Electronic Supplementary Information

# Circularly Polarized Luminescence and High Photoluminescence Quantum Yields from Rigid Carbon-bridged Stilbene and 2,2'-Dialkoxy-1,1'-binaphthyl Conjugates and Co-polymers

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**Contents**

## 1. Synthesis of precursors

**COPV1-(Bpin)$_2$** A mixture of **COPV1-Br$_2$** (157 mg, 0.374 mmol), bis(pinacolato)diboron (486.1 mg, 1.89 mmol), $PdCl_2$(dppf)-$CH_2Cl_2$ adduct (41.1 mg, 0.0411 mmol), and potassium acetate (398 mg, 3.74 mmol) in 1,4-dioxane (6 mL) were stirred at 80 °C for 16 h. Water was added to the mixture, which was then extracted with dichloromethane. The organic layer was dried with $MgSO_4$ and concentrated in vacuo. Silica gel column chromatography (eluent: hexane/dichloromethane = 3/2) afforded the title compound as a white solid (179 mg, 94%). Mp >300 ˚C. $^1$H NMR (400 MHz, $CDCl_3$, δ in ppm): 1.37 (s, 24H), 1.53 (s, 12H), 7.42 (d, *J* = 8.0 Hz, 2H), 7.79 (d, *J* = 8.0 Hz, 2H), 7.85 (s, 2H); $^{13}$C{$^1$H} NMR (100 MHz, $CDCl_3$, δ in ppm): 158.6, 157.7, 141.2, 134.4, 128.2, 119.5, 84.1, 45.5, 25.3, 24.8. HRMS(APCI+) *m/z* calcd for $C_{32}H_{42}B_2O_4^+$([M$^+$]): 512.3275, Found: 512.3276.

**CzCOPV1-Br.** To a microwave reactor purged with argon gas was charged with **COPV1-Br$_2$** (997 mg, 2.38 mmol), carbazole (525 mg, 3.15 mmol), $Pd_2(dba)_3$ (51 mg, 0.056 mmol), *t*-$Bu_3PHBF_4$ (40 mg, 0.0 mmol), NaO*t*-Bu (557 mg, 5.8 mmol) and dry toluene (12 mL). The resulting mixture was stirred at 300 W and 140 °C for 3 min. After cooling to ambient temperature, the reaction mixture was passed through a short plug of silica gel. The solvent was removed under reduced pressure. The residue was purified on silica gel column chromatography (hexane/$CH_2Cl_2$ = 10/3) to furnish the product (742 mg, 1.47 mmol, 66% yield) as a white solid. Mp 282.5-284 ˚C. $^1$H NMR (400 MHz, $CDCl_3$, δ in ppm): 8.13 (d, *J* = 7.7 Hz, 2H), 7.53 (d, *J* = 1.4 Hz, 1H), 7.44 (d, *J* = 7.7 Hz, 2H), 7.37-7.32 (m, 4H), 7.28 (t, *J* = 7.5 Hz, 2H), 7.18 (dd, *J* = 7.7, 1.8 Hz, 2H), 6.85 (d, *J* = 7.7 Hz, 1H), 1.29 (s, 6H), 1.26 (s, 6H). $^{13}$C{$^1$H} NMR (150 MHz, $CDCl_3$, δ in ppm): 161.1, 160.9, 156.0, 155.5, 141.8, 137.0, 136.7, 135.3, 130.2, 126.3, 126.2, 126.0, 124.0, 121.5, 121.0, 120.8, 120.5, 120.4, 119.7, 110.2, 45.4, 45.3, 24.1. HRMS(APCI+) *m/z* calcd for $C_{32}H_{26}BrN^+$([M$^+$]): 503.1249, Found:503.1238.

**CzCOPV1-Bpin.** To a microwave reactor purged with argon gas was charged with **CzCOPV1-Br** (251 mg, 0.498 mmol), bis(pinacolato)diboron (189 mg, 0.746 mmol), $Pd(OAc)_2$ (15 mg, $6.7 \times 10^{-3}$ mmol), XPhos (48 mg, 0.101 mmol) and potassium acetate (155.6 mg, 1.58 mmol) in DMSO (5 mL). The mixture was stirred at 300 W and 110 °C for 3 min. Water was added to the mixture, which was then filtered to afford a crude product. Silica gel column chromatography (eluent: hexane/$CH_2Cl_2$= 1/2) afforded the title compound as a white solid (158 mg, 0.284 mmol, 57%). Mp >300 ˚C. $^1$H NMR (400 MHz, $CDCl_3$, δ in ppm) 8.17 (d, *J* = 7.7 Hz, 2H), 7.89 (s, 1H), 7.82 (dd, *J* = 7.2, 0.9 Hz, 1H), 7.58 (m, 2H), 7.50-7.40 (m, 6H), 7.32-7.28 (m, 3H), 1.62 (s, 6H), 1.59 (s, 6H), 1.39 (s, 12H). $^{13}$C{$^1$H}

NMR (150 MHz, $CDCl_3$, δ in ppm): 161.4, 158.4, 157.2, 157.0, 141.6, 141.1, 137.4, 135.2, 134.5, 129.5, 128.7, 128.3, 126.4, 126.0, 123.8, 121.5, 120.8, 120.7, 120.3, 119.4, 110.4, 84.2, 45.8, 45.6, 25.4, 24.9. HRMS (APCI+) *m/z* calcd for $C_{38}H_{38}BNO_2^+$([$M^+$]): 551.3007, Found: 551. 2997.

## 2. NMR Charts

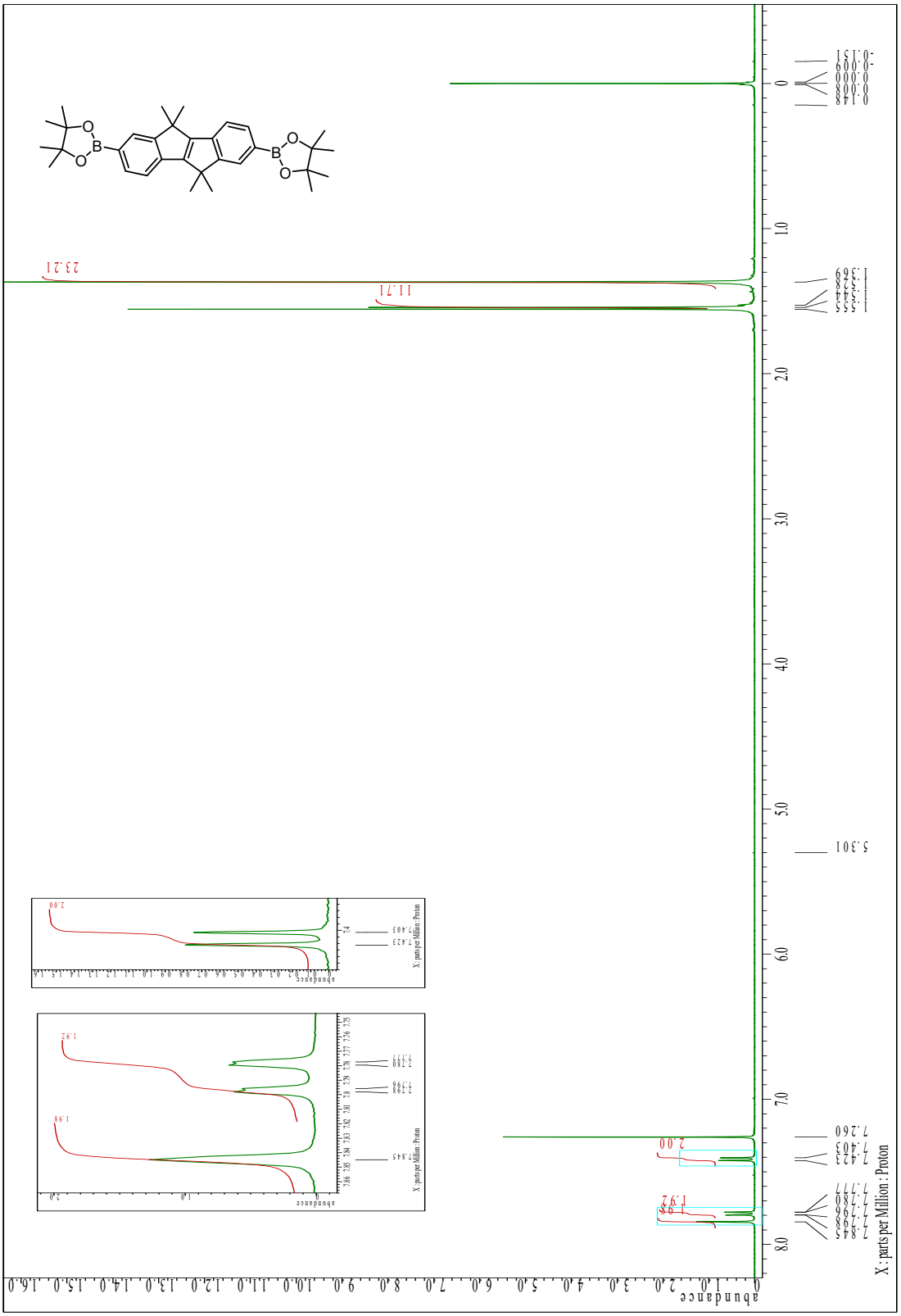

**Figure S1.** $^{1}$H NMR of **COPV1-(Bpin)$_2$**

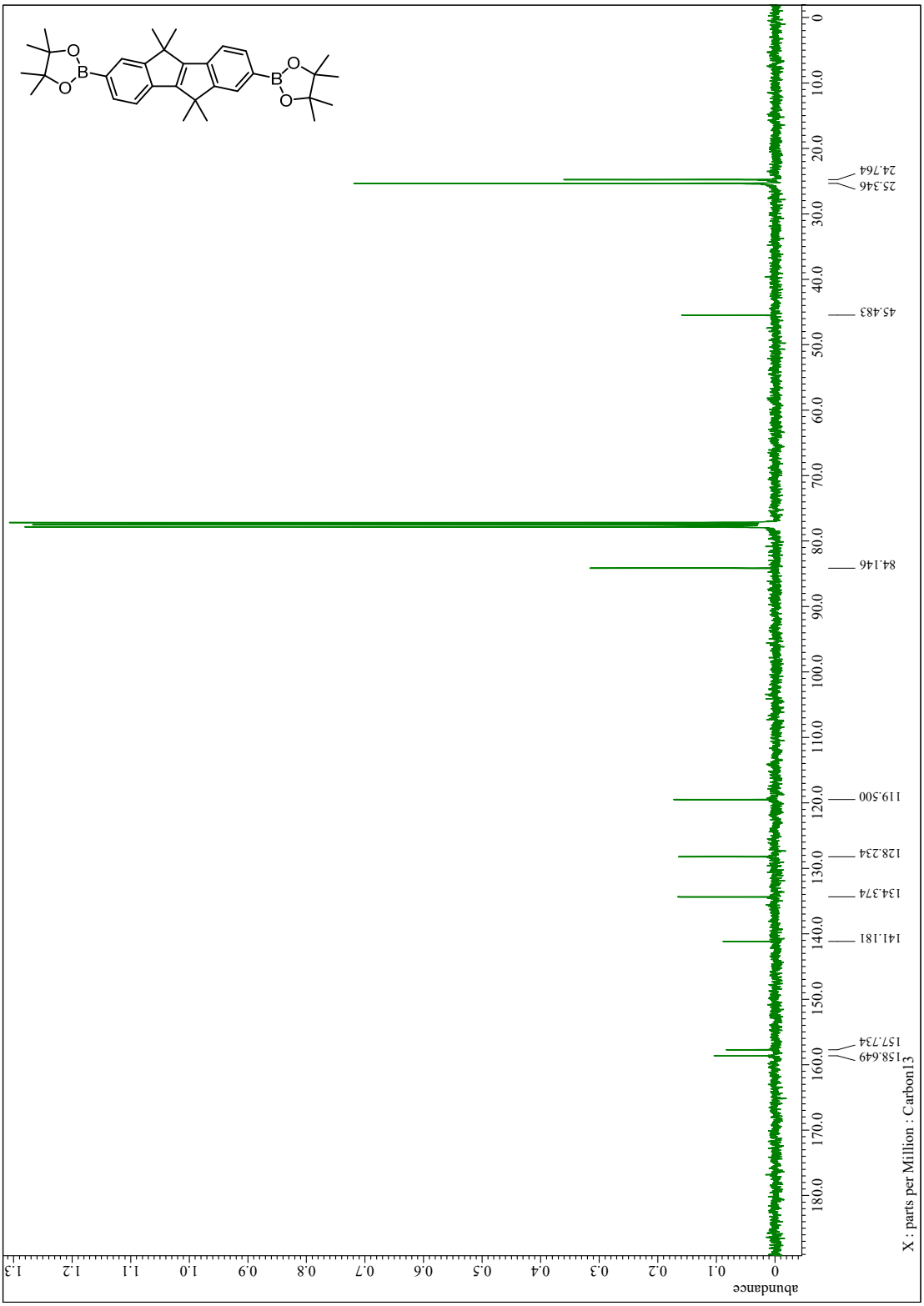


**Figure S2.** $^{13}$C NMR of **COPV1-(Bpin)$_2$**

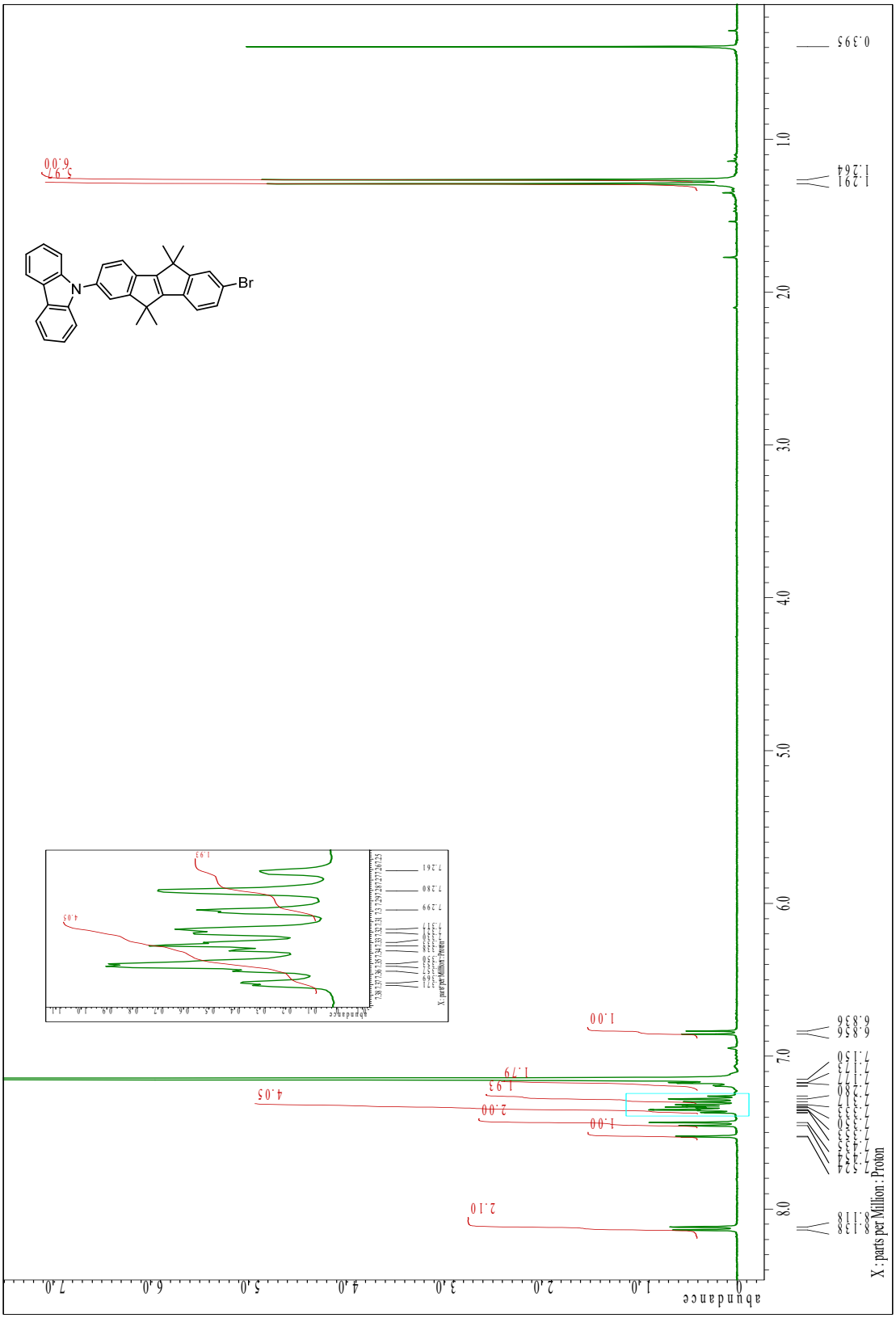


**Figure S3.** $^{1}$H NMR of **Cz-COPV1-Br**

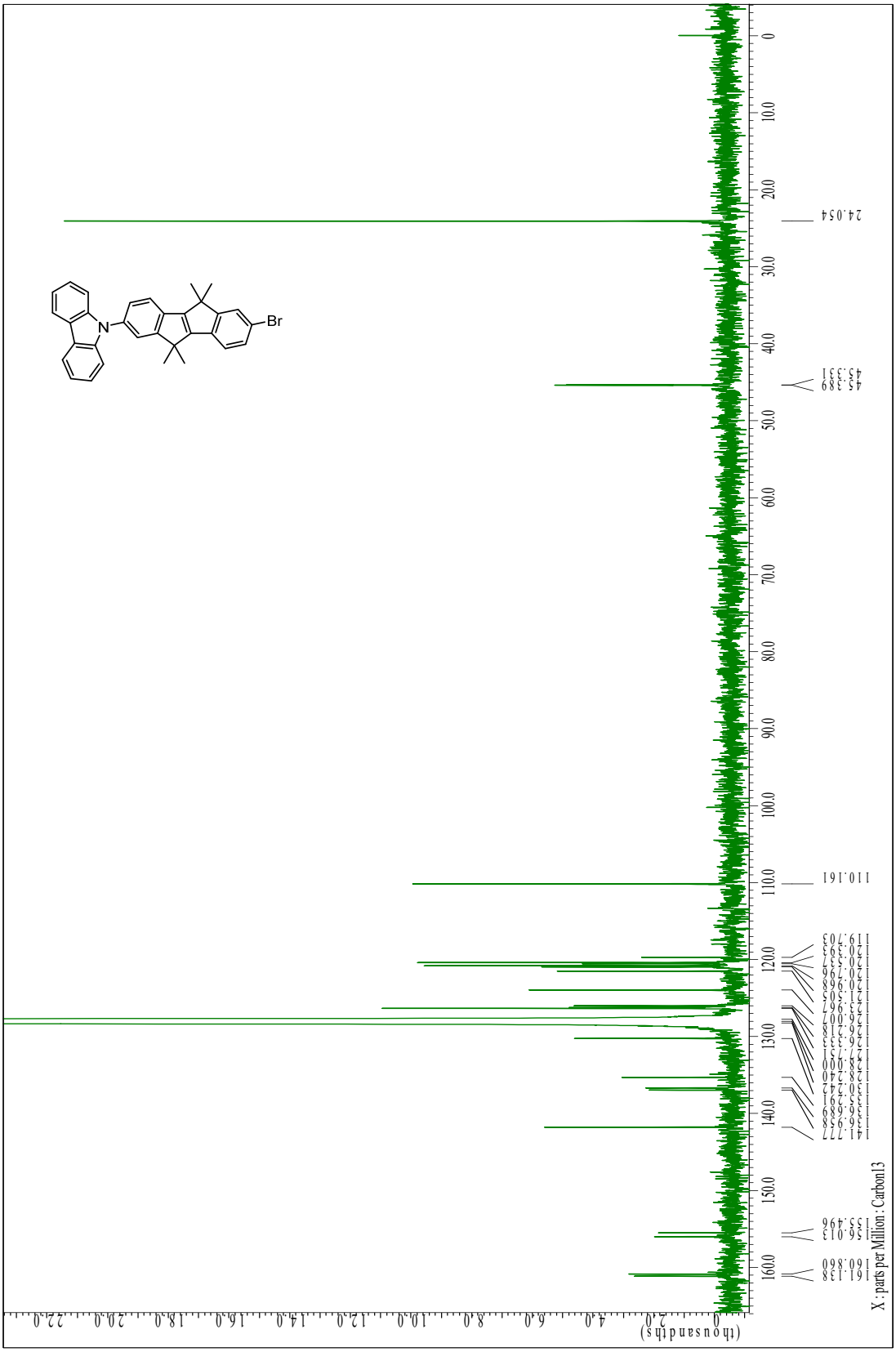


**Figure S4.** $^{13}$C NMR of **Cz-COPV1-Br**

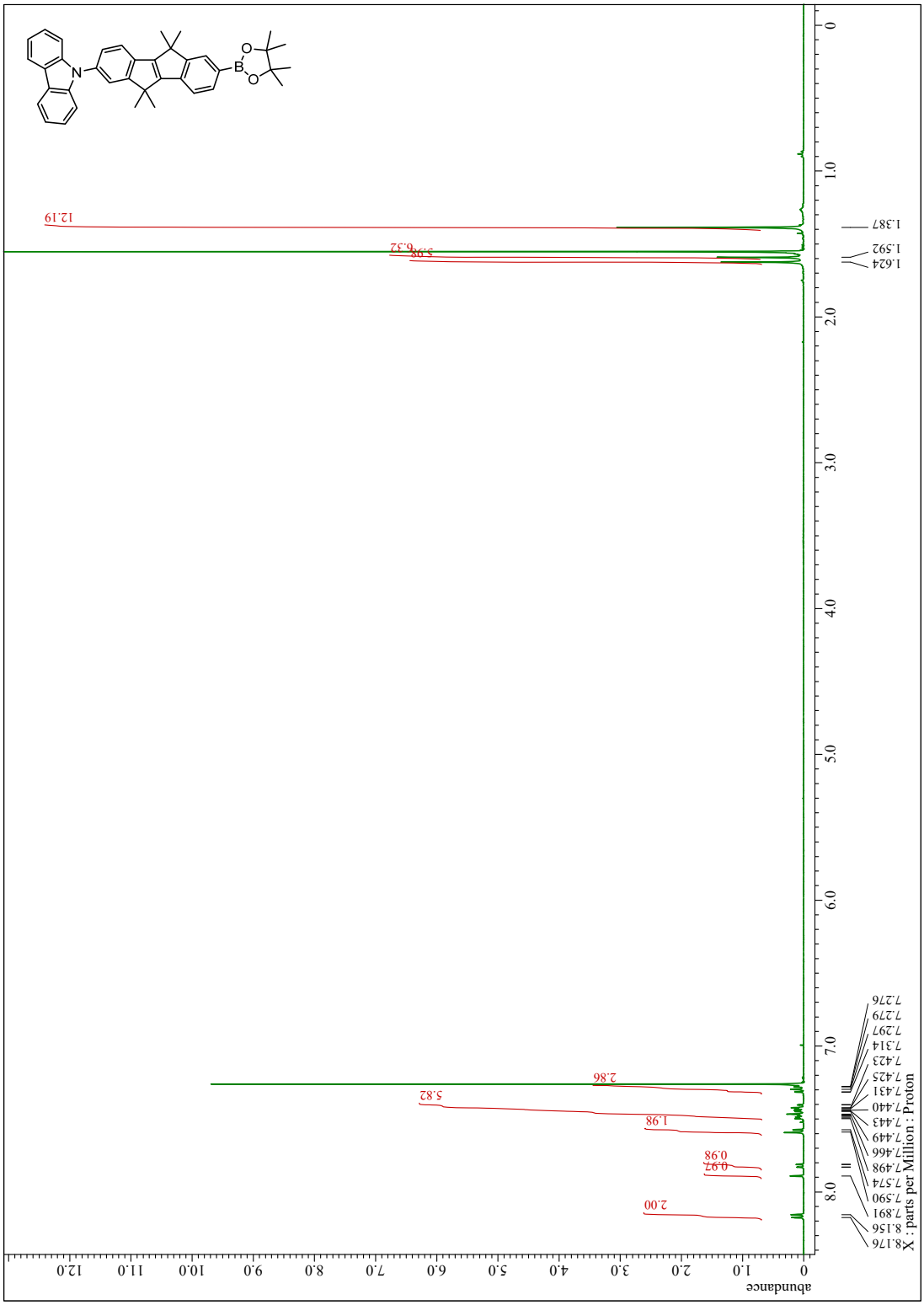


**Figure S5.** $^{1}$H NMR of **Cz-COPV1-Bpin**

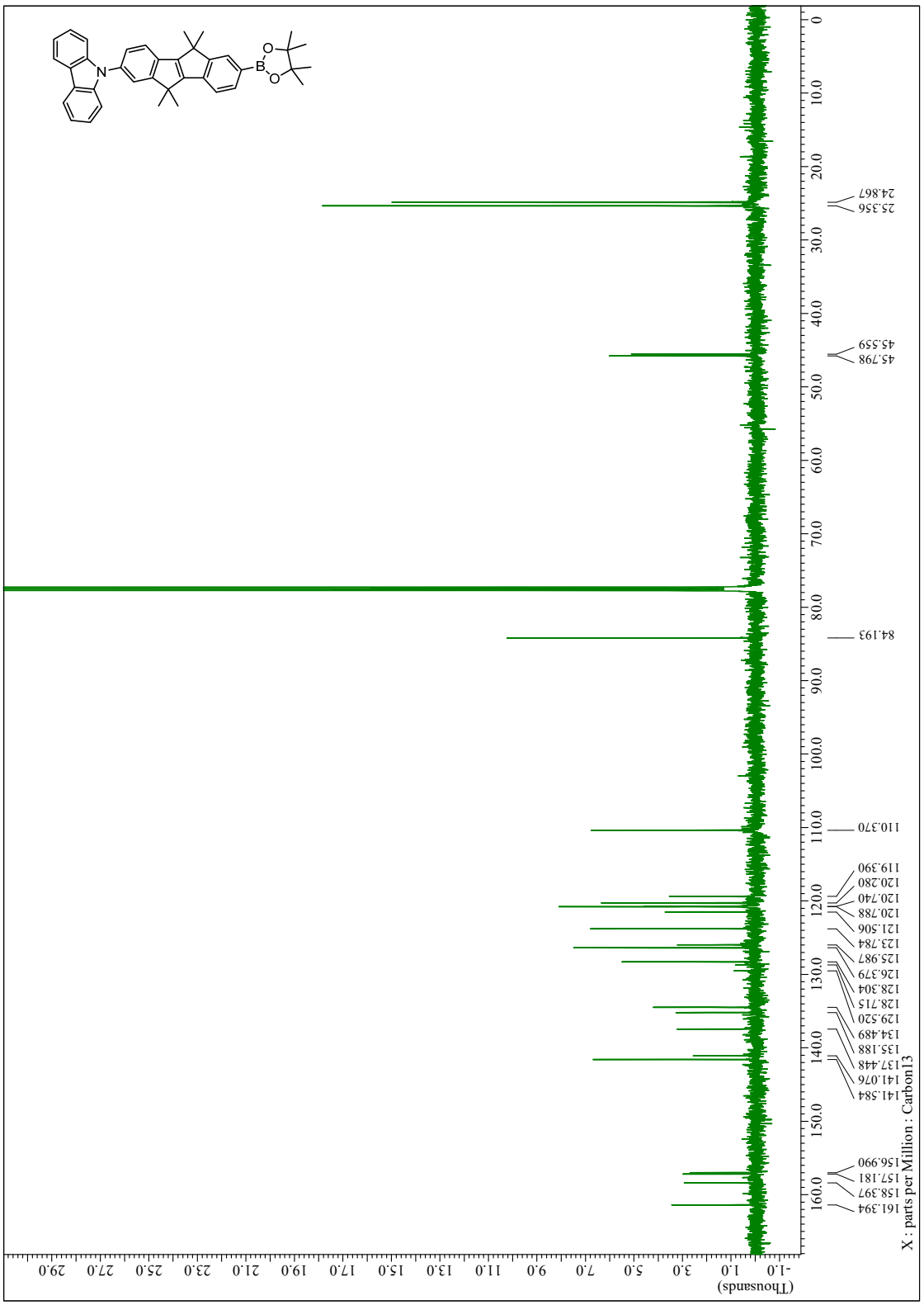


**Figure S6.** $^{13}$C NMR of **Cz-COPV1-Bpin**

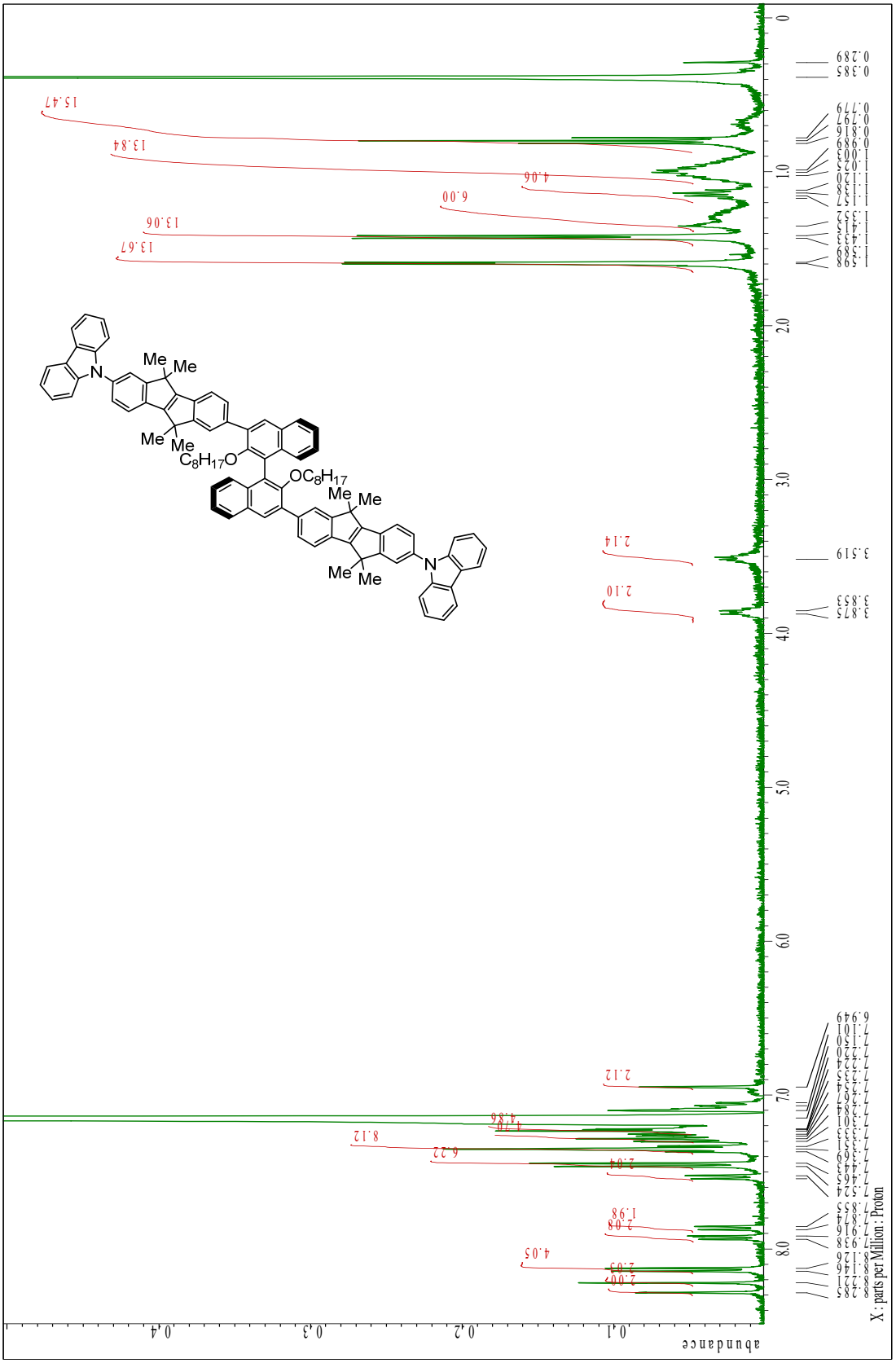


**Figure S7.** $^{1}$H NMR of **(*S*)-3,3'-(CzCOPV1)$_2$-binaph**

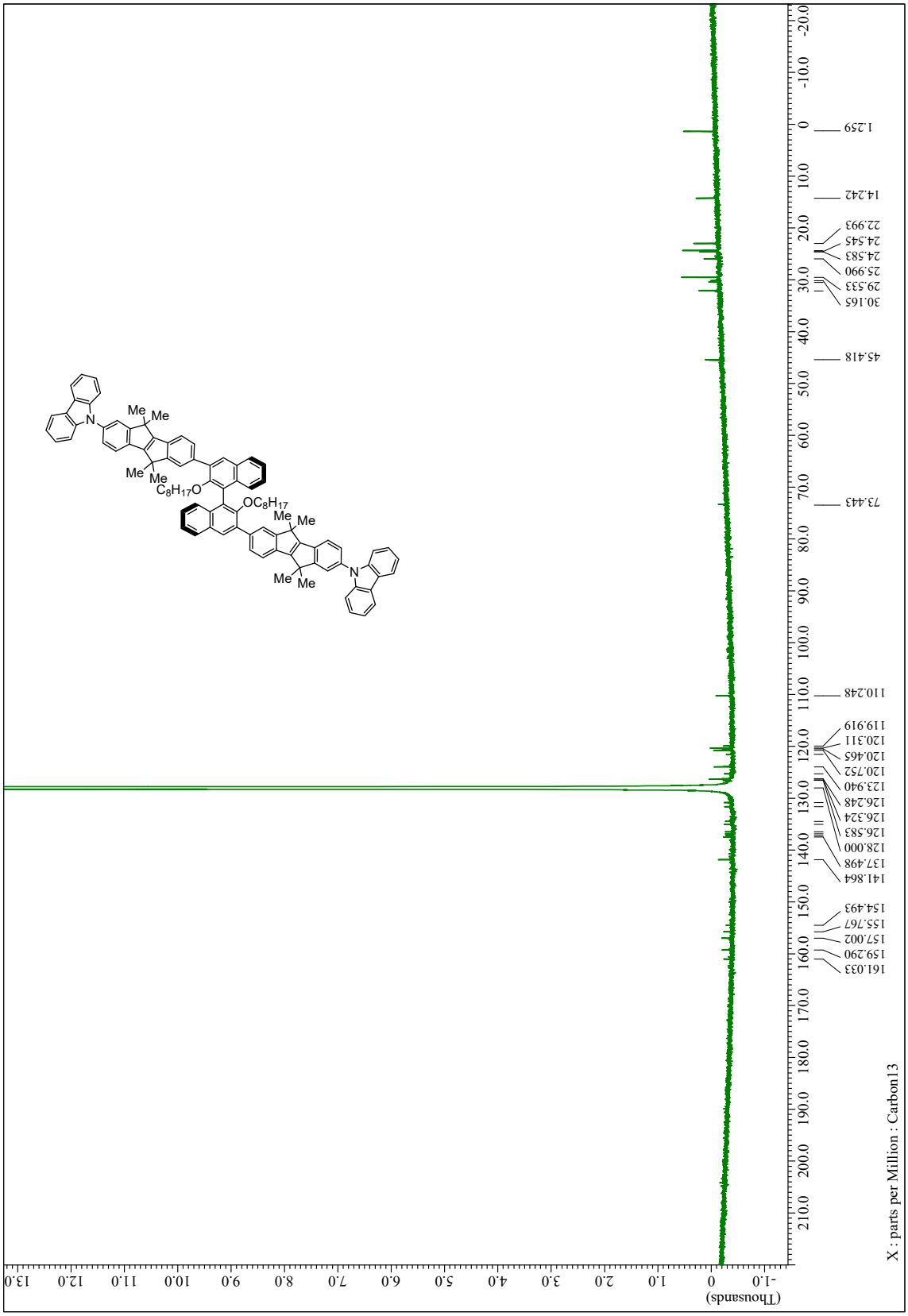


**Figure S8.** $^{13}$C NMR of **(*S*)-3,3'-(CzCOPV1)$_2$-binaph**

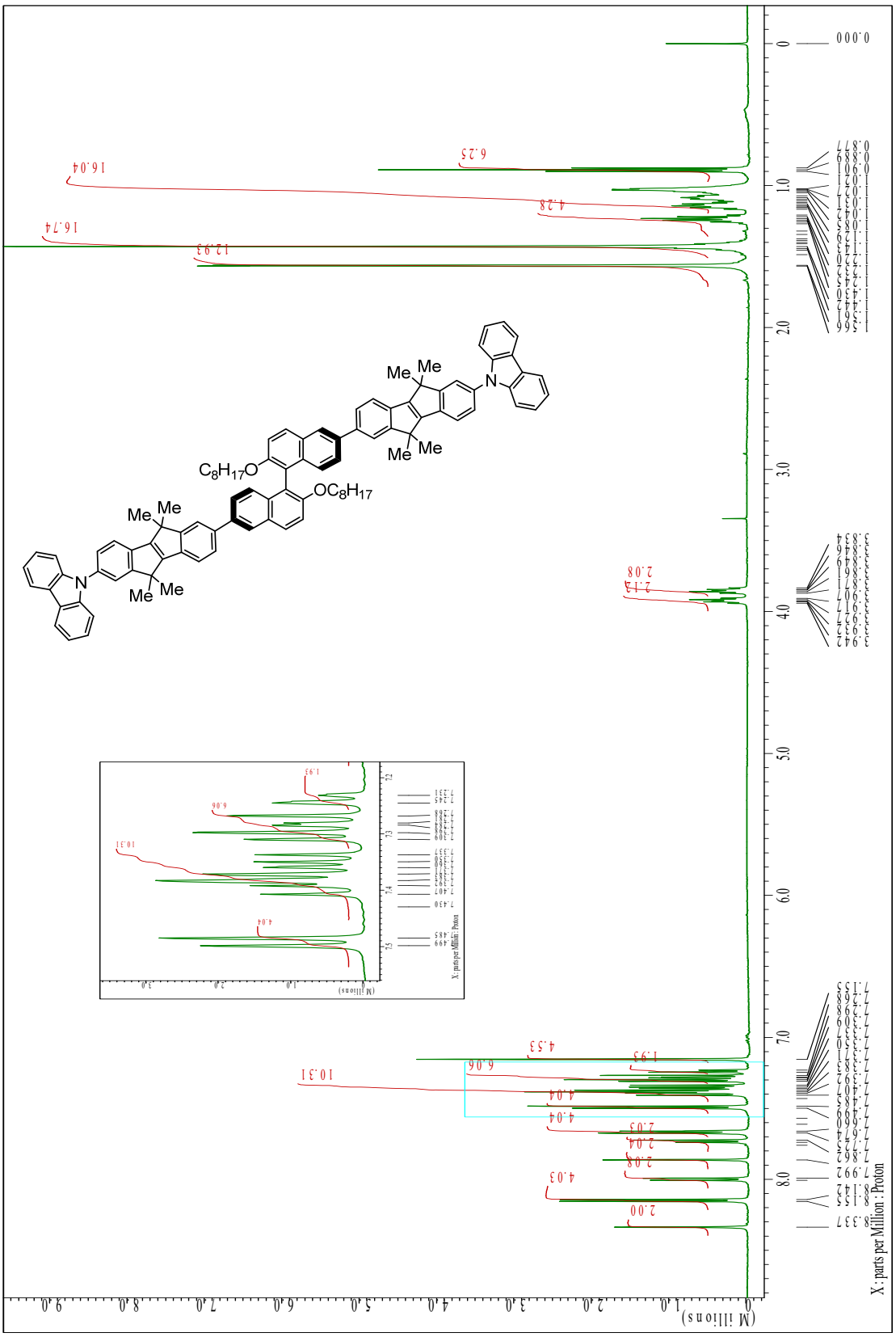


**Figure S9.** $^{1}$H NMR of **(*S*)-6,6'-(CzCOPV1)$_2$-binaph**

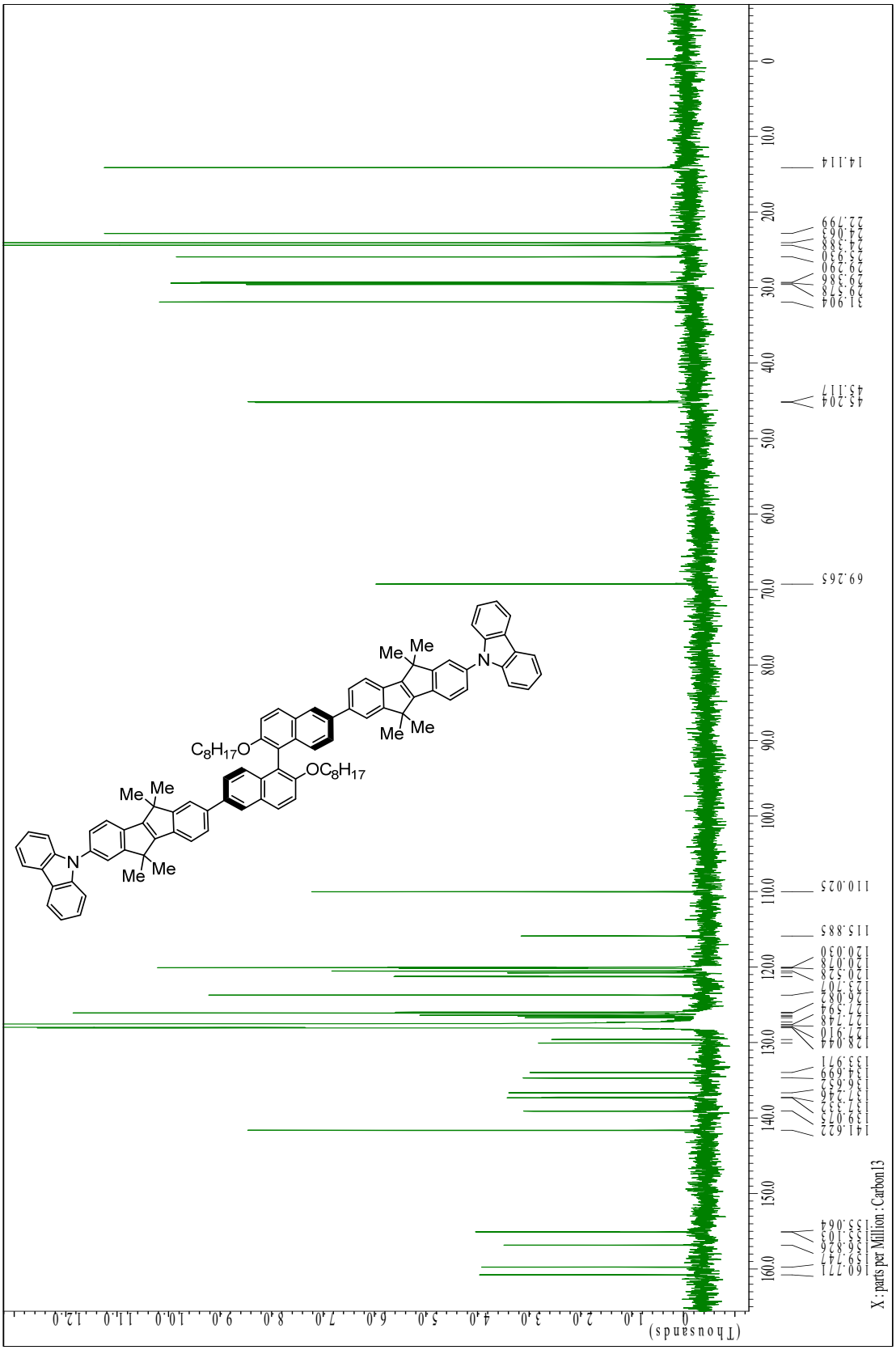


**Figure S10.** $^{13}$C NMR of **(*S*)-6,6'-(CzCOPV1)$_2$-binaph**

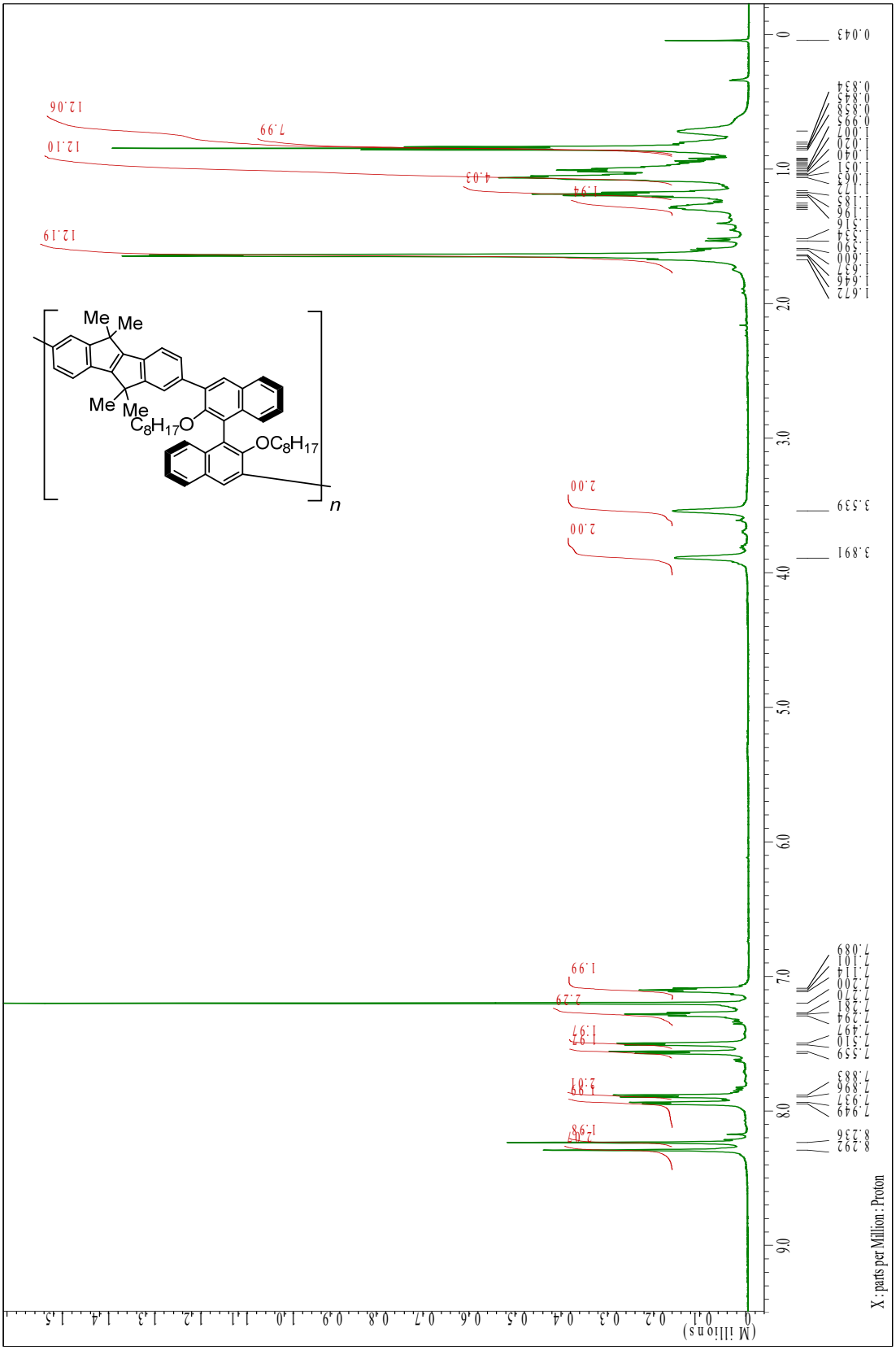


**Figure S11.** $^{1}$H NMR of **poly-[(*S*)-3,3'-COPV1-binaph]**

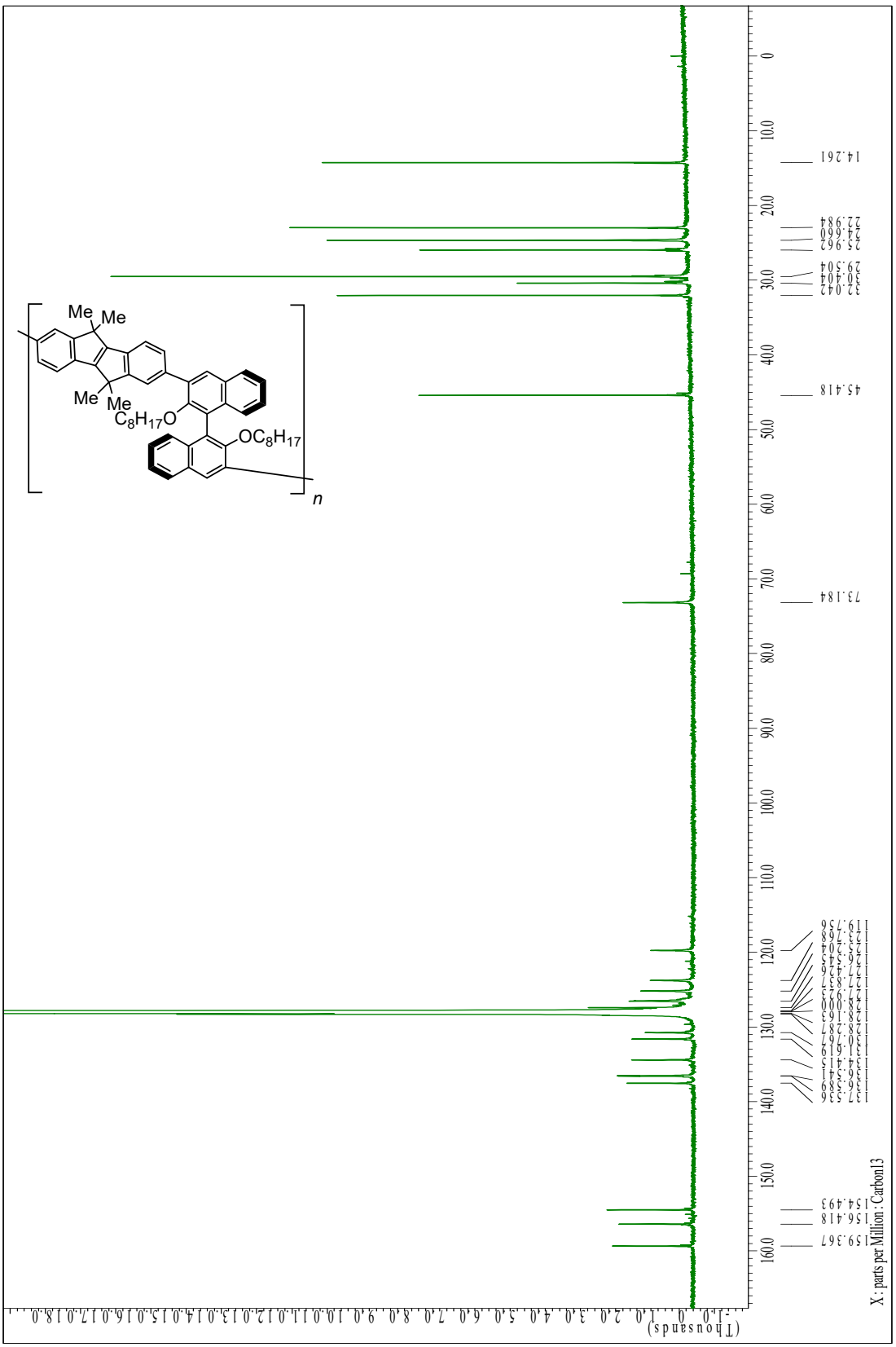


**Figure S12.** $^{13}$C NMR of **poly-[(*S*)-3,3'-COPV1-binaph]**

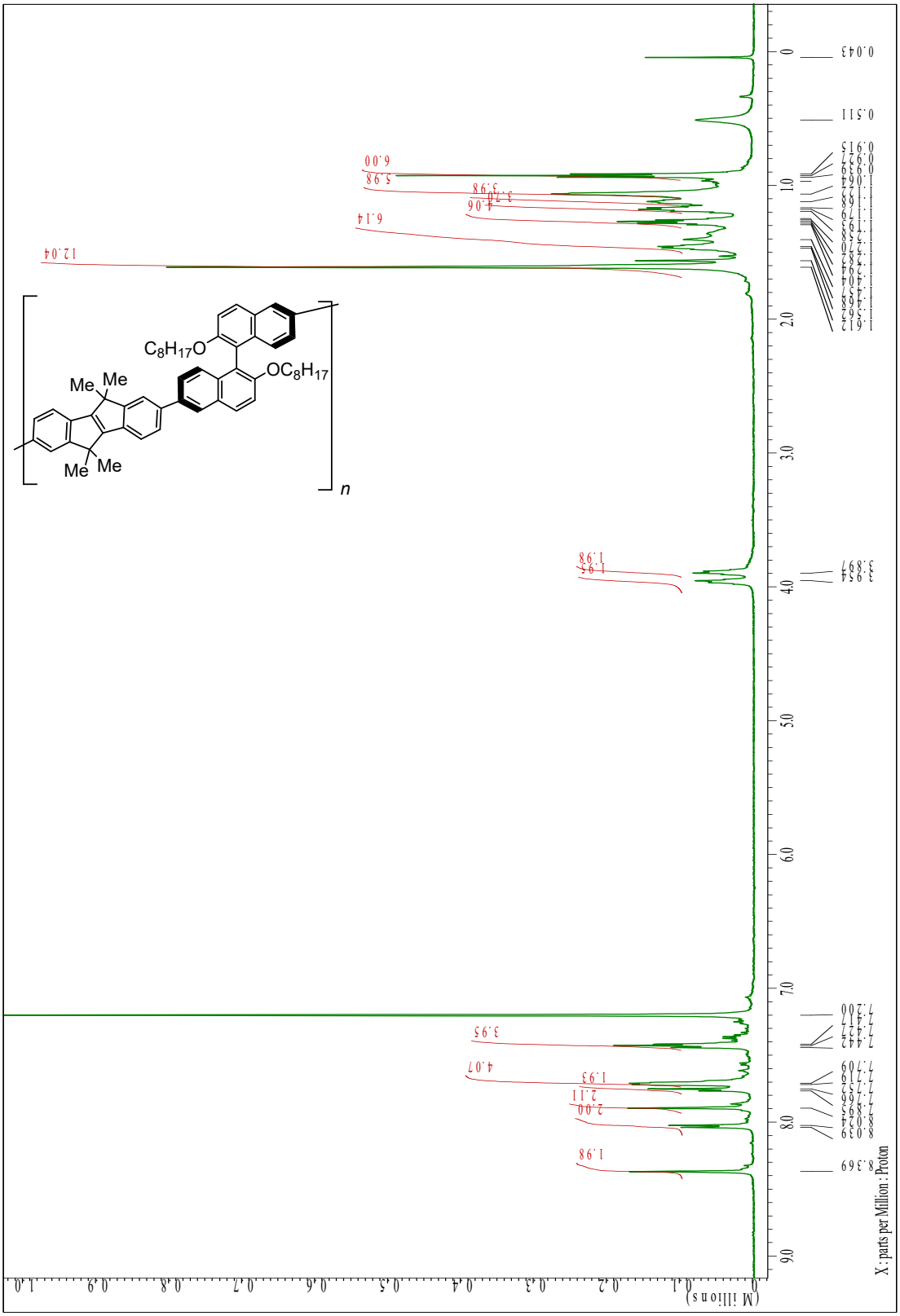


**Figure S13.** $^{1}$H NMR of **poly-[(*S*)-6,6'-COPV1-binaph]**

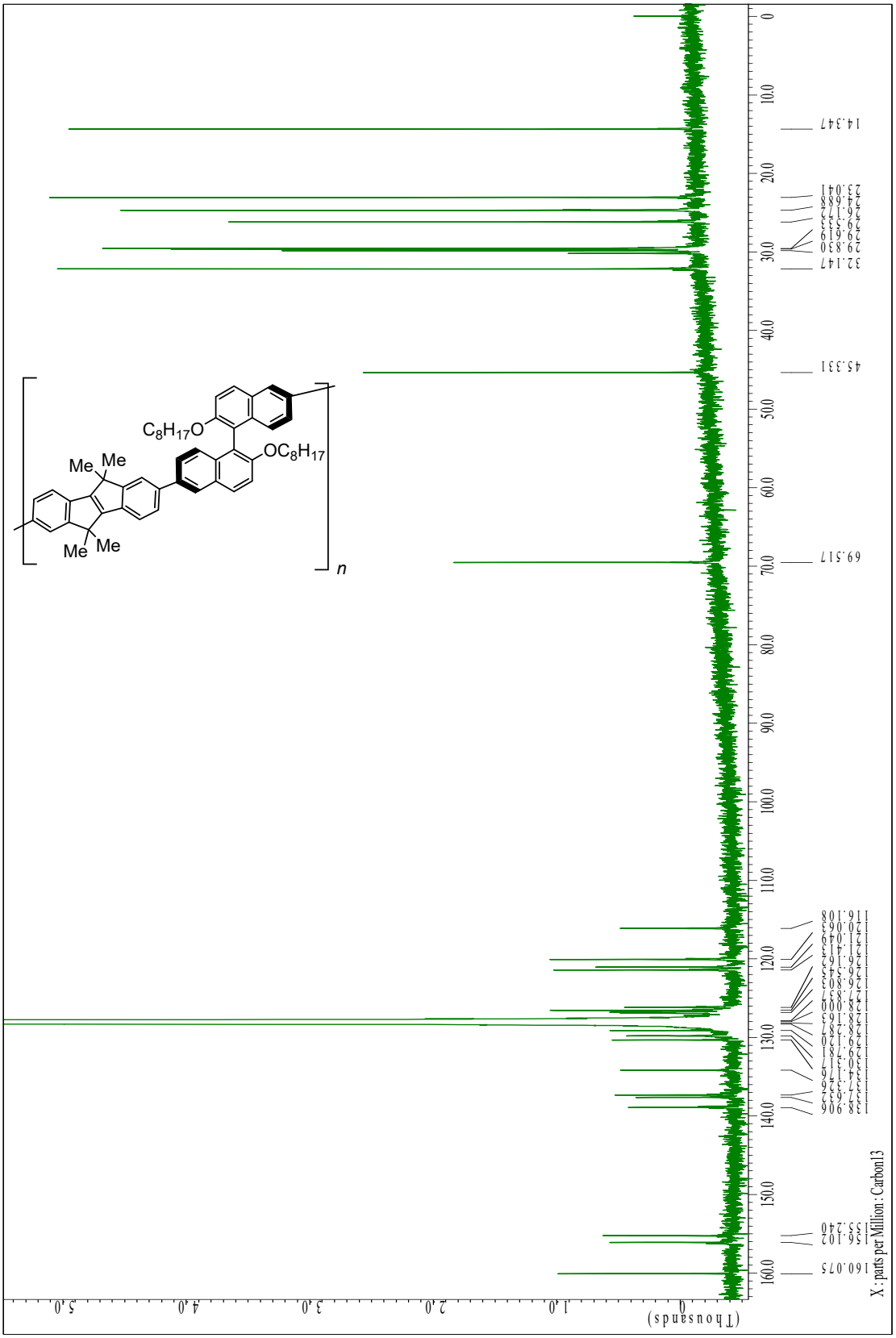


**Figure S14.** $^{13}$C NMR of **poly-[(*S*)-6,6'-COPV1-binaph]**

## 3. Calculations

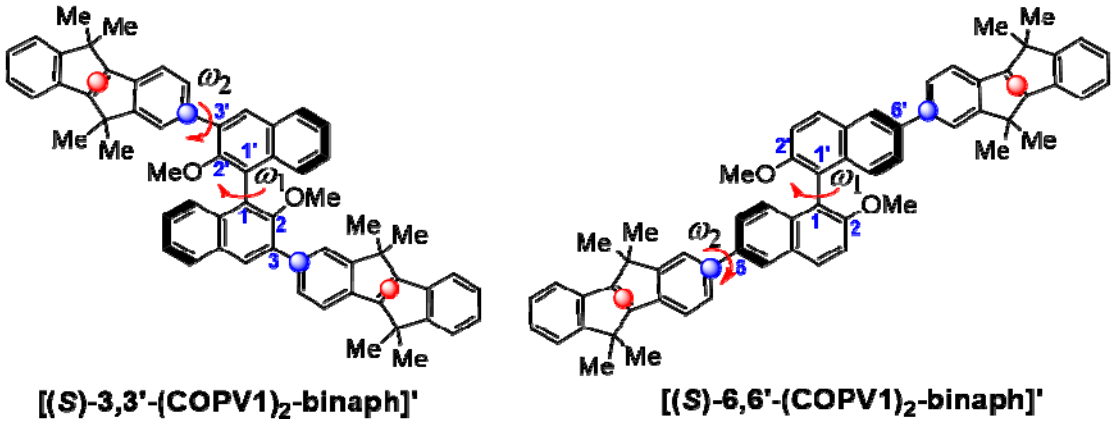


**Figure S15.** Structures of model compounds for calculations.

**Table S1.** Optimized coordinates of a model compound **[(*S*)-3,3'-(COPV1)$_2$-binaph]'** and in the $S_0$ state.

Total energy = −2545.6089624 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.050028 | 3.053370 | 1.556208 |
| 2 | 1 | 0 | 1.602813 | 4.369451 | 2.199279 |
| 3 | 6 | 0 | 1.236713 | 3.345760 | 2.201919 |
| 4 | 6 | 0 | 0.266790 | 0.700255 | 2.281111 |
| 5 | 6 | 0 | 1.967253 | 2.371341 | 2.924384 |
| 6 | 6 | 0 | -0.419542 | 1.699043 | 1.603964 |
| 7 | 6 | 0 | 1.473671 | 1.029175 | 2.984939 |
| 8 | 6 | 0 | 3.163591 | 2.707060 | 3.614717 |
| 9 | 1 | 0 | 1.829139 | -0.935380 | 3.822463 |
| 10 | 6 | 0 | 3.846337 | 1.762630 | 4.345417 |
| 11 | 1 | 0 | 3.525859 | 3.731068 | 3.558062 |
| 12 | 1 | 0 | 4.758883 | 2.030623 | 4.871111 |
| 13 | 6 | 0 | 3.352953 | 0.438307 | 4.418577 |
| 14 | 1 | 0 | 3.889159 | -0.303462 | 5.004560 |
| 15 | 6 | 0 | 2.199196 | 0.081622 | 3.756176 |
| 16 | 6 | 0 | 0.419542 | -1.699043 | 1.603964 |
| 17 | 6 | 0 | -0.266790 | -0.700255 | 2.281111 |
| 18 | 6 | 0 | -1.236713 | -3.345760 | 2.201919 |
| 19 | 6 | 0 | -1.473671 | -1.029175 | 2.984939 |
| 20 | 6 | 0 | -0.050028 | -3.053370 | 1.556208 |
| 21 | 6 | 0 | -1.967253 | -2.371341 | 2.924384 |
| 22 | 6 | 0 | -2.199196 | -0.081622 | 3.756176 |
| 23 | 1 | 0 | -3.525859 | -3.731068 | 3.558062 |
| 24 | 1 | 0 | -1.602813 | -4.369451 | 2.199279 |
| 25 | 6 | 0 | -3.352953 | -0.438307 | 4.418577 |
| 26 | 1 | 0 | -1.829139 | 0.935380 | 3.822463 |

| | | | | | |
|---|---|---|---|---|---|
| 27 | 1 | 0 | -3.889159 | 0.303462 | 5.004560 |
| 28 | 6 | 0 | -3.846337 | -1.762630 | 4.345417 |
| 29 | 1 | 0 | -4.758883 | -2.030623 | 4.871111 |
| 30 | 6 | 0 | -3.163591 | -2.707060 | 3.614717 |
| 31 | 8 | 0 | -1.628470 | 1.386395 | 1.012991 |
| 32 | 8 | 0 | 1.628470 | -1.386395 | 1.012991 |
| 33 | 6 | 0 | -1.617258 | 1.229997 | -0.405053 |
| 34 | 1 | 0 | -1.075945 | 0.319982 | -0.691646 |
| 35 | 1 | 0 | -1.170513 | 2.097320 | -0.904556 |
| 36 | 1 | 0 | -2.661897 | 1.137367 | -0.710976 |
| 37 | 6 | 0 | 1.617258 | -1.229997 | -0.405053 |
| 38 | 1 | 0 | 2.661897 | -1.137367 | -0.710976 |
| 39 | 1 | 0 | 1.075945 | -0.319982 | -0.691646 |
| 40 | 1 | 0 | 1.170513 | -2.097320 | -0.904556 |
| 41 | 1 | 0 | -3.844605 | 5.460444 | 0.596192 |
| 42 | 6 | 0 | -2.775000 | 5.355403 | 0.435264 |
| 43 | 6 | 0 | -0.002868 | 5.061243 | 0.053293 |
| 44 | 6 | 0 | -2.075294 | 6.266593 | -0.360563 |
| 45 | 6 | 0 | -2.086039 | 4.300732 | 1.036203 |
| 46 | 6 | 0 | -0.699505 | 4.135670 | 0.862798 |
| 47 | 6 | 0 | -0.678083 | 6.109133 | -0.548314 |
| 48 | 1 | 0 | -2.626843 | 3.593013 | 1.654066 |
| 49 | 1 | 0 | 1.065552 | 4.928702 | -0.101160 |
| 50 | 6 | 0 | -2.479712 | 7.443569 | -1.114842 |
| 51 | 6 | 0 | -1.402579 | 7.988215 | -1.737991 |
| 52 | 6 | 0 | -1.806007 | 9.167733 | -2.491522 |
| 53 | 6 | 0 | -3.163591 | 11.281345 | -3.702806 |
| 54 | 6 | 0 | -3.203992 | 9.325858 | -2.299832 |
| 55 | 6 | 0 | -1.097589 | 10.070242 | -3.289397 |
| 56 | 6 | 0 | -1.788332 | 11.126663 | -3.892124 |
| 57 | 6 | 0 | -3.878373 | 10.376941 | -2.902370 |
| 58 | 1 | 0 | -0.027589 | 9.959179 | -3.443138 |
| 59 | 1 | 0 | -1.247800 | 11.834930 | -4.514720 |
| 60 | 1 | 0 | -4.949252 | 10.506903 | -2.761586 |
| 61 | 1 | 0 | -3.684729 | 12.107863 | -4.178417 |
| 62 | 6 | 0 | -3.754260 | 8.218054 | -1.390077 |
| 63 | 6 | 0 | -0.127557 | 7.214043 | -1.462285 |
| 64 | 1 | 0 | 3.844605 | -5.460444 | 0.596192 |
| 65 | 6 | 0 | 2.775000 | -5.355403 | 0.435264 |
| 66 | 6 | 0 | 0.002868 | -5.061243 | 0.053293 |
| 67 | 6 | 0 | 2.075294 | -6.266593 | -0.360563 |
| 68 | 6 | 0 | 2.086039 | -4.300732 | 1.036203 |
| 69 | 6 | 0 | 0.699505 | -4.135670 | 0.862798 |
| 70 | 6 | 0 | 0.678083 | -6.109133 | -0.548314 |
| 71 | 1 | 0 | 2.626843 | -3.593013 | 1.654066 |
| 72 | 1 | 0 | -1.065552 | -4.928702 | -0.101160 |
| 73 | 6 | 0 | 2.479712 | -7.443569 | -1.114842 |
| 74 | 6 | 0 | 1.402579 | -7.988215 | -1.737991 |
| 75 | 6 | 0 | 1.806007 | -9.167733 | -2.491522 |
| 76 | 6 | 0 | 3.163591 | -11.281345 | -3.702806 |
| 77 | 6 | 0 | 3.203992 | -9.325858 | -2.299832 |
| 78 | 6 | 0 | 1.097589 | -10.070242 | -3.289397 |
| 79 | 6 | 0 | 1.788332 | -11.126663 | -3.892124 |
| 80 | 6 | 0 | 3.878373 | -10.376941 | -2.902370 |

| | | | | | |
|---|---|---|---|---|---|
| 81 | 1 | 0 | 0.027589 | -9.959179 | -3.443138 |
| 82 | 1 | 0 | 1.247800 | -11.834930 | -4.514720 |
| 83 | 1 | 0 | 4.949252 | -10.506903 | -2.761586 |
| 84 | 1 | 0 | 3.684729 | -12.107863 | -4.178417 |
| 85 | 6 | 0 | 3.754260 | -8.218054 | -1.390077 |
| 86 | 6 | 0 | 0.127557 | -7.214043 | -1.462285 |
| 87 | 6 | 0 | -0.477005 | -6.624606 | -2.756896 |
| 88 | 1 | 0 | -1.352644 | -6.006217 | -2.528231 |
| 89 | 1 | 0 | -0.796292 | -7.424203 | -3.435188 |
| 90 | 1 | 0 | 0.253578 | -6.002308 | -3.283473 |
| 91 | 6 | 0 | -0.922662 | -8.079176 | -0.729152 |
| 92 | 1 | 0 | -1.805545 | -7.481752 | -0.474009 |
| 93 | 1 | 0 | -0.511793 | -8.495154 | 0.196218 |
| 94 | 1 | 0 | -1.250239 | -8.911800 | -1.362223 |
| 95 | 6 | 0 | 4.803155 | -7.354383 | -2.126989 |
| 96 | 1 | 0 | 5.131456 | -6.520324 | -1.496116 |
| 97 | 1 | 0 | 4.390922 | -6.940950 | -3.052932 |
| 98 | 1 | 0 | 5.685704 | -7.952136 | -2.382242 |
| 99 | 6 | 0 | 4.360899 | -8.803359 | -0.094463 |
| 100 | 1 | 0 | 4.679612 | -8.001507 | 0.581443 |
| 101 | 1 | 0 | 5.237283 | -9.420864 | -0.322516 |
| 102 | 1 | 0 | 3.632101 | -9.425978 | 0.434044 |
| 103 | 6 | 0 | 0.477005 | 6.624606 | -2.756896 |
| 104 | 1 | 0 | 0.796292 | 7.424203 | -3.435188 |
| 105 | 1 | 0 | -0.253578 | 6.002308 | -3.283473 |
| 106 | 1 | 0 | 1.352644 | 6.006217 | -2.528231 |
| 107 | 6 | 0 | 0.922662 | 8.079176 | -0.729152 |
| 108 | 1 | 0 | 0.511793 | 8.495154 | 0.196218 |
| 109 | 1 | 0 | 1.250239 | 8.911800 | -1.362223 |
| 110 | 1 | 0 | 1.805545 | 7.481752 | -0.474009 |
| 111 | 6 | 0 | -4.803155 | 7.354383 | -2.126989 |
| 112 | 1 | 0 | -5.685704 | 7.952136 | -2.382242 |
| 113 | 1 | 0 | -5.131456 | 6.520324 | -1.496116 |
| 114 | 1 | 0 | -4.390922 | 6.940950 | -3.052932 |
| 115 | 6 | 0 | -4.360899 | 8.803359 | -0.094463 |
| 116 | 1 | 0 | -5.237283 | 9.420864 | -0.322516 |
| 117 | 1 | 0 | -3.632101 | 9.425978 | 0.434044 |
| 118 | 1 | 0 | -4.679612 | 8.001507 | 0.581443 |

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**Table S2.** Optimized coordinates of a model compound **[(*S*)-3,3'-(COPV1)$_2$-binaph]'** and in the $S_1$ state.

Total energy = −2545.6031367 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.606334 | 2.991973 | 1.471899 |
| 2 | 1 | 0 | 0.702022 | 4.599431 | 2.049651 |
| 3 | 6 | 0 | 0.543957 | 3.524823 | 2.069255 |
| 4 | 6 | 0 | 0.110383 | 0.738728 | 2.211731 |
| 5 | 6 | 0 | 1.465552 | 2.732625 | 2.779755 |

| | | | | | |
|---|---|---|---|---|---|
| 6 | 6 | 0 | -0.790449 | 1.573187 | 1.561060 |
| 7 | 6 | 0 | 1.249033 | 1.316778 | 2.883439 |
| 8 | 6 | 0 | 2.596572 | 3.309039 | 3.429025 |
| 9 | 1 | 0 | 1.983441 | -0.511813 | 3.764464 |
| 10 | 6 | 0 | 3.464618 | 2.532365 | 4.163566 |
| 11 | 1 | 0 | 2.755260 | 4.381341 | 3.338246 |
| 12 | 1 | 0 | 4.320256 | 2.986875 | 4.656563 |
| 13 | 6 | 0 | 3.235884 | 1.144200 | 4.287311 |
| 14 | 1 | 0 | 3.911589 | 0.535629 | 4.882238 |
| 15 | 6 | 0 | 2.152516 | 0.554191 | 3.659374 |
| 16 | 6 | 0 | 0.790449 | -1.573187 | 1.561060 |
| 17 | 6 | 0 | -0.110383 | -0.738728 | 2.211731 |
| 18 | 6 | 0 | -0.543957 | -3.524823 | 2.069255 |
| 19 | 6 | 0 | -1.249033 | -1.316778 | 2.883439 |
| 20 | 6 | 0 | 0.606334 | -2.991973 | 1.471899 |
| 21 | 6 | 0 | -1.465552 | -2.732625 | 2.779755 |
| 22 | 6 | 0 | -2.152516 | -0.554191 | 3.659374 |
| 23 | 1 | 0 | -2.755260 | -4.381341 | 3.338246 |
| 24 | 1 | 0 | -0.702022 | -4.599431 | 2.049651 |
| 25 | 6 | 0 | -3.235884 | -1.144200 | 4.287311 |
| 26 | 1 | 0 | -1.983441 | 0.511813 | 3.764464 |
| 27 | 1 | 0 | -3.911589 | -0.535629 | 4.882238 |
| 28 | 6 | 0 | -3.464618 | -2.532365 | 4.163566 |
| 29 | 1 | 0 | -4.320256 | -2.986875 | 4.656563 |
| 30 | 6 | 0 | -2.596572 | -3.309039 | 3.429025 |
| 31 | 8 | 0 | -1.919376 | 1.010099 | 0.990455 |
| 32 | 8 | 0 | 1.919376 | -1.010099 | 0.990455 |
| 33 | 6 | 0 | -1.845752 | 0.731705 | -0.405605 |
| 34 | 1 | 0 | -1.148565 | -0.090992 | -0.603735 |
| 35 | 1 | 0 | -1.543078 | 1.617350 | -0.977861 |
| 36 | 1 | 0 | -2.850442 | 0.430863 | -0.712579 |
| 37 | 6 | 0 | 1.845752 | -0.731705 | -0.405605 |
| 38 | 1 | 0 | 2.850442 | -0.430863 | -0.712579 |
| 39 | 1 | 0 | 1.148565 | 0.090992 | -0.603735 |
| 40 | 1 | 0 | 1.543078 | -1.617350 | -0.977861 |
| 41 | 1 | 0 | -4.921928 | 4.372821 | 0.310635 |
| 42 | 6 | 0 | -3.853543 | 4.560083 | 0.244494 |
| 43 | 6 | 0 | -1.076508 | 5.044919 | 0.119710 |
| 44 | 6 | 0 | -3.363731 | 5.701240 | -0.422315 |
| 45 | 6 | 0 | -2.963881 | 3.676235 | 0.833580 |
| 46 | 6 | 0 | -1.556758 | 3.885821 | 0.793884 |
| 47 | 6 | 0 | -1.950838 | 5.926198 | -0.474831 |
| 48 | 1 | 0 | -3.343134 | 2.805687 | 1.352991 |
| 49 | 1 | 0 | -0.004191 | 5.207389 | 0.052529 |
| 50 | 6 | 0 | -3.994798 | 6.776662 | -1.122648 |
| 51 | 6 | 0 | -3.042606 | 7.652650 | -1.610932 |
| 52 | 6 | 0 | -3.680440 | 8.728924 | -2.317574 |
| 53 | 6 | 0 | -5.455505 | 10.513323 | -3.530270 |
| 54 | 6 | 0 | -5.090267 | 8.502449 | -2.258632 |
| 55 | 6 | 0 | -3.177393 | 9.857201 | -2.989844 |
| 56 | 6 | 0 | -4.073691 | 10.739263 | -3.590388 |
| 57 | 6 | 0 | -5.966581 | 9.388776 | -2.860863 |
| 58 | 1 | 0 | -2.108075 | 10.041619 | -3.042038 |
| 59 | 1 | 0 | -3.696554 | 11.614703 | -4.112567 |

| | | | | | |
|---|---|---|---|---|---|
| 60 | 1 | 0 | -7.041139 | 9.224647 | -2.821218 |
| 61 | 1 | 0 | -6.137303 | 11.213538 | -4.004918 |
| 62 | 6 | 0 | -5.401624 | 7.217373 | -1.477752 |
| 63 | 6 | 0 | -1.635992 | 7.212272 | -1.257005 |
| 64 | 1 | 0 | 4.921928 | -4.372821 | 0.310635 |
| 65 | 6 | 0 | 3.853543 | -4.560083 | 0.244494 |
| 66 | 6 | 0 | 1.076508 | -5.044919 | 0.119710 |
| 67 | 6 | 0 | 3.363731 | -5.701240 | -0.422315 |
| 68 | 6 | 0 | 2.963881 | -3.676235 | 0.833580 |
| 69 | 6 | 0 | 1.556758 | -3.885821 | 0.793884 |
| 70 | 6 | 0 | 1.950838 | -5.926198 | -0.474831 |
| 71 | 1 | 0 | 3.343134 | -2.805687 | 1.352991 |
| 72 | 1 | 0 | 0.004191 | -5.207389 | 0.052529 |
| 73 | 6 | 0 | 3.994798 | -6.776662 | -1.122648 |
| 74 | 6 | 0 | 3.042606 | -7.652650 | -1.610932 |
| 75 | 6 | 0 | 3.680440 | -8.728924 | -2.317574 |
| 76 | 6 | 0 | 5.455505 | -10.513323 | -3.530270 |
| 77 | 6 | 0 | 5.090267 | -8.502449 | -2.258632 |
| 78 | 6 | 0 | 3.177393 | -9.857201 | -2.989844 |
| 79 | 6 | 0 | 4.073691 | -10.739263 | -3.590388 |
| 80 | 6 | 0 | 5.966581 | -9.388776 | -2.860863 |
| 81 | 1 | 0 | 2.108075 | -10.041619 | -3.042038 |
| 82 | 1 | 0 | 3.696554 | -11.614703 | -4.112567 |
| 83 | 1 | 0 | 7.041139 | -9.224647 | -2.821218 |
| 84 | 1 | 0 | 6.137303 | -11.213538 | -4.004918 |
| 85 | 6 | 0 | 5.401624 | -7.217373 | -1.477752 |
| 86 | 6 | 0 | 1.635992 | -7.212272 | -1.257005 |
| 87 | 6 | 0 | 0.790449 | -6.915282 | -2.517269 |
| 88 | 1 | 0 | -0.192366 | -6.519532 | -2.236286 |
| 89 | 1 | 0 | 0.632501 | -7.827557 | -3.103967 |
| 90 | 1 | 0 | 1.284900 | -6.178120 | -3.157704 |
| 91 | 6 | 0 | 0.914009 | -8.249316 | -0.365572 |
| 92 | 1 | 0 | -0.066358 | -7.870956 | -0.053589 |
| 93 | 1 | 0 | 1.497310 | -8.468042 | 0.534317 |
| 94 | 1 | 0 | 0.757046 | -9.188111 | -0.909126 |
| 95 | 6 | 0 | 6.122212 | -6.177866 | -2.367168 |
| 96 | 1 | 0 | 6.272750 | -5.239232 | -1.821942 |
| 97 | 1 | 0 | 5.540475 | -5.960415 | -3.268465 |
| 98 | 1 | 0 | 7.105375 | -6.551109 | -2.676160 |
| 99 | 6 | 0 | 6.245292 | -7.514269 | -0.216321 |
| 100 | 1 | 0 | 6.397162 | -6.602194 | 0.371878 |
| 101 | 1 | 0 | 7.230604 | -7.905063 | -0.495310 |
| 102 | 1 | 0 | 5.752098 | -8.254214 | 0.421760 |
| 103 | 6 | 0 | -0.790449 | 6.915282 | -2.517269 |
| 104 | 1 | 0 | -0.632501 | 7.827557 | -3.103967 |
| 105 | 1 | 0 | -1.284900 | 6.178120 | -3.157704 |
| 106 | 1 | 0 | 0.192366 | 6.519532 | -2.236286 |
| 107 | 6 | 0 | -0.914009 | 8.249316 | -0.365572 |
| 108 | 1 | 0 | -1.497310 | 8.468042 | 0.534317 |
| 109 | 1 | 0 | -0.757046 | 9.188111 | -0.909126 |
| 110 | 1 | 0 | 0.066358 | 7.870956 | -0.053589 |
| 111 | 6 | 0 | -6.122212 | 6.177866 | -2.367168 |
| 112 | 1 | 0 | -7.105375 | 6.551109 | -2.676160 |
| 113 | 1 | 0 | -6.272750 | 5.239232 | -1.821942 |

| | | | | | |
|---|---|---|---|---|---|
| 114 | 1 | 0 | -5.540475 | 5.960415 | -3.268465 |
| 115 | 6 | 0 | -6.245292 | 7.514269 | -0.216321 |
| 116 | 1 | 0 | -7.230604 | 7.905063 | -0.495310 |
| 117 | 1 | 0 | -5.752098 | 8.254214 | 0.421760 |
| 118 | 1 | 0 | -6.397162 | 6.602194 | 0.371878 |

**Table S3.** Optimized coordinates of a model compound **[(*S*)-6,6'-(COPV1)$_2$-binaph]'** and in the $S_0$ state.

Total energy = −2545.6219593 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -1.481532 | 5.044264 | -3.406458 |
| 2 | 6 | 0 | -1.537583 | 4.371999 | -2.558147 |
| 3 | 1 | 0 | -3.419827 | 3.564321 | -3.163867 |
| 4 | 6 | 0 | -2.626018 | 3.541551 | -2.420897 |
| 5 | 6 | 0 | -0.555767 | 3.487855 | -0.500418 |
| 6 | 6 | 0 | -2.736671 | 2.651622 | -1.324786 |
| 7 | 6 | 0 | -0.498046 | 4.349026 | -1.593589 |
| 8 | 6 | 0 | -1.681605 | 2.625579 | -0.353872 |
| 9 | 6 | 0 | -3.852670 | 1.789175 | -1.173644 |
| 10 | 1 | 0 | -1.034336 | 1.687126 | 1.489037 |
| 11 | 6 | 0 | -3.965348 | 0.912004 | -0.108646 |
| 12 | 1 | 0 | -4.622044 | 1.809591 | -1.941905 |
| 13 | 6 | 0 | -2.908931 | 0.896283 | 0.850935 |
| 14 | 1 | 0 | -2.989564 | 0.235997 | 1.709840 |
| 15 | 6 | 0 | -1.814372 | 1.717384 | 0.735316 |
| 16 | 6 | 0 | 0.498035 | 4.349009 | 1.593591 |
| 17 | 6 | 0 | 0.555763 | 3.487853 | 0.500411 |
| 18 | 6 | 0 | 2.626009 | 3.541534 | 2.420899 |
| 19 | 6 | 0 | 1.681607 | 2.625583 | 0.353857 |
| 20 | 6 | 0 | 1.537570 | 4.371974 | 2.558155 |
| 21 | 6 | 0 | 2.736669 | 2.651618 | 1.324776 |
| 22 | 6 | 0 | 1.814381 | 1.717404 | -0.735341 |
| 23 | 1 | 0 | 1.481510 | 5.044230 | 3.406473 |
| 24 | 1 | 0 | 4.622039 | 1.809581 | 1.941894 |
| 25 | 1 | 0 | 3.419816 | 3.564295 | 3.163870 |
| 26 | 6 | 0 | 2.908943 | 0.896306 | -0.850966 |
| 27 | 1 | 0 | 1.034350 | 1.687154 | -1.489066 |
| 28 | 1 | 0 | 2.989582 | 0.236034 | -1.709880 |
| 29 | 6 | 0 | 3.965354 | 0.912017 | 0.108620 |
| 30 | 6 | 0 | 3.852668 | 1.789175 | 1.173630 |
| 31 | 8 | 0 | 0.606111 | 5.150099 | -1.673586 |
| 32 | 8 | 0 | -0.606128 | 5.150077 | 1.673599 |
| 33 | 6 | 0 | 0.732693 | 6.039708 | -2.769308 |
| 34 | 1 | 0 | -0.081098 | 6.776880 | -2.792742 |
| 35 | 1 | 0 | 0.762724 | 5.505137 | -3.728231 |
| 36 | 1 | 0 | 1.681480 | 6.558777 | -2.620236 |
| 37 | 6 | 0 | -0.732719 | 6.039657 | 2.769350 |
| 38 | 1 | 0 | -0.762735 | 5.505057 | 3.728256 |

| | | | | | |
|---|---|---|---|---|---|
| 39 | 1 | 0 | -1.681516 | 6.558712 | 2.620295 |
| 40 | 1 | 0 | 0.081062 | 6.776839 | 2.792799 |
| 41 | 1 | 0 | 5.922728 | -3.151574 | -1.085659 |
| 42 | 6 | 0 | 6.075921 | -2.149942 | -0.692955 |
| 43 | 6 | 0 | 6.429238 | 0.446350 | 0.337426 |
| 44 | 6 | 0 | 7.347363 | -1.712131 | -0.314489 |
| 45 | 6 | 0 | 4.988620 | -1.285986 | -0.552279 |
| 46 | 6 | 0 | 5.136773 | 0.015043 | -0.038466 |
| 47 | 6 | 0 | 7.514095 | -0.401418 | 0.204247 |
| 48 | 1 | 0 | 3.996820 | -1.637862 | -0.821709 |
| 49 | 1 | 0 | 6.562815 | 1.460471 | 0.706245 |
| 50 | 6 | 0 | 8.661276 | -2.336570 | -0.333516 |
| 51 | 6 | 0 | 9.594342 | -1.470250 | 0.140048 |
| 52 | 6 | 0 | 10.910055 | -2.094747 | 0.120411 |
| 53 | 6 | 0 | 13.104440 | -3.793907 | -0.157466 |
| 54 | 6 | 0 | 10.740643 | -3.406638 | -0.395901 |
| 55 | 6 | 0 | 12.178805 | -1.643257 | 0.493962 |
| 56 | 6 | 0 | 13.272313 | -2.503607 | 0.350413 |
| 57 | 6 | 0 | 11.831880 | -4.250836 | -0.533731 |
| 58 | 1 | 0 | 12.320583 | -0.641345 | 0.890141 |
| 59 | 1 | 0 | 14.263812 | -2.163156 | 0.637712 |
| 60 | 1 | 0 | 11.712372 | -5.257611 | -0.928281 |
| 61 | 1 | 0 | 13.964825 | -4.449408 | -0.262444 |
| 62 | 6 | 0 | 8.990224 | -0.136710 | 0.537325 |
| 63 | 6 | 0 | 9.265747 | -3.668939 | -0.732999 |
| 64 | 6 | 0 | 8.694873 | -4.833491 | 0.107767 |
| 65 | 1 | 0 | 7.623228 | -4.961464 | -0.083688 |
| 66 | 1 | 0 | 8.830776 | -4.648578 | 1.178041 |
| 67 | 1 | 0 | 9.197395 | -5.774614 | -0.143631 |
| 68 | 6 | 0 | 9.075702 | -3.955981 | -2.239843 |
| 69 | 1 | 0 | 9.484581 | -3.143593 | -2.848939 |
| 70 | 1 | 0 | 8.012387 | -4.063838 | -2.483083 |
| 71 | 1 | 0 | 9.582866 | -4.885351 | -2.523516 |
| 72 | 6 | 0 | 9.557929 | 1.025317 | -0.308986 |
| 73 | 1 | 0 | 9.420245 | 0.835870 | -1.378217 |
| 74 | 1 | 0 | 10.629767 | 1.155568 | -0.119994 |
| 75 | 1 | 0 | 9.054199 | 1.966567 | -0.060700 |
| 76 | 6 | 0 | 9.183162 | 0.155735 | 2.042627 |
| 77 | 1 | 0 | 8.676067 | 1.085969 | 2.323684 |
| 78 | 1 | 0 | 10.246828 | 0.265014 | 2.283716 |
| 79 | 1 | 0 | 8.775773 | -0.654597 | 2.655499 |
| 80 | 1 | 0 | -5.922715 | -3.151601 | 1.085598 |
| 81 | 6 | 0 | -6.075911 | -2.149963 | 0.692912 |
| 82 | 6 | 0 | -6.429234 | 0.446344 | -0.337429 |
| 83 | 6 | 0 | -7.347356 | -1.712143 | 0.314469 |
| 84 | 6 | 0 | -4.988609 | -1.286007 | 0.552233 |
| 85 | 6 | 0 | -5.136767 | 0.015029 | 0.038441 |
| 86 | 6 | 0 | -7.514092 | -0.401423 | -0.204248 |
| 87 | 1 | 0 | -3.996806 | -1.637889 | 0.821645 |
| 88 | 1 | 0 | -6.562813 | 1.460470 | -0.706234 |
| 89 | 6 | 0 | -8.661271 | -2.336579 | 0.333506 |
| 90 | 6 | 0 | -9.594342 | -1.470250 | -0.140032 |
| 91 | 6 | 0 | -10.910056 | -2.094744 | -0.120385 |
| 92 | 6 | 0 | -13.104442 | -3.793900 | 0.157502 |

| | | | | | |
|---|---|---|---|---|---|
| 93 | 6 | 0 | -10.740640 | -3.406643 | 0.395905 |
| 94 | 6 | 0 | -12.178810 | -1.643244 | -0.493910 |
| 95 | 6 | 0 | -13.272319 | -2.503593 | -0.350356 |
| 96 | 6 | 0 | -11.831877 | -4.250839 | 0.533740 |
| 97 | 1 | 0 | -12.320591 | -0.641326 | -0.890072 |
| 98 | 1 | 0 | -14.263821 | -2.163135 | -0.637634 |
| 99 | 1 | 0 | -11.712367 | -5.257620 | 0.928274 |
| 100 | 1 | 0 | -13.964827 | -4.449400 | 0.262483 |
| 101 | 6 | 0 | -8.990225 | -0.136707 | -0.537301 |
| 102 | 6 | 0 | -9.265739 | -3.668953 | 0.732976 |
| 103 | 6 | 0 | -8.694882 | -4.833491 | -0.107820 |
| 104 | 1 | 0 | -7.623234 | -4.961469 | 0.083614 |
| 105 | 1 | 0 | -8.830802 | -4.648558 | -1.178089 |
| 106 | 1 | 0 | -9.197402 | -5.774617 | 0.143568 |
| 107 | 6 | 0 | -9.075672 | -3.956023 | 2.239812 |
| 108 | 1 | 0 | -9.484538 | -3.143645 | 2.848929 |
| 109 | 1 | 0 | -8.012353 | -4.063888 | 2.483033 |
| 110 | 1 | 0 | -9.582834 | -4.885397 | 2.523476 |
| 111 | 6 | 0 | -9.557914 | 1.025314 | 0.309030 |
| 112 | 1 | 0 | -9.420215 | 0.835854 | 1.378257 |
| 113 | 1 | 0 | -10.629755 | 1.155570 | 0.120055 |
| 114 | 1 | 0 | -9.054185 | 1.966564 | 0.060747 |
| 115 | 6 | 0 | -9.183183 | 0.155755 | -2.042597 |
| 116 | 1 | 0 | -8.676089 | 1.085990 | -2.323652 |
| 117 | 1 | 0 | -10.246853 | 0.265040 | -2.283670 |
| 118 | 1 | 0 | -8.775805 | -0.654572 | -2.655483 |

**Table S4.** Optimized coordinates of a model compound **[(*S*)-6,6'-(COPV1)$_2$-binaph]'** and in the $S_1$ state.

Total energy = −2545.6133841 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -1.475553 | 6.116922 | -3.209760 |
| 2 | 6 | 0 | -1.560410 | 5.363293 | -2.435481 |
| 3 | 1 | 0 | -3.476132 | 4.704681 | -3.112062 |
| 4 | 6 | 0 | -2.683657 | 4.570483 | -2.379608 |
| 5 | 6 | 0 | -0.616209 | 4.225276 | -0.488456 |
| 6 | 6 | 0 | -2.832994 | 3.577045 | -1.381213 |
| 7 | 6 | 0 | -0.522021 | 5.194292 | -1.484748 |
| 8 | 6 | 0 | -1.779579 | 3.403496 | -0.423451 |
| 9 | 6 | 0 | -3.986011 | 2.753874 | -1.315245 |
| 10 | 1 | 0 | -1.177786 | 2.254145 | 1.313514 |
| 11 | 6 | 0 | -4.138991 | 1.778251 | -0.344607 |
| 12 | 1 | 0 | -4.752815 | 2.886322 | -2.074718 |
| 13 | 6 | 0 | -3.085106 | 1.618293 | 0.604490 |
| 14 | 1 | 0 | -3.195691 | 0.878968 | 1.392763 |
| 15 | 6 | 0 | -1.954234 | 2.396802 | 0.569014 |
| 16 | 6 | 0 | 0.534303 | 4.902703 | 1.631357 |
| 17 | 6 | 0 | 0.497831 | 4.071199 | 0.496819 |

| | | | | | |
|---|---|---|---|---|---|
| 18 | 6 | 0 | 2.568837 | 3.851297 | 2.408532 |
| 19 | 6 | 0 | 1.519905 | 3.112907 | 0.311956 |
| 20 | 6 | 0 | 1.572153 | 4.784629 | 2.585695 |
| 21 | 6 | 0 | 2.584890 | 2.990058 | 1.274195 |
| 22 | 6 | 0 | 1.559203 | 2.231196 | -0.816601 |
| 23 | 1 | 0 | 1.589235 | 5.426450 | 3.458984 |
| 24 | 1 | 0 | 4.356101 | 1.949461 | 1.856646 |
| 25 | 1 | 0 | 3.364579 | 3.764524 | 3.144344 |
| 26 | 6 | 0 | 2.554827 | 1.305618 | -0.971305 |
| 27 | 1 | 0 | 0.780991 | 2.314558 | -1.567989 |
| 28 | 1 | 0 | 2.550788 | 0.688539 | -1.863701 |
| 29 | 6 | 0 | 3.626374 | 1.163502 | -0.027567 |
| 30 | 6 | 0 | 3.597121 | 2.035376 | 1.085073 |
| 31 | 8 | 0 | 0.616264 | 5.949663 | -1.485532 |
| 32 | 8 | 0 | -0.481823 | 5.800954 | 1.741376 |
| 33 | 6 | 0 | 0.783297 | 6.941695 | -2.484290 |
| 34 | 1 | 0 | 0.003656 | 7.713012 | -2.427361 |
| 35 | 1 | 0 | 0.789082 | 6.507837 | -3.493040 |
| 36 | 1 | 0 | 1.754699 | 7.398952 | -2.286745 |
| 37 | 6 | 0 | -0.517209 | 6.671226 | 2.861373 |
| 38 | 1 | 0 | -0.597242 | 6.114083 | 3.803966 |
| 39 | 1 | 0 | -1.409522 | 7.285664 | 2.729646 |
| 40 | 1 | 0 | 0.368175 | 7.319340 | 2.897322 |
| 41 | 1 | 0 | 5.322928 | -2.731615 | -1.926661 |
| 42 | 6 | 0 | 5.501030 | -1.885208 | -1.269077 |
| 43 | 6 | 0 | 5.932097 | 0.303228 | 0.476571 |
| 44 | 6 | 0 | 6.739890 | -1.754531 | -0.583028 |
| 45 | 6 | 0 | 4.517454 | -0.938634 | -1.085981 |
| 46 | 6 | 0 | 4.680810 | 0.187836 | -0.213815 |
| 47 | 6 | 0 | 6.925190 | -0.622093 | 0.298288 |
| 48 | 1 | 0 | 3.567908 | -1.077890 | -1.592174 |
| 49 | 1 | 0 | 6.107731 | 1.163600 | 1.115866 |
| 50 | 6 | 0 | 7.923384 | -2.519849 | -0.554097 |
| 51 | 6 | 0 | 8.865710 | -1.923800 | 0.304091 |
| 52 | 6 | 0 | 10.058535 | -2.695895 | 0.328772 |
| 53 | 6 | 0 | 12.092809 | -4.592443 | -0.035329 |
| 54 | 6 | 0 | 9.866611 | -3.822255 | -0.545112 |
| 55 | 6 | 0 | 11.288960 | -2.546367 | 1.011204 |
| 56 | 6 | 0 | 12.287047 | -3.494534 | 0.820210 |
| 57 | 6 | 0 | 10.874528 | -4.752791 | -0.719636 |
| 58 | 1 | 0 | 11.453270 | -1.702544 | 1.675929 |
| 59 | 1 | 0 | 13.235209 | -3.386089 | 1.341387 |
| 60 | 1 | 0 | 10.734408 | -5.606494 | -1.379852 |
| 61 | 1 | 0 | 12.887804 | -5.321006 | -0.168474 |
| 62 | 6 | 0 | 8.329277 | -0.652505 | 0.929458 |
| 63 | 6 | 0 | 8.467514 | -3.790128 | -1.180806 |
| 64 | 6 | 0 | 7.638372 | -5.033622 | -0.781081 |
| 65 | 1 | 0 | 6.620169 | -4.967591 | -1.182415 |
| 66 | 1 | 0 | 7.570953 | -5.126334 | 0.307395 |
| 67 | 1 | 0 | 8.098620 | -5.947905 | -1.174371 |
| 68 | 6 | 0 | 8.550868 | -3.687007 | -2.722160 |
| 69 | 1 | 0 | 9.137059 | -2.813916 | -3.025504 |
| 70 | 1 | 0 | 7.550065 | -3.596119 | -3.160618 |
| 71 | 1 | 0 | 9.025323 | -4.580961 | -3.144260 |

| | | | | | |
|---|---|---|---|---|---|
| 72 | 6 | 0 | 9.159074 | 0.589585 | 0.523387 |
| 73 | 1 | 0 | 9.219837 | 0.680619 | -0.565548 |
| 74 | 1 | 0 | 10.179294 | 0.521960 | 0.918803 |
| 75 | 1 | 0 | 8.702226 | 1.505594 | 0.917764 |
| 76 | 6 | 0 | 8.251954 | -0.748996 | 2.472197 |
| 77 | 1 | 0 | 7.780374 | 0.148145 | 2.891994 |
| 78 | 1 | 0 | 9.253998 | -0.840222 | 2.907312 |
| 79 | 1 | 0 | 7.664524 | -1.619178 | 2.781257 |
| 80 | 1 | 0 | -8.728539 | 1.082062 | -0.820297 |
| 81 | 6 | 0 | -7.764169 | 0.647199 | -0.571595 |
| 82 | 6 | 0 | -5.251564 | -0.436127 | 0.094047 |
| 83 | 6 | 0 | -7.654971 | -0.694932 | -0.197762 |
| 84 | 6 | 0 | -6.615575 | 1.438520 | -0.609585 |
| 85 | 6 | 0 | -5.347498 | 0.922026 | -0.286037 |
| 86 | 6 | 0 | -6.383562 | -1.230221 | 0.136554 |
| 87 | 1 | 0 | -6.704952 | 2.489385 | -0.869962 |
| 88 | 1 | 0 | -4.275767 | -0.856589 | 0.324902 |
| 89 | 6 | 0 | -8.623927 | -1.770553 | -0.058458 |
| 90 | 6 | 0 | -7.998601 | -2.911116 | 0.334402 |
| 91 | 6 | 0 | -8.967922 | -3.989209 | 0.471592 |
| 92 | 6 | 0 | -11.244227 | -5.599019 | 0.552083 |
| 93 | 6 | 0 | -10.239377 | -3.450929 | 0.139614 |
| 94 | 6 | 0 | -8.846109 | -5.331445 | 0.841733 |
| 95 | 6 | 0 | -9.994054 | -6.129650 | 0.878719 |
| 96 | 6 | 0 | -11.370559 | -4.251696 | 0.179898 |
| 97 | 1 | 0 | -7.878433 | -5.754378 | 1.097767 |
| 98 | 1 | 0 | -9.911328 | -7.174937 | 1.165093 |
| 99 | 1 | 0 | -12.348997 | -3.848711 | -0.072650 |
| 100 | 1 | 0 | -12.125957 | -6.233326 | 0.586053 |
| 101 | 6 | 0 | -6.504034 | -2.716456 | 0.505695 |
| 102 | 6 | 0 | -10.117885 | -1.966063 | -0.232097 |
| 103 | 6 | 0 | -10.929864 | -1.075491 | 0.735641 |
| 104 | 1 | 0 | -10.773998 | -0.014287 | 0.509697 |
| 105 | 1 | 0 | -10.631834 | -1.250819 | 1.774186 |
| 106 | 1 | 0 | -12.002005 | -1.285445 | 0.647003 |
| 107 | 6 | 0 | -10.563563 | -1.713246 | -1.690399 |
| 108 | 1 | 0 | -10.003575 | -2.344998 | -2.387137 |
| 109 | 1 | 0 | -10.399240 | -0.666300 | -1.970427 |
| 110 | 1 | 0 | -11.630753 | -1.931659 | -1.812174 |
| 111 | 6 | 0 | -5.694513 | -3.605008 | -0.466002 |
| 112 | 1 | 0 | -5.995308 | -3.427581 | -1.503385 |
| 113 | 1 | 0 | -5.849909 | -4.666579 | -0.241693 |
| 114 | 1 | 0 | -4.622247 | -3.395087 | -0.379883 |
| 115 | 6 | 0 | -6.054624 | -2.971867 | 1.962340 |
| 116 | 1 | 0 | -4.987028 | -2.754056 | 2.081424 |
| 117 | 1 | 0 | -6.218325 | -4.019194 | 2.241054 |
| 118 | 1 | 0 | -6.612600 | -2.341273 | 2.661791 |

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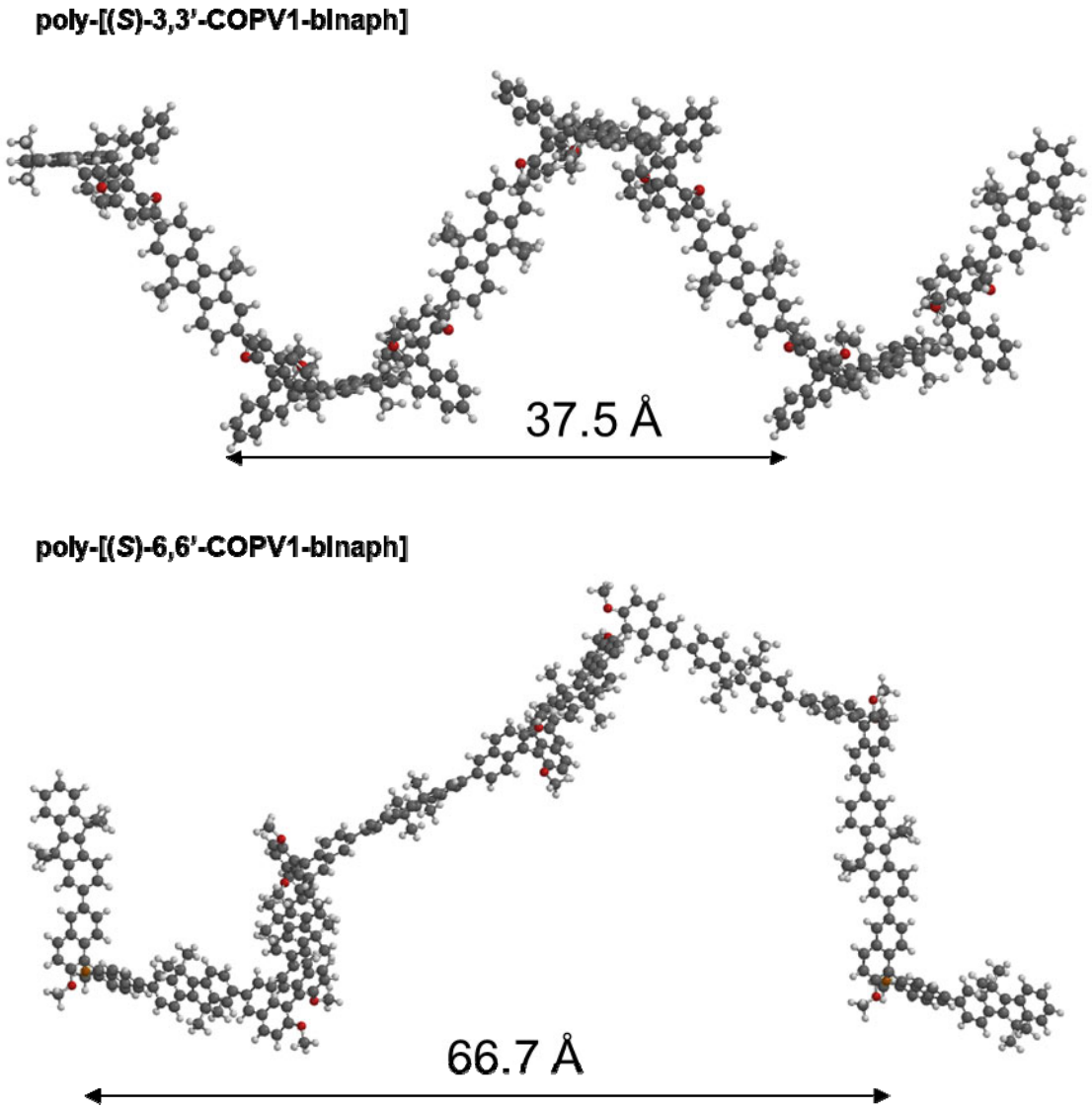


**Figure S16.** One of the possible structures of polymers generated based on the structures of model monomers (optimized using MMFF calculations). The values of pitch of the helix are also shown.