Supporting Information

A new heteropentacyclic system via coupling sterically crowded *o*-benzoquinone with *o*-phenylenediamines

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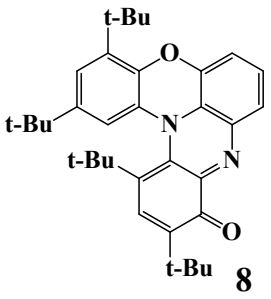
1. Reaction conditions



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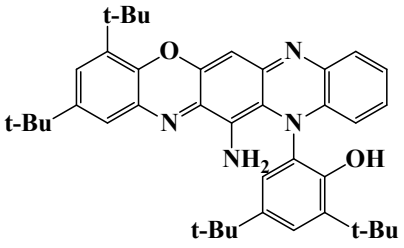

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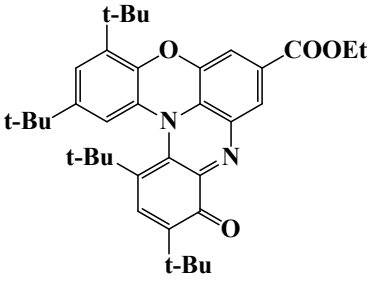

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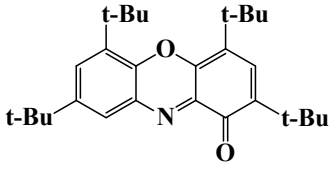

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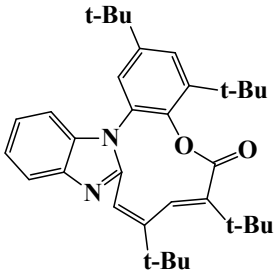

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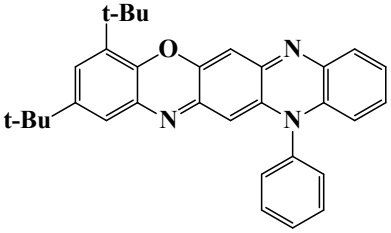
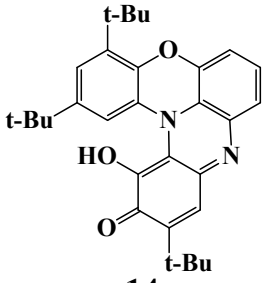


7 ($R^1 = R^2 = H$)



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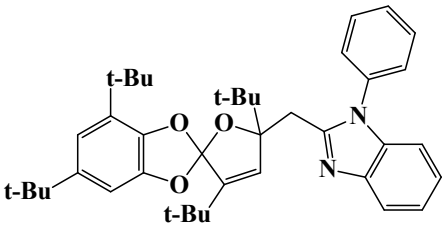

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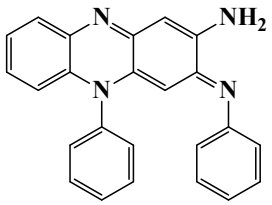

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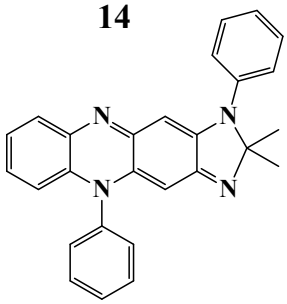

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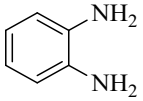
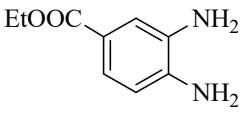
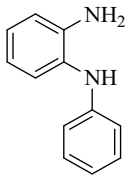
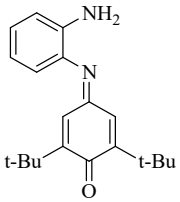
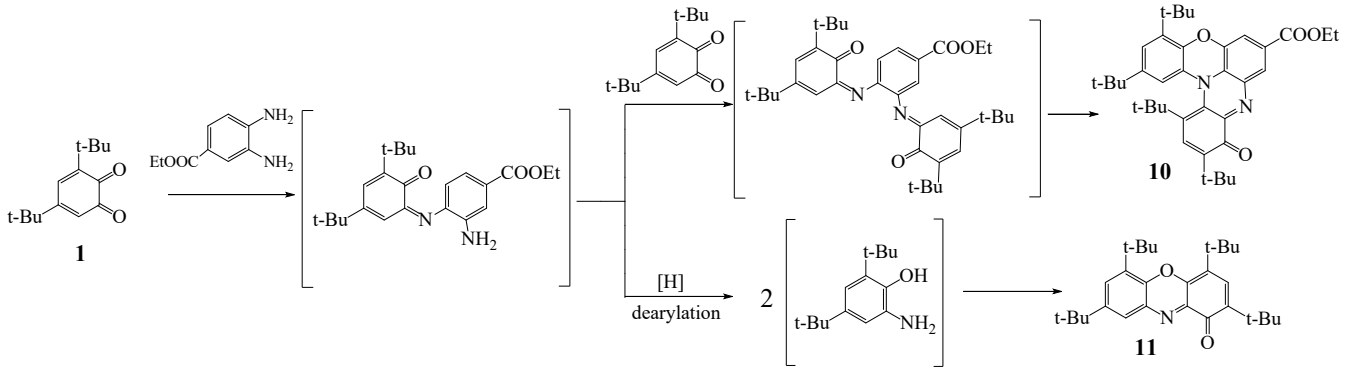
Table S1. New compounds and reaction conditions.

Amine	Solventь	The ratio of reagents, (quinone:amine)	Reaction time, h.	Reaction product	Yield, %
	toluene	1:1	3	**9**	63
			12		15
	isopropanol	1:1	3	**8**	20
				9	32
			12	**8**	22

				9	5
	toluene	2:1	3	**12**	8
			12		52
	isopropanol	2:1	6	**8**	55
	toluene	1:1	3	**10**	47
				11	30
	isopropanol	1:1	3	**10**	5
			12	**11**	27
	toluene	2:1	3	**10**	35
			12	**11**	41
	isopropanol	2:1	3	**11**	48
			12		
	toluene	1:1	3	**17**	37
			12	**18**	16
	isopropanol	1:1	6	**7** ($R^1 = R^2 = H$)	5
			6	**16**	11
			3	**17**	33
	toluene	2:1	6	**7** ($R^1 = R^2 = H$)	7
			3	**17**	28
			12	**18**	14
	isopropanol	2:1	6	**7** ($R^1 = R^2 = H$)	20
			6	**16**	30
			3	**17**	25
			12	**18**	23
	toluene	1:1	8	**14**	39
		2:1	12	**14**	35



Scheme S1. Proposed mechanism of 2,4,6,8-tetra-*tert*-butyl-1H-phenoxazin-1-one **11** formation (a detailed mechanism for the formation of compound **11** is described in ref. 16 of Manuscript).

2. UV spectra

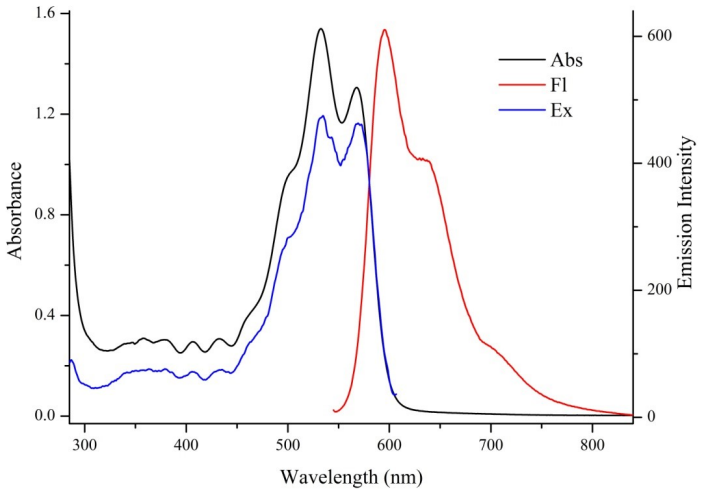


Fig. S1. UV/vis, fluorescence emission (λ_{ex} = 540 nm) and fluorescence excitation (λ_{obs} = 610 nm) spectra of compound **7** ($R^1 = R^2 = H$) (toluene, $T = 293$ K).

3. X-ray study. Molecular geometries. Crystallographic parameters.

Table S2. Crystal data and structure refinement for **8**, **12, 14, 16, 19**.

Parameter	8	12	14	16	19
CCDC Number	2212812	2212829	2212830	2212813	2212831
Empirical formula	$C_{34}H_{42}N_2O_2$	$C_{34}H_{44}N_2O_2$	$C_{30}H_{34}N_2O_3$	$C_{40}H_{50}N_2O_3$	$C_{45}H_{46}CuF_6N_4O_4$
Formula weight	510.69	512.71	470.59	606.82	884.40
Temperature/K	100.01(10)	100.01(11)	99.97(10)	100(2)	100.00(10)
Crystal system	triclinic	monoclinic	monoclinic	triclinic	triclinic
Space group	P-1	I2/a	$P2_1/n$	P-1	P-1
a/Å	9.8617(2)	25.6592(2)	9.2984(2)	10.5024(3)	11.1926(2)
b/Å	11.5168(3)	9.84500(10)	28.6077(5)	12.2437(4)	12.9957(2)
c/Å	15.4591(4)	25.3024(2)	10.9273(3)	15.5391(4)	16.3508(3)
α/°	109.621(2)	90	90	85.566(2)	69.645(2)
β/°	98.038(2)	107.2240(10)	114.557(3)	74.703(3)	88.219(2)
γ/°	93.739(2)	90	90	73.479(3)	89.750(2)
Volume/Å^3	1625.69(7)	6105.12(10)	2643.81(12)	1847.78(10)	2228.67(7)
Z	2	8	4	2	2
ρ_{calc}g/cm^3	1.043	1.116	1.182	1.091	1.318
μ/mm^{-1}	0.497	0.529	0.602	0.529	1.296
F(000)	552.0	2224.0	1008.0	656.0	918.0
Crystal size/mm^3	0.513 × 0.492 × 0.341	0.372 × 0.157 × 0.127	0.381 × 0.239 × 0.209	0.298 × 0.246 × 0.239	0.34 × 0.182 × 0.159
Radiation	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	CuKα (λ = 1.54184)	Cu Kα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.162 to 152.166	7.316 to 152.454	9.42 to 152.558	5.896 to 152.476	7.256 to 152.84
Index ranges	-12 ≤ h ≤ 11, -14 ≤ k ≤ 14, -19 ≤ l ≤ 19	-32 ≤ h ≤ 31, -9 ≤ k ≤ 12, -31 ≤ l ≤ 30	-11 ≤ h ≤ 11, -36 ≤ k ≤ 35, -13 ≤ l ≤ 13	-13 ≤ h ≤ 11, -15 ≤ k ≤ 15, -19 ≤ l ≤ 19	-14 ≤ h ≤ 14, -16 ≤ k ≤ 14, -20 ≤ l ≤ 20
Reflections collected	33958	31952	35368	31832	45994
Independent reflections	6785 [R_{int} = 0.0364, R_{sigma} = 0.0238]	6321 [R_{int} = 0.0160, R_{sigma} = 0.0115]	5437 [R_{int} = 0.0285, R_{sigma} = 0.0164]	7682 [R_{int} = 0.0433, R_{sigma} = 0.0339]	9301 [R_{int} = 0.0401, R_{sigma} = 0.0294]
Data/restraints/parameters	6785/0/355	6321/60/387	5437/0/363	7682/0/419	9301/0/599
Goodness-of-fit on F^2	1.054	1.046	1.026	1.065	1.104
Final R indexes [I>=2σ (I)]	R_1 = 0.0544, wR_2 = 0.1449	R_1 = 0.0374, wR_2 = 0.0956	R_1 = 0.0381, wR_2 = 0.0941	R_1 = 0.0463, wR_2 = 0.1213	R_1 = 0.0459, wR_2 = 0.1240
Final R indexes [all data]	R_1 = 0.0571, wR_2 = 0.1472	R_1 = 0.0387, wR_2 = 0.0968	R_1 = 0.0415, wR_2 = 0.0971	R_1 = 0.0503, wR_2 = 0.1253	R_1 = 0.0477, wR_2 = 0.1255
Largest diff. peak/hole / e Å^{-3}	0.28/-0.27	0.28/-0.27	0.29/-0.20	0.33/-0.29	0.87/-0.56

Table S3. X-ray determined bond lengths of **8**

Bond lengths, Å			
	8		
O15-C14	1.3757(11)	C11-C31	1.5340(14)
O15-C17	1.3987(11)	C8-C7	1.3873(15)
O16-C14	1.1998(12)	C4-C5	1.3966(15)
N1-C9	1.3898(13)	C22-C27	1.5396(13)
N1-C18	1.4277(12)	C20-C23	1.5358(13)
N1-C2	1.3864(12)	C27-C29	1.5359(14)
N3-C2	1.3115(13)	C27-C30	1.5342(15)
N3-C4	1.3911(13)	C27-C28	1.5340(14)
C14-C13	1.4984(13)	C7-C6	1.4045(16)
C9-C8	1.3915(14)	C35-C37	1.5325(14)
C9-C4	1.4041(13)	C35-C36	1.5380(16)
C18-C17	1.4003(13)	C35-C38	1.5331(16)
C18-C19	1.3847(13)	C31-C32	1.5348(15)
C2-C10	1.4694(14)	C31-C34	1.5350(17)
C17-C22	1.3967(13)	C31-C33	1.5289(16)
C12-C13	1.3432(14)	C5-C6	1.3846(16)
C12-C11	1.4815(14)	C23-C25	1.5244(17)
C13-C35	1.5300(13)	C23-C24	1.5245(18)
C21-C22	1.4041(13)	C23-C26	1.5382(17)
C21-C20	1.3921(15)	C23-C24A	1.600(10)
C19-C20	1.3917(14)	C23-C25A	1.538(10)
C11-C10	1.3361(14)	C23-C26A	1.470(10)

Table S4. Valence Angles for **8.**

C6-O1-C14	112.77(12)	C33-C31-C34	107.45(14)
C7-N1-C13	125.08(12)	C33-C31-C32	107.81(14)
C1-N1-C7	117.69(13)	O2-C11-C10	124.35(15)
C1-N1-C13	113.51(12)	O2-C11-C12	119.18(14)
C12-N2-C2	118.10(14)	C10-C11-C12	116.46(13)
C16-C17-C19	119.44(13)	C13-C14-O1	118.60(13)
C18-C17-C16	118.12(13)	C13-C14-C15	121.72(14)
C18-C17-C19	122.45(13)	C15-C14-O1	119.68(13)
C15-C16-C17	123.73(14)	C7-C8-C9	115.93(14)
N1-C7-C12	113.30(13)	C7-C8-C23	128.65(14)
C8-C7-N1	126.78(14)	C9-C8-C23	115.30(13)
C8-C7-C12	119.86(14)	C1-C6-O1	118.17(13)
C18-C13-N1	122.67(13)	C5-C6-O1	121.03(15)
C18-C13-C14	120.57(14)	C5-C6-C1	120.73(15)
C14-C13-N1	116.58(13)	C8-C23-C24	111.62(13)
C17-C18-C13	119.84(13)	C8-C23-C26	107.67(12)
C16-C15-C31	122.39(14)	C25-C23-C8	113.89(12)
C14-C15-C16	116.00(13)	C25-C23-C24	109.11(13)
C14-C15-C31	121.61(13)	C25-C23-C26	105.79(13)
C10-C9-C8	128.03(14)	C24-C23-C26	108.46(13)
C22-C19-C17	112.46(12)	N1-C1-C2	120.63(14)
C22-C19-C21	108.30(13)	C6-C1-N1	118.53(14)
C20-C19-C17	109.12(13)	C6-C1-C2	120.83(14)
C20-C19-C22	108.02(13)	N2-C2-C1	120.13(14)
C20-C19-C21	109.43(14)	N2-C2-C3	121.21(15)
C21-C19-C17	109.47(12)	C1-C2-C3	118.62(16)
C9-C10-C11	117.27(14)	C10-C27-C30	109.27(13)
C9-C10-C27	122.99(14)	C10-C27-C28	109.33(13)
C11-C10-C27	119.74(13)	C28-C27-C30	110.55(14)
N2-C12-C7	124.04(14)	C29-C27-C10	111.51(13)
N2-C12-C11	116.22(14)	C29-C27-C30	107.89(14)
C7-C12-C11	119.62(13)	C29-C27-C28	108.27(14)
C15-C31-C34	110.15(13)	C6-C5-C4	118.60(16)
C15-C31-C32	109.55(13)	C4-C3-C2	119.78(16)
C32-C31-C34	110.02(13)	C3-C4-C5	121.34(15)
C33-C31-C15	111.81(13)		

Table S5. X-ray determined bond lengths of **12**

Bond lengths, Å			
O15-C14	1.3757(11)	C11-C31	1.5340(14)
O15-C17	1.3987(11)	C8-C7	1.3873(15)
O16-C14	1.1998(12)	C4-C5	1.3966(15)
N1-C9	1.3898(13)	C22-C27	1.5396(13)
N1-C18	1.4277(12)	C20-C23	1.5358(13)
N1-C2	1.3864(12)	C27-C29	1.5359(14)
N3-C2	1.3115(13)	C27-C30	1.5342(15)
N3-C4	1.3911(13)	C27-C28	1.5340(14)
C14-C13	1.4984(13)	C7-C6	1.4045(16)
C9-C8	1.3915(14)	C35-C37	1.5325(14)
C9-C4	1.4041(13)	C35-C36	1.5380(16)
C18-C17	1.4003(13)	C35-C38	1.5331(16)
C18-C19	1.3847(13)	C31-C32	1.5348(15)
C2-C10	1.4694(14)	C31-C34	1.5350(17)
C17-C22	1.3967(13)	C31-C33	1.5289(16)
C12-C13	1.3432(14)	C5-C6	1.3846(16)
C12-C11	1.4815(14)	C23-C25	1.5244(17)
C13-C35	1.5300(13)	C23-C24	1.5245(18)
C21-C22	1.4041(13)	C23-C26	1.5382(17)
C21-C20	1.3921(15)	C23-C24A	1.600(10)
C19-C20	1.3917(14)	C23-C25A	1.538(10)
C11-C10	1.3361(14)	C23-C26A	1.470(10)

Table S6. Valence Angles for**12.**

C14-O15-C17	117.36(7)	C19-C20-C21	117.96(9)
C9-N1-C18	124.75(8)	C19-C20-C23	118.92(9)
C2-N1-C9	106.35(8)	C11-C10-C2	121.80(9)
C2-N1-C18	128.08(8)	C29-C27-C22	109.90(8)
C2-N3-C4	104.98(8)	C30-C27-C22	110.47(8)
O15-C14-C13	111.92(8)	C30-C27-C29	109.98(9)
O16-C14-O15	121.70(8)	C30-C27-C28	107.37(10)
O16-C14-C13	126.38(9)	C28-C27-C22	111.65(9)
N1-C9-C8	132.25(9)	C28-C27-C29	107.40(9)
N1-C9-C4	105.03(8)	C8-C7-C6	121.28(10)
C8-C9-C4	122.71(9)	C13-C35-C37	111.78(9)
C17-C18-N1	121.21(8)	C13-C35-C36	107.68(9)
C19-C18-N1	118.32(9)	C13-C35-C38	111.15(9)
C19-C18-C17	120.35(9)	C37-C35-C36	108.05(9)
N1-C2-C10	121.08(9)	C37-C35-C38	107.53(9)
N3-C2-N1	113.14(9)	C38-C35-C36	110.62(10)
N3-C2-C10	125.78(9)	C11-C31-C32	110.72(9)
O15-C17-C18	118.84(8)	C11-C31-C34	110.77(9)
C22-C17-O15	119.92(8)	C32-C31-C34	107.46(10)
C22-C17-C18	121.05(9)	C33-C31-C11	108.66(10)
C13-C12-C11	129.78(9)	C33-C31-C32	109.95(10)
C14-C13-C35-	115.74(8)	C33-C31-C34	109.26(11)
C12-C13-C14	121.08(9)	C6-C5-C4	117.87(10)
C12-C13-C35	123.16(9)	C20-C23-C26	111.92(10)
C20-C21-C22	123.50(9)	C20-C23-C24A	112.7(4)
C18-C19-C20	120.53(9)	C20-C23-C25A	106.8(4)
C12-C11-C31	115.86(8)	C25-C23-C20	109.10(9)
C10-C11-C12	121.72(9)	C25-C23-C24	110.30(12)
C10-C11-C31	122.35(9)	C25-C23-C26	107.98(11)
C7-C8-C9	116.69(9)	C24-C23-C20	108.99(9)
N3-C4-C9	110.50(9)	C24-C23-C26	108.54(12)
N3-C4-C5	129.67(9)	C25A-C23-C24A	103.8(7)
C5-C4-C9	119.81(10)	C26A-C23-C20	111.3(5)
C17-C22-C21	116.60(9)	C26A-C23-C24A	107.6(8)
C17-C22-C27	121.84(9)	C26A-C23-C25A	114.4(8)
C21-C22-C27	121.55(9)	C5-C6-C7	121.62(10)
C21-C20-C23	123.12(9)		

Table S7. X-ray determined bond lengths of **14**.

Bond lengths, Å			
O2-C1	1.3486(13)	C14-C13	1.3961(15)
O3-C2	1.2436(13)	C14-C15	1.3964(16)
O1-C13	1.3980(13)	C14-C19	1.5346(15)
O1-C11	1.3866(13)	C3-C2	1.4848(14)
N1-C18	1.4266(13)	C3-C4	1.3484(15)
N1-C12	1.3886(13)	C3-C27	1.5291(15)
N1-C6	1.3953(14)	C4-C5	1.4475(15)
N2-C7	1.3881(15)	C11-C10	1.3743(15)
N2-C5	1.3083(14)	C7-C8	1.4054(15)
C18-C17	1.3870(15)	C10-C9	1.4022(17)
C18-C13	1.3929(15)	C27-C30	1.5335(15)
C16-C17	1.3875(15)	C27-C29	1.5389(15)
C16-C15	1.3955(16)	C27-C28	1.5368(16)
C16-C23	1.5352(15)	C23-C24	1.5313(16)
C1-C6	1.3634(15)	C23-C26	1.5329(18)
C1-C2	1.4498(15)	C23-C25	1.5304(17)
C12-C11	1.3898(16)	C8-C9	1.3777(17)
C12-C7	1.4028(15)	C19-C21	1.5340(17)
C6-C5	1.4591(14)	C19-C22	1.5399(17)

Table S8. Valence Angles for**14.**

C11-O1-C13	113.83(8)	C3-C4-C5	123.38(10)
C12-N1-C18	115.12(9)	O1-C11-C12	118.70(9)
C12-N1-C6	117.91(9)	C10-C11-O1	120.62(10)
C6-N1-C18	125.17(9)	C10-C11-C12	120.60(10)
C5-N2-C7	117.42(9)	N2-C7-C12	120.97(10)
C17-C18-N``1	121.93(10)	N2-C7-C8	120.59(10)
C17-C18-C13	120.72(10)	C12-C7-C8	118.43(10)
C13-C18-N1	117.11(9)	C11-C10-C9	119.14(11)
C17-C16-C15	118.29(10)	N2-C5-C6	124.44(10)
C17-C16-C23	121.16(10)	N2-C5-C4	117.10(10)
C15-C16-C23	120.48(10)	C4-C5-C6	118.38(9)
O2-C1-C6	120.64(10)	C16-C15-C14	123.54(10)
O2-C1-C2	117.88(9)	C3-C27-C30	111.05(9)
C6-C1-C2	121.46(10)	C3-C27-C29	109.79(9)
N1-C12-C11	118.73(10)	C3-C27-C28	109.91(9)
N1-C12-C7	120.57(10)	C30-C27-C29	107.73(9)
C11-C12-C7	120.69(10)	C30-C27-C28	108.54(10)
N1-C6-C5	116.13(9)	C28-C27-C29	109.78(10)
C1-C6-N1	124.44(10)	C24-C23-C16	110.87(9)
C1-C6-C5	119.37(10)	C24-C23-C26	107.87(10)
C18-C17-C16	119.77(10)	C26-C23-C16	111.41(10)
C13-C14-C15	116.35(10)	C25-23-C16	107.99(9)
C13-C14-C19	121.68(10)	C25-C23-C24	109.58(11)
C15-C14-C19	121.97(10)	C25-C23-C26	109.11(13)
C18-C13-O1	119.14(10)	C9-C8-C7	120.10(11)
C18-C13-C14	121.20(10)	C8-C9-C10	121.03(10)
C14-C13-O1	119.66(10)	C14-C19-C22	110.44(9)
C2-C3-C27	119.31(9)	C21-C19-C14	109.25(10)
C4-C3-C2	117.70(10)	C21-C19-C22	110.34(10)
C4-C3-C27	122.94(10)	C20-C19-C14	111.31(10)
O3-C2-C1	118.11(10)	C20-C19-C21	107.59(10)
O3-C2-C3	122.61(10)	C20-C19-C22	107.86(10)
C1-C2-C3	119.27(9)		

Table S9. X-ray determined bond lengths of **16.**

Bond lengths, Å			
O3-C23	1.3735(14)	C7-C6	1.3937(17)
O3-C22	1.4385(14)	C2-C3	1.3954(18)
O2-C28	1.3850(13)	C15-C14	1.5535(15)
O2-C22	1.4319(13)	C15-C16	1.5593(16)
O1-C22	1.3924(15)	C25-C24	1.4044(17)
O1-C15	1.4524(13)	C25-C37	1.5357(15)
N1-C1	1.3805(15)	C33-C36	1.5369(17)
N1-C8	1.4323(15)	C33-C34	1.5392(17)
N1-C7	1.3829(16)	C33-C35	1.5297(16)
N2-C1	1.3119(16)	C16-C17	1.5403(16)
N2-C2	1.3880(16)	C16-C18	1.5367(16)
C1-C14	1.4974(16)	C16-C19	1.5360(18)
C27-C28	1.3845(16)	C37-C39	1.5314(18)
C27-C26	1.4112(16)	C37-C40	1.5389(18)
C27-C33	1.5309(15)	C37-C38	1.5366(19)
C28-C23	1.3820(16)	C9-C10	1.3906(19)
C8-C9	1.3879(17)	C13-C12	1.3905(19)
C8-C13	1.3883(18)	C29-C31	1.5300(17)
C23-C24	1.3739(16)	C29-C30	1.539(2)
C26-C25	1.3987(17)	C29-C32	1.5276(19)
C22-C21	1.5095(15)	C10-C11	1.385(2)
C21-C20	1.3265(17)	C6-C5	1.388(2)
C21-C29	1.5163(17)	C3-C4	1.385(2)
C20-C15	1.4994(16)	C12-C11	1.389(2)
C7-C2	1.4032(17)	C5-C4	1.401(2)

Table S10. Valence Angles for**16.**

C23-O3-C22	105.80(8)	C20-C15-C14	110.87(10)
C28-O2-C22	106.09(8)	C20-C15-C16	114.29(9)
C22-O1-C15	110.39(8)	C14-C15-C16	112.09(9)
C1-N1-C8	129.72(10)	C1-C14-C15	112.21(9)
C1-N1-C7	106.29(10)	C26-C25-C24	119.06(10)
C7-N1-C8	123.86(10)	C26-C25-C37	122.04(11)
C1-N2-C2	105.40(10)	C24-C25-C37	118.77(11)
N1-C1-C14	123.01(11)	C23-C24-C25	117.20(11)
N2-C1-N1	112.93(10)	C27-C33-C36	110.14(9)
N2-C1-C14	123.99(10)	C27-C33-C34	108.50(10)
C28-C27-C26	114.25(10)	C36-C33-C34	109.81(10)
C28-C27-C33	121.83(10)	C35-C33-C27	111.62(9)
C26-C27-C33	123.91(10)	C35-C33-C36	108.07(10)
C27-C28-O2	128.79(10)	C35-C33-C34	108.67(10)
C23-C28-O2	108.59(10)	C17-C16-C15	108.96(10)
C23-C28-C27	122.62(10)	C18-C16-C15	110.45(10)
C9-C8-N1	119.13(11)	C18-C16-C17	109.39(10)

C9-C8-C13	120.95(11)	C19-C16-C15	110.85(10)
C13-C8-N1	119.81(11)	C19-C16-C17	108.32(10)
O3-C23-C28	109.78(10)	C19-C16-C18	108.84(11)
O3-C23-C24	127.44(11)	C25-C37-C40	108.25(10)
C24-C23-C28	122.78(11)	C25-C37-C38	110.20(11)
C25-C26-C27	124.08(11)	C39-C37-C25	112.35(10)
O3-C22-C21	112.80(10)	C39-C37-C40	108.65(12)
O2-C22-O3	105.73(8)	C39-C37-C38	108.15(11)
O2-C22-C21	113.51(9)	C38-C37-C40	109.20(12)
O1-C22-O3	108.50(9)	C8-C9-C10	119.52(12)
O1-C22-O2	109.01(9)	C8-C13-C12	118.83(12)
O1-C22-C21	107.17(9)	C21-C29-C31	109.34(10)
C22-C21-C29	124.11(10)	C21-C29-C30	111.20(10)
C20-C21-C22	106.82(10)	C21-C29-C32	109.94(12)
C20-C21-C29	129.04(11)	C31-C29-C30	107.30(12)
C21-C20-C15	112.42(10)	C32-C29-C31	109.49(12)
N1-C7-C2	105.62(10)	C32-C29-C30	109.53(14)
N1-C7-C6	131.90(12)	C11-C10-C9	120.17(12)
C6-C7-C2	122.47(12)	C5-C6-C7	116.55(13)
N2-C2-C7	109.74(11)	C4-C3-C2	118.09(13)
N2-C2-C3	130.31(12)	C11-C12-C13	120.76(12)
C3-C2-C7	119.95(12)	C10-C11-C12	119.75(12)
O1-C15-C20	102.77(9)	C6-C5-C4	121.74(13)
O1-C15-C14	107.99(9)	C3-C4-C5	121.19(13)
O1-C15-C16	108.20(9)		

Table S11. X-ray determined bond lengths of **19.**

Bond lengths, Å			
Cu-O4	2.2260(14)	C18-C5	1.430(3)
Cu-O2	1.9328(14)	C18-C1	1.411(3)
Cu-O3	1.9863(14)	C13-C12	1.385(3)
Cu-N1	2.0195(16)	C13-C14	1.393(3)
CuN4	1.9693(16)	C10-C11	1.406(3)
O1-C8	1.364(2)	C10-C9	1.395(3)
O1 C9	1.387(2)	C3-C2	1.412(3)
N1-C17	1.323(2)	C11-C12	1.401(3)
N1-C18	1.368(2)	C9-C14	1.404(3)
N2-C6	1.329(3)	C4-C5	1.417(3)
N2-C5	1.358(3)	C4-C3	1.366(3)
N4-C16	1.324(2)	C17-C16	1.461(2)
N3-C15	1.304(3)	C15-C16	1.456(3)
N3-C14	1.388(2)	C15-C8	1.462(3)
C6-C17	1.442(3)	C8-C7	1.357(3)
C6-C7	1.438(3)		

Table S12. Valence Angles for**19.**

O2-Cu-O4	91.40(6)	C10-C9-C14	121.85(17)
O2-Cu-O3	89.34(6)	N3-C14-C13	117.94(17)
O2-Cu-N1	165.35(6)	N3-C14-C9	122.31(17)
O2-Cu-N4	83.10(6)	C13-C14-C9	119.71(17)
O3-Cu-O4	85.09(6)	C3-C4-C5	120.22(18)
O3-Cu-N1	104.27(6)	O4-C44-C45	115.77(19)
N1-Cu-O4	95.07(6)	O4-C44-C43	128.8(2)
N4-Cu-O4	122.93(6)	C43-C44-C45	115.43(18)
N4-Cu-O3	150.98(7)	C8-C7-C6	119.80(17)
N4-Cu-N1	82.36(7)	C29-C30-C31	124.42(18)
C8-O1-C9	119.69(15)	C28-C29-C37	119.58(17)
C44-O4-Cu	119.31(14)	C30-C29-C28	117.20(17)
C28-O2-Cu	112.33(12)	C30-C29-C37	123.20(17)
C42-O3-Cu	123.39(14)	N2-C5-C18	122.24(17)
C17-N1-Cu	110.21(12)	N2-C5-C4	118.72(17)
C17-N1-C18	118.58(16)	C4-C5-C18	119.04(18)
C18-N1-Cu	130.92(13)	C10-C19-C20	109.68(16)
C6-N2-C5	117.40(16)	C10-C19-C22	111.76(16)
C16-N4-Cu	113.86(13)	C20-C19-C22	107.97(16)
C16-N4-C27	133.89(17)	C21-C19-C10	110.42(16)
C27-N4-Cu	112.25(12)	C21-C19-C20	109.98(16)
C15-N3-C14	117.68(16)	C21-C19-C22	106.97(17)
N2-C6-C17	120.92(17)	C4-C3-C2	120.49(18)
N2-C6-C7	119.48(17)	C12-C23-C26	109.71(17)
C7-C6-C17	119.59(17)	C25-C23-C12	112.48(17)
N1-C17-C6	121.59(17)	C25-C23-C24	108.42(18)
N1-C17-C16	118.37(16)	C25-C23-C26	108.31(18)
C6-C17-C16	119.95(17)	C24-C23-C12	108.82(17)
N3-C15-C16	119.83(17)	C24-C23-C26	109.04(18)
N3-C15-C8	122.76(17)	C1-C2-C3	121.08(19)
C16-C15-C8	117.30(16)	C34-C33-C31	108.60(16)
C31-C32-C27	120.50(18)	C36-C33-C31	111.71(17)
C32-C31-C30	118.18(18)	C36-C33-C34	107.93(19)
C32-C31-C33	122.39(17)	C35-C33-C31	111.26(17)
C30-C31-C33	119.41(17)	C35-C33-C34	109.3(2)
N4-C16-C17	113.56(16)	C35-C33-C36	107.9(2)
N4-C16-C15	128.63(17)	C2-C1-C18	119.41(18)
C15-C16-C17	117.64(16)	O3-C42-C43	128.7(2)
O1-C8-C15	118.05(16)	O3-C42-C41	113.0(2)
C7-C8-O1	118.41(17)	C43-C42-C41	118.3(2)
C7-C8-C15	123.54(17)	F3-C45-F2	107.02(18)
N1-C18-C5	119.01(17)	F3-C45-C44	112.47(18)
N1-C18-C1	121.29(17)	F1-C45-F3	107.82(19)
C1-C18-C5	119.67(17)	F1-C45-F2	107.44(19)
C12-C13-C14	121.05(18)	F1-C45-C44	111.97(18)

C11-C10-C19	121.92(17)	F2-C45-C44	109.87(18)
C9-C10-C11	115.69(17)	C42-C43-C44	121.55(19)
C9-C10-C19	122.38(17)	C29-C37-C38	109.84(16)
N4-C27-C32	127.29(17)	C29-C37-C39	109.19(16)
N4-C27-C28	111.70(16)	C29-C37-C40	111.59(17)
C32-C27-C28	120.48(17)	C39-C37-C38	110.18(18)
C12-C11-C10	124.35(18)	C40-C37-C38	107.09(17)
C13-C12-C11	117.33(17)	C40-C37-C39	108.92(17)
C13-C12-C23	119.44(17)	F5-C41-F6	105.9(2)
C11-C12-C23	123.22(17)	F5-C41-C42	114.0(2)
O2-C28-C27	119.53(17)	F6-C41-C42	110.5(2)
O2-C28-C29	121.86(17)	F4-C41-F5	108.3(2)
C29-C28-C27	118.61(17)	F4-C41-F6	107.4(2)
O1-C9-C10	119.27(16)	F4-C41-C42	110.50(19)
O1-C9-C14	118.88(16)		

4. NMR spectra

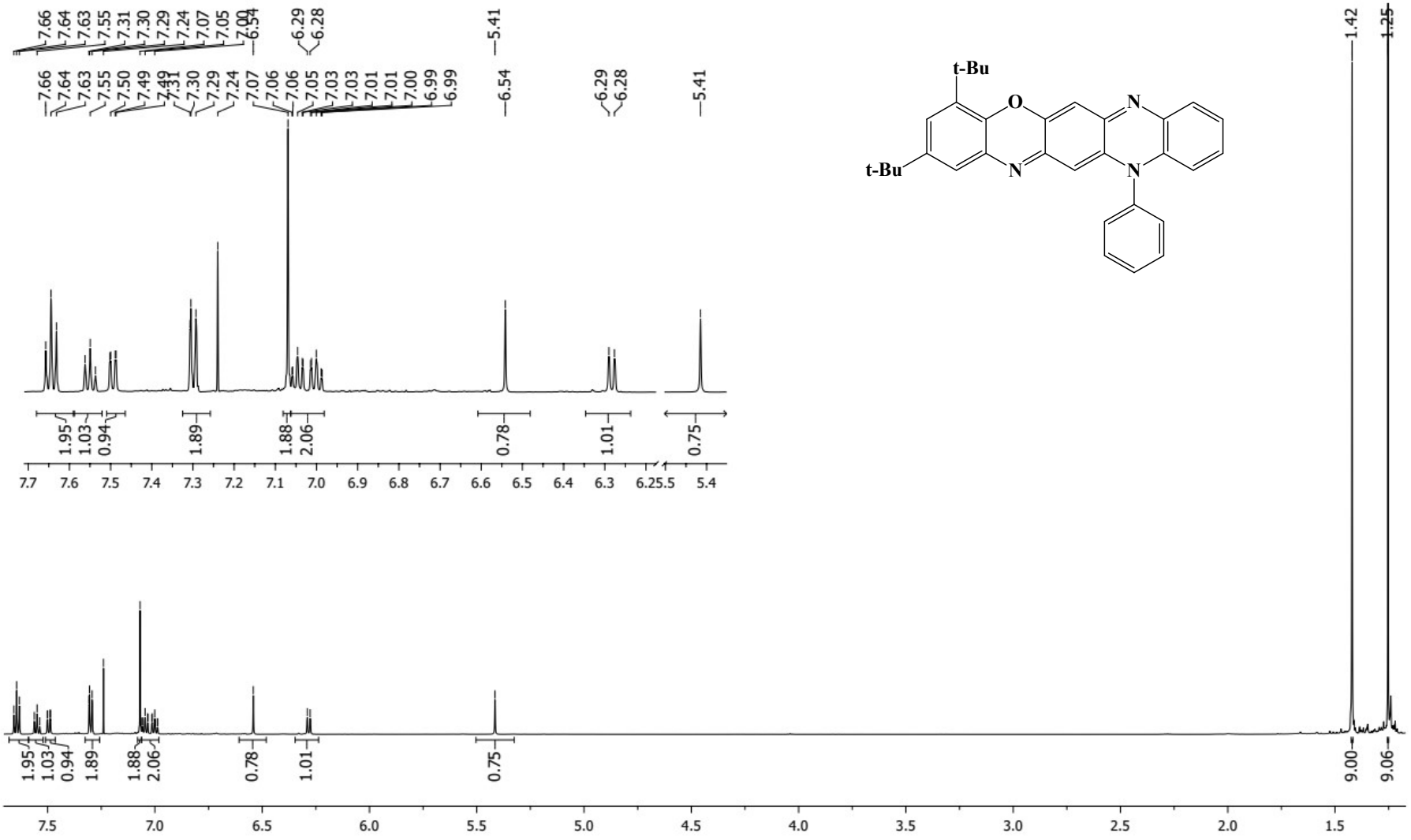


Fig. S2. ^{1}H NMR spectrum of 2,4-di-*tert*-butyl-12-phenyl-12H-quinoxalino[2,3-b]phenoxazine **7** ($R^1 = R^2 = H$).

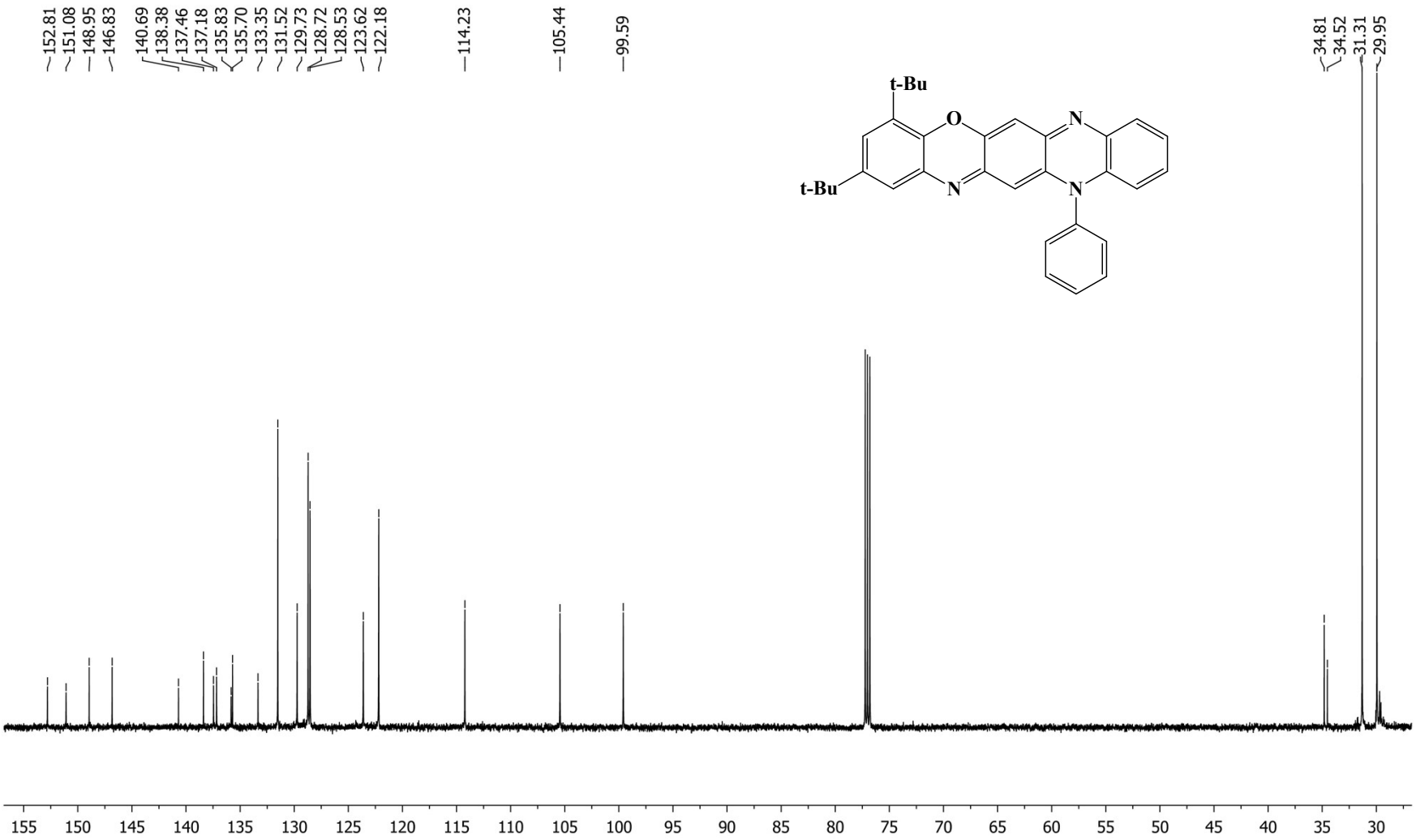


Fig. S3. ^{13}C NMR spectrum of 2,4-di-*tert*-butyl-12-phenyl-12H-quinoxalino[2,3-b]phenoxazine **7** ($R^1 = R^2 = H$).

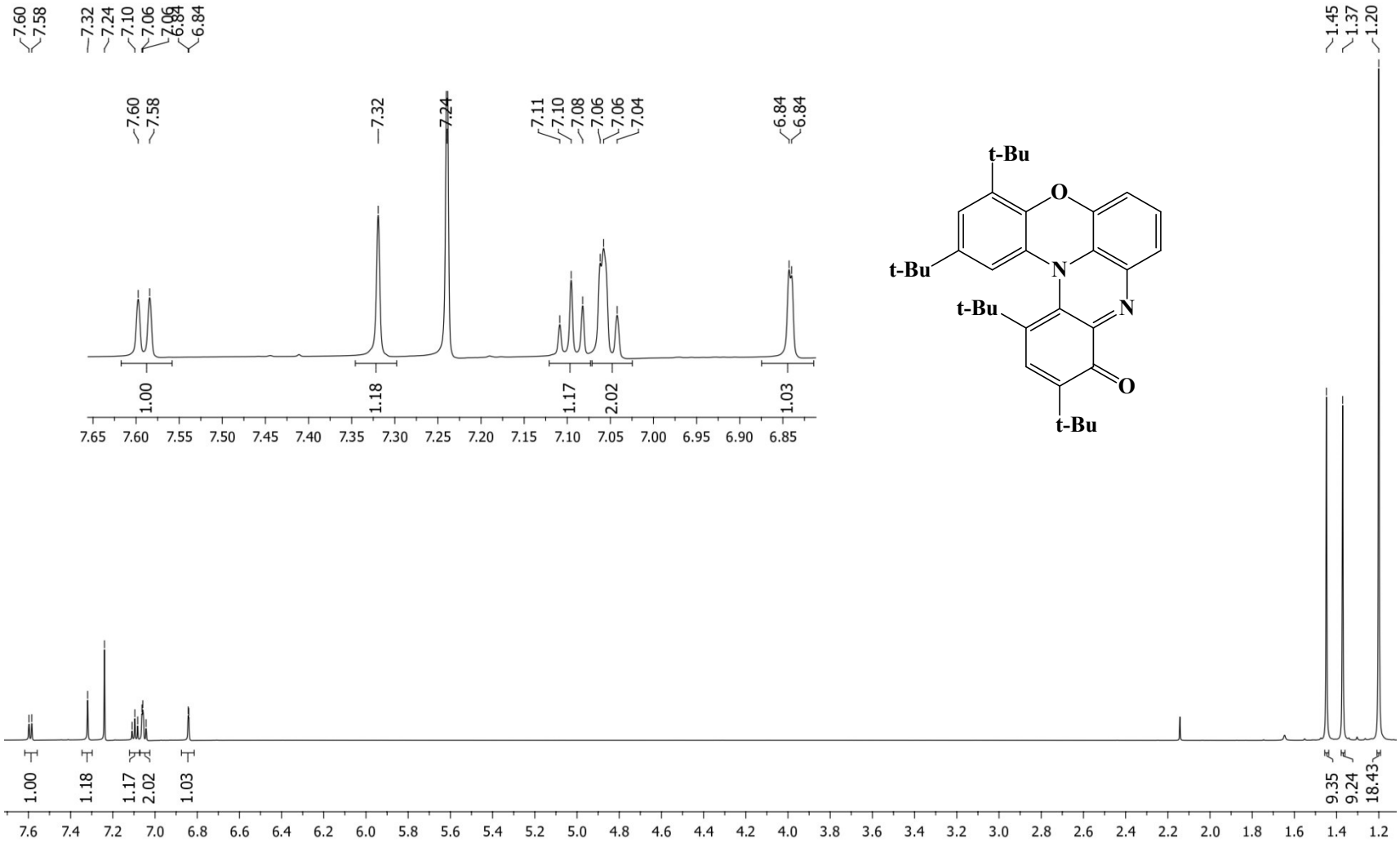


Fig. S4. ^{1}H NMR spectrum of 2,4,11,13-tetra-*tert*-butyl-10H-quinoxalino[3,2,1-kl]phenoxazin-10-one **8**.

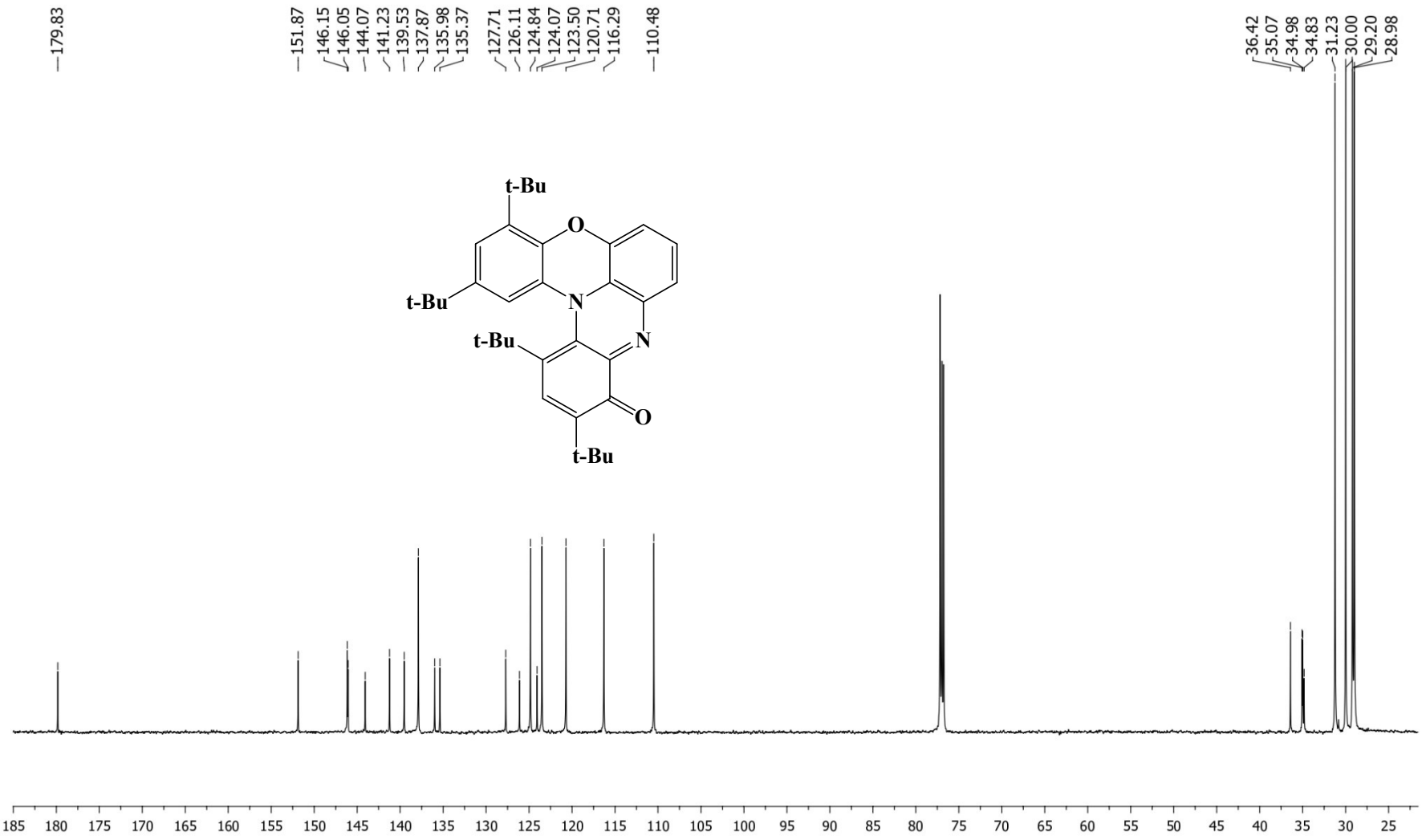


Fig. S5. ^{13}C NMR spectrum of 2,4,11,13-tetra-*tert*-butyl-10H-quinoxalino[3,2,1-kl]phenoxazin-10-one **8**.

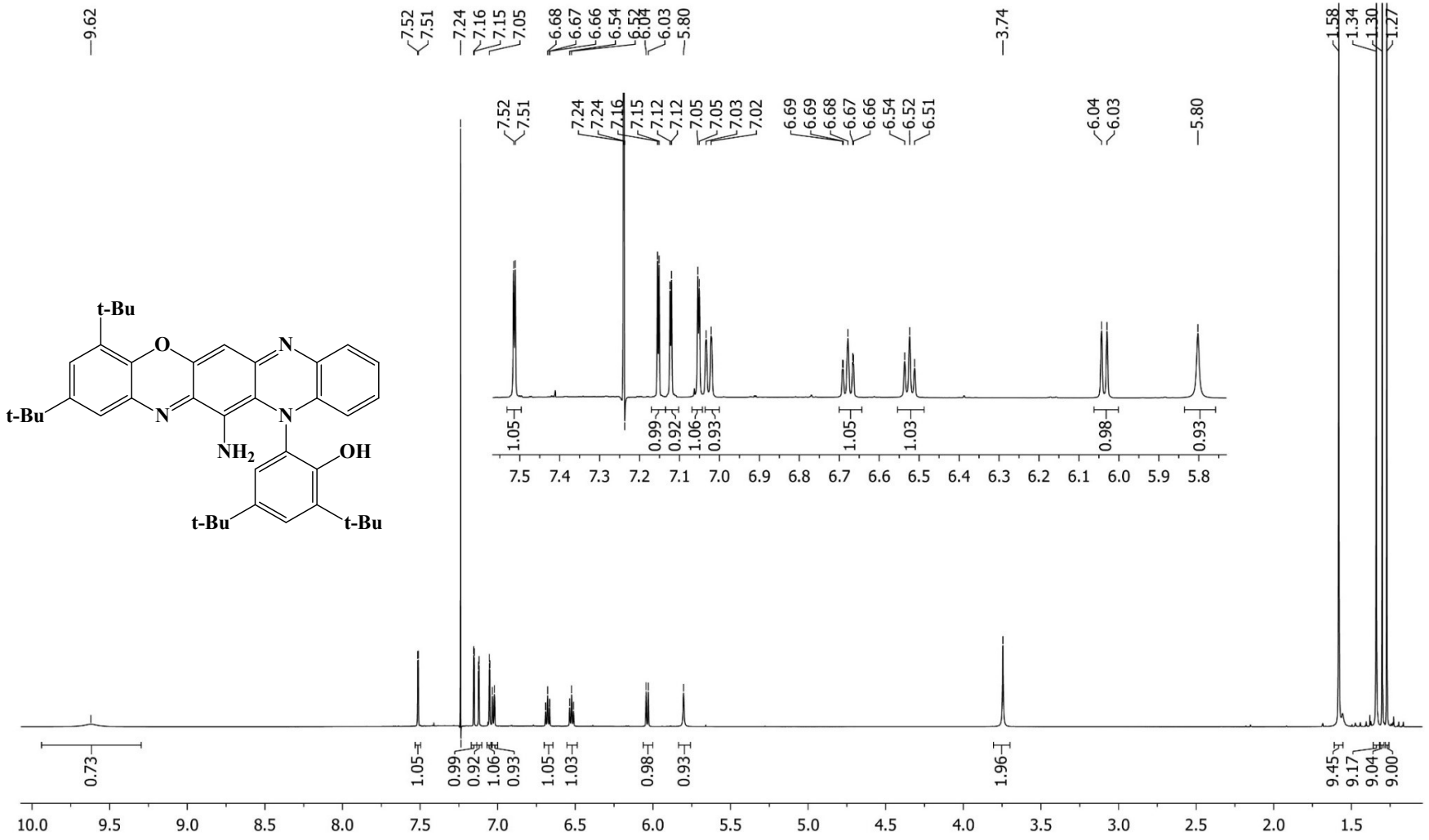


Fig. S6. ^{1}H NMR spectrum of 2-(13-amino-2,4-di-*tert*-butyl-12H-quinoxalino[2,3-b]phenoxazin-12-yl)-4,6-di-*tert*-butylphenol **9**.

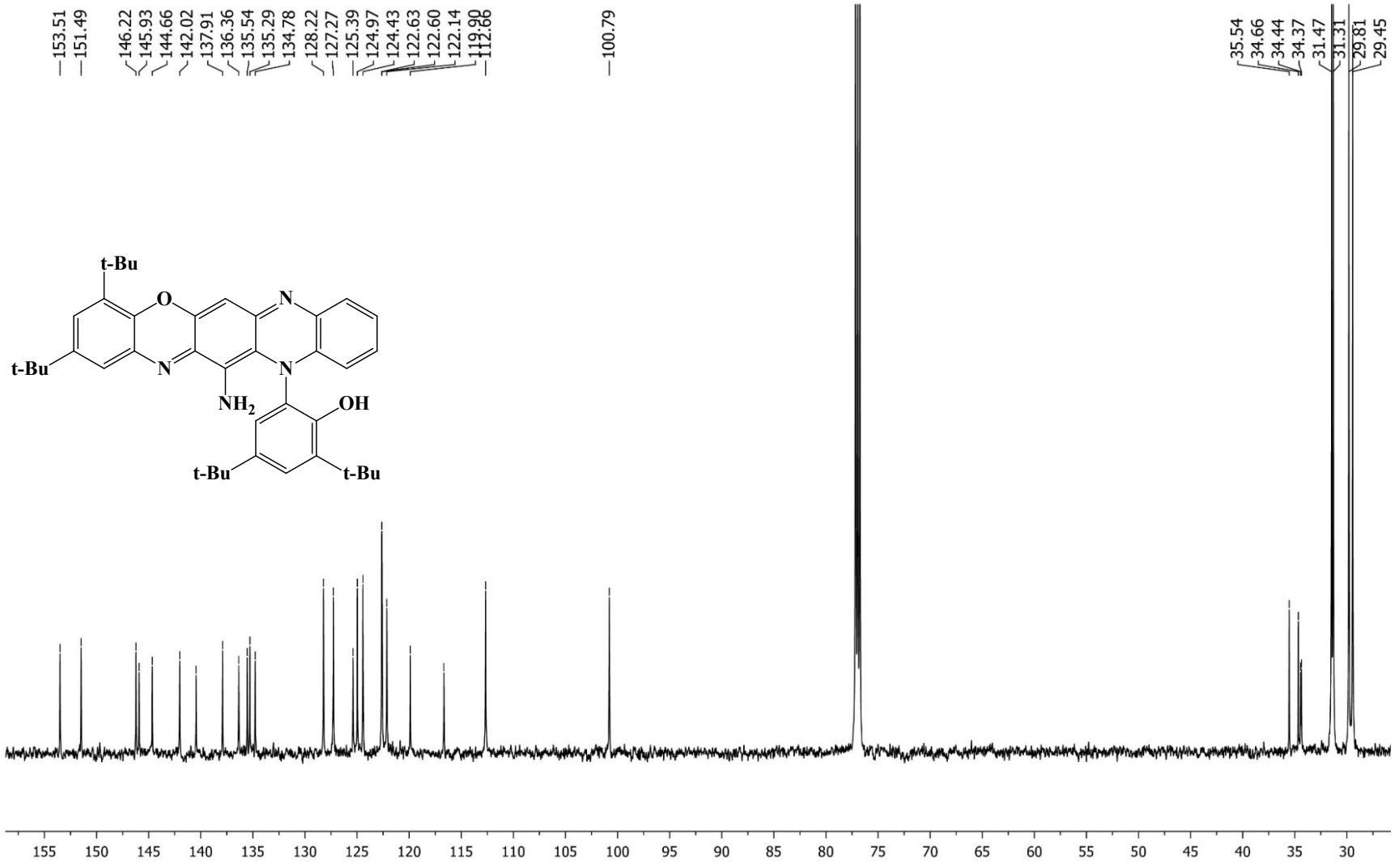


Fig. S7. ^{13}C NMR spectrum of 2-(13-amino-2,4-di-*tert*-butyl-12H-quinoxalino[2,3-b]phenoxazin-12-yl)-4,6-di-*tert*-butylphenol **9**.

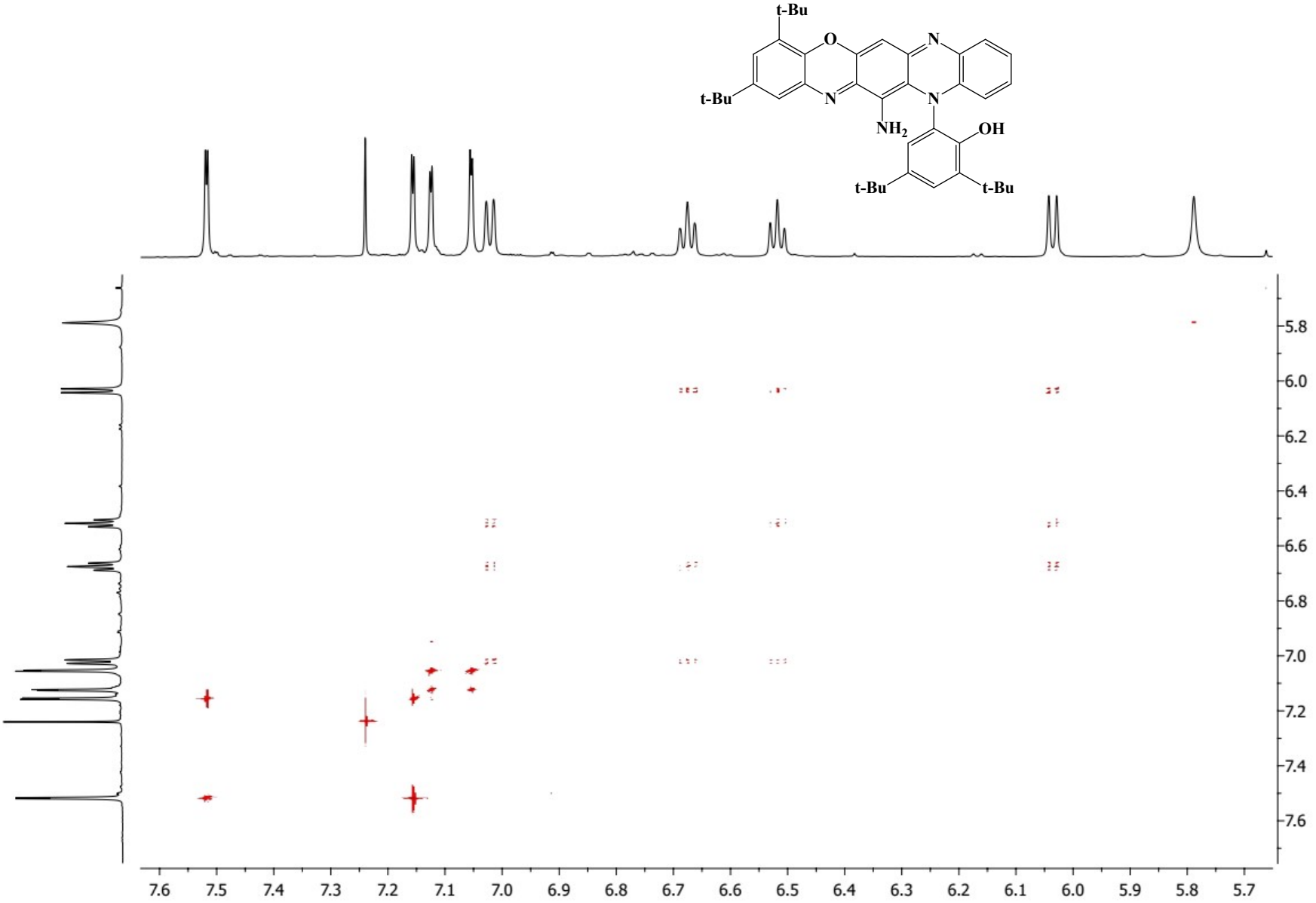


Fig. S8. COSY ^{1}H-^{1}H NMR spectrum of **9**, aromatic protons region.

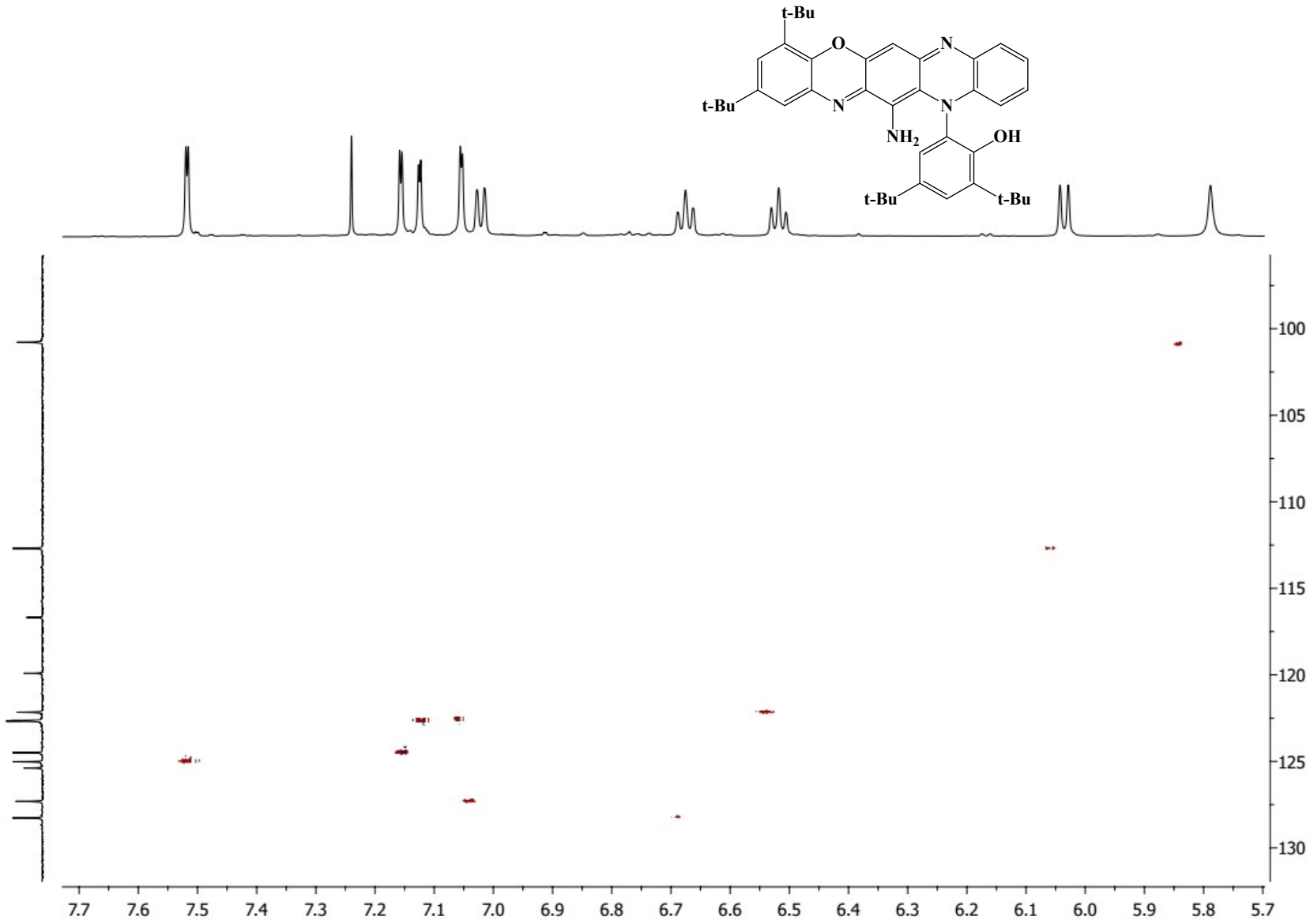


Fig. S9. HSQC ^{1}H-^{13}C NMR spectrum of **9**, aromatic protons region

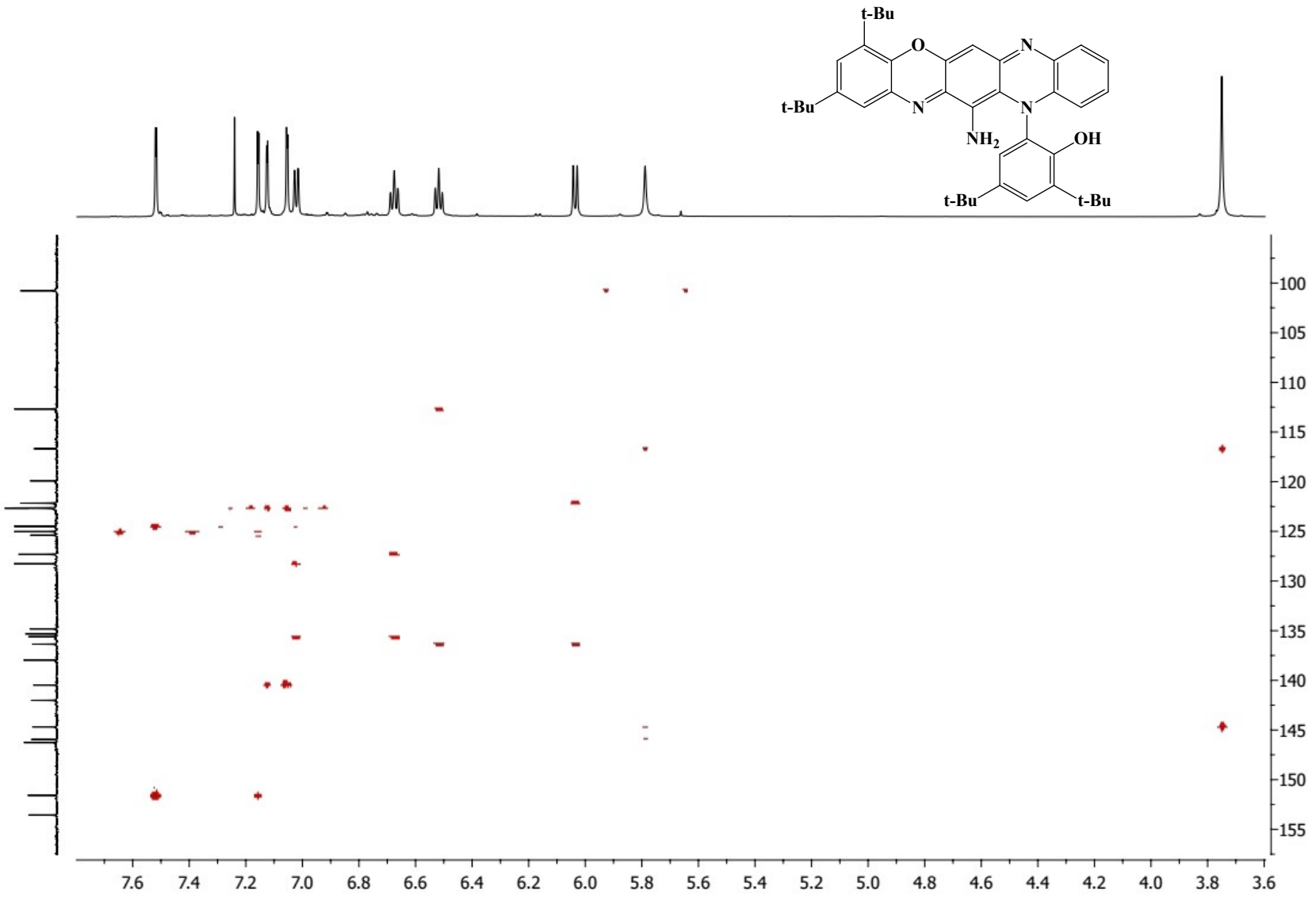


Fig. S10. HMBC ^{1}H-^{13}C NMR spectrum of **9**.

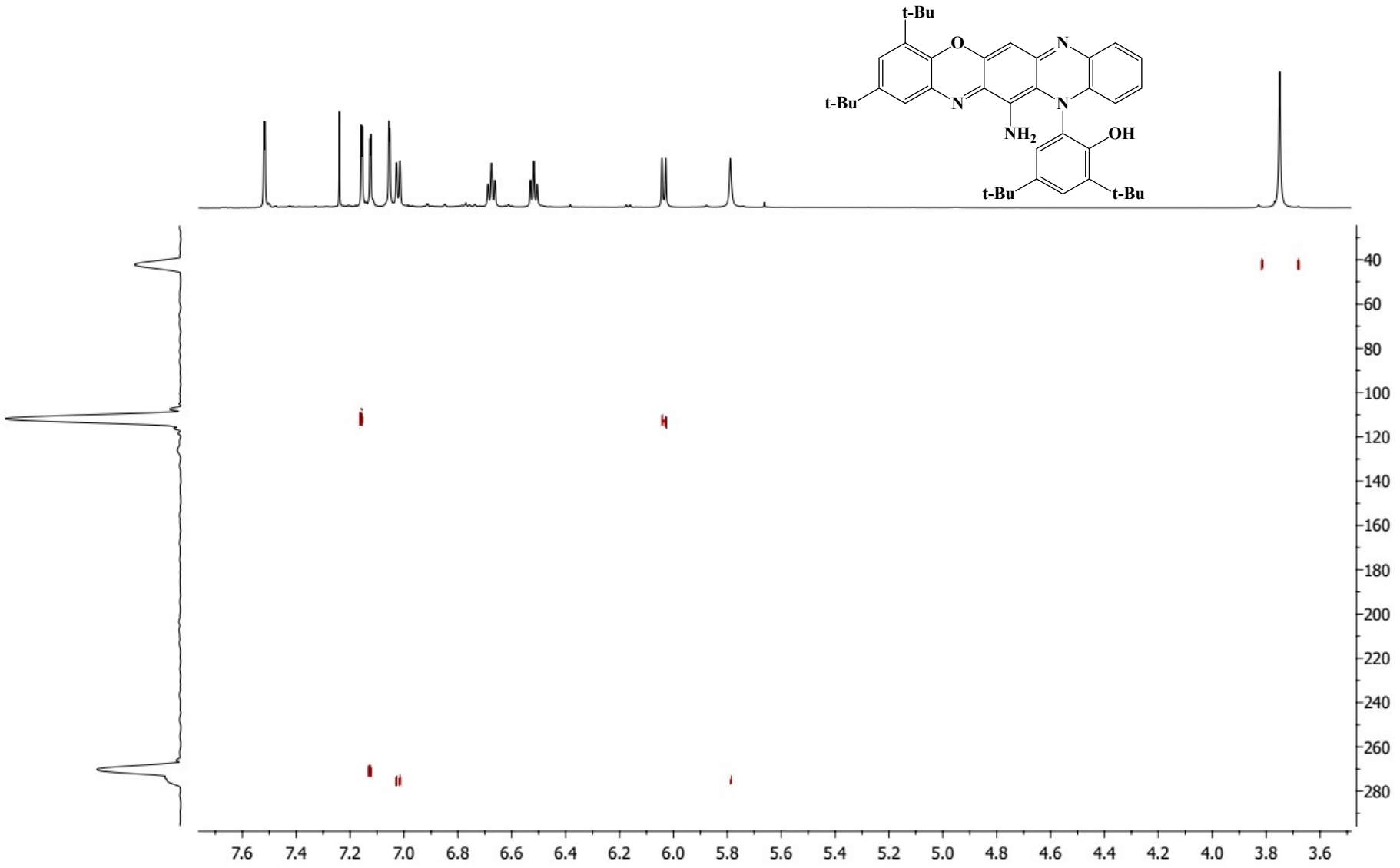


Fig. S11. HMBC ^{1}H-^{15}N NMR spectrum of **9**.

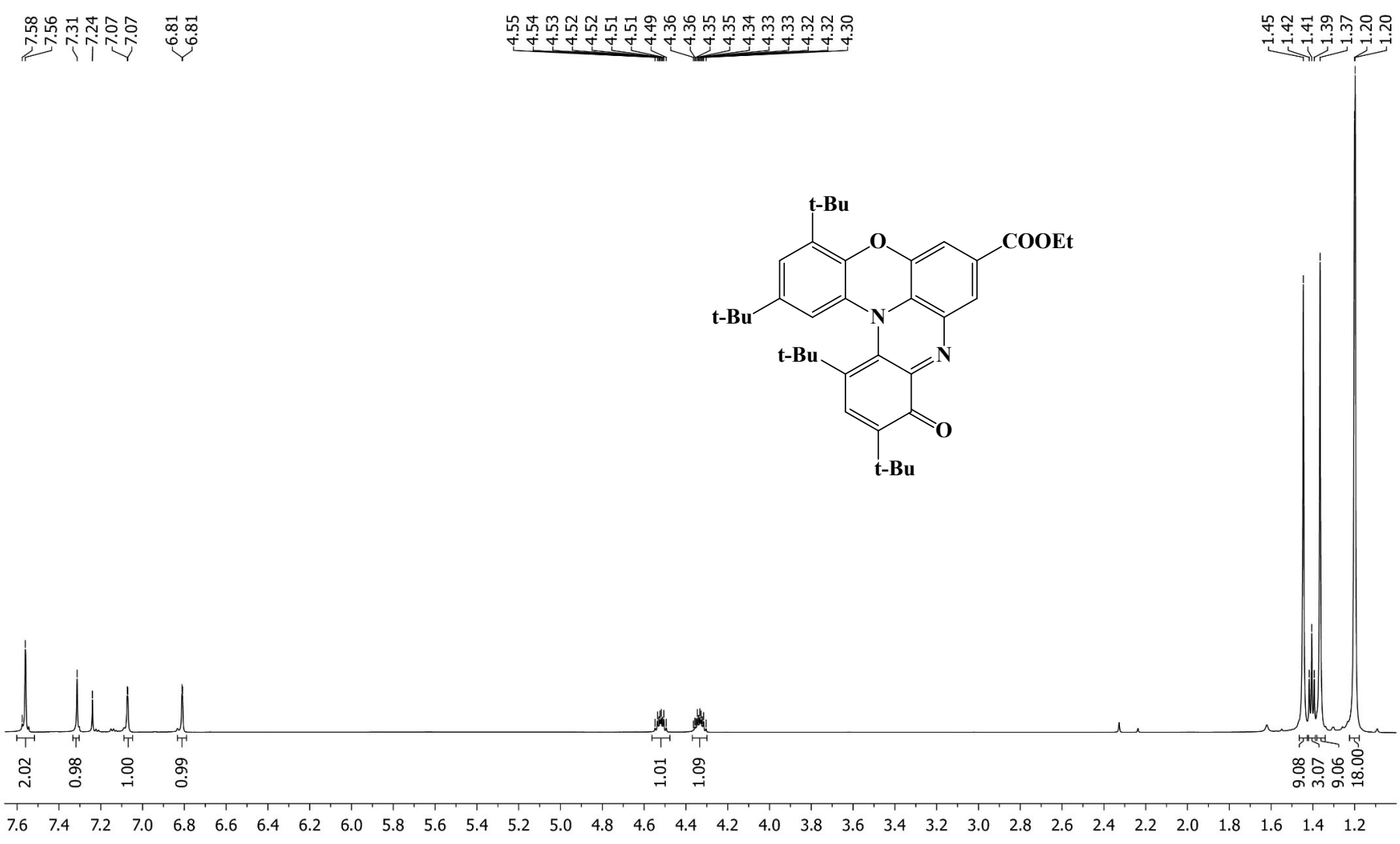


Fig. S12. ^{1}H NMR spectrum of ethyl 2,4,11,13-tetra-*tert*-butyl-10-oxo-10H-quinoxalino[3,2,1-kl]phenoxazine-7-carboxylate **10**.

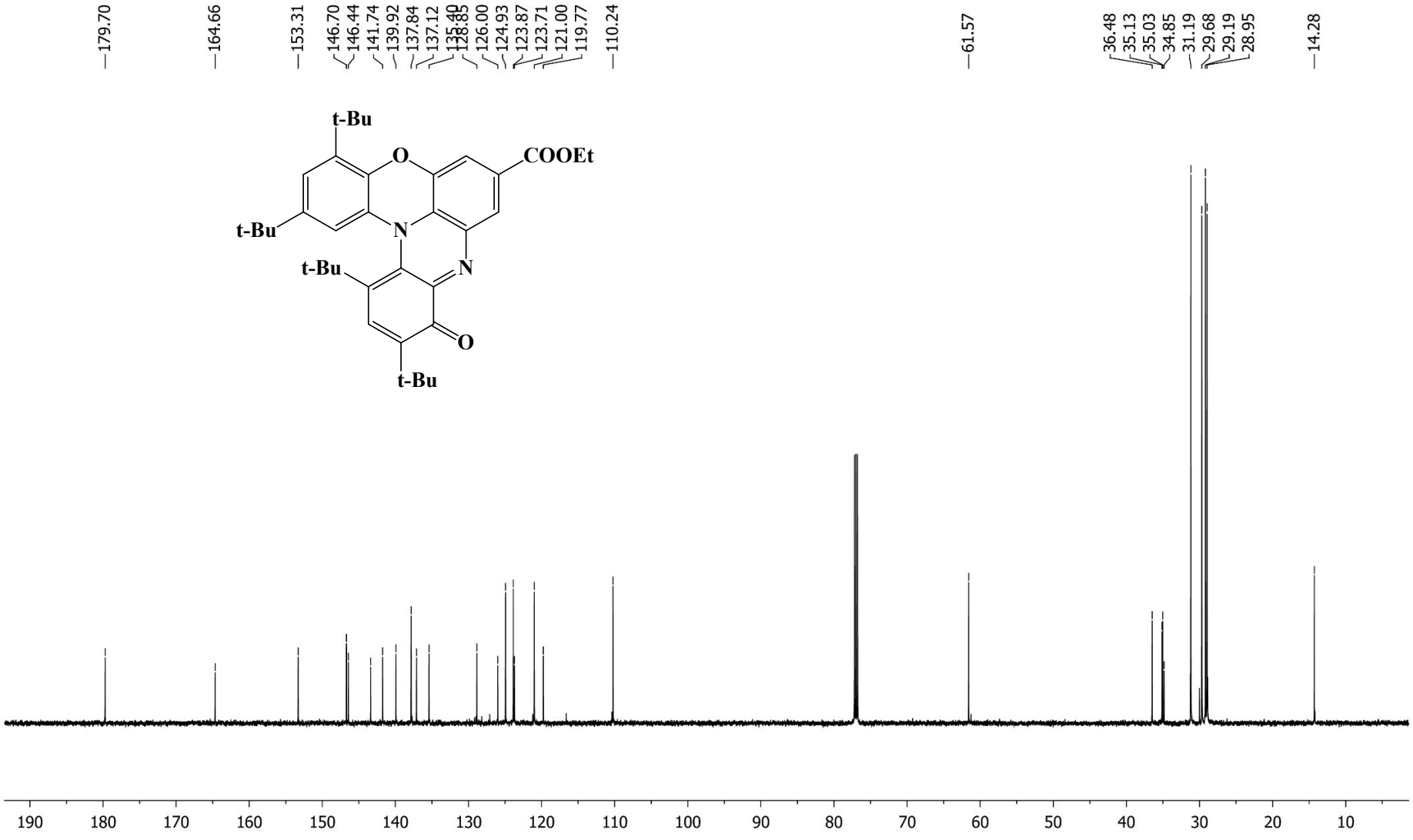


Fig. S13. ^{13}C NMR spectrum of 2,4,11,13-tetra-*tert*-butyl-10-oxo-10H-quinoxalino[3,2,1-kl]phenoxazine-7-carboxylate **10**.

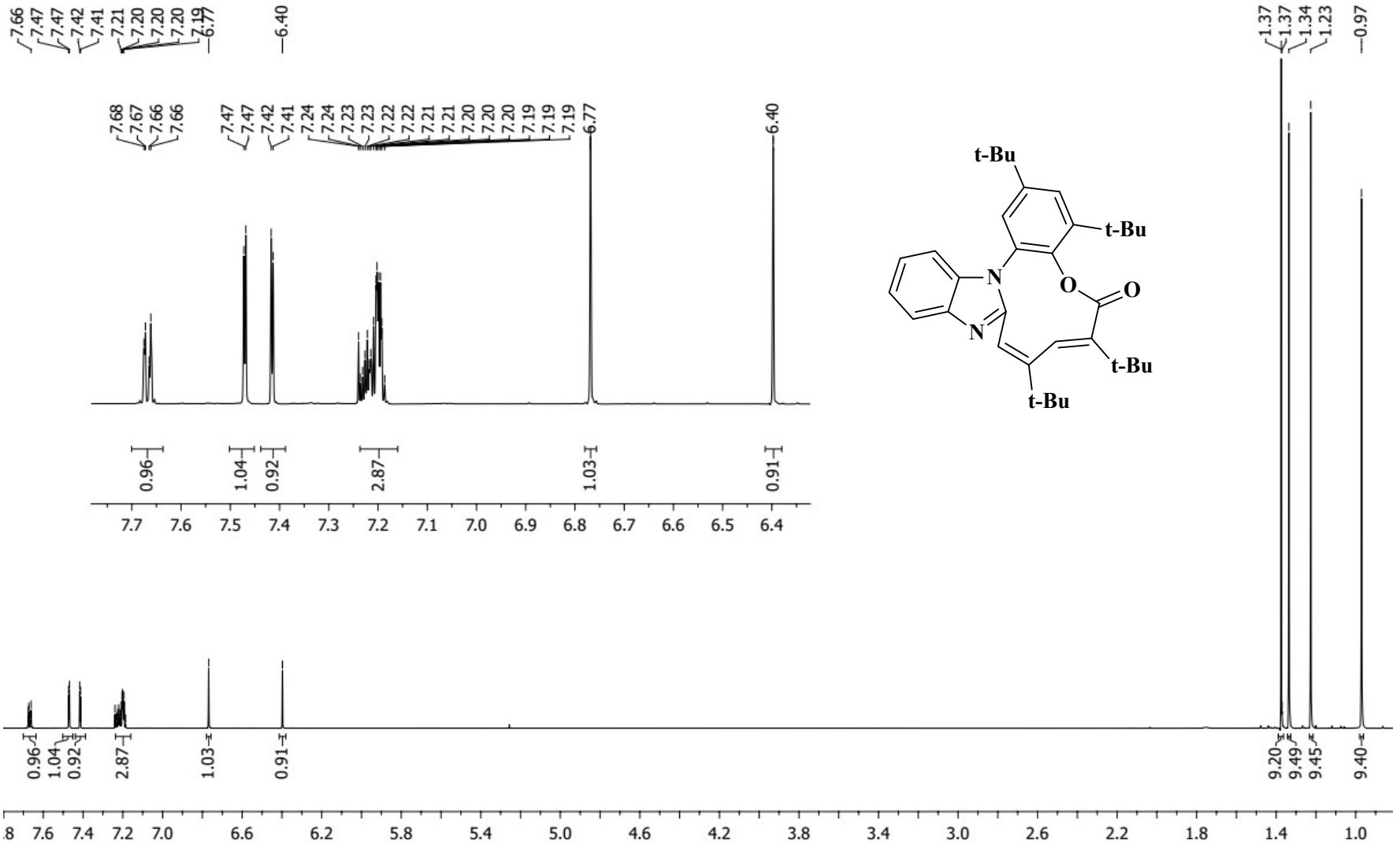


Fig. S14. [1]H NMR spectrum of 2,4,7,9-tetra-*tert*-butyl-6H-benzo[b]benzo[4,5]imidazo[1,2-d][1,4]oxazecin-6-one **12**.

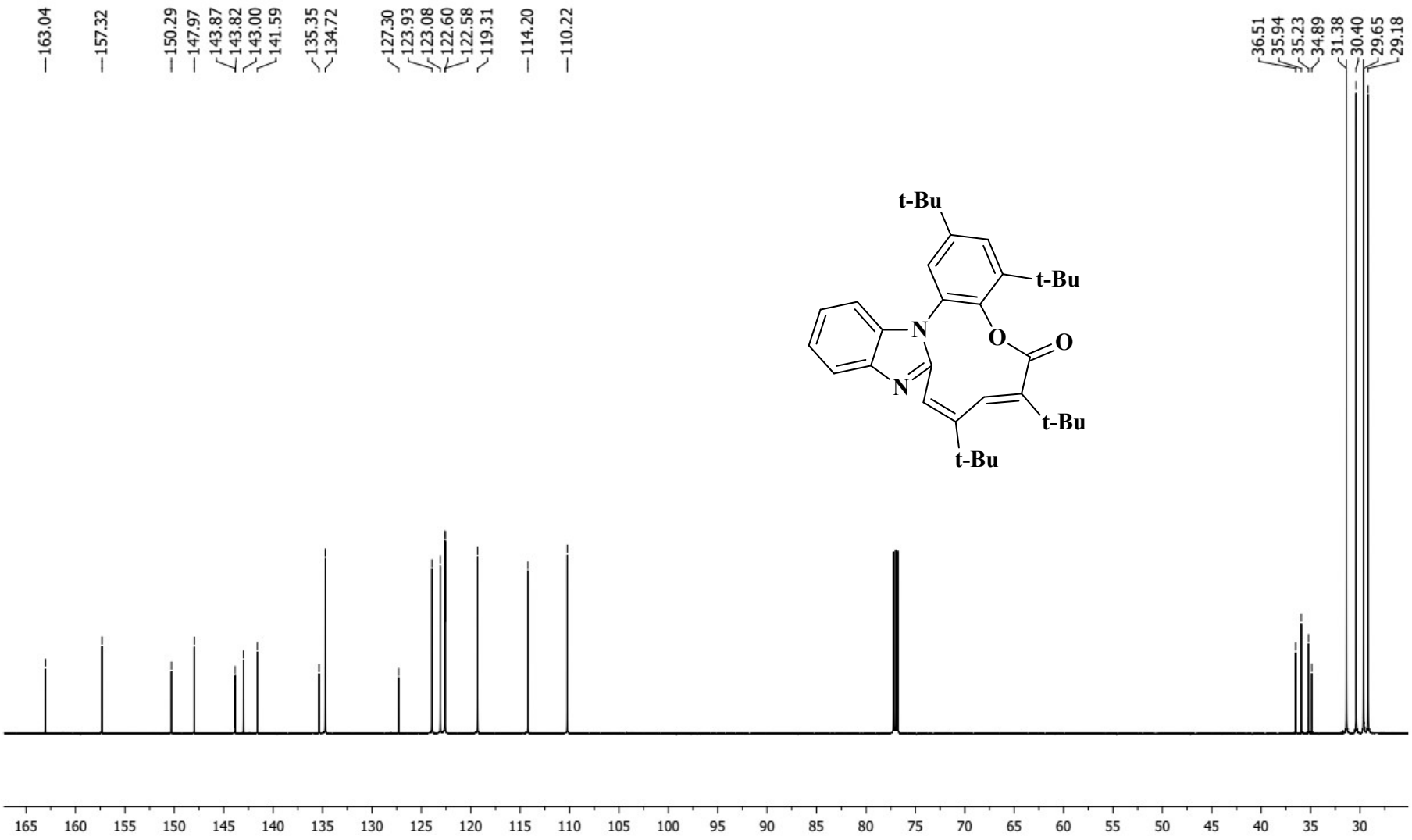


Fig. S15. ^{13}C NMR spectrum of 2,4,7,9-tetra-*tert*-butyl-6H-benzo[b]benzo[4,5]imidazo[1,2-d][1,4]oxazecin-6-one **12**.

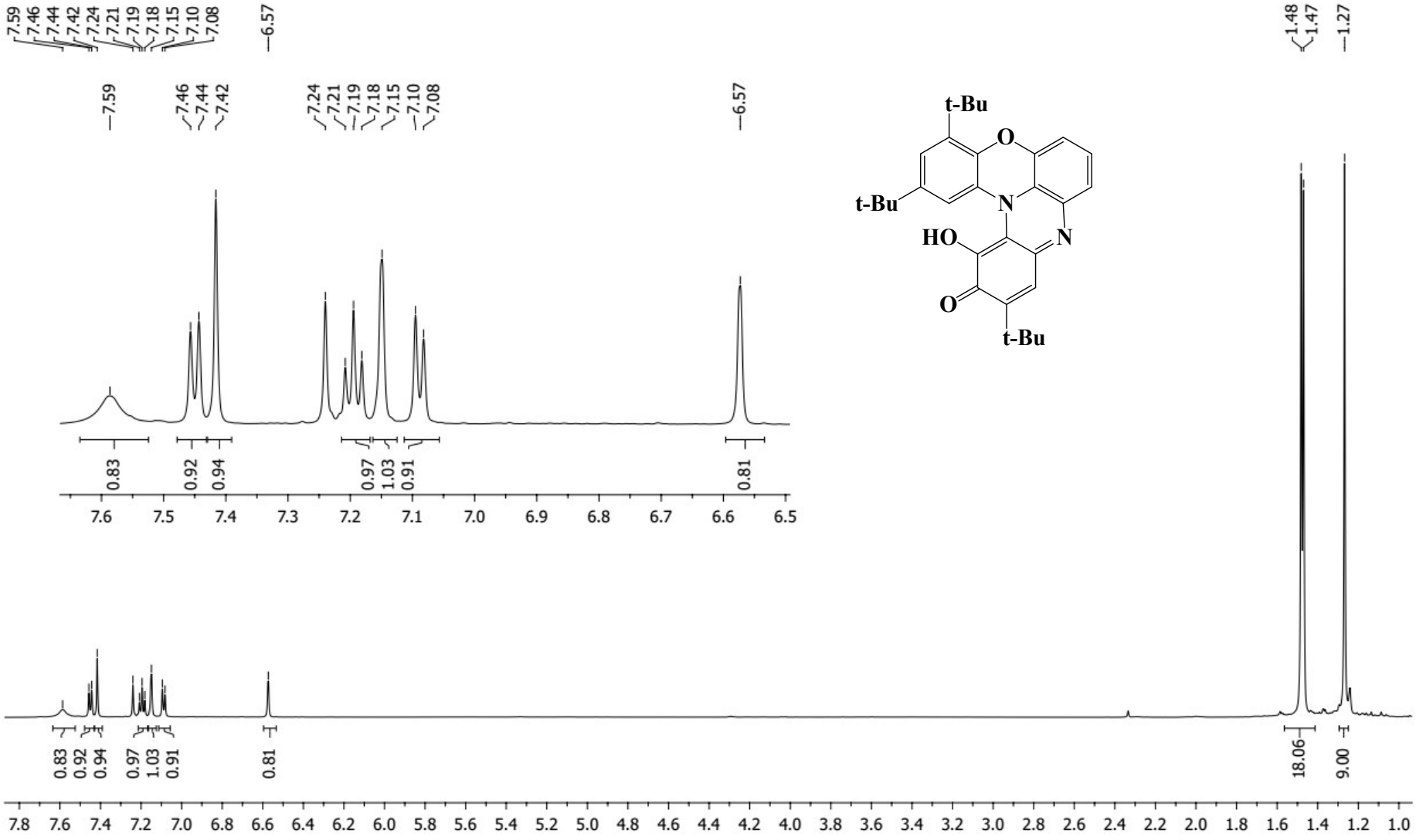


Fig. S16. ^{1}H NMR spectrum of 2,4,11-tri-*tert*-butyl-13-hydroxy-12H-quinoxalino[3,2,1-kl]phenoxazin-12-one **14**.

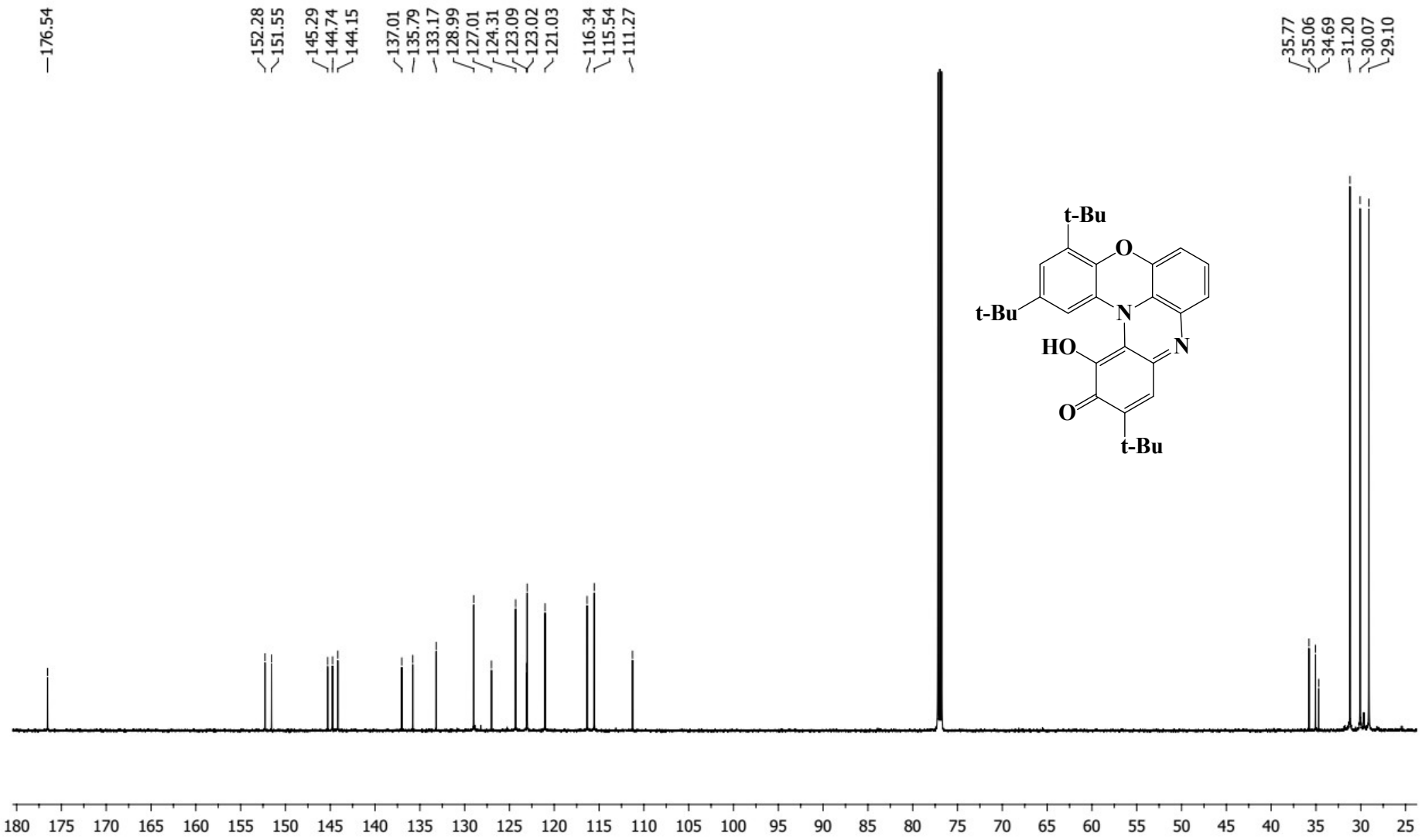


Fig. S17. ^{13}C NMR spectrum of 2,4,11-tri-*tert*-butyl-13-hydroxy-12H-quinoxalino[3,2,1-kl]phenoxazin-12-one **14**.

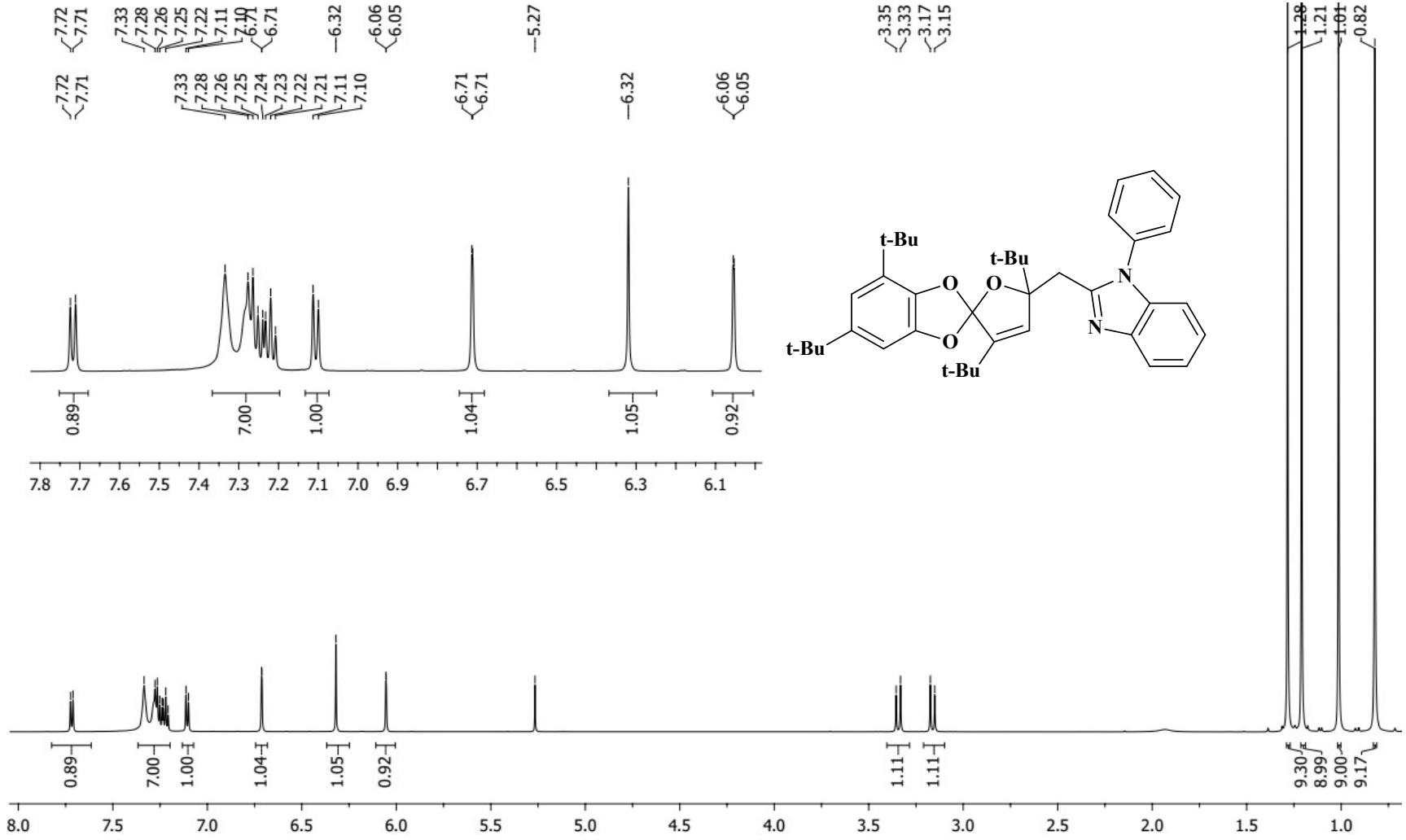


Fig. S18. [1]H NMR spectrum of 1-phenyl-2-((3',4,5',6-tetra-*tert*-butyl-5'H-spiro[benzo[d][1,3]dioxole-2,2'-furan]-5'-yl)methyl)-1H-benzo[d]imidazole **16**.

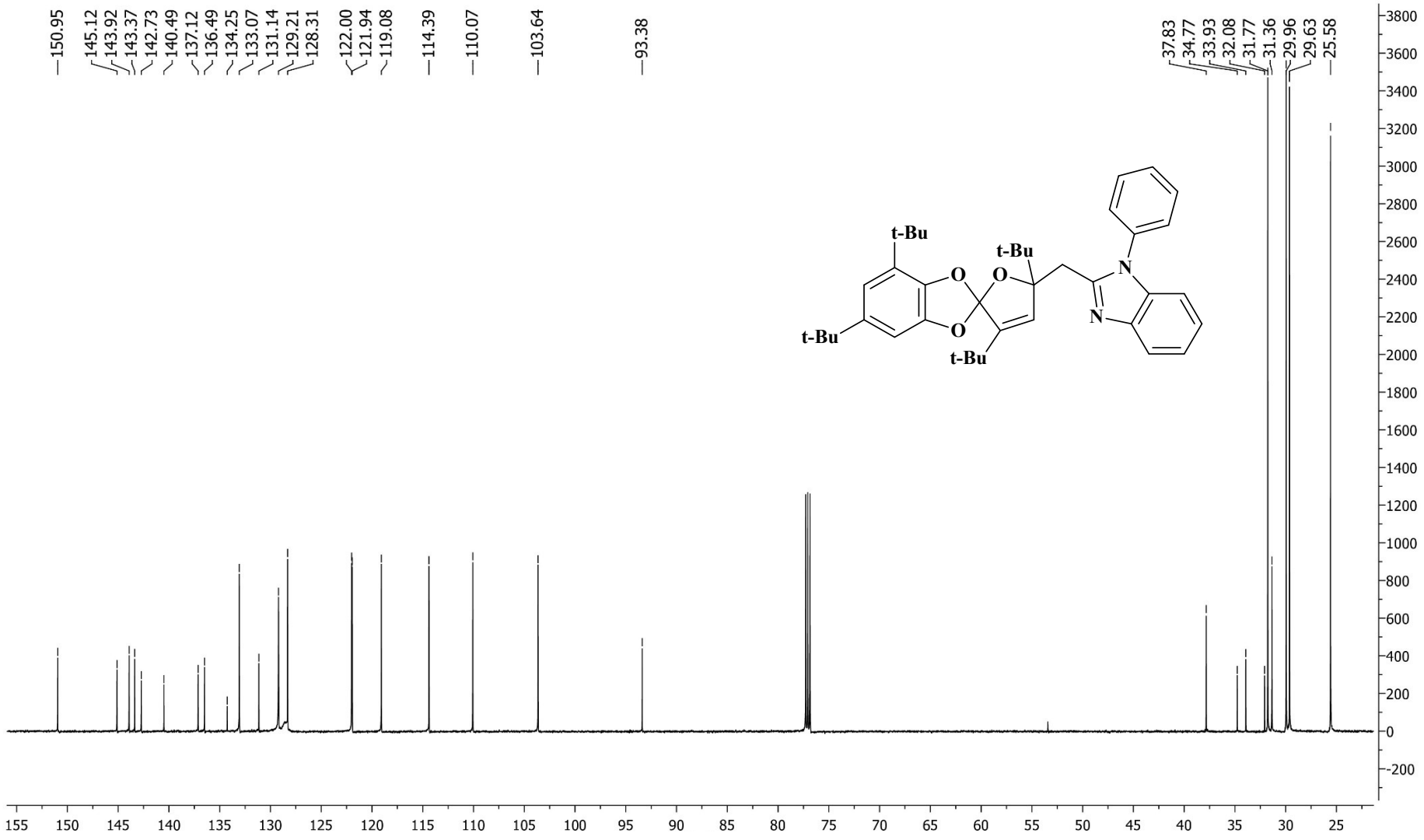


Fig. S19. ^{13}C NMR spectrum of 1-phenyl-2-((3',4,5',6-tetra-*tert*-butyl-5'H-spiro[benzo[d][1,3]dioxole-2,2'-furan]-5'-yl)methyl)-1H-benzo[d]imidazole **16**.

5. HRMS spectra

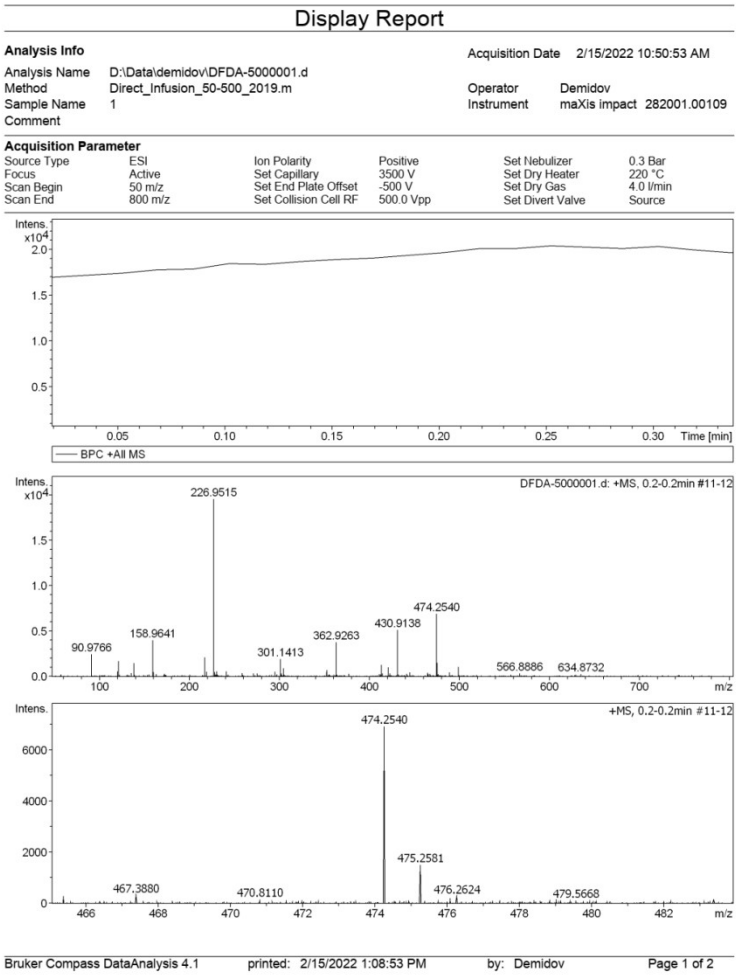
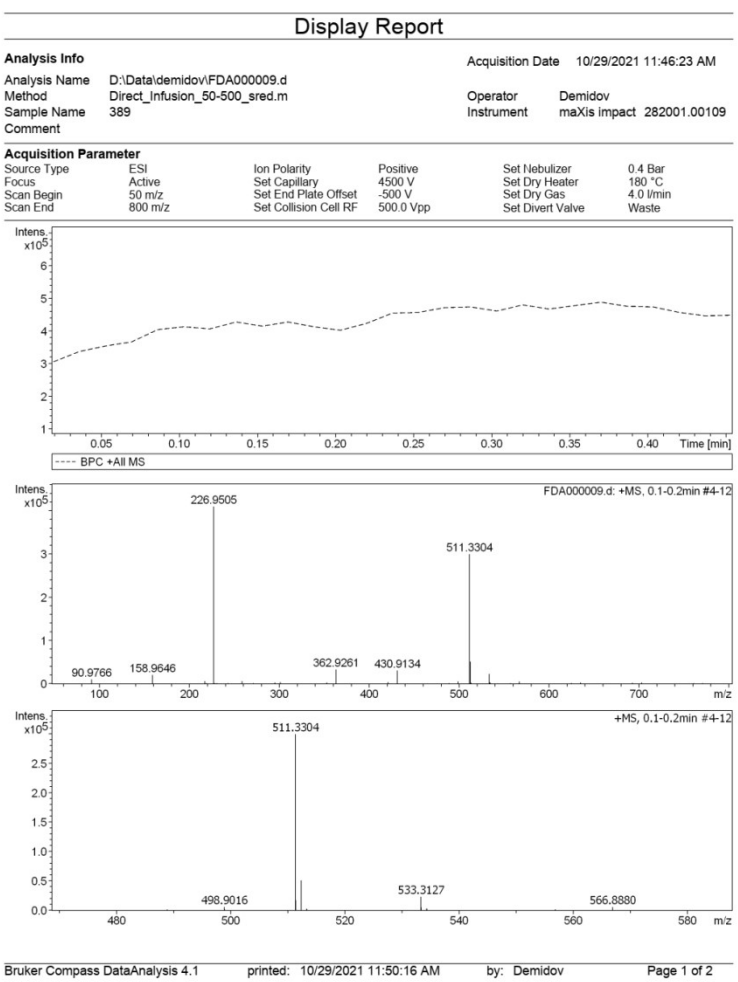


Fig. S20. HRMS spectrum of 2,4-di-*tert*-butyl-12-phenyl-12H-quinoxalino[2,3-b]phenoxazine **7** ($R^1 = R^2 = H$)



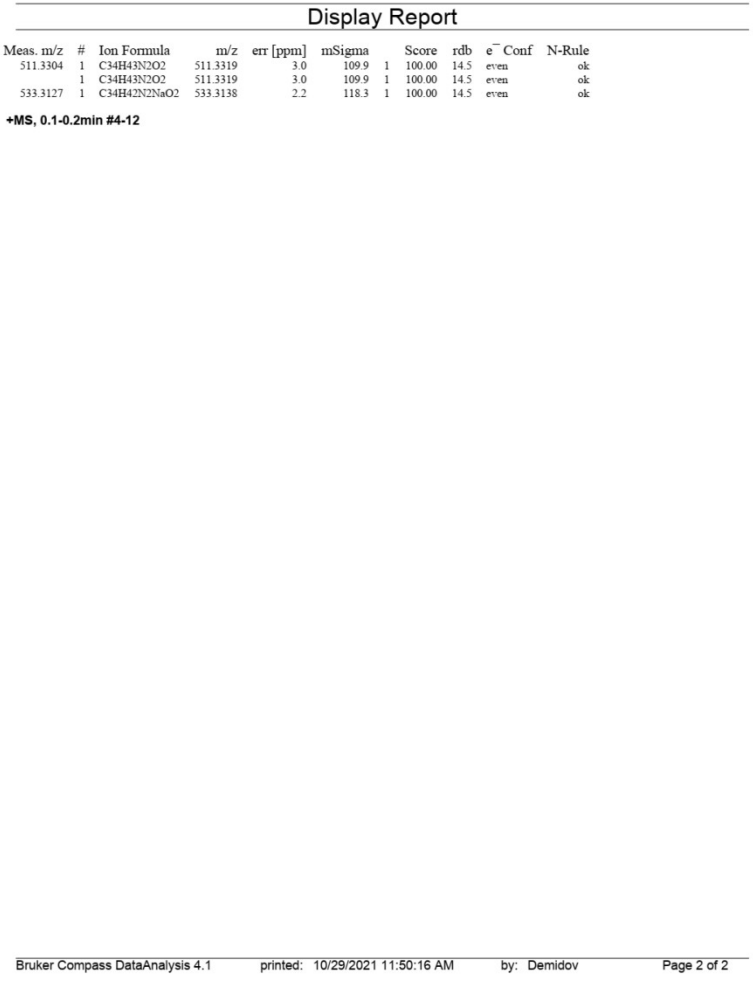
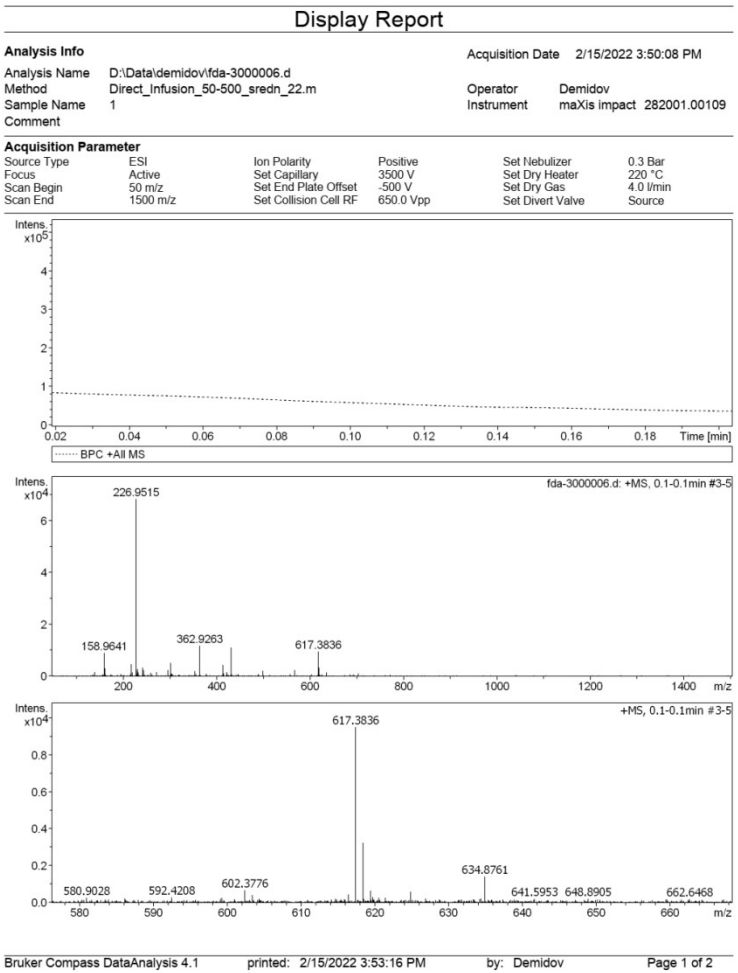


Fig. S21. HRMS spectrum of 2,4,11,13-tetra-*tert*-butyl-10H-quinoxalino[3,2,1-kl]phenoxazin-10-one **8**



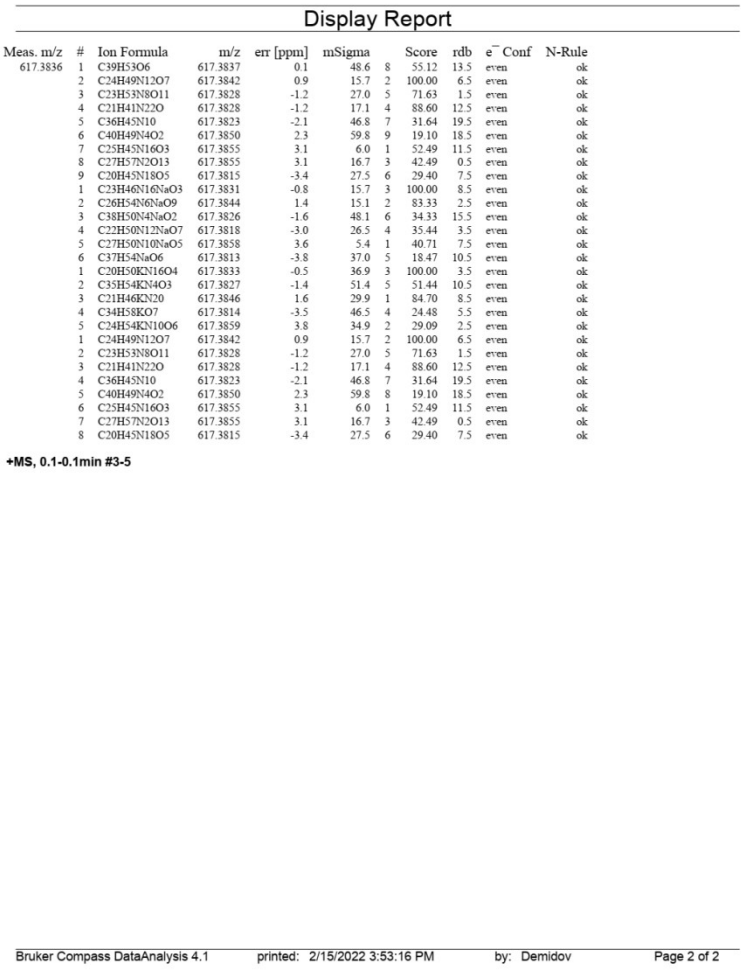
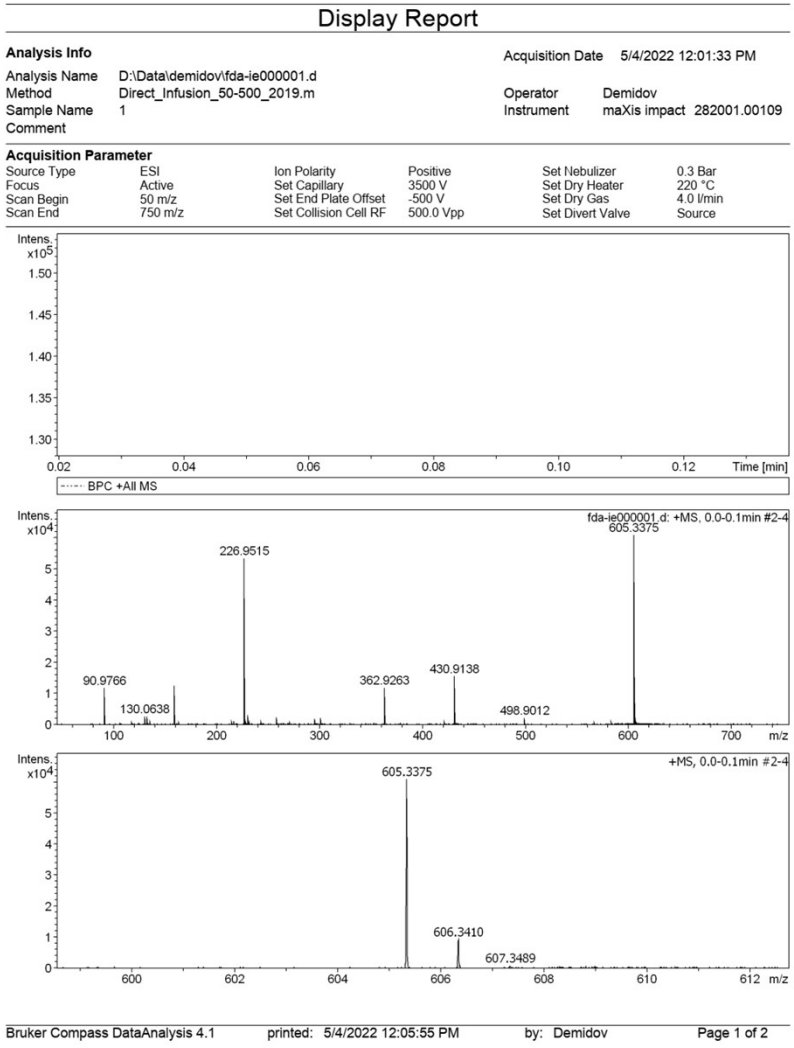


Fig. S22. HRMS spectrum of 2-(13-amino-2,4-di-*tert*-butyl-12H-quinoxalino[2,3-b]phenoxazin-12-yl)-4,6-di-*tert*-butylphenol **9**.



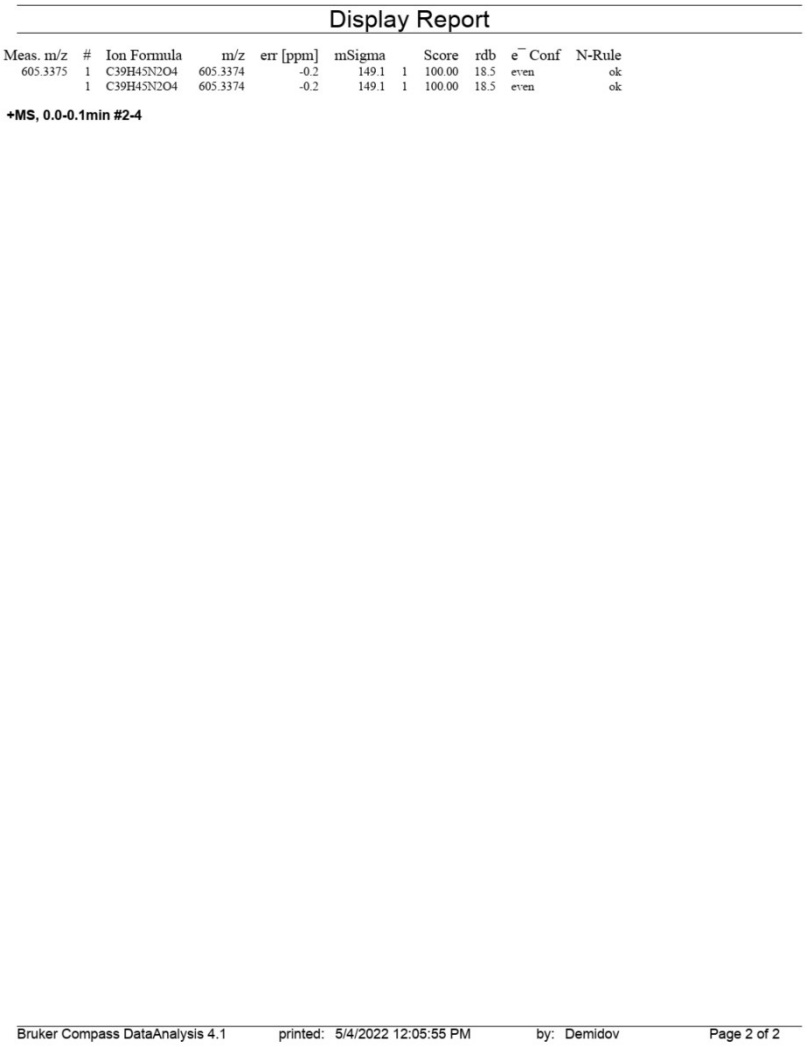
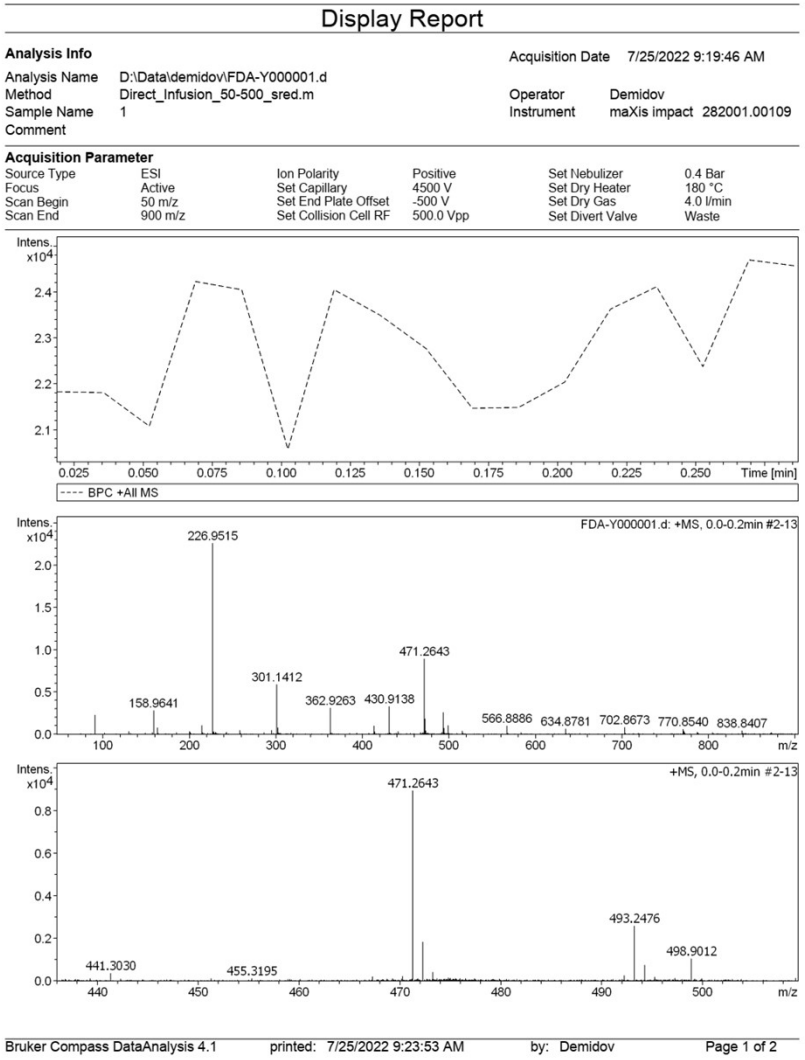


Fig. S23. HRMS spectrum of ethyl 2,4,11,13-tetra-*tert*-butyl-10-oxo-10H-quinoxalino[3,2,1-kl]phenoxazine-7-carboxylate **10**

Fig. S24. HRMS spectrum of 2,4,7,9-tetra-*tert*-butyl-6H-benzo[b]benzo[4,5]imidazo[1,2-d][1,4]oxazecin-6-one **12**.



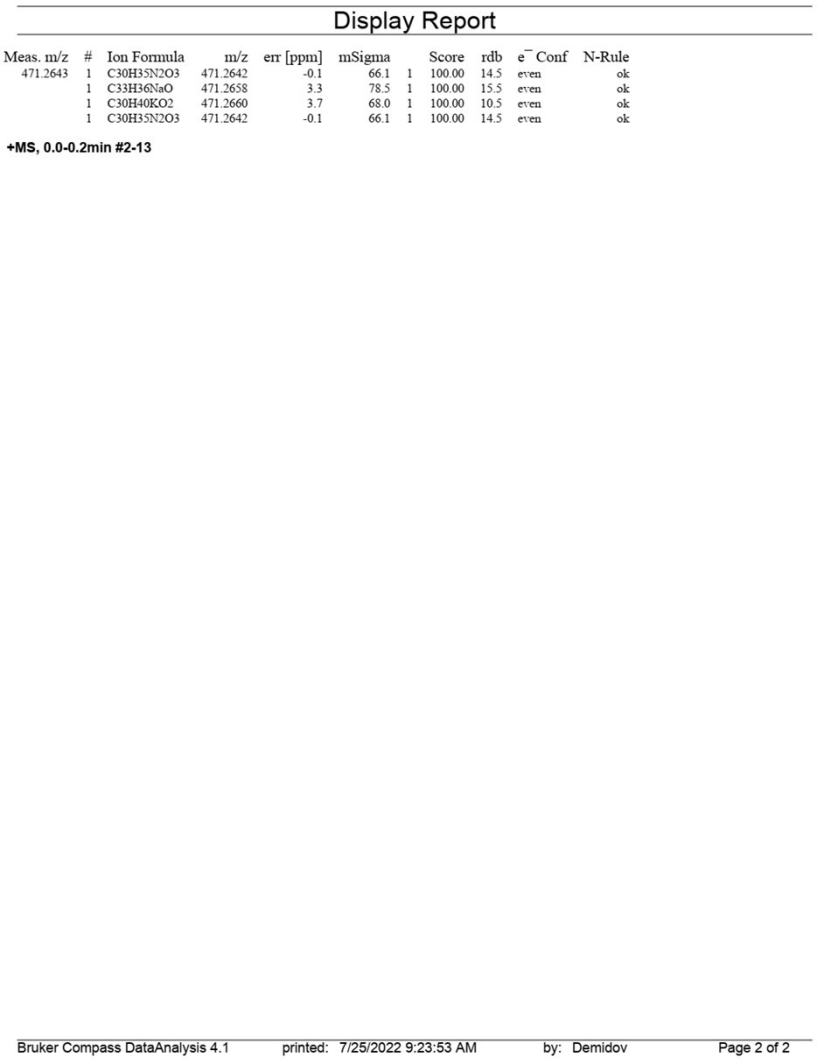
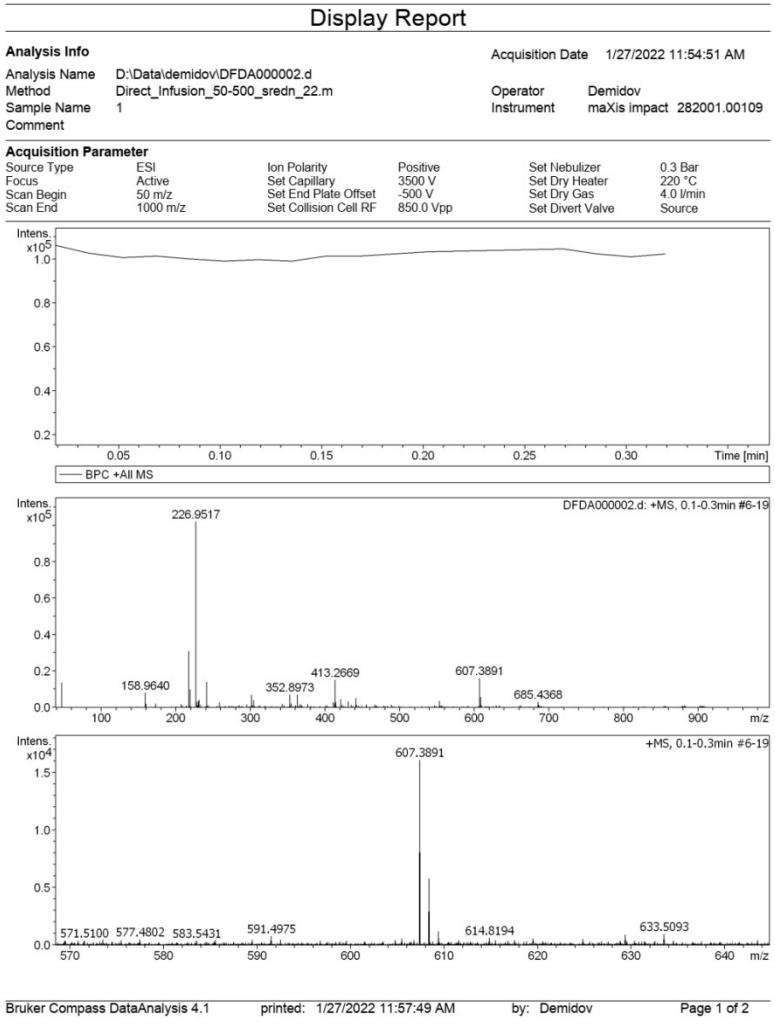


Fig. S25. HRMS spectrum of 2,4,11-tri-*tert*-butyl-13-hydroxy-12H-quinoxalino[3,2,1-kl]phenoxazin-12-one **14**.



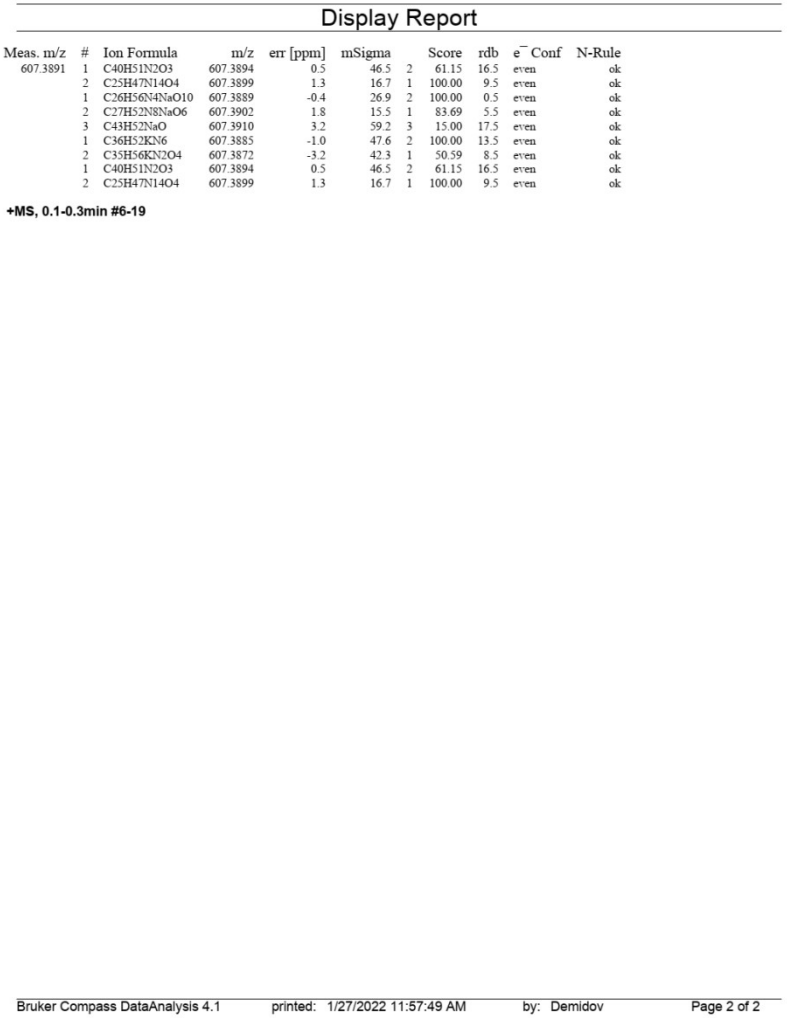


Fig. S26. HRMS spectrum of 1-phenyl-2-((3',4,5',6-tetra-*tert*-butyl-5'H-spiro[benzo[d][1,3]dioxole-2,2'-furan]-5'-yl)methyl)-1H-benzo[d]imidazole **16**.

6. DFT calculations

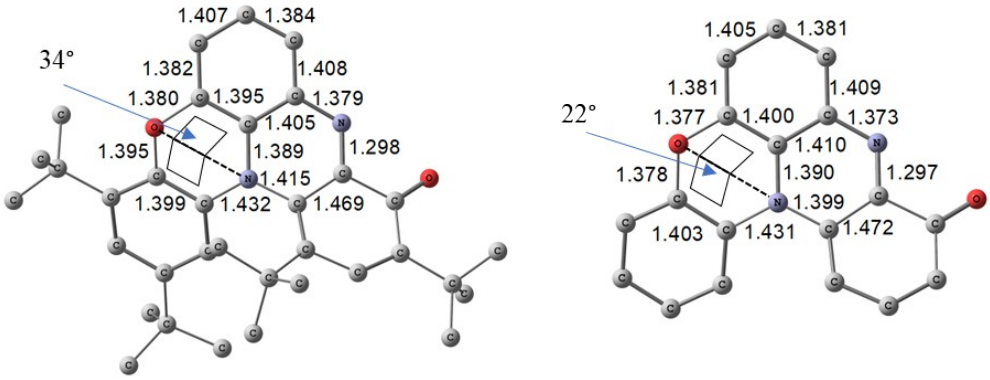


Fig. S27. Optimized geometry in **8** and **8'** by DFT (B3LYP/6-311++G(d,p)) method.

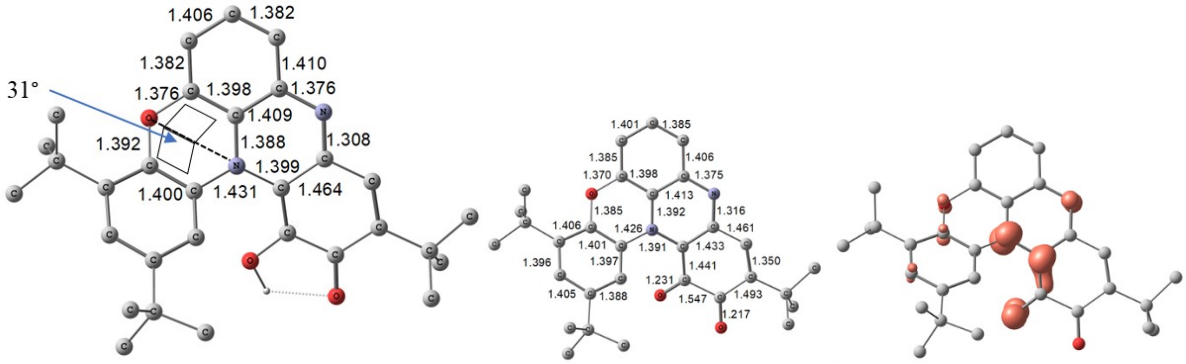


Fig. S28. Optimized geometry in **14** and it monoradical **15** (the spin density is shown on the right) by DFT (B3LYP/6-311++G(d,p)) method.

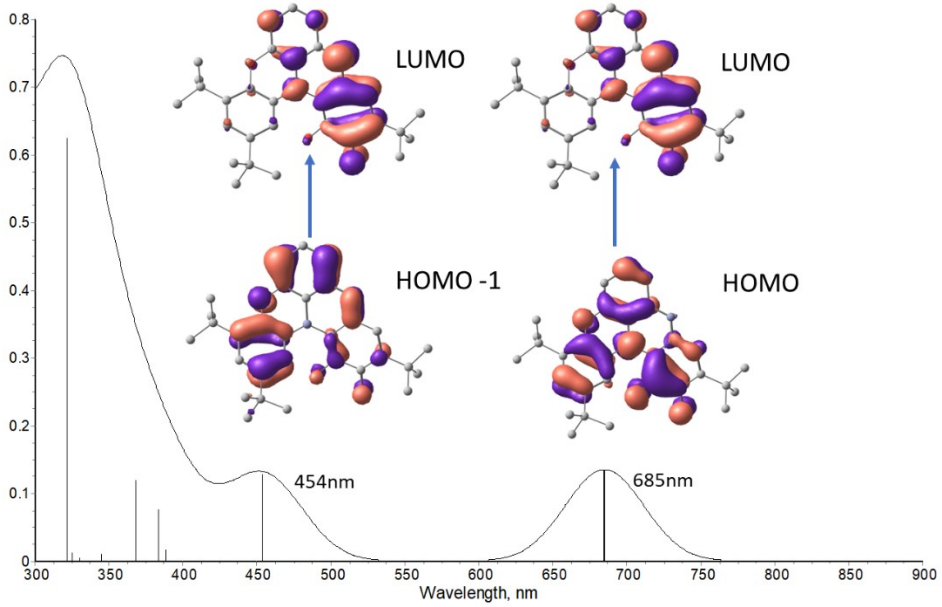


Fig. S29. The TD DFT (B3LYP/6-311++G(d,p), SMD, (solvent - toluene) calculated UV/vis spectra of **14**.

8, E_{tot}= -1581.28055406 a.u., ω1=24 cm^{-1}

Sum of electronic and zero-point Energies = -1580.598016 a.u.

Sum of electronic and thermal Energies = -1580.560591 a.u.

Sum of electronic and thermal Enthalpies = -1580.559647 a.u.

Sum of electronic and thermal Free Energies = -1580.663840 a.u.

8	-2.651659000	1.883892000	0.554238000
8	4.113081000	1.527503000	-1.889160000
7	-0.095823000	1.007954000	0.200019000
7	1.805448000	2.661672000	-0.998758000
6	-2.026706000	-2.068787000	-0.710620000
6	-3.315620000	-1.578705000	-0.456243000
1	-4.152423000	-2.241491000	-0.616878000
6	1.275509000	0.674651000	0.303287000
6	-1.164914000	0.080775000	-0.016523000
6	-0.948594000	-1.217127000	-0.476731000
1	0.067753000	-1.538759000	-0.647607000
6	-3.583585000	-0.272122000	-0.032109000
6	3.224347000	-0.620610000	0.816117000
1	3.625366000	-1.418861000	1.424327000
6	-1.849017000	-3.499549000	-1.256501000
6	4.033021000	-0.128646000	-0.166580000
6	2.129603000	1.474804000	-0.584816000
6	-5.028455000	0.223375000	0.199111000
6	3.510419000	0.979067000	-0.973764000
6	-2.468118000	0.557493000	0.164158000
6	1.856832000	-0.242181000	1.143348000
6	-1.716594000	2.771997000	0.063140000
6	1.292665000	-0.853199000	2.450941000
6	-0.408838000	2.322323000	-0.120374000
6	0.570541000	3.172580000	-0.659886000
6	5.438994000	-0.683088000	-0.452085000
6	-0.035958000	-0.233468000	2.926085000
1	0.015771000	0.857120000	2.969784000
1	-0.246632000	-0.592138000	3.937740000
1	-0.883548000	-0.518110000	2.305838000
6	-0.370197000	-3.858979000	-1.485365000
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1	-0.298333000	-4.877774000	-1.876255000
1	0.210368000	-3.823404000	-0.559483000
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1	0.355651000	-2.636065000	1.589686000
1	0.793907000	-2.797865000	3.291844000
1	2.045253000	-2.884072000	2.050657000
6	-5.359470000	1.369086000	-0.786321000
1	-4.710864000	2.232565000	-0.643752000

1	-6.393846000	1.696573000	-0.640837000
1	-5.257826000	1.032710000	-1.822435000
6	2.321712000	-0.558535000	3.577712000
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1	1.941408000	-0.949569000	4.525859000
1	2.476879000	0.517748000	3.695090000
6	-2.040788000	4.091258000	-0.193263000
1	-3.052128000	4.437212000	-0.017508000
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1	-1.944300000	-4.465270000	0.710751000
1	-2.327216000	-5.537132000	-0.644179000
1	-3.513202000	-4.351926000	-0.093334000
6	-5.200211000	0.710103000	1.657678000
1	-4.987554000	-0.098171000	2.364098000
1	-6.233465000	1.032372000	1.821363000
1	-4.544857000	1.548217000	1.892491000
6	6.491841000	0.436629000	-0.270037000
1	6.311815000	1.269875000	-0.948755000
1	7.493528000	0.042448000	-0.470166000
1	6.481588000	0.817816000	0.756030000
6	0.238708000	4.517252000	-0.914931000
1	1.003817000	5.170615000	-1.316098000
6	5.504782000	-1.225162000	-1.900558000
1	4.778496000	-2.030709000	-2.049909000
1	6.501028000	-1.633068000	-2.100505000
1	5.304731000	-0.441266000	-2.630554000
6	-1.046130000	4.967238000	-0.665176000
1	-1.303381000	6.002582000	-0.853623000
6	-2.584986000	-3.623312000	-2.611103000
1	-3.657039000	-3.435785000	-2.513017000
1	-2.460398000	-4.631703000	-3.018382000
1	-2.186202000	-2.912858000	-3.341098000
6	-6.062542000	-0.895502000	-0.034489000
1	-6.048443000	-1.265907000	-1.063210000
1	-7.063505000	-0.498097000	0.154017000
1	-5.915181000	-1.742904000	0.640993000
6	5.810557000	-1.836732000	0.497337000
1	5.824106000	-1.522447000	1.545437000
1	6.814735000	-2.193823000	0.252624000
1	5.129763000	-2.688236000	0.401117000

8', E_{tot}= -952.116949496 a.u., ω1=54 cm^{-1}

Sum of electronic and zero-point Energies = -951.880564 a.u.

Sum of electronic and thermal Energies = -951.865760 a.u.

Sum of electronic and thermal Enthalpies = -951.864816 a.u.

Sum of electronic and thermal Free Energies = -951.922161 a.u.

8	-2.624477000	1.082946000	0.578185000
8	4.528482000	0.074986000	-0.685313000
7	-0.196540000	-0.221500000	0.111171000
7	2.102457000	1.316038000	-0.336417000
6	-2.741962000	-2.862524000	-0.691880000
6	-3.917024000	-2.184433000	-0.375933000
1	-4.878714000	-2.672001000	-0.481452000
6	1.063352000	-0.811895000	0.256751000
6	-1.427362000	-0.931675000	-0.053891000
6	-1.506601000	-2.239778000	-0.539382000
1	-0.605038000	-2.770646000	-0.806397000
6	-3.855571000	-0.862228000	0.052871000
6	2.623908000	-2.598772000	0.742992000
1	2.754753000	-3.603193000	1.133850000
6	3.716623000	-1.914547000	0.299181000
6	2.201167000	0.040787000	-0.123613000
6	3.592827000	-0.571515000	-0.221727000
6	-2.622770000	-0.240588000	0.196144000
6	1.292381000	-2.083933000	0.712044000
6	-1.502385000	1.814013000	0.257710000
6	-0.277544000	1.165622000	0.058990000
6	0.885226000	1.929328000	-0.172127000
6	-1.583566000	3.192106000	0.207314000
1	-2.542437000	3.666980000	0.376745000
6	0.793130000	3.334302000	-0.221647000
1	1.701356000	3.896515000	-0.398940000
6	-0.427494000	3.952702000	-0.034309000
1	-0.502191000	5.032713000	-0.065893000
1	-4.750405000	-0.291769000	0.270625000
1	-2.779212000	-3.880162000	-1.061478000
1	0.484828000	-2.708799000	1.062673000
1	4.705589000	-2.356708000	0.307089000

14, E_{tot}= -1499.2706063 a.u., ω1=24 cm^{-1}

Sum of electronic and zero-point Energies = -1498.694488 a.u.

Sum of electronic and thermal Energies = -1498.661831 a.u.

Sum of electronic and thermal Enthalpies = -1498.660886 a.u.

Sum of electronic and thermal Free Energies = -1498.755232 a.u.

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8	-3.585899000	-1.930838000	1.511121000
8	2.471292000	1.940183000	0.573626000
7	-0.049880000	0.950035000	0.128563000
7	-2.073538000	2.657652000	-0.826292000
6	1.065017000	0.056636000	0.048477000

6	2.034566000	-2.105068000	-0.434554000
6	-1.867645000	-0.520267000	0.916583000
6	0.220651000	2.281400000	-0.157591000
6	-1.391657000	0.568557000	0.238877000
6	0.921992000	-1.272622000	-0.346836000
1	-0.063311000	-1.640388000	-0.581171000
6	3.487282000	-0.219541000	0.229510000
6	2.339378000	0.585515000	0.283608000
6	-4.229724000	-0.092311000	0.086316000
6	-3.273864000	-0.912650000	0.865093000
6	-3.748566000	1.038114000	-0.487228000
1	-4.388884000	1.731390000	-1.015254000
6	1.515092000	2.771114000	0.036512000
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6	1.810537000	4.094019000	-0.234735000
1	2.814408000	4.460252000	-0.058238000
6	-2.367028000	1.460402000	-0.389709000
6	3.285870000	-1.560400000	-0.117633000
1	4.148229000	-2.208635000	-0.160459000
6	-5.699139000	-0.519089000	-0.007813000
6	1.926423000	-3.584943000	-0.850544000
6	-0.484677000	4.477795000	-0.913939000
1	-1.276882000	5.122515000	-1.274120000
6	-6.517574000	0.451285000	-0.878486000
1	-6.540097000	1.462098000	-0.461305000
1	-7.550811000	0.098353000	-0.934611000
1	-6.134263000	0.509956000	-1.901453000
6	0.799001000	4.947432000	-0.708712000
1	1.035999000	5.984932000	-0.911087000
6	4.897115000	0.336038000	0.531994000
6	-6.330180000	-0.545418000	1.405437000
1	-5.826337000	-1.258590000	2.056936000
1	-7.384054000	-0.831441000	1.331147000
1	-6.284499000	0.443746000	1.871518000
6	2.385109000	-4.479893000	0.323841000
1	3.422093000	-4.280701000	0.606262000
1	2.312895000	-5.536656000	0.047036000
1	1.760711000	-4.317849000	1.207182000
6	-5.788512000	-1.926424000	-0.646845000
1	-5.358103000	-1.927208000	-1.653236000
1	-6.838224000	-2.223832000	-0.733108000
1	-5.269766000	-2.673642000	-0.047048000
6	4.942384000	0.936039000	1.957485000
1	4.252168000	1.770555000	2.076591000
1	5.952083000	1.298629000	2.175137000

1	4.691851000	0.177575000	2.705305000
6	5.279506000	1.412242000	-0.511630000
1	5.270445000	0.993912000	-1.522628000
1	6.290498000	1.781495000	-0.311637000
1	4.600787000	2.264110000	-0.489974000
6	5.972158000	-0.766668000	0.467244000
1	5.789700000	-1.564997000	1.192026000
1	6.945229000	-0.327432000	0.703235000
1	6.049942000	-1.213288000	-0.527831000
6	0.487750000	-3.983094000	-1.225589000
1	-0.202439000	-3.870877000	-0.385207000
1	0.466493000	-5.034249000	-1.526625000
1	0.106277000	-3.394776000	-2.065440000
6	2.829915000	-3.848464000	-2.076823000
1	2.530720000	-3.227492000	-2.926497000
1	2.755796000	-4.896895000	-2.382619000
1	3.881519000	-3.640803000	-1.864710000
1	-1.709674000	-2.003744000	2.011535000

Excitation energies and oscillator strengths for the first ten transitions in **14**:

Excited State 1: Singlet-A 1.8101 eV 684.95 nm f=0.1354 <S**2>=0.000
126 ->127 0.70041

Excited State 2: Singlet-A 2.7308 eV 454.03 nm f=0.1287 <S**2>=0.000
123 ->127 -0.11004
125 ->127 0.68188

Excited State 3: Singlet-A 3.1887 eV 388.83 nm f=0.0169 <S**2>=0.000
121 ->127 0.57015
122 ->127 0.31637
123 ->127 -0.20963
124 ->127 0.12307

Excited State 4: Singlet-A 3.2286 eV 384.01 nm f=0.0773 <S**2>=0.000
122 ->127 -0.11049
123 ->127 0.13721
124 ->127 0.66623
126 ->128 -0.12363

Excited State 5: Singlet-A 3.3630 eV 368.68 nm f=0.1200 <S**2>=0.000
121 ->127 0.27543
123 ->127 0.59633
126 ->128 0.21759

Excited State 6: Singlet-A 3.5910 eV 345.27 nm f=0.0102 <S**2>=0.000
120 ->127 0.13718
121 ->127 -0.27250
122 ->127 0.59686
123 ->127 0.19327

Excited State 7: Singlet-A 3.7513 eV 330.51 nm f=0.0053 <S**2>=0.000

119 ->127 -0.12784
120 ->127 0.67004
122 ->127 -0.12890
Excited State 8: Singlet-A 3.8086 eV 325.54 nm f=0.0127 <S**2>=0.000
126 ->129 0.69591
Excited State 9: Singlet-A 3.8523 eV 321.84 nm f=0.6248 <S**2>=0.000
123 ->127 -0.15327
124 ->127 0.13599
125 ->127 -0.13166
126 ->128 0.63409
Excited State 10: Singlet-A 4.3188 eV 287.08 nm f=0.0767 <S**2>=0.000
124 ->129 -0.10114
125 ->129 -0.12844
126 ->130 0.65320
126 ->131 -0.17176