)
C(15)	13155(2)	9472(2)	11974(1)	70(1)
C(16)	13168(2)	8411(2)	11789(1)	71(1)
C(17)	11844(2)	7935(2)	11514(1)	67(1)
C(18)	10510(2)	8526(2)	11430(1)	54(1)
C(25)	13416(3)	16003(2)	10084(1)	84(1)
C(26)	14415(3)	15747(2)	11229(1)	85(1)
N(1)	7795(2)	9875(1)	10947(1)	46(1)
N(2)	5979(2)	8582(1)	10497(1)	58(1)
N(3)	13343(2)	15433(2)	10685(1)	72(1)
O(1)	9254(2)	11476(1)	11414(1)	53(1)
Cl(1)	5276(1)	8267(1)	9266(1)	69(1)
B(1)	8901(2)	10317(2)	11561(1)	49(1)

Table S33. Bond lengths [Å] and angles [°] for **15**.

C(1)-O(1)	1.328(2)
C(1)-C(2)	1.368(3)
C(1)-C(6)	1.461(3)
C(2)-C(3)	1.404(3)
C(2)-H(2)	0.9300
C(3)-N(1)	1.373(2)
C(3)-C(4)	1.404(3)
C(4)-C(12)	1.359(3)
C(4)-H(4)	0.9300
C(5)-N(2)	1.312(3)
C(5)-N(1)	1.344(2)
C(5)-H(5)	0.9300
C(6)-C(7)	1.394(3)
C(6)-C(11)	1.396(3)
C(7)-C(8)	1.372(3)
C(7)-H(7)	0.9300
C(8)-C(9)	1.399(3)
C(8)-H(8)	0.9300
C(9)-N(3)	1.372(3)

C(9)-C(10)	1.404(3)
C(10)-C(11)	1.370(3)
C(10)-H(10)	0.9300
C(11)-H(11)	0.9300
C(12)-N(2)	1.344(3)
C(12)-Cl(1)	1.724(2)
C(19)-C(24)	1.375(3)
C(19)-C(20)	1.387(3)
C(19)-B(1)	1.619(3)
C(24)-C(23)	1.400(3)
C(24)-H(24)	0.9300
C(23)-C(22)	1.363(4)
C(23)-H(23)	0.9300
C(22)-C(21)	1.356(4)
C(22)-H(22)	0.9300
C(21)-C(20)	1.394(3)
C(21)-H(21)	0.9300
C(20)-H(20)	0.9300
C(13)-C(18)	1.390(3)
C(13)-C(14)	1.395(3)
C(13)-B(1)	1.616(3)
C(14)-C(15)	1.389(3)
C(14)-H(14)	0.9300
C(15)-C(16)	1.360(4)
C(15)-H(15)	0.9300
C(16)-C(17)	1.375(3)
C(16)-H(16)	0.9300
C(17)-C(18)	1.383(3)
C(17)-H(17)	0.9300
C(18)-H(18)	0.9300
C(25)-N(3)	1.447(3)
C(25)-H(25)	0.9600
C(25)-H(25A)	0.9600
C(25)-H(25B)	0.9600
C(26)-N(3)	1.445(3)
C(26)-H(26)	0.9600
C(26)-H(26A)	0.9600
C(26)-H(26B)	0.9600
N(1)-B(1)	1.613(3)
O(1)-B(1)	1.498(3)

O(1)-C(1)-C(2)	120.75(17)
O(1)-C(1)-C(6)	115.99(16)
C(2)-C(1)-C(6)	123.26(16)
C(1)-C(2)-C(3)	122.06(16)
C(1)-C(2)-H(2)	119.0
C(3)-C(2)-H(2)	119.0
N(1)-C(3)-C(2)	118.97(16)
N(1)-C(3)-C(4)	117.59(17)
C(2)-C(3)-C(4)	123.44(16)
C(12)-C(4)-C(3)	117.84(17)
C(12)-C(4)-H(4)	121.1
C(3)-C(4)-H(4)	121.1
N(2)-C(5)-N(1)	126.74(18)
N(2)-C(5)-H(5)	116.6
N(1)-C(5)-H(5)	116.6
C(7)-C(6)-C(11)	116.41(18)
C(7)-C(6)-C(1)	121.29(17)
C(11)-C(6)-C(1)	122.26(18)
C(8)-C(7)-C(6)	122.14(18)
C(8)-C(7)-H(7)	118.9
C(6)-C(7)-H(7)	118.9
C(7)-C(8)-C(9)	121.31(19)
C(7)-C(8)-H(8)	119.3
C(9)-C(8)-H(8)	119.3
N(3)-C(9)-C(8)	121.95(19)
N(3)-C(9)-C(10)	121.34(19)
C(8)-C(9)-C(10)	116.72(19)
C(11)-C(10)-C(9)	121.31(19)
C(11)-C(10)-H(10)	119.3
C(9)-C(10)-H(10)	119.3
C(10)-C(11)-C(6)	122.1(2)
C(10)-C(11)-H(11)	119.0
C(6)-C(11)-H(11)	119.0
N(2)-C(12)-C(4)	124.90(17)
N(2)-C(12)-Cl(1)	115.55(15)
C(4)-C(12)-Cl(1)	119.54(15)
C(24)-C(19)-C(20)	115.98(19)
C(24)-C(19)-B(1)	121.22(18)
C(20)-C(19)-B(1)	122.73(18)

C(19)-C(24)-C(23)	121.8(2)
C(19)-C(24)-H(24)	119.1
C(23)-C(24)-H(24)	119.1
C(22)-C(23)-C(24)	120.4(2)
C(22)-C(23)-H(23)	119.8
C(24)-C(23)-H(23)	119.8
C(21)-C(22)-C(23)	119.5(2)
C(21)-C(22)-H(22)	120.2
C(23)-C(22)-H(22)	120.2
C(22)-C(21)-C(20)	119.8(2)
C(22)-C(21)-H(21)	120.1
C(20)-C(21)-H(21)	120.1
C(19)-C(20)-C(21)	122.5(2)
C(19)-C(20)-H(20)	118.7
C(21)-C(20)-H(20)	118.7
C(18)-C(13)-C(14)	115.78(18)
C(18)-C(13)-B(1)	123.97(17)
C(14)-C(13)-B(1)	120.21(18)
C(15)-C(14)-C(13)	122.2(2)
C(15)-C(14)-H(14)	118.9
C(13)-C(14)-H(14)	118.9
C(16)-C(15)-C(14)	120.2(2)
C(16)-C(15)-H(15)	119.9
C(14)-C(15)-H(15)	119.9
C(15)-C(16)-C(17)	119.3(2)
C(15)-C(16)-H(16)	120.3
C(17)-C(16)-H(16)	120.3
C(16)-C(17)-C(18)	120.4(2)
C(16)-C(17)-H(17)	119.8
C(18)-C(17)-H(17)	119.8
C(17)-C(18)-C(13)	122.1(2)
C(17)-C(18)-H(18)	119.0
C(13)-C(18)-H(18)	119.0
N(3)-C(25)-H(25)	109.5
N(3)-C(25)-H(25A)	109.5
H(25)-C(25)-H(25A)	109.5
N(3)-C(25)-H(25B)	109.5
H(25)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
N(3)-C(26)-H(26)	109.5

N(3)-C(26)-H(26A)	109.5
H(26)-C(26)-H(26A)	109.5
N(3)-C(26)-H(26B)	109.5
H(26)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(5)-N(1)-C(3)	118.41(16)
C(5)-N(1)-B(1)	123.58(15)
C(3)-N(1)-B(1)	117.67(15)
C(5)-N(2)-C(12)	114.38(17)
C(9)-N(3)-C(26)	120.3(2)
C(9)-N(3)-C(25)	121.7(2)
C(26)-N(3)-C(25)	117.4(2)
C(1)-O(1)-B(1)	119.15(14)
O(1)-B(1)-N(1)	106.22(15)
O(1)-B(1)-C(13)	109.32(16)
N(1)-B(1)-C(13)	107.90(15)
O(1)-B(1)-C(19)	109.19(14)
N(1)-B(1)-C(19)	109.47(16)
C(13)-B(1)-C(19)	114.41(16)

Symmetry transformations used to generate equivalent atoms:

Table S34. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **15**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	51(1)	46(1)	44(1)	2(1)	15(1)	6(1)
C(2)	55(1)	52(1)	43(1)	2(1)	16(1)	-1(1)
C(3)	45(1)	48(1)	44(1)	1(1)	14(1)	6(1)
C(4)	51(1)	54(1)	44(1)	-1(1)	12(1)	2(1)
C(5)	58(1)	61(1)	54(1)	5(1)	18(1)	-4(1)
C(6)	52(1)	43(1)	50(1)	2(1)	15(1)	4(1)
C(7)	69(1)	53(1)	46(1)	-1(1)	18(1)	-2(1)
C(8)	64(1)	58(1)	54(1)	-9(1)	12(1)	-3(1)
C(9)	53(1)	48(1)	63(1)	0(1)	12(1)	2(1)
C(10)	78(1)	60(1)	56(1)	14(1)	7(1)	-12(1)
C(11)	70(1)	58(1)	50(1)	6(1)	4(1)	-9(1)
C(12)	43(1)	54(1)	56(1)	-6(1)	7(1)	6(1)

C(19)	56(1)	58(1)	45(1)	-6(1)	17(1)	-9(1)
C(24)	82(2)	66(1)	69(1)	-12(1)	34(1)	-5(1)
C(23)	90(2)	89(2)	93(2)	-34(2)	47(2)	-9(1)
C(22)	76(2)	115(2)	53(1)	-25(1)	31(1)	-34(1)
C(21)	91(2)	97(2)	54(1)	4(1)	29(1)	-20(1)
C(20)	84(2)	71(1)	57(1)	5(1)	29(1)	-4(1)
C(13)	54(1)	55(1)	35(1)	5(1)	14(1)	-3(1)
C(14)	67(1)	64(1)	48(1)	-1(1)	6(1)	-8(1)
C(15)	56(1)	94(2)	59(1)	3(1)	1(1)	-11(1)
C(16)	57(1)	82(2)	73(2)	9(1)	10(1)	8(1)
C(17)	66(1)	62(1)	76(1)	2(1)	17(1)	6(1)
C(18)	54(1)	55(1)	54(1)	2(1)	12(1)	-4(1)
C(25)	79(2)	70(2)	105(2)	24(1)	19(1)	-12(1)
C(26)	67(1)	74(2)	113(2)	-11(1)	1(1)	-12(1)
N(1)	48(1)	49(1)	45(1)	0(1)	14(1)	0(1)
N(2)	55(1)	65(1)	56(1)	0(1)	12(1)	-9(1)
N(3)	70(1)	61(1)	83(1)	5(1)	11(1)	-17(1)
O(1)	69(1)	48(1)	44(1)	-2(1)	21(1)	-4(1)
Cl(1)	65(1)	76(1)	64(1)	-13(1)	3(1)	-9(1)
B(1)	60(1)	48(1)	41(1)	1(1)	16(1)	-4(1)

Table S35. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **15**.

	x	y	z	U(eq)
H(2)	9375	11271	9911	59
H(4)	7371	9957	9394	59
H(5)	6575	8879	11393	68
H(7)	11261	12835	11738	66
H(8)	12853	14276	11682	70
H(10)	11693	14399	9768	78
H(11)	10178	12918	9828	71
H(24)	7217	11800	12134	85
H(23)	5896	11742	13021	105
H(22)	5791	10164	13599	95
H(21)	7107	8664	13327	95

H(20)	8500	8739	12467	83
H(14)	11824	10785	12027	71
H(15)	14047	9803	12155	84
H(16)	14064	8012	11848	85
H(17)	11846	7211	11385	81
H(18)	9629	8189	11241	65
H(25)	12407	16149	9882	126
H(25A)	13939	15561	9804	126
H(25B)	13951	16677	10167	126
H(26)	15109	15159	11341	128
H(26A)	13881	15912	11589	128
H(26B)	14968	16377	11119	128

Table S36. Torsion angles [°] for **15**.

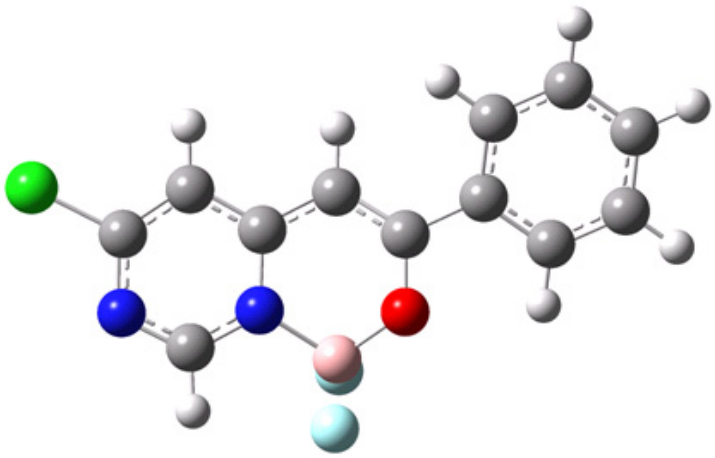
O(1)-C(1)-C(2)-C(3)	5.5(3)
C(6)-C(1)-C(2)-C(3)	-174.02(16)
C(1)-C(2)-C(3)-N(1)	-13.0(3)
C(1)-C(2)-C(3)-C(4)	167.14(17)
N(1)-C(3)-C(4)-C(12)	1.0(2)
C(2)-C(3)-C(4)-C(12)	-179.11(16)
O(1)-C(1)-C(6)-C(7)	16.4(2)
C(2)-C(1)-C(6)-C(7)	-164.07(18)
O(1)-C(1)-C(6)-C(11)	-165.66(17)
C(2)-C(1)-C(6)-C(11)	13.9(3)
C(11)-C(6)-C(7)-C(8)	-0.9(3)
C(1)-C(6)-C(7)-C(8)	177.19(17)
C(6)-C(7)-C(8)-C(9)	2.1(3)
C(7)-C(8)-C(9)-N(3)	177.70(18)
C(7)-C(8)-C(9)-C(10)	-2.0(3)
N(3)-C(9)-C(10)-C(11)	-179.0(2)
C(8)-C(9)-C(10)-C(11)	0.7(3)
C(9)-C(10)-C(11)-C(6)	0.5(3)
C(7)-C(6)-C(11)-C(10)	-0.4(3)
C(1)-C(6)-C(11)-C(10)	-178.47(19)
C(3)-C(4)-C(12)-N(2)	1.8(3)
C(3)-C(4)-C(12)-Cl(1)	-179.46(13)
C(20)-C(19)-C(24)-C(23)	0.5(3)

B(1)-C(19)-C(24)-C(23)	177.5(2)
C(19)-C(24)-C(23)-C(22)	-1.8(4)
C(24)-C(23)-C(22)-C(21)	1.7(4)
C(23)-C(22)-C(21)-C(20)	-0.4(4)
C(24)-C(19)-C(20)-C(21)	0.8(3)
B(1)-C(19)-C(20)-C(21)	-176.1(2)
C(22)-C(21)-C(20)-C(19)	-0.9(4)
C(18)-C(13)-C(14)-C(15)	-0.1(3)
B(1)-C(13)-C(14)-C(15)	177.67(17)
C(13)-C(14)-C(15)-C(16)	-0.6(3)
C(14)-C(15)-C(16)-C(17)	0.8(3)
C(15)-C(16)-C(17)-C(18)	-0.3(3)
C(16)-C(17)-C(18)-C(13)	-0.4(3)
C(14)-C(13)-C(18)-C(17)	0.6(3)
B(1)-C(13)-C(18)-C(17)	-177.09(18)
N(2)-C(5)-N(1)-C(3)	3.7(3)
N(2)-C(5)-N(1)-B(1)	-169.49(18)
C(2)-C(3)-N(1)-C(5)	176.60(16)
C(4)-C(3)-N(1)-C(5)	-3.5(2)
C(2)-C(3)-N(1)-B(1)	-9.8(2)
C(4)-C(3)-N(1)-B(1)	170.11(15)
N(1)-C(5)-N(2)-C(12)	-1.0(3)
C(4)-C(12)-N(2)-C(5)	-1.9(3)
Cl(1)-C(12)-N(2)-C(5)	179.34(14)
C(8)-C(9)-N(3)-C(26)	13.1(3)
C(10)-C(9)-N(3)-C(26)	-167.3(2)
C(8)-C(9)-N(3)-C(25)	-176.0(2)
C(10)-C(9)-N(3)-C(25)	3.6(3)
C(2)-C(1)-O(1)-B(1)	26.4(2)
C(6)-C(1)-O(1)-B(1)	-154.03(16)
C(1)-O(1)-B(1)-N(1)	-43.7(2)
C(1)-O(1)-B(1)-C(13)	72.5(2)
C(1)-O(1)-B(1)-C(19)	-161.69(16)
C(5)-N(1)-B(1)-O(1)	-151.56(15)
C(3)-N(1)-B(1)-O(1)	35.2(2)
C(5)-N(1)-B(1)-C(13)	91.31(19)
C(3)-N(1)-B(1)-C(13)	-81.97(19)
C(5)-N(1)-B(1)-C(19)	-33.8(2)
C(3)-N(1)-B(1)-C(19)	152.94(15)
C(18)-C(13)-B(1)-O(1)	-146.02(17)

C(14)-C(13)-B(1)-O(1)	36.4(2)
C(18)-C(13)-B(1)-N(1)	-30.9(2)
C(14)-C(13)-B(1)-N(1)	151.52(15)
C(18)-C(13)-B(1)-C(19)	91.2(2)
C(14)-C(13)-B(1)-C(19)	-86.4(2)
C(24)-C(19)-B(1)-O(1)	24.2(3)
C(20)-C(19)-B(1)-O(1)	-159.01(19)
C(24)-C(19)-B(1)-N(1)	-91.7(2)
C(20)-C(19)-B(1)-N(1)	85.1(2)
C(24)-C(19)-B(1)-C(13)	147.10(19)
C(20)-C(19)-B(1)-C(13)	-36.1(3)

Symmetry transformations used to generate equivalent atoms:

DFT calculation results of 6.

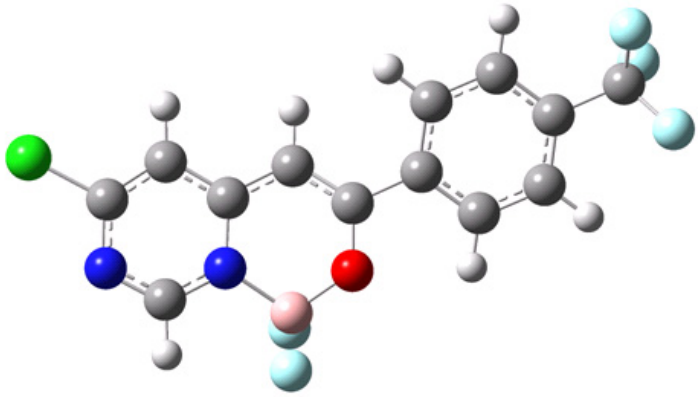


SCF Energy: -1331.77467591

C	0	-2.2217	-1.3194	0.1829
C	0	-3.4683	-0.7766	-0.0333
N	0	-3.7004	0.5211	-0.2938
C	0	-2.6363	1.2967	-0.3051
N	0	-1.3726	0.8877	-0.0798
C	0	-1.1137	-0.4429	0.1407
C	0	0.2307	-0.8649	0.2710
C	0	1.2768	-0.0030	0.0052
O	0	1.0673	1.2760	-0.2605
Cl	0	-4.8786	-1.8076	0.0105
C	0	2.6909	-0.4207	-0.0320

C	0	3.0625	-1.7745	-0.1241
C	0	4.4064	-2.1356	-0.1429
C	0	5.3993	-1.1541	-0.0741
C	0	5.0407	0.1934	0.0079
C	0	3.6975	0.5597	0.0255
B	0	-0.1982	1.9586	0.0588
F	0	-0.4266	2.9735	-0.8439
F	0	-0.1870	2.4097	1.3659
H	0	-2.0779	-2.3763	0.3634
H	0	-2.7610	2.3547	-0.5070
H	0	0.4166	-1.9028	0.5048
H	0	2.3061	-2.5472	-0.2057
H	0	4.6802	-3.1831	-0.2198
H	0	6.4468	-1.4391	-0.0893
H	0	5.8080	0.9594	0.0601
H	0	3.4139	1.6031	0.0935

DFT calculation results of 7.

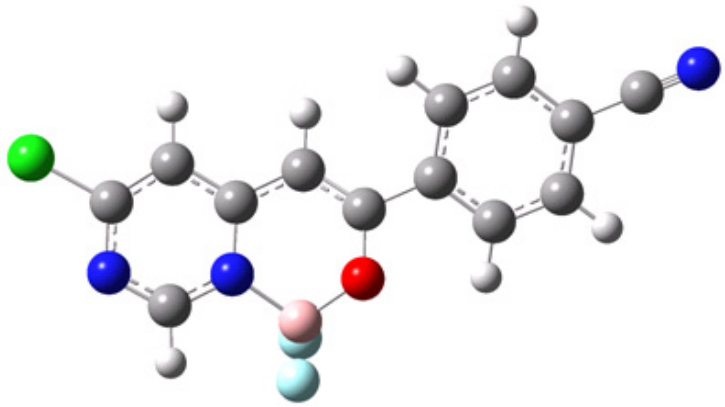


SCF Energy: -1668.80912773

C	0	-3.3962	-1.4587	0.1902
C	0	-4.7032	-1.0829	-0.0329
N	0	-5.0985	0.1723	-0.3001
C	0	-4.1438	1.0796	-0.3130
N	0	-2.8387	0.8380	-0.0817
C	0	-2.4134	-0.4464	0.1469
C	0	-1.0232	-0.6916	0.2814
C	0	-0.1006	0.2966	0.0139
O	0	-0.4667	1.5378	-0.2573

Cl	0	-5.9666	-2.2874	0.0108
C	0	1.3585	0.0623	-0.0182
C	0	1.8984	-1.2305	-0.1296
C	0	3.2751	-1.4206	-0.1491
C	0	4.1319	-0.3191	-0.0626
C	0	3.6084	0.9724	0.0380
C	0	2.2306	1.1613	0.0559
B	0	-1.8126	2.0550	0.0498
F	0	-2.1653	3.0203	-0.8654
F	0	-1.8664	2.5152	1.3515
C	0	5.6213	-0.5321	-0.0263
F	0	6.0689	-0.7012	1.2418
F	0	6.2965	0.5186	-0.5415
F	0	5.9918	-1.6315	-0.7198
H	0	-3.1170	-2.4872	0.3752
H	0	-4.4042	2.1113	-0.5214
H	0	-0.7054	-1.6953	0.5221
H	0	1.2488	-2.0924	-0.2280
H	0	3.6833	-2.4199	-0.2469
H	0	4.2743	1.8259	0.0969
H	0	1.8191	2.1601	0.1326

DFT calculation results of 8.

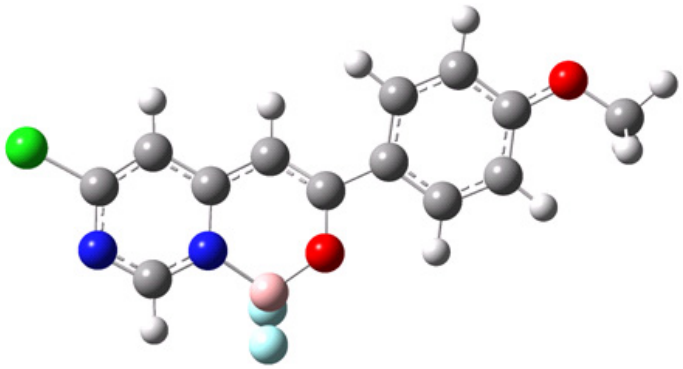


SCF Energy: -1424.01762784

C	0	-2.6934	-1.4165	0.1865
C	0	-3.9824	-0.9808	-0.0367
N	0	-4.3189	0.2912	-0.3021
C	0	-3.3237	1.1541	-0.3135

N	0	-2.0312	0.8523	-0.0820
C	0	-1.6663	-0.4502	0.1460
C	0	-0.2876	-0.7590	0.2825
C	0	0.6780	0.1864	0.0168
O	0	0.3702	1.4427	-0.2576
Cl	0	-5.2989	-2.1261	0.0054
C	0	2.1261	-0.1118	-0.0100
C	0	2.6102	-1.4282	-0.1085
C	0	3.9750	-1.6805	-0.1223
C	0	4.8831	-0.6104	-0.0422
C	0	4.4106	0.7095	0.0464
C	0	3.0431	0.9514	0.0585
B	0	-0.9504	2.0217	0.0505
F	0	-1.2588	3.0022	-0.8639
F	0	-0.9827	2.4817	1.3525
C	0	6.2932	-0.8681	-0.0571
N	0	7.4376	-1.0781	-0.0686
H	0	-2.4621	-2.4570	0.3702
H	0	-3.5363	2.1969	-0.5207
H	0	-0.0174	-1.7760	0.5257
H	0	1.9252	-2.2628	-0.1987
H	0	4.3423	-2.6971	-0.2033
H	0	5.1131	1.5331	0.1065
H	0	2.6724	1.9664	0.1285

DFT calculation results of 9.

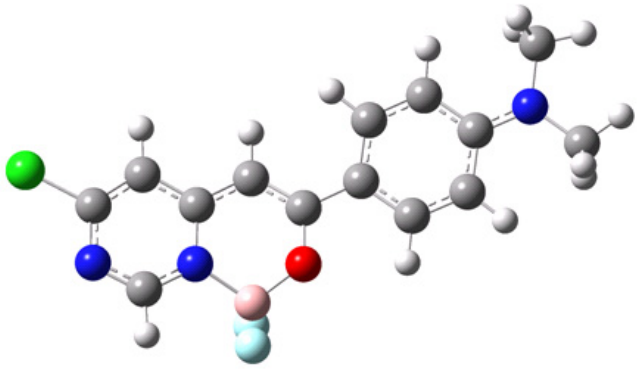


SCF Energy: -1446.30401570

C	0	-2.8972	-1.3817	0.1662
C	0	-4.1681	-0.9084	-0.0618

N	0	-4.4719	0.3769	-0.3173
C	0	-3.4526	1.2102	-0.3106
N	0	-2.1704	0.8722	-0.0732
C	0	-1.8367	-0.4442	0.1417
C	0	-0.4761	-0.7915	0.2850
C	0	0.5287	0.1293	0.0367
O	0	0.2443	1.3963	-0.2245
Cl	0	-5.5197	-2.0184	-0.0424
C	0	1.9560	-0.2050	0.0060
C	0	2.4193	-1.5386	0.0070
C	0	3.7724	-1.8214	-0.0154
C	0	4.7157	-0.7768	-0.0433
C	0	4.2742	0.5550	-0.0515
C	0	2.9103	0.8261	-0.0294
B	0	-1.0600	2.0032	0.0870
F	0	-1.3339	3.0136	-0.8096
F	0	-1.0877	2.4452	1.3982
O	0	6.0142	-1.1588	-0.0640
C	0	7.0261	-0.1498	-0.1054
H	0	-2.6968	-2.4301	0.3417
H	0	-3.6343	2.2612	-0.5065
H	0	-0.2387	-1.8209	0.5091
H	0	1.7186	-2.3658	0.0057
H	0	4.1304	-2.8452	-0.0210
H	0	4.9791	1.3765	-0.0715
H	0	2.5718	1.8553	-0.0316
H	0	7.9759	-0.6837	-0.1219
H	0	6.9837	0.4920	0.7810
H	0	6.9369	0.4646	-1.0077

DFT calculation results of 10.

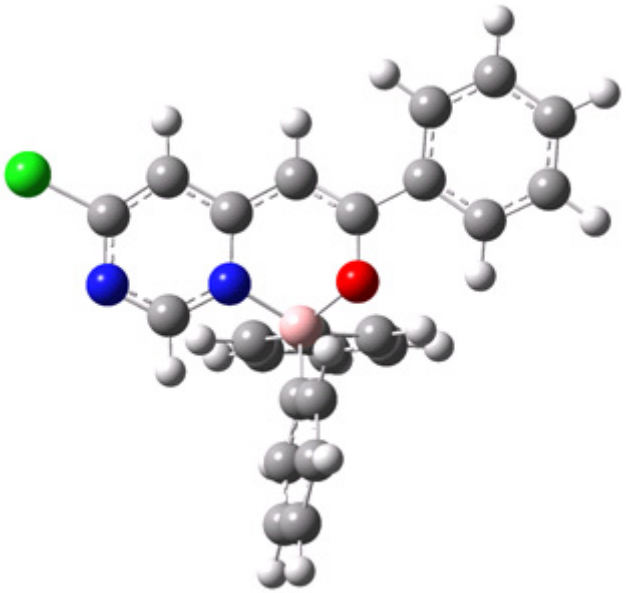


SCF Energy: -1465.75636489

C	0	-3.1499	-1.4478	0.1449
C	0	-4.4421	-1.0443	-0.0828
N	0	-4.8206	0.2259	-0.3248
C	0	-3.8494	1.1142	-0.3024
N	0	-2.5509	0.8483	-0.0642
C	0	-2.1393	-0.4515	0.1350
C	0	-0.7672	-0.7227	0.2786
C	0	0.1924	0.2586	0.0497
O	0	-0.1709	1.5110	-0.1967
Cl	0	-5.7311	-2.2305	-0.0837
C	0	1.6261	0.0094	0.0189
C	0	2.1783	-1.2879	0.0889
C	0	3.5429	-1.5000	0.0627
C	0	4.4535	-0.4115	-0.0393
C	0	3.8970	0.8947	-0.1169
C	0	2.5294	1.0886	-0.0893
B	0	-1.5080	2.0349	0.1176
F	0	-1.8351	3.0445	-0.7646
F	0	-1.5666	2.4582	1.4358
N	0	5.8054	-0.6140	-0.0636
C	0	6.3507	-1.9636	0.0266
C	0	6.7164	0.5170	-0.1985
H	0	-2.8917	-2.4854	0.3091
H	0	-4.0896	2.1558	-0.4855
H	0	-0.4740	-1.7420	0.4817
H	0	1.5318	-2.1566	0.1513
H	0	3.9115	-2.5162	0.1125
H	0	4.5437	1.7591	-0.1942
H	0	2.1357	2.0967	-0.1450

H	0	6.0352	-2.5871	-0.8192
H	0	6.0418	-2.4609	0.9537
H	0	7.4383	-1.9092	0.0196
H	0	6.6197	1.2168	0.6405
H	0	6.5378	1.0701	-1.1286
H	0	7.7412	0.1489	-0.2153

DFT calculation results of 11.

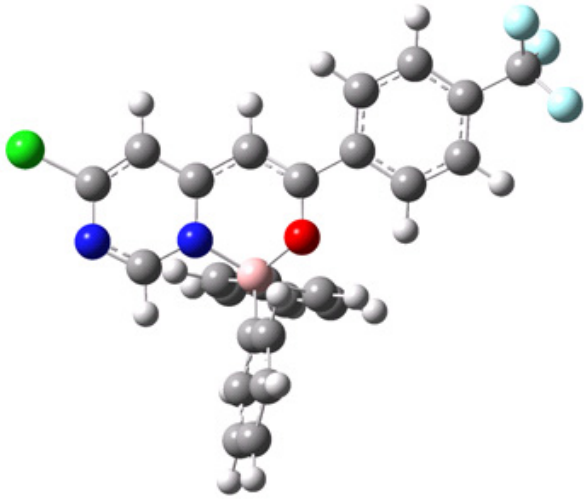


SCF Energy: -1595.29055595

C	0	-1.6149	-2.8355	-0.0647
C	0	-2.9411	-2.5588	-0.3109
N	0	-3.4251	-1.3365	-0.5708
C	0	-2.5376	-0.3576	-0.5456
N	0	-1.2257	-0.4918	-0.2821
C	0	-0.7103	-1.7500	-0.0683
C	0	0.6892	-1.9116	0.0756
C	0	1.5545	-0.8857	-0.2560
O	0	1.1076	0.3255	-0.5186
Cl	0	-4.1106	-3.8614	-0.3103
C	0	3.0154	-1.0586	-0.3982
C	0	3.6208	-2.3287	-0.3968
C	0	5.0012	-2.4528	-0.5250
C	0	5.8003	-1.3145	-0.6644
C	0	5.2091	-0.0492	-0.6781

C	0	3.8286	0.0793	-0.5477
B	0	-0.2511	0.7885	-0.0454
C	0	-0.7083	2.0172	-0.9913
C	0	-0.2082	1.1070	1.5467
C	0	-1.2558	1.2706	3.7580
C	0	-0.7697	3.0596	-3.2082
C	0	-1.3084	0.9284	2.4035
C	0	-0.3807	2.0208	-2.3611
C	0	-0.0851	1.8037	4.2990
C	0	1.0249	1.9926	3.4720
C	0	0.9570	1.6503	2.1203
C	0	-1.5101	4.1324	-2.7040
C	0	-1.4482	3.1118	-0.5105
C	0	-1.8496	4.1552	-1.3505
H	0	-1.2596	-3.8426	0.1081
H	0	-2.8803	0.6521	-0.7421
H	0	1.0592	-2.9011	0.3004
H	0	3.0180	-3.2259	-0.3134
H	0	5.4538	-3.4395	-0.5240
H	0	6.8766	-1.4147	-0.7658
H	0	5.8239	0.8385	-0.7891
H	0	3.3658	1.0587	-0.5603
H	0	-2.1267	1.1156	4.3896
H	0	-0.4960	3.0347	-4.2599
H	0	-2.2344	0.5074	2.0176
H	0	0.2002	1.1968	-2.7682
H	0	-0.0372	2.0678	5.3518
H	0	1.9435	2.4058	3.8809
H	0	1.8329	1.8038	1.4952
H	0	-1.8156	4.9432	-3.3597
H	0	-1.7108	3.1537	0.5434
H	0	-2.4208	4.9870	-0.9466

DFT calculation results of 12.

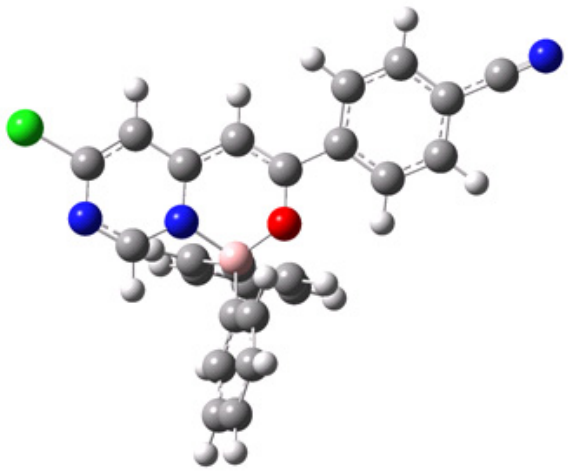


SCF Energy: -1932.32508795

C	0	2.2201	3.0148	-0.0396
C	0	3.5625	2.9499	-0.3446
N	0	4.2160	1.8199	-0.6446
C	0	3.4916	0.7153	-0.6052
N	0	2.1855	0.6430	-0.2914
C	0	1.4961	1.8033	-0.0279
C	0	0.0941	1.7449	0.1820
C	0	-0.6145	0.6036	-0.1314
O	0	-0.0073	-0.5198	-0.4500
Cl	0	4.5151	4.4165	-0.3677
C	0	-2.0934	0.5515	-0.1806
C	0	-2.8797	1.7169	-0.1919
C	0	-4.2664	1.6336	-0.2245
C	0	-4.8893	0.3814	-0.2537
C	0	-4.1206	-0.7845	-0.2576
C	0	-2.7323	-0.6986	-0.2251
B	0	1.4329	-0.7789	-0.0546
C	0	2.0248	-1.8958	-1.0601
C	0	1.5085	-1.1495	1.5238
C	0	2.5205	-1.0411	3.7545
C	0	2.1229	-2.8816	-3.3008
C	0	2.4758	-0.6501	2.4123
C	0	1.6159	-1.9371	-2.4069
C	0	1.5853	-1.9498	4.2496
C	0	0.6115	-2.4648	3.3895
C	0	0.5815	-2.0698	2.0517

C	0	3.0681	-3.8158	-2.8686
C	0	2.9725	-2.8511	-0.6516
C	0	3.4934	-3.7972	-1.5394
C	0	-6.3914	0.2989	-0.2294
F	0	-6.8750	0.4001	1.0328
F	0	-6.8463	-0.8701	-0.7307
F	0	-6.9627	1.2954	-0.9434
H	0	1.7215	3.9522	0.1678
H	0	3.9772	-0.2270	-0.8325
H	0	-0.4128	2.6585	0.4564
H	0	-2.4144	2.6956	-0.1981
H	0	-4.8630	2.5388	-0.2418
H	0	-4.6048	-1.7536	-0.2897
H	0	-2.1313	-1.5993	-0.2313
H	0	3.2831	-0.6313	4.4117
H	0	1.7822	-2.8907	-4.3329
H	0	3.2168	0.0662	2.0646
H	0	0.8776	-1.2205	-2.7582
H	0	1.6136	-2.2543	5.2922
H	0	-0.1225	-3.1748	3.7619
H	0	-0.1821	-2.4865	1.3992
H	0	3.4661	-4.5525	-3.5611
H	0	3.3046	-2.8606	0.3835
H	0	4.2247	-4.5222	-1.1919

DFT calculation results of 13.

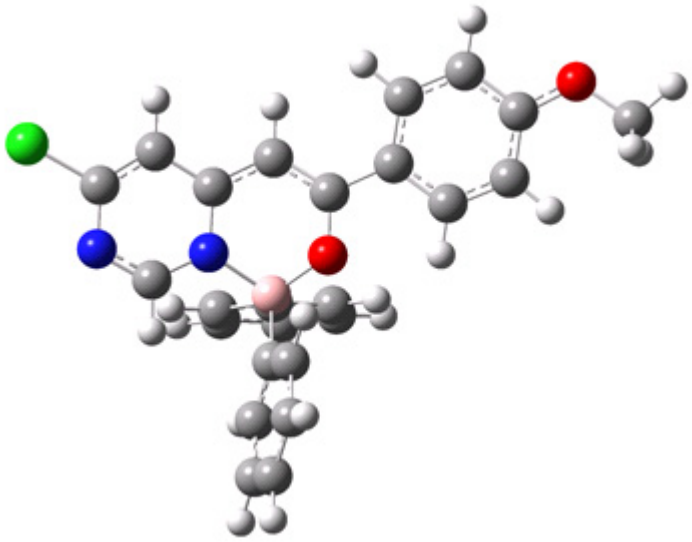


SCF Energy: -1687.53379317

C	0	1.7313	2.9728	-0.0508
C	0	3.0750	2.8499	-0.3344
N	0	3.6846	1.6912	-0.6147
C	0	2.9146	0.6177	-0.5780
N	0	1.6020	0.6027	-0.2838
C	0	0.9586	1.7927	-0.0399
C	0	-0.4489	1.7946	0.1492
C	0	-1.1986	0.6819	-0.1681
O	0	-0.6342	-0.4672	-0.4740
Cl	0	4.0877	4.2749	-0.3545
C	0	-2.6781	0.6888	-0.2395
C	0	-3.4201	1.8833	-0.2278
C	0	-4.8067	1.8568	-0.2848
C	0	-5.4788	0.6245	-0.3627
C	0	-4.7480	-0.5749	-0.3873
C	0	-3.3610	-0.5367	-0.3279
B	0	0.7867	-0.7852	-0.0503
C	0	1.3485	-1.9323	-1.0382
C	0	0.8172	-1.1450	1.5318
C	0	1.7853	-1.0511	3.7824
C	0	1.4633	-2.9213	-3.2767
C	0	1.7823	-0.6710	2.4364
C	0	0.9791	-1.9519	-2.3969
C	0	0.8094	-1.9230	4.2649
C	0	-0.1635	-2.4120	3.3886
C	0	-0.1520	-2.0280	2.0473
C	0	2.3446	-3.9039	-2.8173
C	0	2.2318	-2.9360	-0.6025
C	0	2.7290	-3.9081	-1.4757
C	0	-6.9106	0.5939	-0.4226
N	0	-8.0731	0.5696	-0.4706
H	0	1.2690	3.9319	0.1410
H	0	3.3638	-0.3457	-0.7902
H	0	-0.9201	2.7310	0.4098
H	0	-2.9201	2.8438	-0.1917
H	0	-5.3719	2.7818	-0.2771
H	0	-5.2678	-1.5243	-0.4502
H	0	-2.7919	-1.4575	-0.3466
H	0	2.5476	-0.6619	4.4523

H	0	1.1545	-2.9123	-4.3188
H	0	2.5547	0.0161	2.0986
H	0	0.2905	-1.1975	-2.7696
H	0	0.8055	-2.2193	5.3102
H	0	-0.9291	-3.0931	3.7512
H	0	-0.9162	-2.4235	1.3824
H	0	2.7246	-4.6601	-3.4988
H	0	2.5312	-2.9628	0.4421
H	0	3.4103	-4.6705	-1.1073

DFT calculation results of 14.

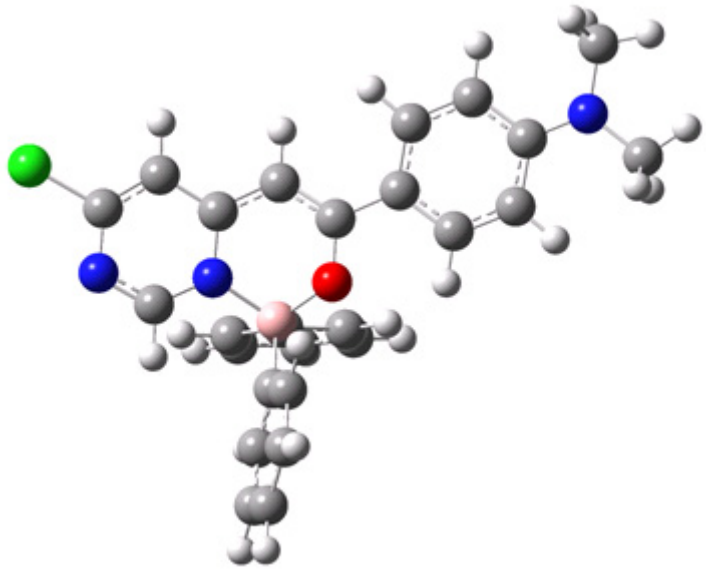


SCF Energy: -1709.81971712

C	0	1.9750	2.9200	-0.1413
C	0	3.3019	2.7297	-0.4501
N	0	3.8567	1.5391	-0.7215
C	0	3.0394	0.5040	-0.6434
N	0	1.7355	0.5521	-0.3183
C	0	1.1445	1.7754	-0.0891
C	0	-0.2498	1.8442	0.1299
C	0	-1.0646	0.7563	-0.1413
O	0	-0.5446	-0.4207	-0.4331
Cl	0	4.3799	4.1090	-0.5217
C	0	-2.5319	0.8207	-0.1892
C	0	-3.2465	2.0259	-0.0176
C	0	-4.6286	2.0469	-0.0614

C	0	-5.3506	0.8600	-0.2870
C	0	-4.6585	-0.3466	-0.4679
C	0	-3.2683	-0.3544	-0.4170
B	0	0.8630	-0.7865	-0.0277
C	0	1.3544	-1.9889	-0.9916
C	0	0.9206	-1.0963	1.5662
C	0	2.0988	-1.2125	3.7143
C	0	1.3992	-3.0202	-3.2144
C	0	2.0623	-0.8777	2.3575
C	0	0.9842	-2.0056	-2.3506
C	0	0.9788	-1.7790	4.3247
C	0	-0.1704	-2.0075	3.5643
C	0	-0.1915	-1.6718	2.2092
C	0	2.2090	-4.0552	-2.7386
C	0	2.1640	-3.0455	-0.5396
C	0	2.5913	-4.0646	-1.3966
O	0	-6.6988	0.9884	-0.3132
C	0	-7.4942	-0.1770	-0.5405
H	0	1.5614	3.9031	0.0395
H	0	3.4391	-0.4831	-0.8472
H	0	-0.6716	2.8116	0.3599
H	0	-2.7226	2.9606	0.1466
H	0	-5.1787	2.9723	0.0710
H	0	-5.1890	-1.2738	-0.6448
H	0	-2.7352	-1.2871	-0.5570
H	0	2.9993	-1.0260	4.2937
H	0	1.0921	-3.0058	-4.2571
H	0	2.9508	-0.4297	1.9173
H	0	0.3501	-1.2108	-2.7358
H	0	1.0002	-2.0376	5.3798
H	0	-1.0504	-2.4464	4.0277
H	0	-1.0970	-1.8553	1.6366
H	0	2.5351	-4.8470	-3.4074
H	0	2.4621	-3.0770	0.5052
H	0	3.2169	-4.8672	-1.0146
H	0	-8.5296	0.1626	-0.5220
H	0	-7.3409	-0.9226	0.2471
H	0	-7.2744	-0.6243	-1.5159

DFT calculation results of 15.



SCF Energy: -1729.27164887

C	0	2.0357	2.9996	-0.1474
C	0	3.3696	2.9031	-0.4592
N	0	4.0090	1.7548	-0.7361
C	0	3.2661	0.6654	-0.6567
N	0	1.9630	0.6192	-0.3288
C	0	1.2832	1.7985	-0.0983
C	0	-0.1071	1.7689	0.1222
C	0	-0.8494	0.6217	-0.1411
O	0	-0.2414	-0.5157	-0.4300
Cl	0	4.3497	4.3564	-0.5306
C	0	-2.3074	0.5814	-0.1819
C	0	-3.1126	1.7280	-0.0149
C	0	-4.4925	1.6597	-0.0480
C	0	-5.1619	0.4227	-0.2597
C	0	-4.3509	-0.7309	-0.4374
C	0	-2.9719	-0.6443	-0.3982
B	0	1.1892	-0.7744	-0.0301
C	0	1.7615	-1.9446	-0.9916
C	0	1.2777	-1.0755	1.5651
C	0	2.4863	-1.1299	3.6992
C	0	1.8658	-2.9808	-3.2107
C	0	2.4176	-0.8015	2.3422
C	0	1.3856	-1.9940	-2.3483

C	0	1.4017	-1.7463	4.3251
C	0	0.2551	-2.0299	3.5796
C	0	0.2018	-1.6997	2.2238
C	0	2.7492	-3.9541	-2.7356
C	0	2.6461	-2.9397	-0.5406
C	0	3.1391	-3.9302	-1.3959
N	0	-6.5278	0.3476	-0.2925
C	0	-7.3365	1.5455	-0.1012
C	0	-7.1881	-0.9327	-0.5182
H	0	1.5551	3.9511	0.0377
H	0	3.7343	-0.2909	-0.8626
H	0	-0.5968	2.7048	0.3489
H	0	-2.6576	2.7005	0.1389
H	0	-5.0608	2.5710	0.0855
H	0	-4.8074	-1.6981	-0.6036
H	0	-2.3794	-1.5412	-0.5365
H	0	3.3843	-0.8999	4.2670
H	0	1.5523	-2.9928	-4.2515
H	0	3.2789	-0.3137	1.8900
H	0	0.6947	-1.2477	-2.7327
H	0	1.4482	-2.0006	5.3805
H	0	-0.5981	-2.5075	4.0549
H	0	-0.7013	-1.9262	1.6629
H	0	3.1263	-4.7243	-3.4030
H	0	2.9515	-2.9452	0.5025
H	0	3.8217	-4.6852	-1.0144
H	0	-7.1377	2.2967	-0.8755
H	0	-7.1528	2.0056	0.8774
H	0	-8.3904	1.2761	-0.1548
H	0	-6.9442	-1.6581	0.2677
H	0	-6.9067	-1.3677	-1.4849
H	0	-8.2668	-0.7824	-0.5164

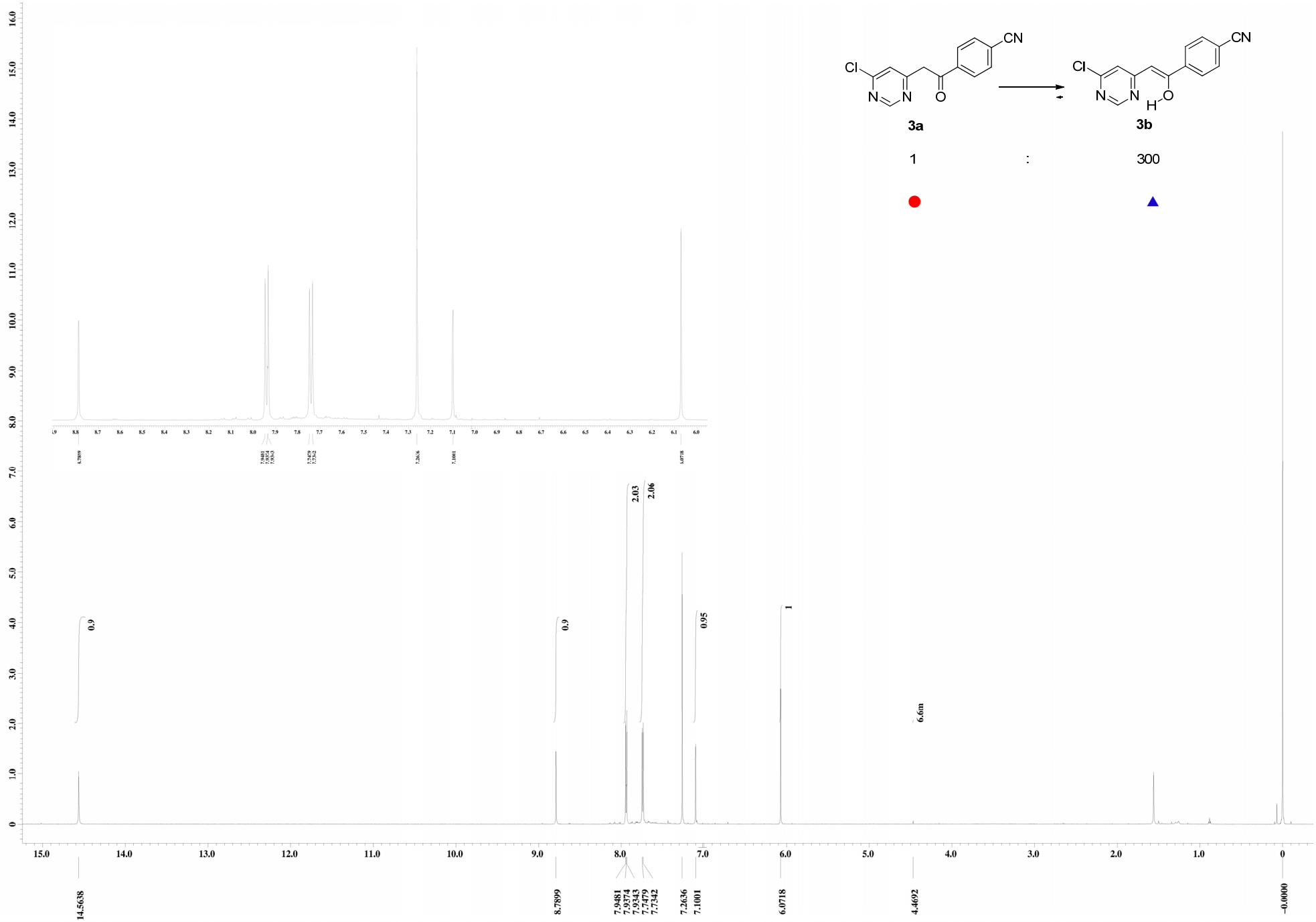


Figure S13. ^{1}H NMR spectra of **3**.

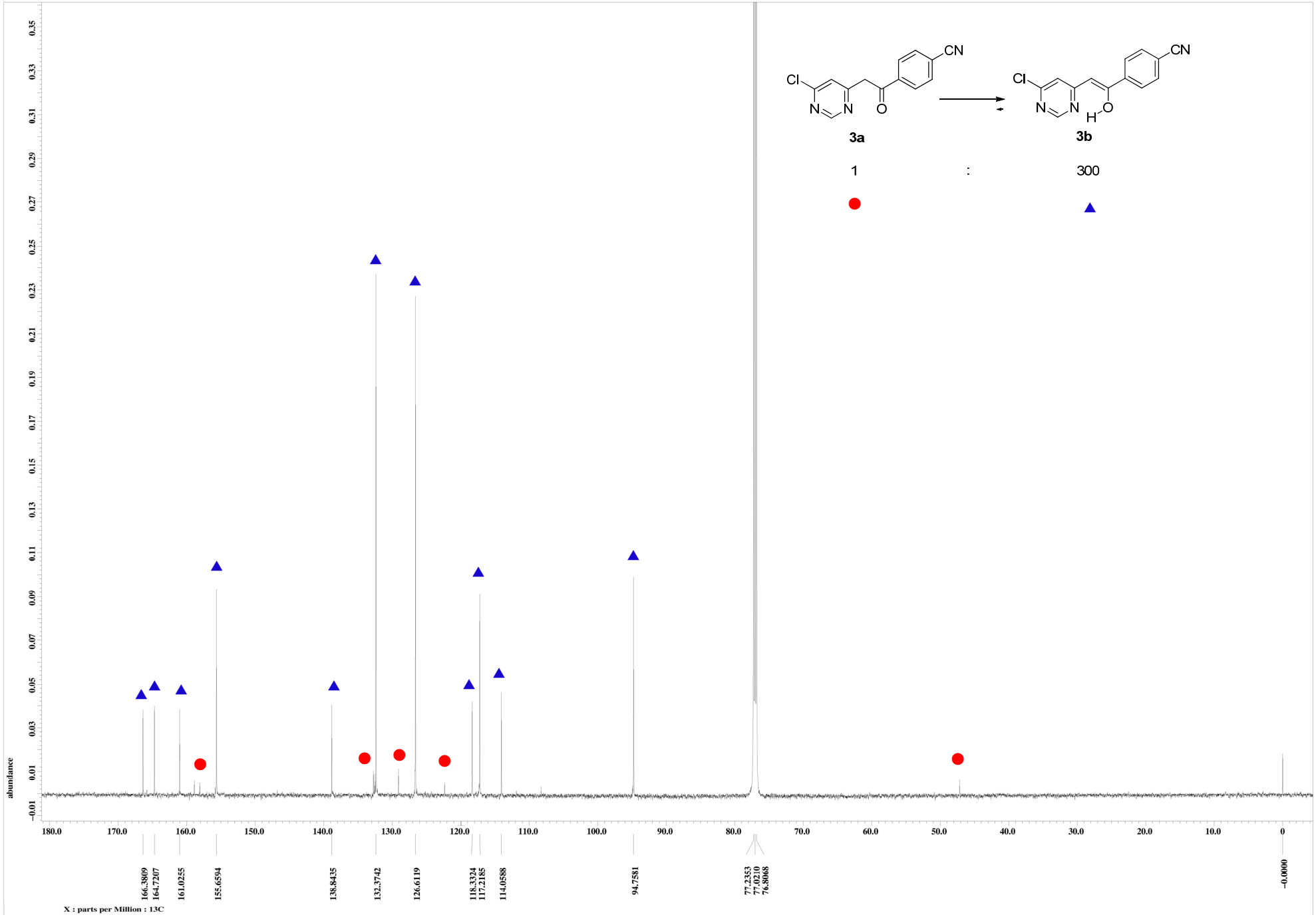


Figure S14. ^{13}C NMR spectra of **3**.

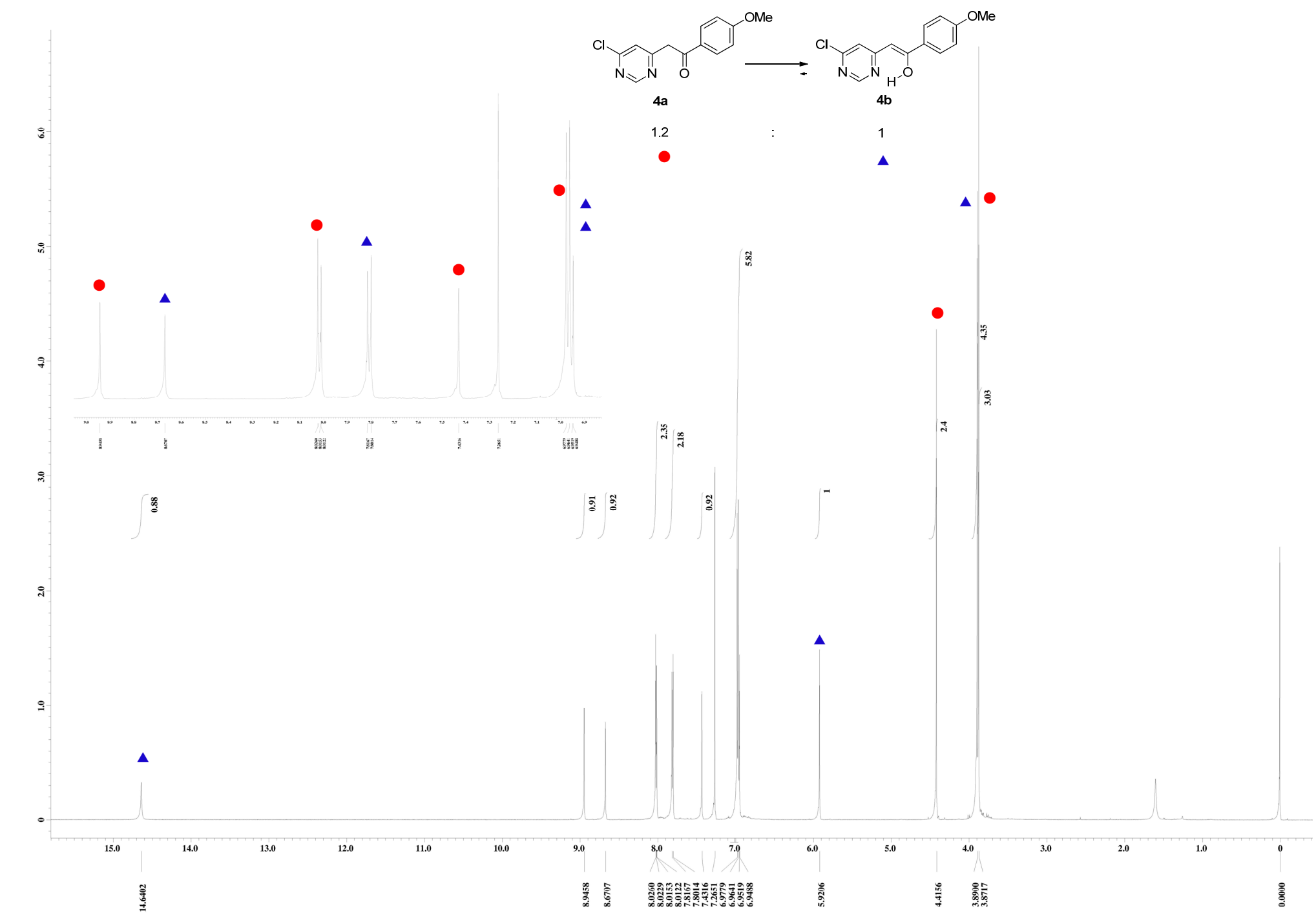


Figure S15. ^{1}H NMR spectra of **4**.

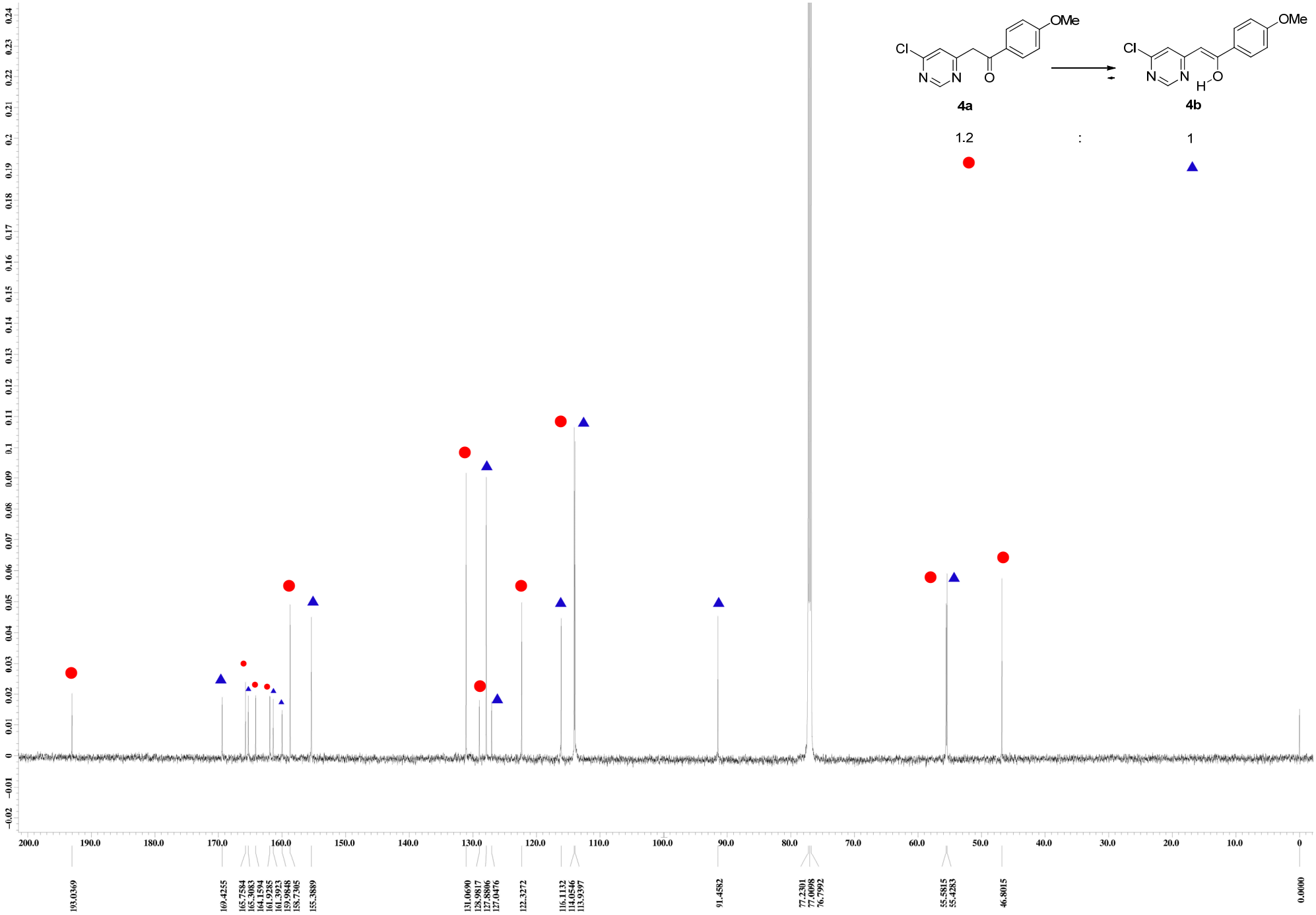


Figure S16. ^{13}C NMR spectra of **4**.

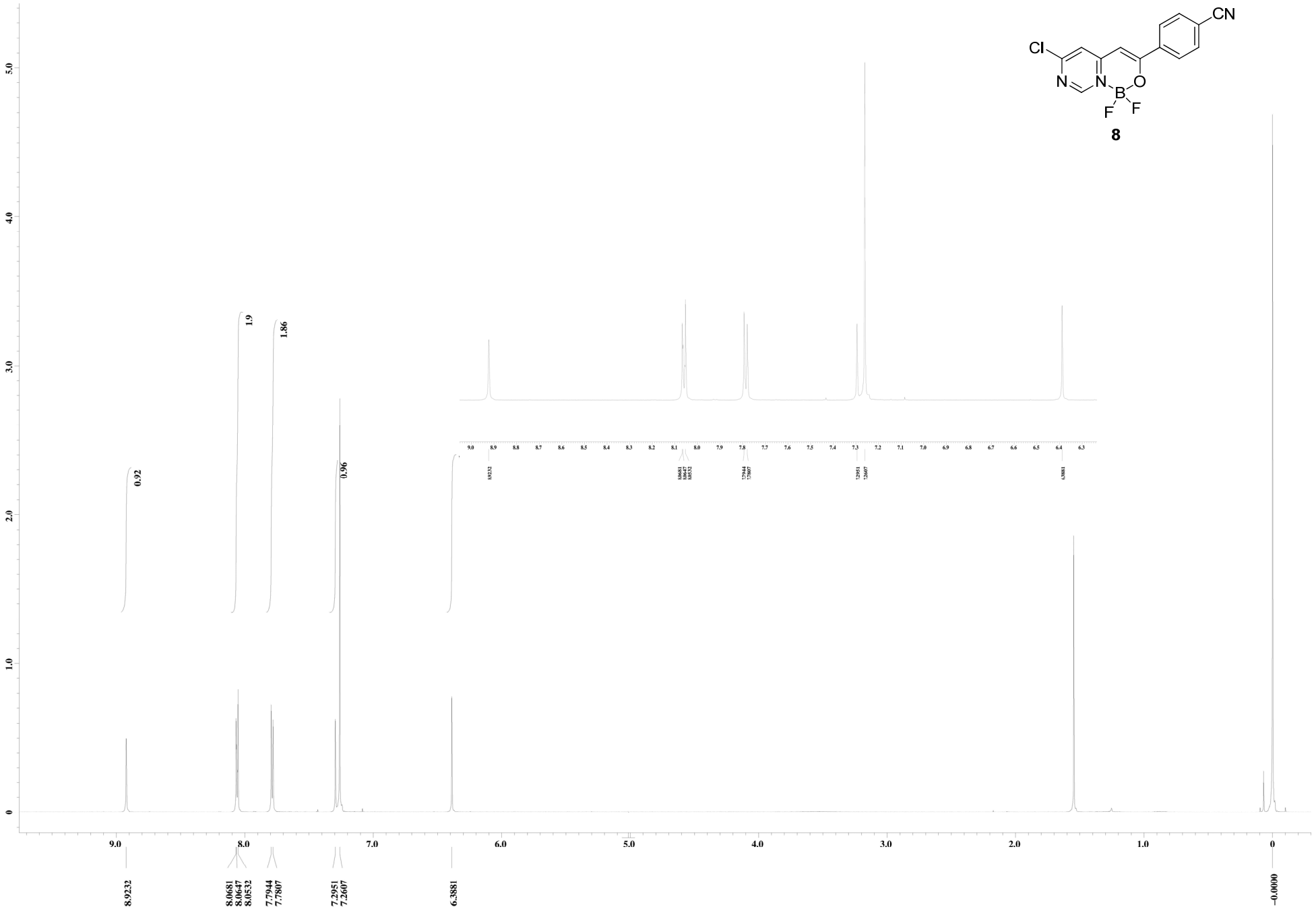


Figure S17. ^{1}H NMR spectra of **8**.

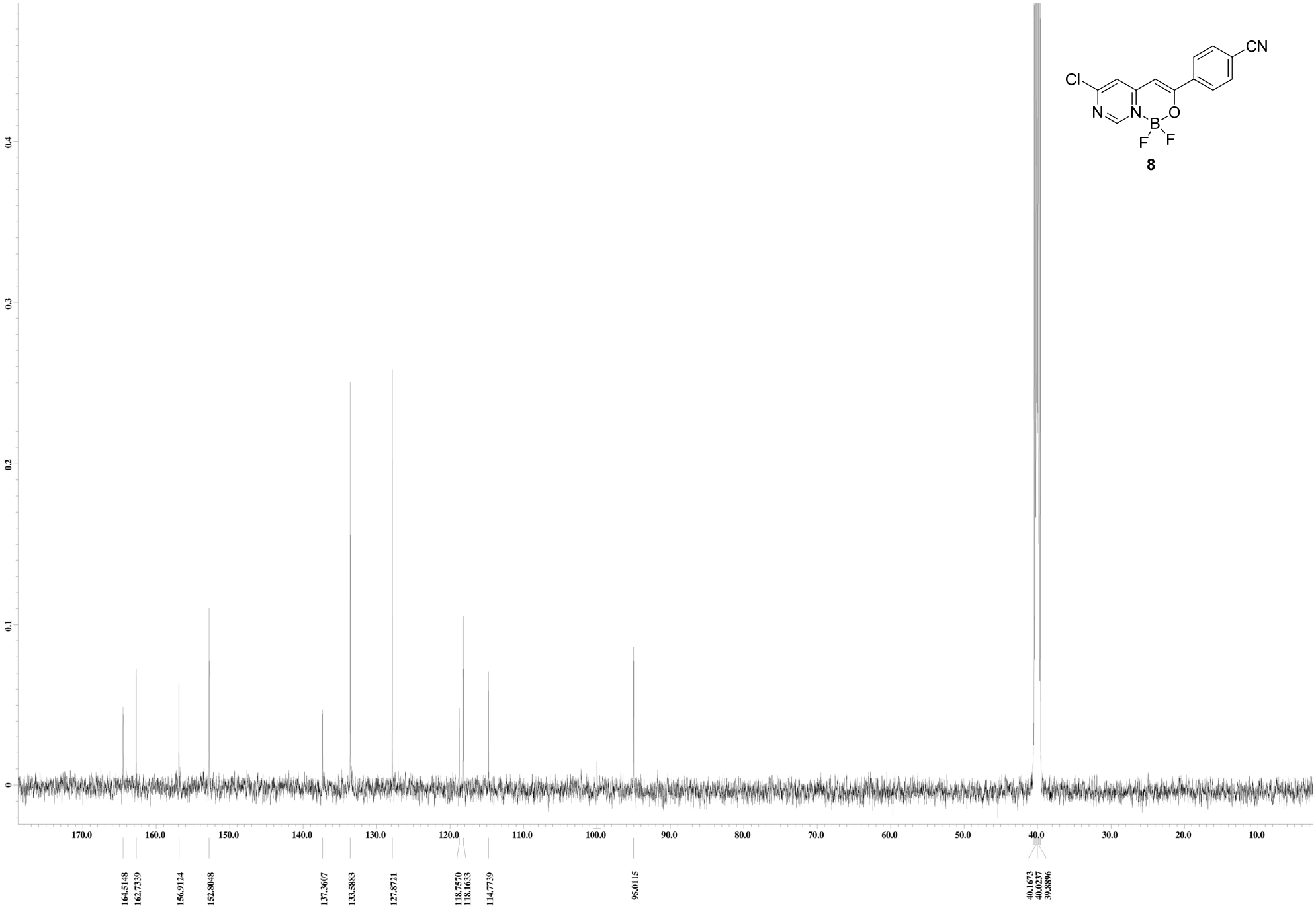


Figure S18. ^{13}C NMR spectra of **8**.

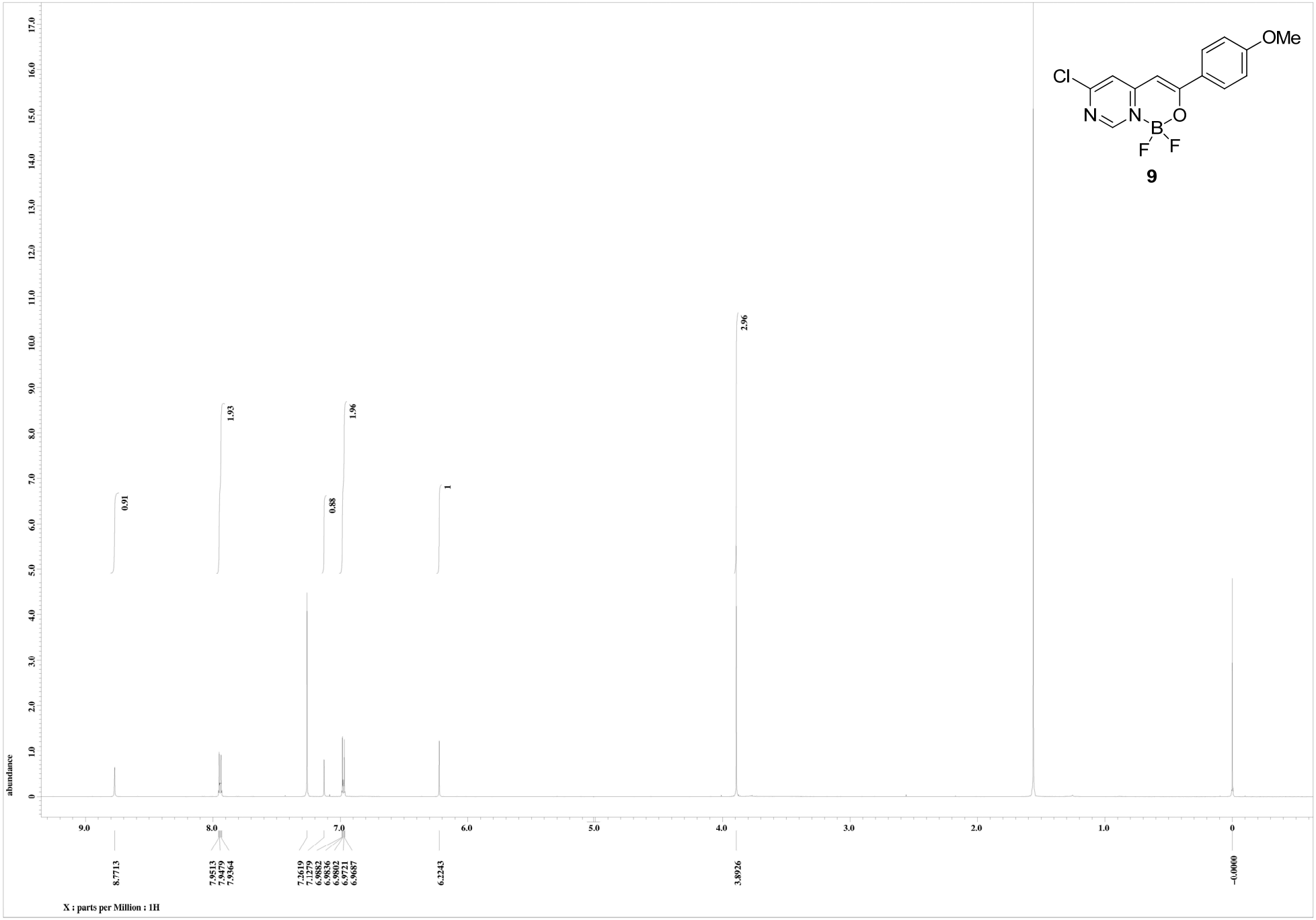


Figure S19. ^{1}H NMR spectra of **9**.

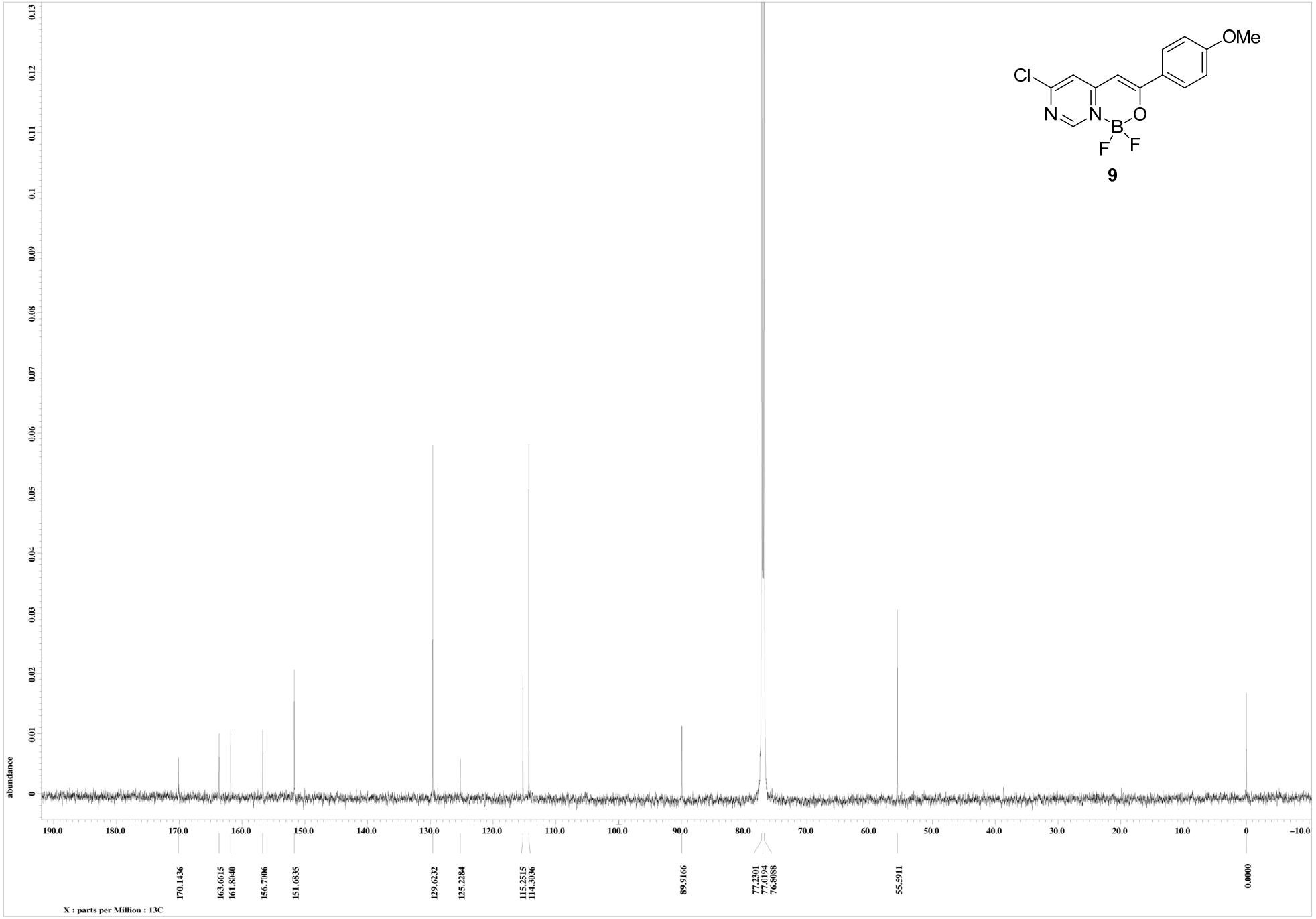


Figure S20. ^{13}C NMR spectra of **9**.

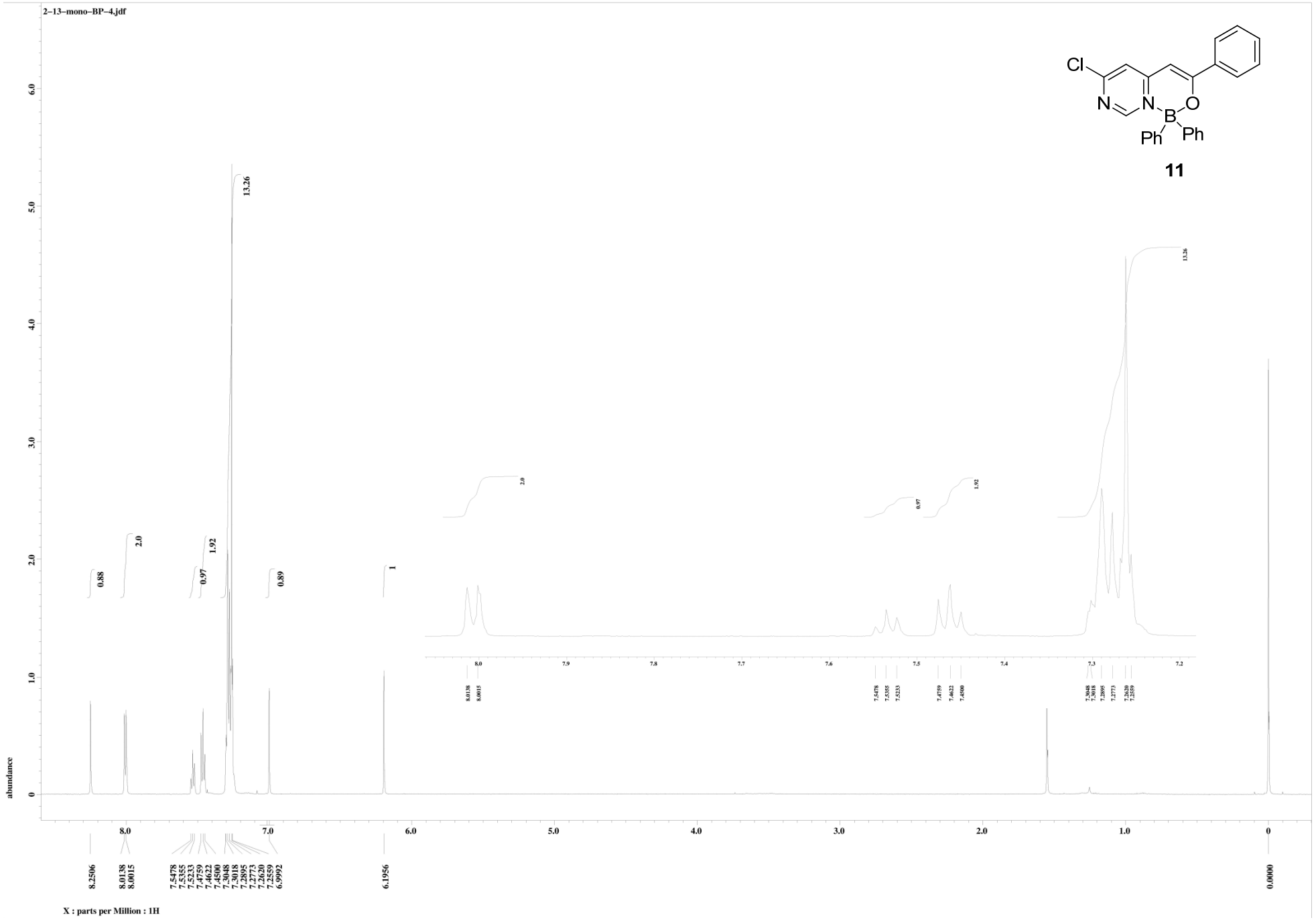


Figure S21. ^{1}H NMR spectra of **11**.

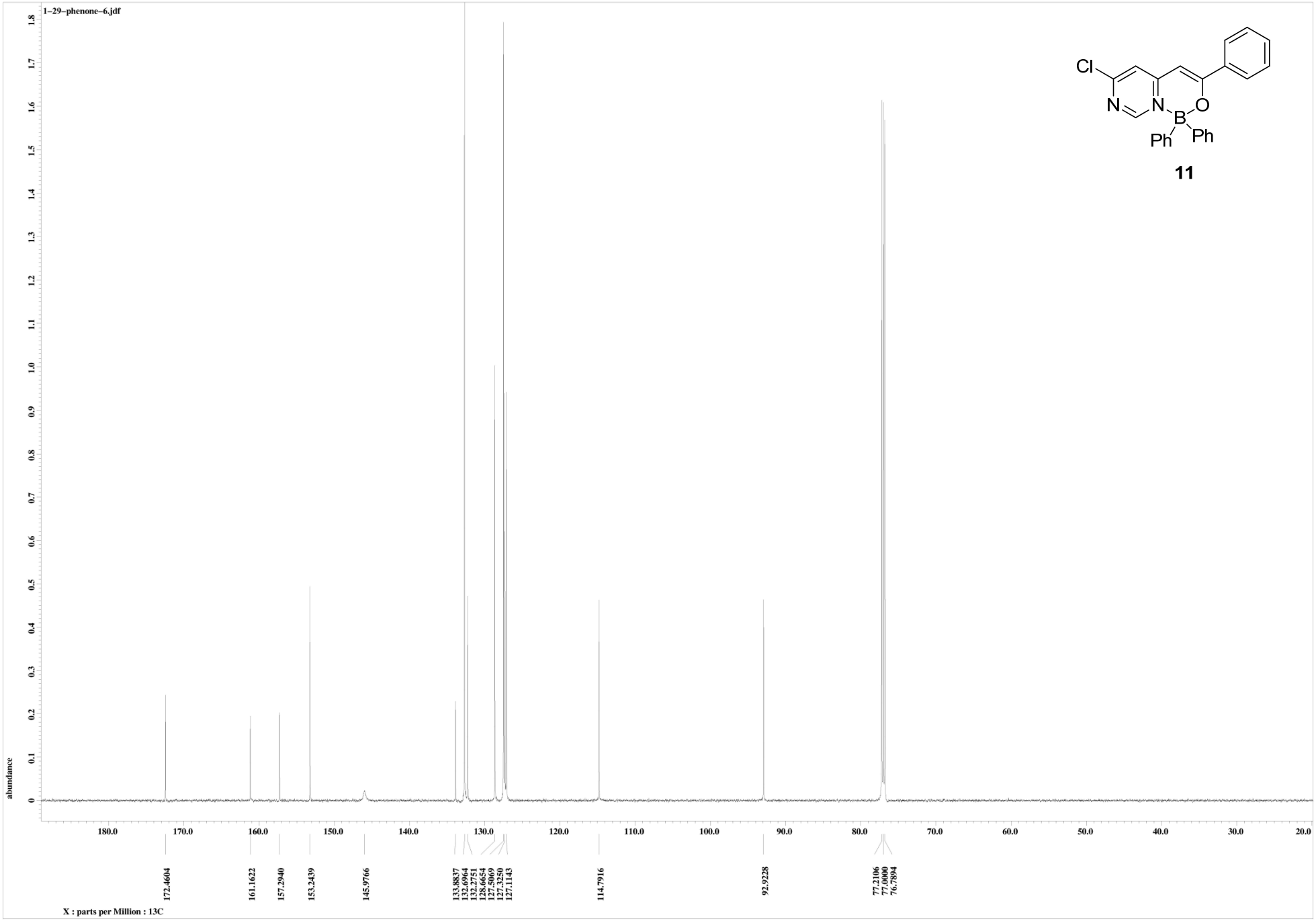


Figure S22. ^{13}C NMR spectra of **11**.

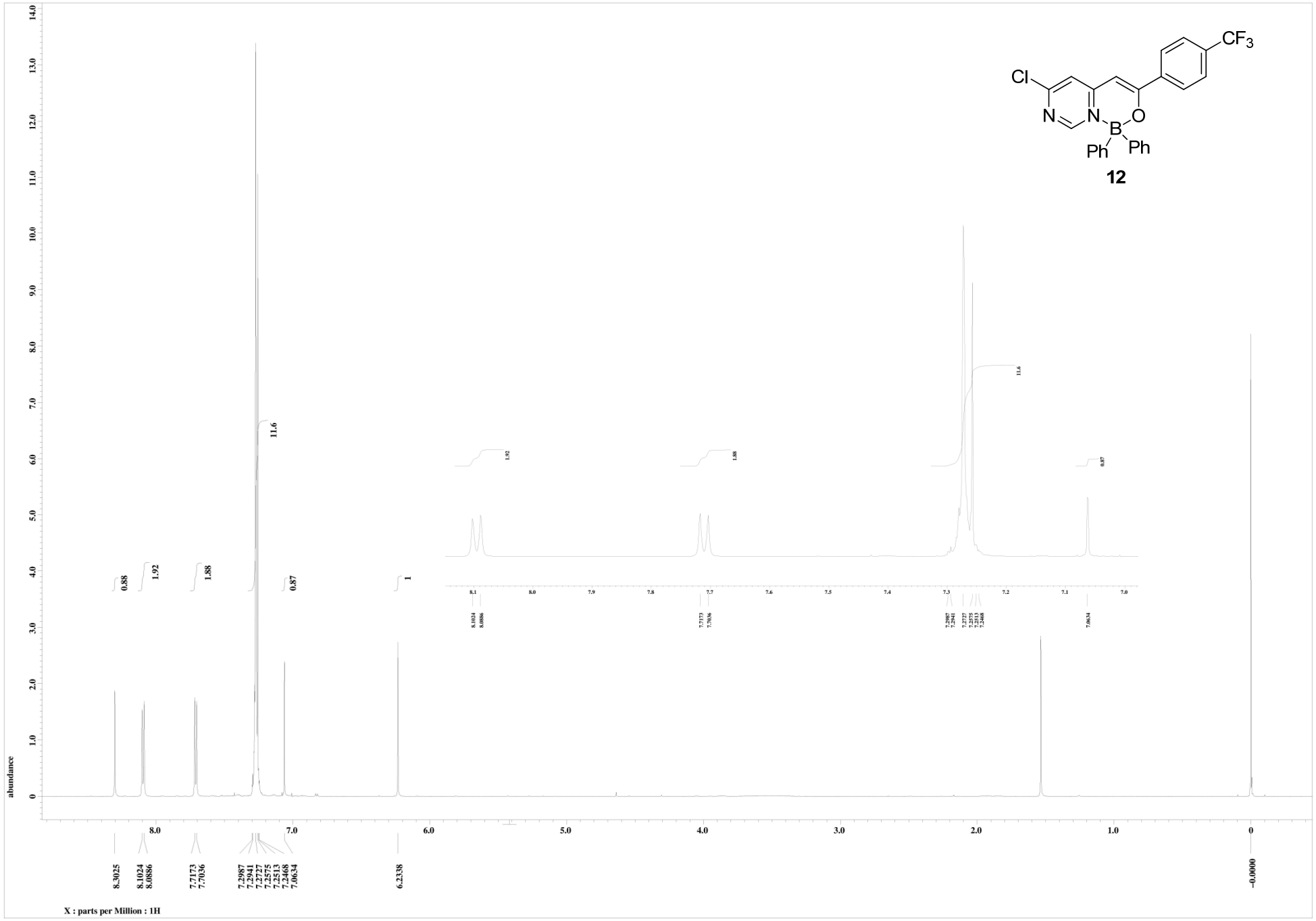


Figure S23. ^{1}H NMR spectra of **12**.

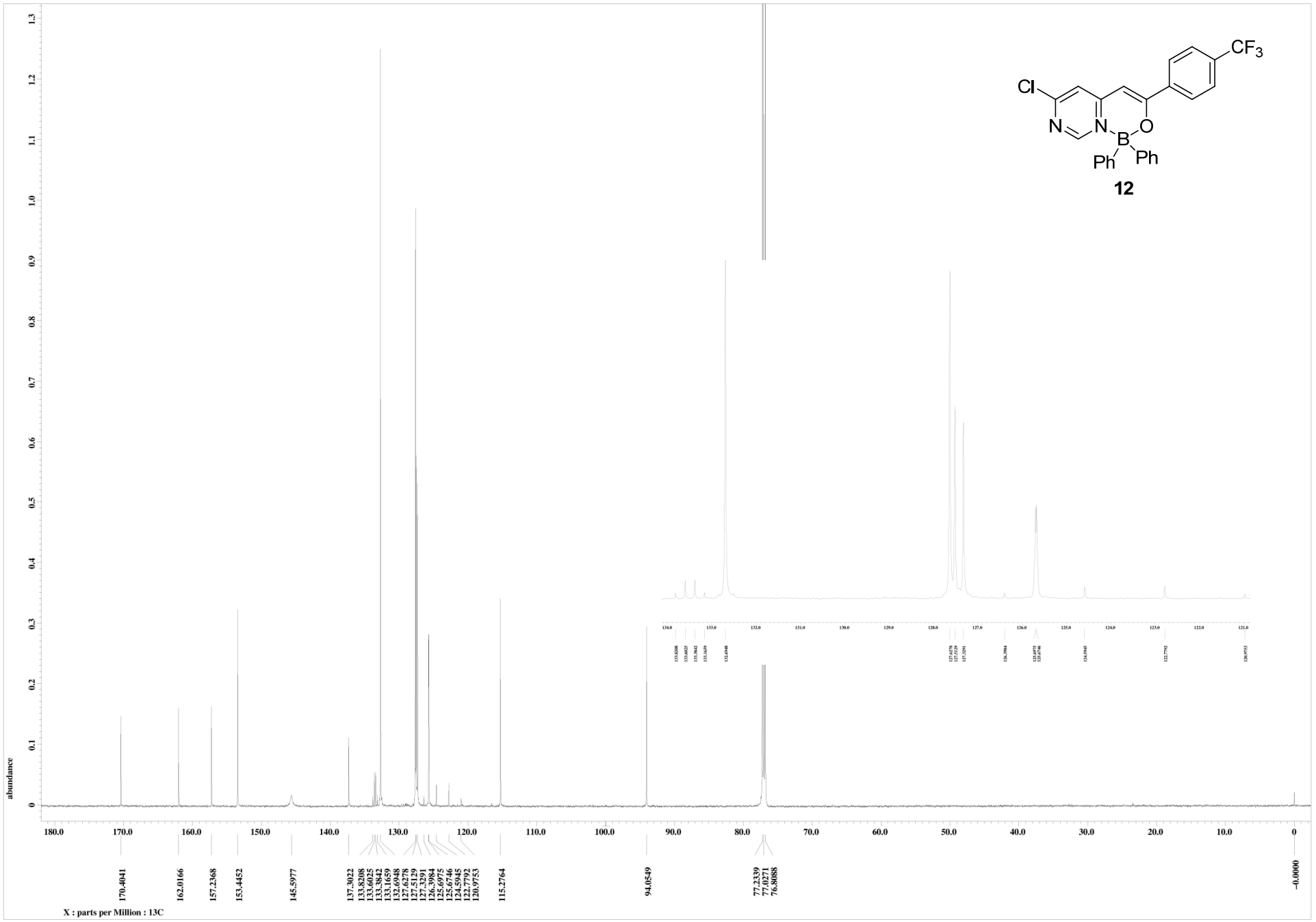


Figure S24. ^{13}C NMR spectra of **12**.

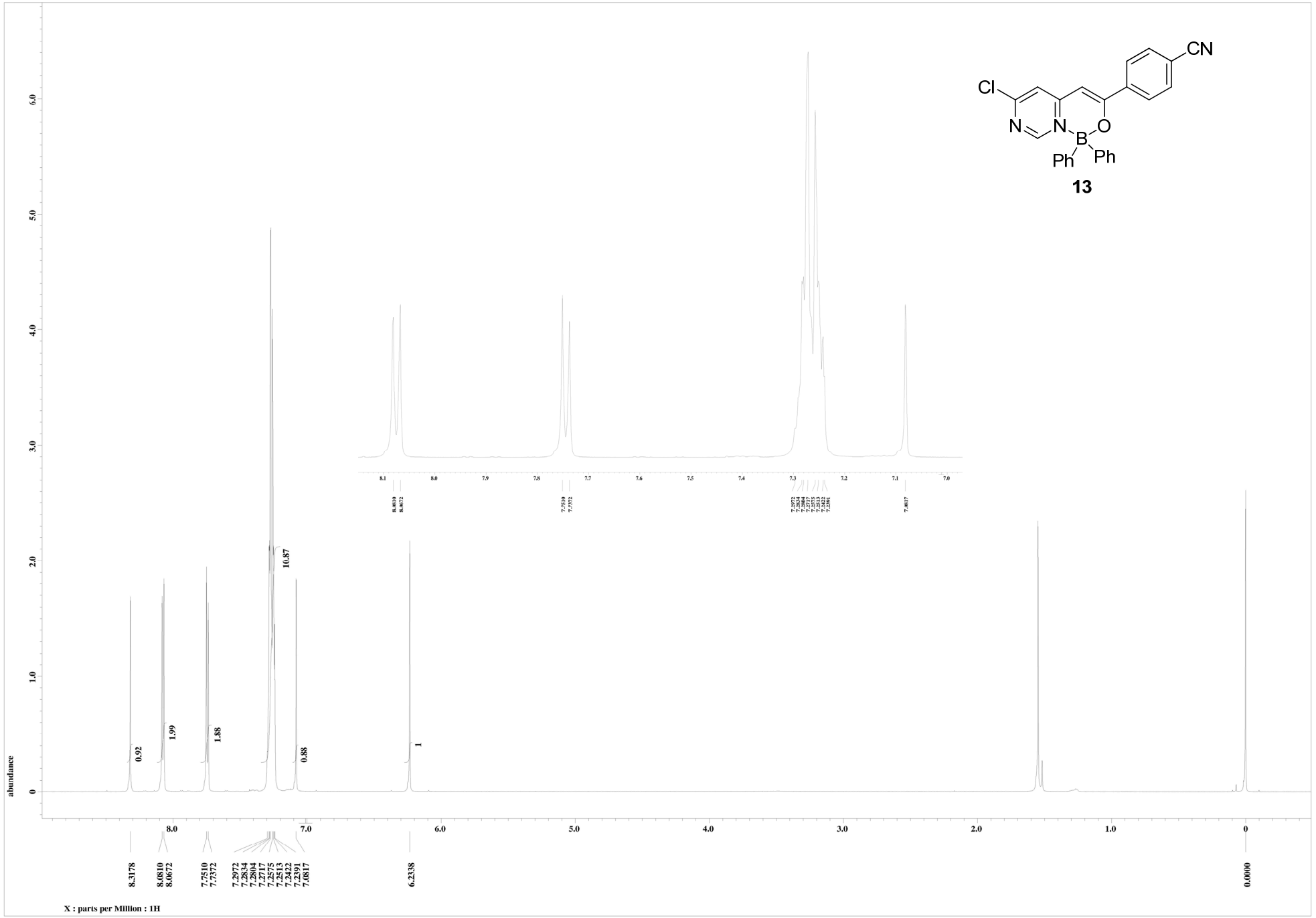


Figure S25. ^{1}H NMR spectra of **13**.

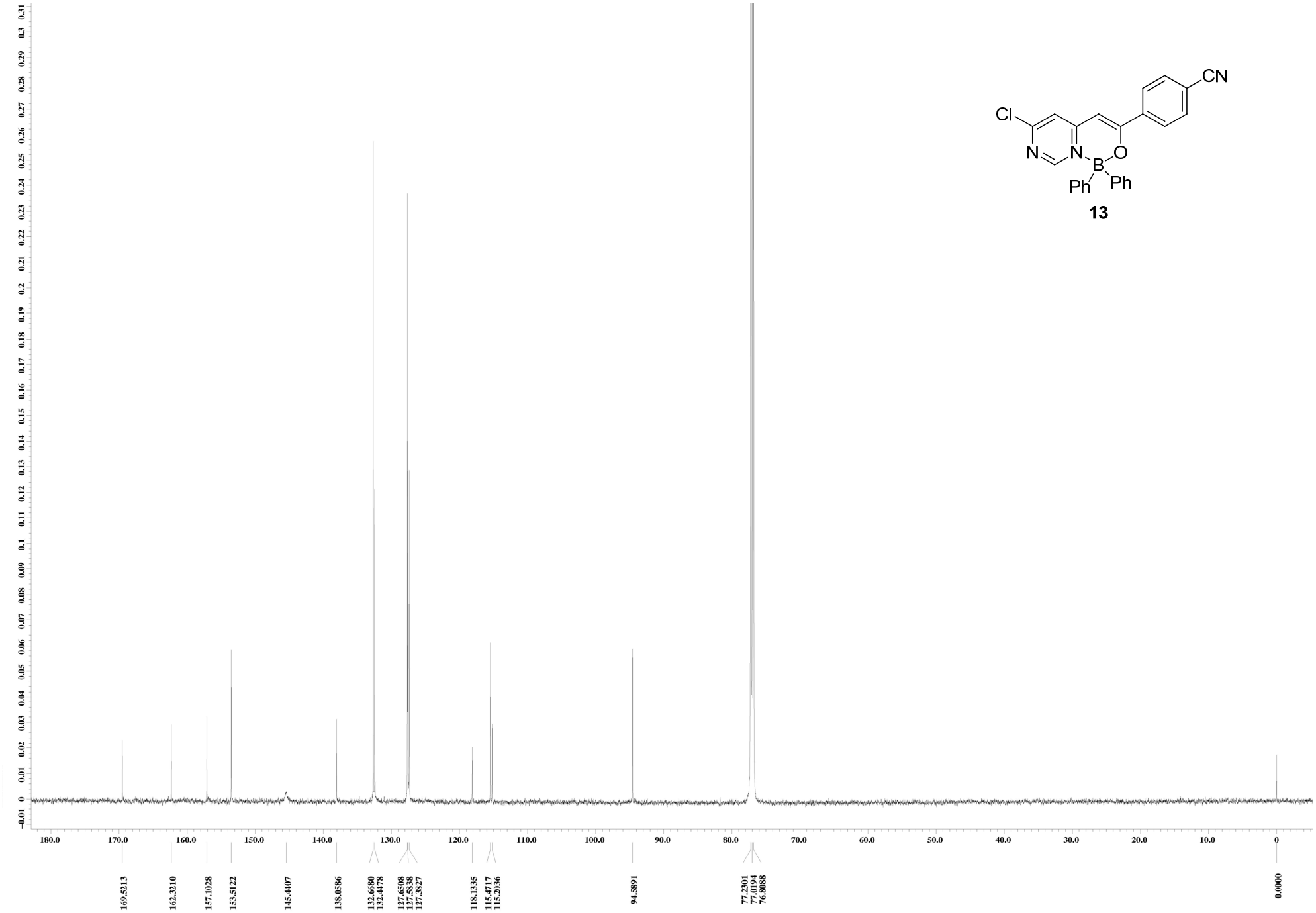


Figure S26. ^{13}C NMR spectra of **13**.

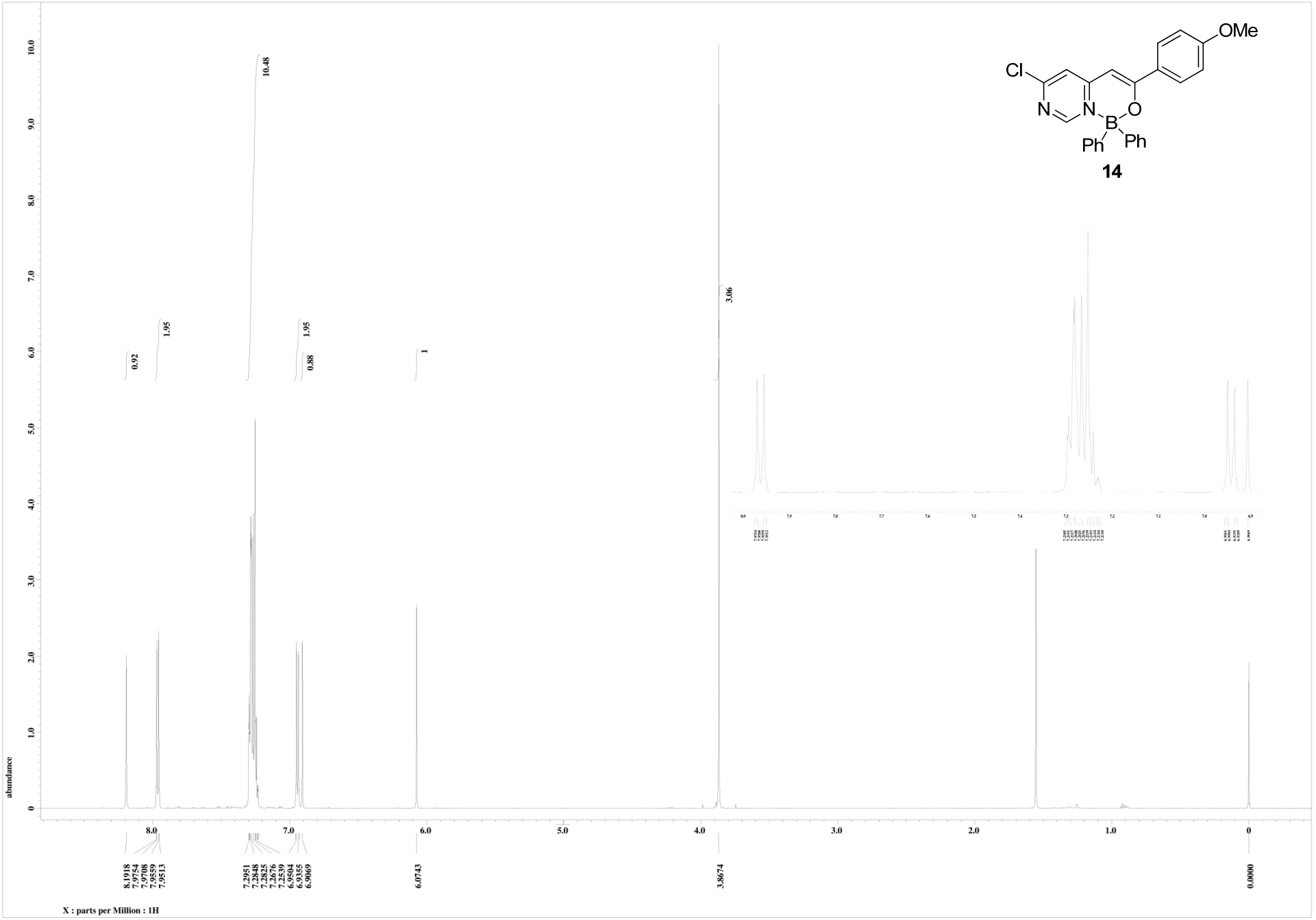


Figure S27. ^{1}H NMR spectra of **14**.

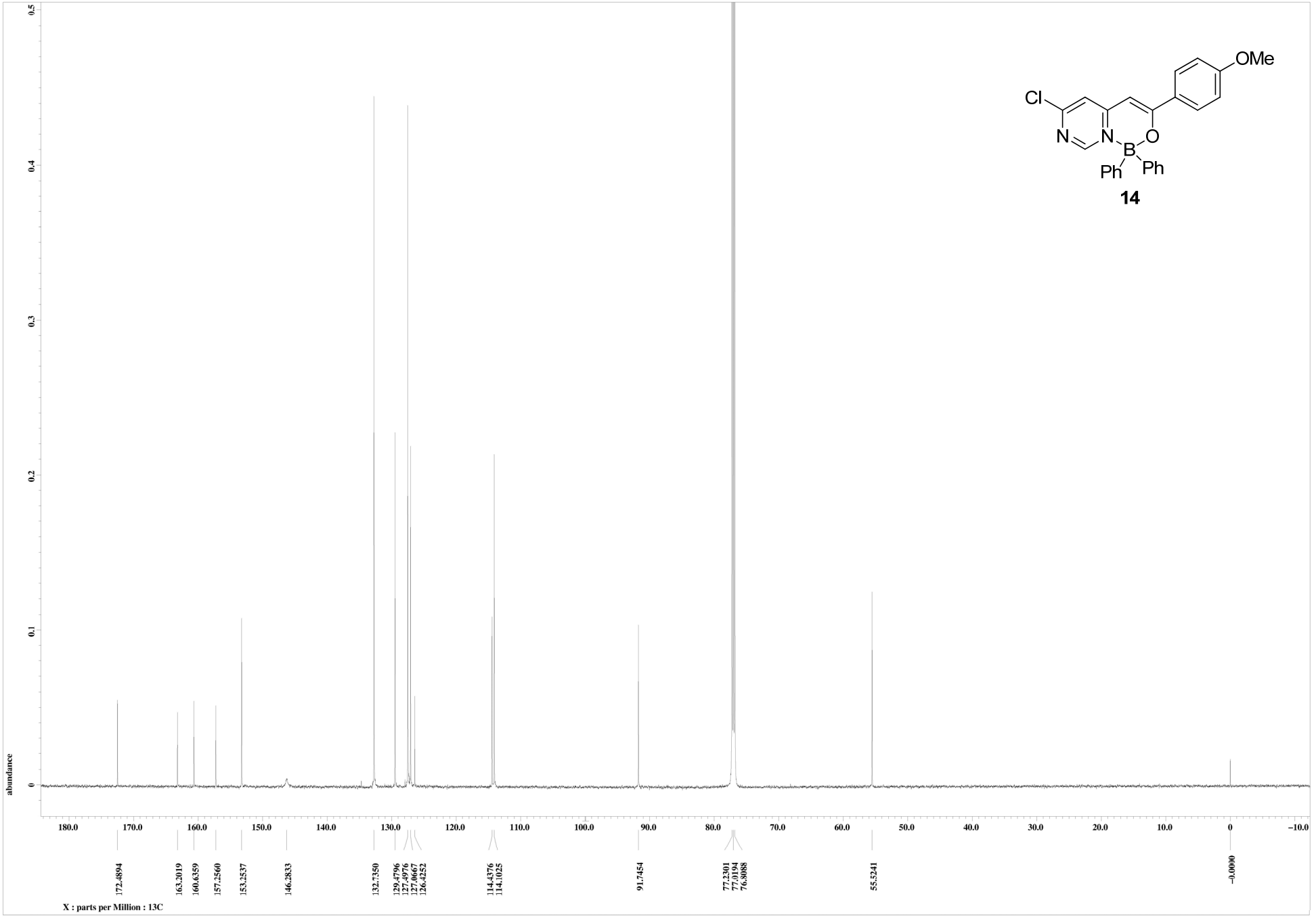


Figure S28. ^{13}C NMR spectra of **14**.

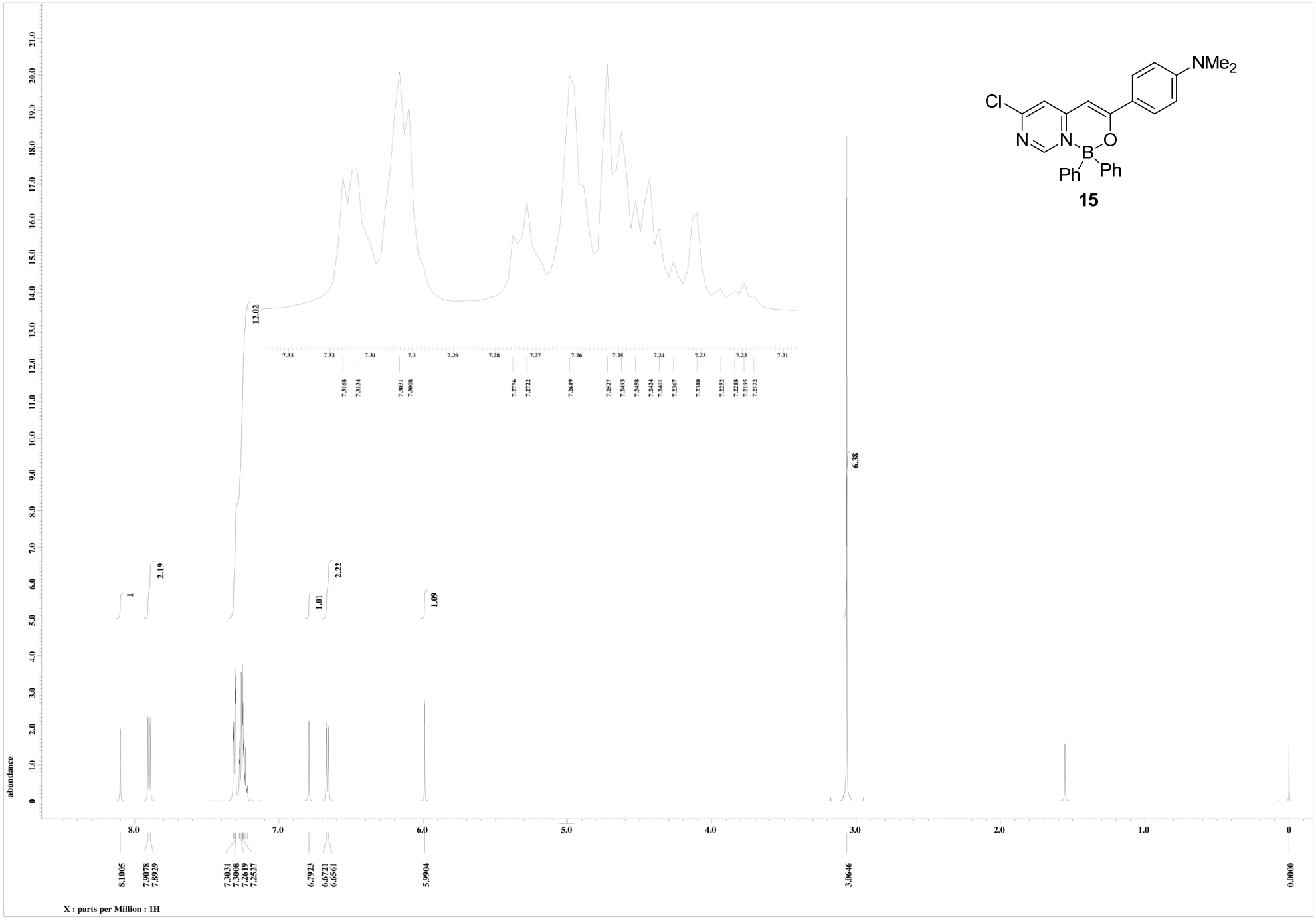


Figure S29. ^{1}H NMR spectra of **15**.

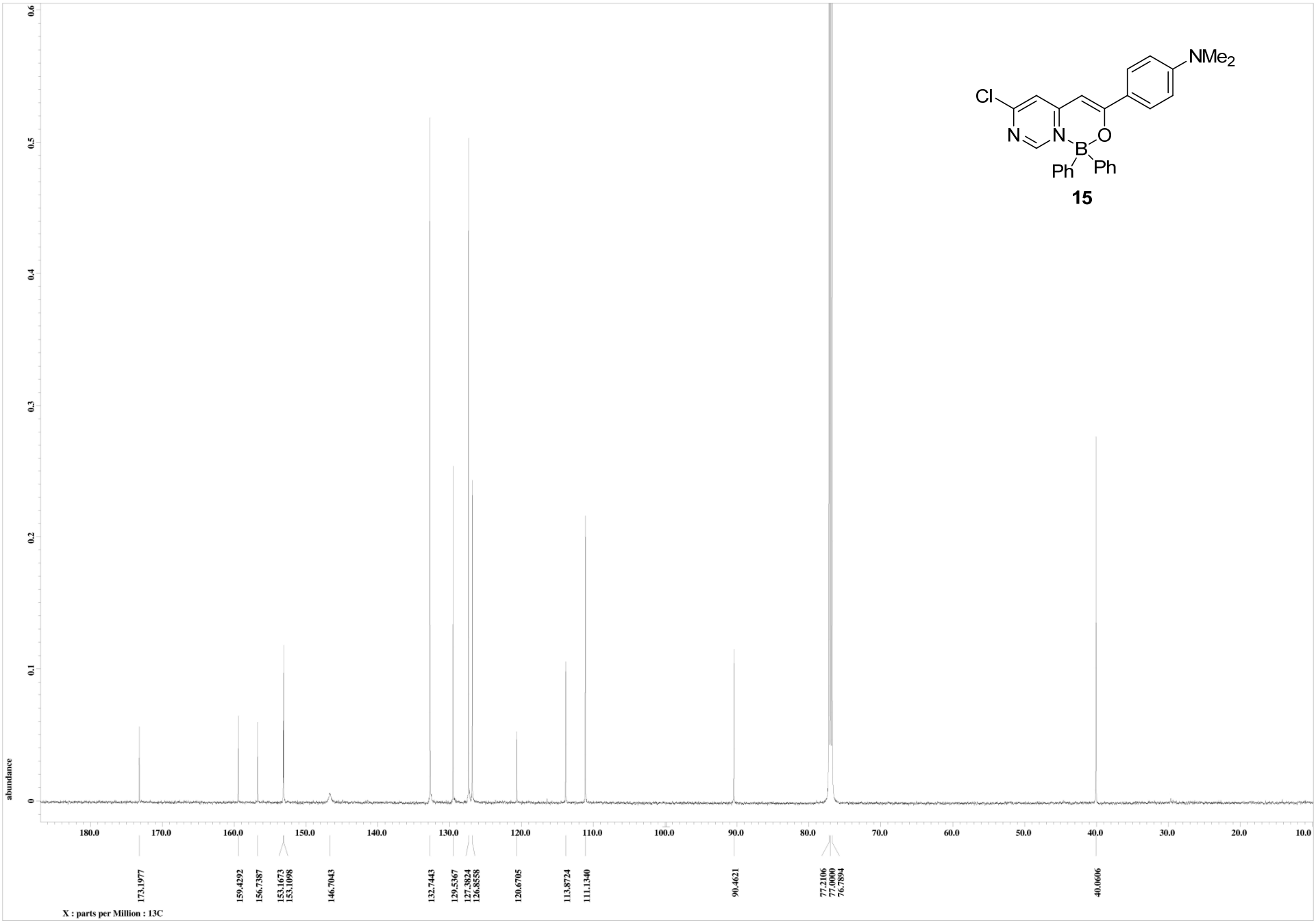


Figure S30. ^{13}C NMR spectra of **15**.