Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Copper-Catalyzed Aerobic Oxidative Coupling of *o*-Phenylenediamines with 2-Aryl/Heteroarylethylamines: Direct Access to Construct Quinoxalines

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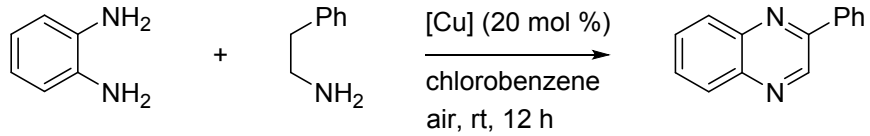
Table S1: The reactions of **1a** and **2a** catalyzed by different Copper-catalysts[a]

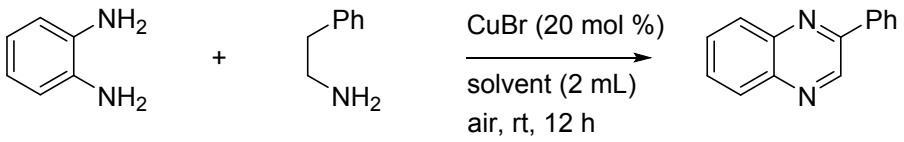


1a **2a** **3a**

Entry	[Cu] (20 mol %)	Yield (%)[b]
1	$Cu(acac)_2$	32
2	$Cu(CO_2CF_3)_2 .xH_2O$	37
3	$Cu(OTf)_2$	48
4	$Cu(ClO_4)_2 .6H_2O$	55
5	$Cu(BF_4)_2 .xH_2O$	23
6	$Cu_2(OH)PO_4$	18
7	$Cu_2P_2O_7 .xH_2O$	20
8	CuO	31
9	CuF_2	25
10	$CuSO_4$	23
11	CuCN	39
12	CuOAc	42
13	$Cu(OH)_2$	21
14	$Cu(NO_3)_2.3H_2O$	19

[a] Reaction conditions: **1a** (1.0 mmol), **2a** (1.2 mmol), catalyst (20 mol %), chlorobenzene (2 mL), air atmosphere, room temperature, 12 h. [b] Isolated yields.

Table S2: The reactions of **1a** and **2a** in different solvents[a]

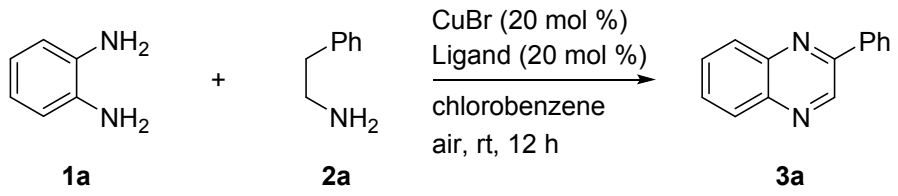


1a **2a** **3a**

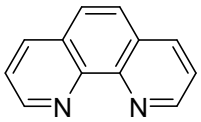
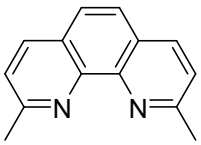
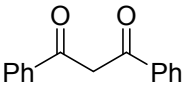
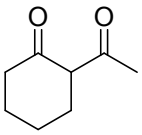
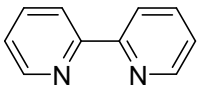
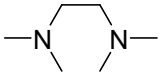
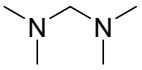
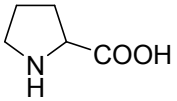
Entry	Solvent	Yield (%)[b]
1	chlorobenzene	73
2	toluene	60
3	acetonitrile	24
4	N,N-dimethylacetamide	trace
5	N,N-dimethylformamide	trace
6	acetone	35
7	1,4-dioxane	42
8	tetrahydrofuran	51
9	N-methylpyrrolidone	trace
10	dimethyl sufoxide	trace
11	benzene	53
12	ethyl acetate	45
13	1,2-dichloroethane	64
14	ethanol	trace
15	water	trace

[a] Reaction conditions: **1a** (1.0 mmol), **2a** (1.2 mmol), CuBr (20 mol %), solvent (2 mL), air atmosphere, room temperature, 12 h. [b] Isolated yields.

Table S3: The effect of different ligands on the reactions of **1a** and **2a**[a]



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

Entry	Ligand	Yield (%)[b]
1	none	73
2	Terpyridine	38
3		43
4		43
5		52
6		59
7		45
8		56
9		41
10		54

[a] Reaction conditions: **1a** (1.0 mmol), **2a** (1.2 mmol), CuBr (20 mol %), ligand (20 mol %), chlorobenzene (2 mL), air atmosphere, room temperature, 12 h. [b] Isolated yields.

Single Crystal X-ray Diffraction (SCXRD) Analysis:

SCXRD of grown crystals was carried out using an Oxford diffractometer (MoKα X-ray source λ = 0.71073 Å). The crystal structures were solved by direct method using WinGX software. The refinement was done using full-matrix least-square technique employing SHELX-97 program. The hydrogen atoms for all the compounds were refined with isotropic thermal parameters. The non-hydrogen atoms were refined for anisotropic displacement parameters.

2-(4-Nitrophenyl)quinoxaline (3e):

Fig. S1 depicts the displacement ellipsoid style plot of the title compound at 50 % probability level. The crystallographic parameters along with discrepancy indices are tabulated in Table S4. Table S5 displays the refined fractional atomic positions and isotropic displacement parameters for **2-(4-Nitrophenyl)quinoxaline**. Table S6 contains the anisotropic displacement parameters of non hydrogen atoms for **2-(4-Nitrophenyl)quinoxaline**. Table S7 and S8 summarize the bond length and bond angle of **2-(4-Nitrophenyl)quinoxaline**, respectively. Hydrogen atom coordinate with isotropic displacement parameters are listed in Table S9. The crystal structure of **2-(4-Nitrophenyl)quinoxaline** is novel and submitted to Cambridge Crystallographic Data Centre (CCDC No: 1506177).

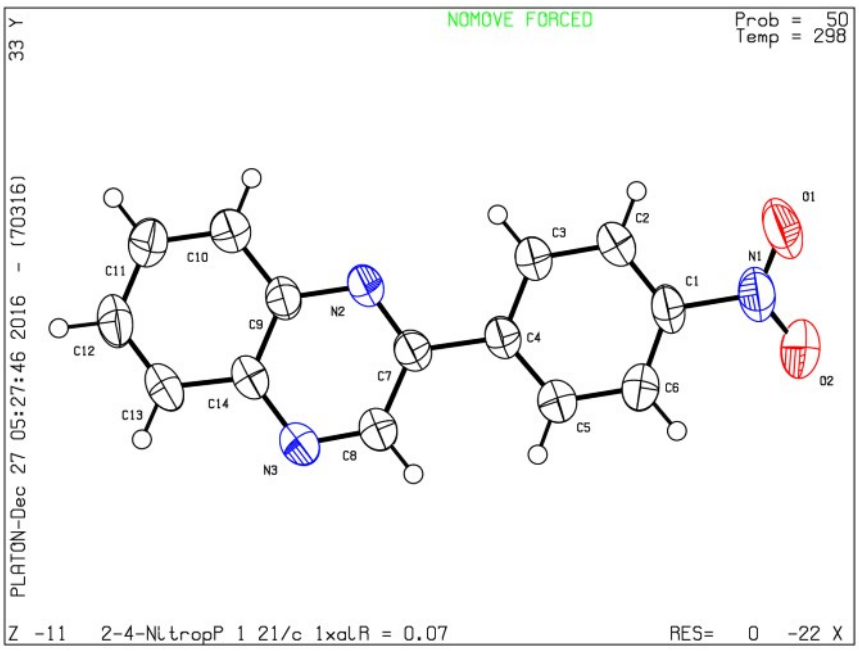


Figure S1: X-Ray Crystal Structure of **2-(4-Nitrophenyl)quinoxaline**.

Table S4. Crystal data and structure refinement for **2-(4-Nitrophenyl)quinoxaline**.

CCDC No.	1506177
Empirical formula	$C_{14}H_9N_3O_2$
Formula weight	251.24
Temperature/K	298.15
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	6.3758(4)
b/Å	12.4522(7)
c/Å	14.7628(10)
α/°	90.000(5)
β/°	79.702(6)
γ/°	90.000(5)
Volume/Å^3	1153.18(13)
Z	4
ρ_{calc}g/cm^3	1.447
μ/mm^{-1}	0.101
F(000)	520.0
Crystal size/mm^3	0.02 × 0.02 × 0.02
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.494 to 58.544
Index ranges	$-8 \leq h \leq 8$, $-16 \leq k \leq 16$, $-19 \leq l \leq 18$
Reflections collected	15229

Independent reflections	2853 [R_{int} = 0.0562, R_{sigma} = 0.0620]
Data/restraints/parameters	2853/0/173
Goodness-of-fit on F^2	1.045
Final R indexes [I>=2σ (I)]	R_1 = 0.0678, wR_2 = 0.1177
Final R indexes [all data]	R_1 = 0.1536, wR_2 = 0.1505
Largest diff. peak/hole / e $Å^{-3}$	0.16/-0.16

Table S5. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **2-(4-Nitrophenyl)quinoxaline**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***Z***	**U(eq)**
O1	10814(3)	2375.2(18)	-1017.8(14)	88.2(7)
O2	9951(3)	713.7(19)	-889.0(16)	111.0(9)
N1	9568(3)	1661(2)	-741.6(14)	67.0(7)
N2	644(3)	3737.8(15)	1112.2(12)	49.0(5)
N3	-1811(3)	2286.9(16)	2324.7(14)	63.1(6)
C1	7464(3)	1950(2)	-217.2(16)	51.7(6)
C2	6741(4)	2975(2)	-260.2(16)	57.4(7)
C3	4748(3)	3228.3(19)	218.2(16)	54.8(7)
C4	3496(3)	2465.3(18)	745.0(14)	44.5(6)
C5	4294(4)	1442(2)	778.7(17)	65.9(8)
C6	6284(4)	1177(2)	295.3(18)	69.4(8)
C7	1346(3)	2770.3(18)	1252.8(15)	45.2(6)
C8	83(4)	2056(2)	1866.7(17)	60.8(7)
C9	-1323(3)	4010.6(17)	1579.6(15)	46.3(6)
C10	-2160(4)	5029.5(19)	1441.0(18)	65.0(8)
C11	-4137(4)	5307(2)	1894.2(18)	67.6(8)
C12	-5358(4)	4589(2)	2497.1(17)	61.2(7)
C13	-4597(3)	3602(2)	2645.5(16)	56.5(7)
C14	-2561(3)	3285.1(19)	2183.4(15)	45.8(6)

Table S6. Anisotropic Displacement Parameters (Å2×103) for **2-(4-Nitrophenyl)quinoxaline**. The Anisotropic displacement factor exponent takes the form: -2π2[h2a*2U11+2hka*b*U12+…].

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
O1	44.3(12)	107.2(17)	101.2(16)	-4.7(12)	19.2(11)	-1.3(11)
O2	87.2(16)	92.4(17)	131(2)	6.4(14)	40.5(14)	37.6(13)
N1	47.0(15)	87.7(18)	60.8(15)	0.6(13)	4.8(11)	16.5(13)
N2	37.5(11)	51.6(12)	53.3(13)	0.3(9)	3.8(9)	-1.2(9)
N3	47.6(13)	65.7(14)	68.5(15)	16.9(11)	9.4(11)	3.6(11)
C1	33.4(13)	71.1(18)	47.4(15)	-0.7(12)	1.5(11)	8.3(12)

C2	41.9(14)	61.4(17)	62.6(17)	4.8(13)	7.8(12)	-1.4(12)
C3	41.4(14)	53.8(15)	63.9(17)	1.2(13)	4.7(12)	2.9(11)
C4	35.3(13)	53.4(15)	43.3(13)	0.3(11)	-3(1)	1.5(10)
C5	53.5(17)	60.2(17)	75.3(19)	14.7(14)	12.3(14)	10.1(13)
C6	55.1(17)	66.5(18)	79(2)	11.4(14)	10.2(14)	20.7(14)
C7	38.3(13)	51.5(14)	44.4(14)	1.7(11)	-3.2(10)	-0.6(11)
C8	45.9(15)	61.9(17)	68.2(17)	14.9(13)	7.3(13)	7.6(12)
C9	36.8(13)	49.9(14)	49.2(15)	-5.2(11)	0.3(11)	0.0(11)
C10	55.1(17)	52.7(16)	78.7(19)	2.6(13)	10.8(14)	2.2(13)
C11	56.7(17)	55.9(16)	83(2)	-6.6(14)	6.0(14)	10.9(13)
C12	43.3(15)	72.2(18)	62.1(17)	-13.6(14)	6.6(12)	7.2(14)
C13	39.7(15)	70.6(18)	53.5(16)	-1.7(13)	7.2(12)	-6.0(13)
C14	35.7(13)	56.5(15)	42.9(13)	-2.7(11)	-0.7(10)	-4.0(11)

Table S7. Bond Lengths for **2-(4-Nitrophenyl)quinoxaline**.

Atom	**Atom**	**Length/Å**
O1	N1	1.213(3)
O2	N1	1.216(3)
N1	C1	1.469(3)
N2	C7	1.315(3)
N2	C9	1.362(3)
N3	C8	1.307(3)
N3	C14	1.361(3)
C1	C2	1.362(3)
C1	C6	1.364(3)
C2	C3	1.376(3)
C3	C4	1.386(3)
C4	C5	1.376(3)
C4	C7	1.489(3)
C5	C6	1.380(3)
C7	C8	1.413(3)
C9	C10	1.406(3)
C9	C14	1.407(3)
C10	C11	1.362(3)
C11	C12	1.396(3)
C12	C13	1.353(3)
C13	C14	1.411(3)

Table S8. Bond Angles for **2-(4-Nitrophenyl)quinoxaline**.

Atom	**Atom**	**Atom**	**Angle/°**
O1	N1	O2	123.5(2)
O1	N1	C1	118.6(2)
O2	N1	C1	117.9(2)

C7	N2	C9	117.26(19)
C8	N3	C14	116.06(19)
C2	C1	N1	119.4(2)
C2	C1	C6	121.9(2)
C6	C1	N1	118.6(2)
C1	C2	C3	118.8(2)
C2	C3	C4	121.1(2)
C3	C4	C7	119.6(2)
C5	C4	C3	118.3(2)
C5	C4	C7	122.1(2)
C4	C5	C6	121.0(2)
C1	C6	C5	118.8(2)
N2	C7	C4	117.62(19)
N2	C7	C8	120.4(2)
C8	C7	C4	122.0(2)
N3	C8	C7	124.1(2)
N2	C9	C10	119.4(2)
N2	C9	C14	121.4(2)
C10	C9	C14	119.1(2)
C11	C10	C9	120.0(2)
C10	C11	C12	120.8(2)
C13	C12	C11	120.6(2)
C12	C13	C14	120.1(2)
N3	C14	C9	120.69(19)
N3	C14	C13	120.0(2)
C9	C14	C13	119.3(2)

Table S9. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **2-(4-Nitrophenyl)quinoxaline**.

Atom	***x***	***y***	***z***	**U(eq)**
H2	7578.23	3493.01	-606.62	69
H3	4233.01	3923.42	187.63	66
H5	3479.74	921.99	1132.61	79
H6	6810.89	482.98	318.56	83
H8	635.69	1379.77	1949.86	73
H10	-1364.18	5514.19	1039.63	78
H11	-4680.69	5983.05	1800.91	81
H12	-6706.31	4789.96	2799.74	73
H13	-5418.38	3132.07	3052.73	68

6-Chloro-2-phenylquinoxaline (4f):

Fig. S2 depicts the displacement ellipsoid style plot of **6-Chloro-2-phenylquinoxaline** at 50 % probability level. The crystallographic parameters along with discrepancy indices are tabulated in Table S10. Table S11 displays the refined fractional atomic positions and isotropic displacement parameters for **6-Chloro-2-phenylquinoxaline**. Table S12 contains the anisotropic displacement parameters of non hydrogen atoms for **6-Chloro-2-phenylquinoxaline**. Table S13 and S14 summarize the bond length and bond angle of **6-Chloro-2-phenylquinoxaline**, respectively. Hydrogen atom coordinate with isotropic displacement parameters are listed in Table S15. In 2012, Chen and co-workers have reported the crystal structure of **6-Chloro-2-phenylquinoxaline**.[1]

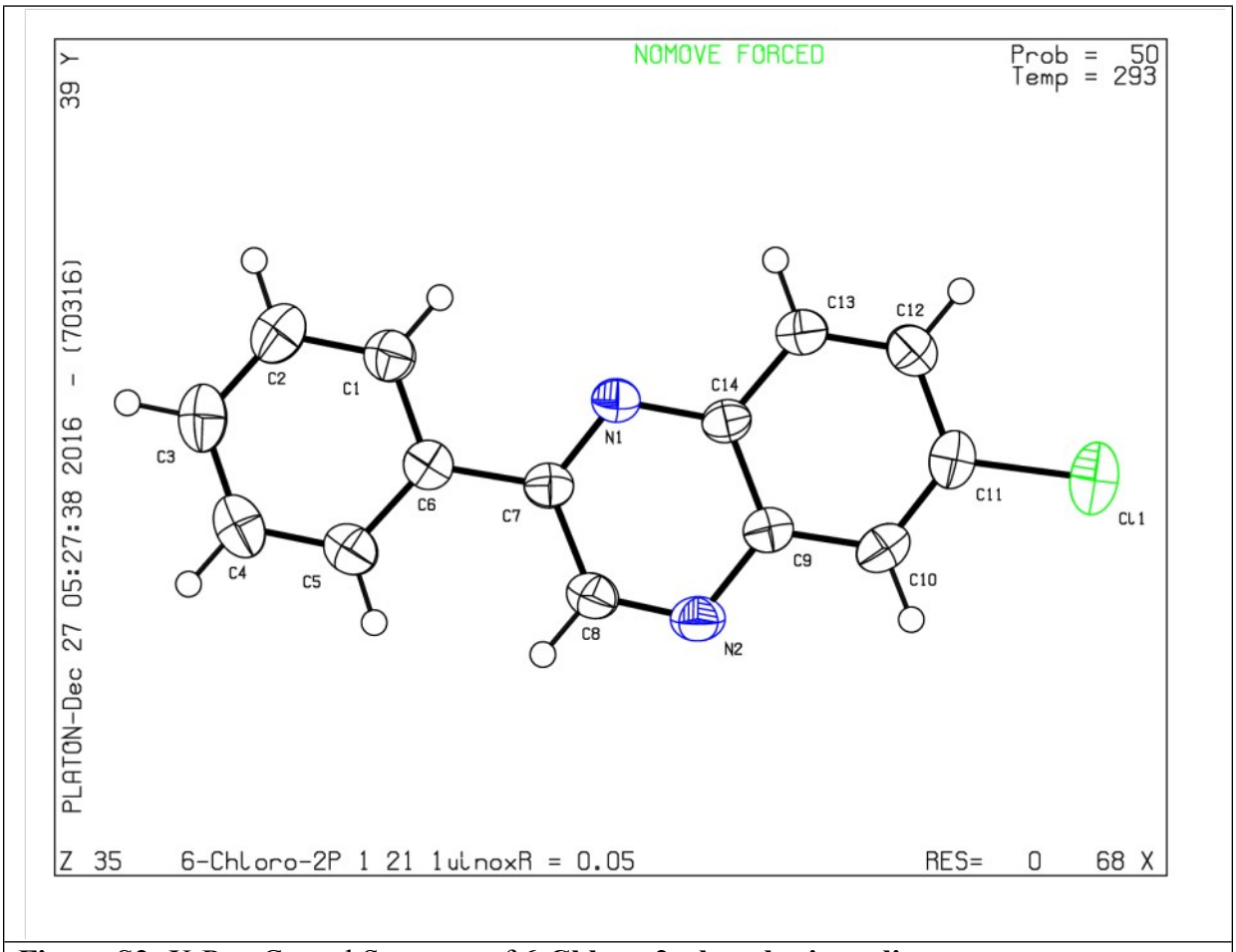


Figure S2: X-Ray Crystal Structure of **6-Chloro-2-phenylquinoxaline.**

Table S10. Crystal data and structure refinement for **6-Chloro-2-phenylquinoxaline.**

CCDC No.	1506178
Empirical formula	$C_{14}H_9ClN_2$
Formula weight	240.68
Temperature/K	293(2)
Crystal system	Monoclinic
Space group	$P2_1$
a/Å	9.5475(13)
b/Å	4.7592(5)
c/Å	12.4973(18)
α/°	90
β/°	103.477(13)
γ/°	90
Volume/Å^3	552.23(13)
Z	2
ρ_{calc}g/cm^3	1.447
μ/mm^{-1}	0.320
F(000)	248.0
Crystal size/mm^3	0.5 × 0.5 × 0.5
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.112 to 58.764
Index ranges	-12 ≤ h ≤ 12, -6 ≤ k ≤ 6, -17 ≤ l ≤ 16
Reflections collected	7467
Independent reflections	2654 [R_{int} = 0.0362, R_{sigma} = 0.0468]
Data/restraints/parameters	2654/1/154
Goodness-of-fit on F^2	1.010
Final R indexes [I>=2σ (I)]	R_1 = 0.0454, wR_2 = 0.0953
Final R indexes [all data]	R_1 = 0.0629, wR_2 = 0.1085
Largest diff. peak/hole / e Å^{-3}	0.17/-0.21
Flack parameter	0.15(5)

Table S11. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **6-Chloro-2-phenylquinoxaline**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***Y***	***Z***	**U(eq)**
Cl1	9042.5(8)	12900(3)	3924.5(7)	56.6(3)
N1	4472(2)	4382(5)	3067.3(18)	32.2(6)
N2	5816(3)	5969(6)	1377.9(19)	41.2(7)
C9	6216(3)	7162(6)	2402(2)	32.3(7)
C14	5536(3)	6352(7)	3242(2)	31.5(6)

C7	4092(3)	3247(7)	2086(2)	32.0(7)
C10	7307(3)	9213(7)	2614(2)	38.8(7)
C6	2934(3)	1111(6)	1878(2)	33.8(6)
C11	7697(3)	10378(6)	3632(3)	37.5(7)
C12	7030(3)	9595(7)	4477(2)	40.9(7)
C1	2243(3)	441(7)	2715(3)	42.7(8)
C5	2483(3)	-263(7)	878(2)	43.5(8)
C8	4791(3)	4098(7)	1241(2)	40.5(8)
C13	5976(3)	7639(8)	4282(2)	39.2(8)
C2	1165(3)	-1537(8)	2552(3)	49.4(9)
C4	1398(3)	-2233(10)	719(3)	51.0(8)
C3	734(3)	-2883(7)	1557(3)	50.7(10)

Table S12. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **6-Chloro-2-phenylquinoxaline**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl1	44.4(4)	43.9(5)	78.5(6)	-0.9(5)	8.4(4)	-8.8(4)
N1	33.4(12)	34.1(14)	29.1(13)	1.5(11)	7.8(9)	2.2(11)
N2	42.8(14)	50.7(18)	31.0(13)	2.6(13)	10.8(10)	-0.8(14)
C9	31.3(14)	34.1(19)	31.7(15)	4.4(12)	8.0(11)	5.5(12)
C14	33.4(14)	31.9(16)	30.0(15)	4.5(13)	9.2(11)	3.6(13)
C7	32.2(13)	33.5(19)	29.5(14)	4.1(14)	5.9(10)	5.1(14)
C10	35.3(15)	41.7(18)	41.5(17)	10.0(15)	13.4(13)	2.6(15)
C6	32.3(14)	31.9(16)	36.5(15)	1.6(14)	6.6(11)	6.3(13)
C11	29.3(14)	31.4(17)	49.5(19)	3.7(14)	4.4(13)	2.3(13)
C12	42.1(17)	41.9(19)	37.6(17)	-4.7(15)	7.2(13)	-0.7(15)
C1	39.9(17)	47(2)	41.2(17)	-2.6(15)	9.8(13)	-2.0(15)
C5	48.7(19)	44(2)	36.7(17)	-2.7(16)	7.7(14)	0.9(17)
C8	42.7(16)	48(2)	30.1(16)	-2.4(14)	7.7(12)	-2.1(16)
C13	41.2(15)	44(2)	33.9(15)	0.6(16)	12.3(12)	-2.0(17)
C2	41.2(17)	50(2)	59(2)	6.2(18)	14.6(15)	-1.8(17)
C4	51.2(18)	47(2)	48.7(19)	-7.8(18)	-1.1(15)	-3(2)
C3	39.5(17)	44(2)	63(2)	0.4(17)	0.4(15)	-5.0(15)

Table S13. Bond Lengths for **6-Chloro-2-phenylquinoxaline**.

Atom	Atom	Length/Å
Cl1	C11	1.734(3)
N1	C14	1.363(4)
N1	C7	1.311(3)
N2	C9	1.370(3)

N2	C8	1.305(4)
C9	C14	1.411(4)
C9	C10	1.407(4)
C14	C13	1.409(4)
C7	C6	1.479(4)
C7	C8	1.433(4)
C10	C11	1.358(4)
C6	C1	1.398(4)
C6	C5	1.387(4)
C11	C12	1.404(4)
C12	C13	1.350(5)
C1	C2	1.374(4)
C5	C4	1.377(5)
C2	C3	1.375(5)
C4	C3	1.379(5)

Table S14. Bond Angles for **6-Chloro-2-phenylquinoxaline**.

Atom	**Atom**	**Atom**	**Angle/°**
C7	N1	C14	117.8(2)
C8	N2	C9	116.3(2)
N2	C9	C14	120.3(3)
N2	C9	C10	119.8(2)
C10	C9	C14	119.9(3)
N1	C14	C9	121.6(3)
N1	C14	C13	119.8(2)
C13	C14	C9	118.5(3)
N1	C7	C6	118.7(2)
N1	C7	C8	119.9(3)
C8	C7	C6	121.4(3)
C11	C10	C9	119.3(3)
C1	C6	C7	119.3(3)
C5	C6	C7	123.0(3)
C5	C6	C1	117.7(3)
C10	C11	Cl1	120.5(2)
C10	C11	C12	121.5(3)
C12	C11	Cl1	118.0(2)
C13	C12	C11	119.7(3)
C2	C1	C6	120.9(3)
C4	C5	C6	121.0(3)
N2	C8	C7	124.0(3)
C12	C13	C14	121.0(3)
C1	C2	C3	120.6(3)

C5	C4	C3	120.5(3)
C2	C3	C4	119.3(3)

Table S15. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **6-Chloro-2-phenylquinoxaline**.

Atom	***x***	***y***	***Z***	**U(eq)**
H10	7756	9766	2063	47
H12	7313	10420	5168	49
H1	2516	1345	3392	51
H5	2921	153	305	52
H8	4495	3265	552	49
H13	5534	7133	4842	47
H2	723	-1968	3121	59
H4	1111	-3131	42	61
H3	3	-4218	1449	61

7-Chloro-2-phenylquinoxaline (4f'):

Fig. S3 depicts the displacement ellipsoid style plot of **7-Chloro-2-phenylquinoxaline** at 50 % probability level. The crystallographic parameters along with discrepancy indices are tabulated in Table S16. Table S17 displays the refined fractional atomic positions and isotropic displacement parameters for **7-Chloro-2-phenylquinoxaline**. Table S18 contains the anisotropic displacement parameters of non hydrogen atoms for **7-Chloro-2-phenylquinoxaline**. Table S19 and S20 summarize the bond length and bond angle of **7-Chloro-2-phenylquinoxaline**, respectively. Hydrogen atom coordinate with isotropic displacement parameters are listed in Table S21. In 2013, Darabi *et al.* have reported the crystal structure of **7-Chloro-2-phenylquinoxaline**.[2]

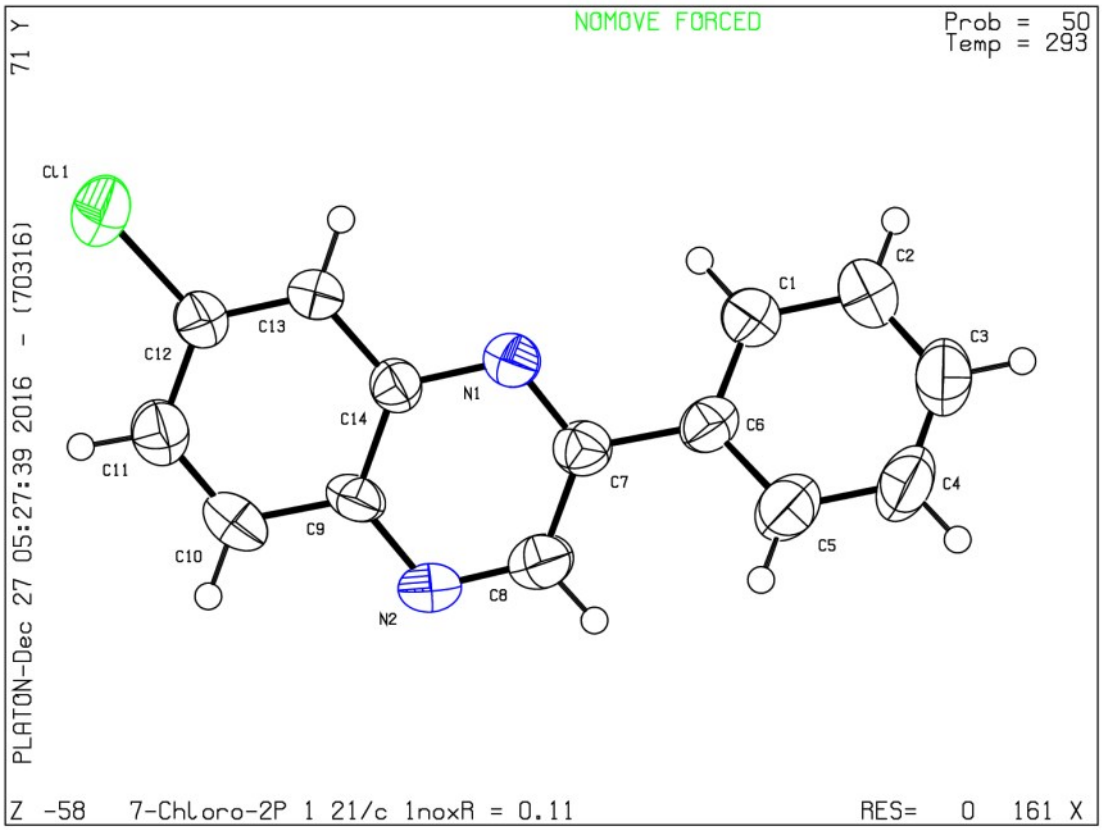


Figure S3: X-Ray Crystal Structure of **7-Chloro-2-phenylquinoxaline.**

Table S16. Crystal data and structure refinement for **7-Chloro-2-phenylquinoxaline.**

CCDC No.	1533362
Empirical formula	$C_{14}H_9ClN_2$
Formula weight	240.68
Temperature/K	293(2)
Crystal system	Monoclinic
Space group	$P2_1/c$
a/Å	3.8983(5)
b/Å	26.209(3)
c/Å	11.0333(11)
α/°	90
β/°	96.286(11)
γ/°	90
Volume/Å^3	1120.5(2)
Z	4
ρ_{calc}g/cm^3	1.427
μ/mm^{-1}	0.316
F(000)	496.0
Crystal size/mm^3	0.5 × 0.5 × 0.5
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.962 to 58.756
Index ranges	$-5 \le h \le 5$, $-34 \le k \le 33$, $-14 \le l \le 15$
Reflections collected	14444
Independent reflections	2831 [R_{int} = 0.1467, R_{sigma} = 0.1847]
Data/restraints/parameters	2831/0/154
Goodness-of-fit on F^2	0.967
Final R indexes [I>=2σ (I)]	R_1 = 0.1109, wR_2 = 0.2407
Final R indexes [all data]	R_1 = 0.2615, wR_2 = 0.3247
Largest diff. peak/hole / e Å^{-3}	0.80/-0.27

Table S17. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **7-Chloro-2-phenylquinoxaline**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***Y***	***Z***	**U(eq)**
Cl1	6472(4)	1109.3(5)	7586.7(16)	69.4(7)
N1	6135(11)	3035.2(16)	7128(4)	46.8(12)
N2	1940(13)	2952.5(17)	4867(4)	54.4(13)
C7	5118(13)	3438(2)	6469(5)	45.4(14)
C14	5050(13)	2571.9(18)	6647(5)	40.3(13)
C6	6254(14)	3947.6(19)	6957(6)	47.0(14)
C9	3014(14)	2532.7(19)	5527(5)	44.8(14)
C13	6116(13)	2123.9(19)	7305(5)	43.5(13)

C12	5109(14)	1665.3(19)	6823(5)	51.2(15)
C11	3087(15)	1622(2)	5692(6)	55.7(16)
C10	2032(15)	2047(2)	5042(6)	56.7(16)
C8	3003(15)	3394(2)	5344(5)	53.2(15)
C1	6886(14)	4024(2)	8194(6)	55.2(16)
C5	6793(16)	4354(2)	6185(6)	69.2(19)
C4	7865(17)	4826(2)	6657(8)	75(2)
C3	8428(19)	4888(2)	7884(8)	80(2)
C2	7971(18)	4493(2)	8663(7)	79(2)

Table S18. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **7-Chloro-2-phenylquinoxaline**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl1	82.1(14)	44.8(10)	79.2(13)	3.9(7)	-0.4(9)	1.2(8)
N1	50(3)	47(3)	42(3)	1(2)	0(2)	-4(2)
N2	65(3)	54(3)	41(3)	7(2)	-9(2)	3(2)
C7	45(3)	47(3)	44(3)	0(3)	3(3)	5(3)
C14	43(3)	39(3)	39(3)	-3(2)	5(3)	-2(2)
C6	45(3)	45(3)	51(4)	9(3)	2(3)	2(2)
C9	45(3)	53(3)	33(3)	-4(2)	-7(3)	-1(3)
C13	49(3)	45(3)	35(3)	0(2)	0(3)	-1(3)
C12	66(4)	42(3)	45(4)	-6(2)	-2(3)	3(3)
C11	61(4)	49(3)	57(4)	-7(3)	8(3)	-3(3)
C10	55(4)	67(4)	45(4)	-13(3)	-6(3)	-6(3)
C8	58(4)	55(4)	47(4)	8(3)	3(3)	7(3)
C1	64(4)	49(3)	50(4)	-2(3)	-2(3)	3(3)
C5	91(5)	52(4)	65(5)	12(3)	12(4)	6(3)
C4	86(5)	40(4)	96(6)	13(4)	1(4)	2(3)
C3	91(6)	45(4)	99(6)	-5(4)	-17(5)	-6(3)
C2	107(6)	56(4)	68(5)	-11(4)	-13(4)	-9(4)

Table S19. Bond Lengths for **7-Chloro-2-phenylquinoxaline**.

Atom	Atom	Length/Å
Cl1	C12	1.737(5)
N1	C7	1.317(6)
N1	C14	1.373(6)
N2	C9	1.360(6)
N2	C8	1.319(6)
C7	C6	1.490(7)
C7	C8	1.417(8)

C14	C9	1.398(7)
C14	C13	1.418(6)
C6	C1	1.374(8)
C6	C5	1.394(7)
C9	C10	1.417(7)
C13	C12	1.355(7)
C12	C11	1.405(8)
C11	C10	1.364(7)
C1	C2	1.381(7)
C5	C4	1.389(8)
C4	C3	1.357(10)
C3	C2	1.369(9)

Table S20. Bond Angles for **7-Chloro-2-phenylquinoxaline**.

Atom	**Atom**	**Atom**	**Angle/°**
C7	N1	C14	115.7(5)
C8	N2	C9	115.5(5)
N1	C7	C6	117.3(5)
N1	C7	C8	122.0(5)
C8	C7	C6	120.7(5)
N1	C14	C9	121.8(5)
N1	C14	C13	118.3(5)
C9	C14	C13	119.9(5)
C1	C6	C7	120.2(5)
C1	C6	C5	118.2(5)
C5	C6	C7	121.5(6)
N2	C9	C14	121.7(5)
N2	C9	C10	118.0(5)
C14	C9	C10	120.2(5)
C12	C13	C14	118.5(5)
C13	C12	Cl1	119.6(4)
C13	C12	C11	122.0(5)
C11	C12	Cl1	118.4(4)
C10	C11	C12	120.6(5)
C11	C10	C9	118.8(6)
N2	C8	C7	123.2(5)
C6	C1	C2	121.1(6)
C4	C5	C6	120.7(6)
C3	C4	C5	119.3(6)
C4	C3	C2	121.2(6)
C3	C2	C1	119.5(7)

Table S21. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **7-Chloro-2-phenylquinoxaline**.

Atom	*x*	*Y*	*z*	U(eq)
H13	7476.05	2144.38	8050.41	52
H11	2462.89	1300.79	5384.87	67
H10	692.04	2018.58	4294.34	68
H8	2332.48	3690.85	4922.3	64
H1	6577.79	3755.97	8723.16	66
H5	6430.34	4308.52	5344.78	83
H4	8194.19	5096.77	6138.23	90
H3	9137.18	5203.76	8201.61	96
H2	8388.56	4539.82	9501.74	94

6-Nitro-2-phenylquinoxaline (4g):

Fig. S4 depicts the displacement ellipsoid style plot of **6-Nitro-2-phenylquinoxaline** at 50 % probability level. The crystallographic parameters along with discrepancy indices are tabulated in Table S22. Table S23 displays the refined fractional atomic positions and isotropic displacement parameters for **6-Nitro-2-phenylquinoxaline**. Table S24 contains the anisotropic displacement parameters of non hydrogen atoms for **6-Nitro-2-phenylquinoxaline**. Table S25 and S26 summarize the bond length and bond angle of **6-Nitro-2-phenylquinoxaline**, respectively. Hydrogen atom coordinate with isotropic displacement parameters are listed in Table S27. In 2013, Darabi *et al.* have reported the crystal structure of **6-Nitro-2-phenylquinoxaline**.[2]

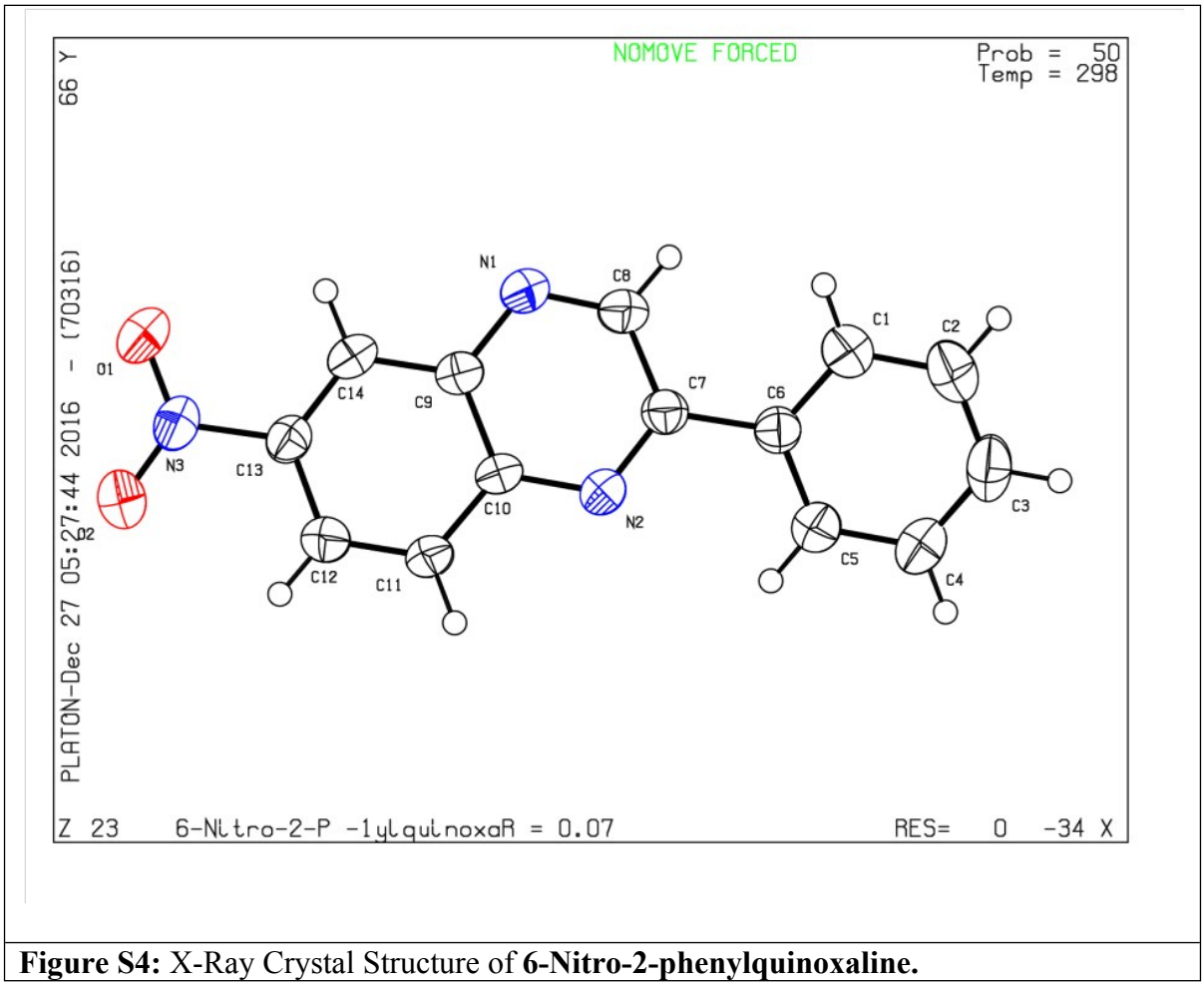


Figure S4: X-Ray Crystal Structure of **6-Nitro-2-phenylquinoxaline.**

Table S22. Crystal data and structure refinement for **6-Nitro-2-phenylquinoxaline**.

CCDC No.	1533364
Empirical formula	$C_{14}H_9N_3O_2$
Formula weight	251.24
Temperature/K	298.15
Crystal system	Triclinic
Space group	P-1
a/Å	3.9286(4)
b/Å	11.3555(15)
c/Å	13.3245(15)
α/°	78.536(11)
β/°	83.012(9)
γ/°	81.083(10)
Volume/Å^3	572.98(12)
Z	2
ρ_{calc}g/cm^3	1.456
μ/mm^{-1}	0.101
F(000)	260.0
Crystal size/mm^3	0.06 × 0.02 × 0.02
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.666 to 58.526
Index ranges	$-4 \le h \le 5$, $-14 \le k \le 15$, $-18 \le l \le 18$
Reflections collected	7787
Independent reflections	2701 [R_{int} = 0.0397, R_{sigma} = 0.0746]
Data/restraints/parameters	2701/0/172
Goodness-of-fit on F^2	1.026
Final R indexes [I>=2σ (I)]	R_1 = 0.0664, wR_2 = 0.1224
Final R indexes [all data]	R_1 = 0.1494, wR_2 = 0.1694
Largest diff. peak/hole / e Å^{-3}	0.20/-0.26

Table S23. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **6-Nitro-2-phenylquinoxaline**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*Y*	*Z*	U(eq)
N2	3003(4)	1869.4(17)	8932.9(15)	39.7(5)
C13	-2696(5)	2358(2)	11671.7(18)	39.0(6)
C14	-2824(6)	3319(2)	10873.9(18)	40.6(6)
C10	1103(5)	2039(2)	9835.9(18)	35.1(6)
C9	-899(5)	3168(2)	9935.9(18)	36.9(6)
C6	4895(6)	2634(2)	7167.9(18)	38.4(6)
C11	1137(5)	1077(2)	10688.4(18)	41.0(6)

N1	-995(5)	4123.7(18)	9123.1(15)	45.2(6)
N3	-4767(5)	2493(2)	12650.9(17)	51.2(6)
C7	2914(5)	2802(2)	8159.4(18)	37.6(6)
C8	855(6)	3927(2)	8277.1(19)	45.3(6)
O2	-5074(5)	1580.1(19)	13292.7(15)	78.9(7)
C12	-748(6)	1231(2)	11595.1(19)	43.7(6)
C1	5821(6)	3612(2)	6429.0(19)	51.4(7)
C5	5842(6)	1478(2)	6948(2)	49.6(7)
O1	-6126(5)	3503.1(19)	12771.7(15)	83.3(7)
C2	7679(6)	3416(3)	5510(2)	59.2(8)
C4	7672(7)	1294(3)	6029(2)	60.3(8)
C3	8610(7)	2267(3)	5311(2)	61.4(8)

Table S24. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **6-Nitro-2-phenylquinoxaline**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N2	38.4(11)	38.3(13)	40.7(12)	-9.2(10)	0.2(9)	-0.3(9)
C13	36.1(13)	40.2(16)	41.3(15)	-12.6(12)	1.3(11)	-4.7(11)
C14	40.1(13)	35.3(15)	47.5(16)	-15.5(12)	-2.7(12)	0.6(10)
C10	34.4(12)	29.6(14)	40.8(14)	-8.7(11)	-4.5(11)	0.7(10)
C9	38.0(13)	32.7(15)	40.4(15)	-8.4(11)	-5.8(11)	-1.9(10)
C6	37.4(13)	39.4(16)	37.5(14)	-6.5(11)	-3.7(11)	-3.2(10)
C11	40.6(13)	33.3(15)	44.9(15)	-6.6(12)	0.5(11)	3.2(10)
N1	52.4(13)	36.7(13)	43.4(13)	-8.8(10)	-1.6(10)	3.5(10)
N3	54.7(14)	54.0(17)	43.1(14)	-15.7(12)	4.8(11)	0.1(11)
C7	36.6(13)	35.4(15)	39.8(14)	-5.8(11)	-2.6(11)	-4.1(10)
C8	53.1(15)	35.7(16)	43.5(15)	-4.8(12)	-5.0(13)	2.3(11)
O2	108.4(17)	59.9(15)	55.2(13)	-4.1(11)	28.2(12)	-7.2(12)
C12	45.9(14)	37.7(16)	44.2(15)	-4.0(12)	-1.6(12)	-1.5(11)
C1	56.4(16)	49.7(18)	46.0(17)	-5.4(14)	-3.6(13)	-6.4(13)
C5	51.8(15)	44.6(17)	49.0(17)	-8.5(13)	4.4(13)	-3.5(12)
O1	110.0(17)	61.2(16)	63.1(14)	-16.9(11)	21.4(12)	21.2(12)
C2	58.8(17)	68(2)	46.4(18)	1.5(15)	1.8(14)	-15.4(15)
C4	63.1(17)	58(2)	55.7(19)	-17.7(15)	8.1(15)	3.8(14)
C3	56.4(17)	82(2)	42.5(17)	-14.6(16)	9.0(13)	-5.3(15)

Table S25. Bond Lengths for **6-Nitro-2-phenylquinoxaline**.

Atom	Atom	Length/Å
N2	C10	1.368(3)
N2	C7	1.322(3)

C13	C14	1.363(3)
C13	N3	1.473(3)
C13	C12	1.401(3)
C14	C9	1.406(3)
C10	C9	1.417(3)
C10	C11	1.411(3)
C9	N1	1.372(3)
C6	C7	1.480(3)
C6	C1	1.392(3)
C6	C5	1.387(3)
C11	C12	1.366(3)
N1	C8	1.303(3)
N3	O2	1.218(3)
N3	O1	1.220(3)
C7	C8	1.429(3)
C1	C2	1.387(3)
C5	C4	1.379(3)
C2	C3	1.367(4)
C4	C3	1.376(4)

Table S26. Bond Angles for **6-Nitro-2-phenylquinoxaline**.

Atom	**Atom**	**Atom**	**Angle/°**
C7	N2	C10	117.4(2)
C14	C13	N3	118.9(2)
C14	C13	C12	122.9(2)
C12	C13	N3	118.2(2)
C13	C14	C9	118.3(2)
N2	C10	C9	121.3(2)
N2	C10	C11	119.6(2)
C11	C10	C9	119.1(2)
C14	C9	C10	120.1(2)
N1	C9	C14	119.2(2)
N1	C9	C10	120.7(2)
C1	C6	C7	121.9(2)
C5	C6	C7	120.0(2)
C5	C6	C1	118.1(2)
C12	C11	C10	120.3(2)
C8	N1	C9	116.2(2)
O2	N3	C13	117.8(2)
O2	N3	O1	123.5(2)
O1	N3	C13	118.8(2)
N2	C7	C6	118.4(2)

N2	C7	C8	120.3(2)
C8	C7	C6	121.3(2)
N1	C8	C7	124.2(2)
C11	C12	C13	119.3(2)
C2	C1	C6	120.1(3)
C4	C5	C6	121.3(2)
C3	C2	C1	120.9(3)
C3	C4	C5	120.0(3)
C2	C3	C4	119.7(3)

Table S27. Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **6-Nitro-2-phenylquinoxaline**.

Atom	***x***	***Y***	***Z***	**U(eq)**
H14	-4149.83	4054.84	10947.79	49
H11	2450.27	333.5	10632.54	49
H8	832.61	4560.26	7714.01	54
H12	-739.32	595.14	12155.62	52
H1	5192.76	4398.5	6552.02	62
H5	5230.28	813.76	7429.74	59
H2	8299.2	4073.32	5021.59	71
H4	8271.58	511.5	5893.72	72
H3	9870.35	2145.36	4694.38	74

6-Methoxy-2-phenylquinoxaline (4j):

Fig. S5 depicts the displacement ellipsoid style plot of **6-Methoxy-2-phenylquinoxaline** at 50 % probability level. The crystallographic parameters along with discrepancy indices are tabulated in Table S28. Table S29 displays the refined fractional atomic positions and isotropic displacement parameters for **6-Methoxy-2-phenylquinoxaline**. Table S30 contains the anisotropic displacement parameters of non hydrogen atoms for **6-Methoxy-2-phenylquinoxaline**. Table S31 and S32 summarize the bond length and bond angle of **6-Methoxy-2-phenylquinoxaline**, respectively. Hydrogen atom coordinate with isotropic displacement parameters are listed in Table S33. In 2013, Nguyen's research group have reported the crystal structure of **6-Methoxy-2-phenylquinoxaline**.[3]

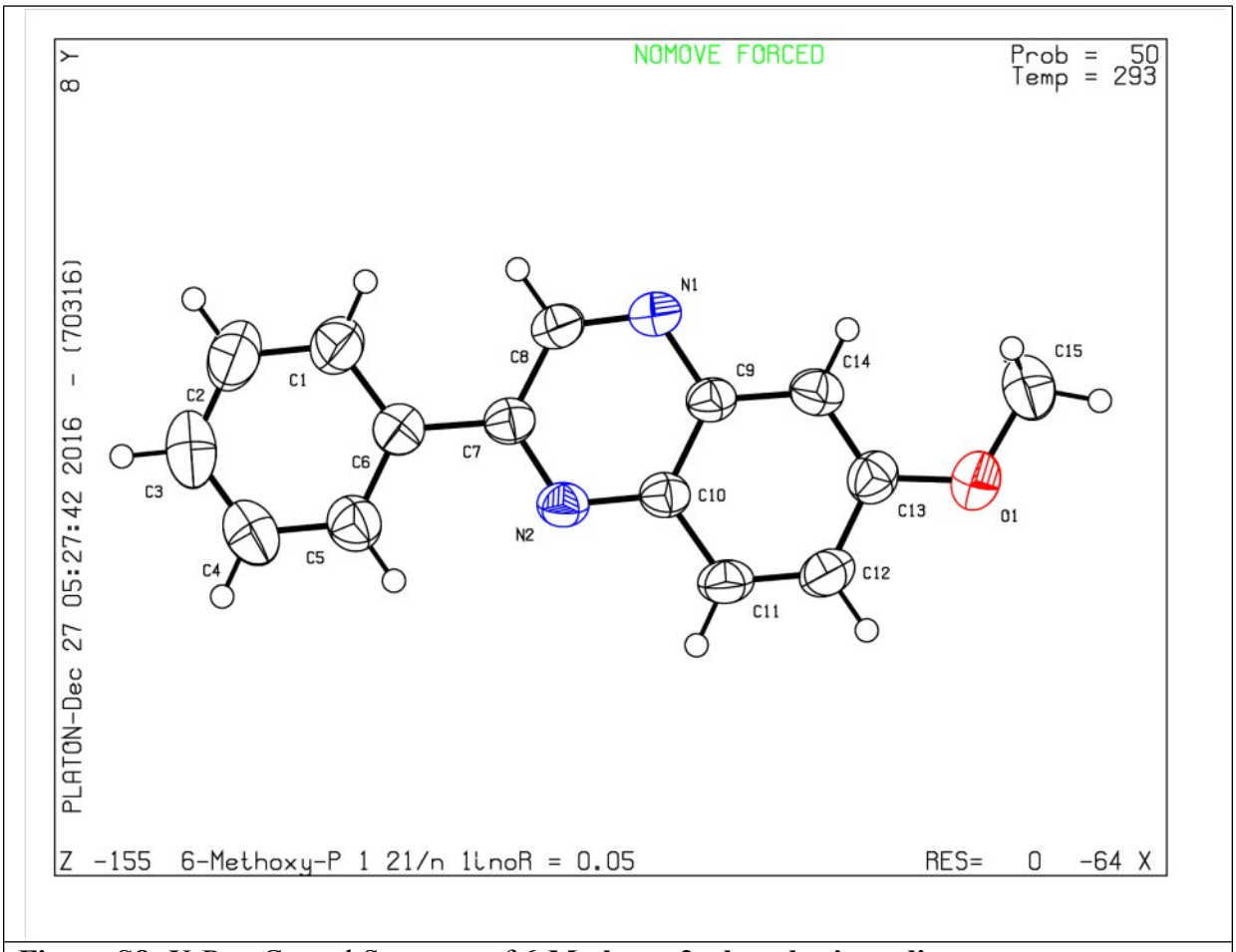


Figure S8: X-Ray Crystal Structure of **6-Methoxy-2-phenylquinoxaline.**

Table S28. Crystal data and structure refinement for **6-Methoxy-2-phenylquinoxaline.**

CCDC No.	1533363
Empirical formula	$C_{15}H_{12}N_2O$
Formula weight	236.27
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	16.0372(12)
b/Å	3.9616(3)
c/Å	18.8895(14)
α/°	90.000(5)
β/°	101.354(6)
γ/°	90.000(5)
Volume/Å^3	1176.62(15)
Z	4
ρ_{calc}g/cm^3	1.334
μ/mm^{-1}	0.086
F(000)	496.0
Crystal size/mm^3	0.5 × 0.5 × 0.5
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.598 to 58.858
Index ranges	$-20 \le h \le 22$, $-5 \le k \le 5$, $-24 \le l \le 25$
Reflections collected	14785
Independent reflections	2969 [R_{int} = 0.0400, R_{sigma} = 0.0448]
Data/restraints/parameters	2969/0/165
Goodness-of-fit on F^2	1.030
Final R indexes [I>=2σ (I)]	R_1 = 0.0547, wR_2 = 0.1110
Final R indexes [all data]	R_1 = 0.1164, wR_2 = 0.1419
Largest diff. peak/hole / e Å^{-3}	0.16/-0.13

Table S29. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **6-Methoxy-2-phenylquinoxaline**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***Y***	***z***	**U(eq)**
O1	958.4(8)	3965(4)	4792.9(7)	67.2(4)
N2	3605.1(8)	5373(3)	3343.6(7)	45.0(4)
N1	3897.8(8)	2058(4)	4688.5(7)	51.1(4)
C10	2970.4(10)	4967(4)	3721.5(8)	41.3(4)
C7	4363(1)	4165(4)	3635.6(8)	41.7(4)
C9	3115.8(10)	3345(4)	4399.0(8)	41.2(4)
C8	4489.1(11)	2481(4)	4307.8(9)	49.8(4)
C14	2449.9(10)	2998(4)	4780.5(9)	48.0(4)

C6	5066.0(11)	4627(4)	3241.7(9)	45.8(4)
C11	2147.3(10)	6200(4)	3436.0(9)	50.9(5)
C13	1664.8(11)	4195(4)	4485.6(9)	49.6(4)
C12	1514.7(11)	5834(5)	3811.0(9)	53.8(5)
C5	4903.8(12)	6037(5)	2557.2(10)	56.9(5)
C15	1046.6(13)	2331(6)	5475.3(10)	73.8(6)
C4	5547.1(14)	6451(5)	2177.1(11)	71.7(6)
C1	5897.7(11)	3700(5)	3537.8(10)	64.1(6)
C3	6360.5(14)	5492(6)	2470.8(13)	79.3(7)
C2	6536.7(13)	4139(6)	3154.3(12)	79.8(7)

Table S30. Anisotropic Displacement Parameters ($Å^2×10^3$) for **6-Methoxy-2-phenylquinoxaline**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	49.2(8)	89.1(10)	66.4(9)	5.4(7)	19.3(6)	9.9(7)
N2	45.5(8)	49.7(8)	37.4(8)	1.1(6)	2.1(6)	2.4(6)
N1	44.6(8)	62.2(10)	44.1(8)	9.1(7)	3.1(6)	8.0(7)
C10	44.3(10)	41.8(9)	35.7(9)	-3.1(7)	3.1(7)	1.0(7)
C7	43.3(9)	41.6(9)	38.0(9)	-4.3(8)	2.3(7)	-0.7(8)
C9	41.5(9)	42.8(9)	37.1(9)	-2.0(7)	2.3(7)	2.7(7)
C8	41.8(10)	58.4(11)	46.4(10)	4.6(9)	1.7(8)	8.3(8)
C14	53.4(11)	50.2(10)	39.0(9)	1.5(8)	5.3(8)	2.9(8)
C6	47.8(10)	44.3(10)	44.4(10)	-7.0(8)	7.0(8)	-2.1(8)
C11	49.5(10)	59.7(12)	39.5(9)	1.9(8)	-1.3(8)	9.8(9)
C13	46.2(10)	52.8(10)	49.9(11)	-6.1(9)	9.7(8)	3.6(8)
C12	44(1)	63.5(12)	50.4(11)	-1.6(9)	1.0(8)	11.8(9)
C5	57.3(12)	59.1(12)	54.9(12)	1.4(10)	12.1(9)	-4.9(9)
C15	72.6(14)	86.5(15)	69.3(14)	8.0(12)	31.4(11)	3.5(12)
C4	79.8(15)	76.7(15)	63.9(13)	5.0(11)	26.8(11)	-10.8(12)
C1	49.5(11)	87.6(15)	54.7(12)	-5.4(11)	8.8(9)	3.9(10)
C3	71.6(15)	92.4(17)	83.8(17)	-14.1(14)	39.6(13)	-16.4(13)
C2	50.6(12)	109.7(19)	81.5(16)	-14.1(14)	19.1(11)	0.9(12)

Table S31. Bond Lengths for **6-Methoxy-2-phenylquinoxaline**.

Atom	Atom	Length/Å
O1	C13	1.3739(19)
O1	C15	1.424(2)
N2	C10	1.3629(18)
N2	C7	1.3218(19)

N1	C9	1.3646(19)
N1	C8	1.309(2)
C10	C9	1.410(2)
C10	C11	1.411(2)
C7	C8	1.413(2)
C7	C6	1.479(2)
C9	C14	1.408(2)
C14	C13	1.358(2)
C6	C5	1.385(2)
C6	C1	1.390(2)
C11	C12	1.355(2)
C13	C12	1.408(2)
C5	C4	1.378(2)
C4	C3	1.367(3)
C1	C2	1.377(2)
C3	C2	1.375(3)

Table S32. Bond Angles for **6-Methoxy-2-phenylquinoxaline**.

Atom	**Atom**	**Atom**	**Angle/°**
C13	O1	C15	117.98(14)
C7	N2	C10	117.32(14)
C8	N1	C9	116.11(14)
N2	C10	C9	121.48(14)
N2	C10	C11	119.85(15)
C9	C10	C11	118.67(15)
N2	C7	C8	120.21(15)
N2	C7	C6	118.33(15)
C8	C7	C6	121.46(15)
N1	C9	C10	120.59(15)
N1	C9	C14	119.24(15)
C14	C9	C10	120.17(15)
N1	C8	C7	124.27(15)
C13	C14	C9	119.44(16)
C5	C6	C7	119.84(16)
C5	C6	C1	118.10(17)
C1	C6	C7	122.06(16)
C12	C11	C10	120.23(16)
O1	C13	C12	113.86(15)
C14	C13	O1	125.35(16)
C14	C13	C12	120.79(16)
C11	C12	C13	120.69(16)

C4	C5	C6	120.80(19)
C3	C4	C5	120.5(2)
C2	C1	C6	120.61(19)
C4	C3	C2	119.5(2)
C3	C2	C1	120.4(2)

Table S33. Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **6-Methoxy-2-phenylquinoxaline**.

Atom	***x***	***Y***	***z***	**U(eq)**
H8	5027.32	1616.59	4491.53	60
H14	2546.7	1958.8	5230.73	58
H11	2038.93	7268.11	2988.85	61
H12	975.62	6673.34	3620.94	65
H5	4353.99	6711.24	2351.68	68
H15A	1229.61	44.83	5434.32	111
H15B	509.17	2337.18	5626.7	111
H15C	1460.34	3509.92	5824.8	111
H4	5427.02	7390.49	1717.05	86
H1	6023.69	2775.43	3999.04	77
H3	6791.6	5752.57	2210.18	95
H2	7090.78	3516.12	3359.03	96

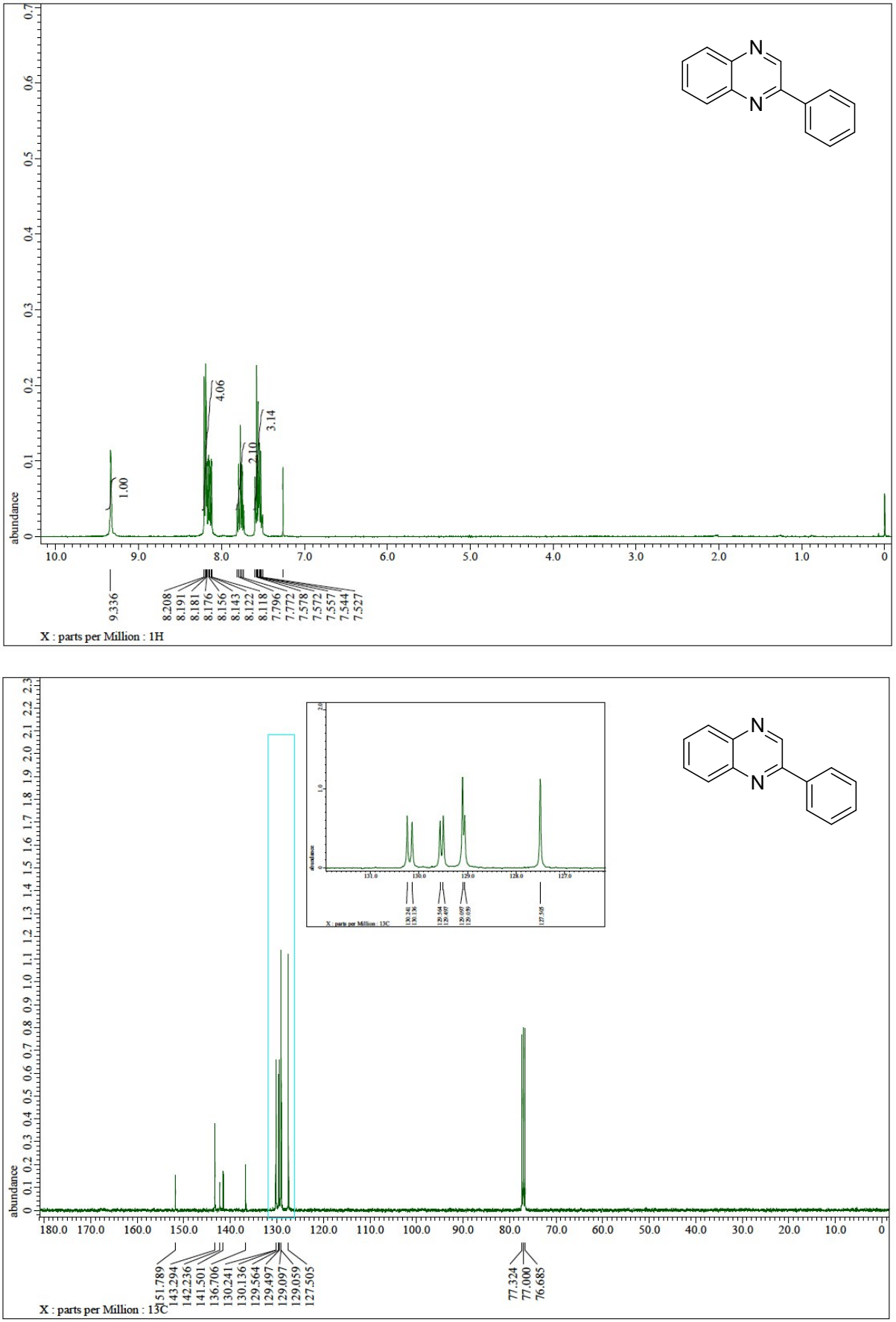


Figure S9. ^{1}H NMR of **3a** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3a** (100 MHz, $CDCl_3$).

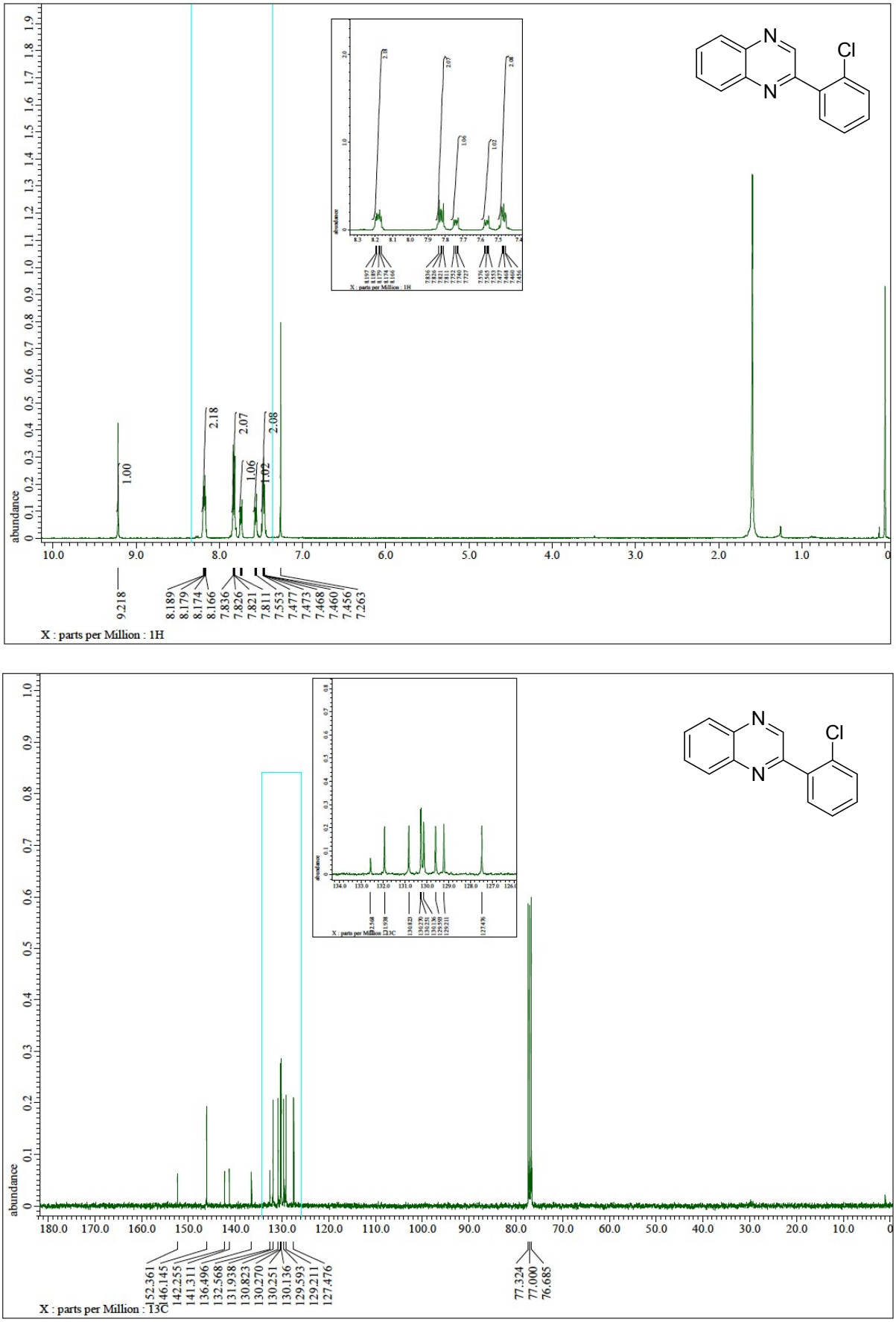
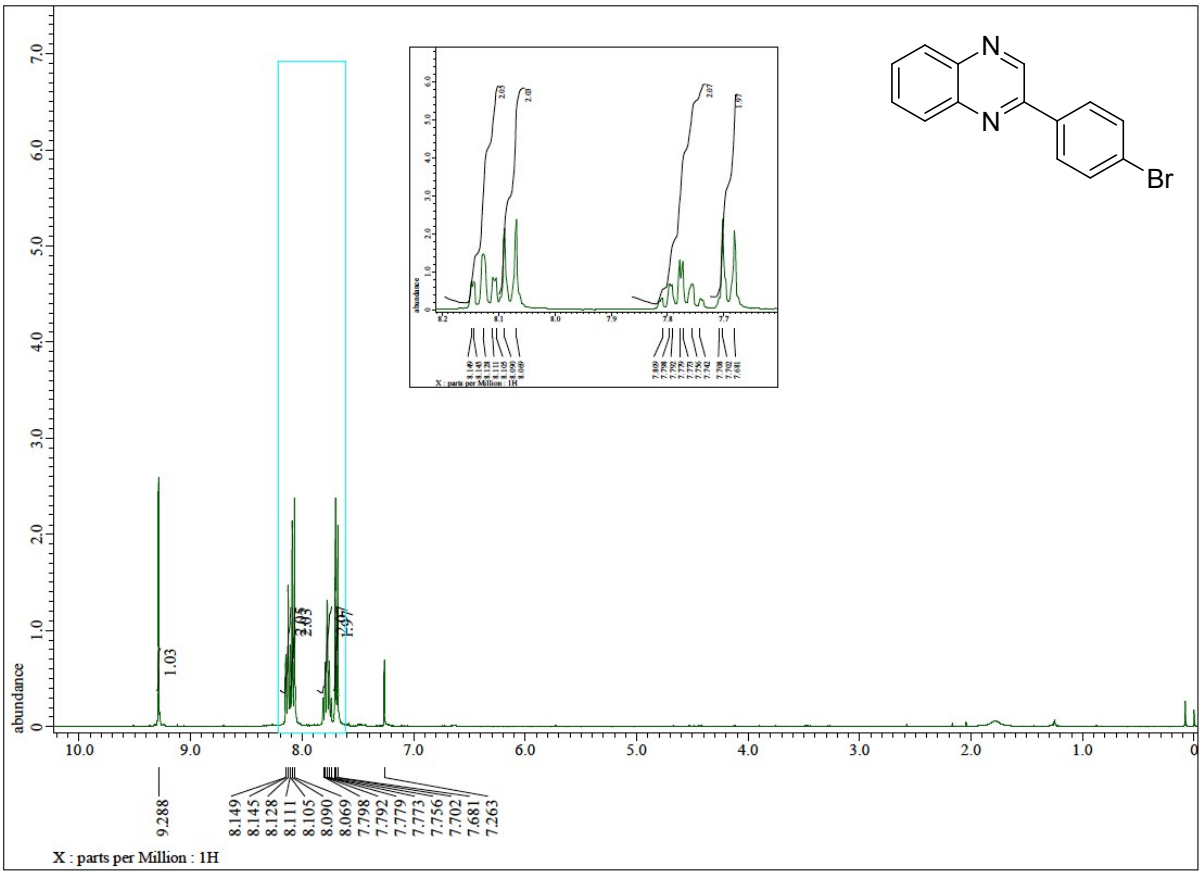


Figure S10. ^{1}H NMR of **3b** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3b** (100 MHz, $CDCl_3$).



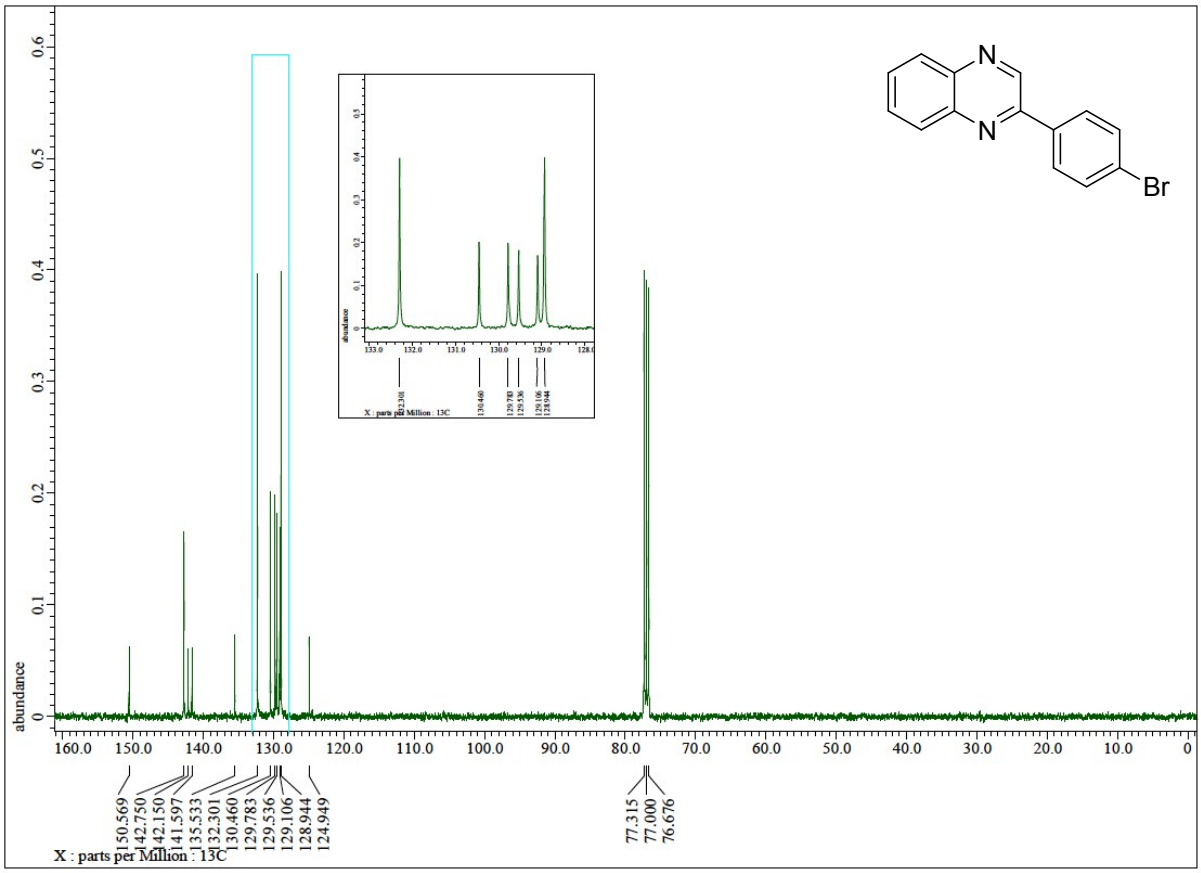
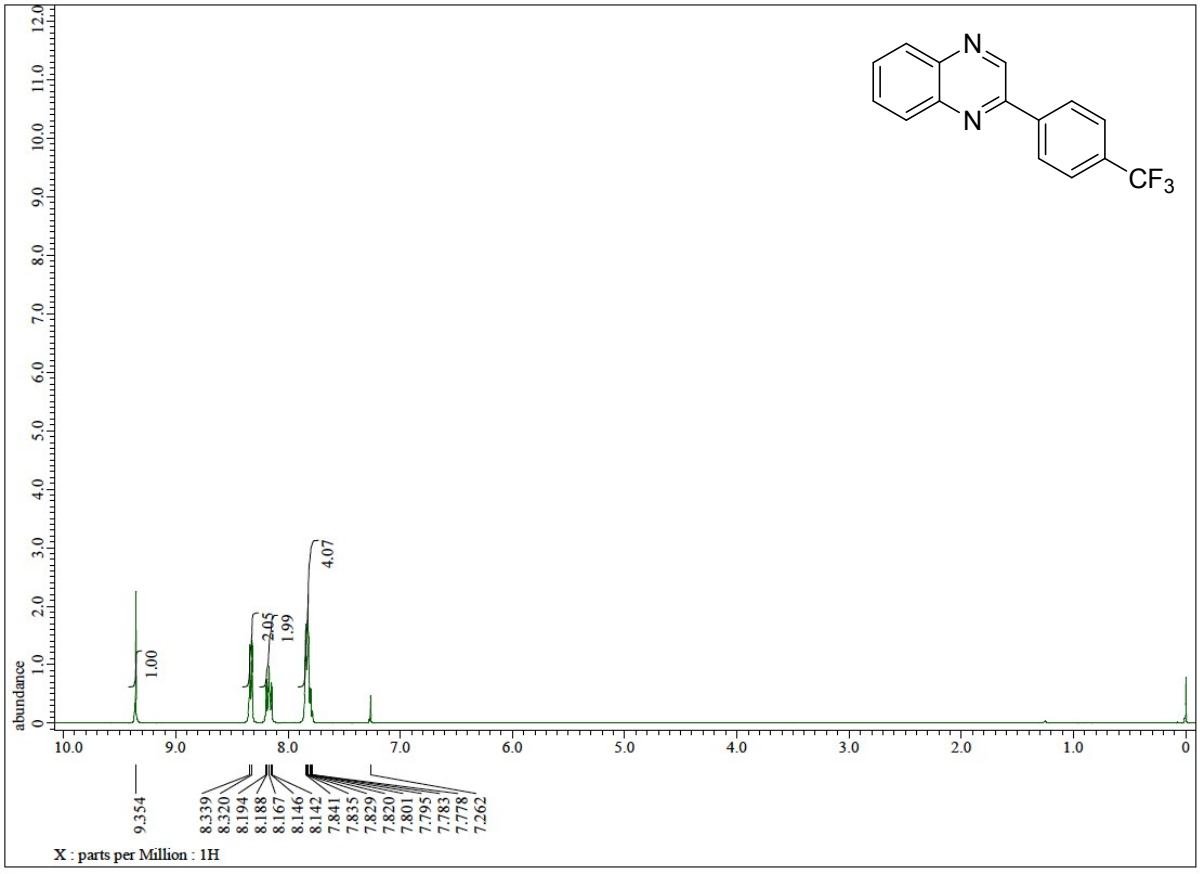


Figure S11. ^{1}H NMR of **3c** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3c** (100 MHz, $CDCl_3$).



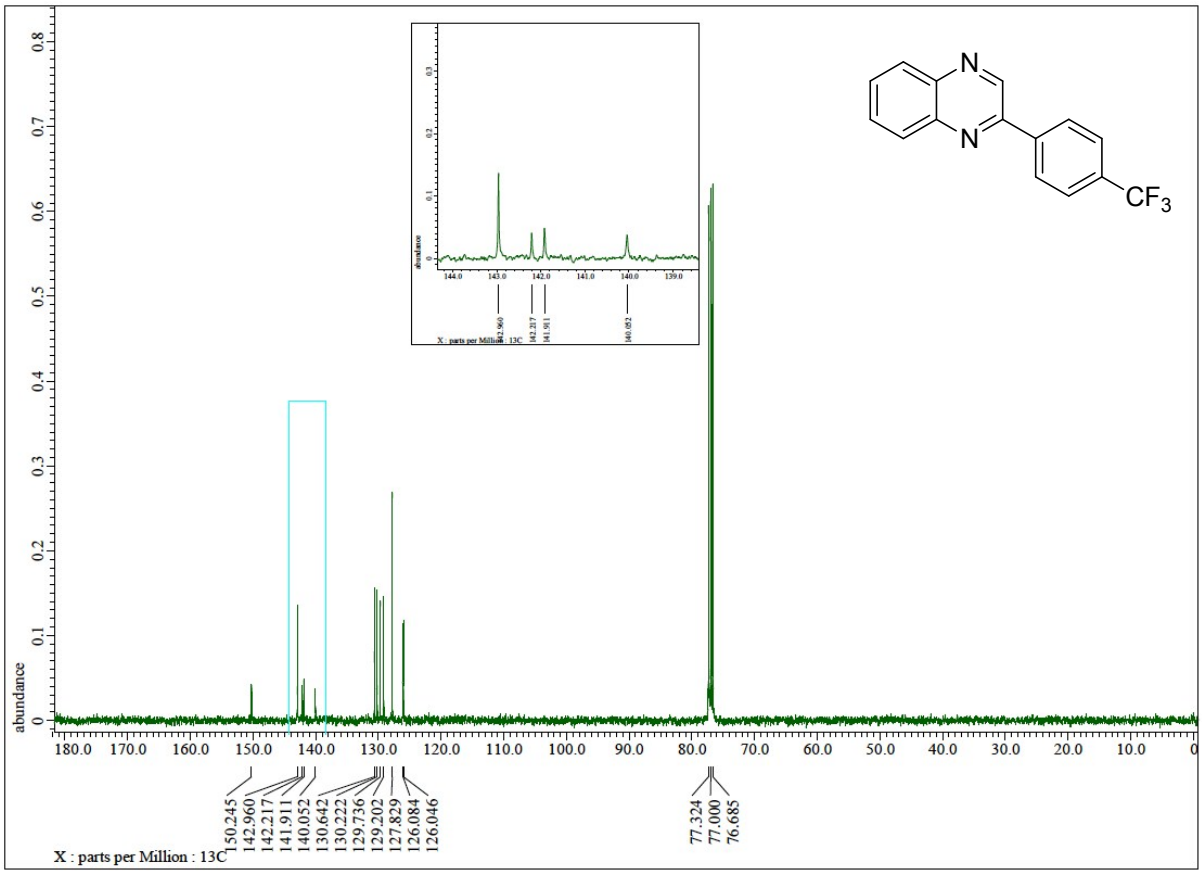
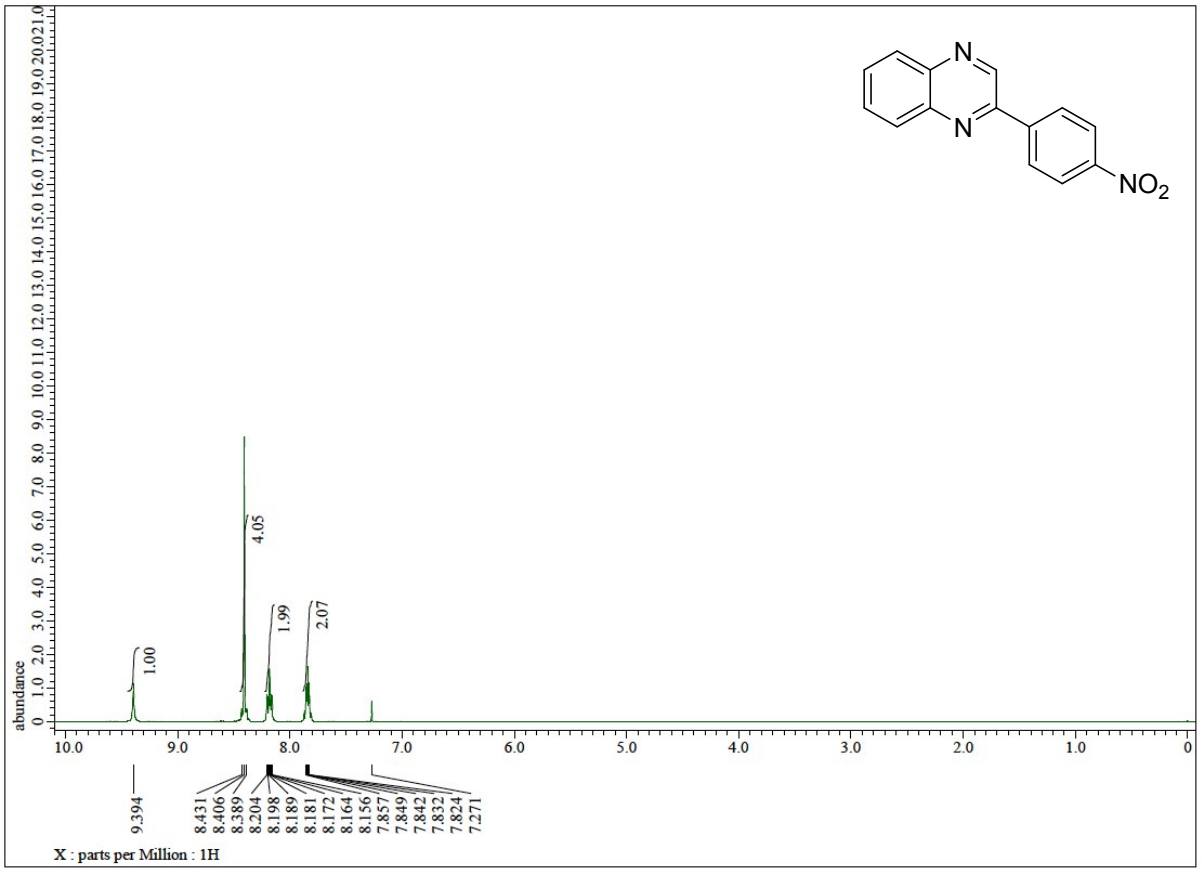


Figure S12. ^{1}H NMR of **3d** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3d** (100 MHz, $CDCl_3$).



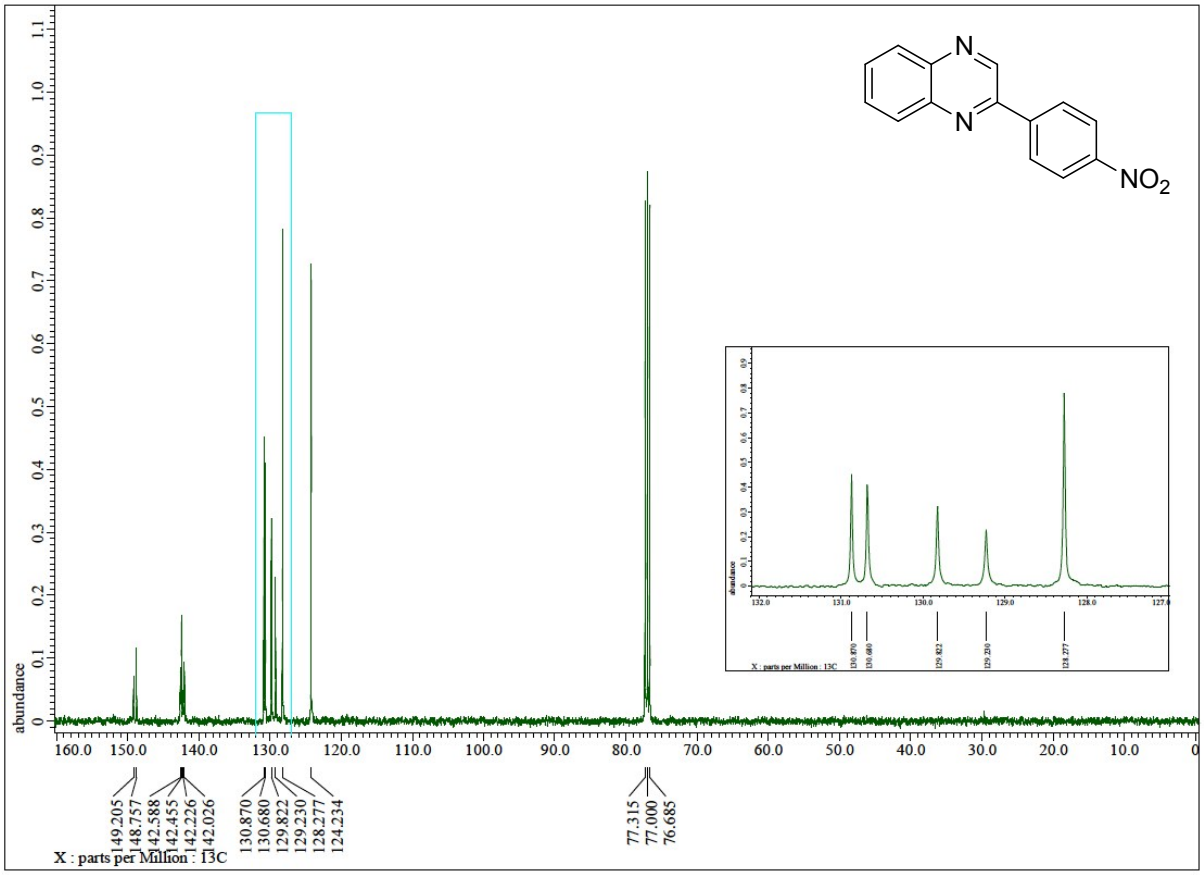


Figure S13. ^{1}H NMR of **3e** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3e** (100 MHz, $CDCl_3$).

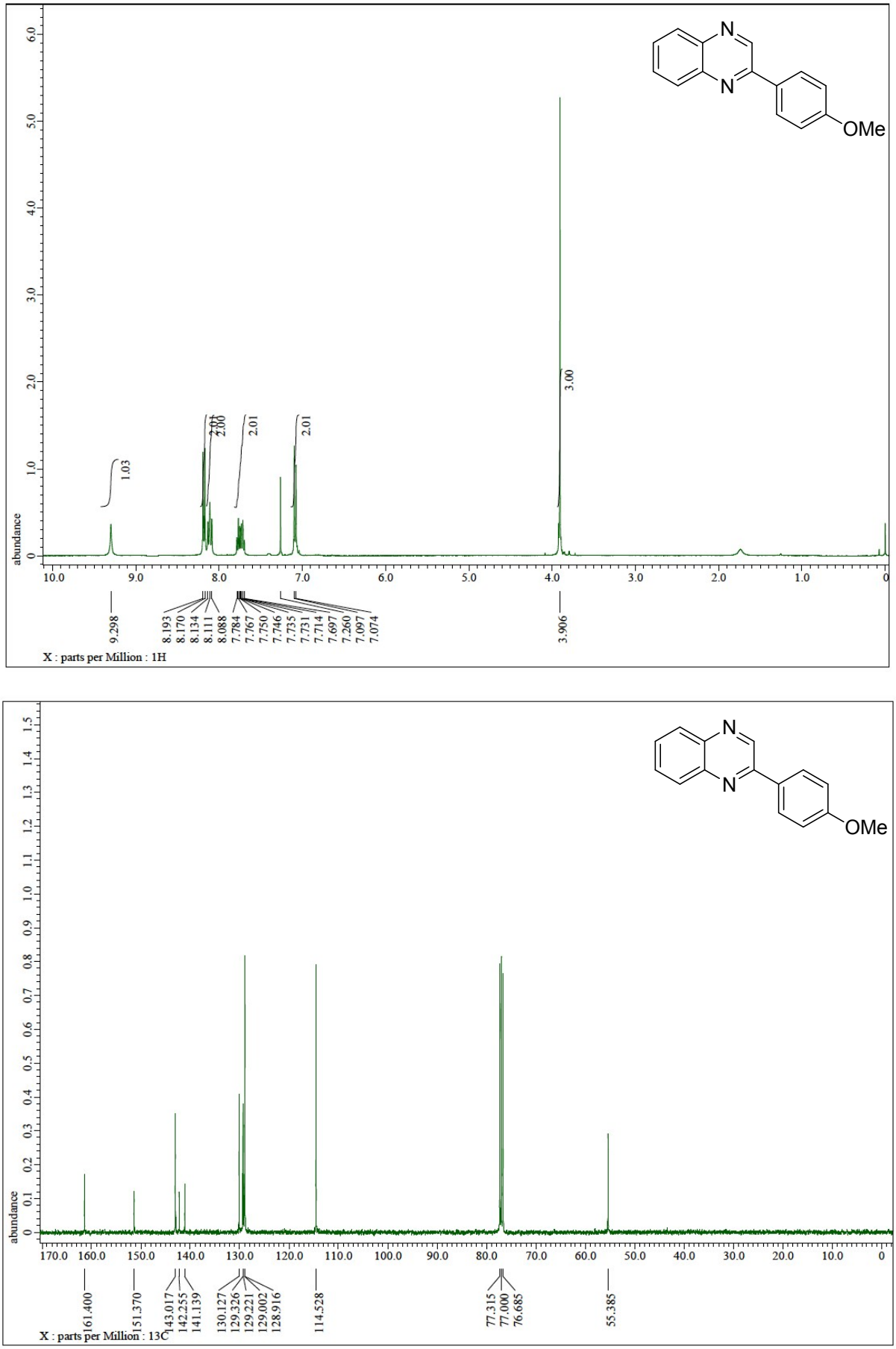


Figure S14. ^{1}H NMR of **3f** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3f** (100 MHz, $CDCl_3$).

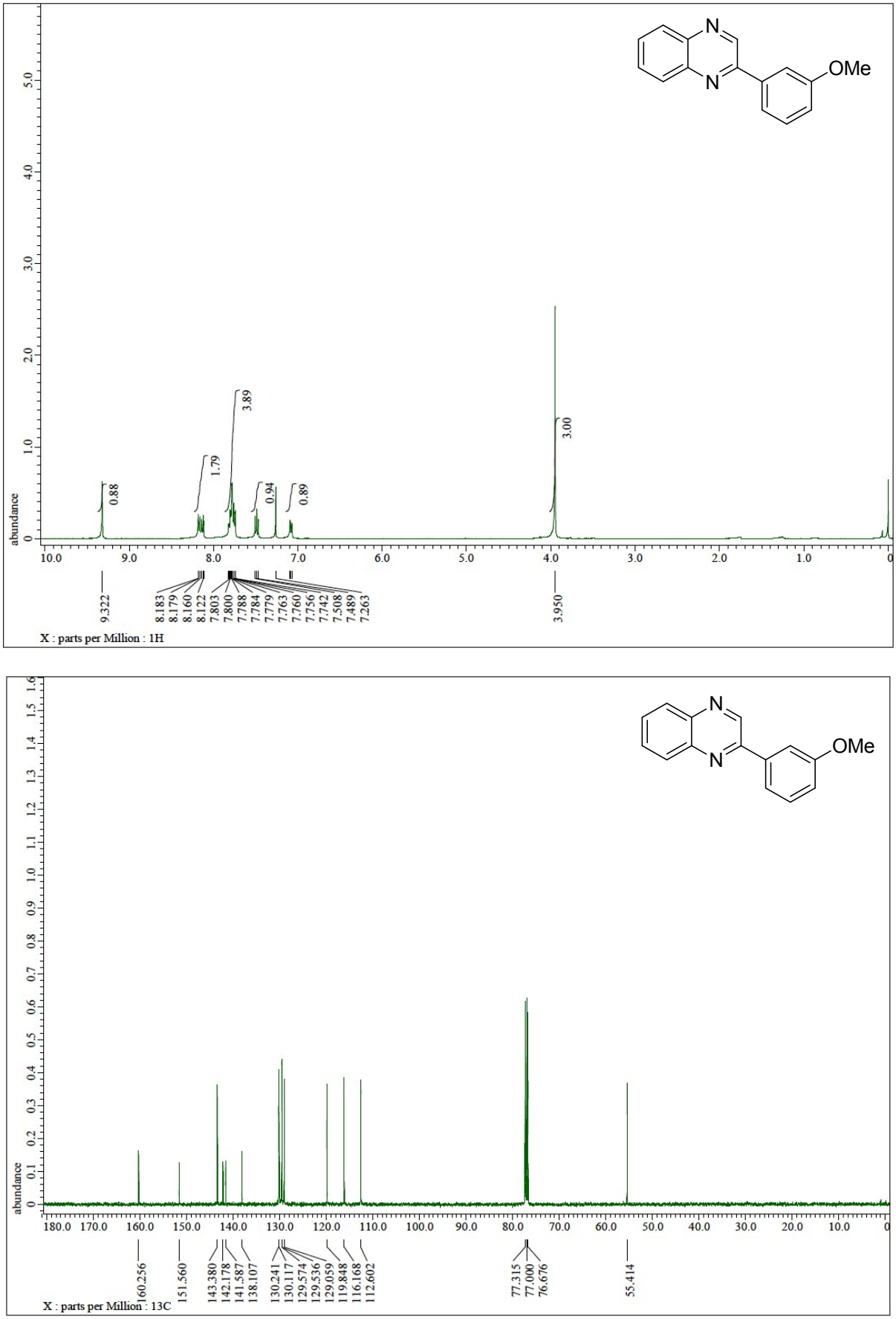


Figure S15. ^{1}H NMR of **3g** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3g** (100 MHz, $CDCl_3$).

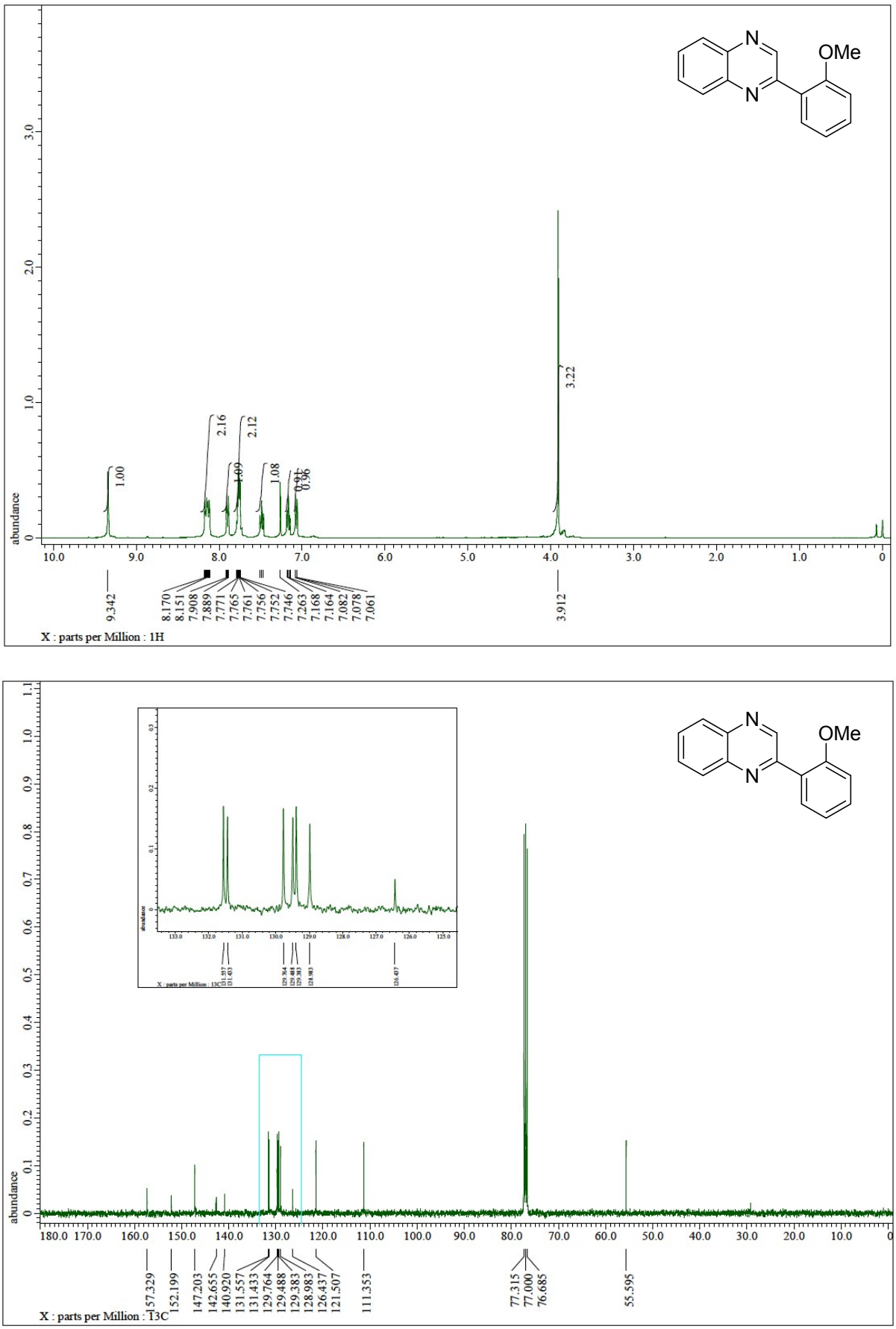


Figure S16. ^{1}H NMR of **3h** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3h** (100 MHz, $CDCl_3$).

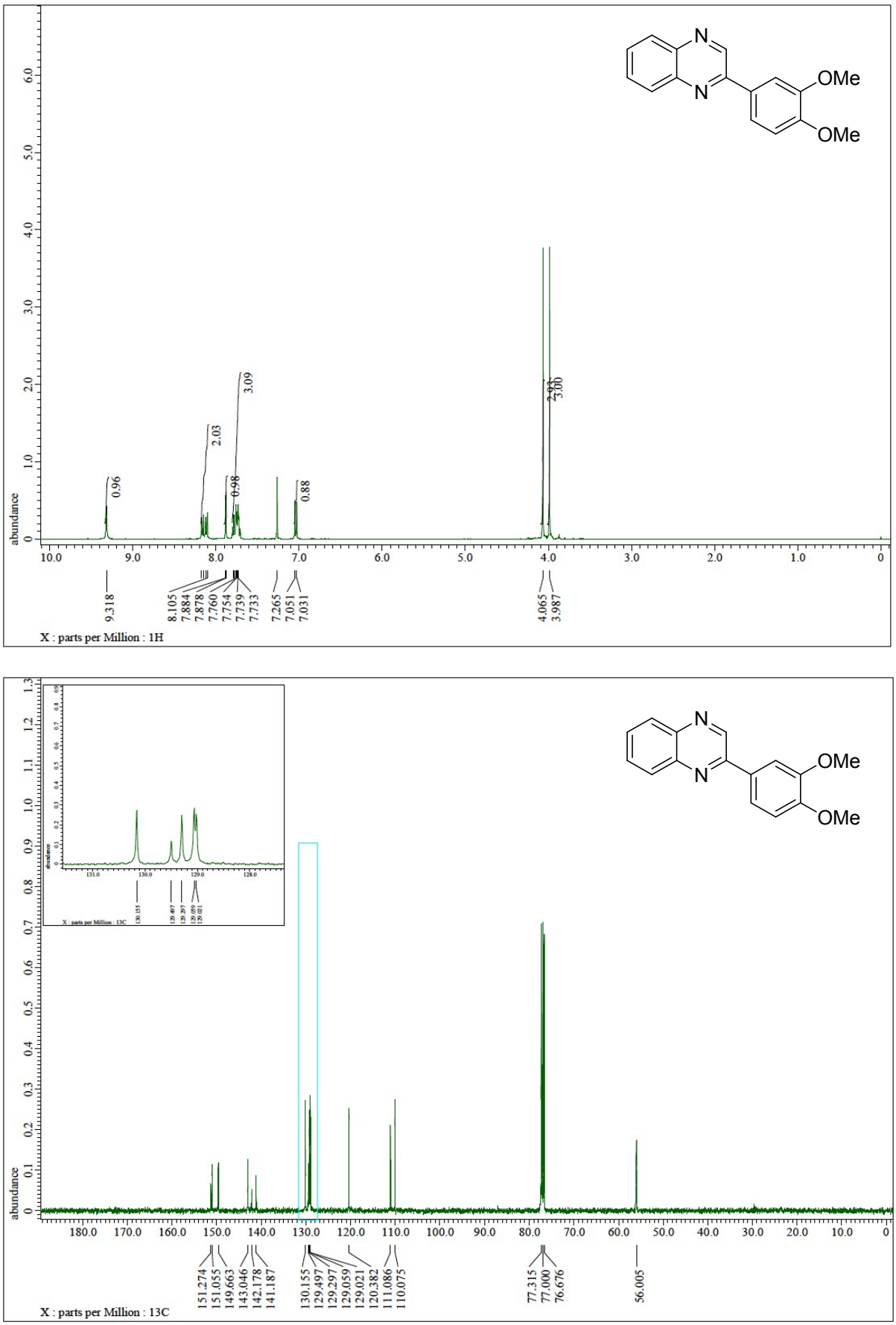


Figure S17. ^{1}H NMR of **3i** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3ai** (100 MHz, $CDCl_3$).

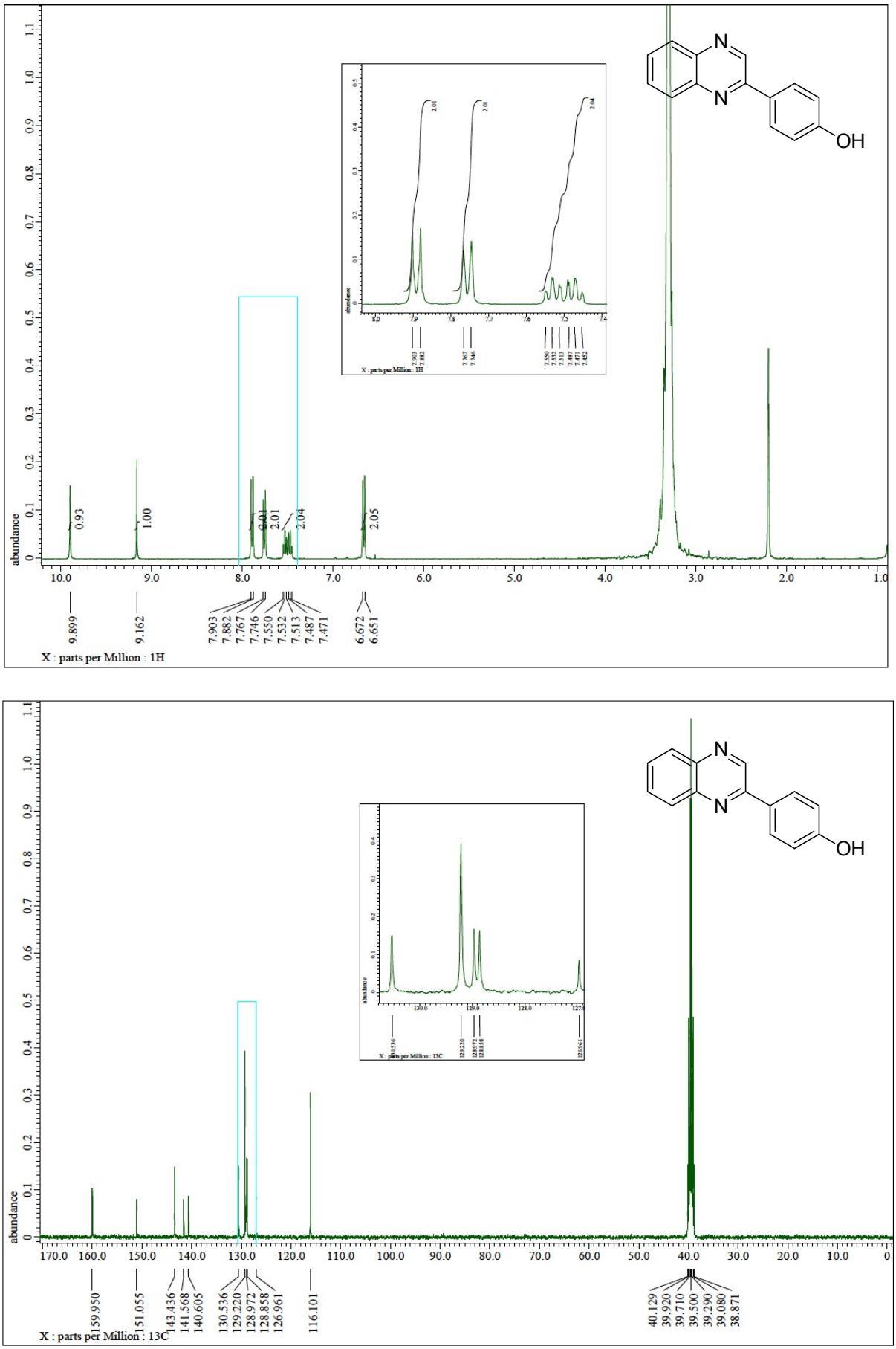


Figure S18. ^{1}H NMR of **3j** (400 MHz) and ^{13}C NMR of **3j** (100 MHz)- DMSO-d6

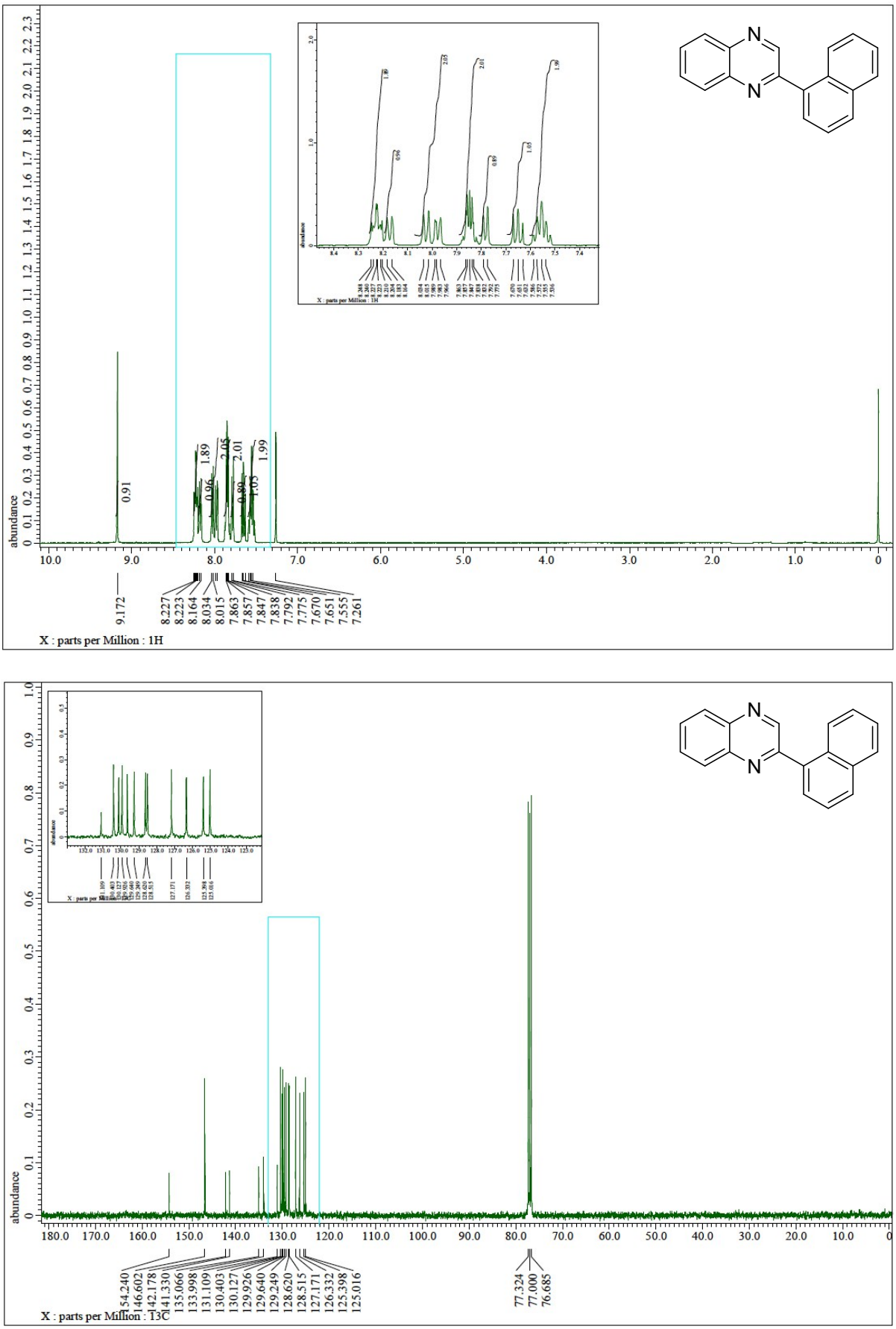


Figure S19. ^{1}H NMR of **3k** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3k** (100 MHz, $CDCl_3$).

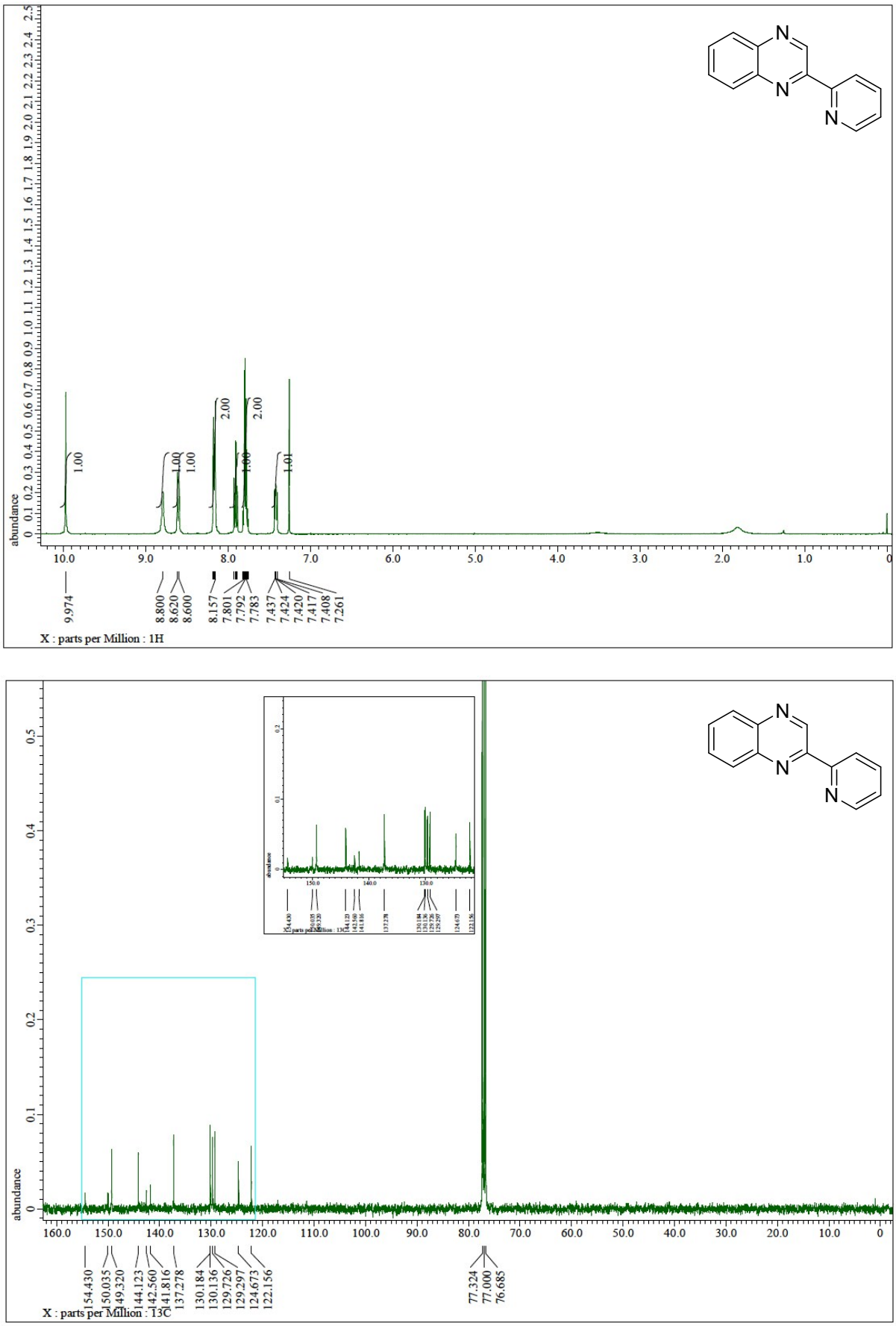


Figure S20. ^{1}H NMR of **3l** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3l** (100 MHz, $CDCl_3$).

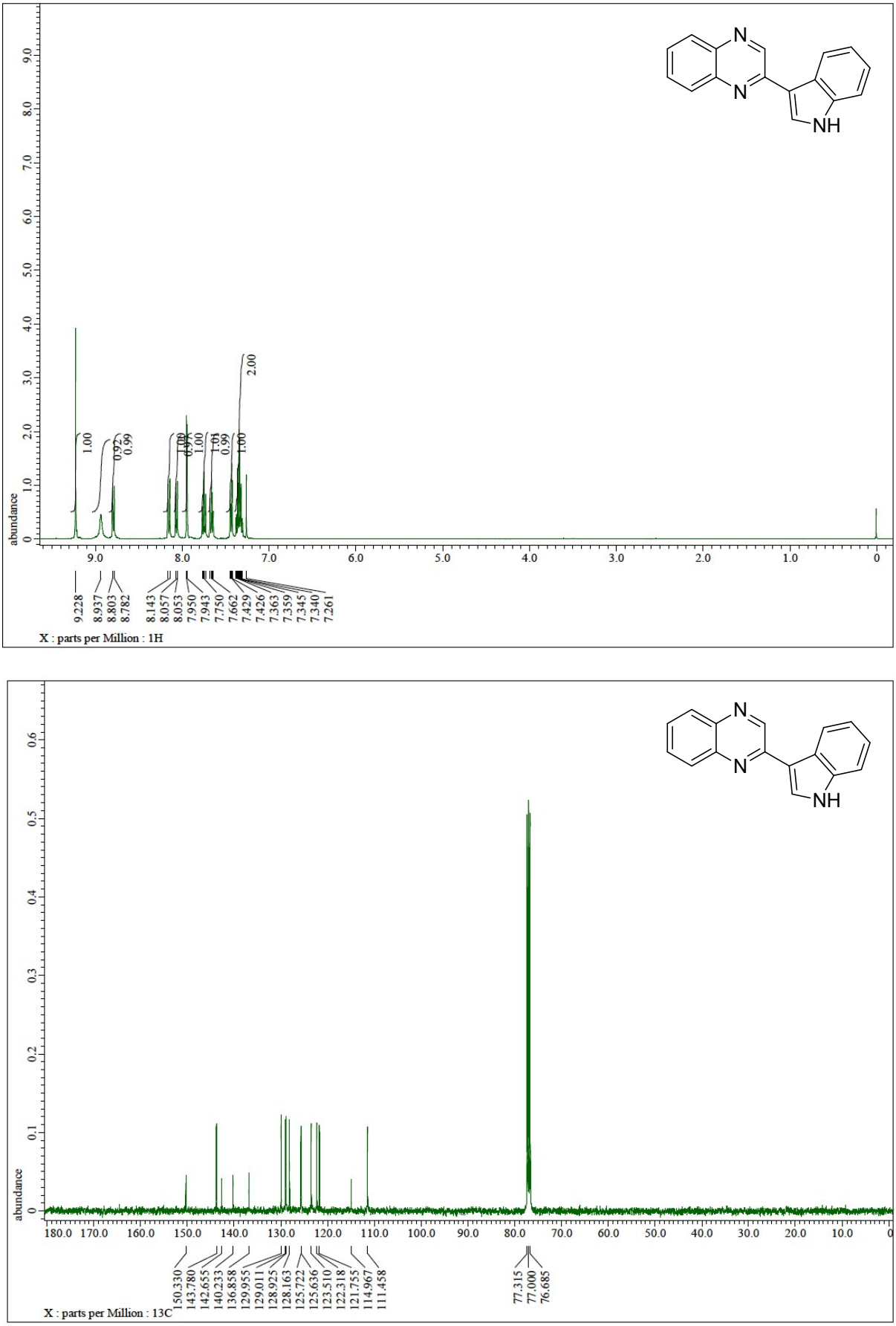
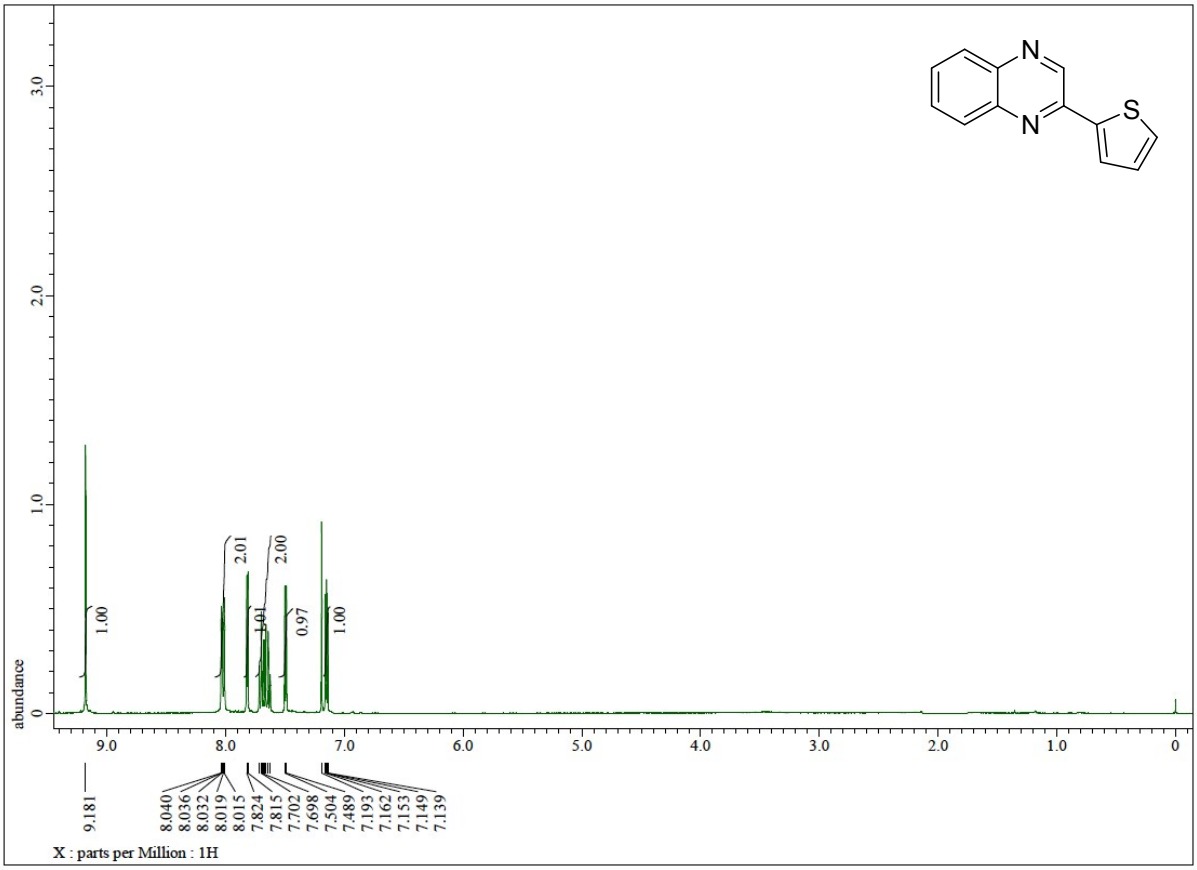


Figure S21. ^{1}H NMR of **3m** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3m** (100 MHz, $CDCl_3$).



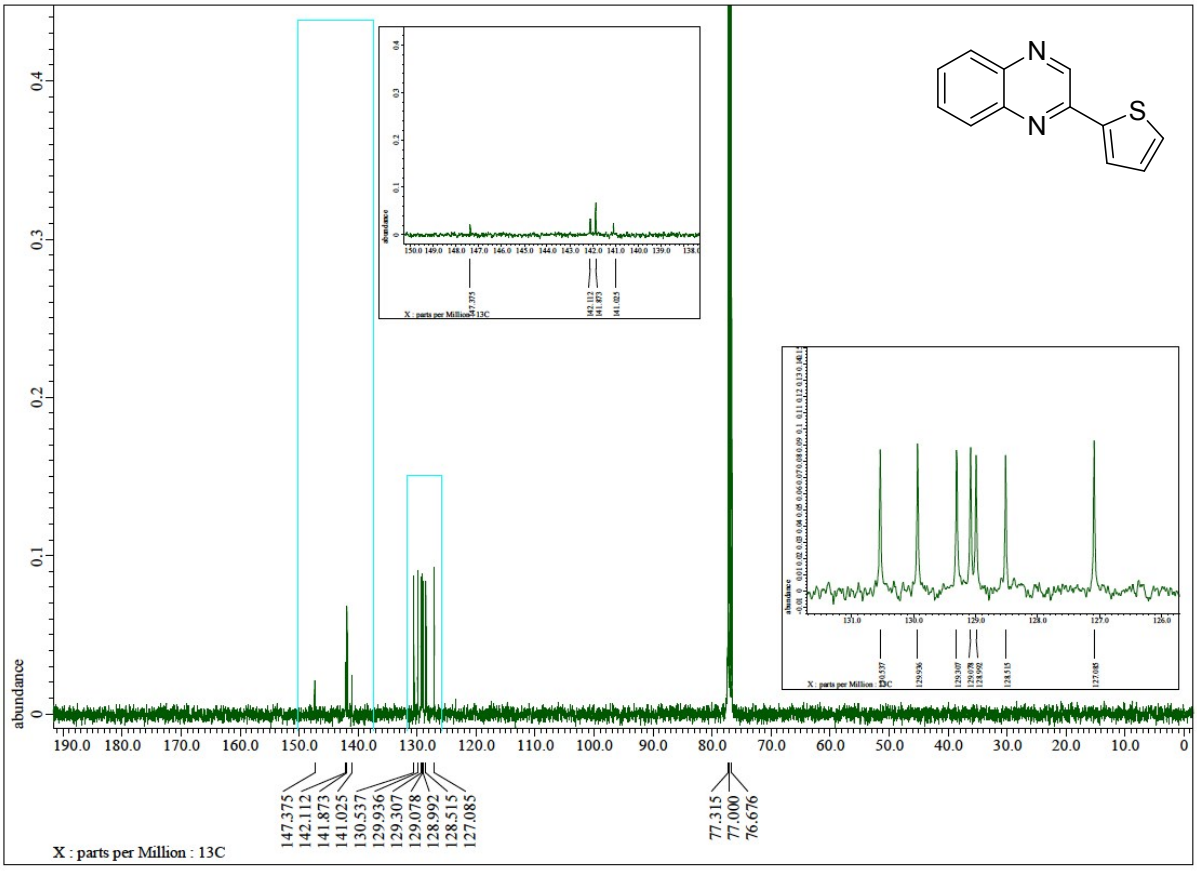


Figure S22. ^{1}H NMR of **3n** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3n** (100 MHz, $CDCl_3$).

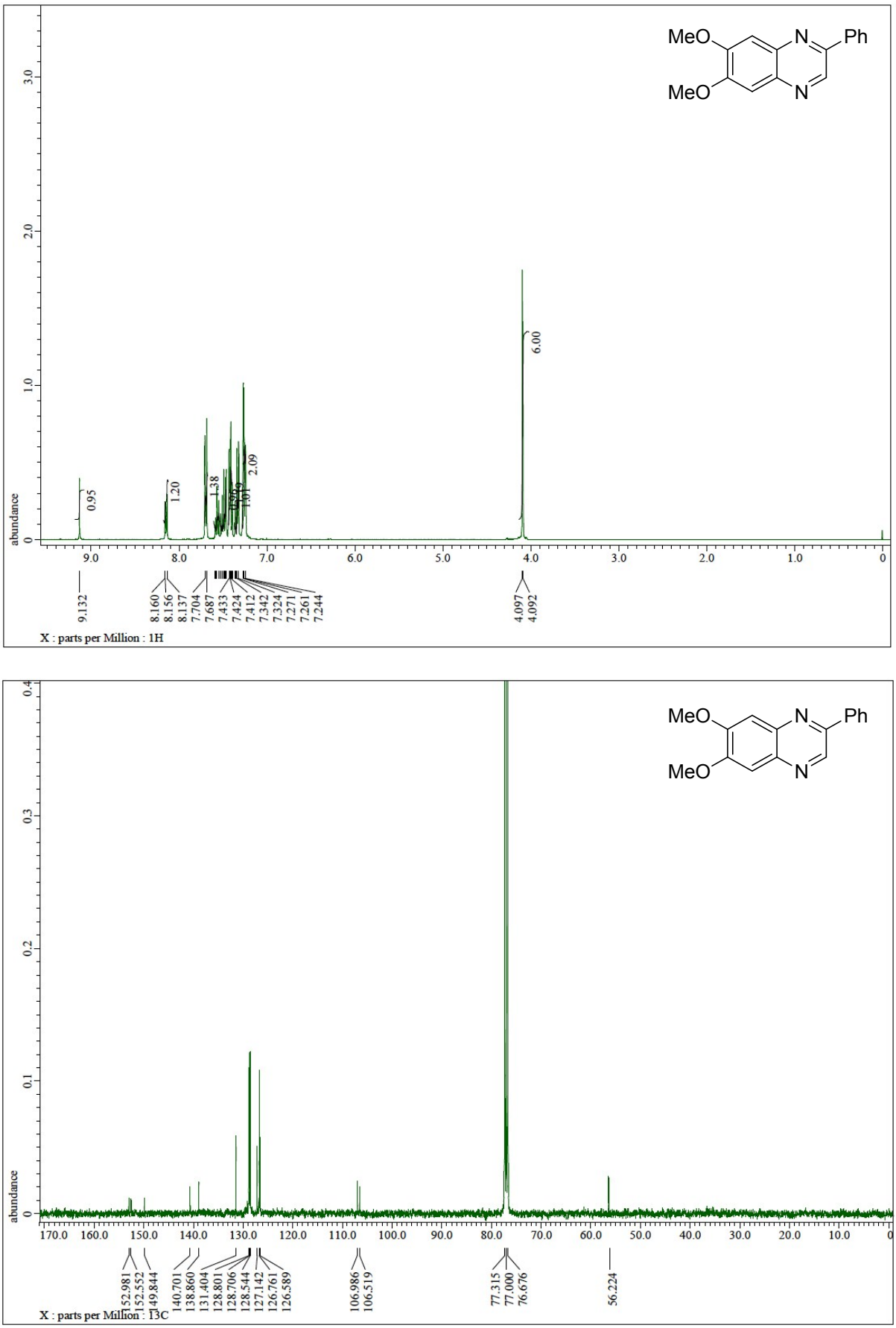


Figure S23. ^{1}H NMR of **4b** (400 MHz, $CDCl_3$) and ^{13}C NMR of **4b** (100 MHz, $CDCl_3$).

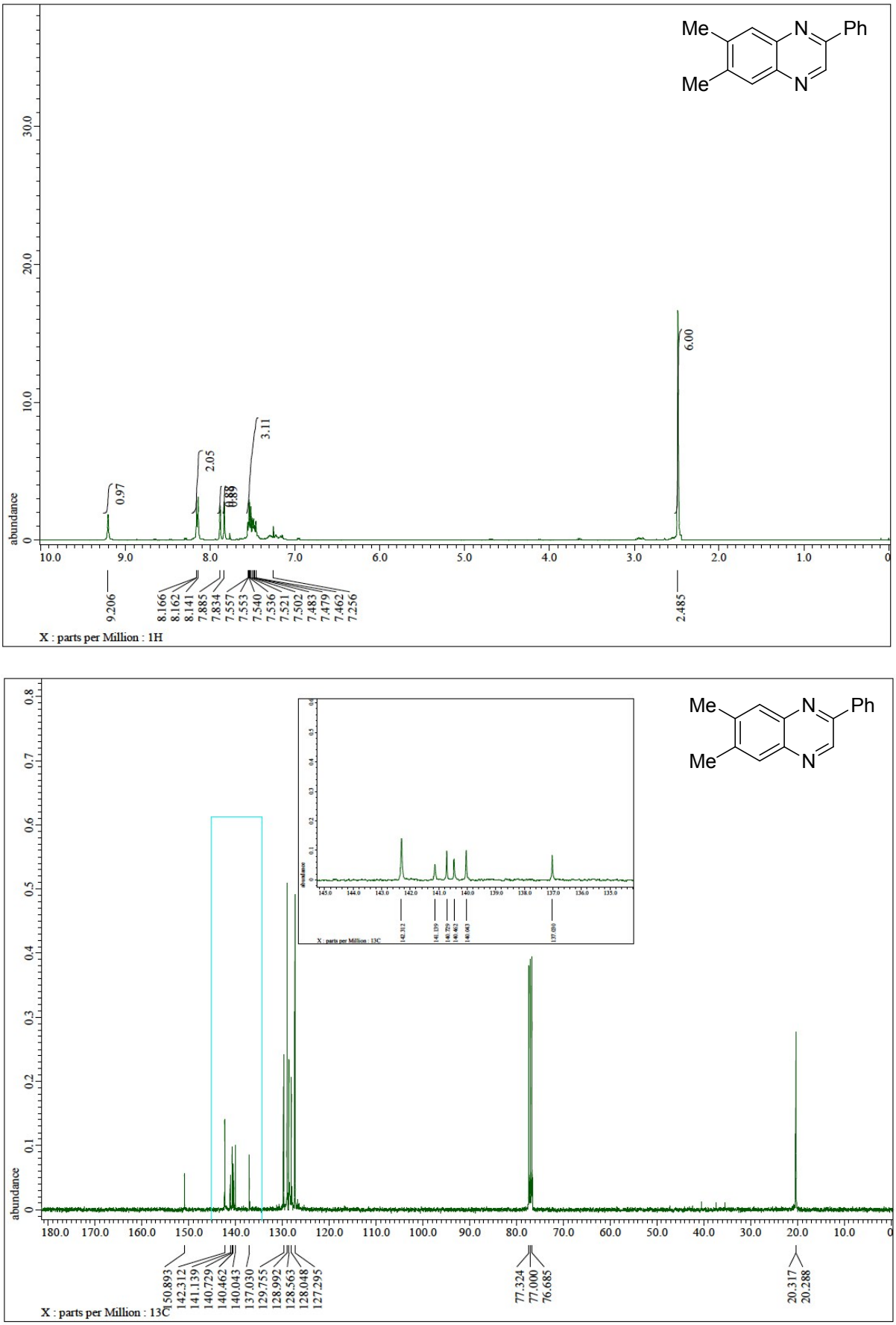


Figure S24. ^{1}H NMR of **4c** (400 MHz, $CDCl_3$) and ^{13}C NMR of **4c** (100 MHz, $CDCl_3$).

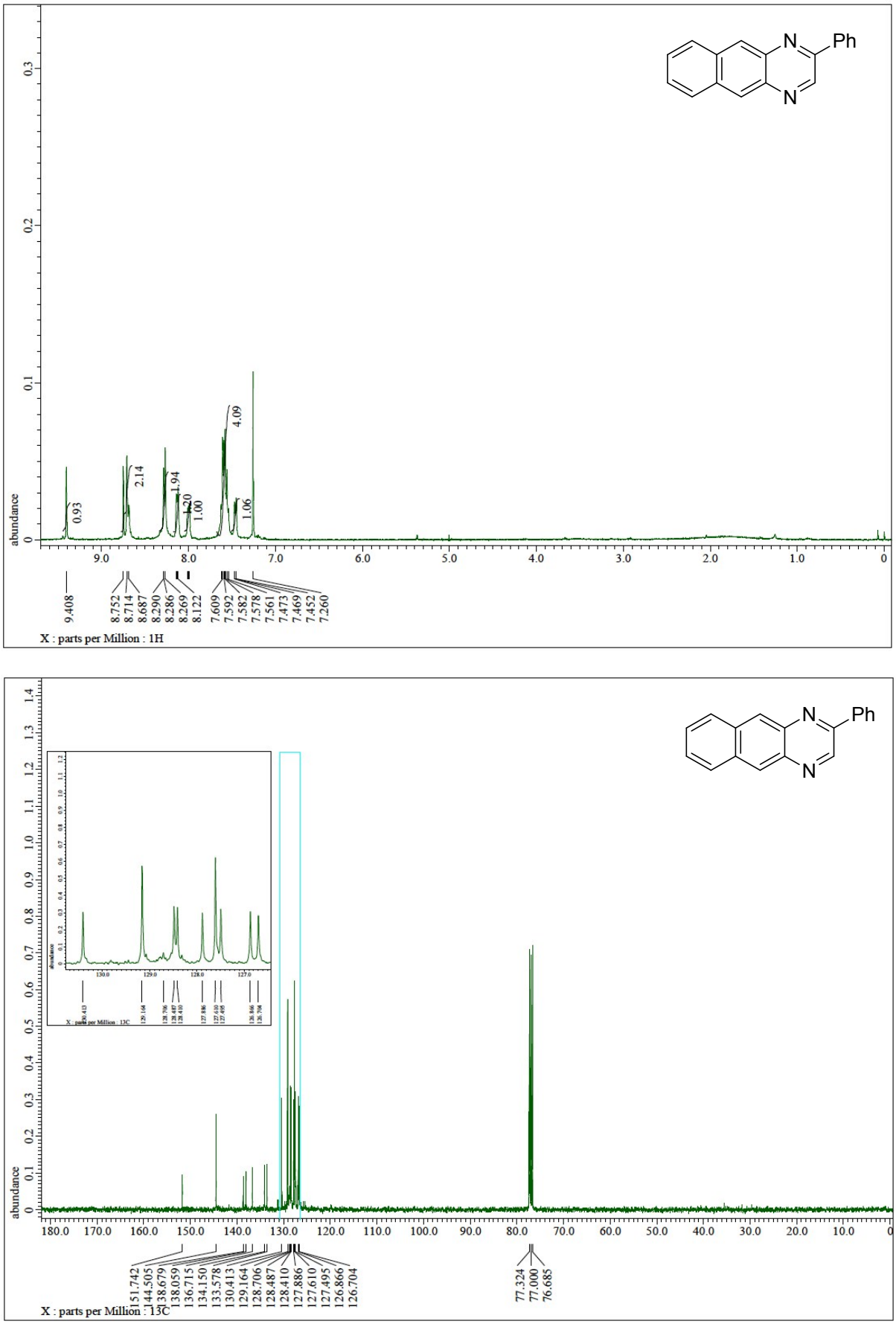


Figure S25. ^{1}H NMR of **4d** (400 MHz, $CDCl_3$) and ^{13}C NMR of **4d** (100 MHz, $CDCl_3$)

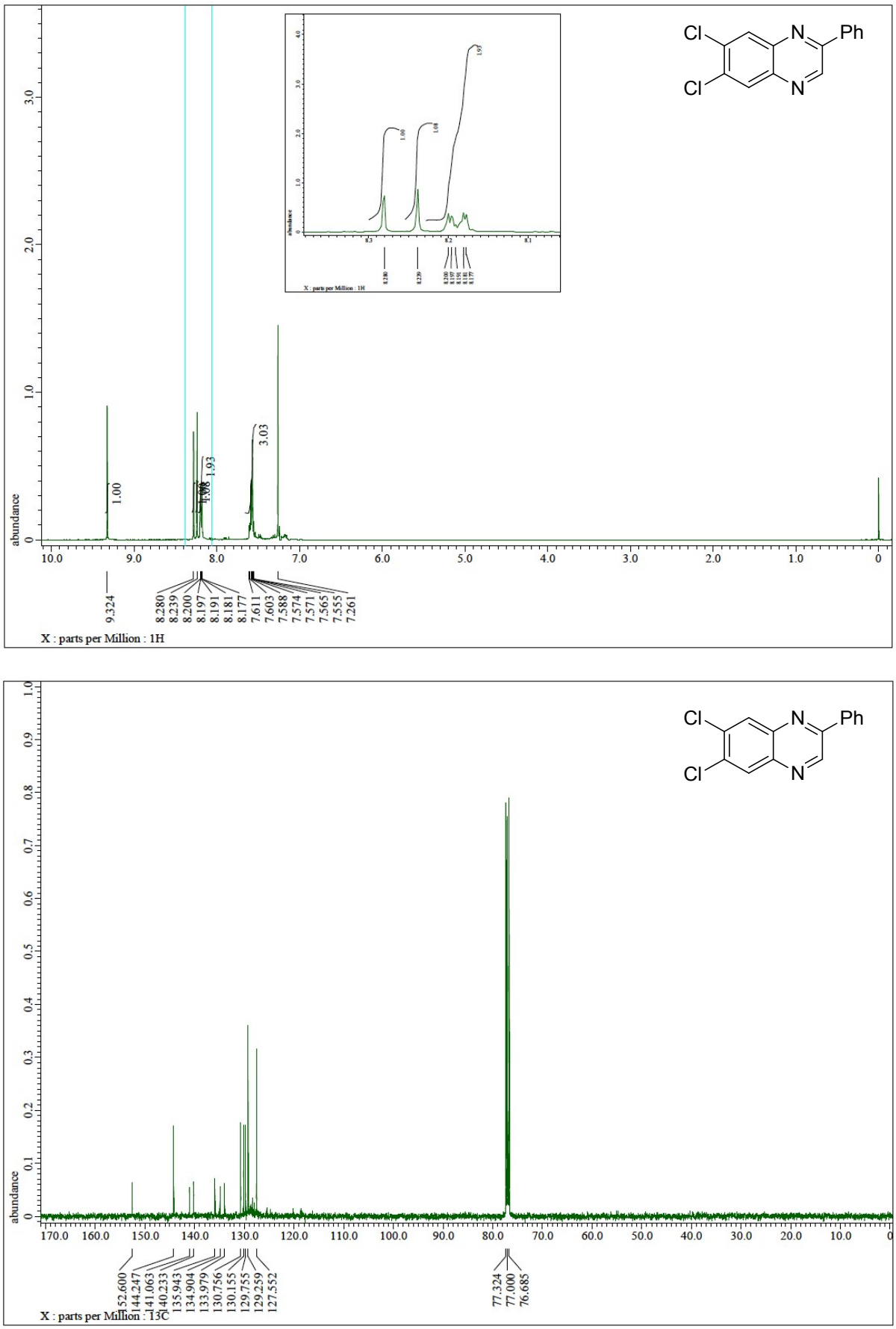


Figure S26. ^{1}H NMR of **4e** (400 MHz, $CDCl_3$) and ^{13}C NMR of **4e** (100 MHz, $CDCl_3$).

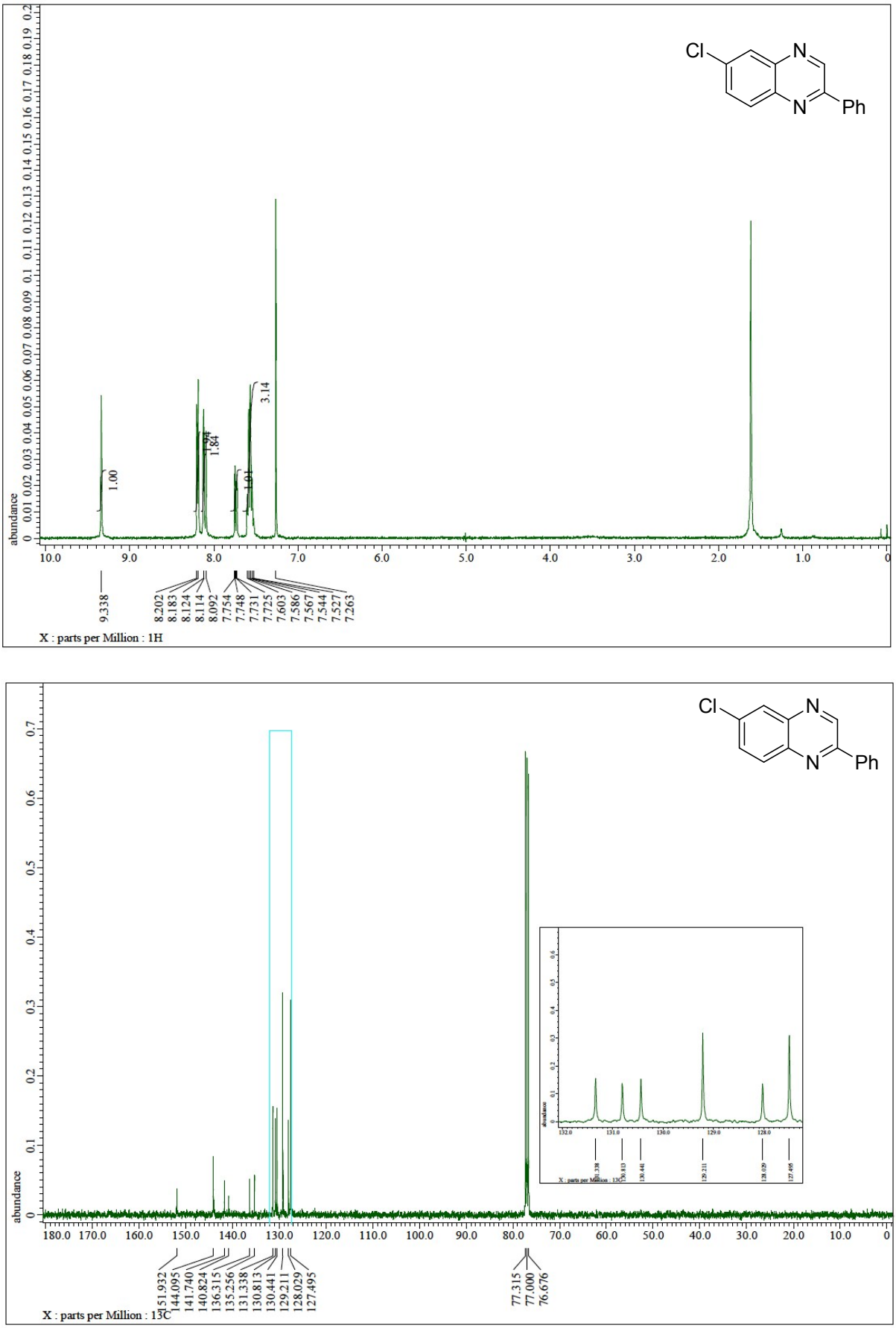
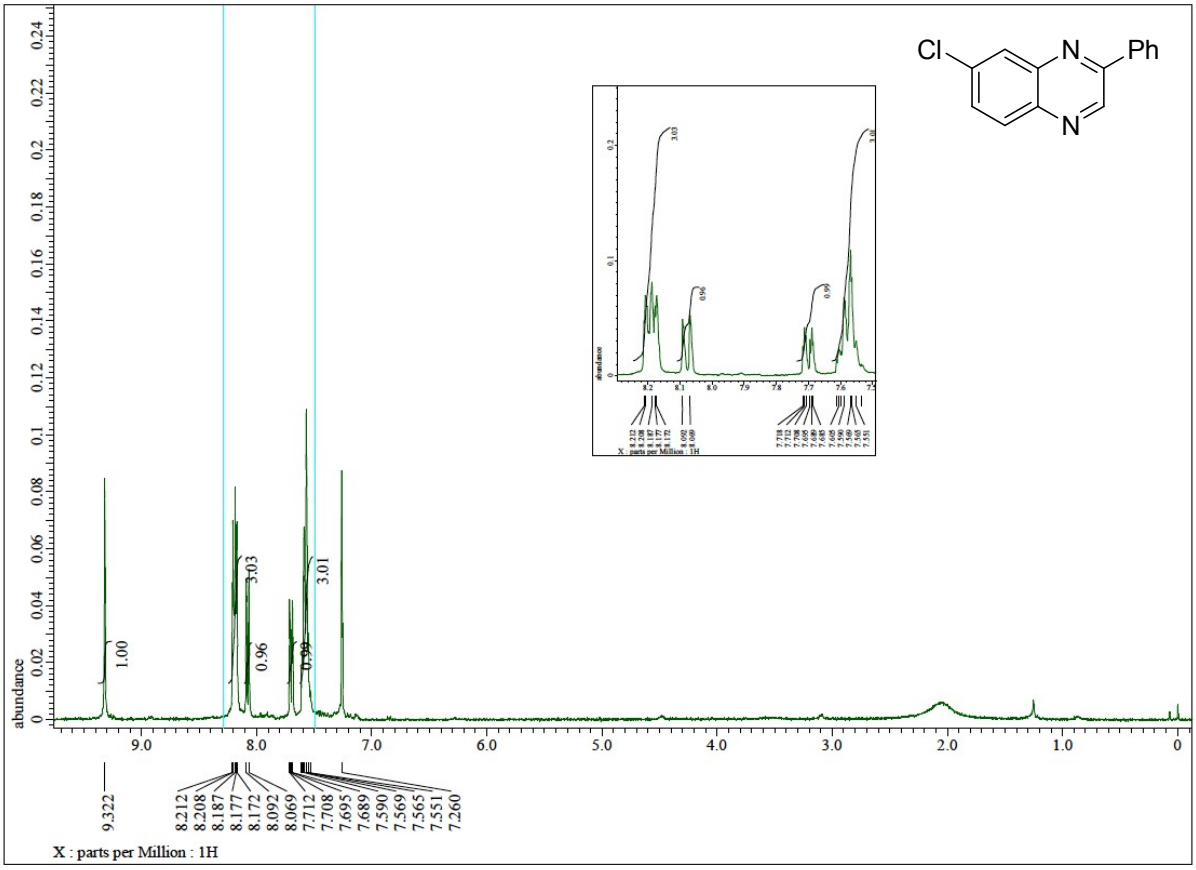


Figure S27. ^{1}H NMR of **4f** (400 MHz, $CDCl_3$) and ^{13}C NMR of **4f** (100 MHz, $CDCl_3$).



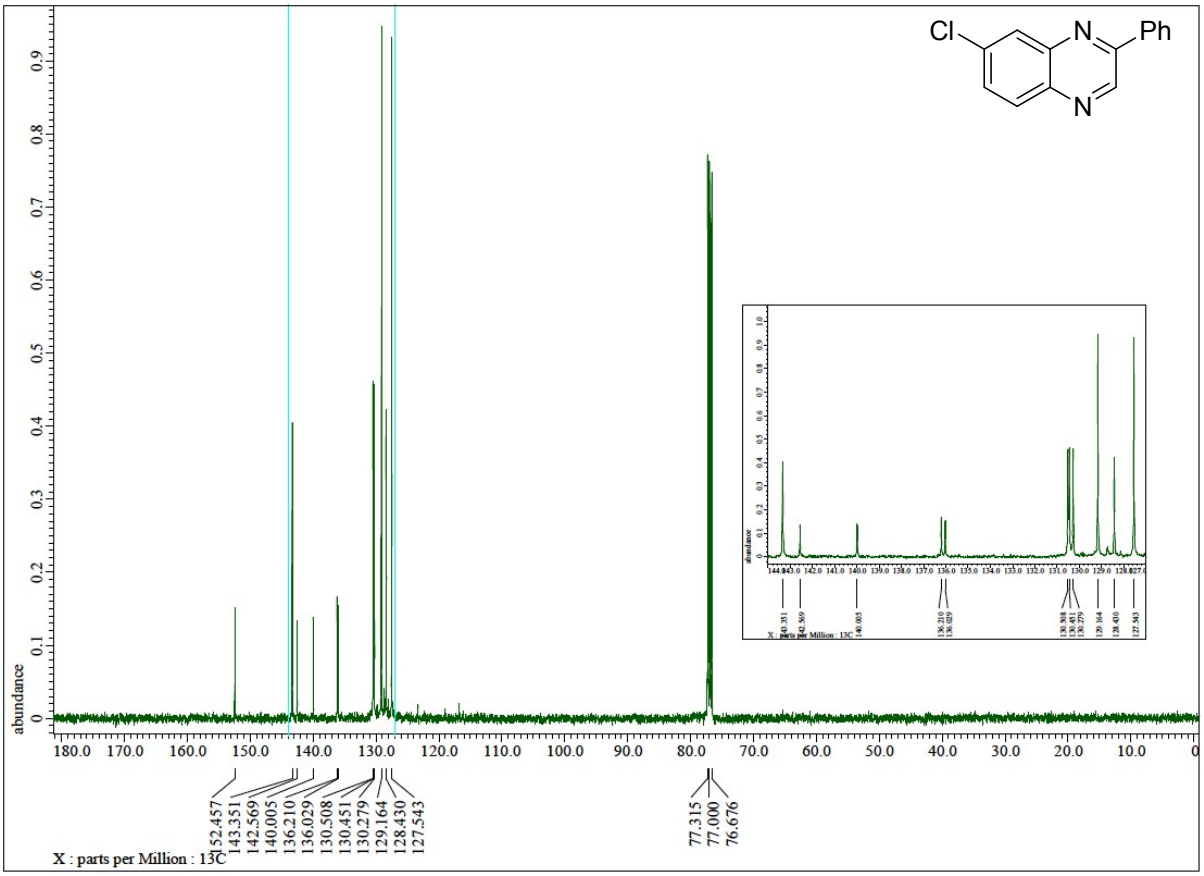


Figure S28. ^{1}H NMR of **4f'** (400 MHz, $CDCl_3$) and ^{13}C NMR of **4f'** (100 MHz, $CDCl_3$).

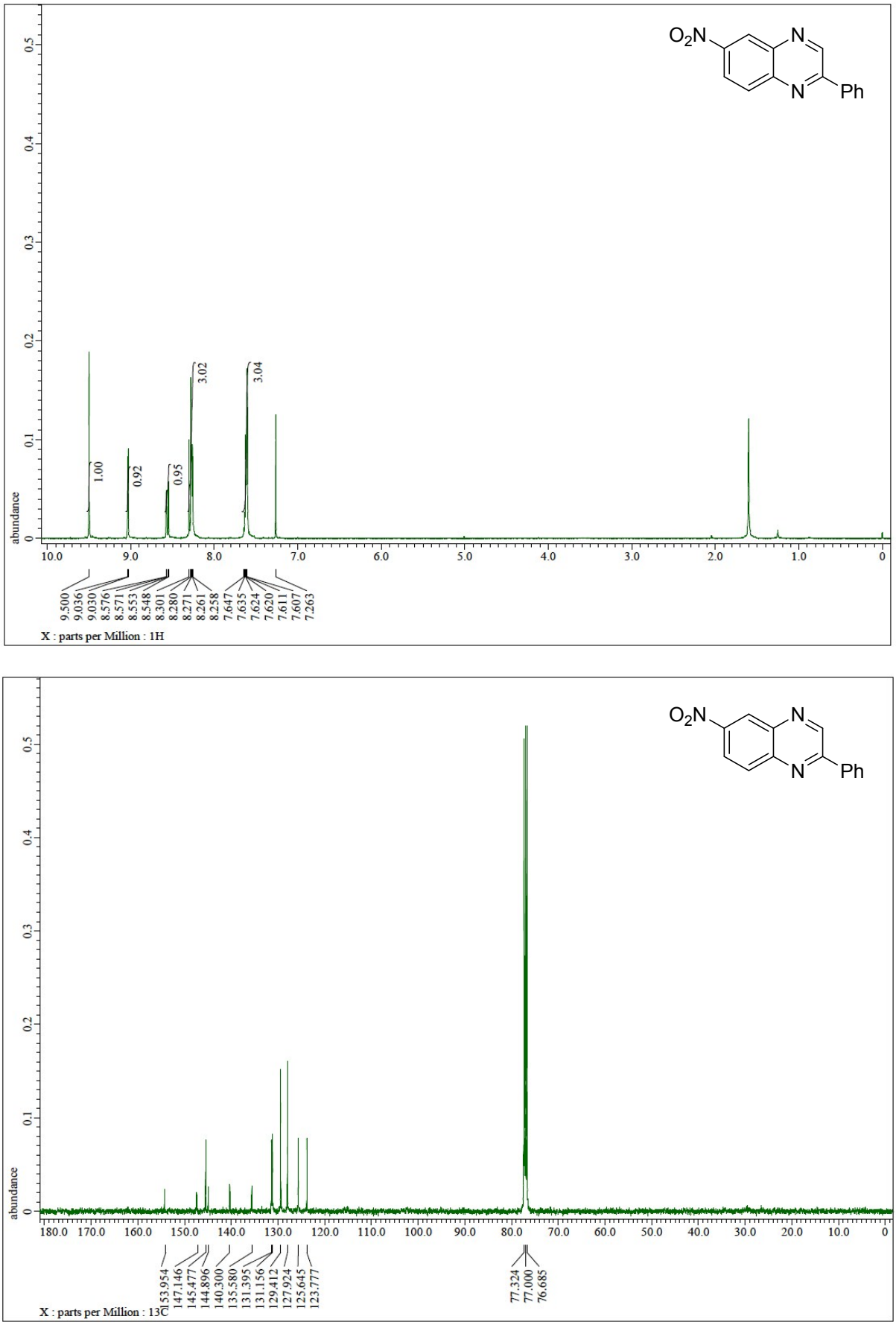


Figure S29. ^{1}H NMR of **4g** (400 MHz, $CDCl_3$) and ^{13}C NMR of **4g** (100 MHz, $CDCl_3$).

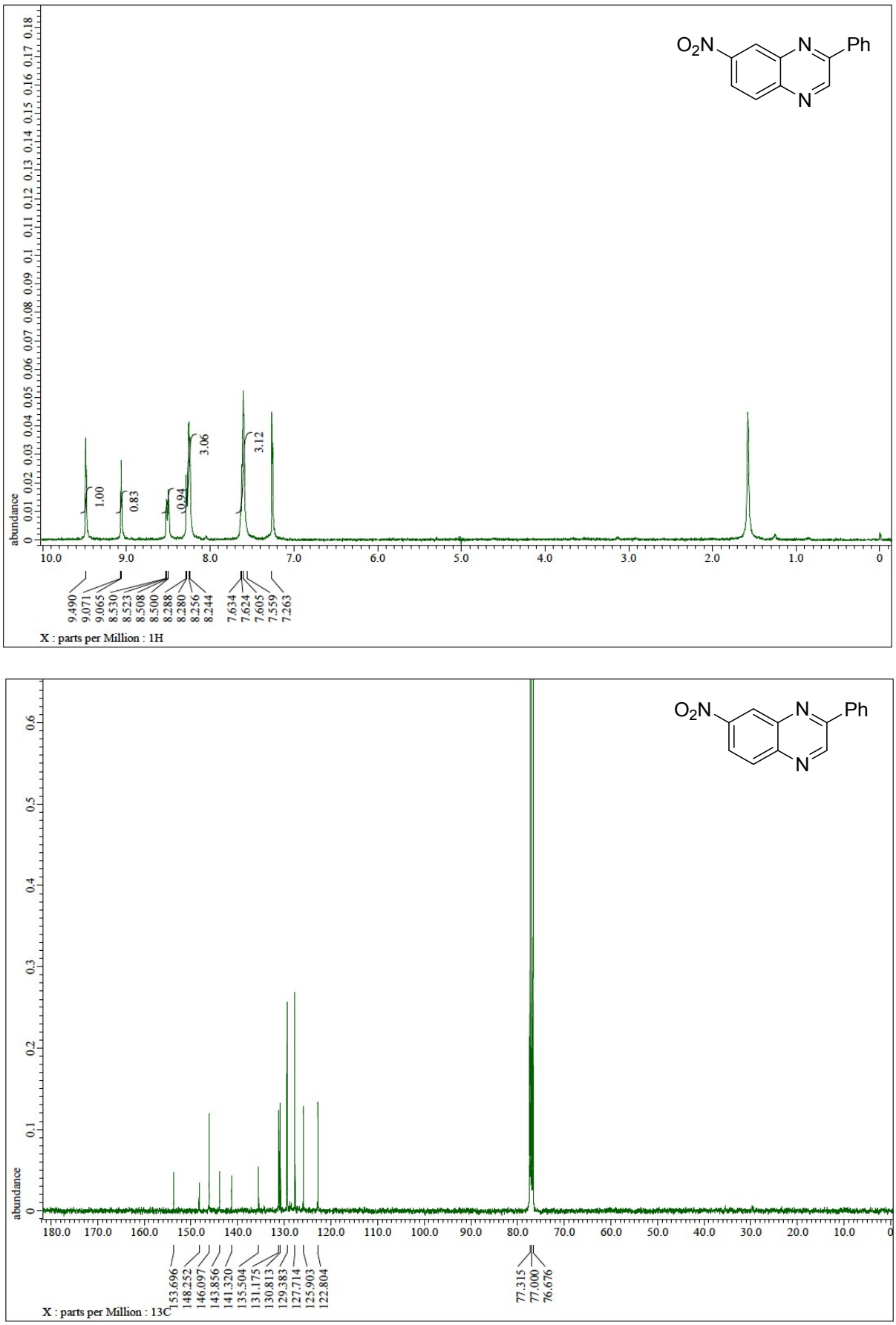
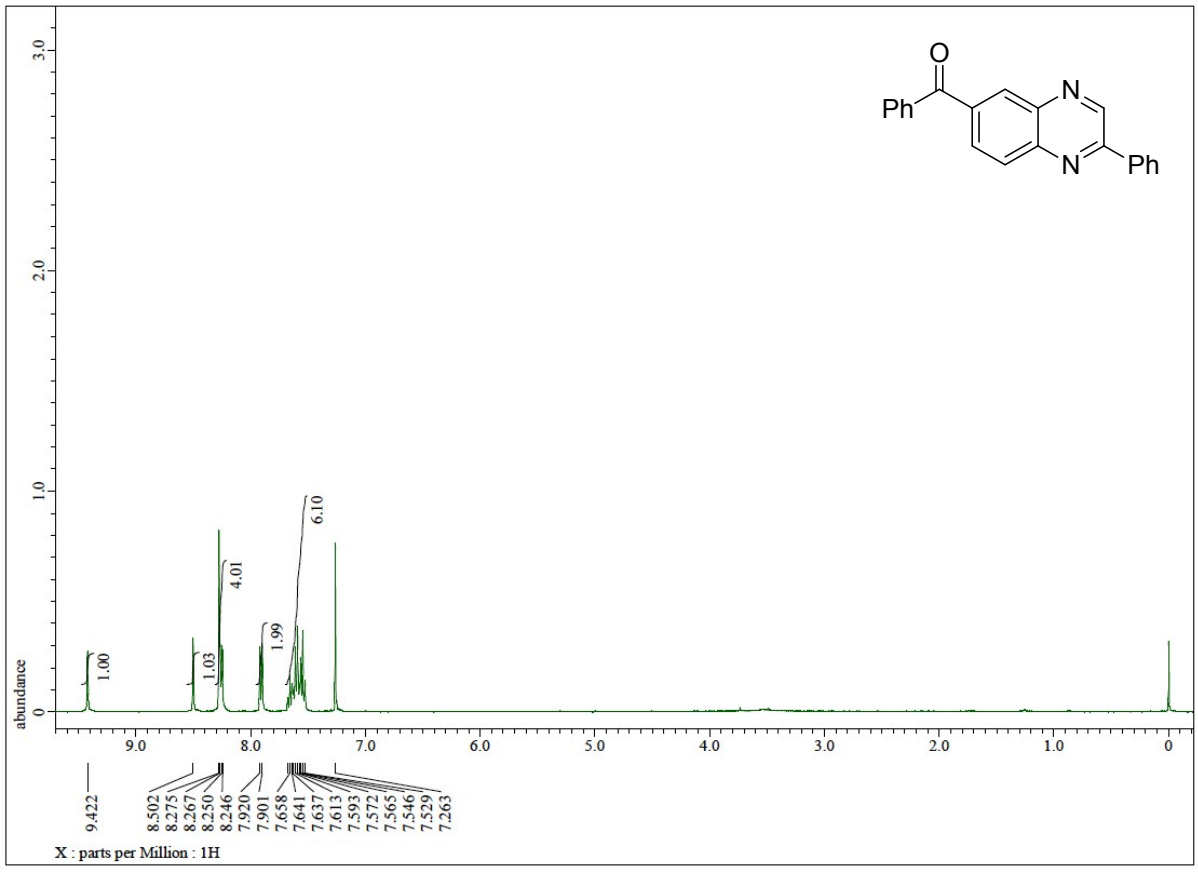


Figure S30. ^{1}H NMR of **4g'** (400 MHz, $CDCl_3$) and ^{13}C NMR of **4g'** (100 MHz, $CDCl_3$).



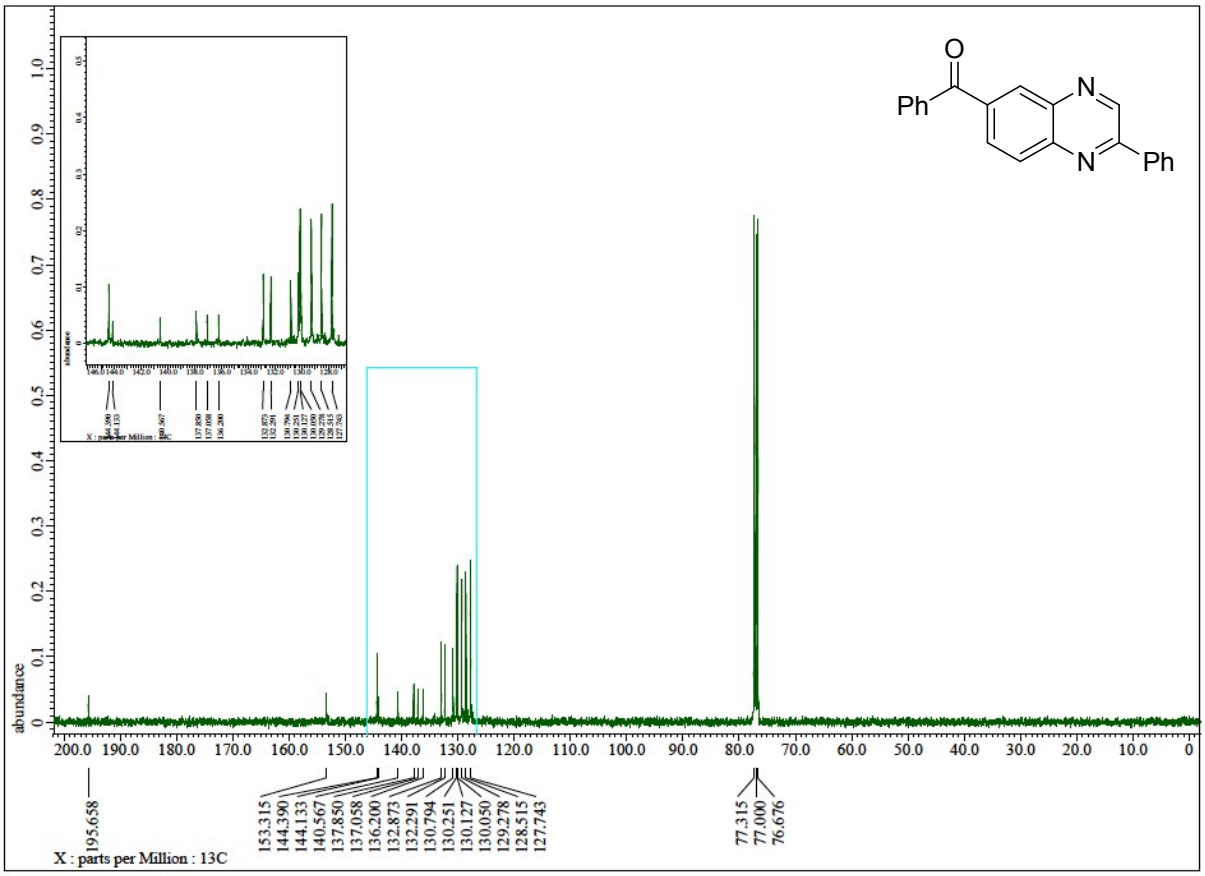


Figure S31. ^{1}H NMR of **4h** (400 MHz, $CDCl_3$) and ^{13}C NMR of **4h** (100 MHz, $CDCl_3$).

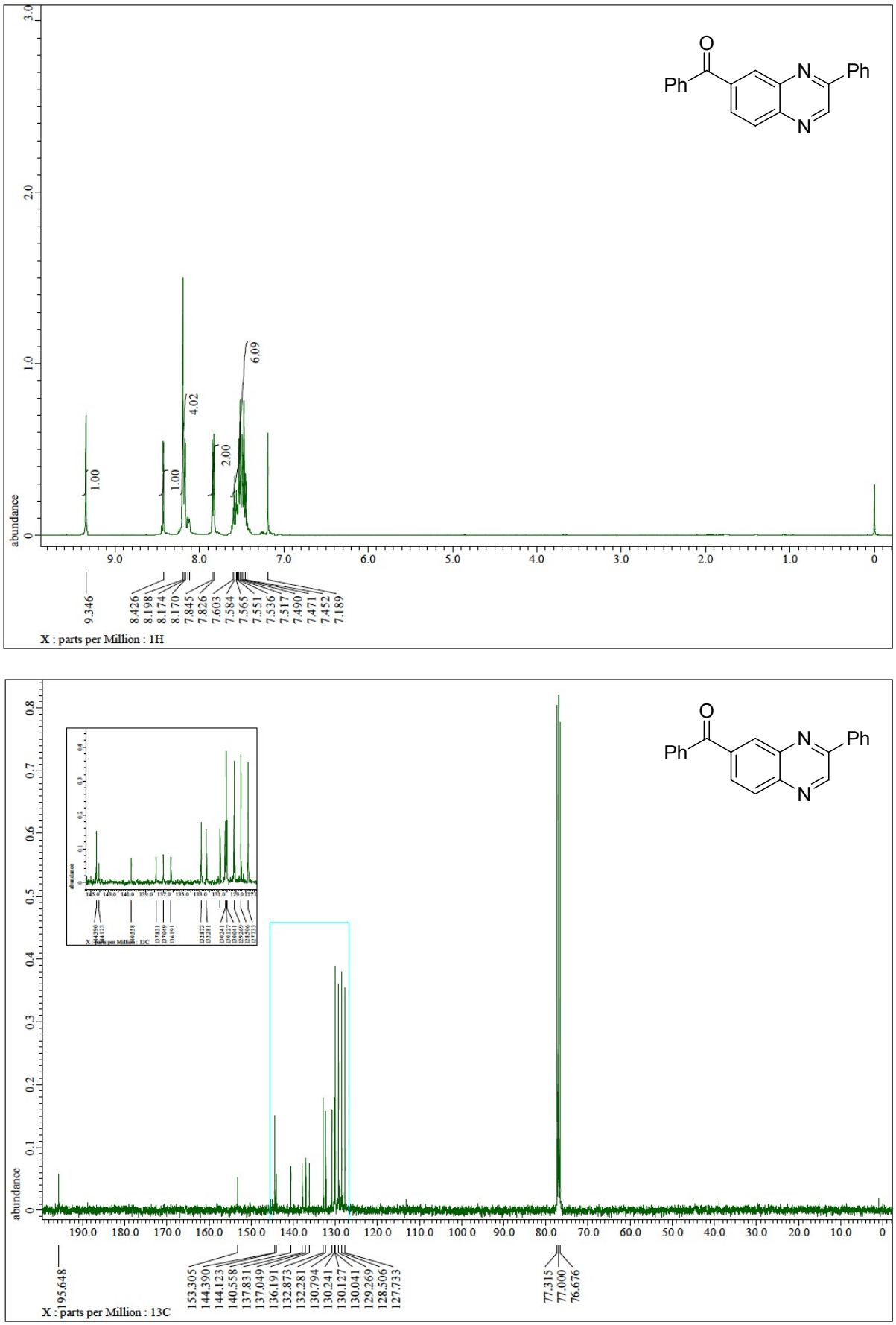


Figure S32. ^{1}H NMR of **4h'** (400 MHz, $CDCl_3$) and ^{13}C NMR of **4h'** (100 MHz, $CDCl_3$).

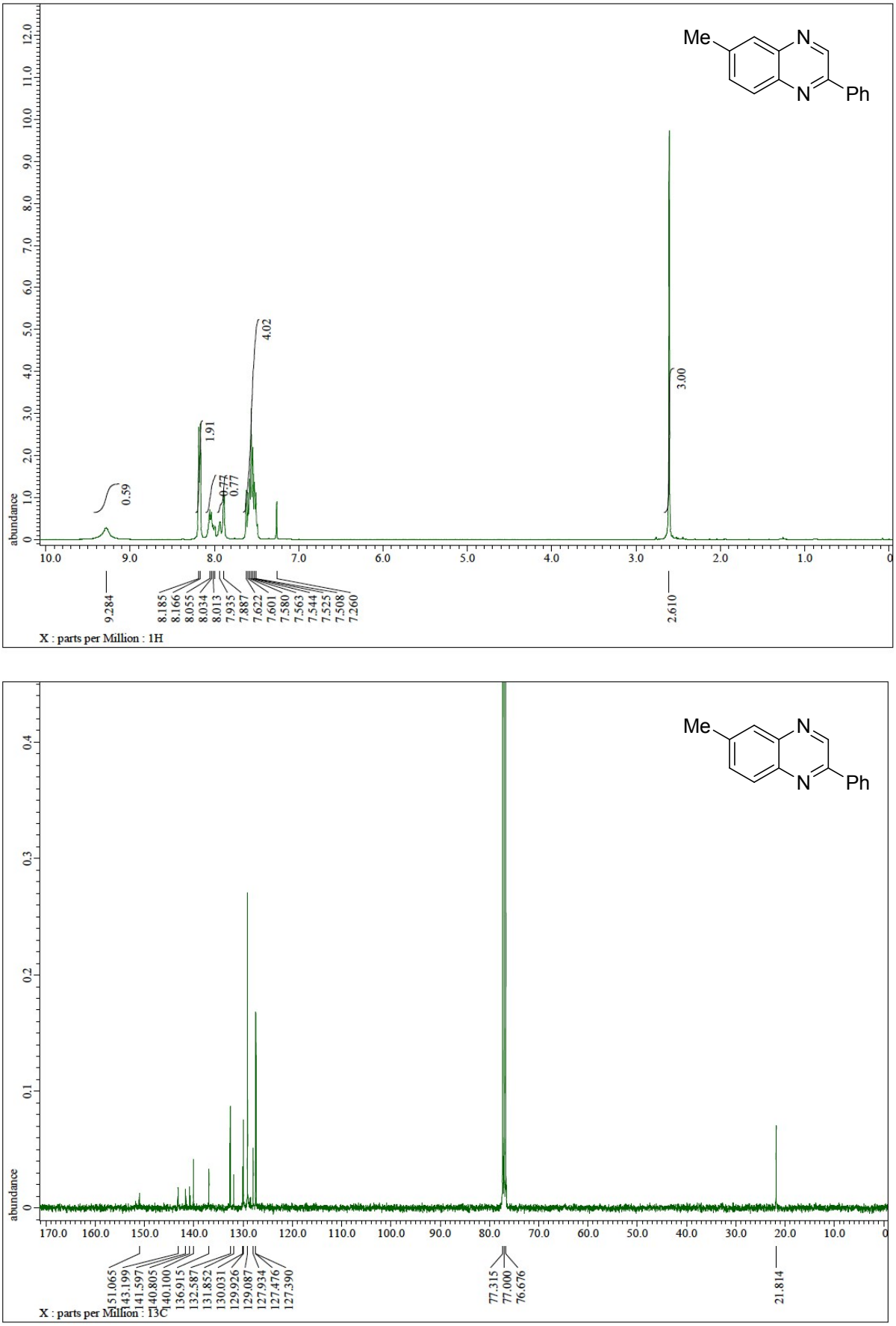
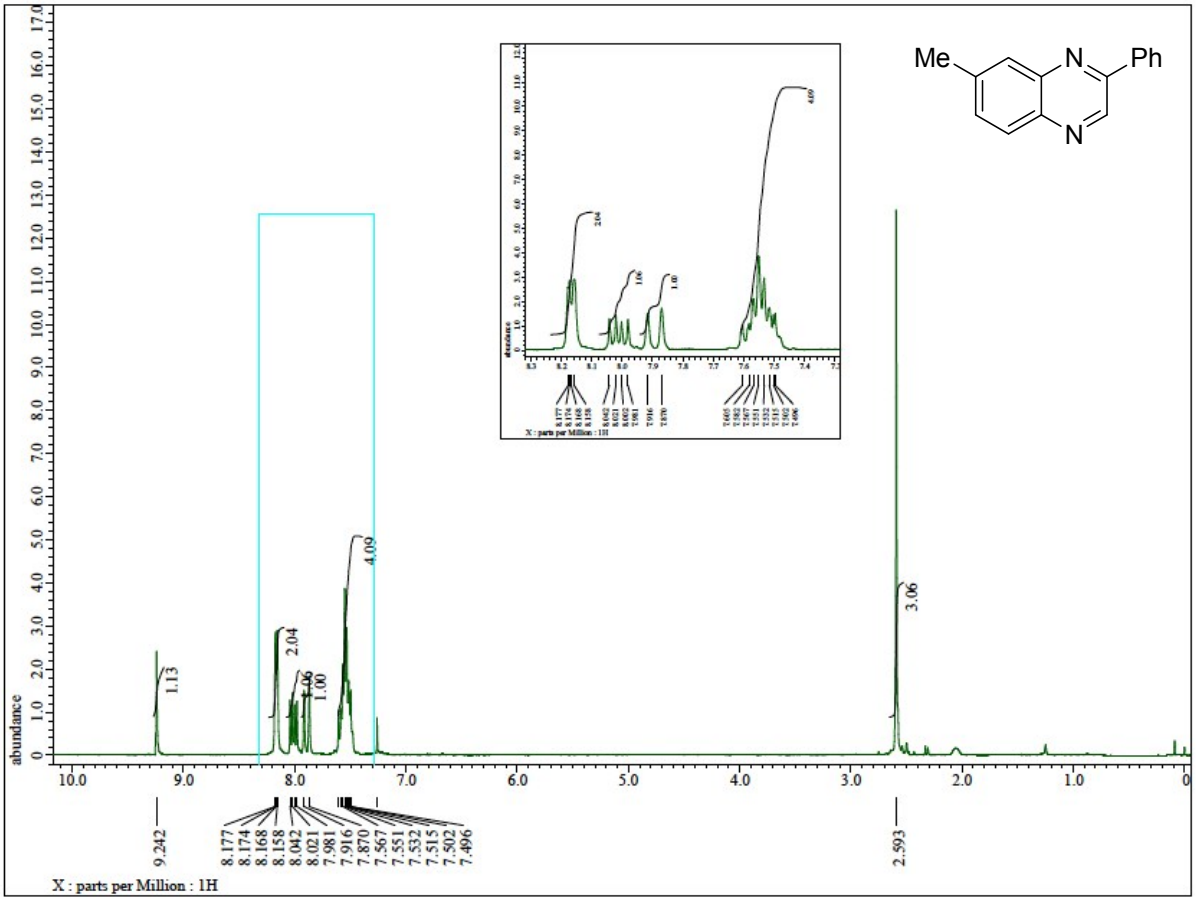


Figure S33. ^{1}H NMR of **4i** (400 MHz, $CDCl_3$) and ^{13}C NMR of **4i** (100 MHz, $CDCl_3$).



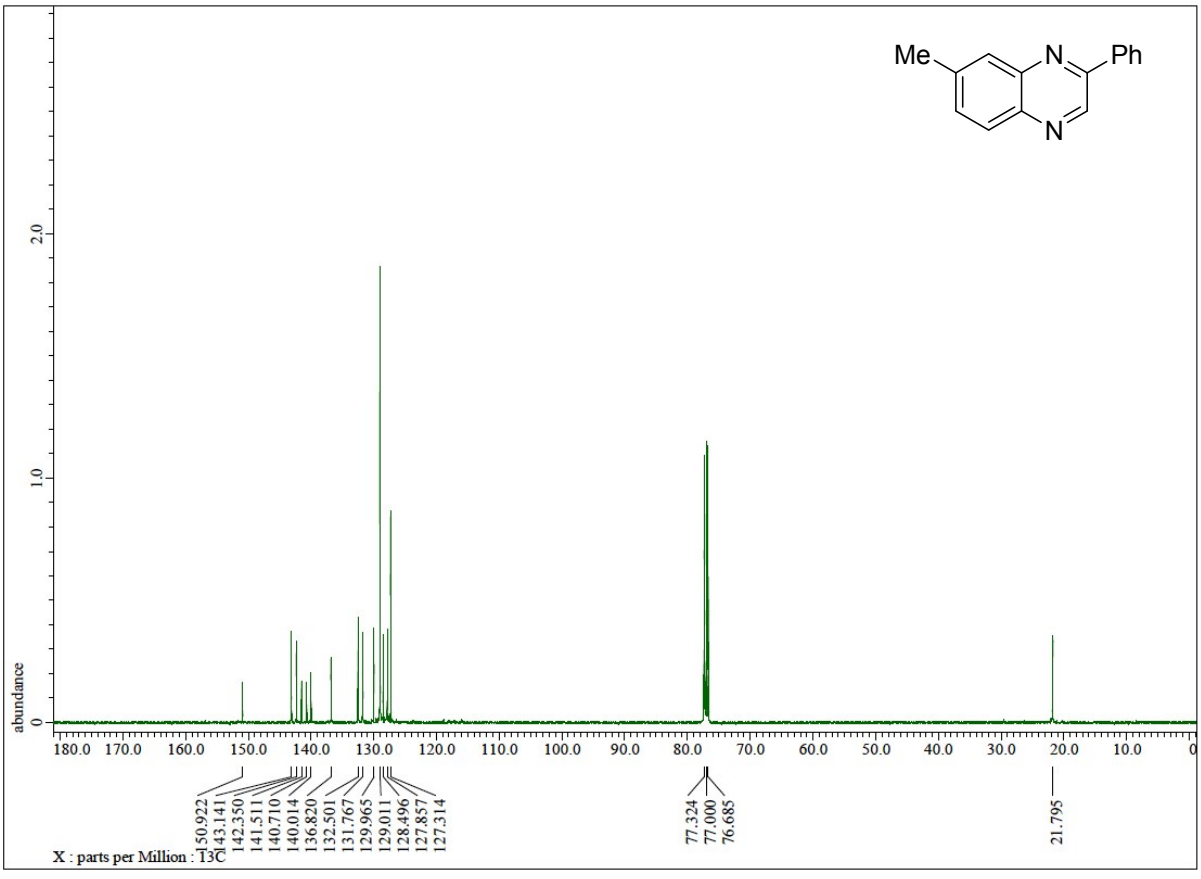


Figure S34. ^{1}H NMR of **4i'** (400 MHz, $CDCl_3$) and ^{13}C NMR of **4i'** (100 MHz, $CDCl_3$).

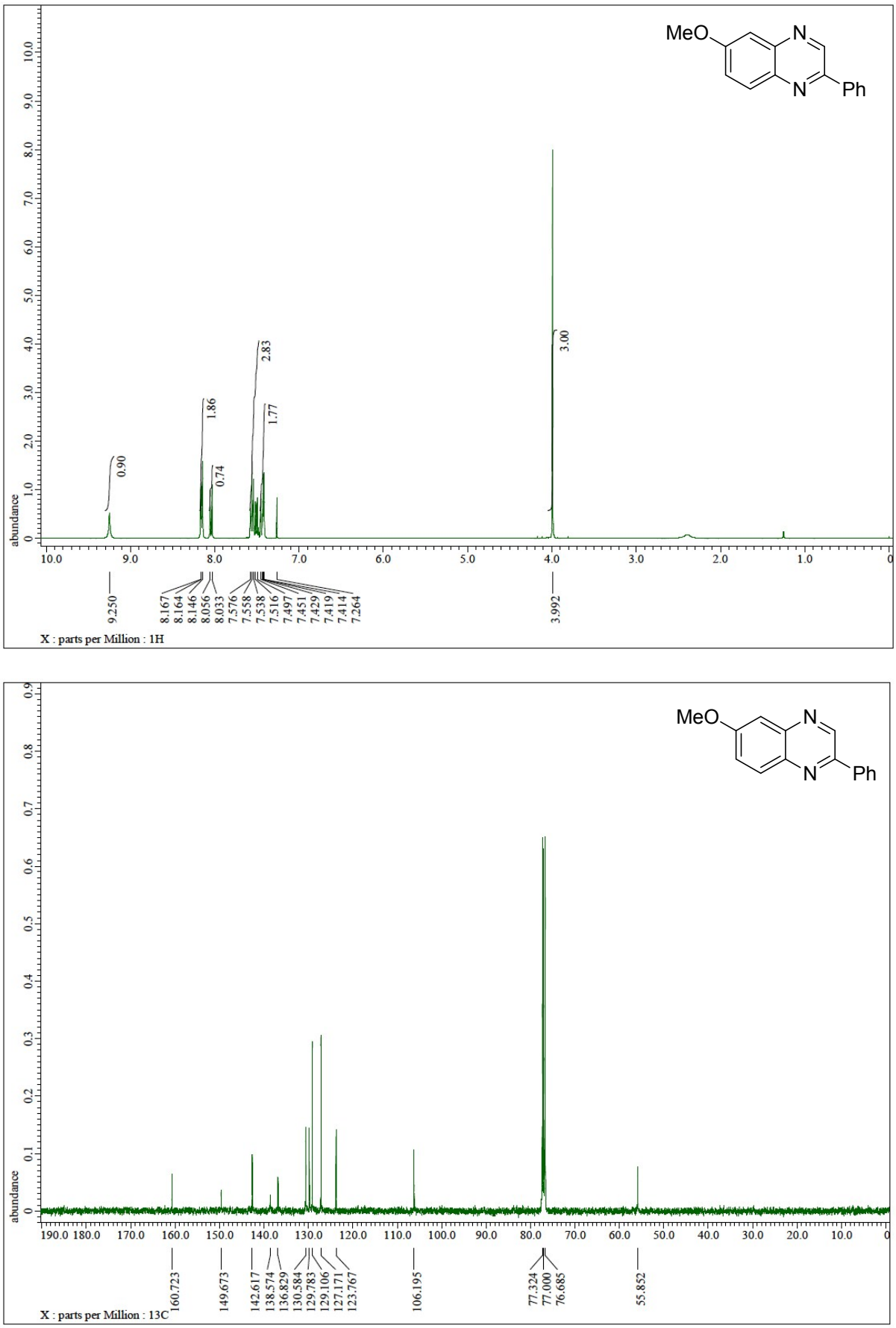


Figure S35. ^{1}H NMR of **4j** (400 MHz, $CDCl_3$) and ^{13}C NMR of **4j** (100 MHz, $CDCl_3$).

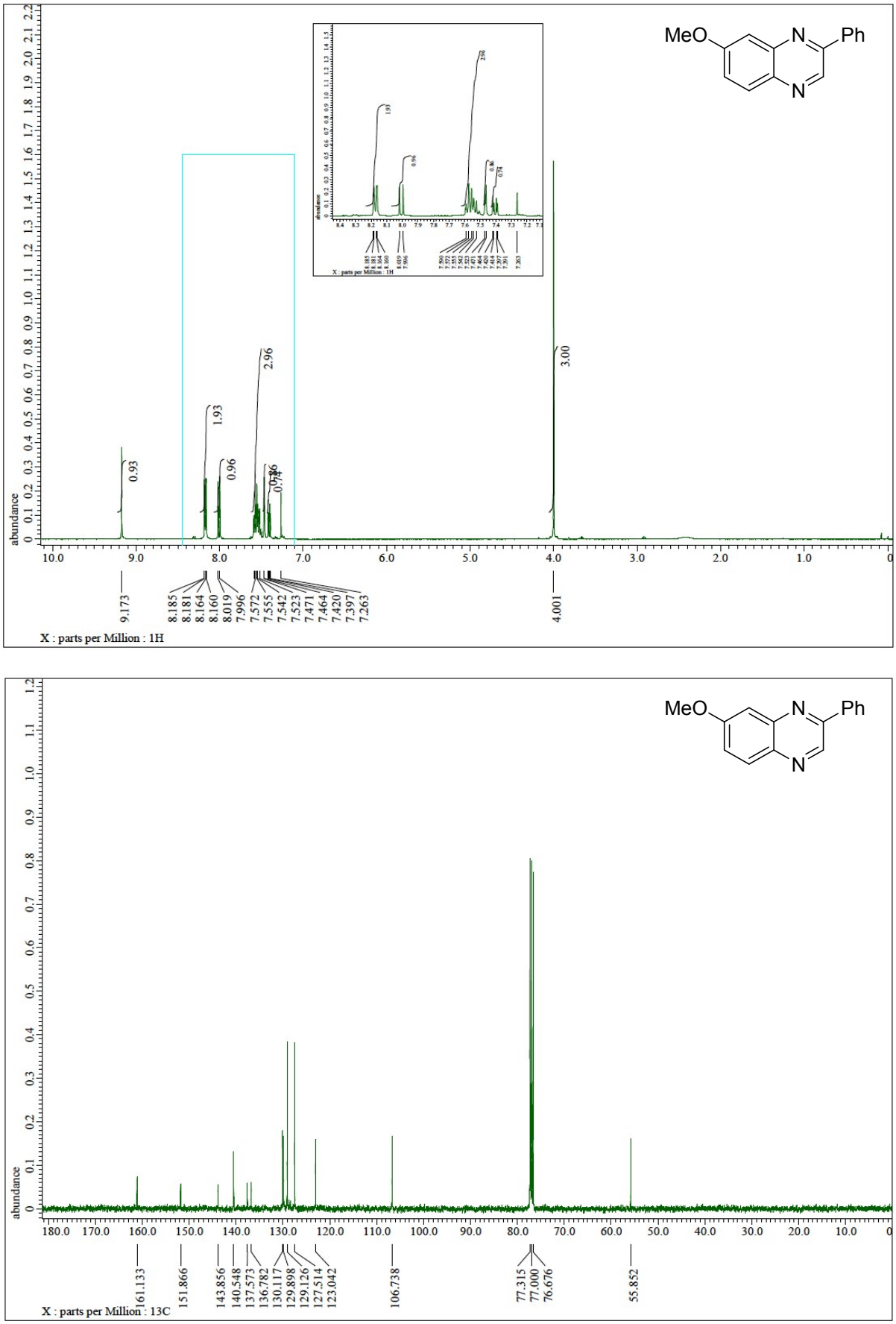


Figure S36. ^{1}H NMR of **4j'** (400 MHz, $CDCl_3$) and ^{13}C NMR of **4j'** (100 MHz, $CDCl_3$).

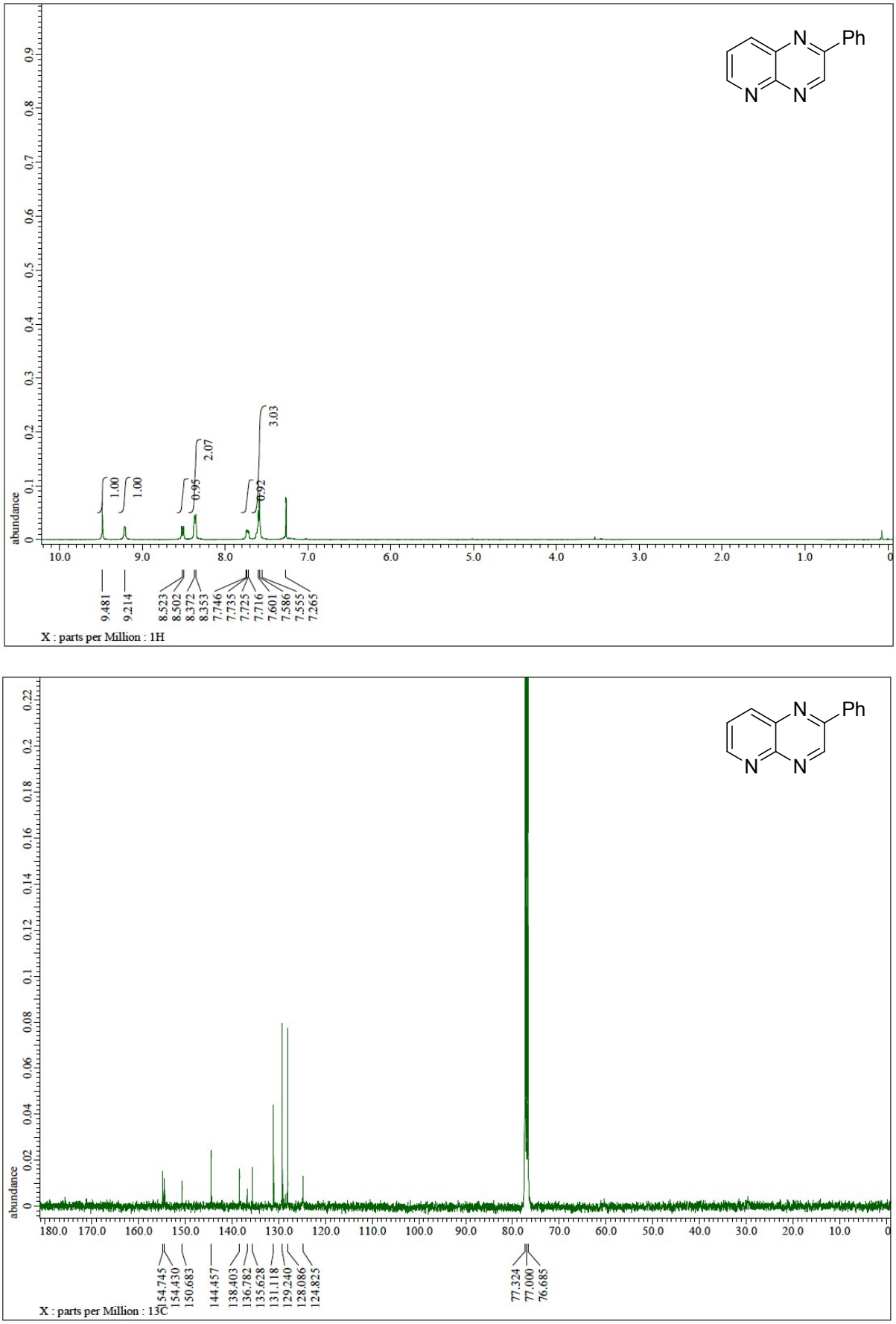


Figure S37. ^{1}H NMR of **4k** (400 MHz, $CDCl_3$) and ^{13}C NMR of **4k** (100 MHz, $CDCl_3$).

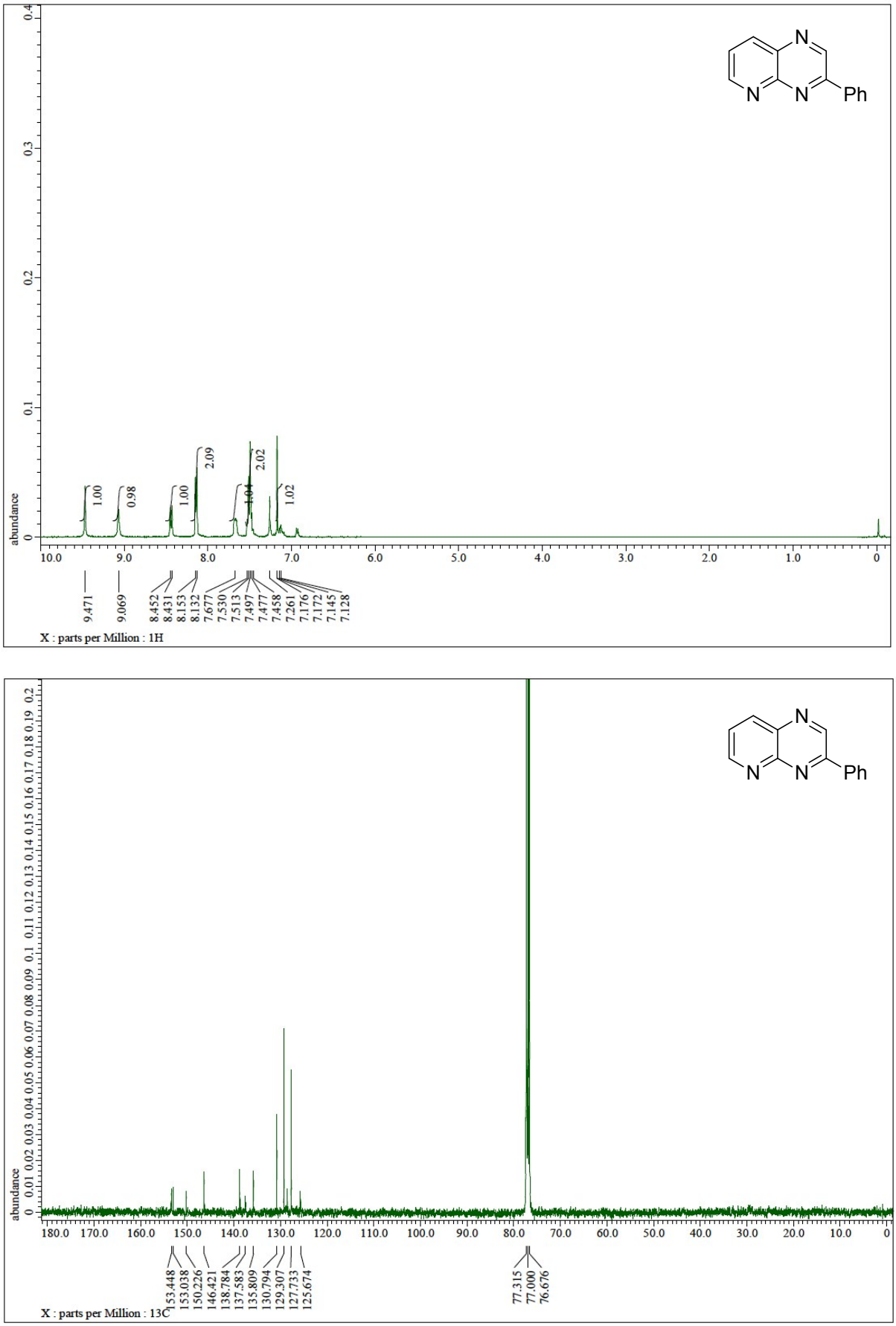


Figure S38. ^{1}H NMR of **4k'** (400 MHz, $CDCl_3$) and ^{13}C NMR of **4k'** (100 MHz, $CDCl_3$).

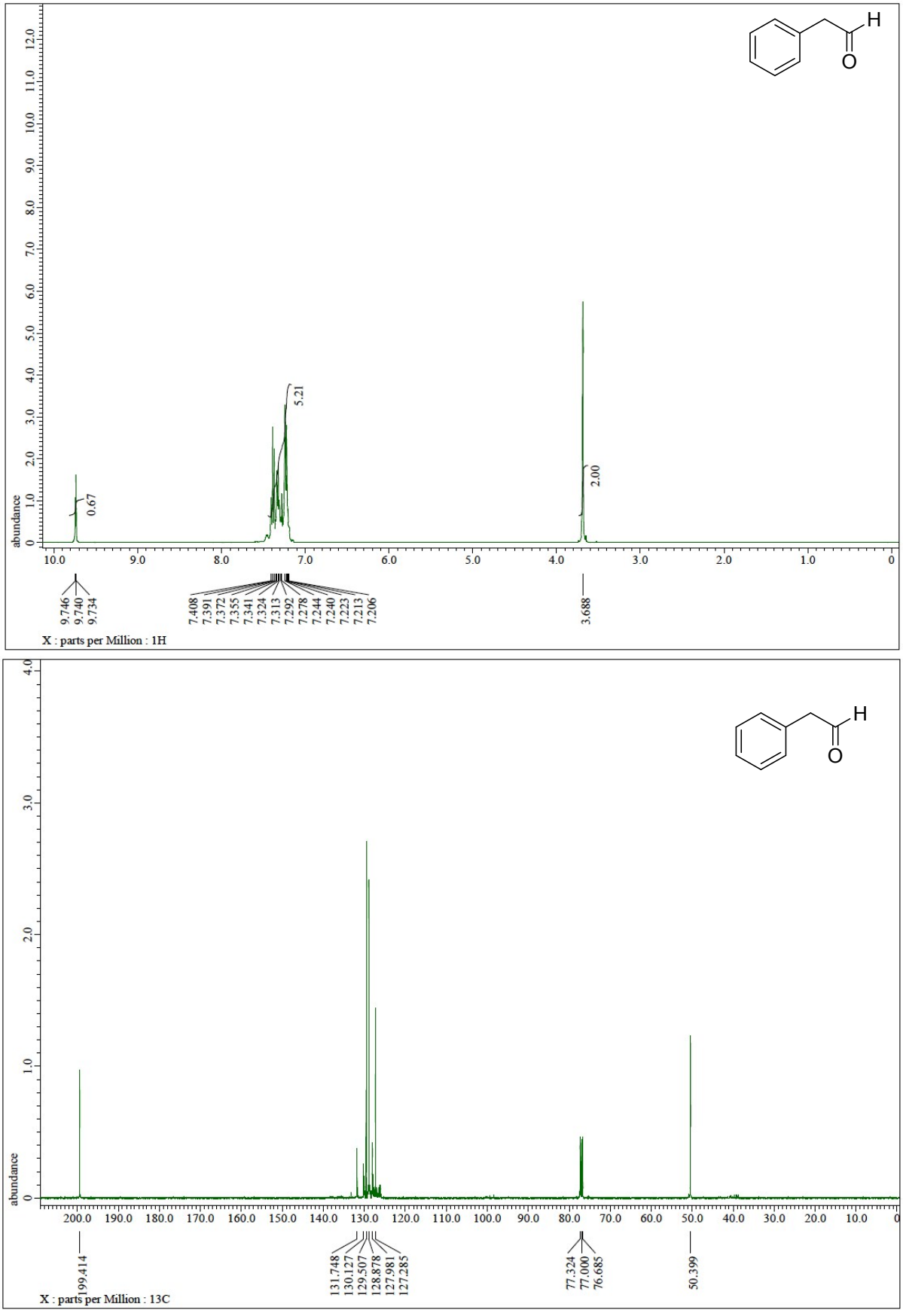


Figure S39. ^{1}H NMR of **5** (400 MHz, $CDCl_3$) and ^{13}C NMR of **5** (100 MHz, $CDCl_3$).

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