

Supplementary Information for
**Structural and electrochemical properties of mononuclear copper(II) complexes
with pentadentate ethylenediamine-based ligands with
pyridine/quinoline/isoquinoline/quinoxaline binding sites**

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*Preparation of copper(II) complexes***Me-PPP-Cu** ([Cu(Me-PPP)](ClO₄)₂)¹

To a solution of **Me-PPP** (8.7 mg, 25 μmol) in ethanol (0.5 mL) was added Cu(ClO₄)₂·6H₂O (9.8 mg, 26 μmol) in ethanol (0.5 mL). After stirring for 5 min, resulting precipitate was collected by filtration and washed with ethanol to afford **Me-PPP-Cu** as a blue powder (13.0 mg, 21.3 μmol, 85%). Single crystals suitable for X-ray crystallography were obtained by recrystallization from acetonitrile and chloroform.

λ_{max} : 678 nm (CH₃CN), 672 nm (CH₃OH).

Anal Calcd. for C₂₂H_{26.5}Cl₂CuN_{5.5}O₈ (**Me-PPP-Cu**·0.5CH₃CN): C, 41.91; H, 4.24; N, 12.22.

Found: C, 41.52; H, 4.26; N, 12.63.

Me-QQQ-Cu ([Cu(Me-QQQ)](ClO₄)₂)²

To a solution of **Me-QQQ** (14.9 mg, 30.0 μmol) in ethanol (0.5 mL) was added Cu(ClO₄)₂·6H₂O (12.0 mg, 32.4 μmol) in ethanol (0.5 mL). After stirring for 5 min, resulting precipitate was collected by filtration and washed with ethanol to afford **Me-QQQ-Cu** as blue powder (18.1 mg, 23.8 μmol, 79%). Single crystals suitable for X-ray crystallography were obtained by recrystallization from acetonitrile.

λ_{max} : 655 nm (CH₃CN), 659 nm (CH₃OH).

Anal Calcd. for C₃₃H₃₃Cl₂CuN₅O₉ (**Me-QQQ-Cu**·H₂O): C, 50.94; H, 4.27; N, 9.00.

Found: C, 50.68; H, 4.34; N, 9.25.

Me-111-Cu

To a solution of **Me-111** (12.5 mg, 25.1 μmol) in ethanol (0.5 mL) was added Cu(ClO₄)₂·6H₂O (10.1 mg, 27.3 μmol) in ethanol (0.5 mL). After stirring for 5 min, resulting precipitate was collected by filtration and washed with ethanol to afford **Me-111-Cu** as a blue powder (14.4 mg, 18.9 μmol, 76%).

λ_{max} : 694 nm (CH₃CN), 687 nm (CH₃OH).

HRMS (ESI) *m/z*: [**Me-111** + Cu^{II} + Cl]⁺ calcd. for C₃₃H₃₁ClCuN₅ 595.15640; found 595.15876.

Me-333-Cu ([Cu(Me-333)](ClO₄)₂)

To a solution of **Me-333** (15.1 mg, 30.3 μmol) in ethanol (0.5 mL) was added Cu(ClO₄)₂·6H₂O (12.0 mg, 32.4 μmol) in ethanol (0.5 mL). After stirring for 5 min, resulting precipitate was collected by filtration and washed with ethanol to afford **Me-333-Cu** as blue powder (17.4 mg, 22.9 μmol, 76%). Single crystals suitable for X-ray crystallography were obtained by recrystallization from acetonitrile.

λ_{max}: 683 nm (CH₃CN), 676 nm (CH₃OH).

Anal Calcd. for C₃₃H₃₆Cl₂CuN₅O_{10.5} (**Me-333-Cu**·2.5H₂O): C, 49.23; H, 4.51; N, 8.70. Found: C, 49.33; H, 4.22; N, 8.80.

Me-XXX-Cu

To a solution of **Me-XXX** (12.2 mg, 24.4 μmol) in ethanol (0.5 mL) was added Cu(ClO₄)₂·6H₂O (9.6 mg, 26 μmol) in ethanol (0.5 mL). After stirring for 5 min, resulting precipitate was collected by filtration and washed with ethanol to afford **Me-XXX** as yellow-green powder (12.3 mg, 61.1 μmol, 66%).

λ_{max}: 641 nm (CH₃CN).

HRMS (ESI) *m/z*: [**Me-XXX** + Cu]⁺ calcd. for C₃₀H₂₈CuN₈ 563.17329; found 563.16825.

Bn-PPP-Cu ([Cu(Bn-PPP)](ClO₄)₂)

To a solution of **Bn-PPP** (12.7 mg, 30.0 μmol) in ethanol (0.5 mL) was added Cu(ClO₄)₂·6H₂O (12.0 mg, 32.4 μmol) in ethanol (0.5 mL). After stirring for 5 min, resulting precipitate was collected by filtration and washed with ethanol to afford **Bn-PPP-Cu** as blue powder (18.6 mg, 27.1 μmol, 90%). Single crystals suitable for X-ray crystallography were obtained by recrystallization from acetonitrile.

λ_{max}: 696 nm (CH₃CN), 690 nm (CH₃OH).

Anal Calcd. for C₂₇H₂₉Cl₂CuN₅O₈ (**Bn-PPP-Cu**): C, 47.27; H, 4.26; N, 10.21. Found: C, 47.14; H, 4.30; N, 10.07.

Bn-QQQ-Cu

To a solution of **Bn-QQQ** (14.6 mg, 25.4 μmol) in ethanol (0.5 mL) was added $\text{Cu}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ (9.8 mg, 26 μmol) in ethanol (0.5 mL). After stirring for 5 min, resulting precipitate was collected by filtration and washed with ethanol to afford **Bn-QQQ-Cu** as a green powder (17.2 mg, 20.6 μmol , 82%).

λ_{max} : 661 nm (CH_3CN), 660 nm (CH_3OH).

HRMS (ESI) m/z : [**Bn-QQQ** + Cu^{I}]⁺ calcd. for $\text{C}_{39}\text{H}_{35}\text{CuN}_5$ 636.21885; found 636.21728.

Bn-111-Cu ([Cu(Bn-111)](ClO₄)₂)

To a solution of **Bn-111** (17.2 mg, 30.0 μmol) in ethanol (2.5 mL) was added $\text{Cu}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ (13.0 mg, 35.0 μmol) in ethanol (2.0 mL). After stirring for 5 min, resulting precipitate was dissolved by addition of DMF. The blue solution was kept at 4 °C to precipitate the complex, which was collected by filtration and washed with ethanol to afford **Bn-111-Cu** as blue crystals suitable for X-ray crystallography (29.2 mg, 35.0 μmol , 43%).

λ_{max} : 703 nm (CH_3CN), 699 nm (CH_3OH).

Anal Calcd. for $\text{C}_{39}\text{H}_{37}\text{Cl}_2\text{CuN}_5\text{O}_9$ (**Bn-111-Cu**· H_2O): C, 54.83; H, 4.37; N, 8.20. Found: C, 54.73; H, 4.34; N, 8.29.

Bn-333-Cu ([Cu(Bn-333)](ClO₄)₂)

To a solution of **Bn-333** (15.4 mg, 26.6 μmol) in ethanol (0.5 mL) was added $\text{Cu}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ (9.85 mg, 26.8 μmol) in ethanol (1.5 mL). After stirring for 5 min, resulting precipitate was collected by filtration and washed with ethanol to afford **Bn-333-Cu** as blue powder (16.0 mg, 19.1 μmol , 72%). Single crystals suitable for X-ray crystallography were obtained by recrystallization from acetonitrile.

λ_{max} : 694 nm (CH_3CN), 692 nm (CH_3OH).

Anal Calcd. for $\text{C}_{39}\text{H}_{37}\text{Cl}_2\text{CuN}_5\text{O}_9$ (**Bn-333-Cu**· H_2O): C, 54.83; H, 4.37; N, 8.20. Found: C, 54.83; H, 4.03; N, 8.25.

Bn-XXX-Cu

To a solution of **Bn-XXX** (14.7 mg, 25.5 μmol) in ethanol (0.5 mL) was added $\text{Cu}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ (9.8 mg, 26 μmol) in ethanol (0.5 mL). After stirring for 5 min, resulting precipitate was collected by filtration and washed with ethanol to afford **Bn-XXX-Cu** as a yellow-green powder (15.4 mg, 18.4 μmol , 74%).

λ_{max} : 636 nm (CH_3CN).

HRMS (ESI) m/z : [**Bn-XXX** + Cu^{I}]⁺ calcd. for $\text{C}_{36}\text{H}_{32}\text{CuN}_8$ 639.20459; found 639.20499.

Ph-PPP-Cu ([Cu(Ph-PPP)(ClO₄)]ClO₄)

To a solution of **Ph-PPP** (10.2 mg, 25.0 μmol) in ethanol (0.5 mL) was added $\text{Cu}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ (9.5 mg, 26 μmol) in ethanol (0.5 mL). After stirring for 5 min, resulting precipitate was collected by filtration and washed with ethanol to afford **Ph-PPP-Cu** as a blue powder (13.4 mg, 19.9 μmol , 80%). Single crystals suitable for X-ray crystallography were obtained from recrystallization from acetonitrile (0.1 mL) in the presence of NaClO_4 (10.8 mg, 76.9 μmol) under ether diffusion condition.

Anal Calcd. for $\text{C}_{26}\text{H}_{27}\text{Cl}_2\text{CuN}_5\text{O}_8$ (**Ph-PPP-Cu**): C, 46.47; H, 4.05; N, 10.42. Found: C, 45.73; H, 3.78; N, 10.28.

On the other hand, recrystallization from acetonitrile (0.2 mL) in the presence of NH_4PF_6 (4.2 mg, 26 μmol) afforded **Ph-PPP-Cu'** ($[\text{Cu}(\text{Ph-PPP})(\text{ClO}_4)]\text{PF}_6$) as single crystals suitable for X-ray crystallography.

λ_{max} : 655 nm (CH_3CN), 633 nm (CH_3OH).

Anal Calcd. for $\text{C}_{26}\text{H}_{30}\text{ClCuF}_6\text{N}_5\text{O}_{5.5}\text{P}$ (**Ph-PPP-Cu'**·1.5 H_2O): C, 41.94; H, 4.06; N, 9.41. Found: C, 41.66; H, 3.71; N, 9.87.

Ph-QQQ-Cu ([Cu(Ph-QQQ)](ClO₄)₂)

To a solution of **Ph-QQQ** (14.3 mg, 25.5 μmol) in ethanol (0.5 mL) was added $\text{Cu}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ (9.4 mg, 25 μmol) in ethanol (0.5 mL). After stirring for 5 min, resulting precipitate was collected by filtration and washed with ethanol to afford **Ph-QQQ-Cu** as a green powder (16.3 mg, 19.8 μmol , 78%). Single crystals suitable for X-

ray crystallography were obtained from recrystallization from acetonitrile (0.1 mL) in the presence of NaClO₄ (3.3 mg, 23 μmol) under ether diffusion condition.

λ_{max} : 643 nm (CH₃CN), 650 nm (CH₃OH).

Anal Calcd. for C₄₀H₃₆Cl₃CuN₆NaO₁₂ (**Ph-QQQ-Cu**·NaClO₄·CH₃CN): C, 48.74; H, 3.68; N, 8.53. Found: C, 48.80; H, 3.70; N, 8.13.

Ph-111-Cu

To a solution of **Ph-111** (14.1 mg, 25.2 μmol) in ethanol (0.5 mL) was added Cu(ClO₄)₂·6H₂O (9.8 mg, 26 μmol) in ethanol (0.5 mL). After stirring for 5 min, resulting precipitate was collected by filtration and washed with ethanol to afford **Ph-111-Cu** as a blue powder (12.0 mg, 14.6 μmol, 58%).

λ_{max} : 674 nm (CH₃CN), 641 nm (CH₃OH).

HRMS (ESI) m/z : [**Ph-111** + Cu^{II} + ClO₄]⁺ calcd. for C₃₈H₃₃ClCuN₅O₄ 721.15171; found 721.14981.

Ph-333-Cu

To a solution of **Ph-333** (13.6 mg, 24.3 μmol) in ethanol (0.5 mL) was added Cu(ClO₄)₂·6H₂O (9.9 mg, 27 μmol) in ethanol (0.5 mL). After stirring for 5 min, resulting precipitate was collected by filtration and washed with ethanol to afford **Ph-333-Cu** as a blue powder (17.4 mg, 21.2 μmol, 88%).

λ_{max} : 650 nm (CH₃CN), 641 nm (CH₃OH).

HRMS (ESI) m/z : [**Ph-333** + Cu^{II} + ClO₄]⁺ calcd. for C₃₈H₃₃ClCuN₅O₄ 721.15171; found 721.14920.

Ph-XXX-Cu

To a solution of **Ph-XXX** (14.0 mg, 24.9 μmol) in ethanol (0.5 mL) was added Cu(ClO₄)₂·6H₂O (9.8 mg, 26 μmol) in ethanol (0.5 mL). After stirring for 5 min, resulting precipitate was collected by filtration and washed with ethanol to afford **Ph-XXX-Cu** as a yellow green powder (12.2 mg, 14.8 μmol, 60%).

HRMS (ESI) m/z : [**Ph-XXX** + Cu]⁺ calcd. for C₃₅H₃₀CuN₈ 625.18894; found 625.19341.

Ph-PPQ-Cu

To a solution of **Ph-PPQ** (22.5 mg, 49.0 μmol) in ethanol (0.5 mL) was added Cu(ClO₄)₂·6H₂O (20.4 mg, 55.1 μmol) in ethanol (0.5 mL). After stirring for 5 min, resulting precipitate was collected by filtration and washed with ethanol to afford **Ph-PPQ-Cu** as a green powder (23.0 mg, 31.8 μmol, 64%). Single crystals suitable for X-ray crystallography were obtained by recrystallization from methanol.

λ_{max} : 714 nm (CH₃CN), 645 nm (CH₃OH).

HRMS (ESI) m/z : [**Ph-PPQ** + Cu]⁺ calcd. for C₃₀H₂₉CuN₅ 522.17190; found 522.16860.

Ph-PQP-Cu

To a solution of **Ph-PQP** (22.7 mg, 49.4 μmol) in ethanol (0.5 mL) was added Cu(ClO₄)₂·6H₂O (20.4 mg, 55.1 μmol) in ethanol (0.5 mL). After stirring for 5 min, resulting precipitate was collected by filtration and washed with ethanol to afford **Ph-PQP-Cu** as a green powder (23.0 mg, 31.8 μmol, 64%).

λ_{max} : 638 nm (CH₃CN), 645 nm (CH₃OH).

HRMS (ESI) m/z : [**Ph-PQP** + Cu]⁺ calcd. for C₃₀H₂₉CuN₅ 522.17190; found 522.16937.

Ph-PQQ-Cu ([Cu(Ph-PQQ)](ClO₄)₂)

To a solution of **Ph-PQQ** (25.5 mg, 50.0 μmol) in ethanol (0.5 mL) was added Cu(ClO₄)₂·6H₂O (20.4 mg, 55.1 μmol) in ethanol (0.5 mL). After stirring for 5 min, resulting precipitate was collected by filtration and washed with ethanol to afford **Ph-PQQ-Cu** as green powder (20.1 mg, 26.0 μmol, 52%). Single crystals suitable for X-ray crystallography were obtained by recrystallization from acetonitrile.

λ_{max} : 742 nm (CH₃CN), 738 nm (CH₃OH).

Anal Calcd. for C₃₄H₃₁Cl₂CuN₅O₈ (**Ph-PQQ-Cu**): C, 52.89; H, 4.05; N, 9.07. Found: C, 52.56; H, 4.06; N, 9.67.

Ph-QQP-Cu ($[\text{Cu}(\text{Ph-QQP})](\text{ClO}_4)_2$)

To a solution of **Ph-QQP** (12.7 mg, 25.0 μmol) in methanol (0.5 mL) was added $\text{Cu}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ (10.9 mg, 29 μmol) in methanol (0.5 mL). The green solution was kept at 4 °C to precipitate the complex, which was collected by filtration. The green powder was recrystallized from acetonitrile (0.6 mL) at 4 °C under ether diffusion conditions to afford **Ph-QQP-Cu** as green crystals suitable for X-ray crystallography (17.7 mg, 22.9 μmol , 92%).

λ_{max} : 636 nm (CH_3CN), 637 nm (CH_3OH).

Anal Calcd. for $\text{C}_{34}\text{H}_{31}\text{Cl}_2\text{CuN}_5\text{O}_8$ (**Ph-QQP-Cu**): C, 52.89; H, 4.05; N, 9.07. Found: C, 53.04; H, 4.10; N, 9.48.

*X-ray crystallography***Table S1.** Crystallographic data for [Cu(**Me-PPP**)](ClO₄)₂·CH₃CN (**Me-PPP-Cu**·CH₃CN) and [Cu(**Me-QQQ**)](ClO₄)₂·1.75CH₃CN (**Me-QQQ-Cu**·1.75CH₃CN)

	Me-PPP-Cu ·CH ₃ CN	Me-QQQ-Cu ·1.75CH ₃ CN
Formula	C ₂₃ H ₂₈ Cl ₂ CuN ₆ O ₈	C _{36.5} H _{36.25} Cl ₂ CuN _{6.75} O ₈
FW	650.96	831.91
Crystal system	triclinic	orthorhombic
Space group	<i>P</i> -1	<i>P</i> 2 ₁ 2 ₁ 2
<i>a</i> , Å	8.300(4)	19.7113(5)
<i>b</i> , Å	11.361(5)	45.9648(14)
<i>c</i> , Å	15.321(6)	8.4267(2)
α , deg	93.883(6)	90
β , deg	96.666(5)	90
γ , deg	105.289(5)	90
<i>V</i> , Å ³	1376.8(10)	7634.8(4)
<i>Z</i>	2	8
<i>D</i> _{calc} , g cm ⁻³	1.570	1.447
μ , mm ⁻¹	1.0449	0.772
2 θ _{max} , deg	55	50.7
temp, K	153	150
no. reflns collected	10754	28038
no. reflns used	6013	13467
no. of params	390	1160
<i>R</i> _{int}	0.0219	0.0354
Final <i>R</i> 1 (<i>I</i> > 2 σ (<i>I</i>)) ^a	0.0476	0.0484
<i>wR</i> 2 (all data) ^b	0.1366	0.1260
GOF	1.043	1.037

^a*R*1 = $\sum ||F_o| - |F_c|| / \sum |F_o|$. ^b*wR*2 = $[\sum w[(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]]^{1/2}$.

Table S2. Crystallographic data for [Cu(**Me-333**)](ClO₄)₂·CH₃OH·0.5CH₃CN·0.5CHCl₃ (**Me-333-Cu**·CH₃OH·0.5CH₃CN·0.5CHCl₃) and [Cu(**Bn-PPP**)](ClO₄)₂ (**Bn-PPP-Cu**)

	Me-333-Cu ·CH ₃ OH ·0.5CH ₃ CN·0.5CHCl ₃	Bn-PPP-Cu
Formula	C _{35.5} H ₃₇ Cl _{3.5} CuN _{5.5} O ₉	C ₂₇ H ₂₉ Cl ₂ CuN ₅ O ₈
FW	872.32	686.01
Crystal system	monoclinic	orthorhombic
Space group	<i>P2₁/c</i>	<i>Pbca</i>
<i>a</i> , Å	18.6631(5)	14.5386(19)
<i>b</i> , Å	15.1459(3)	18.525(3)
<i>c</i> , Å	28.2417(9)	21.715(3)
β, deg	105.021(3)	90
<i>V</i> , Å ³	7710.3(4)	5848.4(15)
<i>Z</i>	8	8
<i>D</i> _{calc} , g cm ⁻³	1.503	1.558
μ, mm ⁻¹	0.870	0.9877
2θ _{max} , deg	60.3	55
temp, K	150	153
no. reflns collected	55167	45067
no. reflns used	18533	6526
no. of params	1028	388
<i>R</i> _{int}	0.0450	0.0481
Final <i>R</i> 1 (<i>I</i> > 2σ(<i>I</i>)) ^a	0.0706	0.0435
<i>wR</i> 2 (all data) ^b	0.2224	0.1122
GOF	1.042	1.052

^a*R*1 = Σ||*F*_o| - |*F*_c||/Σ|*F*_o|. ^b*wR*2 = [Σ*w*[(*F*_o² - *F*_c²)²]/Σ[*w*(*F*_o²)²]^{1/2}.

Table S3. Crystallographic data for [Cu(**Bn-111**)](ClO₄)₂·DMF (**Bn-111-Cu**·DMF) and [Cu(**Bn-333**)](ClO₄)₂·1.25CH₃CN (**Bn-333-Cu**·1.25CH₃CN)

	Bn-111-Cu ·DMF	Bn-333-Cu ·1.25CH ₃ CN
Formula	C ₄₂ H ₄₂ Cl ₂ CuN ₆ O ₉	C _{41.5} H _{38.75} Cl ₂ CuN _{6.25} O ₈
FW	909.28	887.48
Crystal system	triclinic	triclinic
Space group	<i>P</i> -1	<i>P</i> -1
<i>a</i> , Å	11.805(3)	13.425(6)
<i>b</i> , Å	13.196(4)	15.738(7)
<i>c</i> , Å	13.294(4)	19.413(8)
α, deg	86.264(7)	76.205(10)
β, deg	75.769(6)	86.332(9)
γ, deg	88.616(6)	87.694(8)
<i>V</i> , Å ³	2003.0(10)	3974(3)
<i>Z</i>	2	4
<i>D</i> _{calc} , g cm ⁻³	1.507	1.483
μ, mm ⁻¹	0.7442	0.747
2θ _{max} , deg	61.5	55
temp, K	153	153
no. reflns collected	24105	40334
no. reflns used	11187	17833
no. of params	389	1187
<i>R</i> _{int}	0.0242	0.0474
Final <i>R</i> 1 (<i>I</i> > 2σ(<i>I</i>)) ^a	0.0443	0.0635
<i>wR</i> 2 (all data) ^b	0.1267	0.2045
GOF	1.072	1.073

^a*R*1 = Σ||*F*_o| - |*F*_c||/Σ|*F*_o|. ^b*wR*2 = [Σ*w*[(*F*_o² - *F*_c²)²]/Σ[*w*(*F*_o²)²]^{1/2}.

Table S4. Crystallographic data for [Cu(**Ph-PPP**)(ClO₄)]ClO₄ (**Ph-PPP-Cu**) and [Cu(**Ph-PPP**)(ClO₄)]PF₆ (**Ph-PPP-Cu'**)

	Ph-PPP-Cu	Ph-PPP-Cu'
Formula	C ₂₆ H ₂₇ Cl ₂ CuN ₅ O ₈	C ₂₆ H ₂₇ ClCuF ₆ N ₅ O ₄ P
FW	671.98	717.49
Crystal system	monoclinic	monoclinic
Space group	<i>P2₁/c</i>	<i>P2₁/c</i>
<i>a</i> , Å	20.820(4)	21.039(10)
<i>b</i> , Å	7.9052(15)	7.934(4)
<i>c</i> , Å	18.113(4)	18.056(9)
β, deg	110.212(3)	110.078(7)
<i>V</i> , Å ³	2797.6(10)	2831(2)
<i>Z</i>	4	4
<i>D</i> _{calc} , g cm ⁻³	1.595	1.683
μ, mm ⁻¹	1.0306	1.0060
2θ _{max} , deg	55	55
temp, K	153	153
no. reflns collected	20997	18245
no. reflns used	6338	6360
no. of params	403	399
<i>R</i> _{int}	0.0288	0.0365
Final <i>R</i> 1 (<i>I</i> > 2σ(<i>I</i>)) ^a	0.0791	0.0561
<i>wR</i> 2 (all data) ^b	0.2397	0.1684
GOF	1.116	1.036

^a*R*1 = Σ ||*F*_o| - |*F*_c|| / Σ |*F*_o|. ^b*wR*2 = [Σ*w*[(*F*_o² - *F*_c²)] / Σ [*w*(*F*_o²)]]^{1/2}.

Table S5. Crystallographic data for [Cu(**Ph-QQQ**)](ClO₄)₂·NaClO₄·CH₃CN (**Ph-QQQ-Cu**·NaClO₄·CH₃CN) and [Cu(**Ph-PQQ**)](ClO₄)₂·CH₃CN (**Ph-PQQ-Cu**·0.5CH₃CN)

	Ph-QQQ-Cu ·NaClO ₄ ·CH ₃ CN	Ph-PQQ-Cu ·0.5CH ₃ CN
Formula	C ₄₀ H ₃₈ Cl ₃ CuN ₆ NaO ₁₃	C ₃₅ H _{32.5} Cl ₂ CuN _{5.5} O ₈
FW	1003.67	792.60
Crystal system	triclinic	monoclinic
Space group	<i>P</i> -1	<i>I</i> 2/ <i>a</i>
<i>a</i> , Å	10.7240(19)	9.9174(2)
<i>b</i> , Å	13.815(3)	18.90674)
<i>c</i> , Å	15.435(3)	37.0398(7)
α, deg	84.3269(10)	90
β, deg	74.387(8)	91.504(2)
γ, deg	71.884(6)	90
<i>V</i> , Å ³	2092.9(7)	6942.8(2)
<i>Z</i>	2	8
<i>D</i> _{calc} , g cm ⁻³	1.593	1.517
μ, mm ⁻¹	0.7979	0.844
2θ _{max} , deg	55	59
temp, K	153	150
no. reflns collected	17126	26753
no. reflns used	9180	8373
no. of params	578	497
<i>R</i> _{int}	0.0260	0.0240
Final <i>R</i> 1 (<i>I</i> > 2σ(<i>I</i>)) ^a	0.0546	0.0472
<i>wR</i> 2 (all data) ^b	0.1631	0.1402
GOF	1.042	1.066

^a*R*1 = Σ||*F*_o| - |*F*_c||/Σ|*F*_o|. ^b*wR*2 = [Σ*w*[(*F*_o² - *F*_c²)²]/Σ[*w*(*F*_o²)²]^{1/2}.

Table S6. Crystallographic data for [Cu(**Ph-QQP**)](ClO₄)₂ (**Ph-QQP-Cu**) and [Cu(**Ph-PPQ**)](ClO₄)₂·0.75CH₃OH·0.125H₂O (**Ph-PPQ-Cu**·0.75CH₃OH·0.125H₂O)

	Ph-QQP-Cu	Ph-PPQ-Cu ·0.75CH ₃ - OH·0.125H ₂ O
Formula	C ₃₄ H ₃₁ Cl ₂ CuN ₅ O ₈	C _{30.75} H _{32.25} Cl ₂ CuN ₅ O _{8.875}
FW	772.10	748.30
Crystal system	orthorhombic	monoclinic
Space group	<i>Pna</i> 2 ₁	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> , Å	14.734(2)	8.1238(2)
<i>b</i> , Å	21.124(3)	37.8829(8)
<i>c</i> , Å	10.5506(16)	41.6362(12)
β, deg	90	92.788(2)
<i>V</i> , Å ³	3283.8(8)	12798.5(6)
<i>Z</i>	4	16
<i>D</i> _{calc} , g cm ⁻³	1.562	1.553
μ, mm ⁻¹	0.8895	0.912
2θ _{max} , deg	55	50.7
temp, K	153	150
no. reflns collected	26183	23294
no. reflns used	6043	13744
no. of params	451	1879
<i>R</i> _{int}	0.0391	0.0635
Final <i>R</i> 1 (<i>I</i> > 2σ(<i>I</i>)) ^a	0.0413	0.0572
<i>wR</i> 2 (all data) ^b	0.1118	0.1549
GOF	1.042	1.081

^a*R*1 = Σ||*F*_o| - |*F*_c||/Σ|*F*_o|. ^b*wR*2 = [Σ*w*[(*F*_o² - *F*_c²)²]/Σ[*w*(*F*_o²)²]]^{1/2}.

Table S7. Selected Bond Angles (°) for **Me-PPP-Cu**, **Me-QQQ-Cu**, **Me-333-Cu**, **Bn-PPP-Cu**, **Bn-111-Cu** and **Bn-333-Cu**

	Me-PPP -Cu	Me-QQQ -Cu^a	Me-333 -Cu^a	Bn-PPP -Cu	Bn-111 -Cu	Bn-333 -Cu^a
N1-Cu-N2	87.5	85.3	85.9	87.1	87.2	86.2
N1-Cu-N3	82.6	80.6	82.4	83.5	83.3	82.9
N1-Cu-N4	82.3	81.9	82.5	82.8	83.1	83.1
N1-Cu-N5	168.1	163.3	166.6	167.9	167.1	168.1
N2-Cu-N3	107.2	161.9	104.1	106.7	132.7	103.3
N2-Cu-N4	138.8	98.9	139.7	138.3	107.3	143.4
N2-Cu-N5	82.0	79.1	82.5	82.3	81.2	82.8
N3-Cu-N4	110.8	90.4	112.3	112.2	117.2	109.8
N3-Cu-N5	106.0	113.5	107.2	105.2	100.5	103.3
N4-Cu-N5	101.8	106.1	105.9	101.3	105.7	103.8

^a Average values for two crystallographically independent complexes.

Table S8. Selected Bond Angles (°) for **Ph-PPP-Cu**, **Ph-PPP-Cu'**, **Ph-QQQ-Cu**, **Ph-PQQ-Cu** and **Ph-QQP-Cu**

	Ph-PPP -Cu	Ph-PPP -Cu'	Ph-QQQ -Cu	Ph-PQQ -Cu	Ph-QQP -Cu
N1-Cu-N2	84.7	84.8	85.7	86.5	85.3
N1-Cu-N3	82.6	82.4	81.0	131.5	80.7
N1-Cu-N4	83.4	83.6	81.7	82.6	82.7
N1-Cu-N5	161.0	161.2	163.2	161.0	116.5
N2-Cu-N3	91.0	90.0	161.3	131.5	164.2
N2-Cu-N4	100.4	100.0	98.9	100.5	93.6
N2-Cu-N5	76.8	76.9	79.3	80.9	83.8
N3-Cu-N4	161.0	161.3	92.0	124.4	91.8
N3-Cu-N5	101.8	101.8	111.7	95.0	96.1
N4-Cu-N5	95.7	95.4	107.9	113.6	160.2
O1-Cu-N1	111.1	110.3	–	–	–
O1-Cu-N2	161.7	161.7	–	–	–
O1-Cu-N3	82.3	81.5	–	–	–
O1-Cu-N4	90.9	91.8	–	–	–
O1-Cu-N5	87.9	88.4	–	–	–

Table S9. Selected Bond Angles (°) for **Ph-PPQ-Cu**

	Ph-PPQ- Cu-1	Ph-PPQ- Cu-2	Ph-PPQ- Cu-3	Ph-PPQ- Cu-4
N1-Cu-N2	85.0	85.9	85.9	86.6
N1-Cu-N3	84.7	84.2	84.4	83.0
N1-Cu-N4	83.8	84.1	83.5	83.8
N1-Cu-N5	164.3	164.8	163.9	166.9
N2-Cu-N3	102.6	104.2	106.3	98.8
N2-Cu-N4	94.1	64.6	93.0	131.7
N2-Cu-N5	79.8	79.9	78.9	81.8
N3-Cu-N4	158.8	157.0	156.4	126.6
N3-Cu-N5	94.9	94.2	94.7	104.7
N4-Cu-N5	101.0	102.2	102.4	99.4

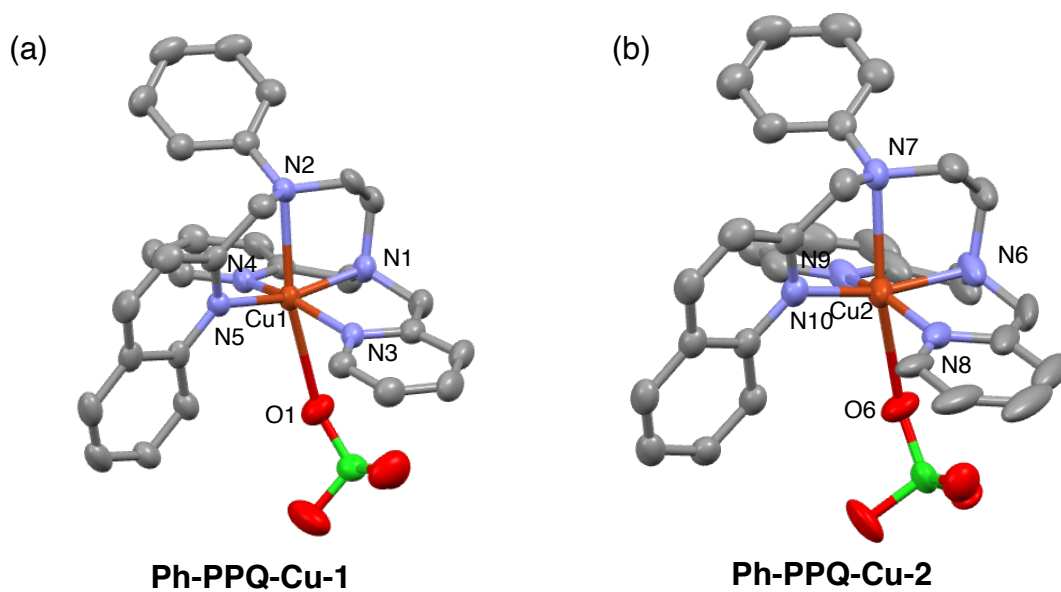
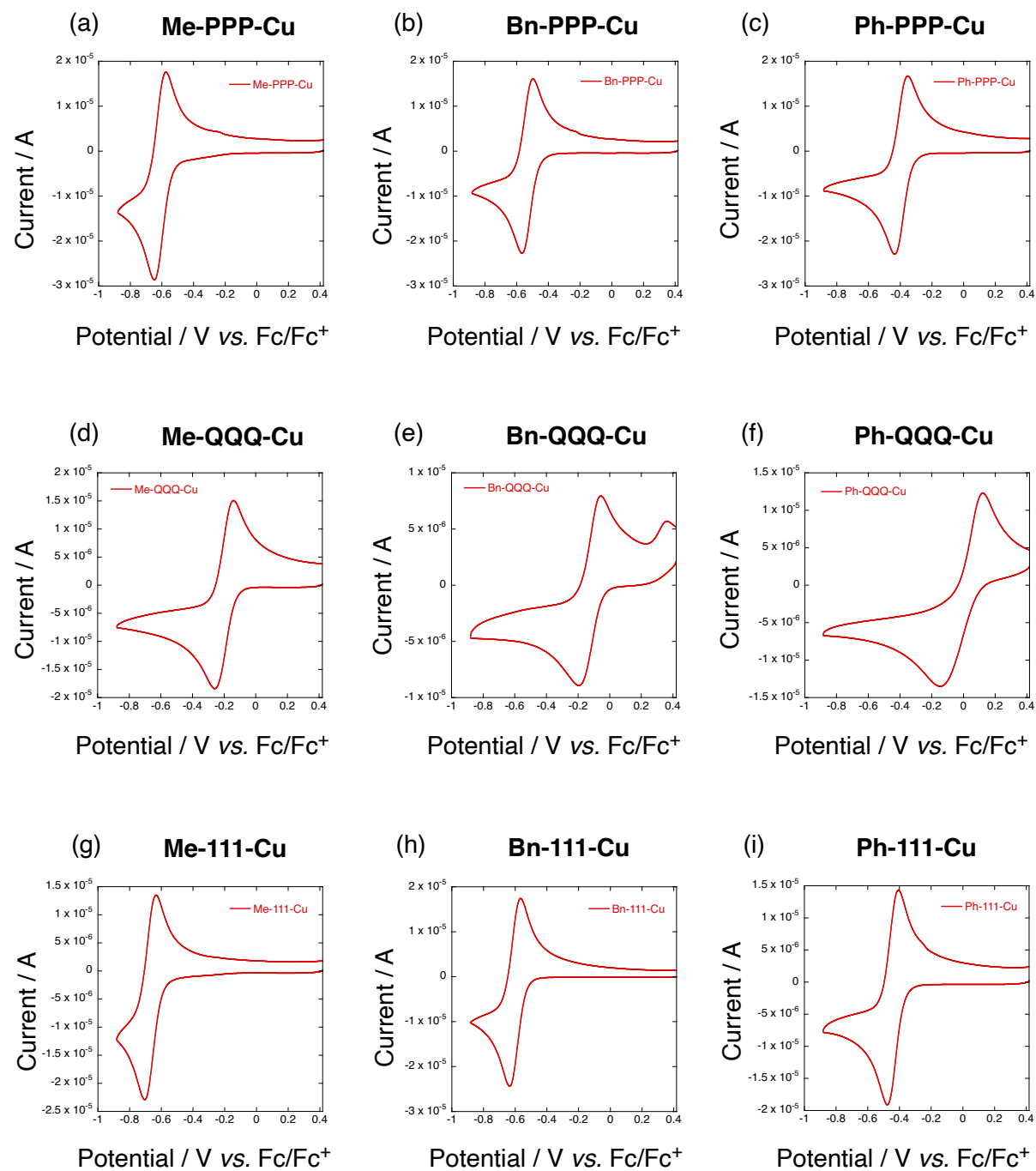


Fig. S2. Perspective view for **Ph-PPQ-Cu** complex in 50% probability. Non-coordinating counter anions, solvents and hydrogen atoms are omitted for clarity.

Cyclic voltammetry

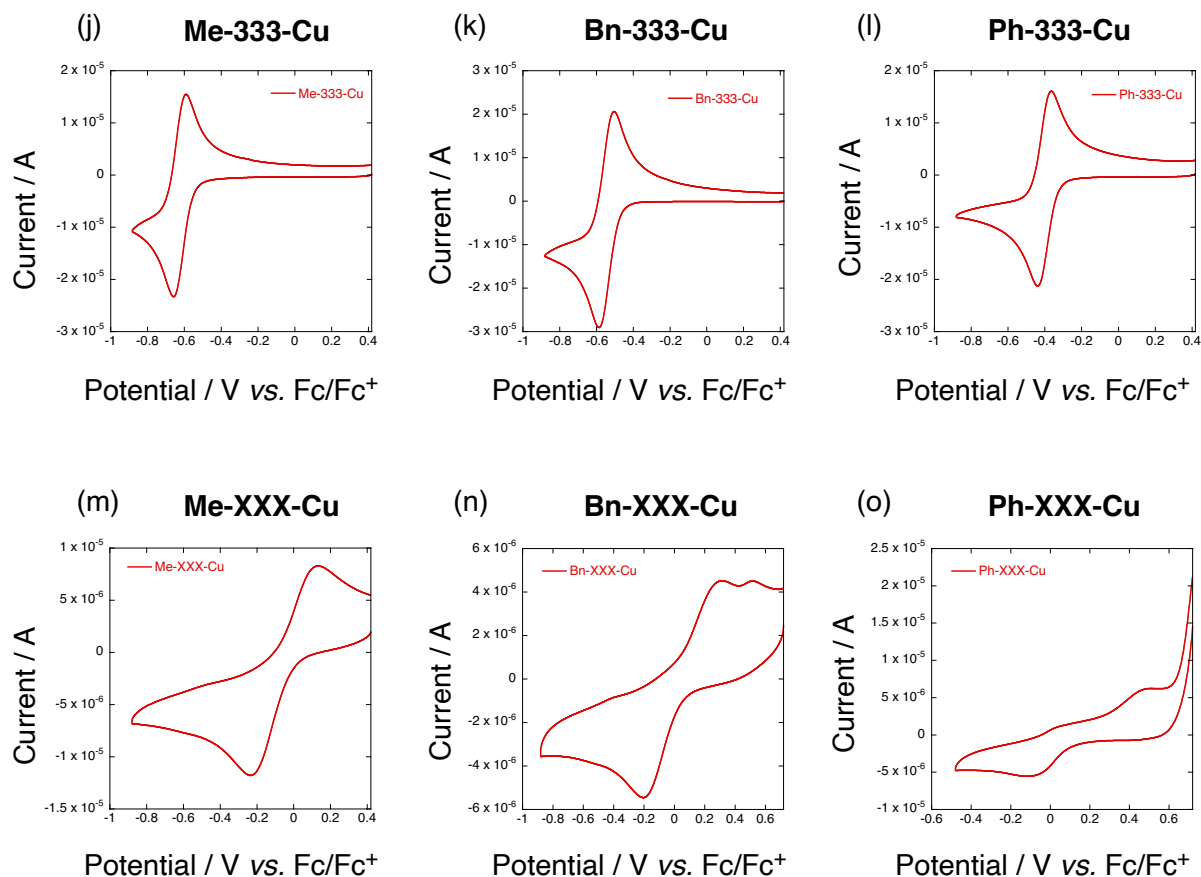


Fig. S3. Cyclic voltammogram of copper(II) complexes in acetonitrile (1 mM, scan rate 100 mV/s). (a) Me-PPP-Cu, (b) Bn-PPP-Cu, (c) Ph-PPP-Cu, (d) Me-QQQ-Cu, (e) Bn-QQQ-Cu, (f) Ph-QQQ-Cu, (g) Me-111-Cu, (h) Bn-111-Cu, (i) Ph-111-Cu, (j) Me-333-Cu, (k) Bn-333-Cu, (l) Ph-333-Cu, (m) Me-XXX-Cu, (n) Bn-XXX-Cu and (o) Ph-XXX-Cu.

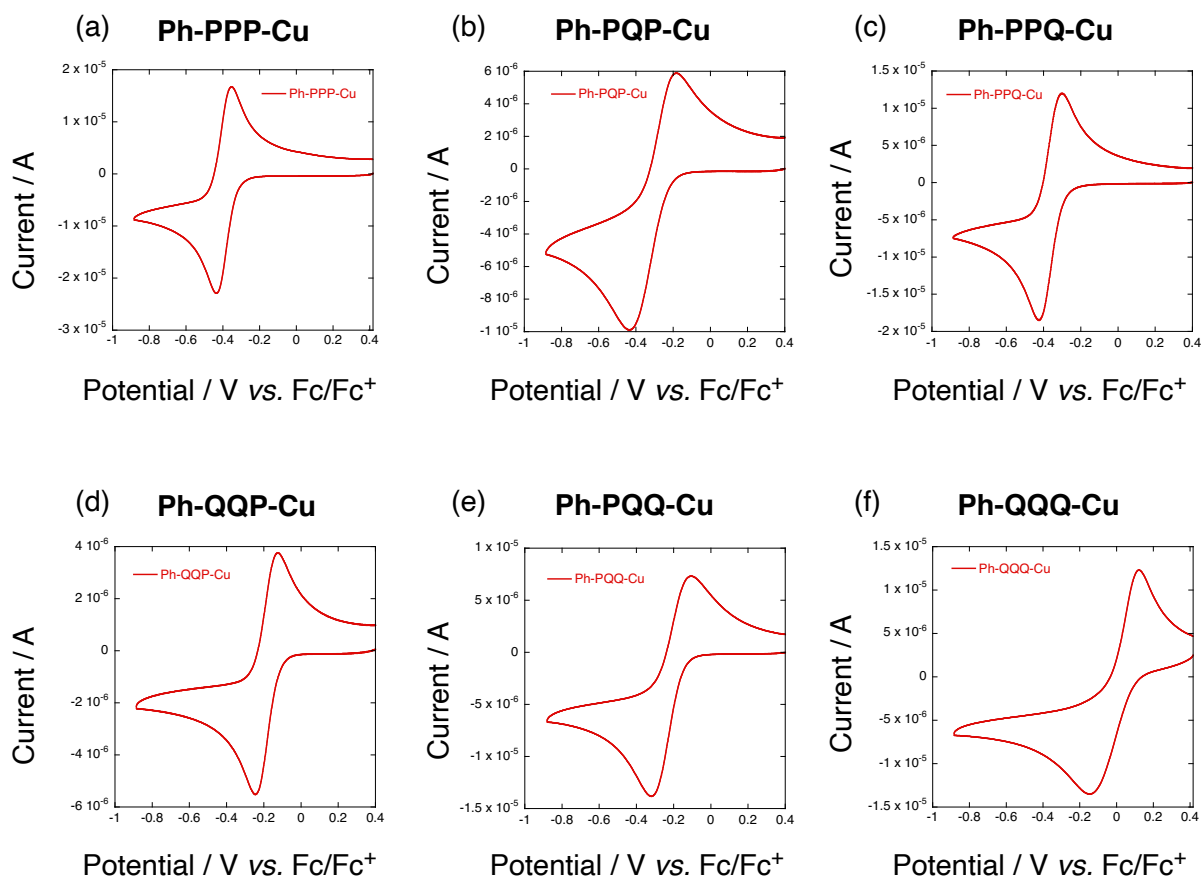


Fig. S4. Cyclic voltammogram of copper(II) complexes in acetonitrile (1 mM, scan rate 100 mV/s). (a) **Ph-PPP-Cu**, (b) **Ph-PQP-Cu**, (c) **Ph-PPQ-Cu**, (d) **Ph-QQP-Cu**, (e) **Ph-PQQ-Cu** and (f) **Ph-QQQ-Cu**.

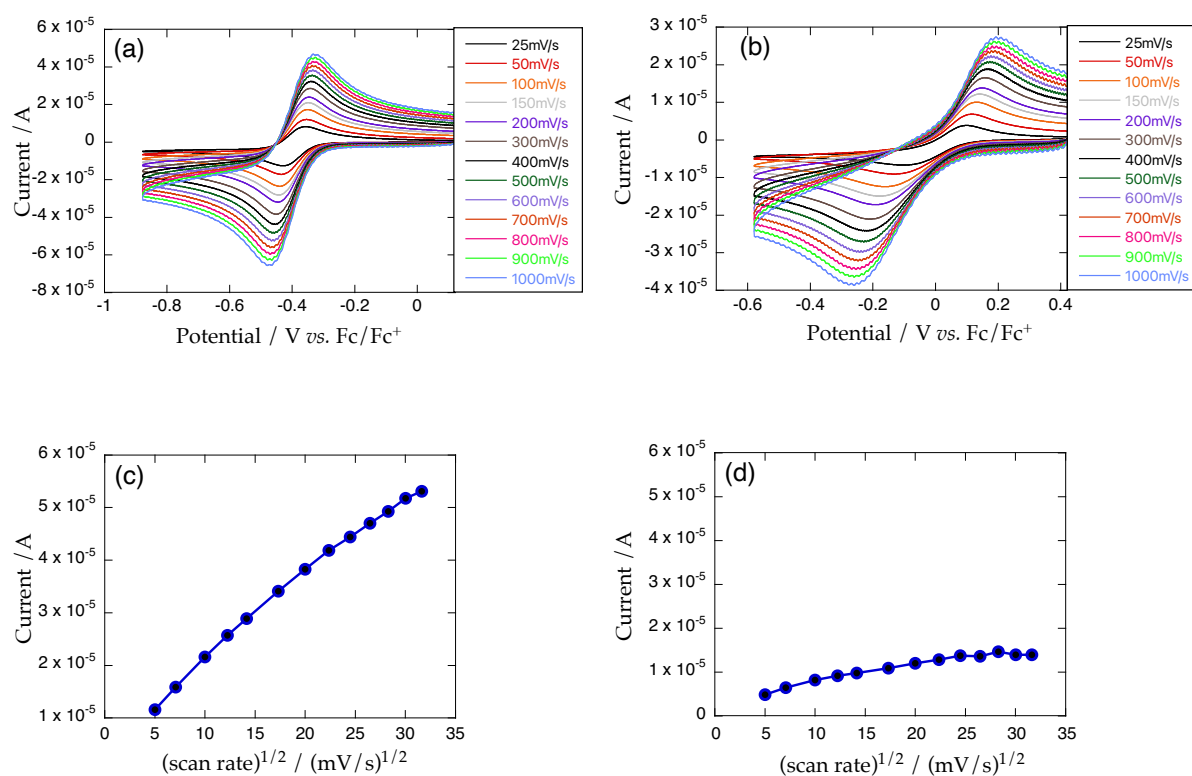
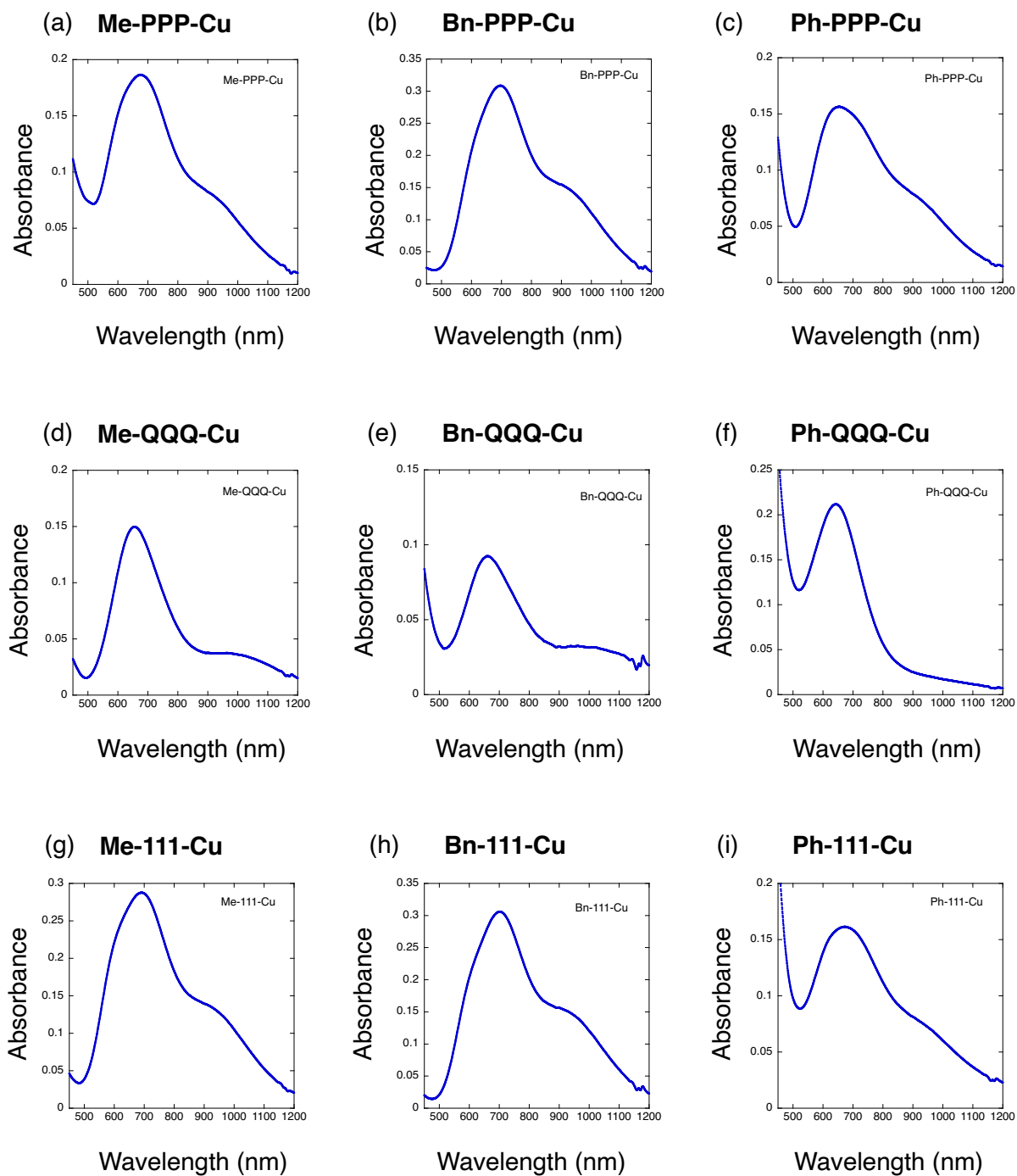


Fig. S5. Cyclic voltammogram of (a) **Ph-PPP-Cu** and (b) **Ph-QQQ-Cu** in acetonitrile at various scan rates (1 mM, scan rate 25-1000 mV/s) and plot for current *vs.* $(\text{scan rate})^{1/2}$ for (c) **Ph-PPP-Cu** and (d) **Ph-QQQ-Cu**.

Absorption spectrum

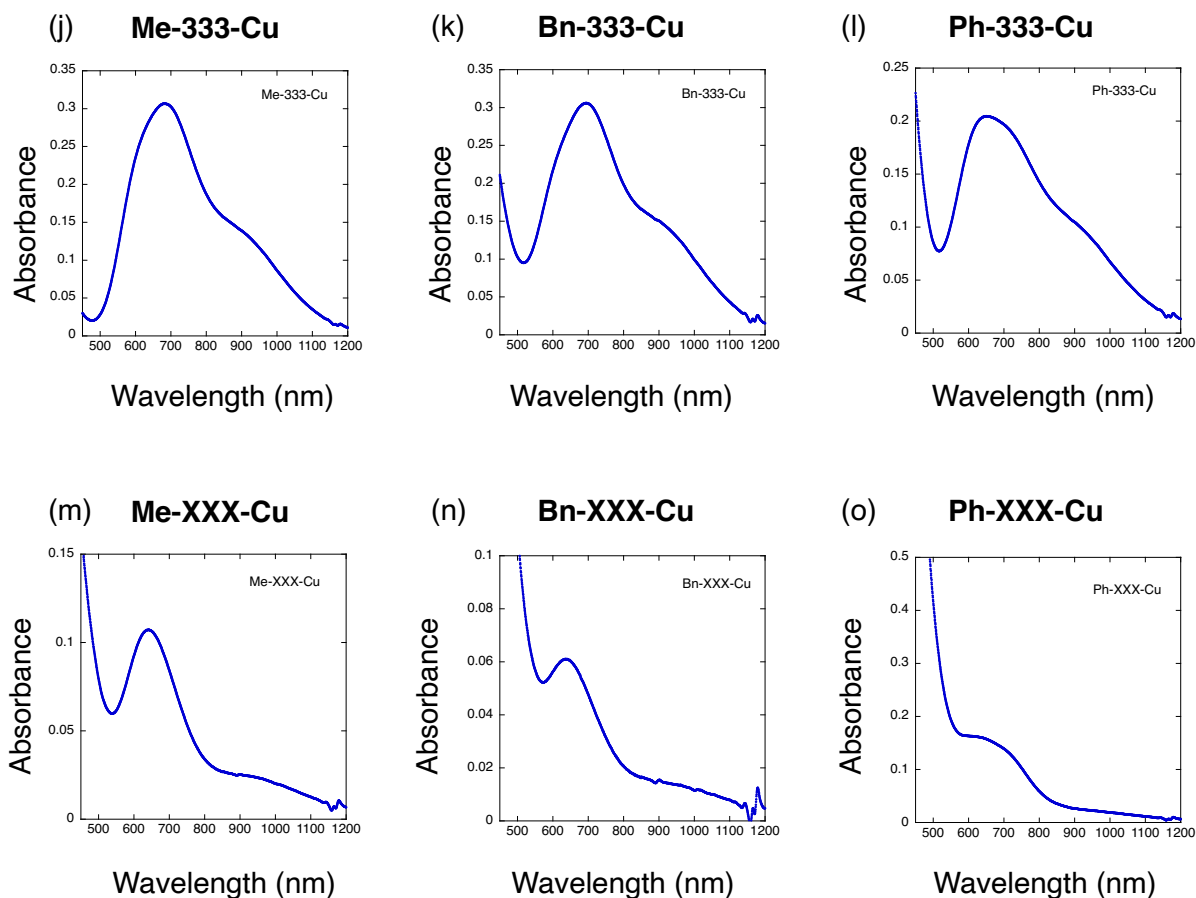


Fig. S6. Absorption spectrum of **R-ArArAr-Cu** in acetonitrile (1 mM). (a) **Me-PPP-Cu**, (b) **Bn-PPP-Cu**, (c) **Ph-PPP-Cu**, (d) **Me-QQQ-Cu**, (e) **Bn-QQQ-Cu**, (f) **Ph-QQQ-Cu**, (g) **Me-111-Cu**, (h) **Bn-111-Cu**, (i) **Ph-111-Cu**, (j) **Me-333-Cu**, (k) **Bn-333-Cu**, (l) **Ph-333-Cu**, (m) **Me-XXX-Cu**, (n) **Bn-XXX-Cu** and (o) **Ph-XXX-Cu**.

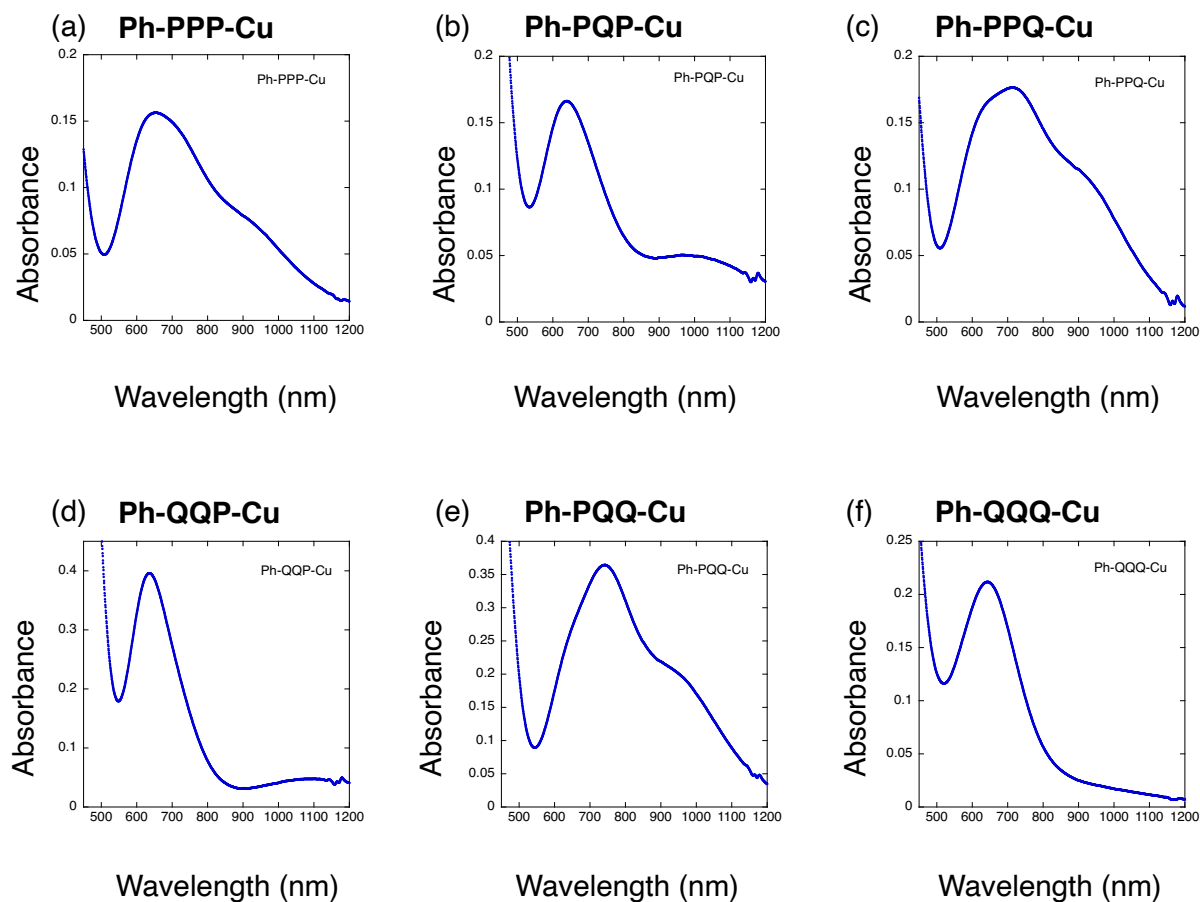
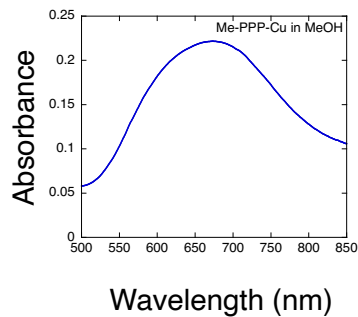
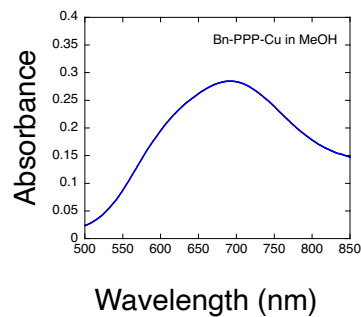
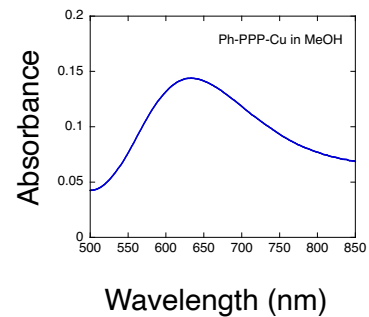
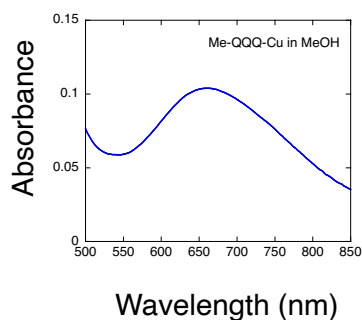
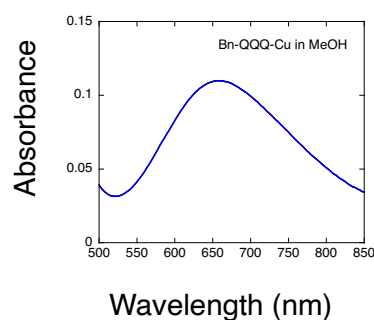
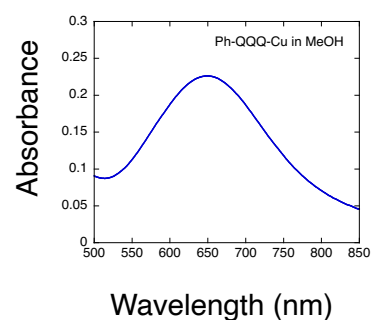
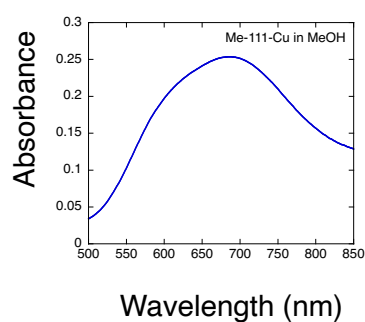
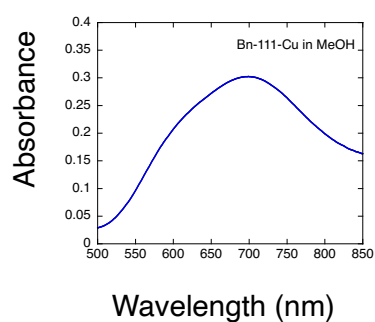
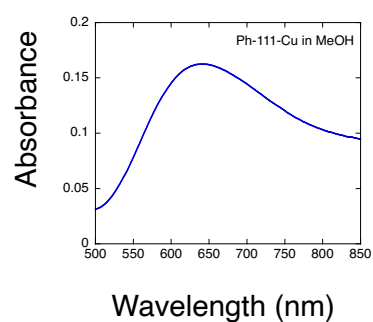


Fig. S7. Absorption spectrum of **Ph-Ar¹Ar²Ar³-Cu** in acetonitrile (1 mM). (a) **Ph-PPP-Cu**, (b) **Ph-PQP-Cu**, (c) **Ph-PPQ-Cu**, (d) **Ph-QQP-Cu**, (e) **Ph-PQQ-Cu** and (f) **Ph-QQQ-Cu**.

(a) **Me-PPP-Cu**(b) **Bn-PPP-Cu**(c) **Ph-PPP-Cu**(d) **Me-QQQ-Cu**(e) **Bn-QQQ-Cu**(f) **Ph-QQQ-Cu**(g) **Me-111-Cu**(h) **Bn-111-Cu**(i) **Ph-111-Cu**

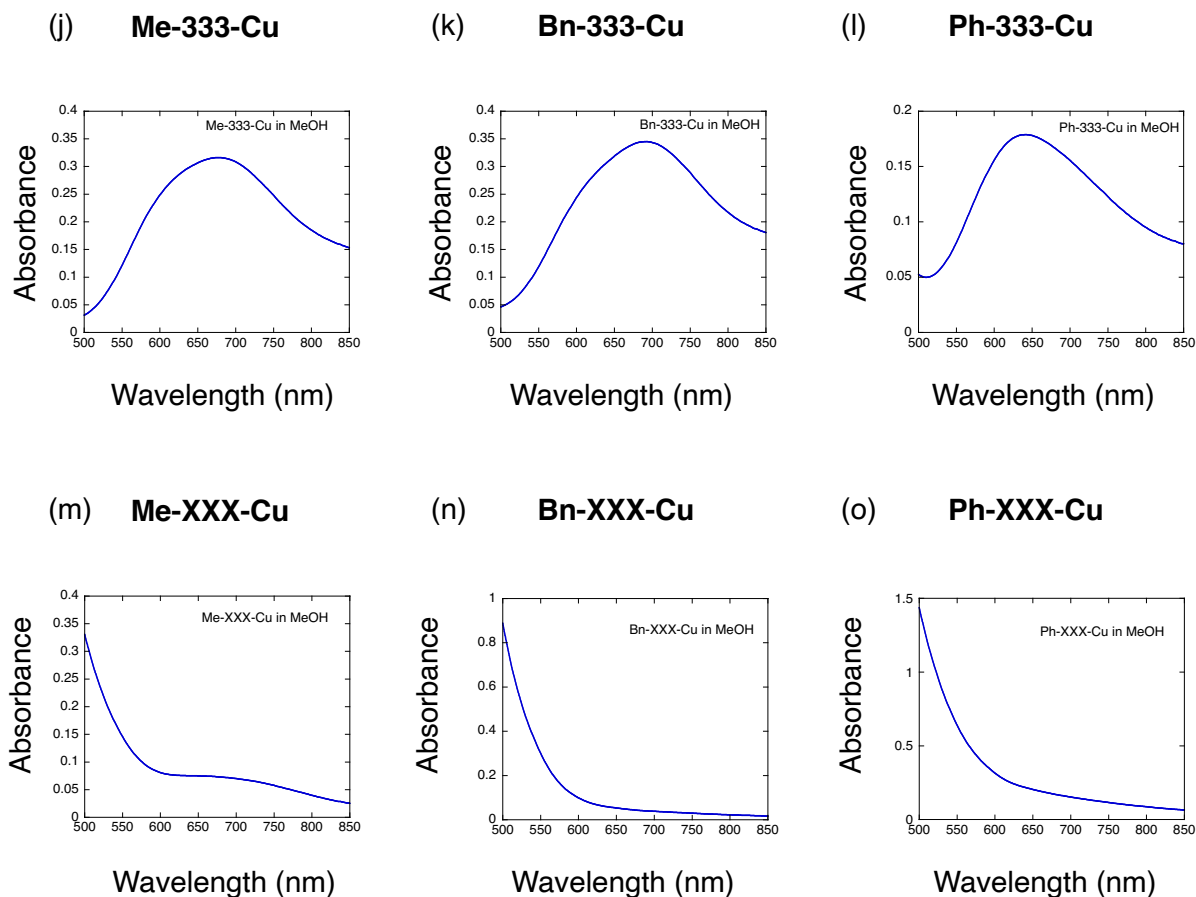


Fig. S8. Absorption spectrum of **R-ArArAr-Cu** in methanol (1 mM). (a) **Me-PPP-Cu**, (b) **Bn-PPP-Cu**, (c) **Ph-PPP-Cu**, (d) **Me-QQQ-Cu**, (e) **Bn-QQQ-Cu**, (f) **Ph-QQQ-Cu**, (g) **Me-111-Cu**, (h) **Bn-111-Cu**, (i) **Ph-111-Cu**, (j) **Me-333-Cu**, (k) **Bn-333-Cu**, (l) **Ph-333-Cu**, (m) **Me-XXX-Cu**, (n) **Bn-XXX-Cu** and (o) **Ph-XXX-Cu**.

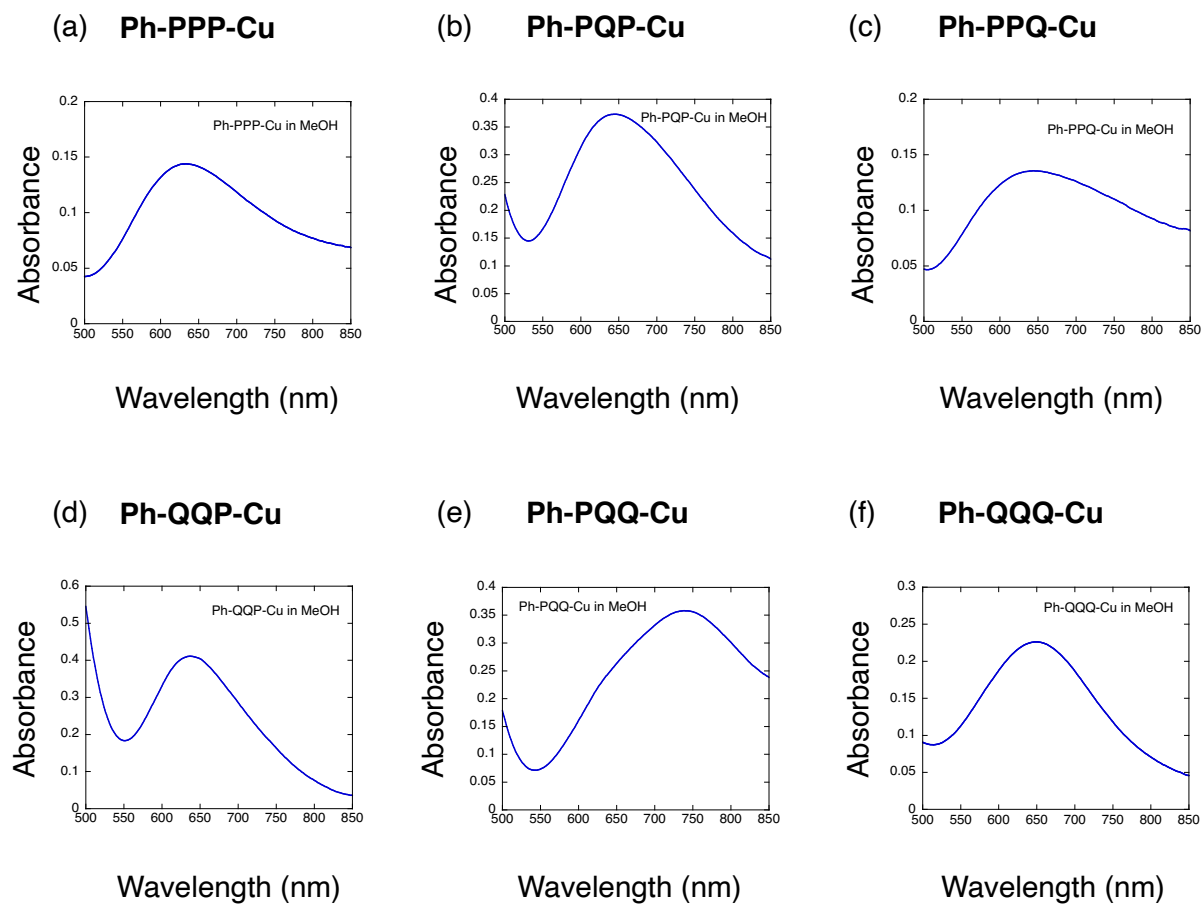


Fig. S9. Absorption spectrum of **Ph-Ar¹Ar²Ar³-Cu** in methanol (1 mM). (a) **Ph-PPP-Cu**, (b) **Ph-PQP-Cu**, (c) **Ph-PPQ-Cu**, (d) **Ph-QQP-Cu**, (e) **Ph-PQQ-Cu** and (f) **Ph-QQQ-Cu**.

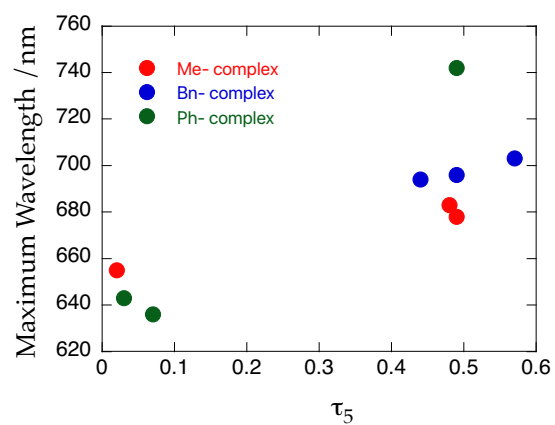
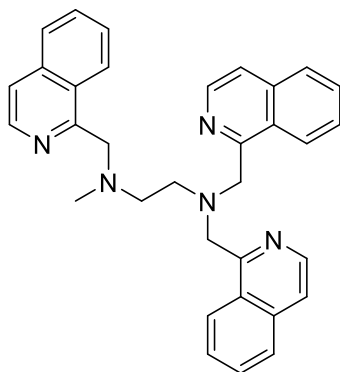
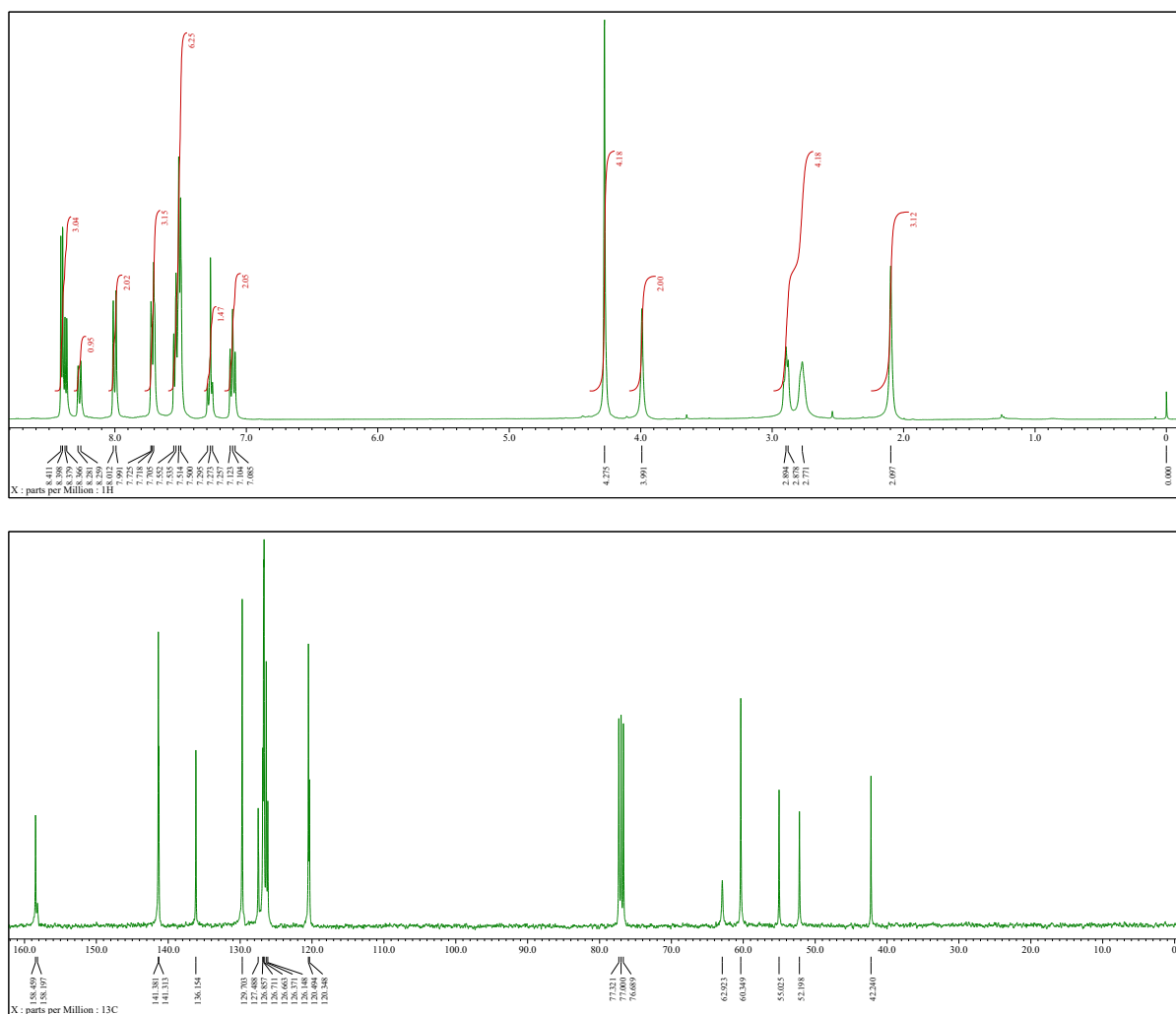
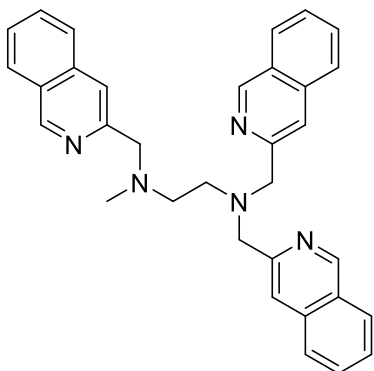
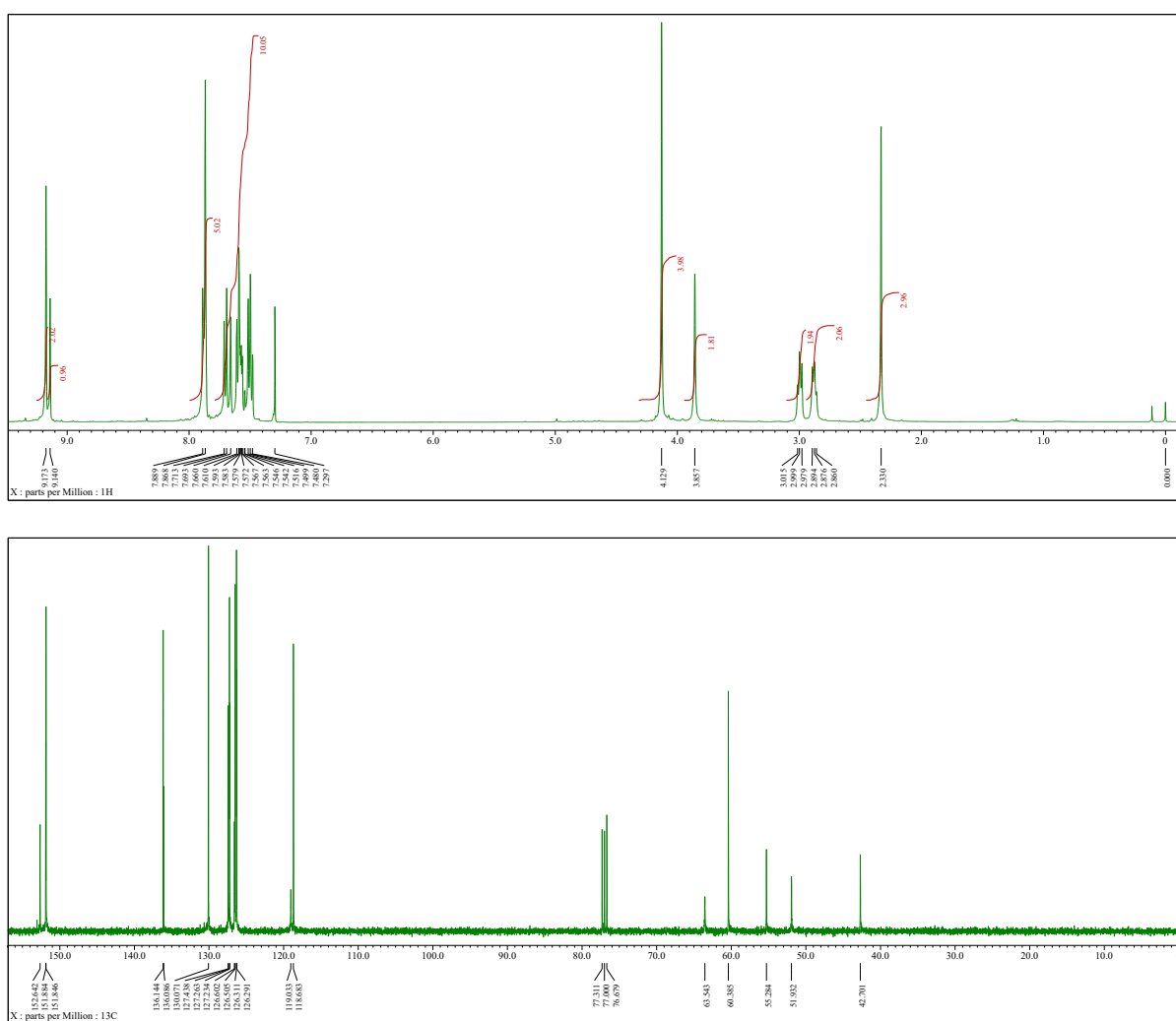


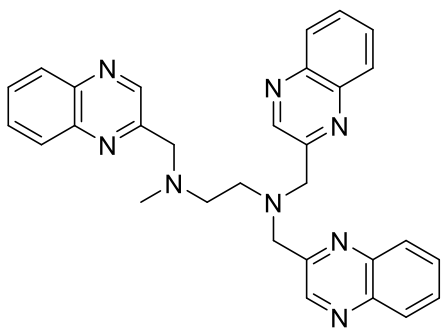
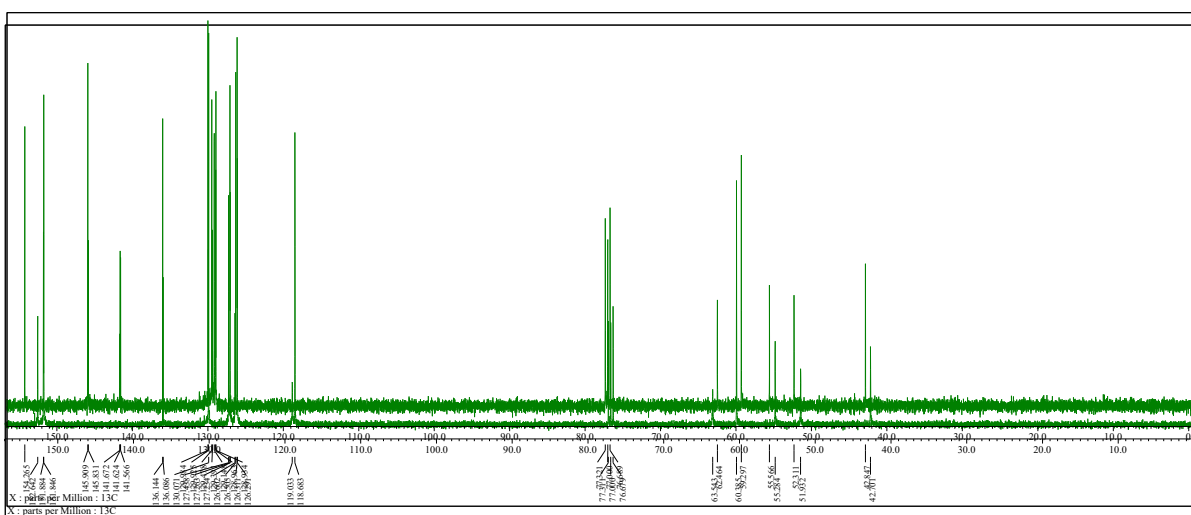
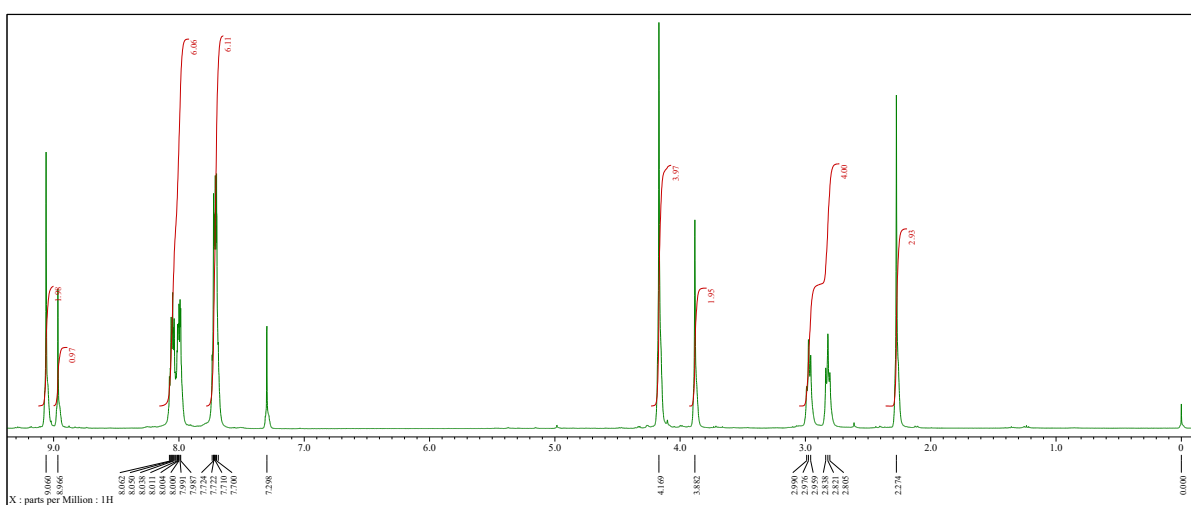
Fig. S10. Plot for absorption maxima of copper complexes measured in acetonitrile against the τ_5 values derived from X-ray crystallography shown in Fig. 2 and 3. The data for **Ph-PPP-Cu** (octahedral geometry) and **Ph-PPQ-Cu** (two geometries with largely different τ_5 values) were not included.

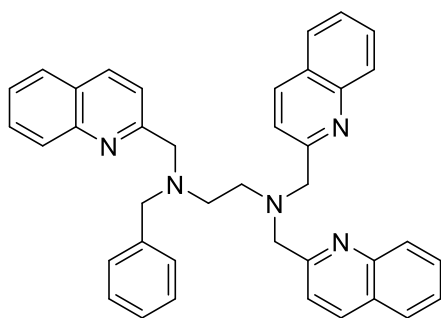
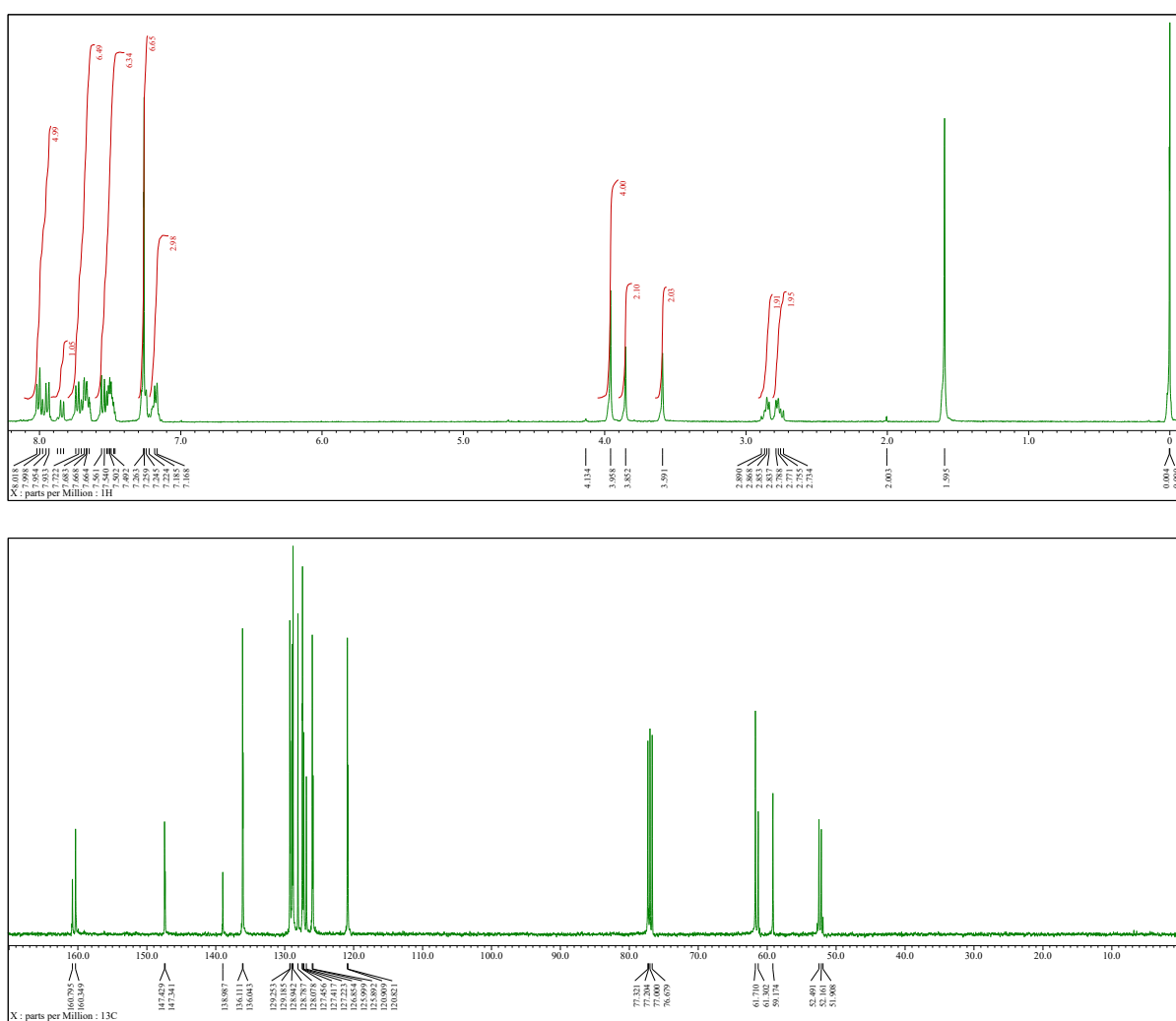
$^1\text{H}/^{13}\text{C}$ NMR spectrum

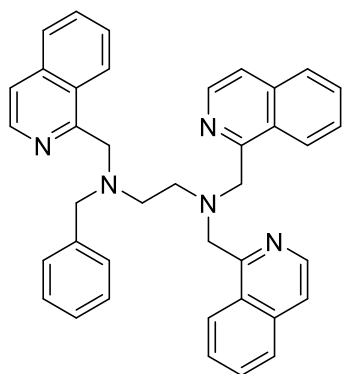
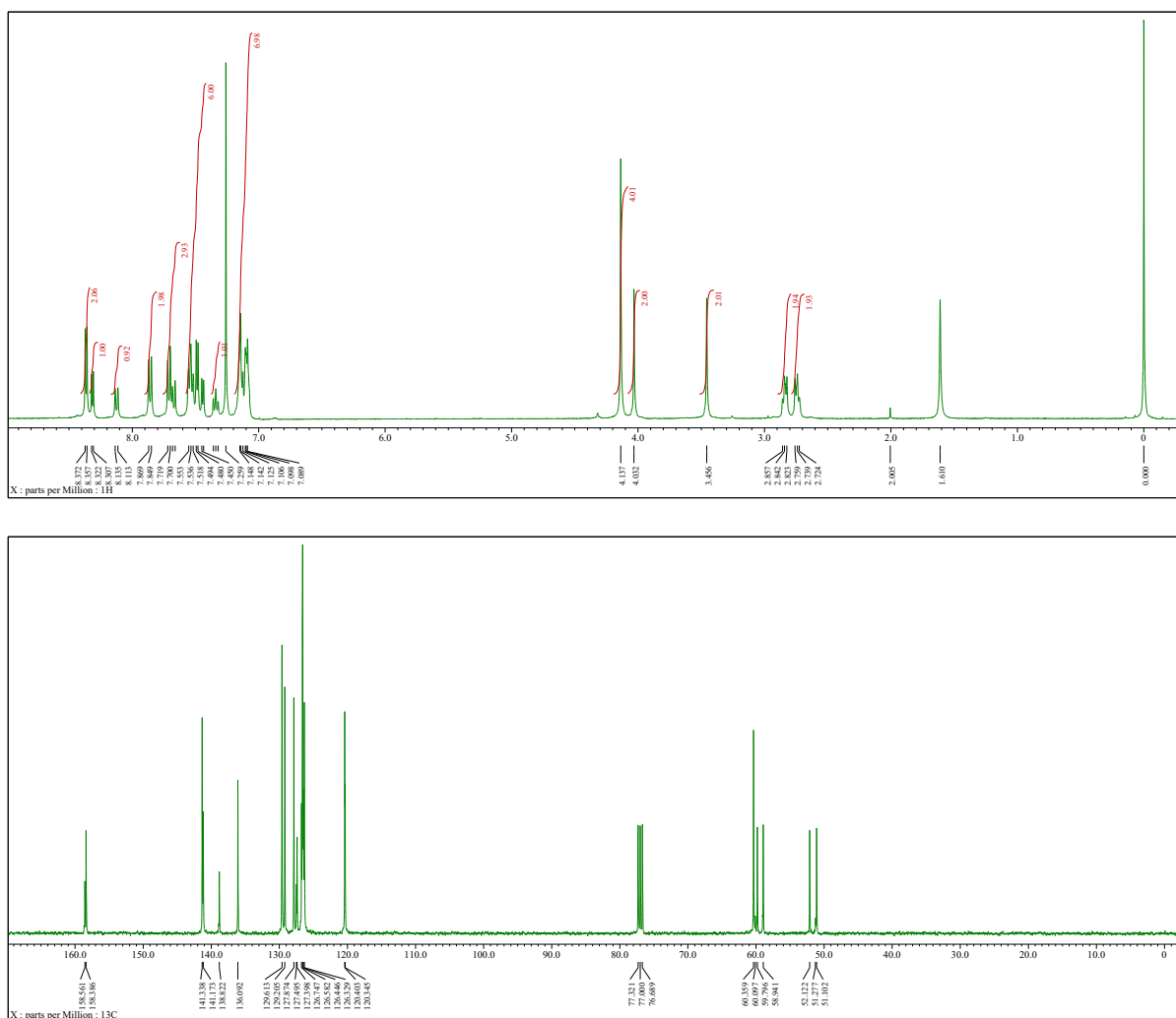
Me-111

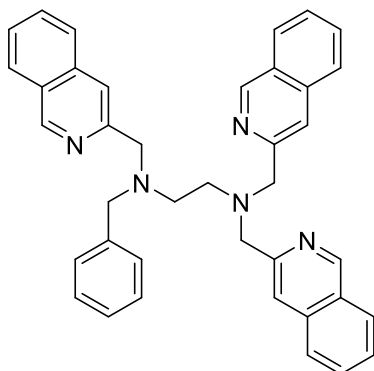
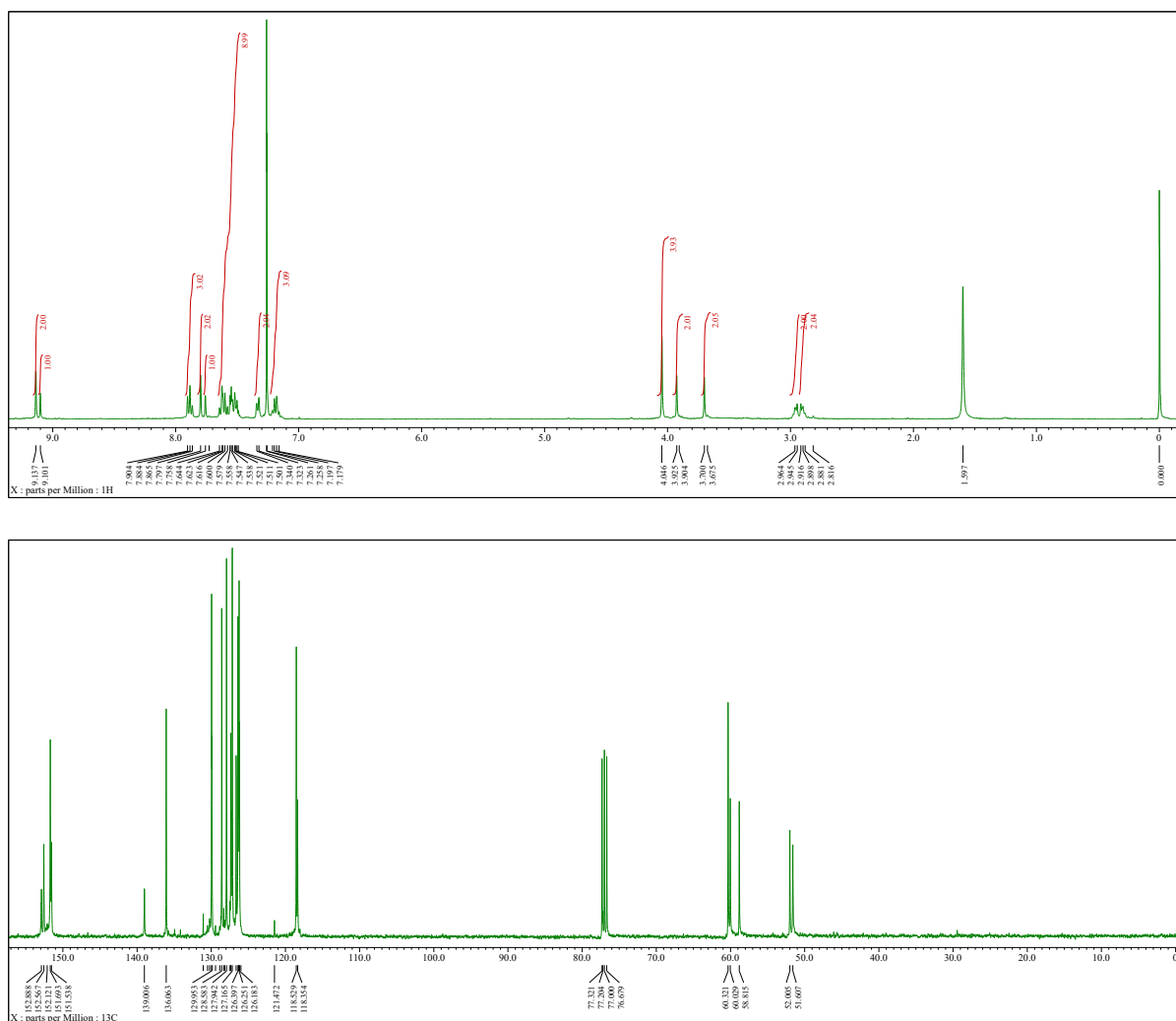
Fig. S11. $^1\text{H}/^{13}\text{C}$ NMR spectrum of Me-111 in CDCl_3 .

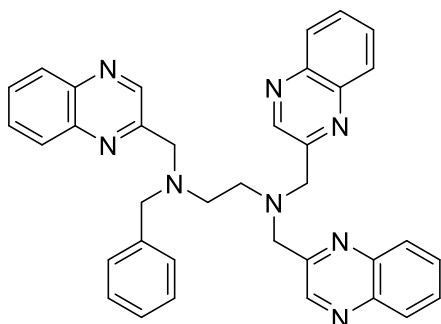
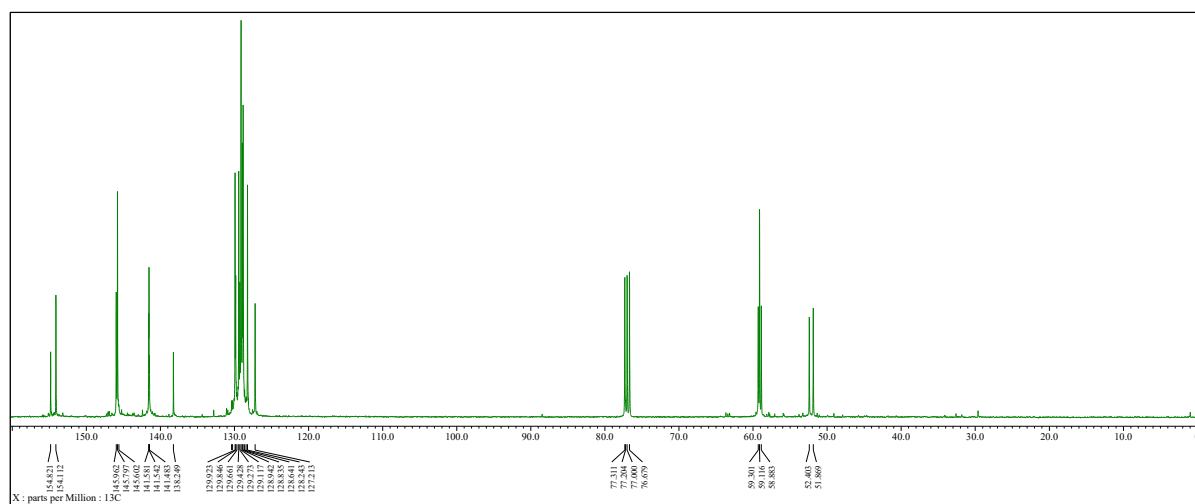
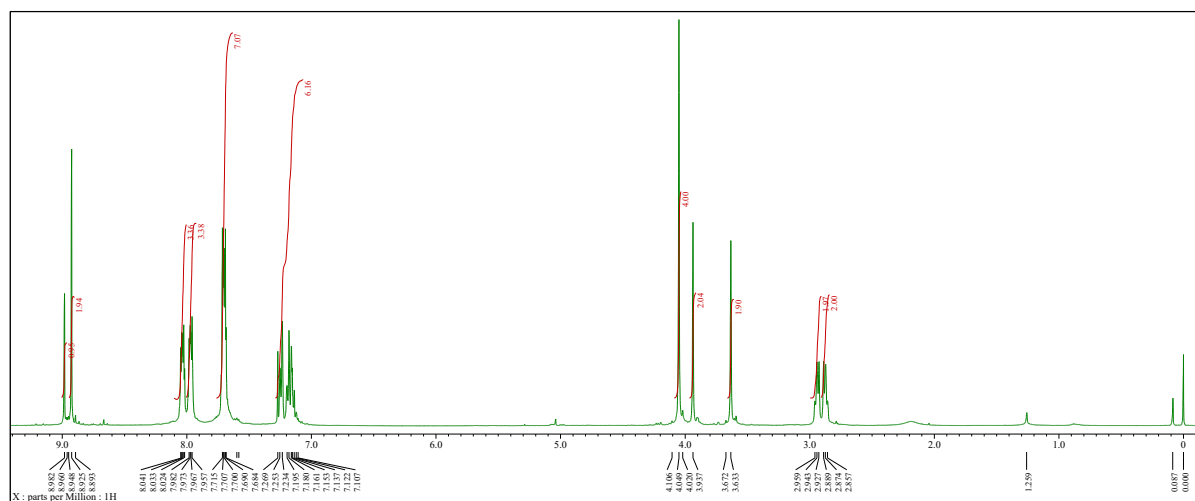
**Me-333****Fig. S12.** $^1\text{H}/^{13}\text{C}$ NMR spectrum of Me-333 in CDCl_3 .

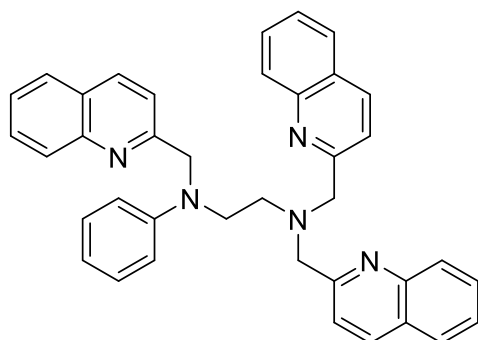
**Me-XXX****Fig. S13.** $^1\text{H}/^{13}\text{C}$ NMR spectrum of Me-XXX in CDCl_3 .

**Bn-QQQ**

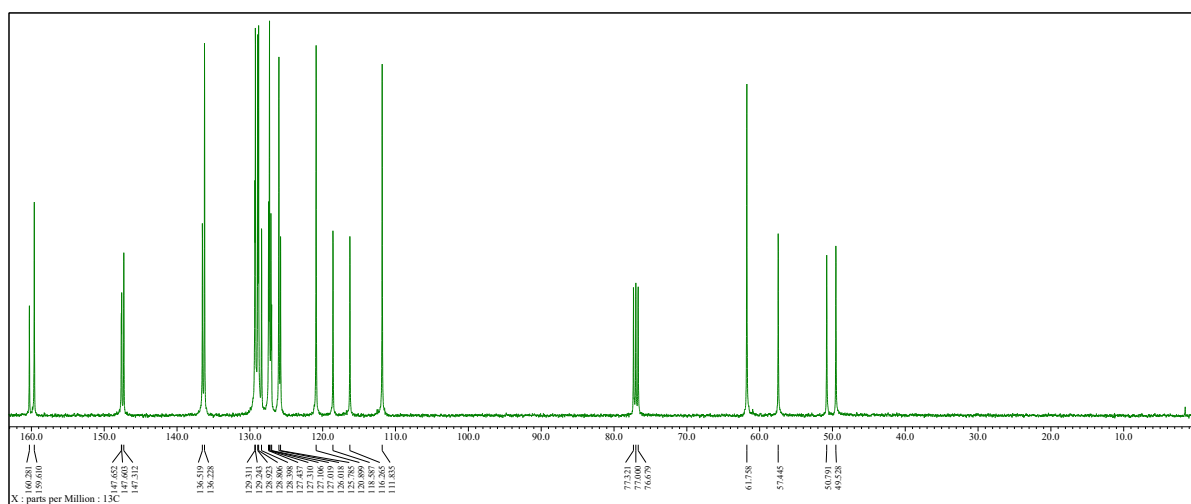
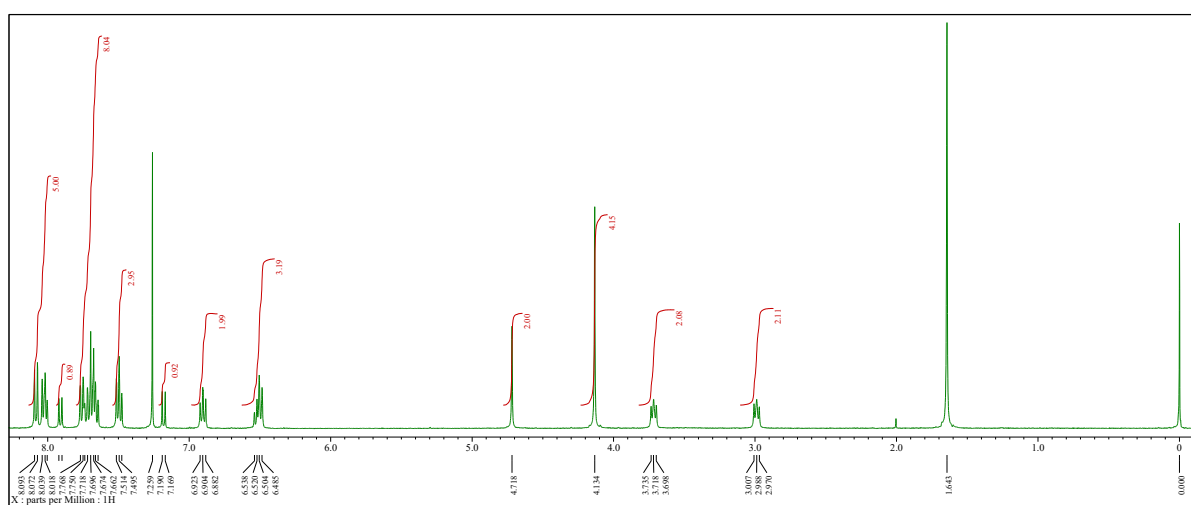
**Bn-111****Fig. S15.** $^1\text{H}/^{13}\text{C}$ NMR spectrum of **Bn-111** in CDCl_3 .

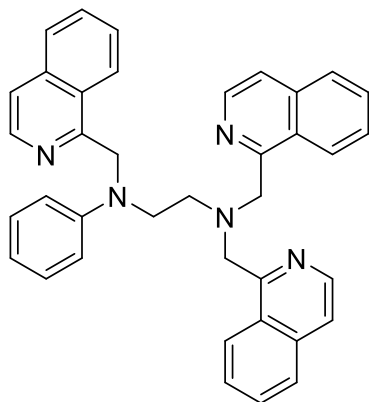
**Bn-333****Fig. S16.** $^1\text{H}/^{13}\text{C}$ NMR spectrum of **Bn-333** in CDCl_3 .

**Bn-XXX****Fig. S17.** $^1\text{H}/^{13}\text{C}$ NMR spectrum of **Bn-XXX** in CDCl_3 .

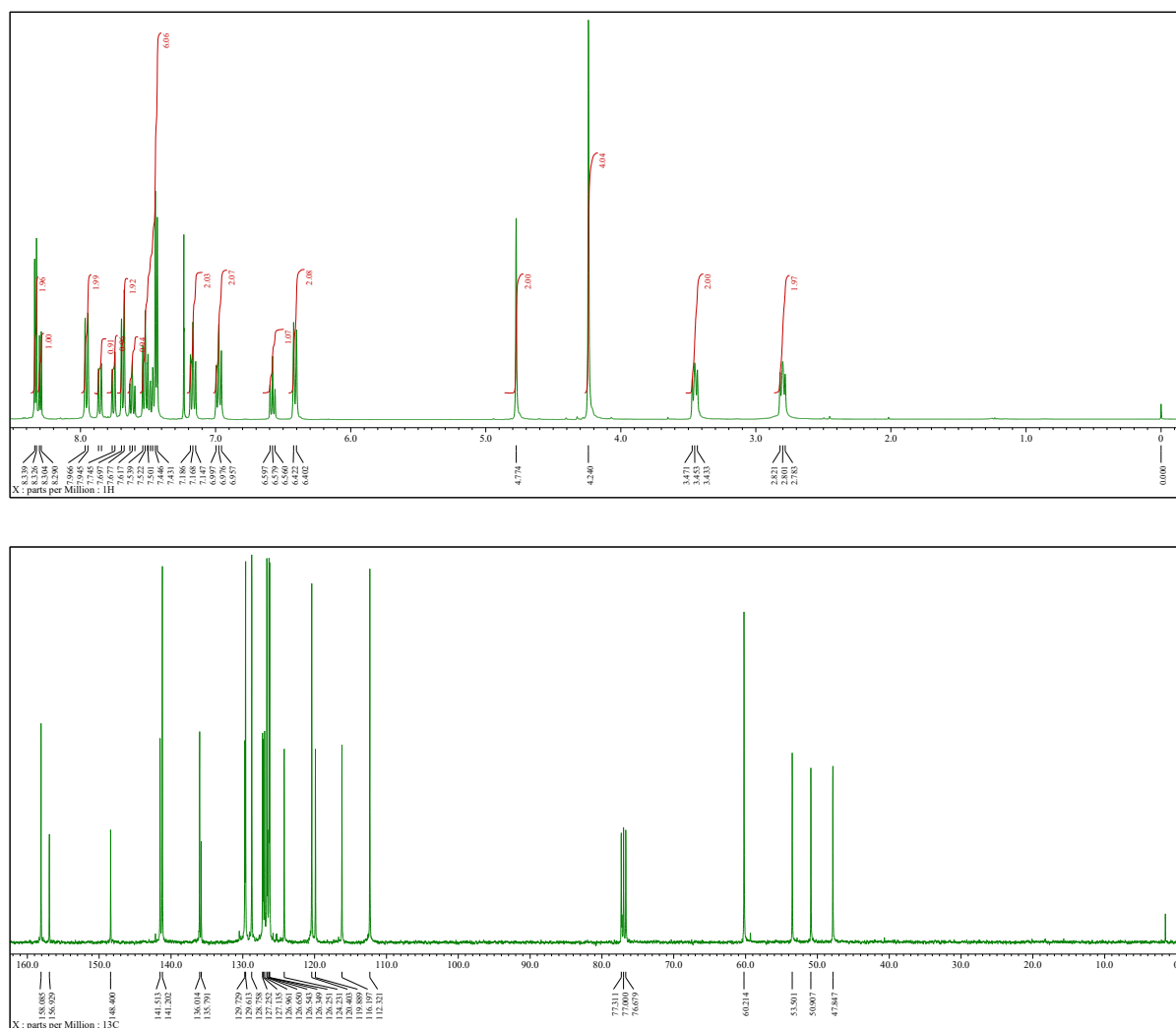


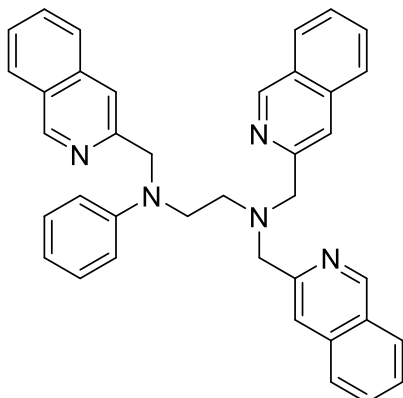
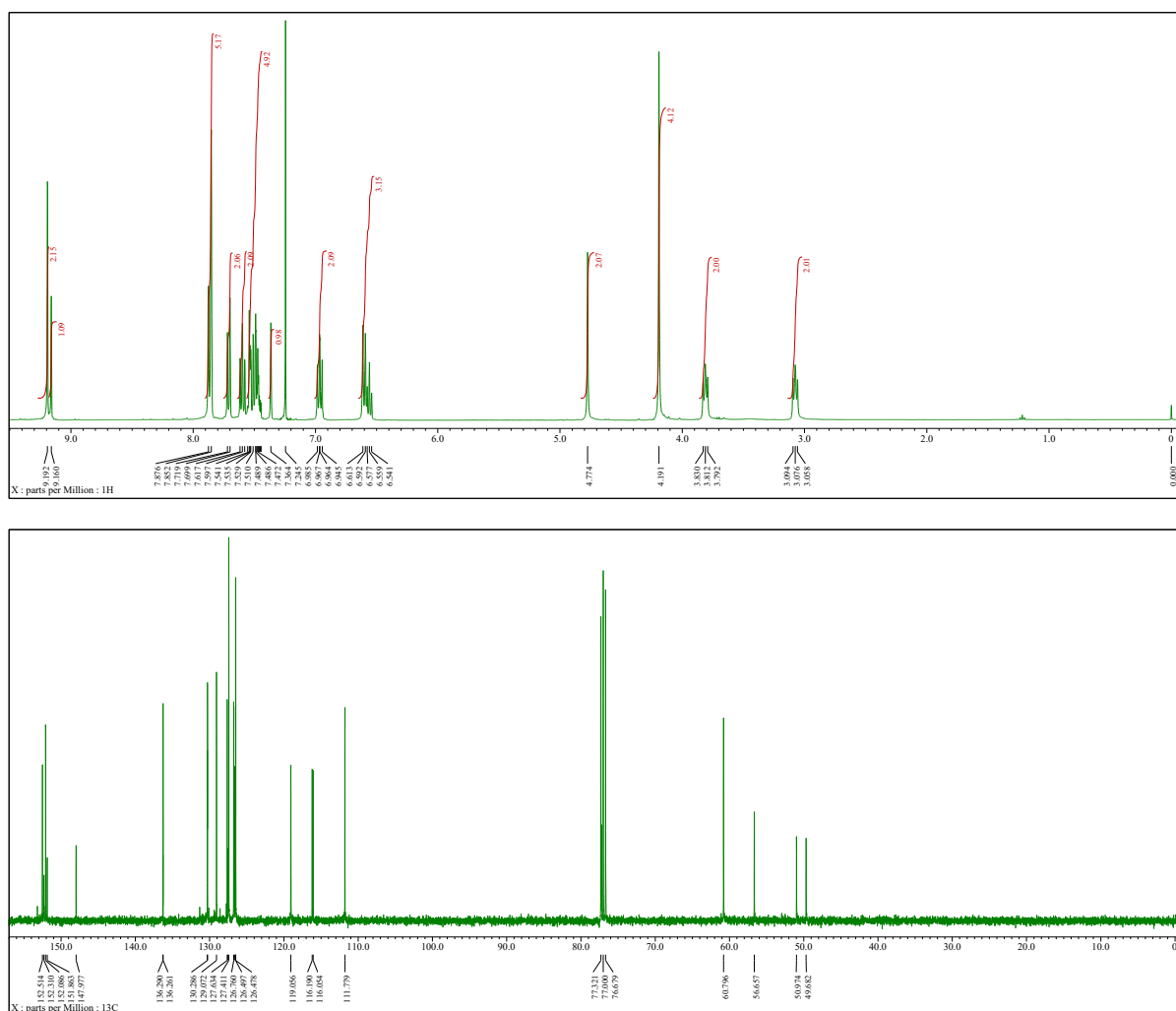
Ph-QQQ

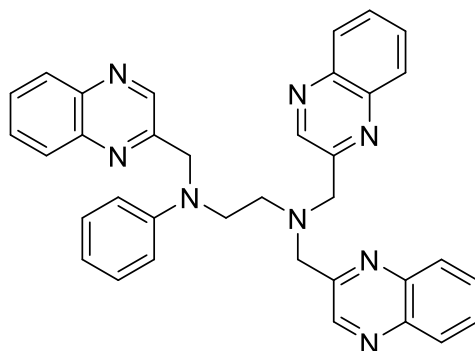
Fig. S18. $^1\text{H}/^{13}\text{C}$ NMR spectrum of Ph-QQQ in CDCl_3 .



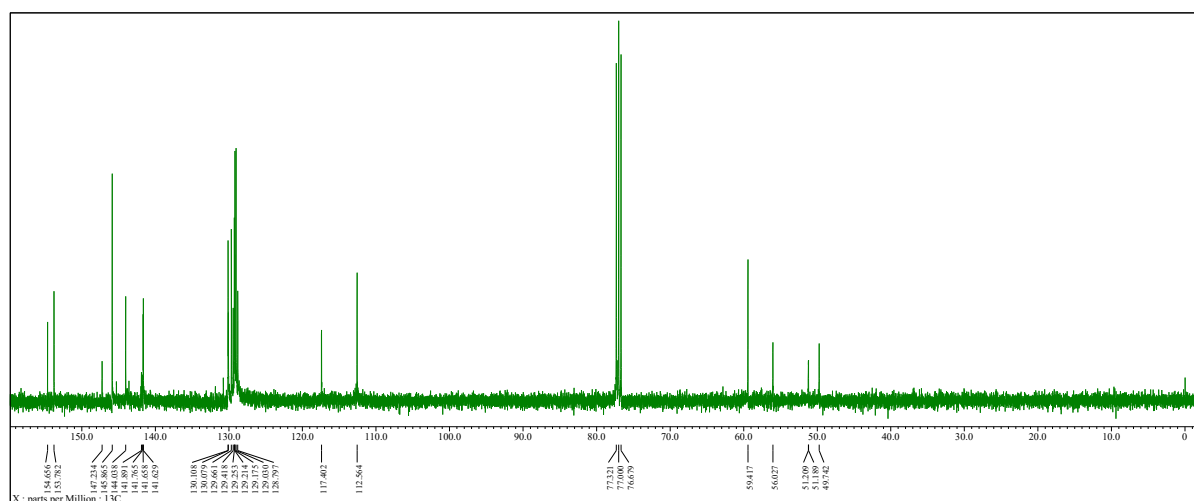
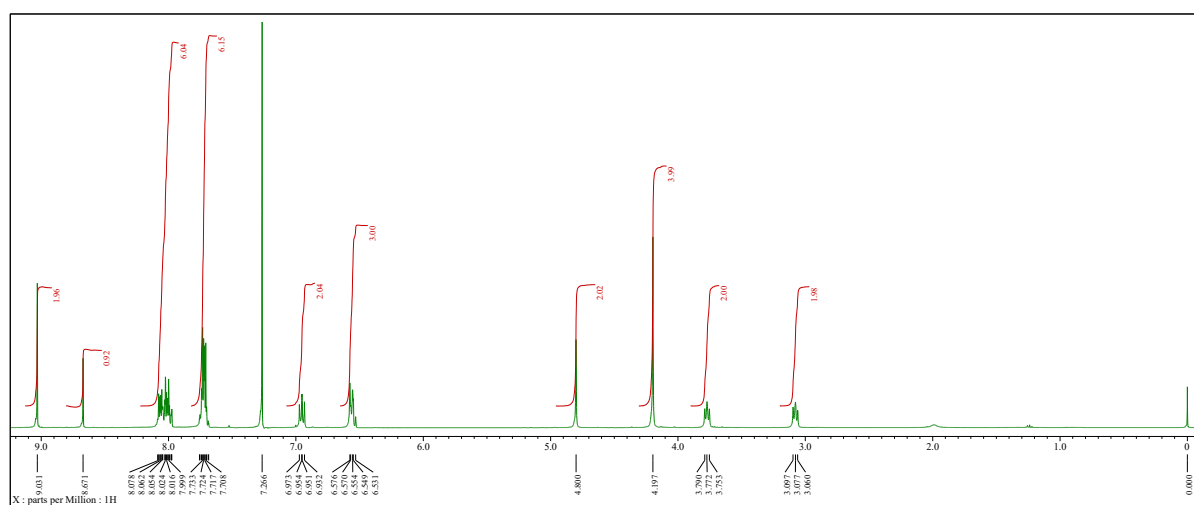
Ph-111

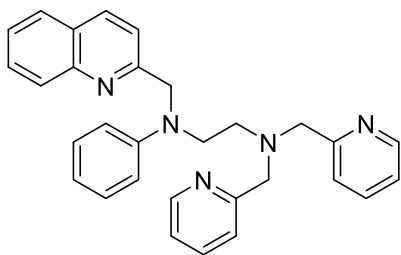
Fig. S19. ¹H/¹³C NMR spectrum of Ph-111 in CDCl₃.

**Ph-333****Fig. S20.** ¹H/¹³C NMR spectrum of Ph-333 in CDCl₃.

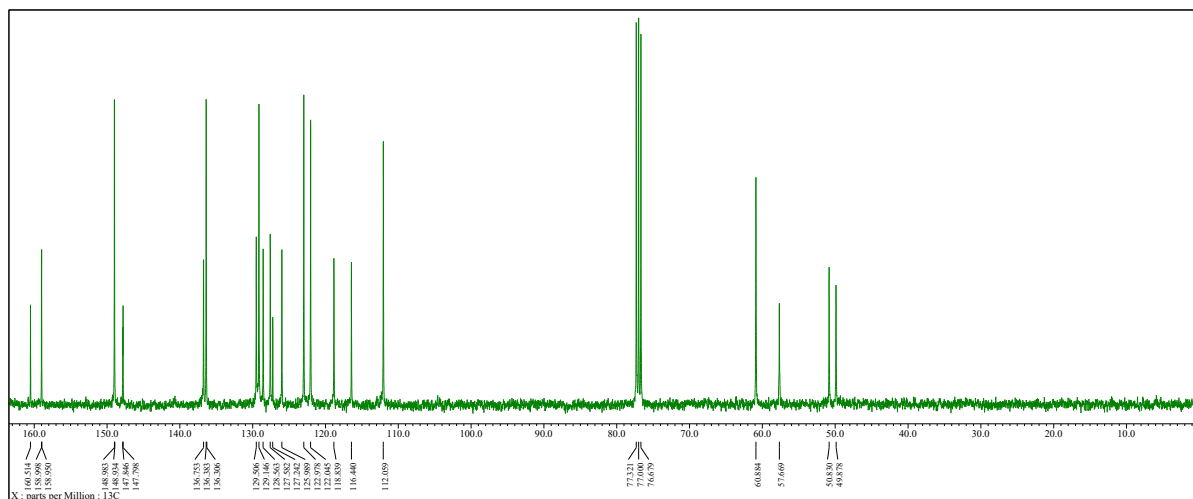
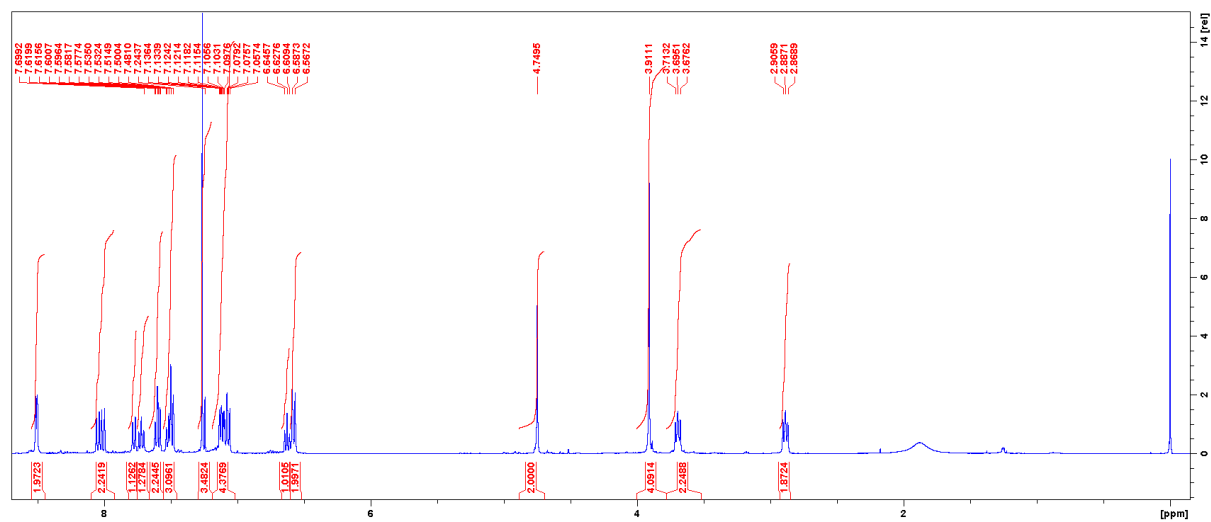


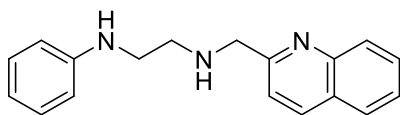
Ph-XXX

Fig. S21. $^1\text{H}/^{13}\text{C}$ NMR spectrum of Ph-XXX in CDCl_3 .



Ph-PPQ

Fig. S23. ¹H/¹³C NMR spectrum of Ph-PPQ in CDCl₃.



N-(2-quinolylmethyl)-*N'*-phenylethylenediamine

Ph-QHH

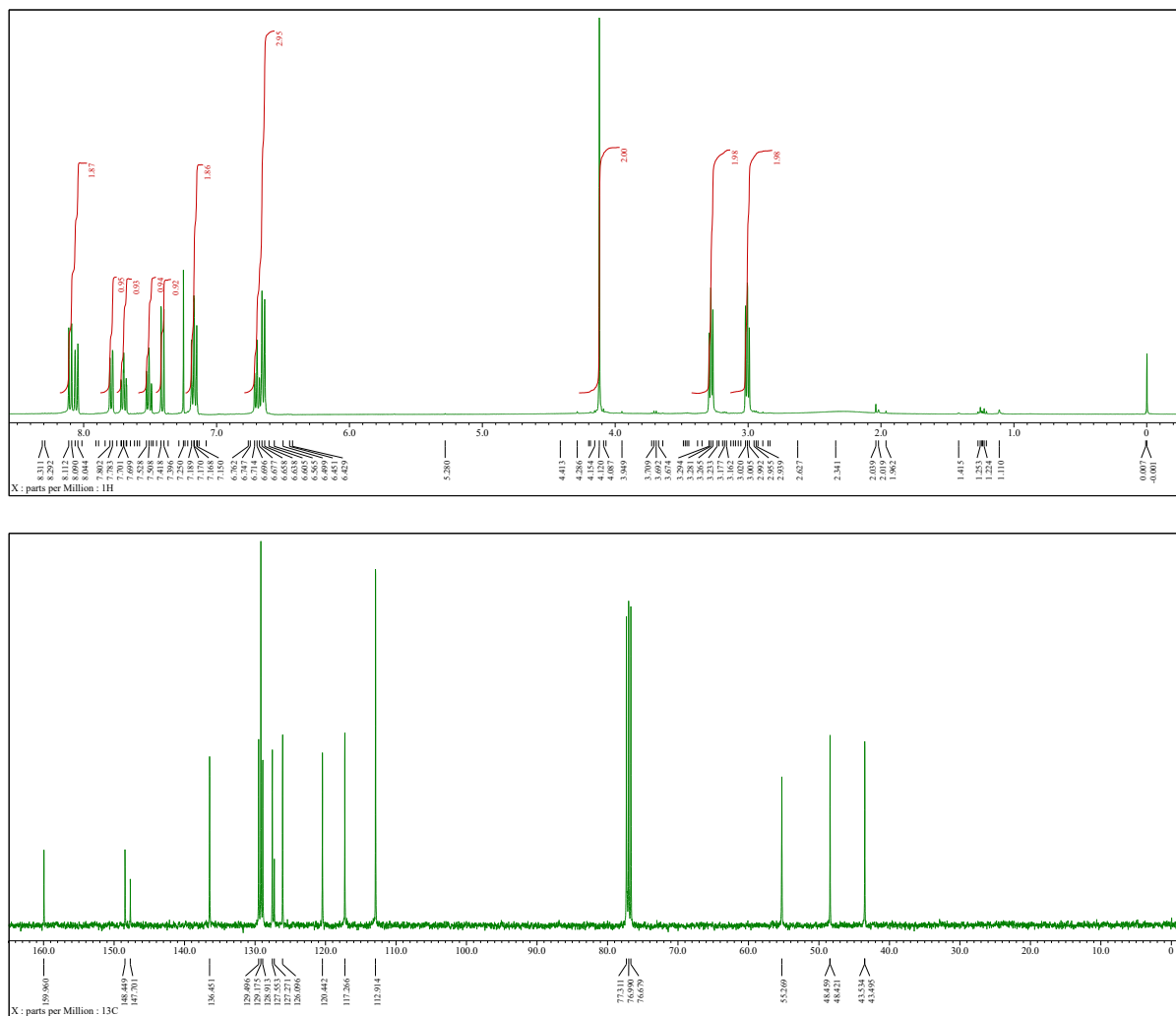
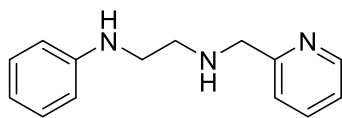


Fig. S24. $^1\text{H}/^{13}\text{C}$ NMR spectrum of **Ph-QHH** in CDCl_3 .



N-(2-pyridylmethyl)-*N'*-phenylethylenediamine

Ph-PHH

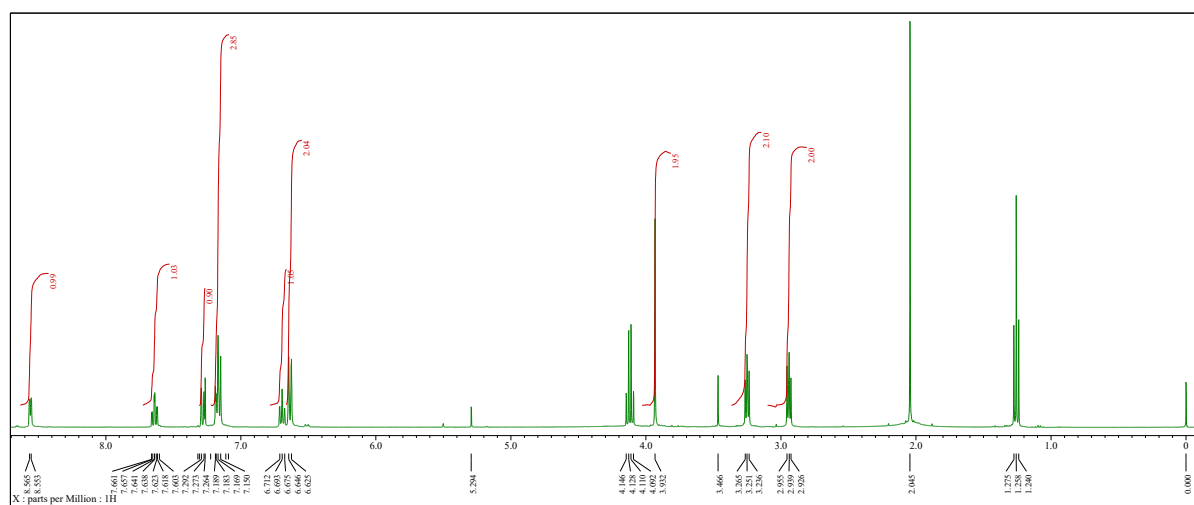
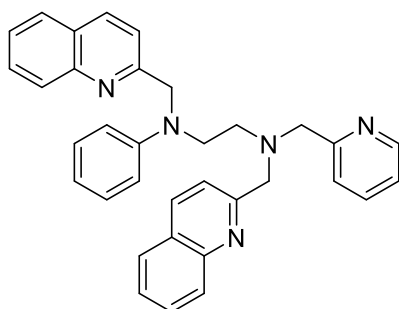
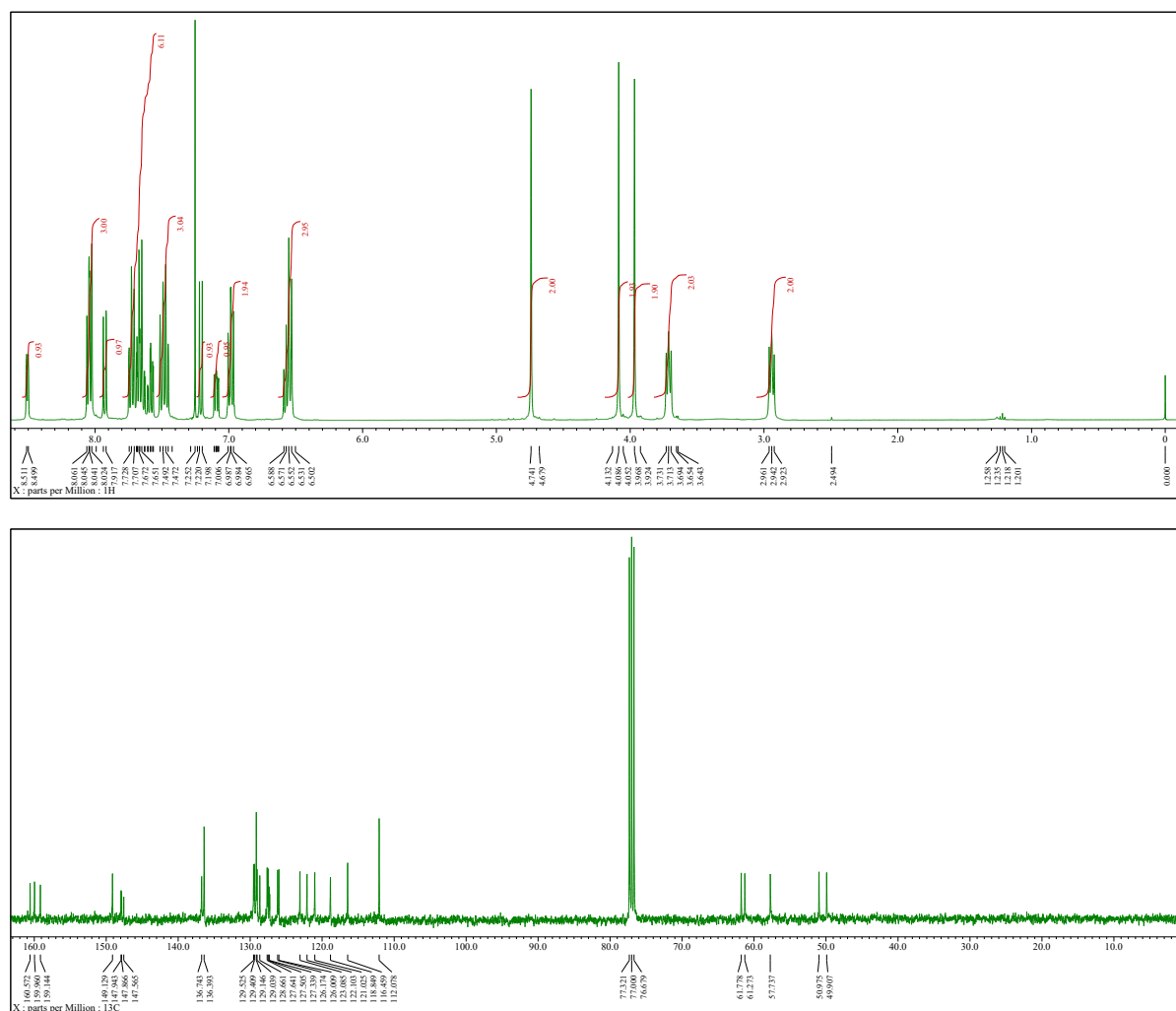
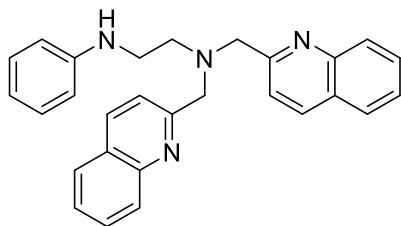


Fig. S26. ¹H NMR spectrum of **Ph-PHH** in CDCl₃.



Ph-PQQ

Fig. S27. $^1\text{H}/^{13}\text{C}$ NMR spectrum of Ph-PQQ in CDCl_3 .



N,N-Bis(2-quinolylmethyl)-*N'*-phenylethylenediamine

Ph-QQH

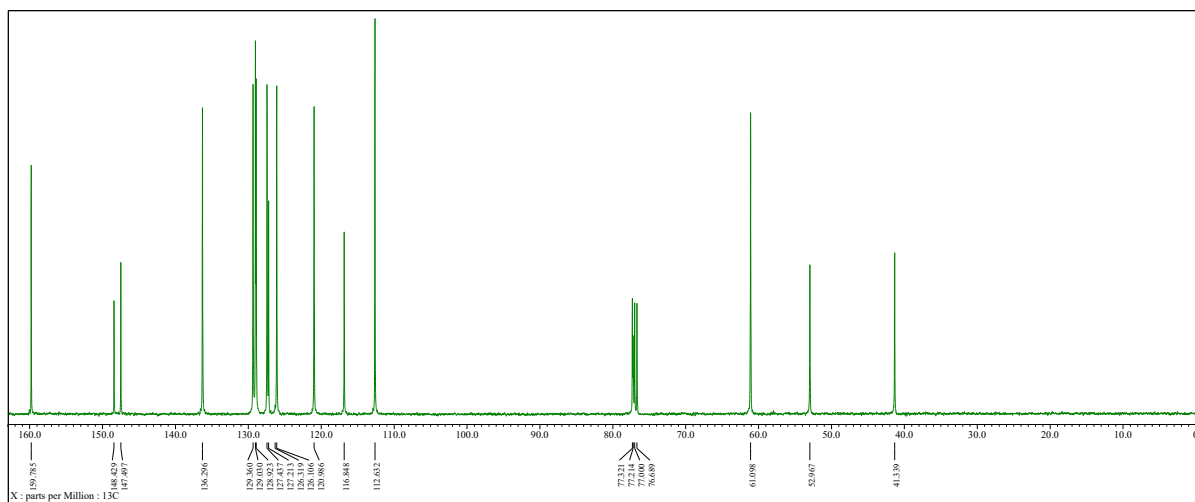
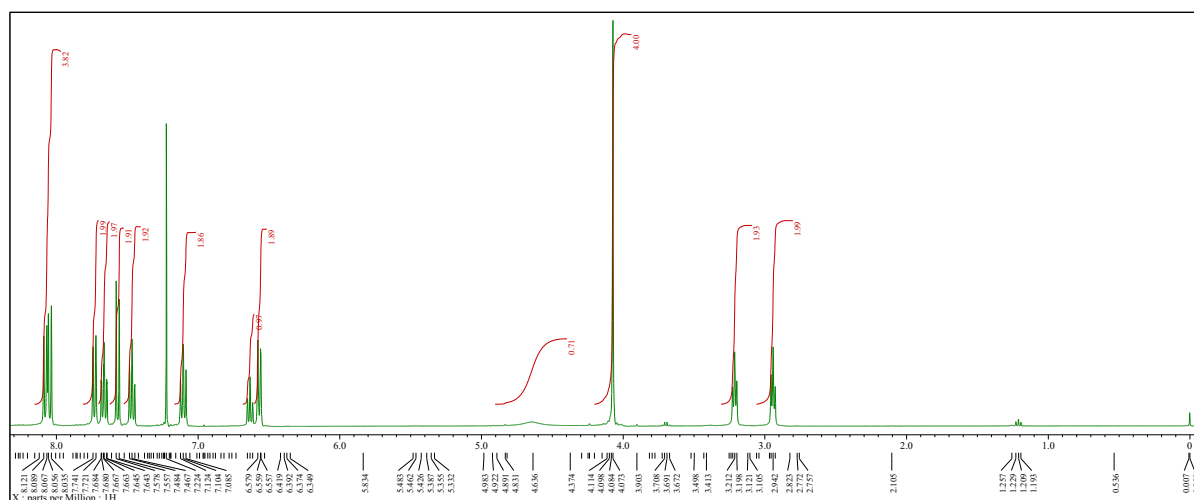
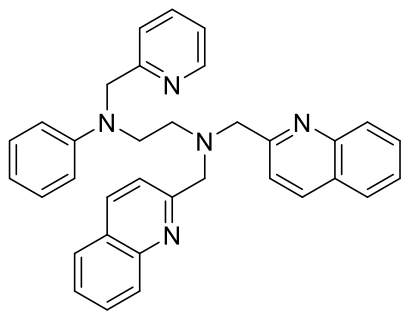
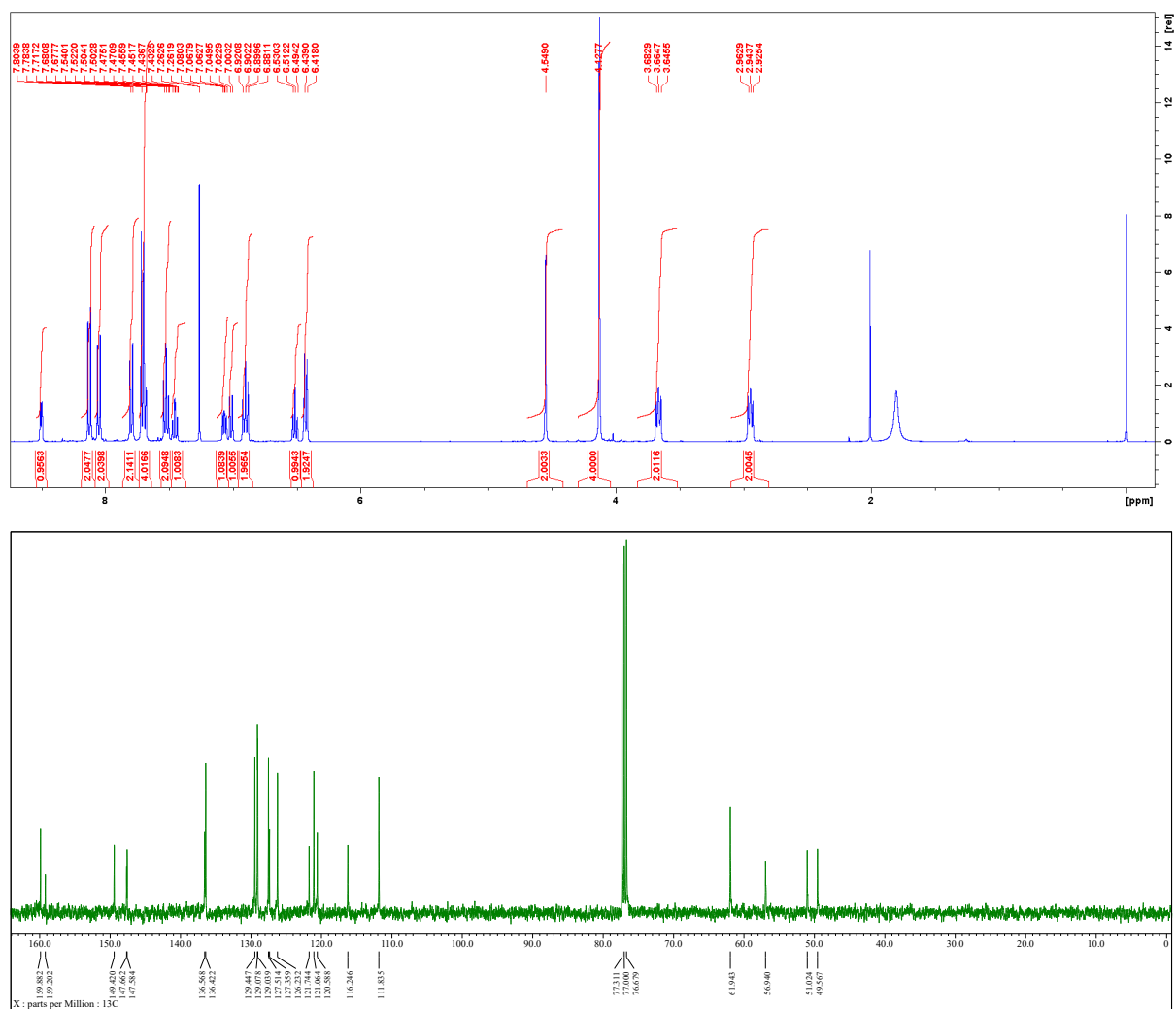


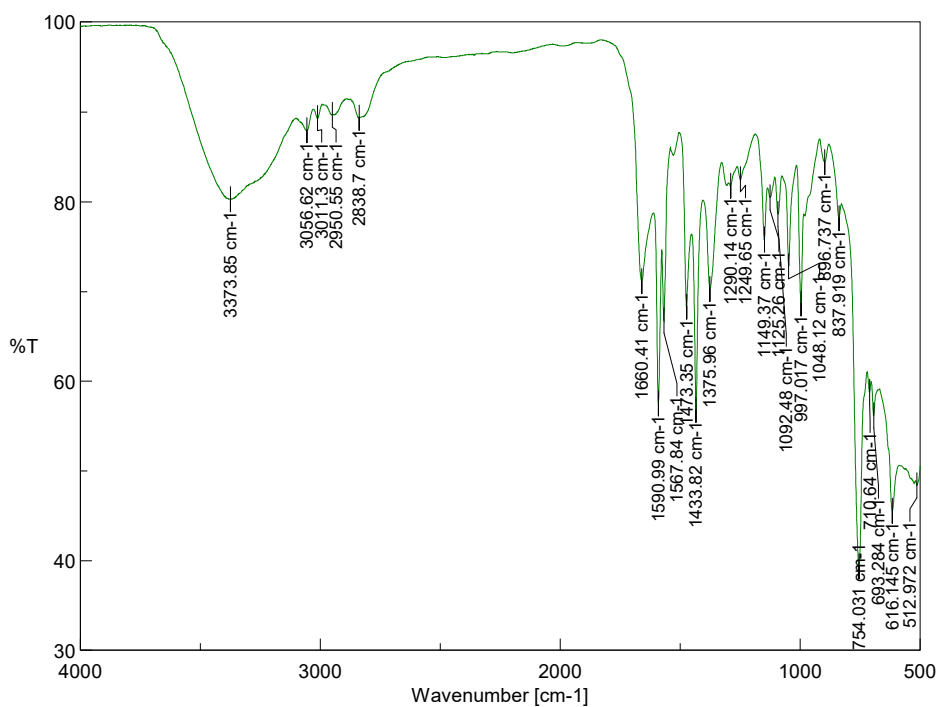
Fig. S28. $^1\text{H}/^{13}\text{C}$ NMR spectrum of Ph-QQH in CDCl_3 .



Ph-QQP

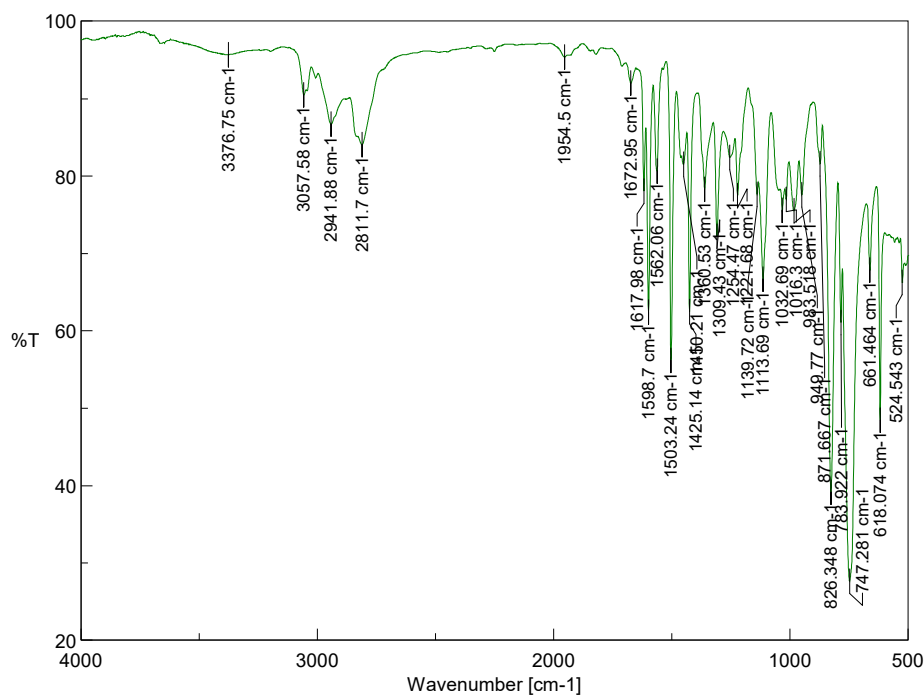
Fig. S29. IR spectrum of Ph-QQP in CDCl_3 .

IR spectrum



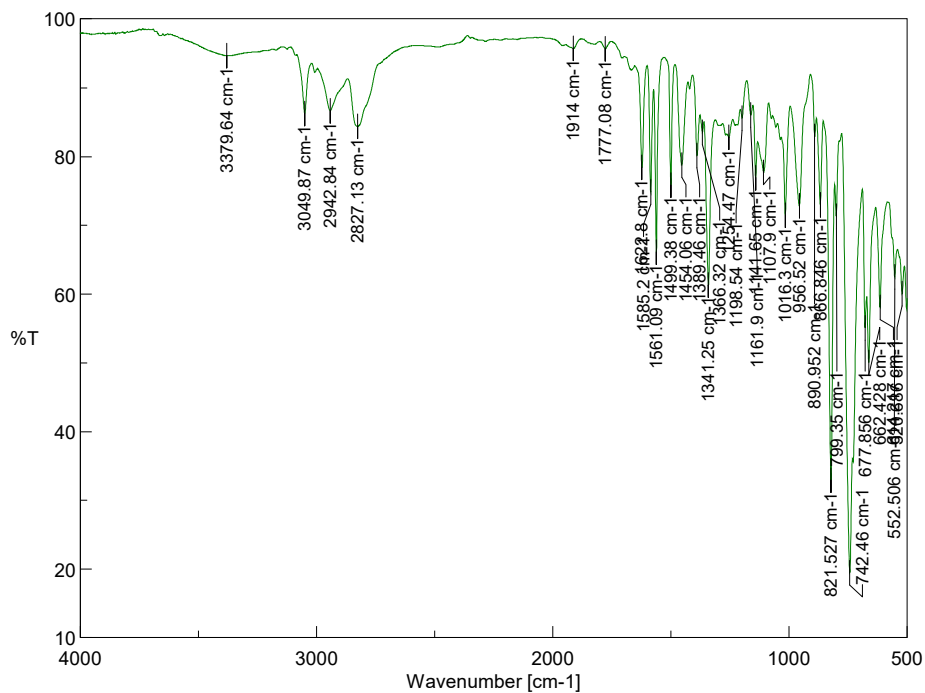
[コメント情報]
試料名

Fig. S30. IR spectrum of Me-PPP.



[コメント情報]
試料名

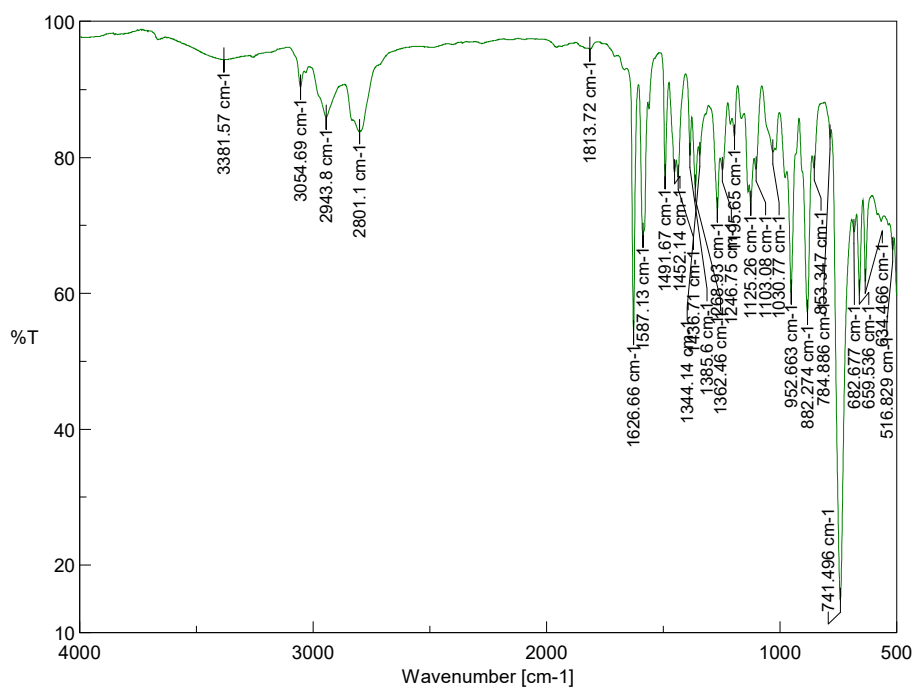
Fig. S31. IR spectrum of Me-QQQ.



[コメント情報]
試料名

Me-111-240913.jws

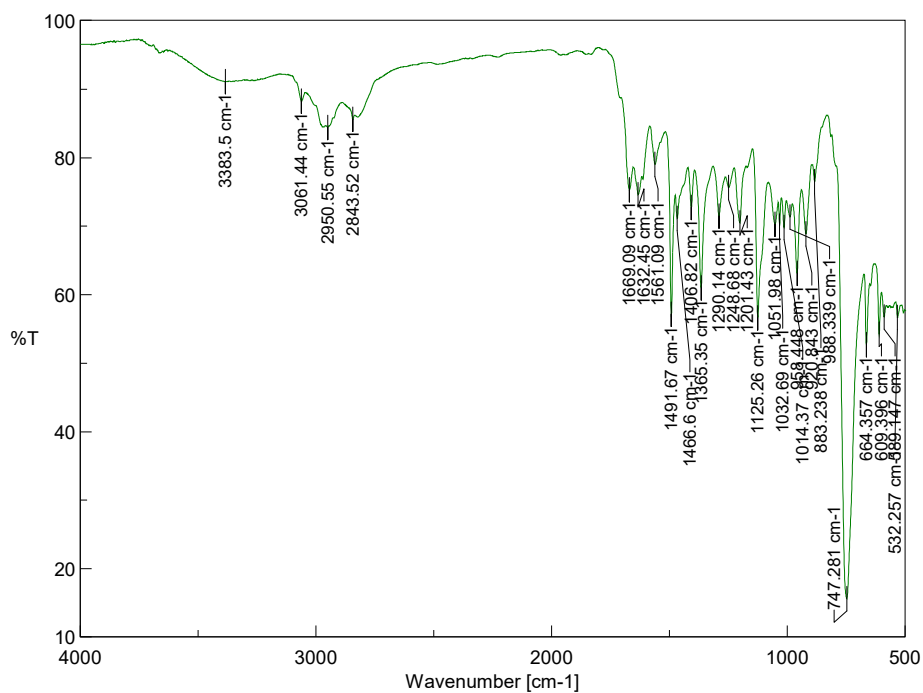
Fig. S32. IR spectrum of Me-111.



[コメント情報]
試料名

Me-333-240913.jws

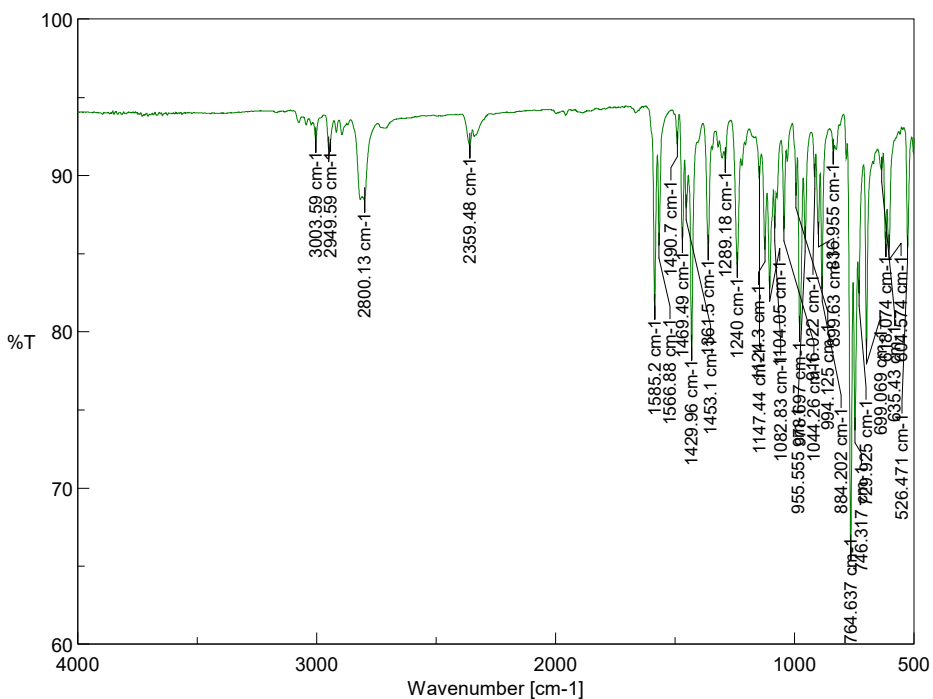
Fig. S33. IR spectrum of Me-333.



[コメント情報]
試料名

Me-XXX-240913.jws

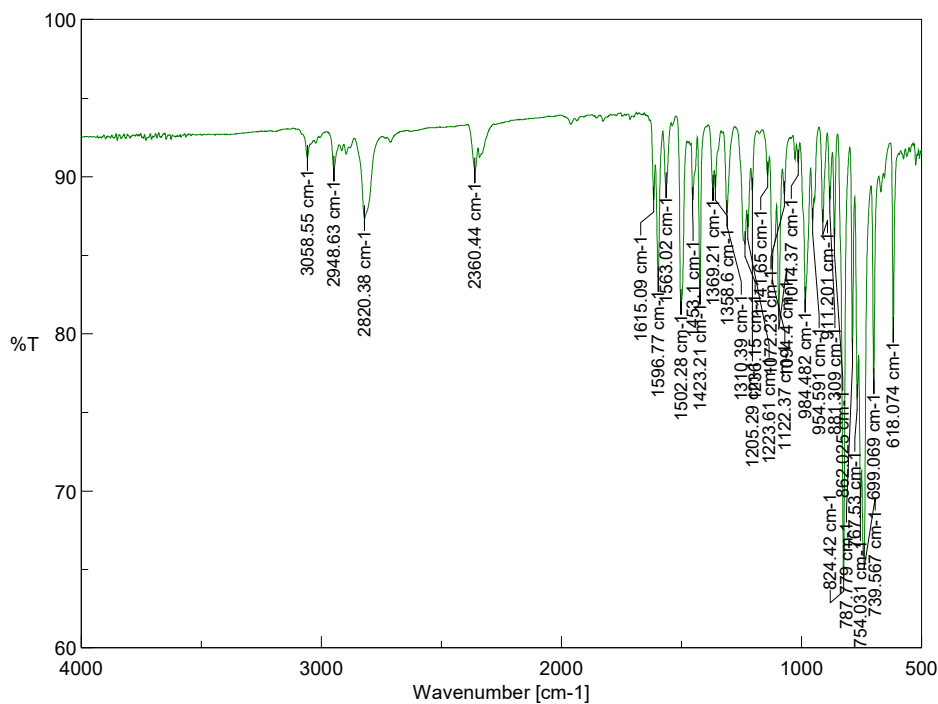
Fig. S34. IR spectrum of Me-XXX.



[コメント情報]
試料名

Bn-TPEN-240913.jws

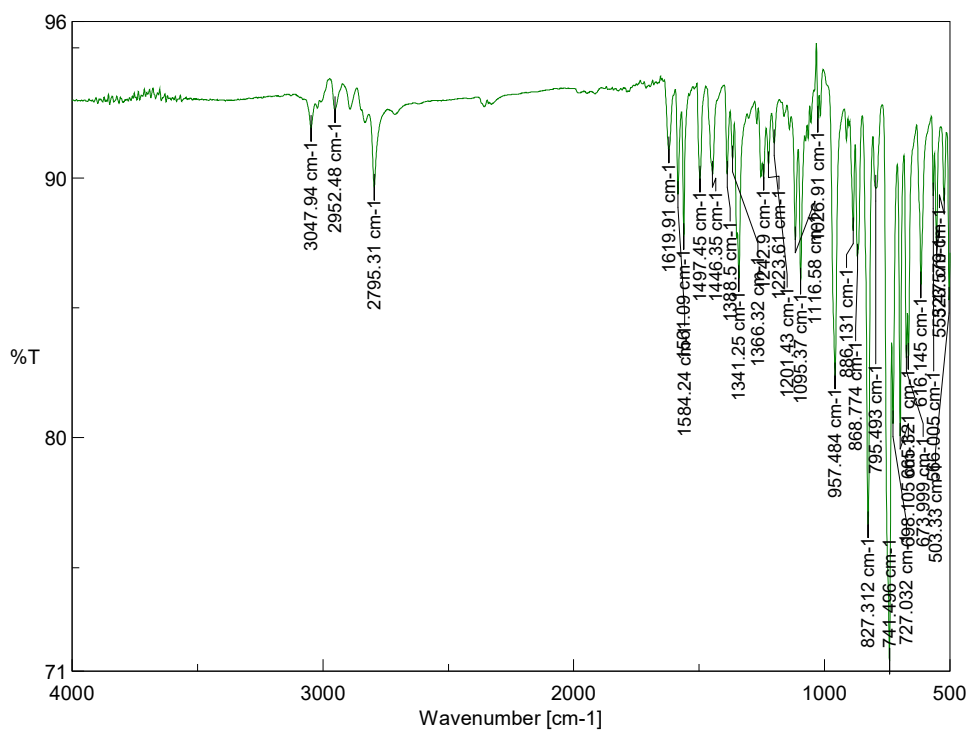
Fig. S35. IR spectrum of Bn-PPP.



[コメント情報]
試料名

Bn-TQEN-240913.jws

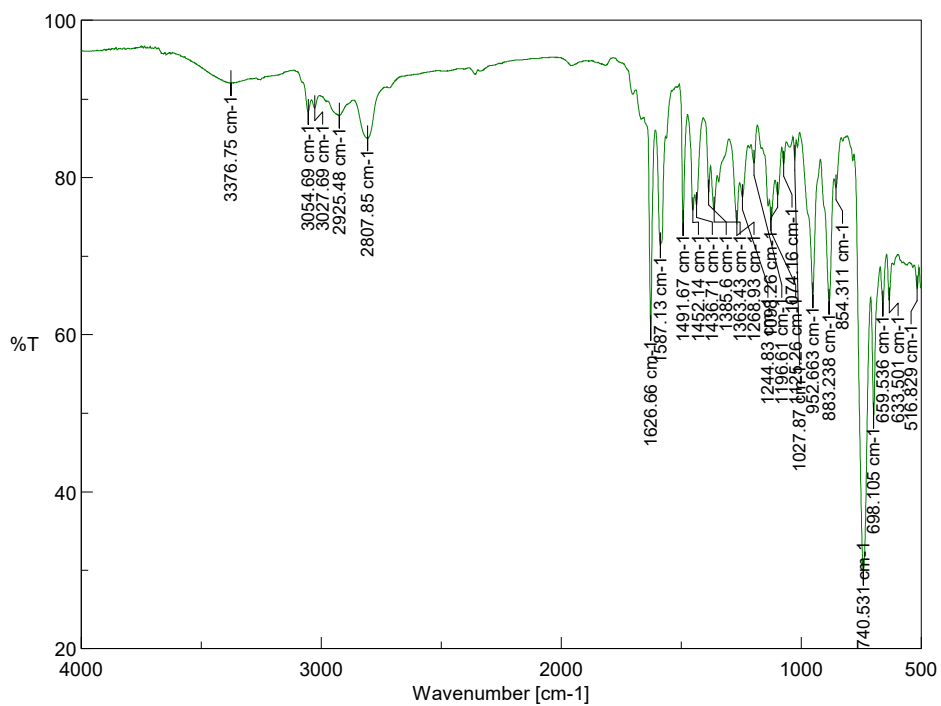
Fig. S36. IR spectrum of **Bn-QQQ**.



[コメント情報]
試料名

Bn-111-240913.jws

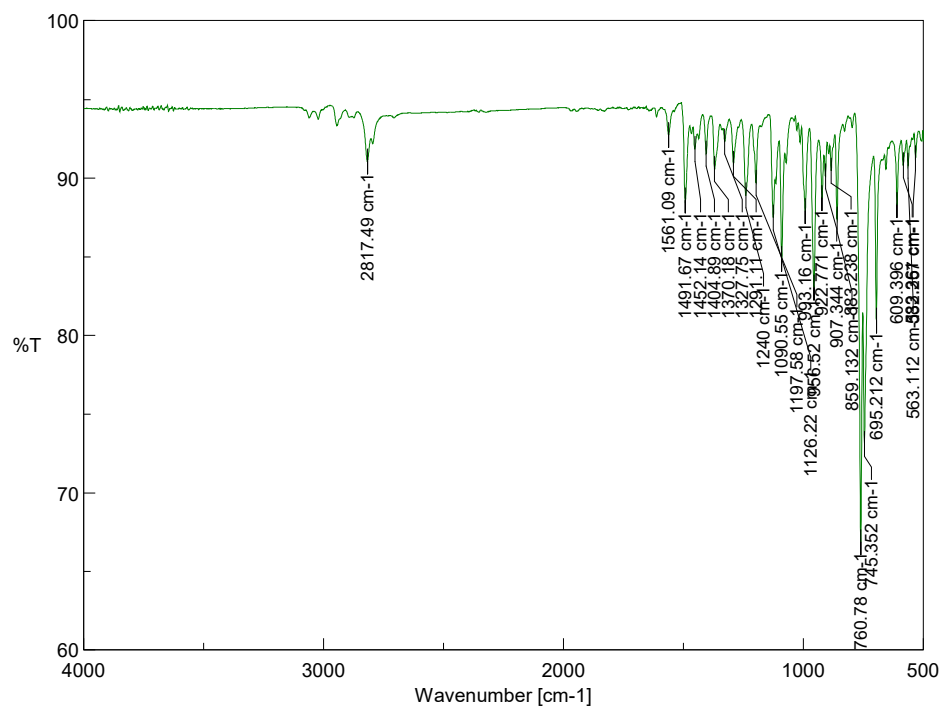
Fig. S37. IR spectrum of **Bn-111**.



[コメント情報]
試料名

Bn-333-240913jws

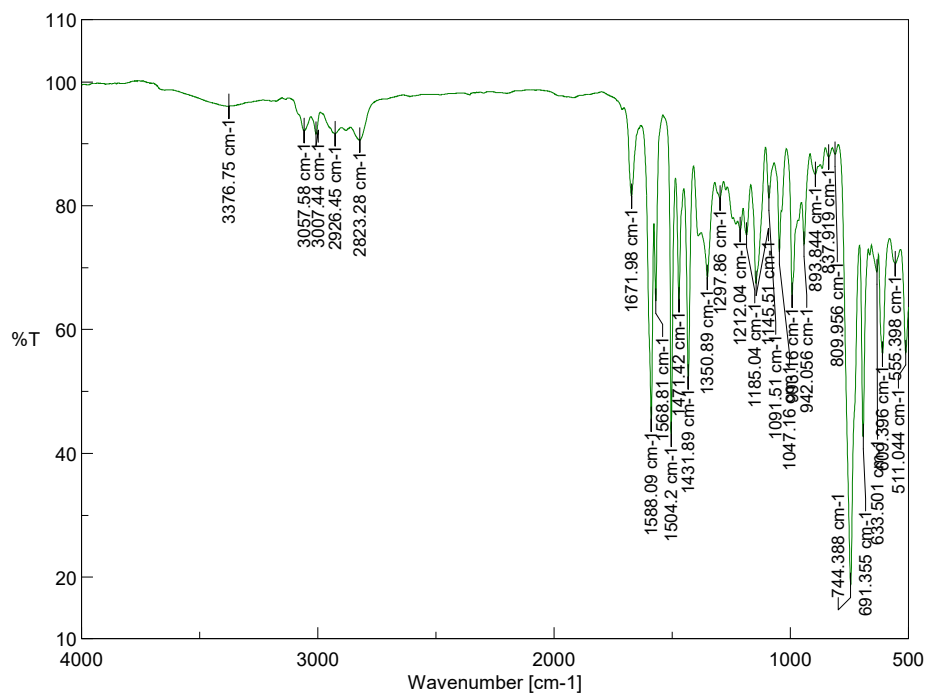
Fig. S38. IR spectrum of **Bn-333**.



[コメント情報]
試料名

Bn-XXX-240913jws

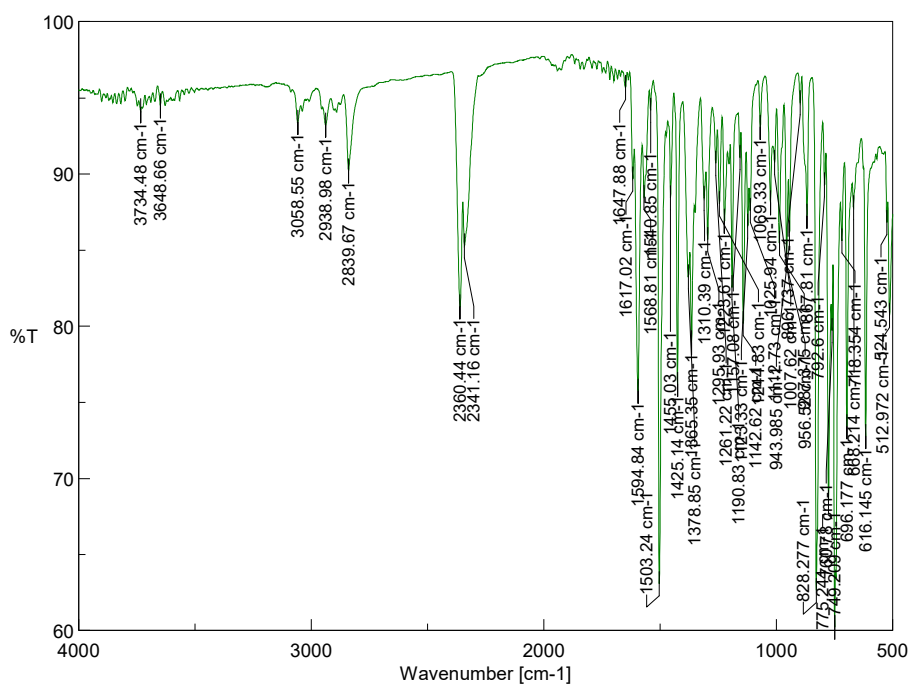
Fig. S39. IR spectrum of **Bn-XXX**.



[コメント情報]
試料名

Ph-PPP-240913.jws

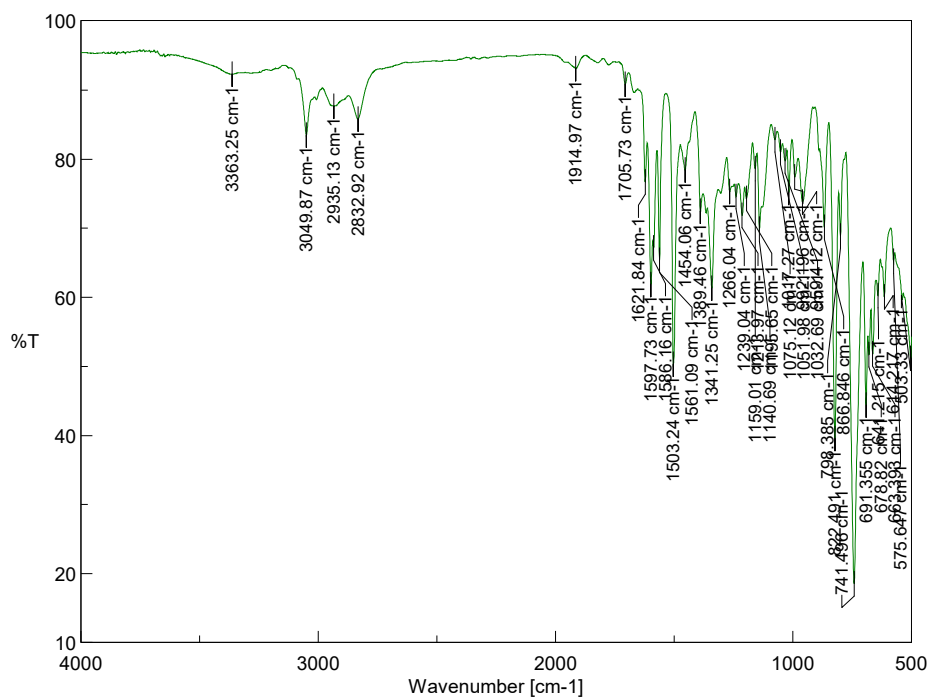
Fig. S40. IR spectrum of Ph-PPP.



[コメント情報]
試料名

Ph-TQEN-240913.jws

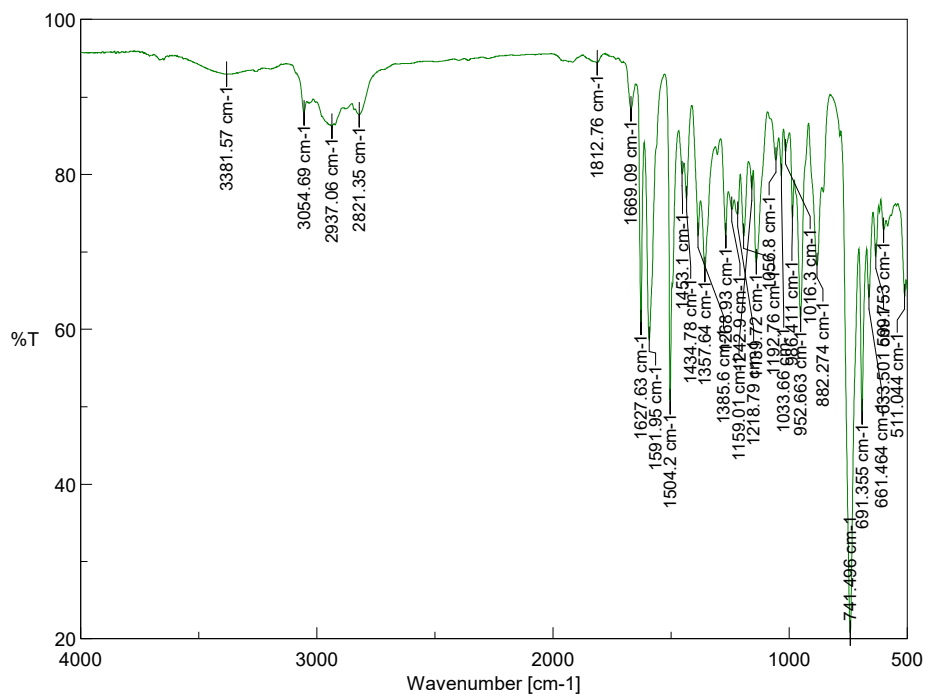
Fig. S41. IR spectrum of Ph-QQQ.



[コメント情報]
試料名

Ph-111-240913.jws

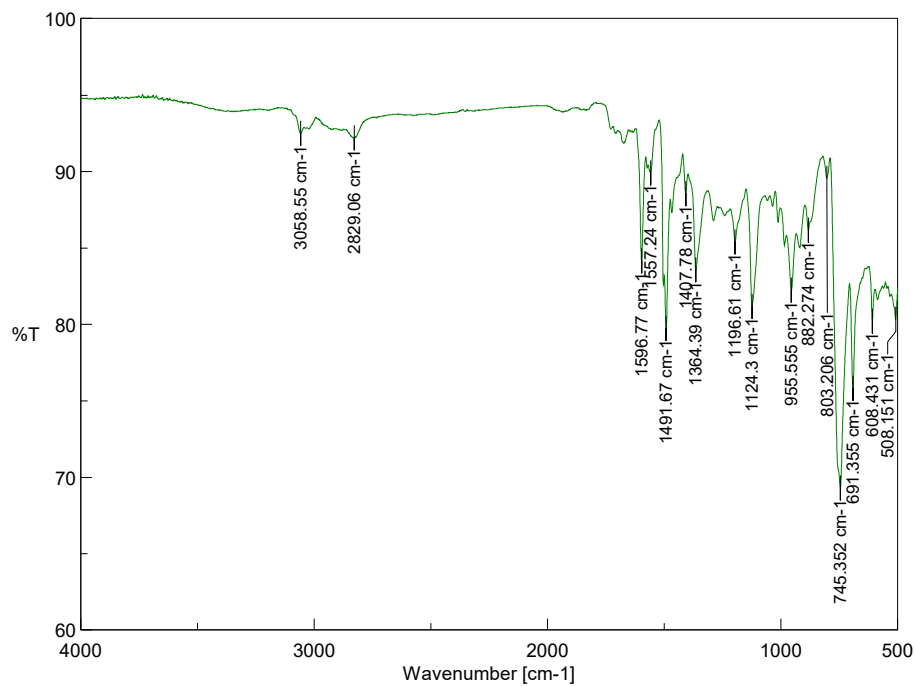
Fig. S42. IR spectrum of Ph-111.



[コメント情報]
試料名

Ph-333-240913.jws

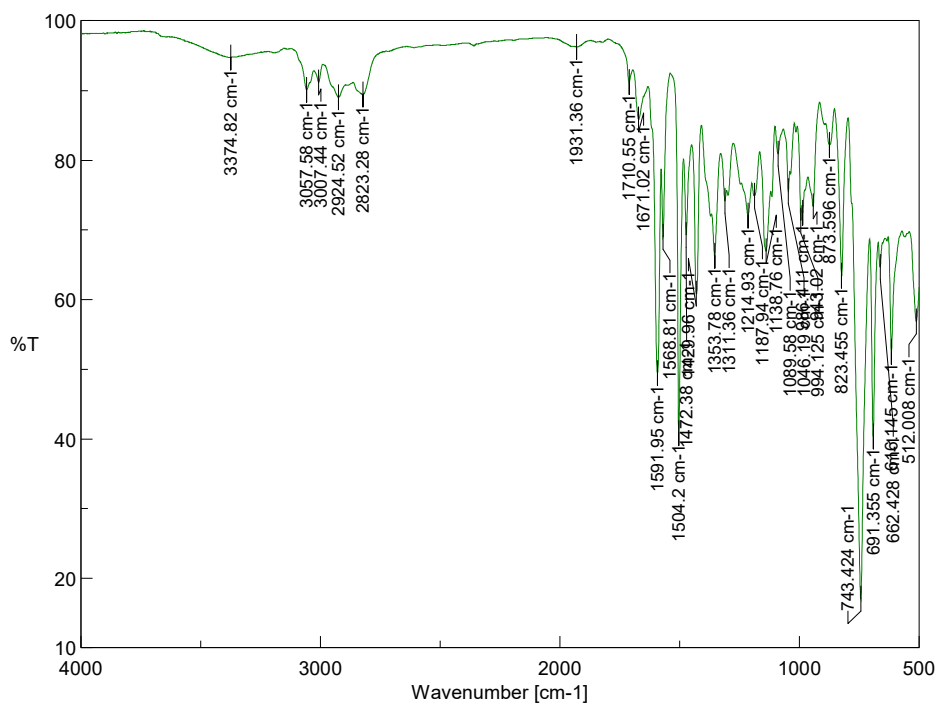
Fig. S43. IR spectrum of Ph-333.



[コメント情報]
試料名

Ph-XXX-240913.jws

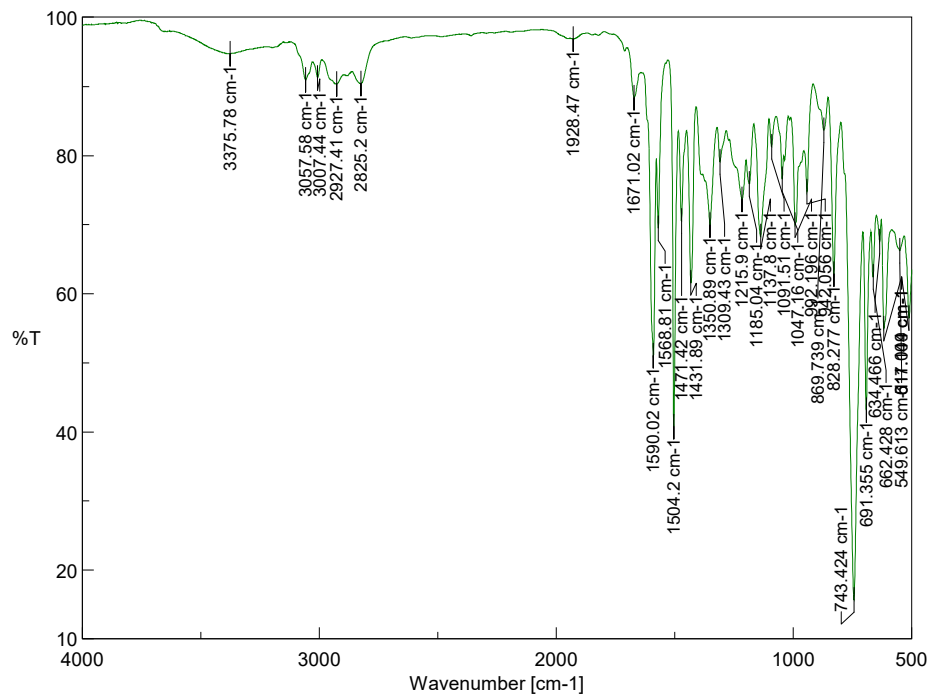
Fig. S44. IR spectrum of Ph-XXX.



[コメント情報]
試料名

Ph-PPQ-240913.jws

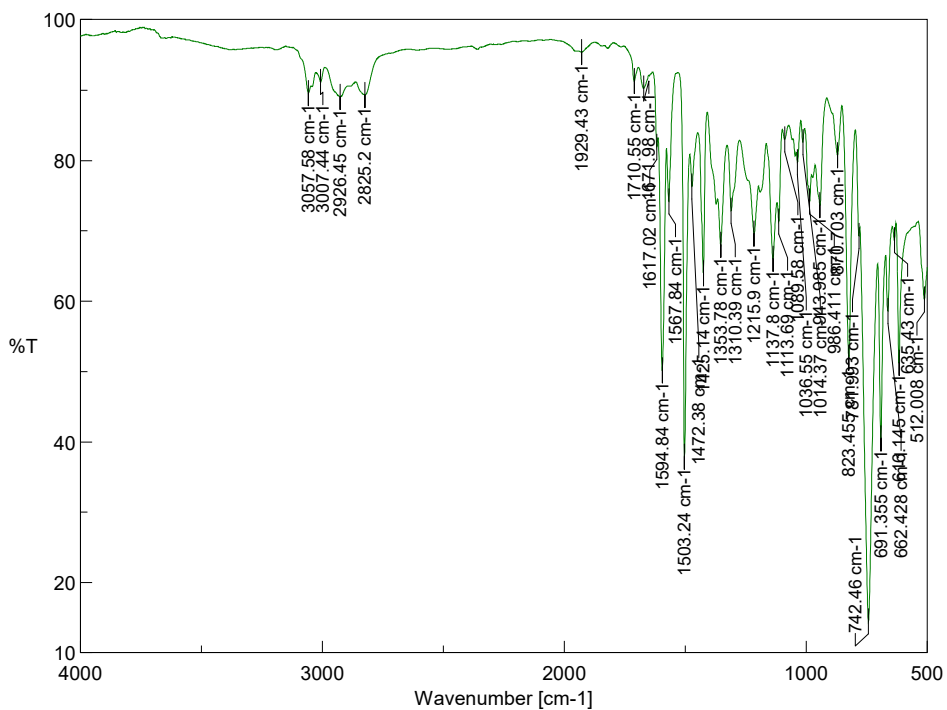
Fig. S45. IR spectrum of Ph-PPQ.



[コメント情報]
試料名

Ph-PQP-240913.jws

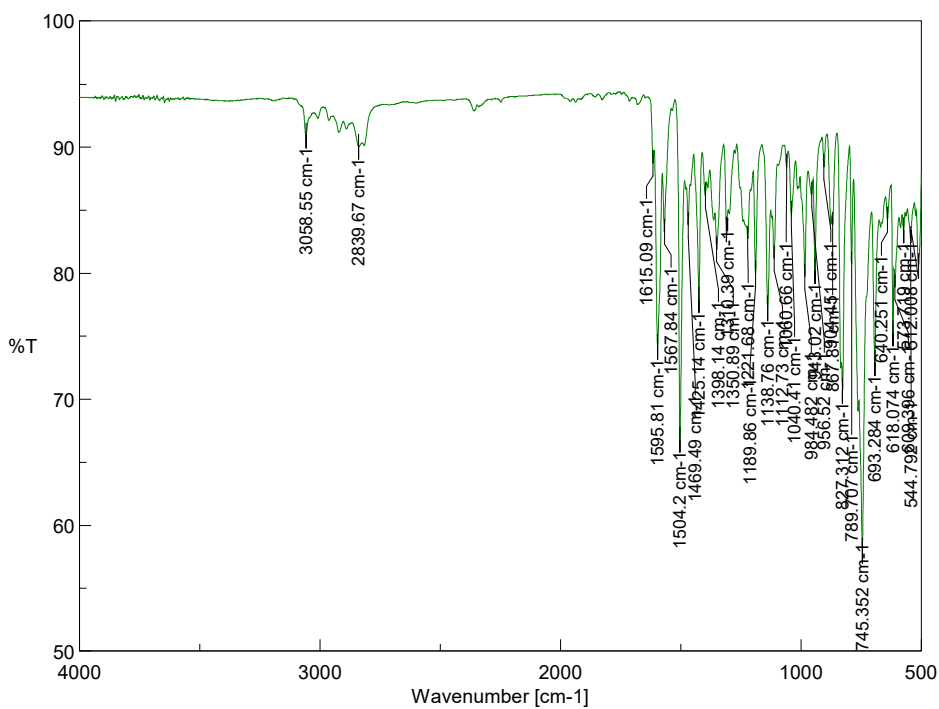
Fig. S46. IR spectrum of Ph-PQP.



[コメント情報]
試料名

Ph-PQQ-240913.jws

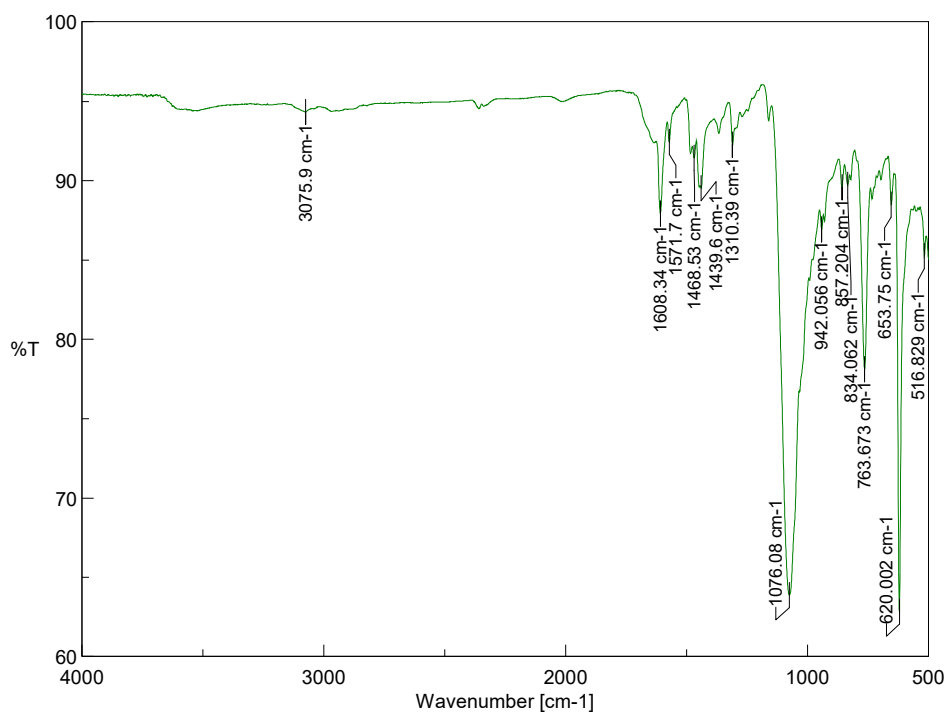
Fig. S47. IR spectrum of Ph-PQQ.



[コメント情報]
試料名

Ph-QQP-240913.jws

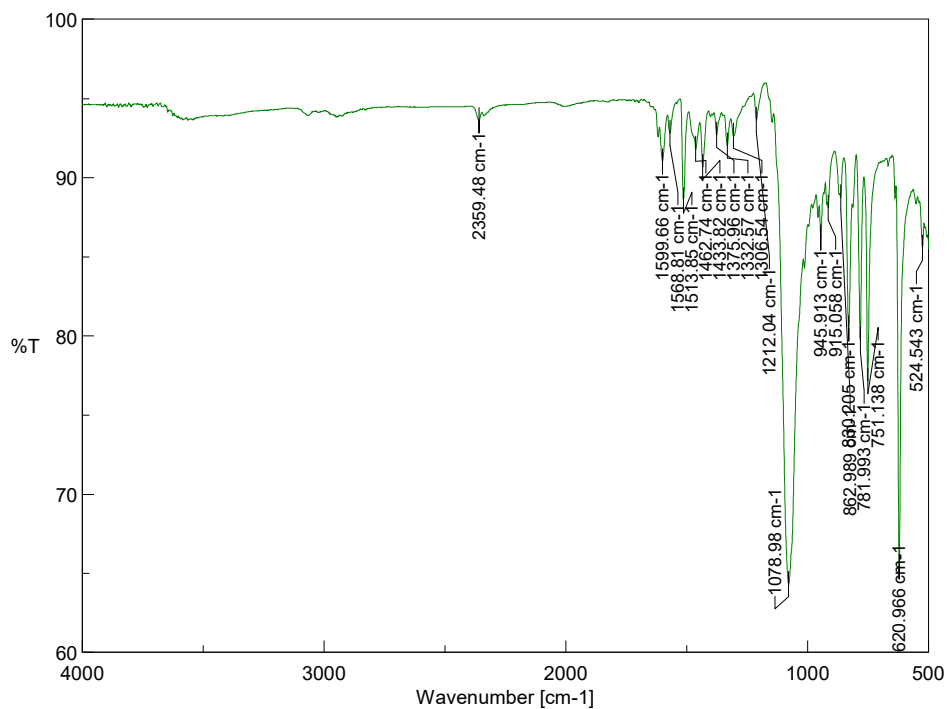
Fig. S48. IR spectrum of Ph-QQP.



[コメント情報]
試料名

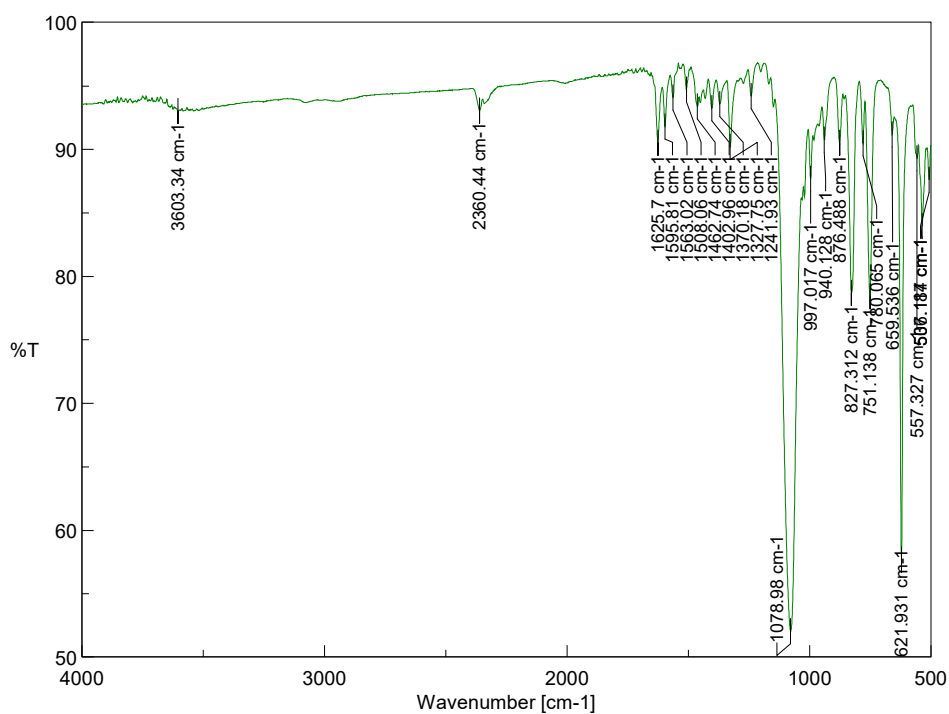
Me-PPP-Cu-240913.jws

Fig. S49. IR spectrum of Me-PPP-Cu.



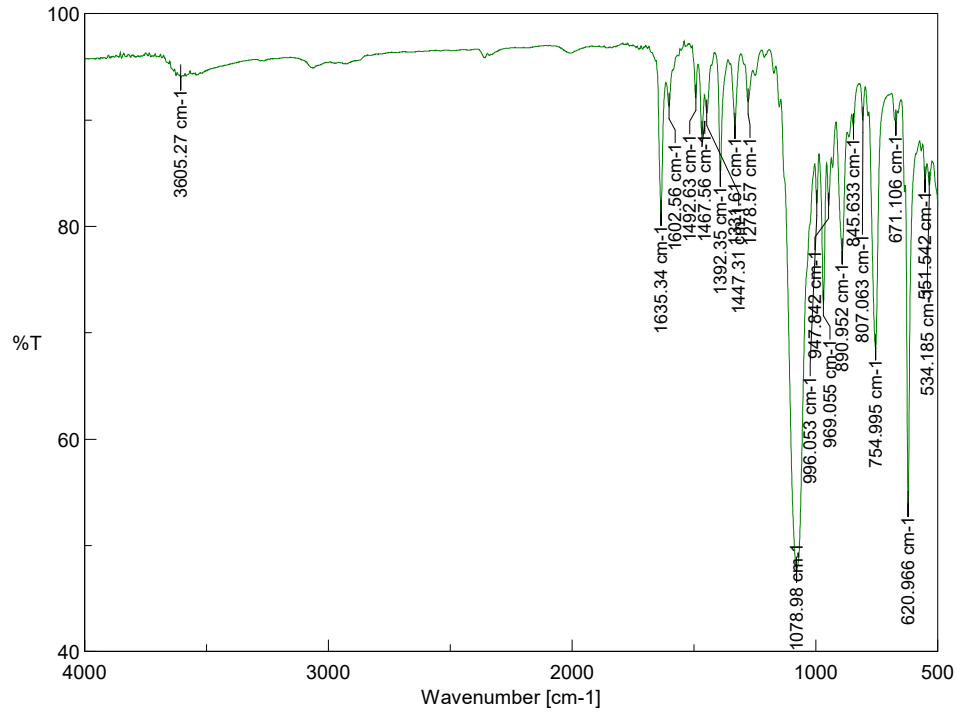
[コメント情報]
試料名

Fig. S50. IR spectrum of Me-**QQQ**-Cu.



[コメント情報]
試料名

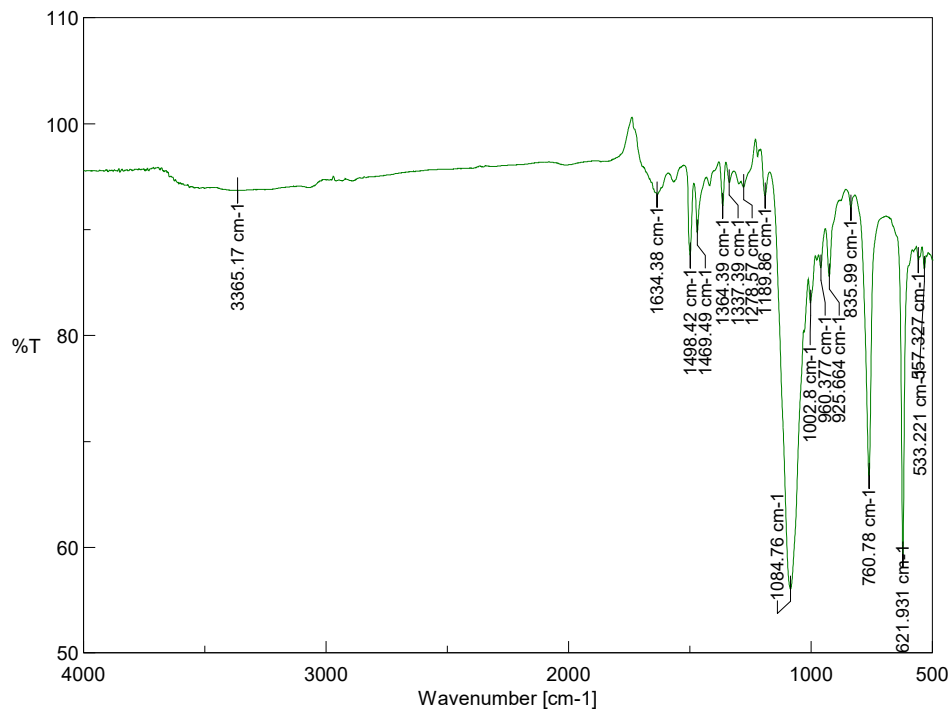
Fig. S51. IR spectrum of Me-**111**-Cu.



[コメント情報]
試料名

Me-333-Cu-240913jws

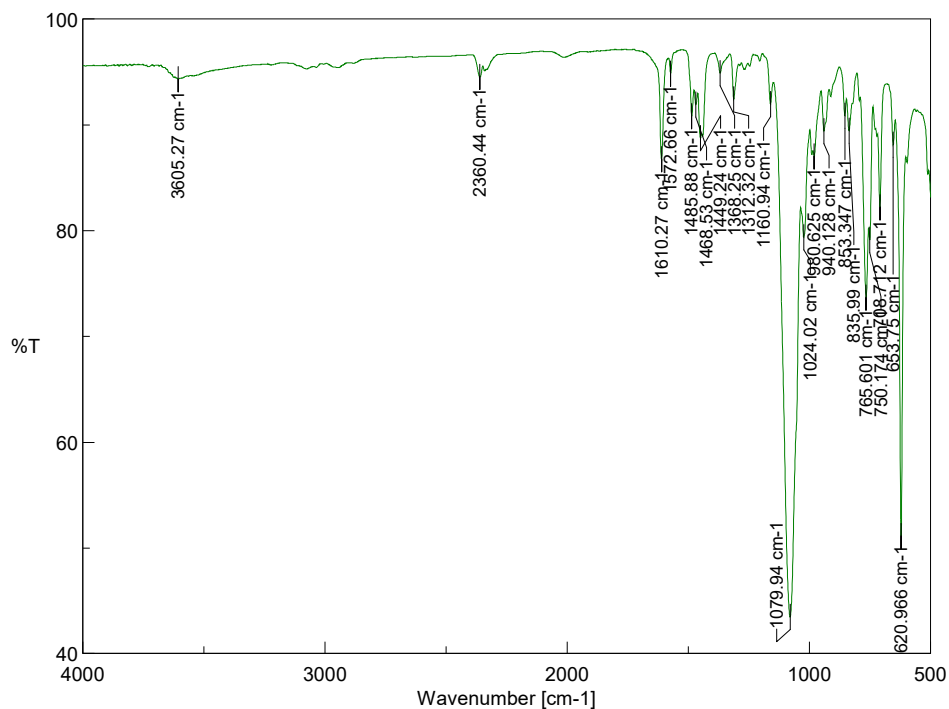
Fig. S52. IR spectrum of Me-333-Cu.



[コメント情報]
試料名

Me-XXX-Cu-240913jws

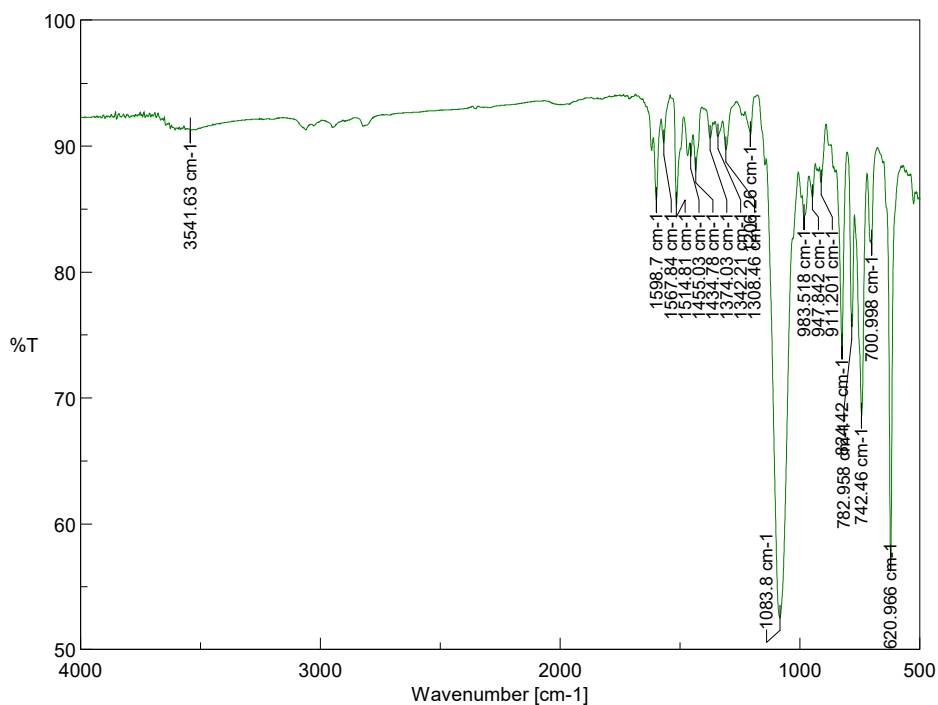
Fig. S53. IR spectrum of Me-XXX-Cu.



[コメント情報]
試料名

— Bn-PPP-Cu-240913.jws

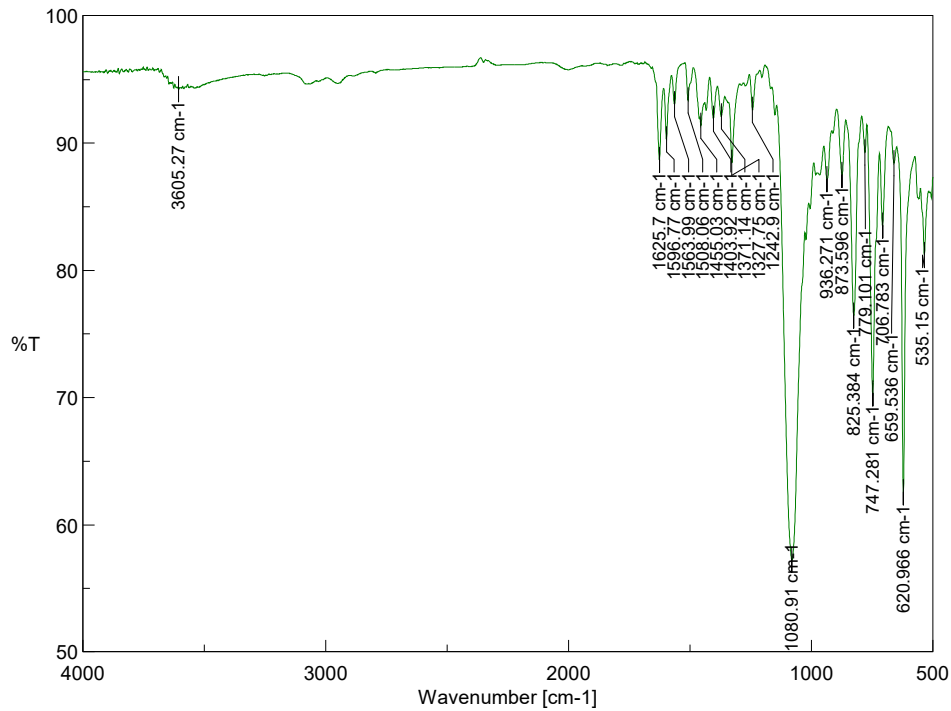
Fig. S54. IR spectrum of Bn-PPP-Cu.



[コメント情報]
試料名

— Bn-QQQ-Cu-240913.jws

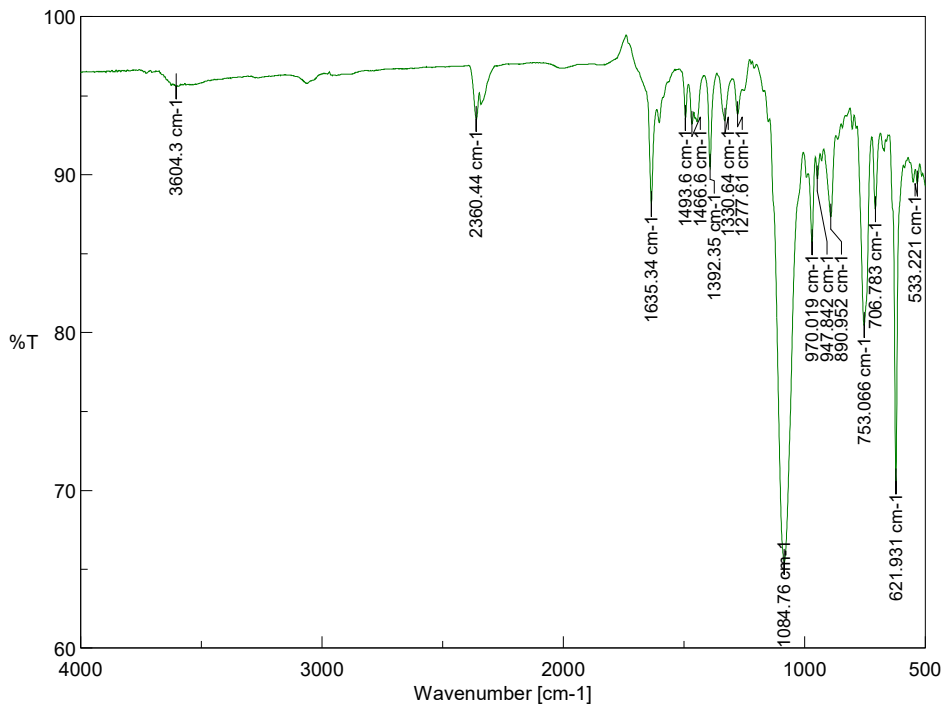
Fig. S55. IR spectrum of Bn-QQQ-Cu.



[コメント情報]
試料名

Bn-111-Cu-240913jws

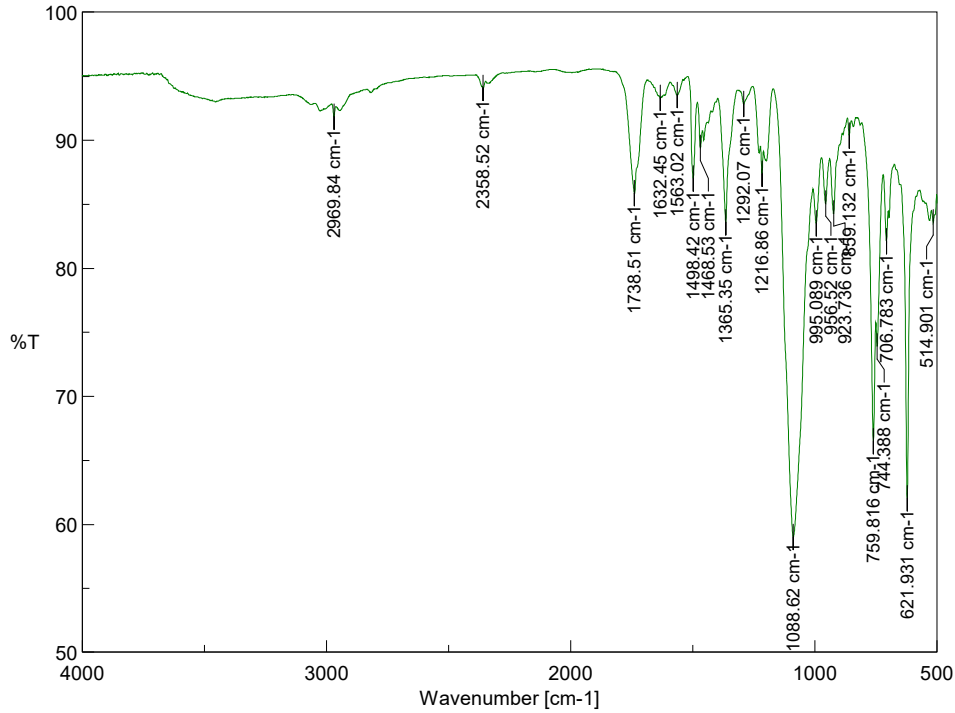
Fig. S56. IR spectrum of Bn-111-Cu.



[コメント情報]
試料名

Bn-333-Cu-240913jws

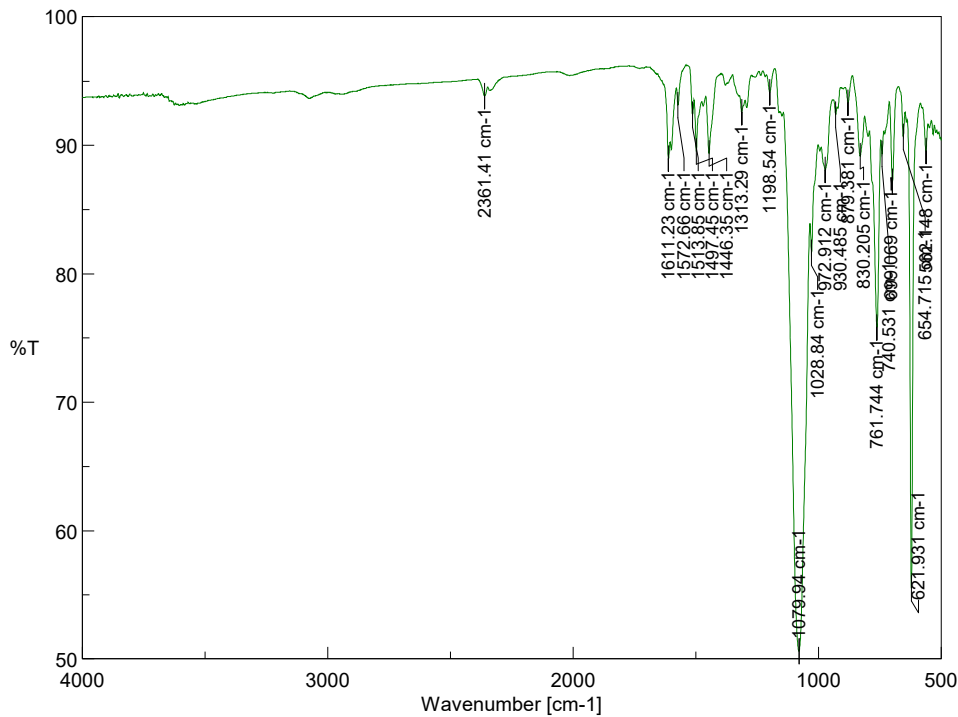
Fig. S57. IR spectrum of Bn-333-Cu.



[コメント情報]
試料名

Bn-XXX-Cu-240913.jws

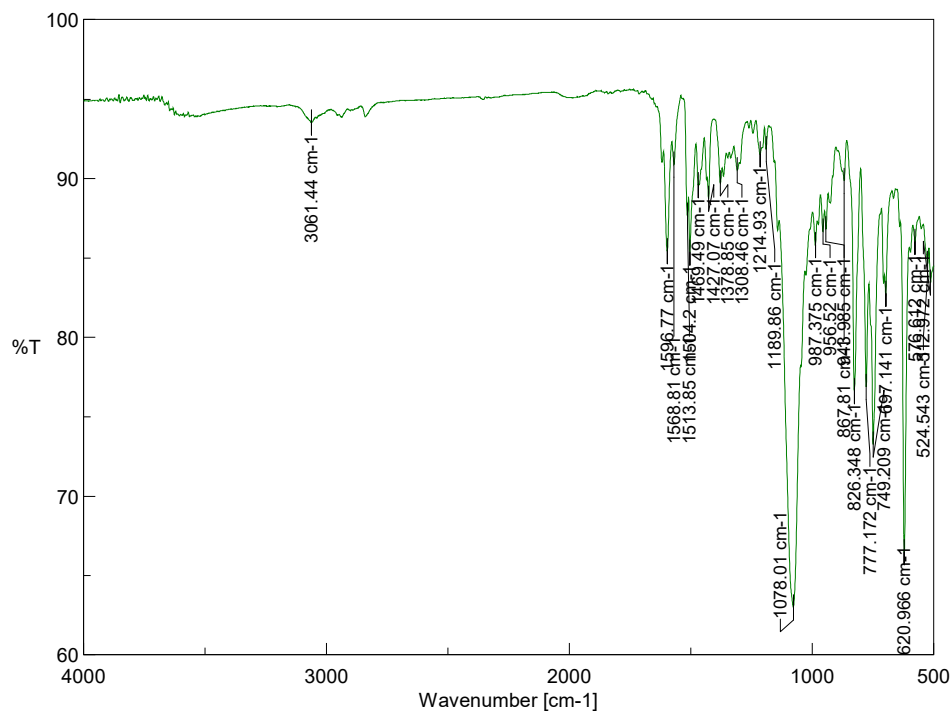
Fig. S58. IR spectrum of Bn-XXX-Cu.



[コメント情報]
試料名

Ph-PPQ-Cu-240913.jws

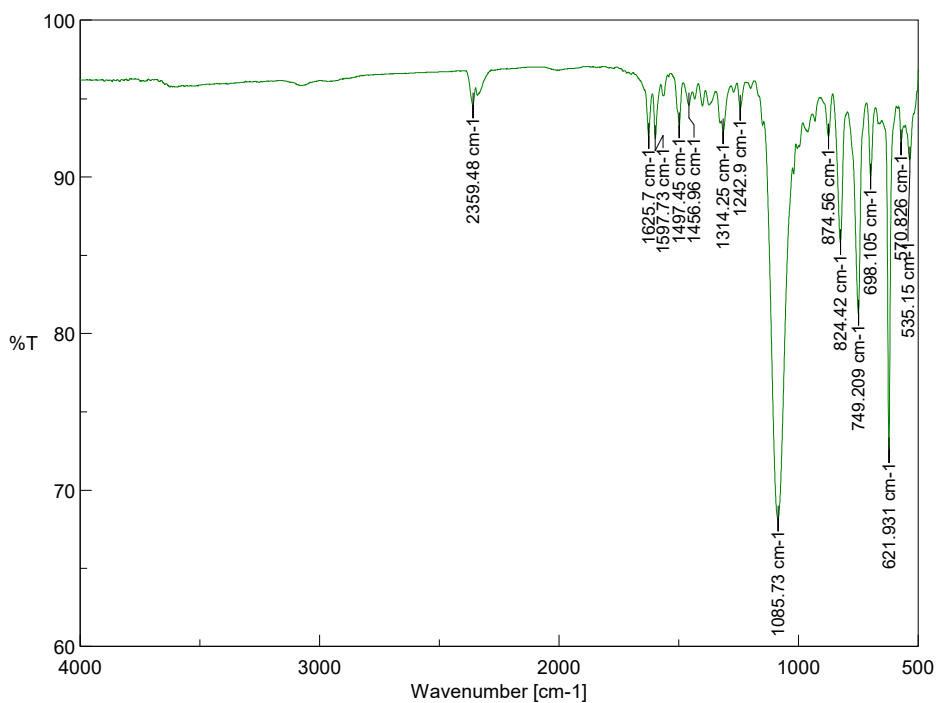
Fig. S59. IR spectrum of Ph-PPQ-Cu.



[コメント情報]
試料名

Ph-QQQ-Cu-240913.jws

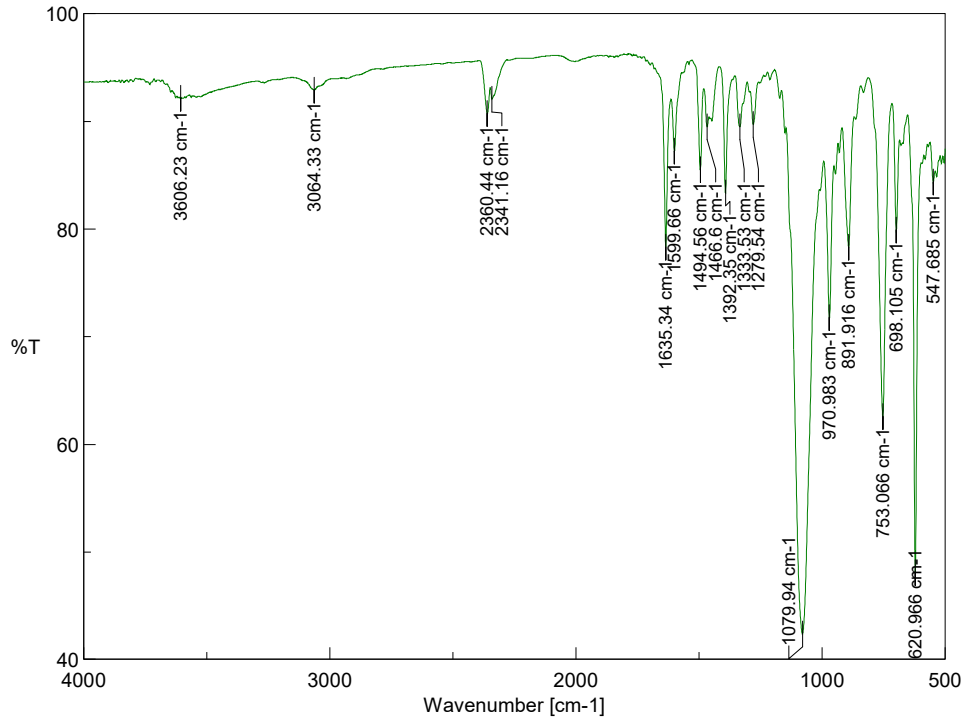
Fig. S60. IR spectrum of Ph-QQQ-Cu.



[コメント情報]
試料名

Ph-111-Cu-240913.jws

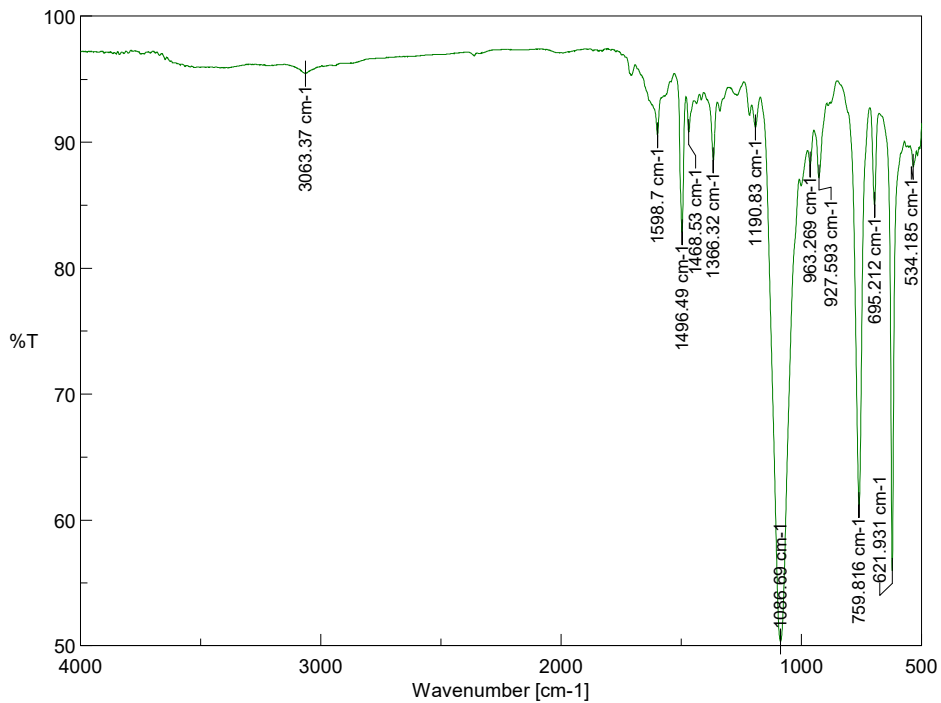
Fig. S61. IR spectrum of Ph-111-Cu.



[コメント情報]
試料名

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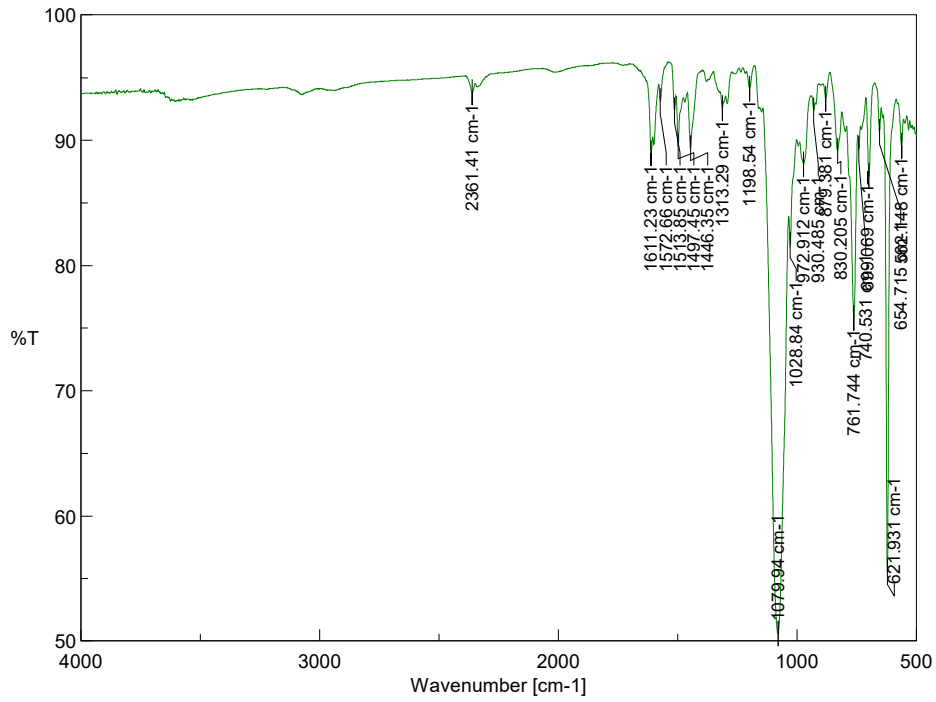
Fig. S62. IR spectrum of Ph-333-Cu.



[コメント情報]
試料名

Ph-XXX-Cu-240913.jws

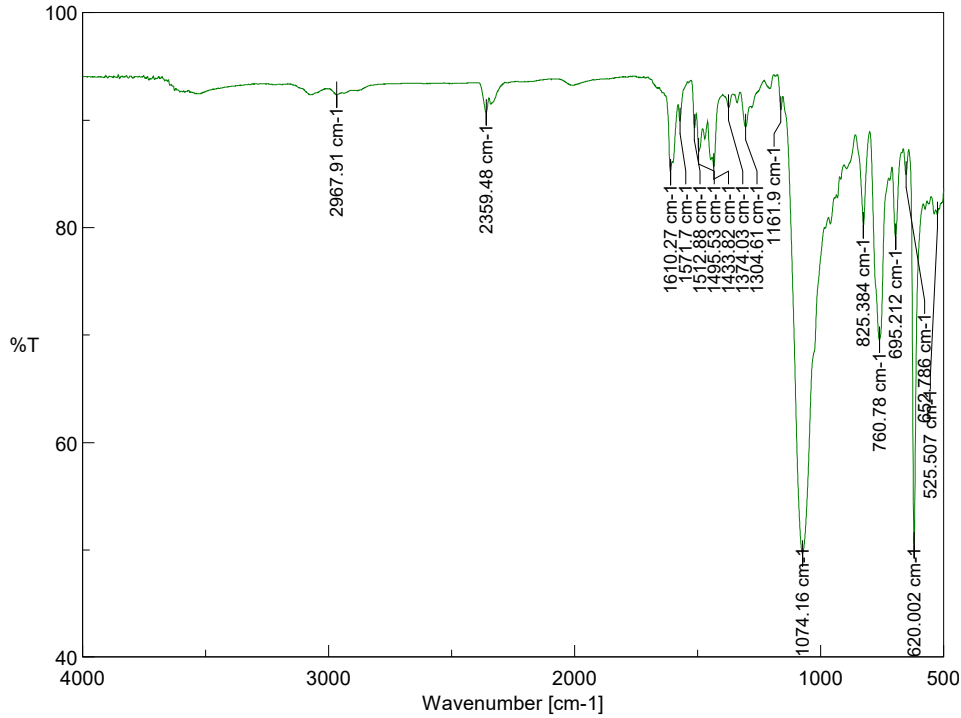
Fig. S63. IR spectrum of Ph-XXX-Cu.



[コメント情報]
試料名

Ph-PPQ-Cu-240913jws

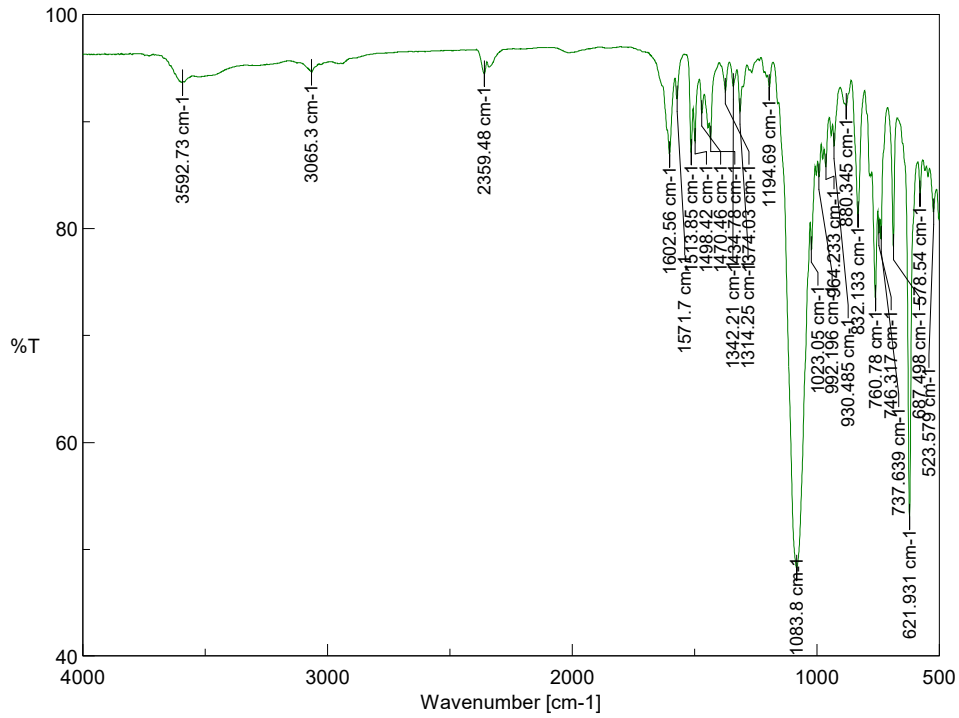
Fig. S64. IR spectrum of Ph-PPQ-Cu.



[コメント情報]
試料名

Ph-PQP-Cu-240913jws

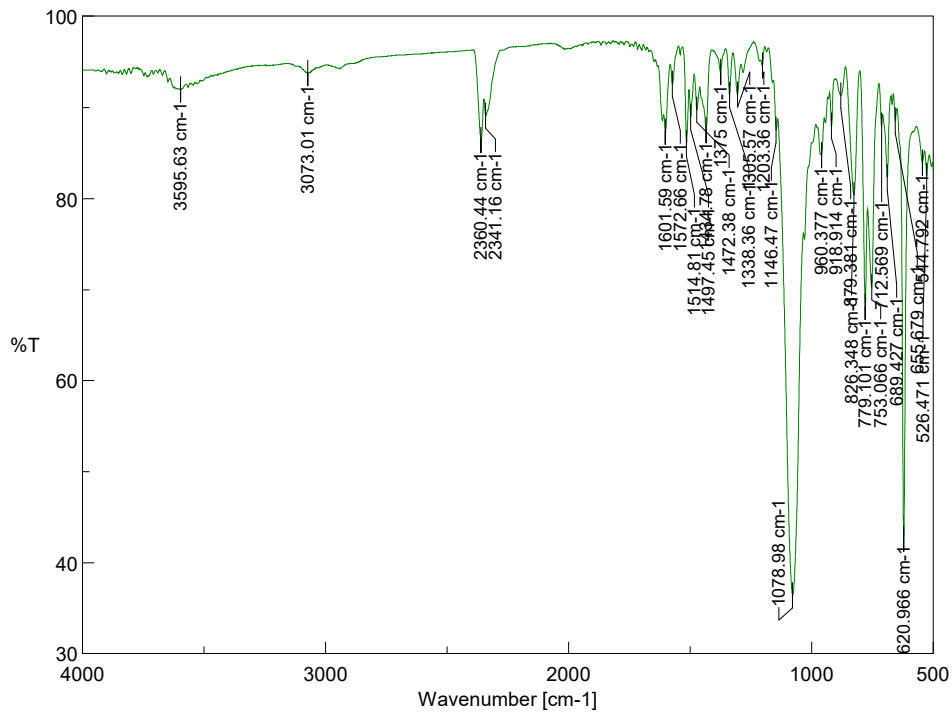
Fig. S65. IR spectrum of Ph-PQP-Cu.



[コメント情報]
試料名

— Ph-PQQ-Cu-240913.jws

Fig. S66. IR spectrum of Ph-PQQ-Cu.



[コメント情報]
試料名

— Ph-QQP-Cu-240917.jws

Fig. S67. IR spectrum of Ph-QQP-Cu.

References

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