Supporting Information

Balancing Interactions in Proline-Based Receptors for Chiral Recognition of L-/D-DOPA

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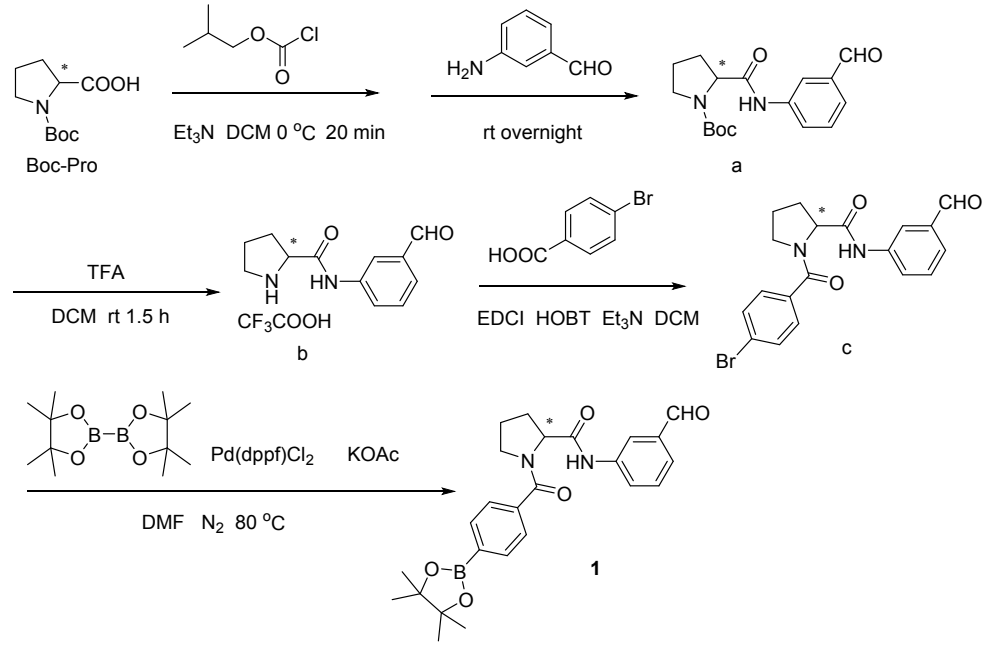
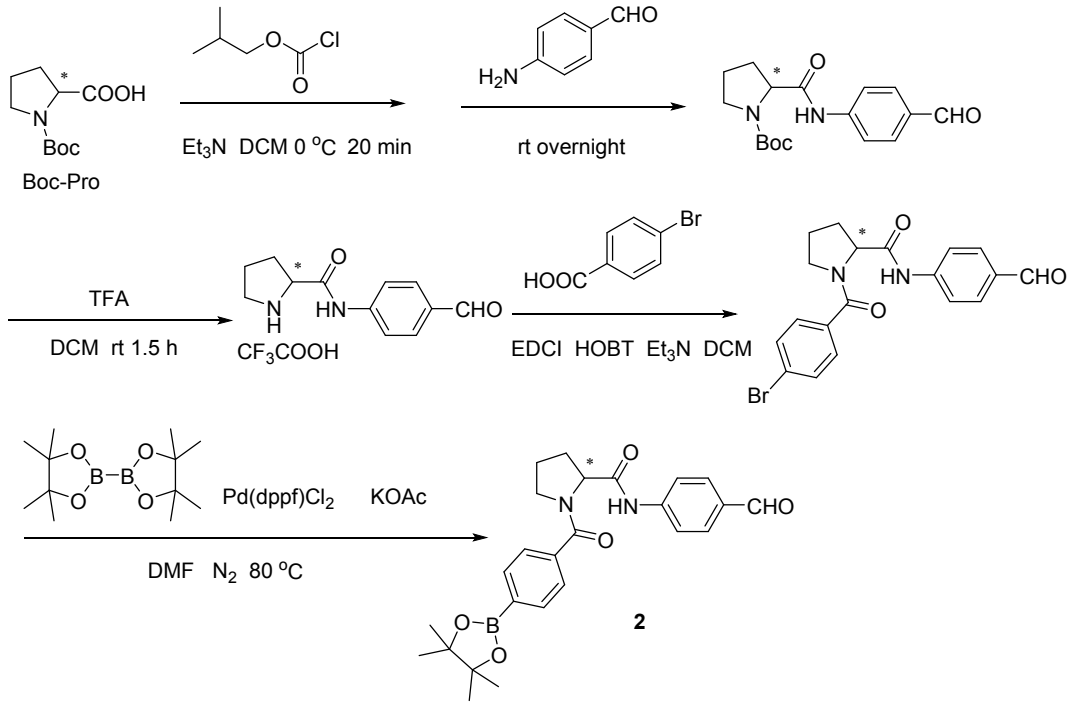
1. Syntheses and characterizations of 1 to 14



Scheme S1. Synthesis of **1**.



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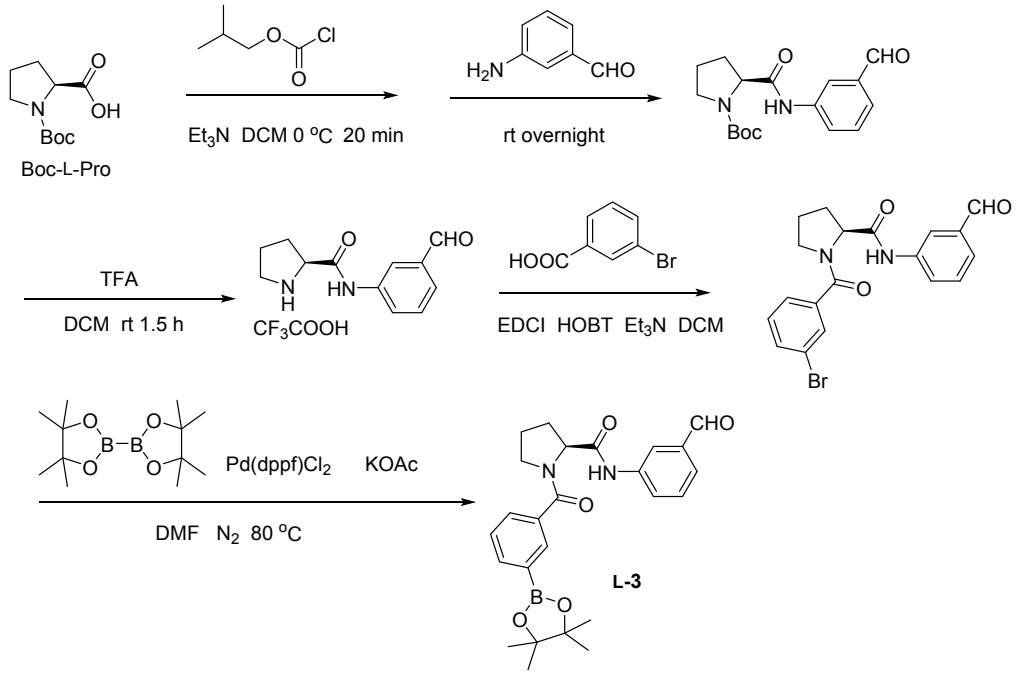
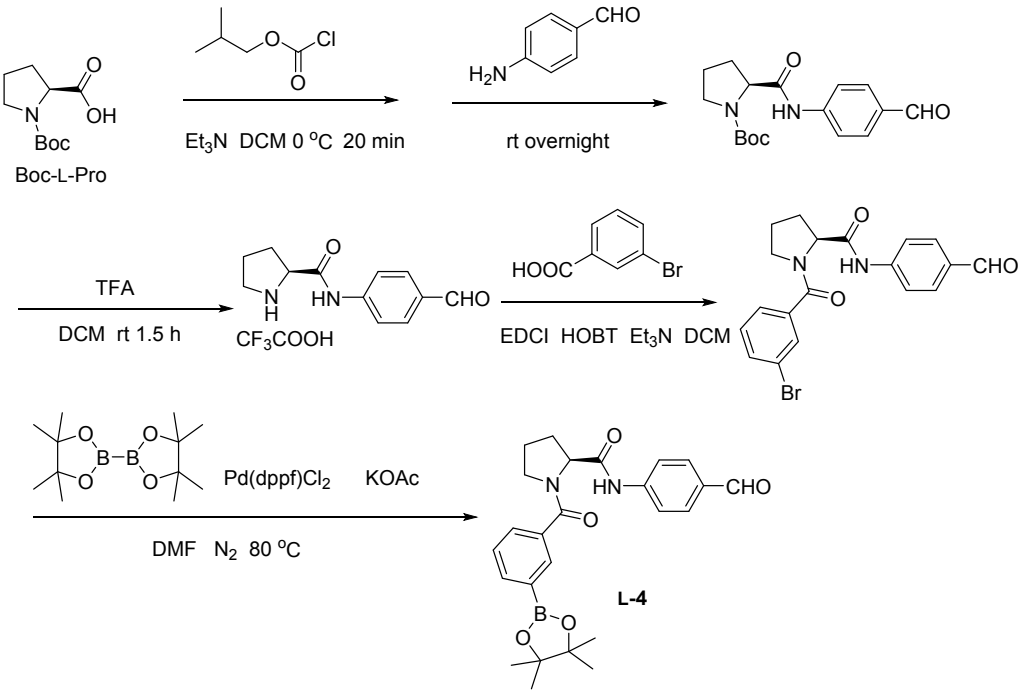


Scheme S3. Synthesis of L-**3**.



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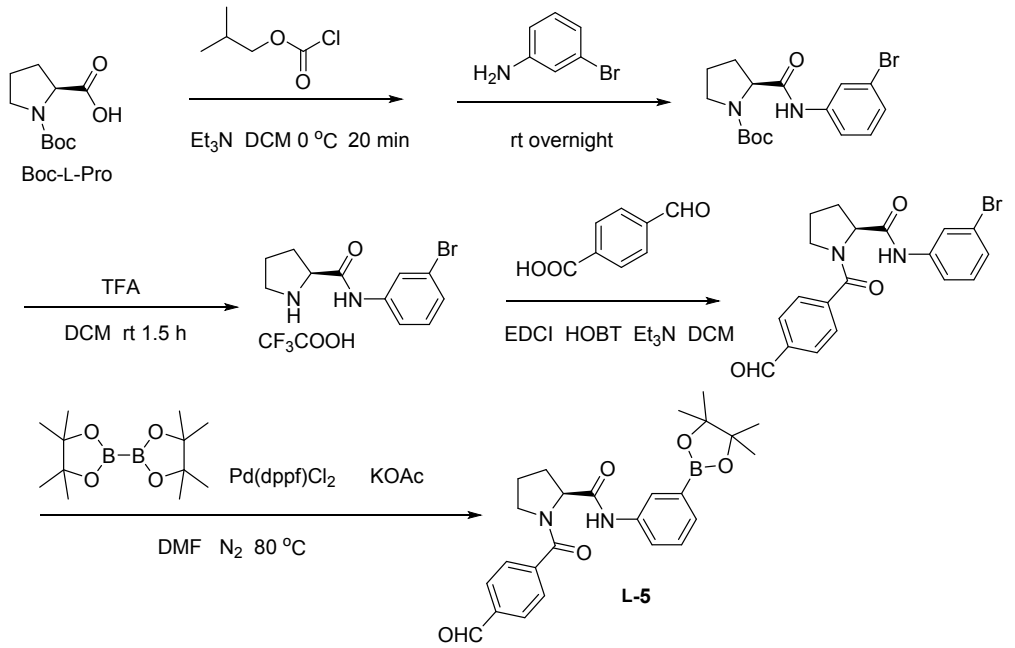
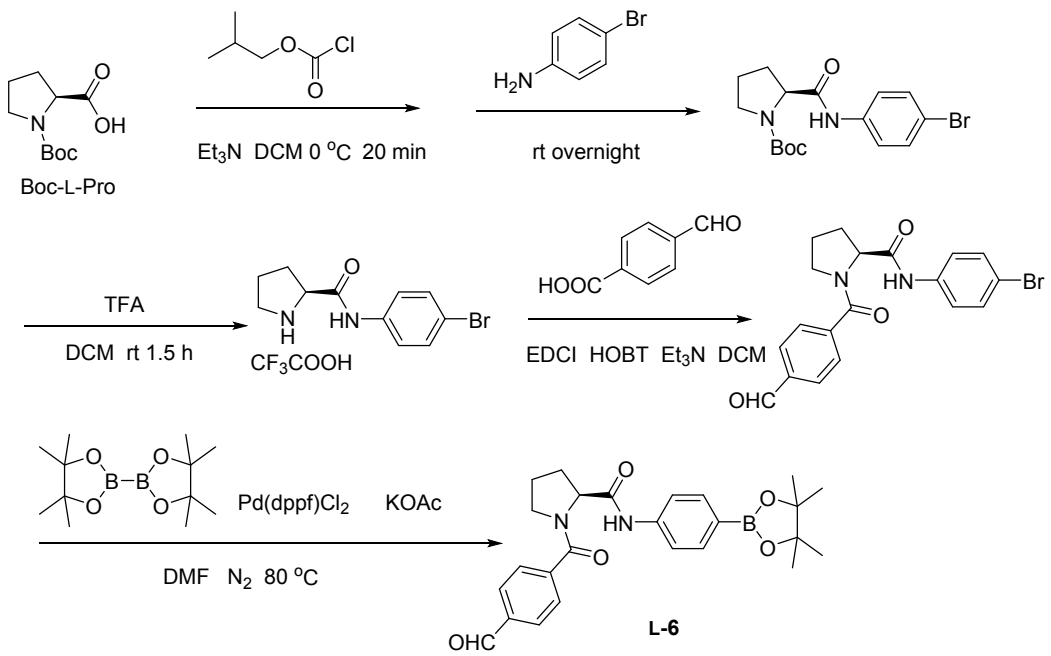
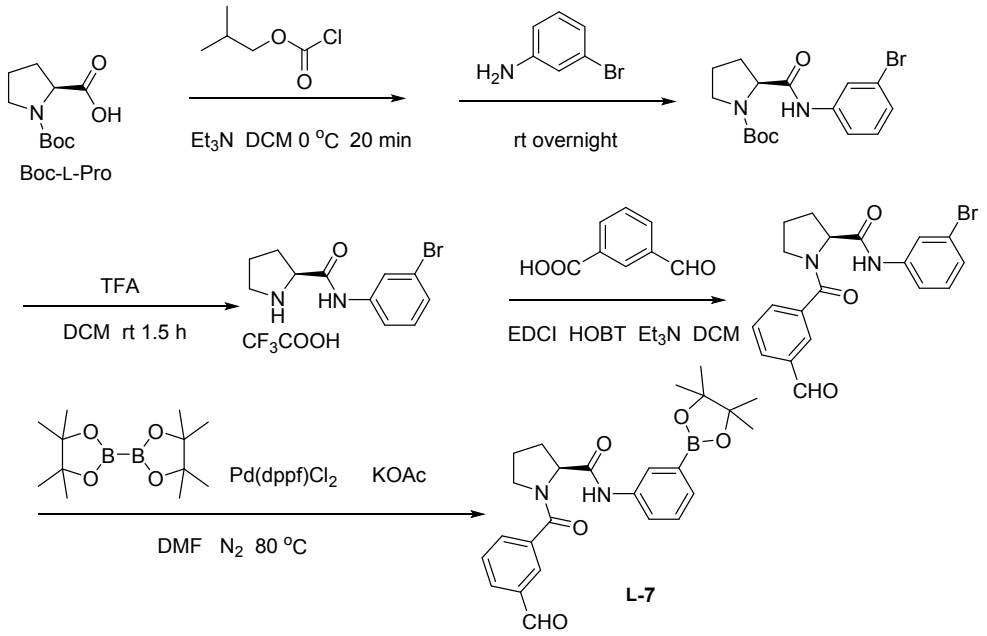


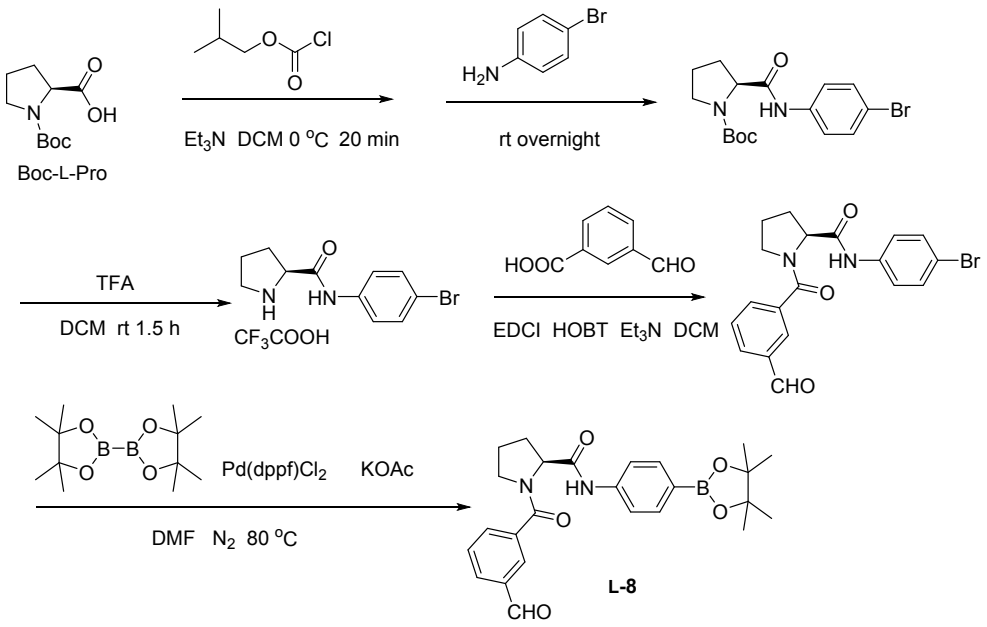
Scheme S5. Synthesis of L-**5**.



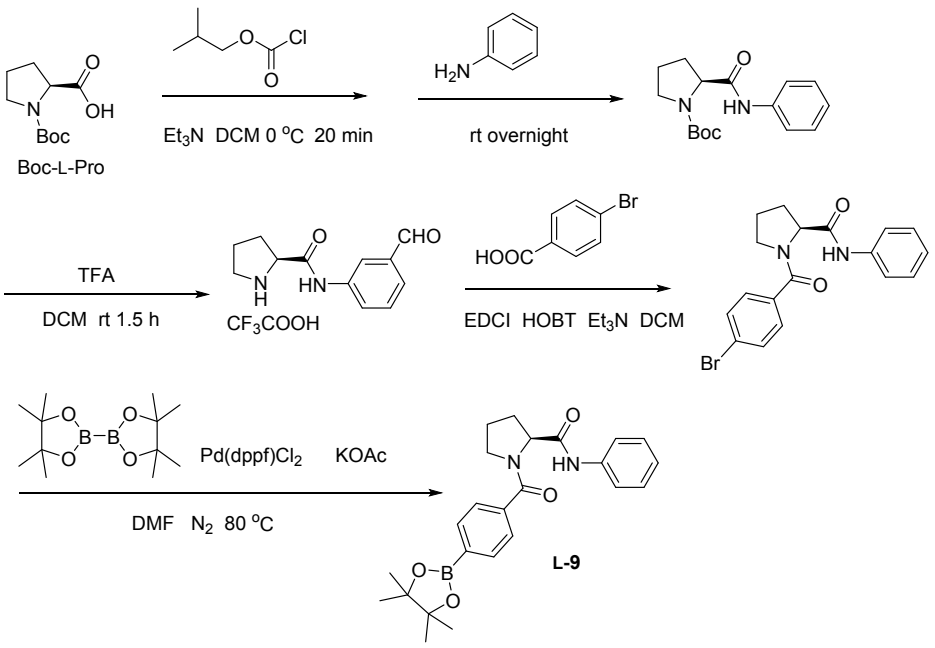
Scheme S6. Synthesis of L-**6**.



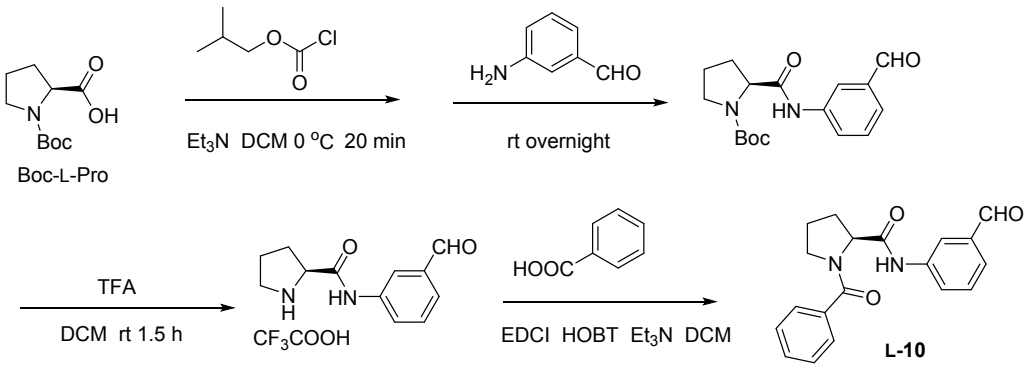
Scheme S7. Synthesis of L-**7**.



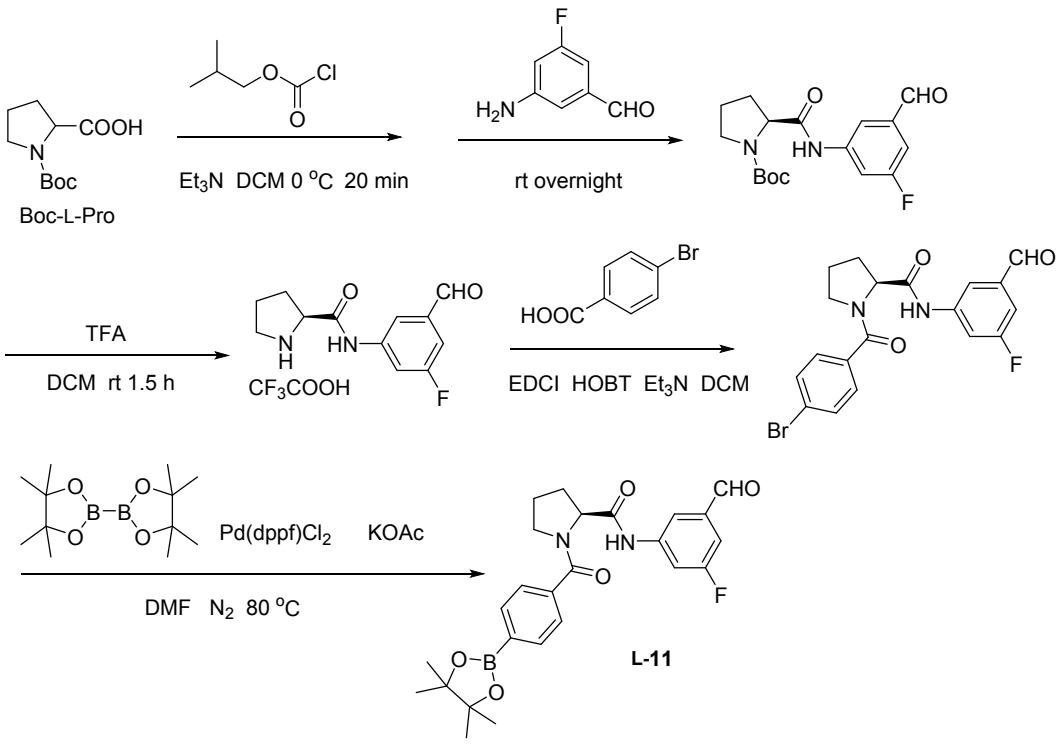
Scheme S8. Synthesis of L-**8**.



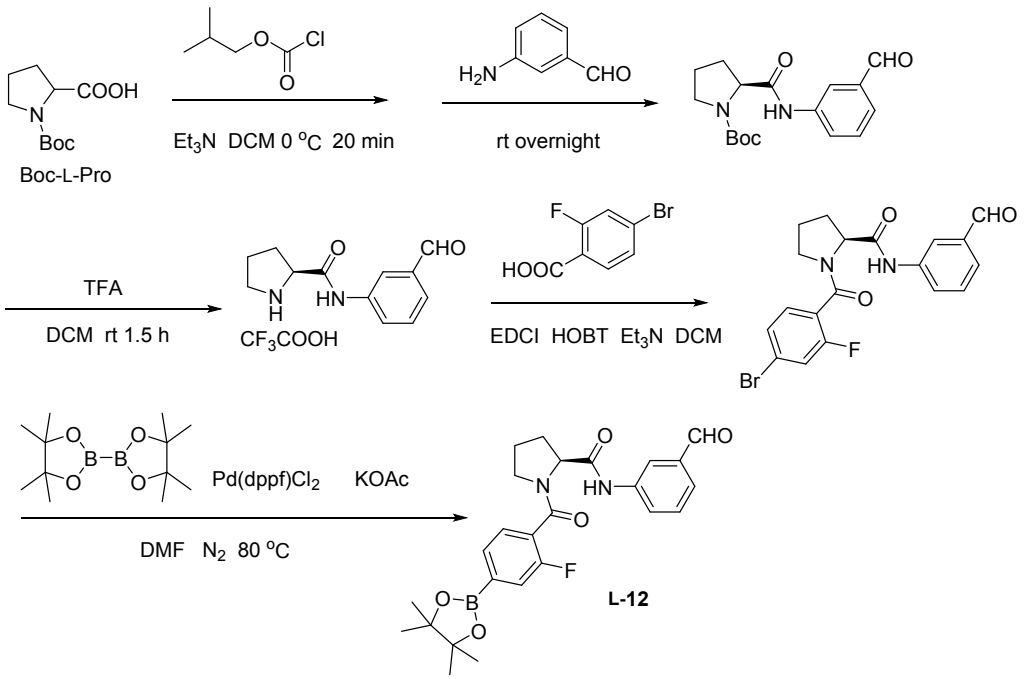
Scheme S9. Synthesis of L-**9**.



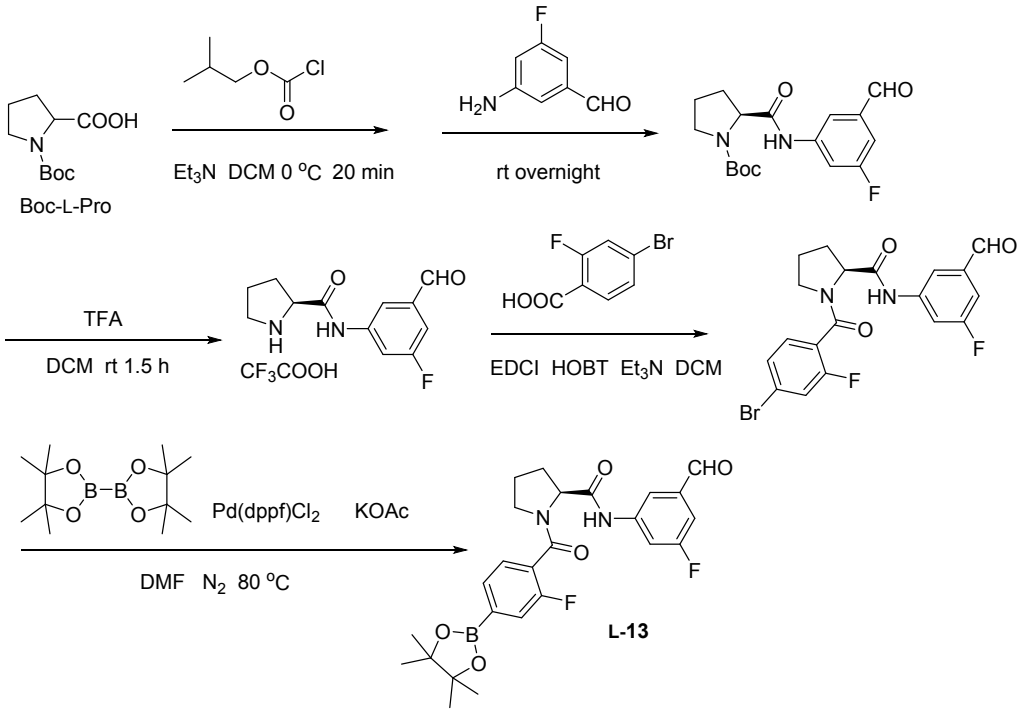
Scheme S10. Synthesis of L-**10**.



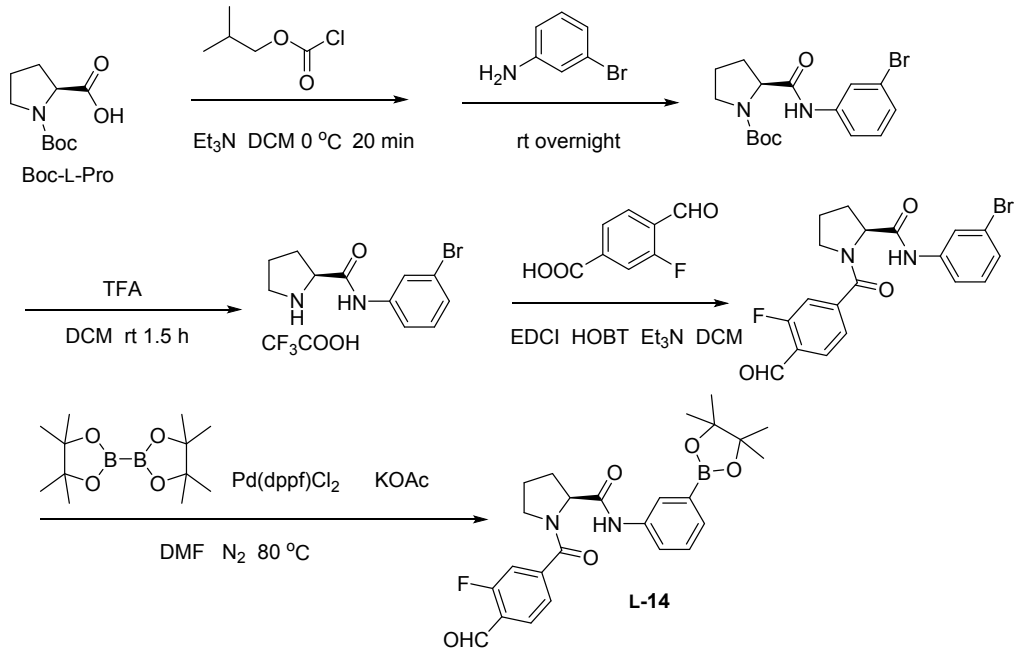
Scheme S11. Synthesis of L-**11**.



Scheme S12. Synthesis of L-**12**.



Scheme S13. Synthesis of L-**13**.



Scheme S14. Synthesis of L-**14**.

2. Spectral analyses of 1 to 11

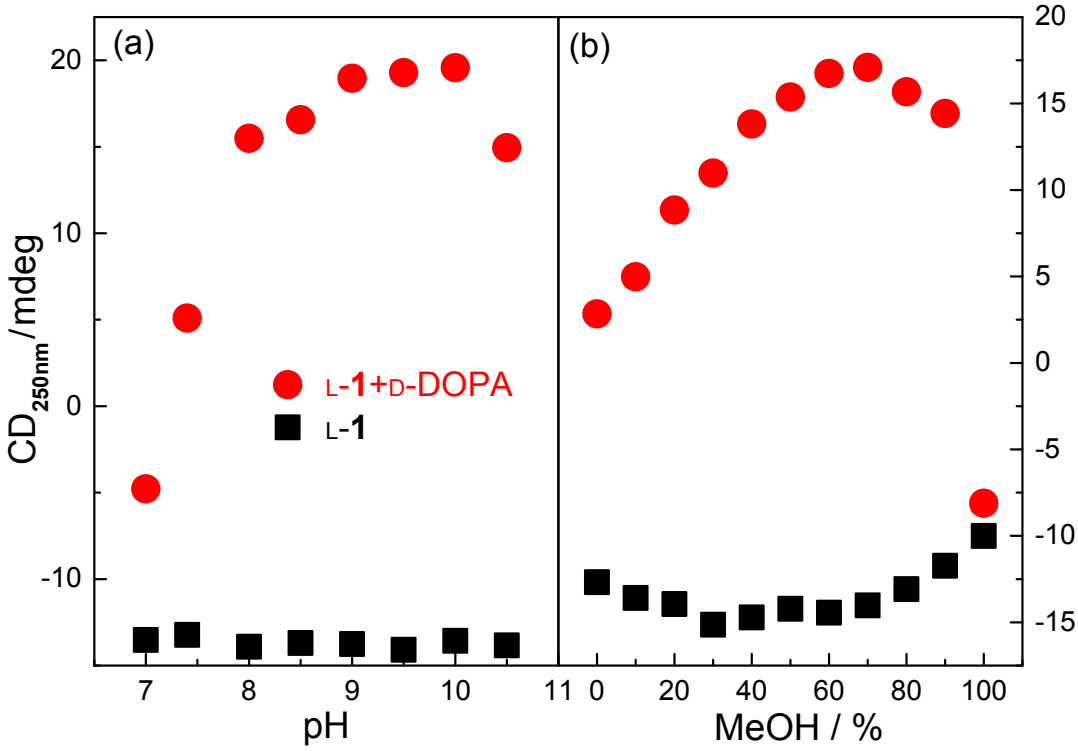


Figure S1. CD intensities at 250 nm of L-**1** and L-**1**/D-DOPA complexes in 7:3 (v/v) MeOH/buffer of different pH (a) and in aqueous MeOH solutions of varying volume fraction of methanol (b). [L-**1**] = 40 μM, [D-DOPA] = 250 μM.

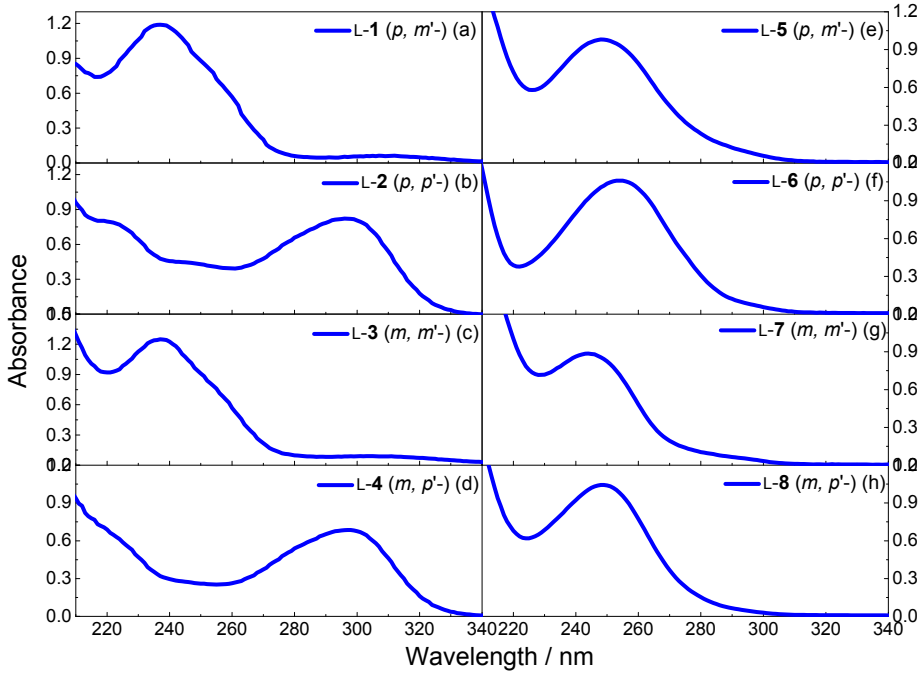


Figure S2. Absorption spectra of L-**1** (a), L-**2** (b), L-**3** (c), L-**4** (d), L-**5** (e), L-**6** (f), L-**7** (g) and L-**8** (h) in 7:3 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. [L-**1**] = [L-**2**] = [L-**3**] = [L-**4**] = [L-**5**] = [L-**6**] = [L-**7**] = [L-**8**] = 40 μM.

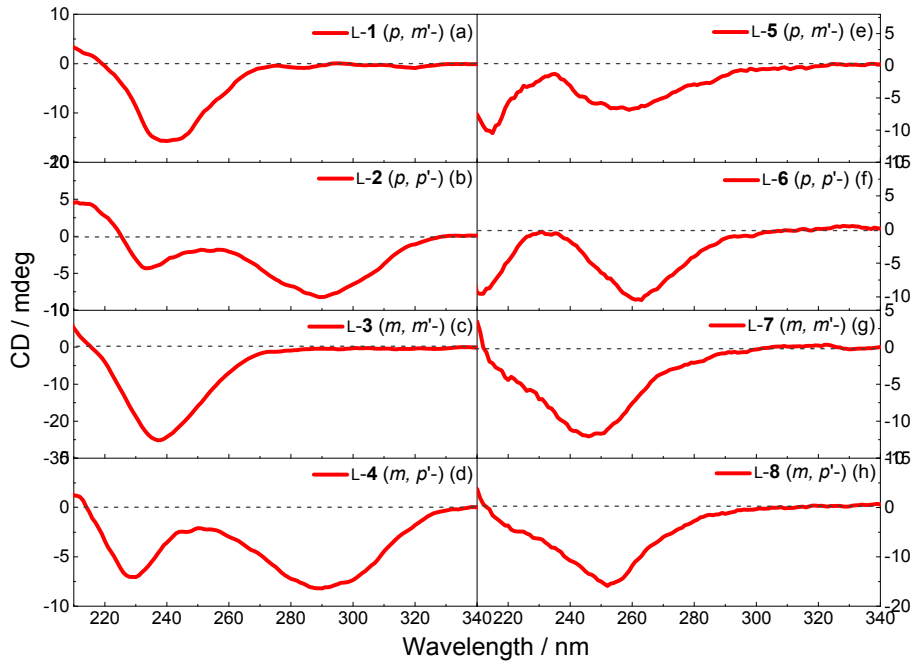


Figure S3. CD spectra of L-**1** (a), L-**2** (b), L-**3** (c), L-**4** (d), L-**5** (e), L-**6** (f), L-**7** (g) and L-**8** (h) in 7:3 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. [L-**1**] = [L-**2**] = [L-**3**] = [L-**4**] = [L-**5**] = [L-**6**] = [L-**7**] = [L-**8**] = 40 μM.

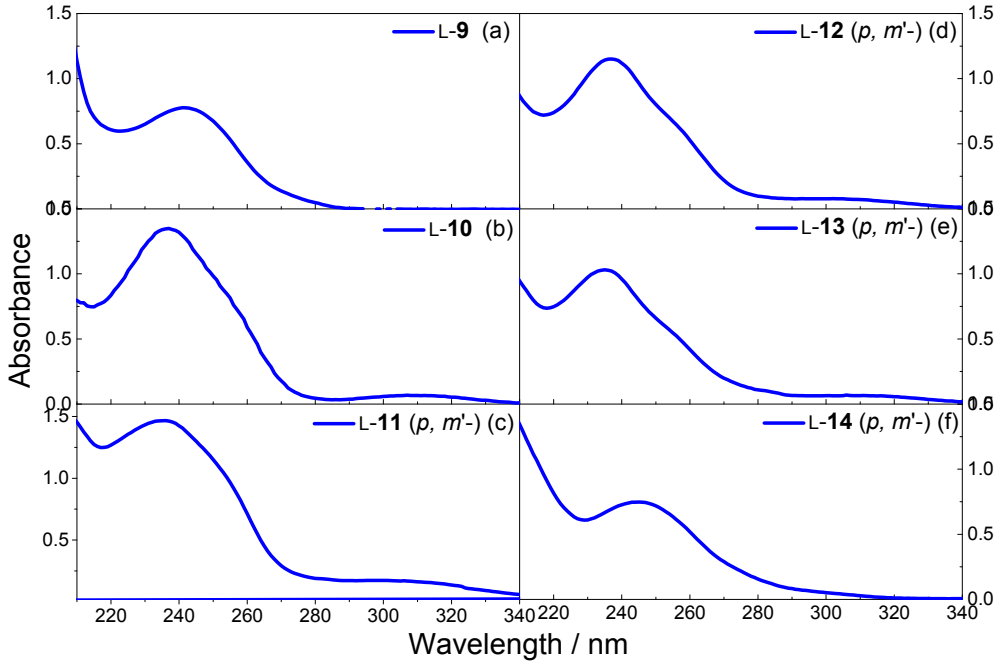


Figure S4. Absorption spectra of L-**9** (a), L-**10** (b), L-**11** (c), L-**12** (d), L-**13** (e) and L-**14** (f) in 7:3 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. [L-**9**] = [L-**10**] = [L-**11**] = [L-**12**] = [L-**13**] = [L-**14**] = 40 μM.

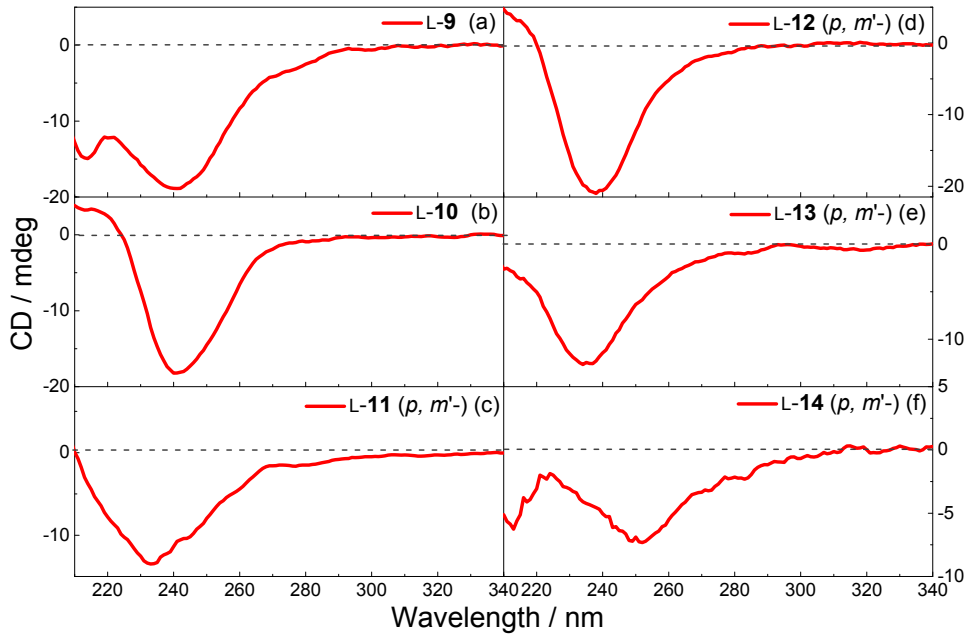


Figure S5. CD spectra of L-**9** (a), L-**10** (b), L-**11** (c), L-**12** (d), L-**13** (e) and L-**14** (f) in 7:3 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. [L-**9**] = [L-**10**] = [L-**11**] = [L-**12**] = [L-**13**] = [L-**14**] = 40 μM.

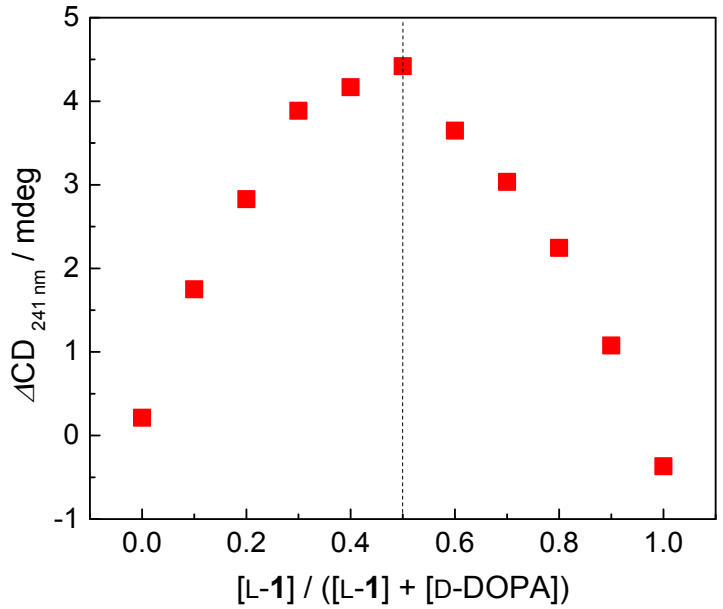


Figure S6. Job plot for interaction of L-**1** with D-DOPA revealing a 1:1 stoichiometry. [L-**1**] + [D-DOPA] = 40 μM.

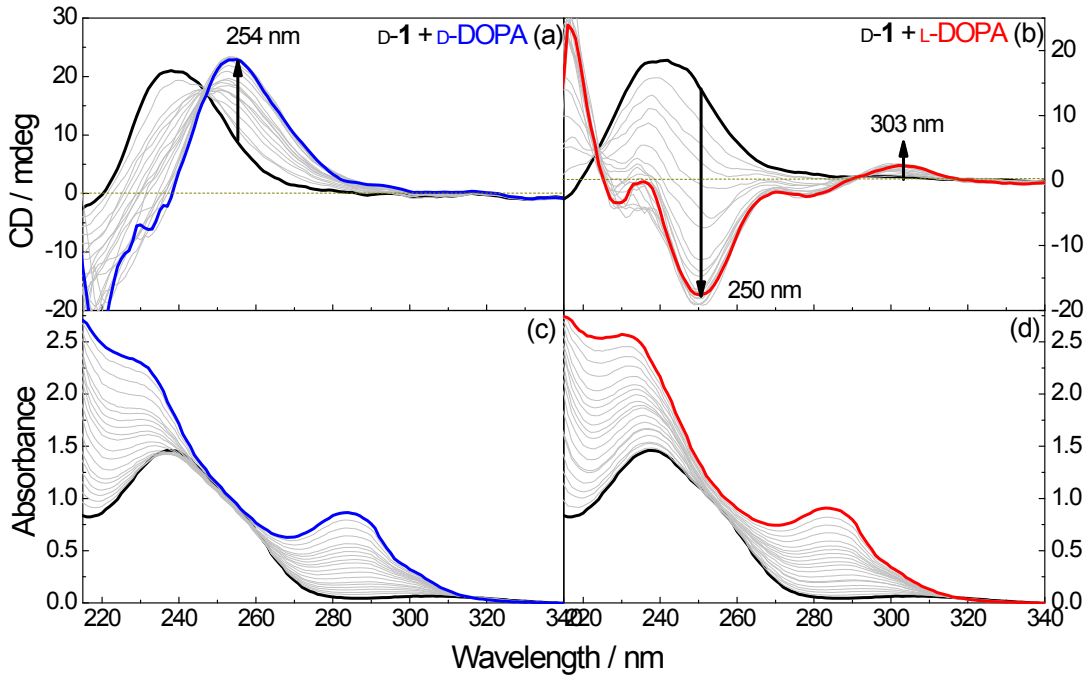


Figure S7. CD (a, b) and absorption (c, d) spectra of D-**1** in the presence of D- (a, c) or L-DOPA (b, d) in 7:3 (v/v) MeOH/0.05M pH 8.0 PBS buffer. [D-**1**] = 40 μM, [L-DOPA] = [D-DOPA] = 0 - 250 μM.

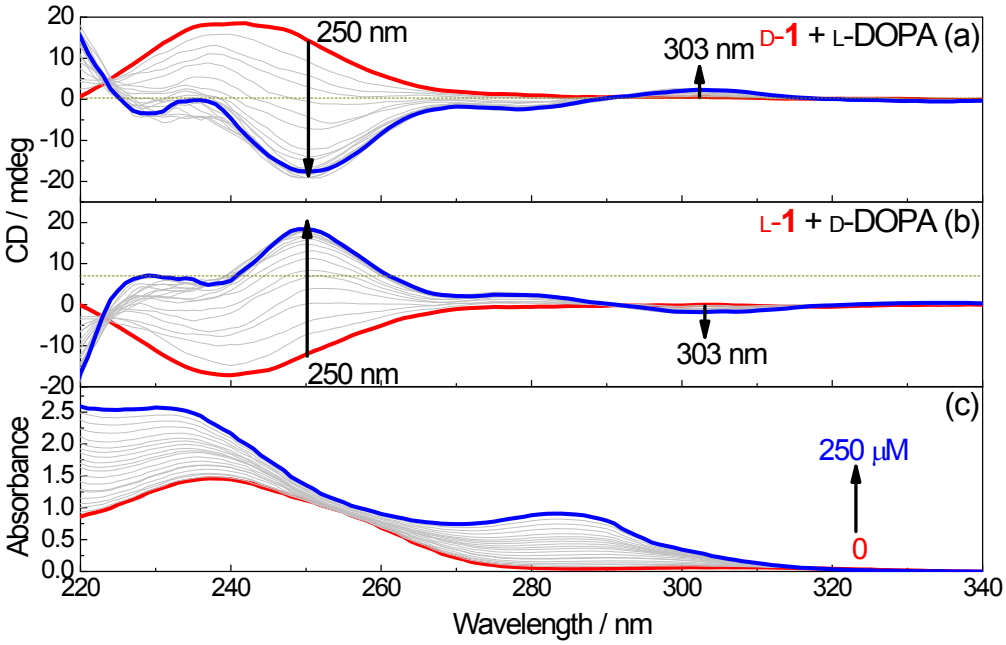


Figure S8. Evolution of CD spectra of D-**1** upon mixing with L-DOPA (a) and of L-**1** with D-DOPA (b) in 7:3 (v/v) MeOH/0.05M pH 8.0 PBS buffer. Shown in (c) are the traces of absorption spectra. [**1**] = 40 μM, [L-DOPA] = [D-DOPA] = 0 - 250 μM.

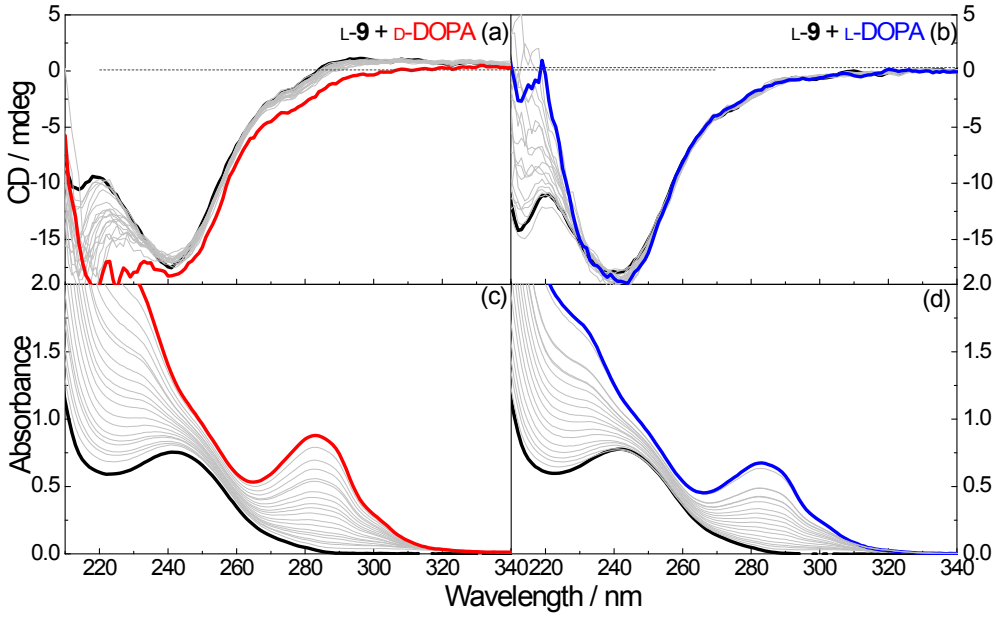


Figure S9. CD (a, b) and absorption (c, d) spectra of L-**9** in the presence of D-DOPA (a, c) and L-DOPA (b, d) in 7:3 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. [L-**9**] = 40 μM, [L-DOPA] = [D-DOPA] = 0 - 250 μM.

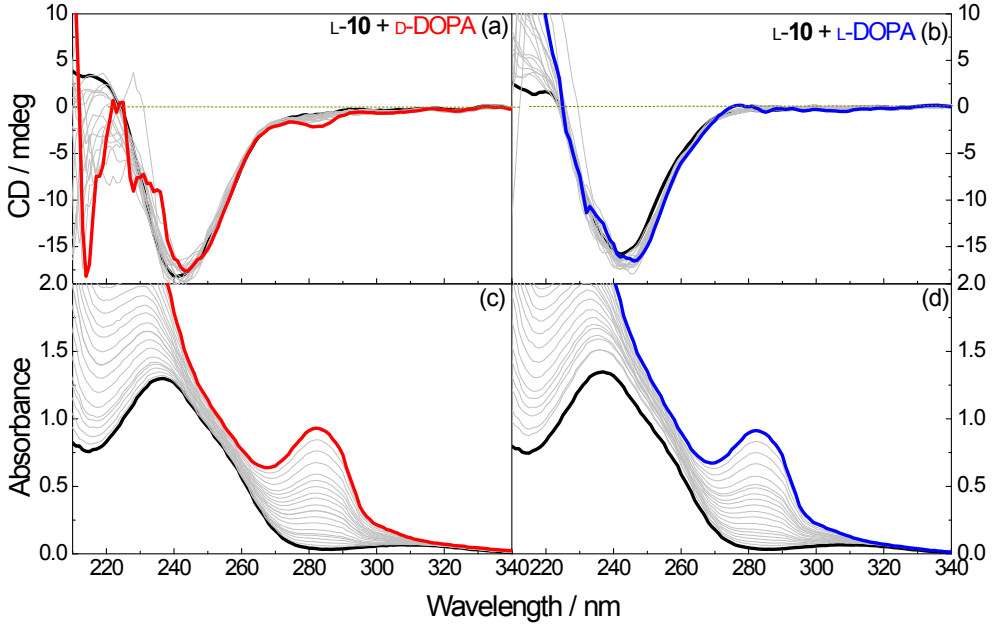


Figure S10. CD (a, b) and absorption (c, d) spectra of L-**10** in the presence of D-DOPA (a, c) and L-DOPA (b, d) in 7:3 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. [L-**10**] = 40 μM, [L-DOPA] = [D-DOPA] = 0 - 250 μM.

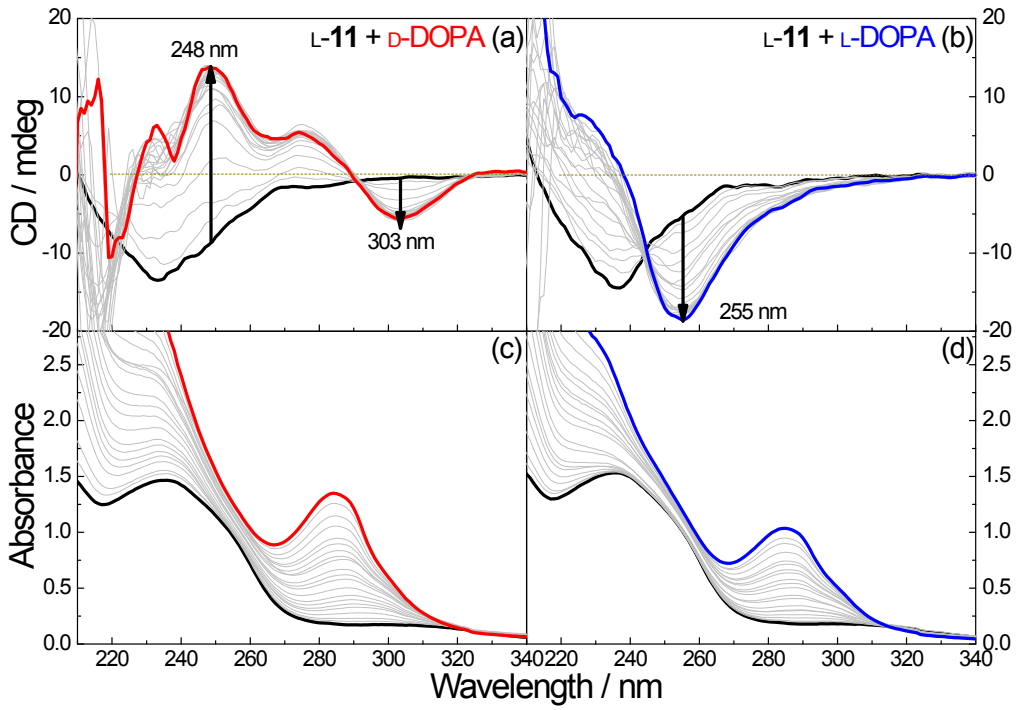


Figure S11. CD (a, b) and absorption (c, d) spectra of L-**11** in the presence of D- (a, c) or L-DOPA (b, d) in 7:3 (v/v) MeOH/0.05M pH 8.0 PBS buffer. [L-**11**] = 40 μM, [L-DOPA] = [D-DOPA] = 0 - 250 μM.

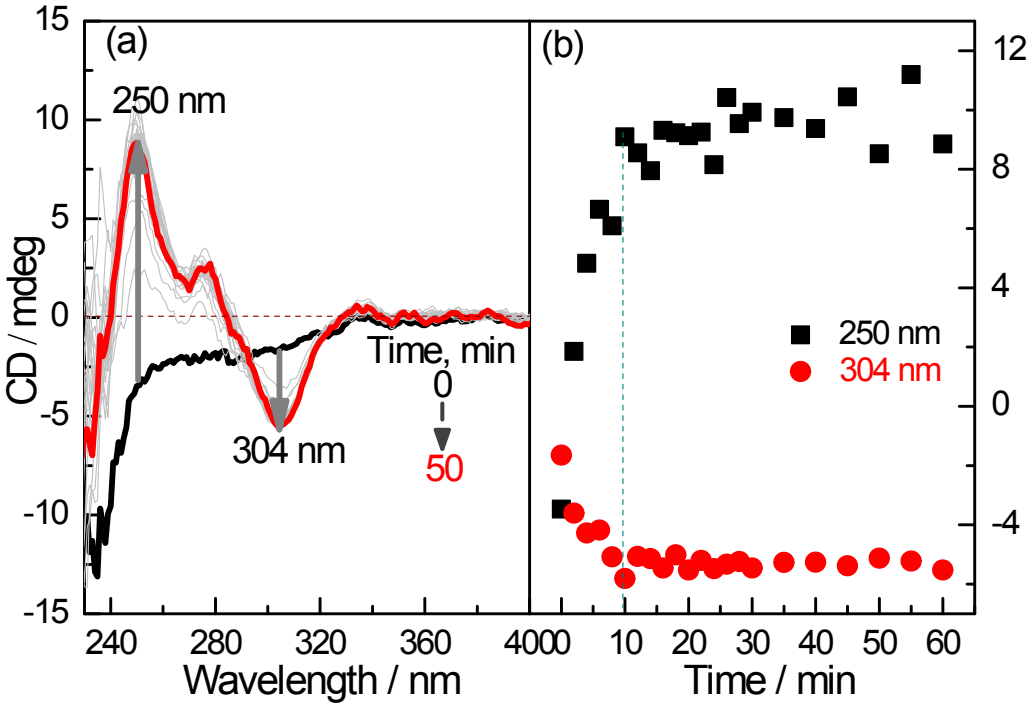


Figure S12. Time profiles of CD spectra (a) and signals (b) of L-**11** in the presence of D-DOPA in 7:3 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. [L-**11**] = 40 μM, [D-DOPA] = 250 μM.

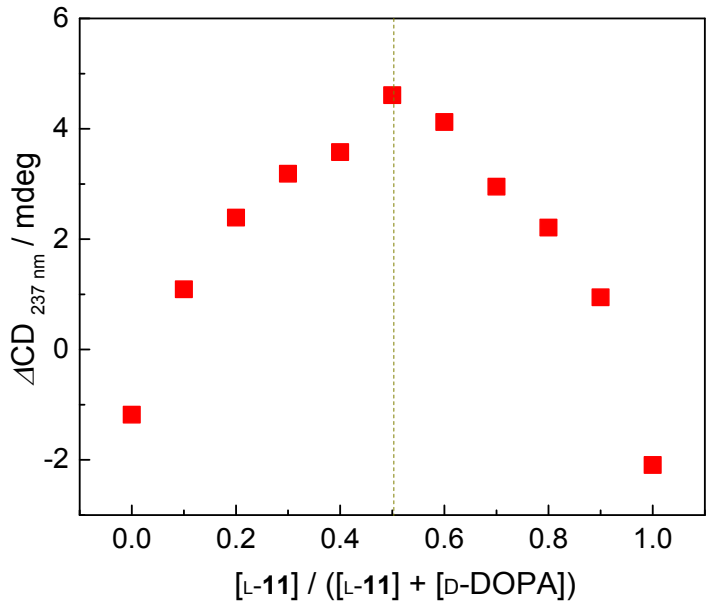


Figure S13. Job plot for the interaction of L-**11** with D-DOPA revealing a 1:1 stoichiometry. [L-**11**] + [D-DOPA] = 40 μM.

3. MS spectra of L-11 in the presence of D-DOPA and L-DOPA

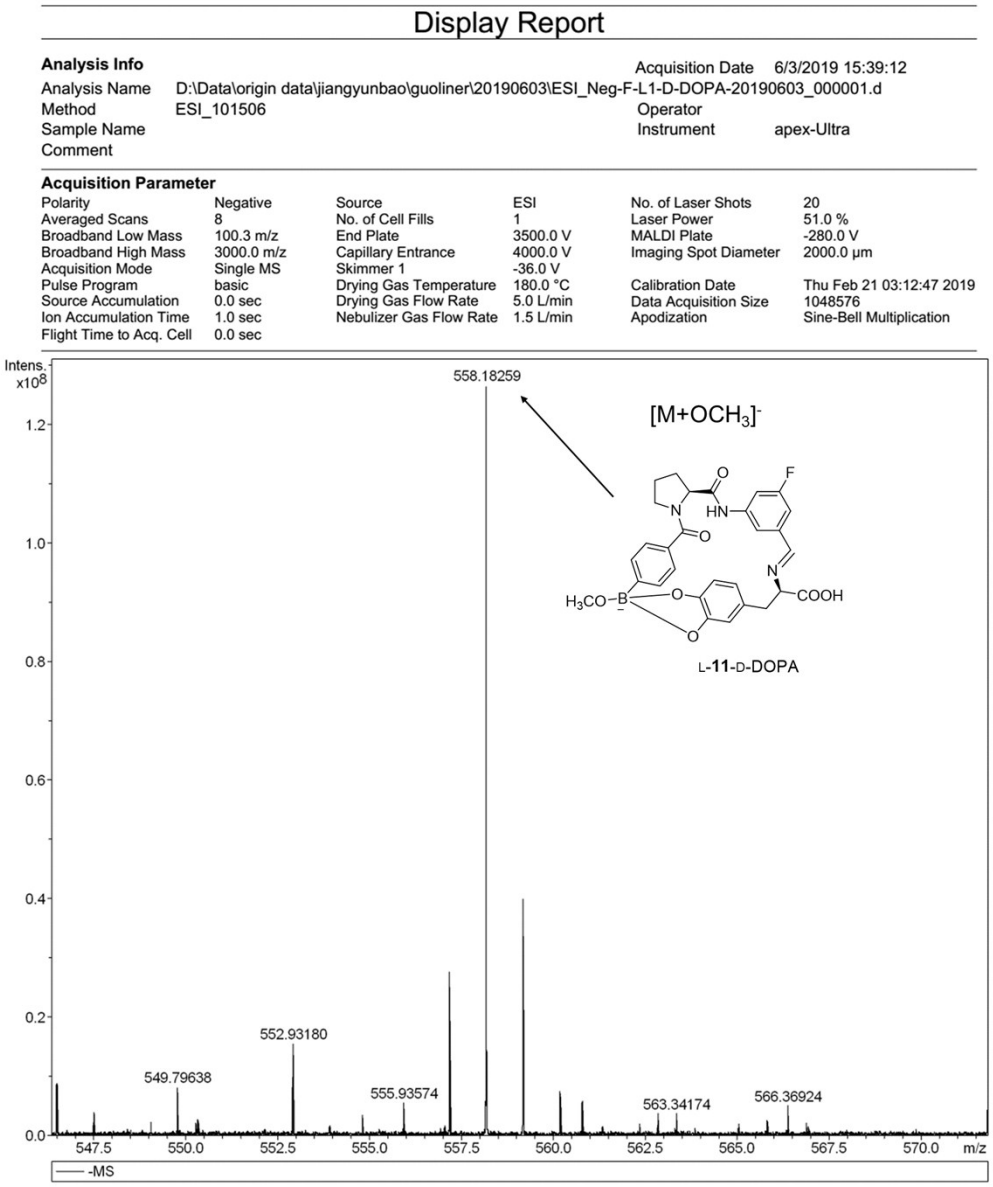


Figure S14. HRMS spectrum of L-**11**/D-DOPA complex. $[M+OCH_3]^-$ calcd for $C_{29}H_{26}BFN_3O_7^-$: *m/z* 558.1853, found *m/z* 558.1826.

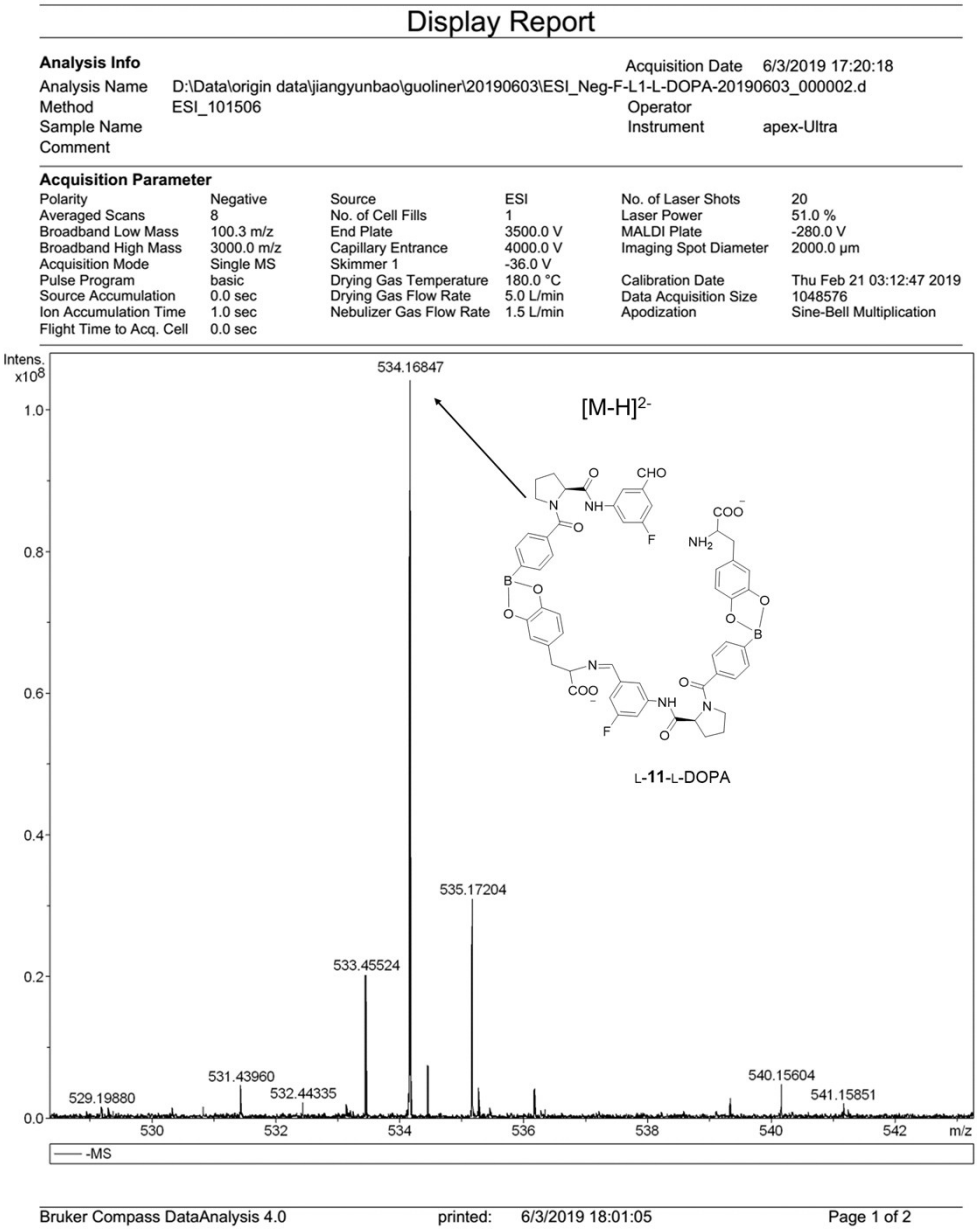


Figure S15. HRMS spectrum of L-**11**/L-DOPA complex. $[M-H]^{2-}$ calcd for $C_{56}H_{45}B_2F_2N_6O_{13}^{2-}$: *m/z* 534.1623, found *m/z* 534.1685.

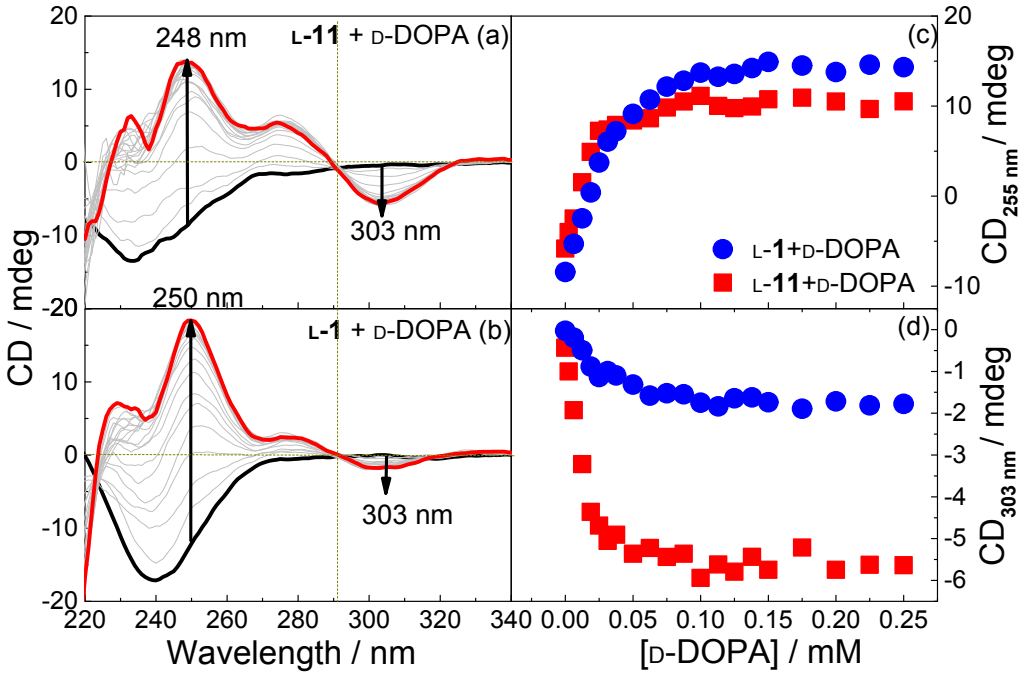


Figure S16. CD spectra (a, b) and CD intensities at 255 nm (c) and 303 nm (d) of L-**1** and L-**11** in the presence of D-DOPA in 7:3 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. [L-**1**] = [L-**11**] = 40 μM. [D-DOPA] = 0 - 250 μM.

4. Spectral titrations of L-12, L-13 and L-14 by DOPA

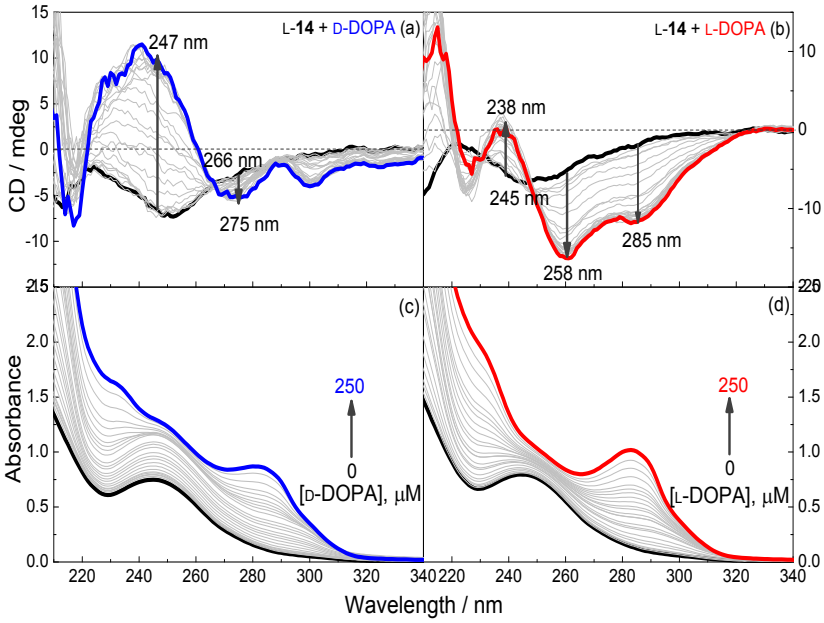


Figure S17. CD (a, b) and absorption (c, d) spectra of L-**14** in the presence of D- (a, c) or L-DOPA (b, d) in 7:3 (v/v) MeOH/0.05M pH 8.0 PBS buffer. [L-**14**] = 50 μM. [D-DOPA] = [L-DOPA] = 0 - 250 μM.

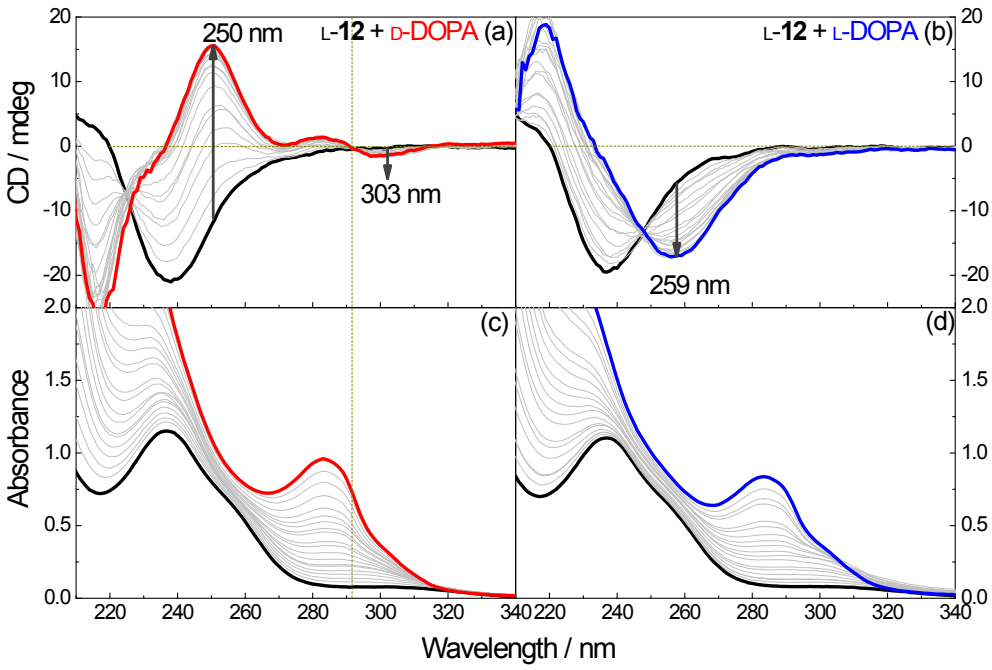


Figure S18. CD (a, b) and absorption (c, d) spectra of L-**12** in the presence of D-DOPA (a, c) and L-DOPA (b, d) in 7:3 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. [L-**12**] = 40 μM. [D-DOPA] = [L-DOPA] = 0 - 250 μM.

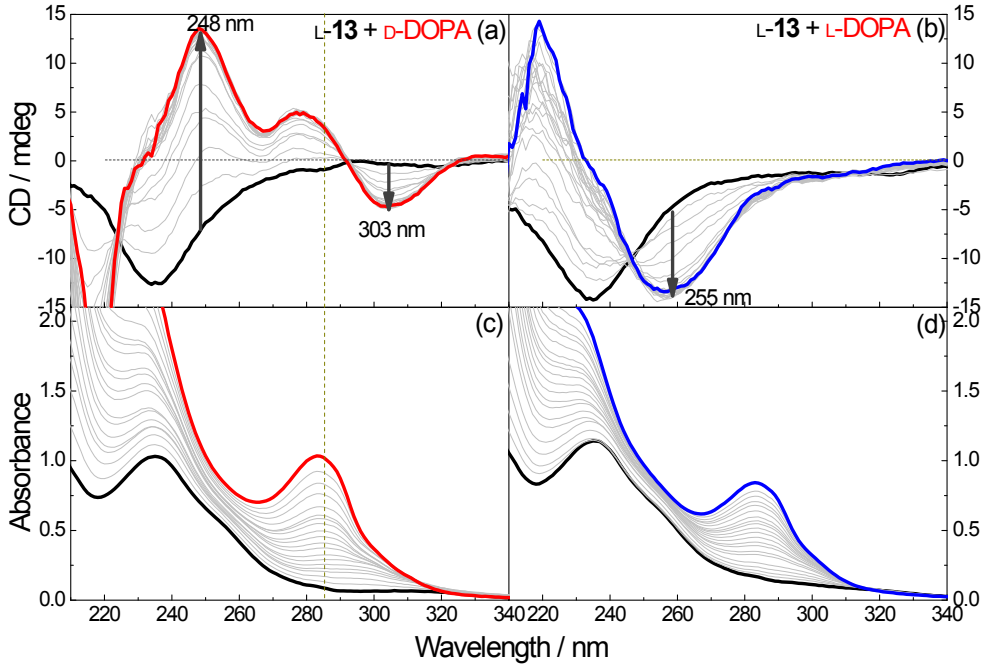


Figure S19. CD (a, b) and absorption (c, d) spectra of L-**13** in the presence of D-DOPA (a, c) and L-DOPA (b, d) in 7:3 (v/v) MeOH / 0.05 M pH 8.0 PBS buffer. [L-**13**] = 40 μM. [D-DOPA] = [L-DOPA] = 0 - 250 μM.

5. ^{1}H NMR and ^{19}F NMR studies

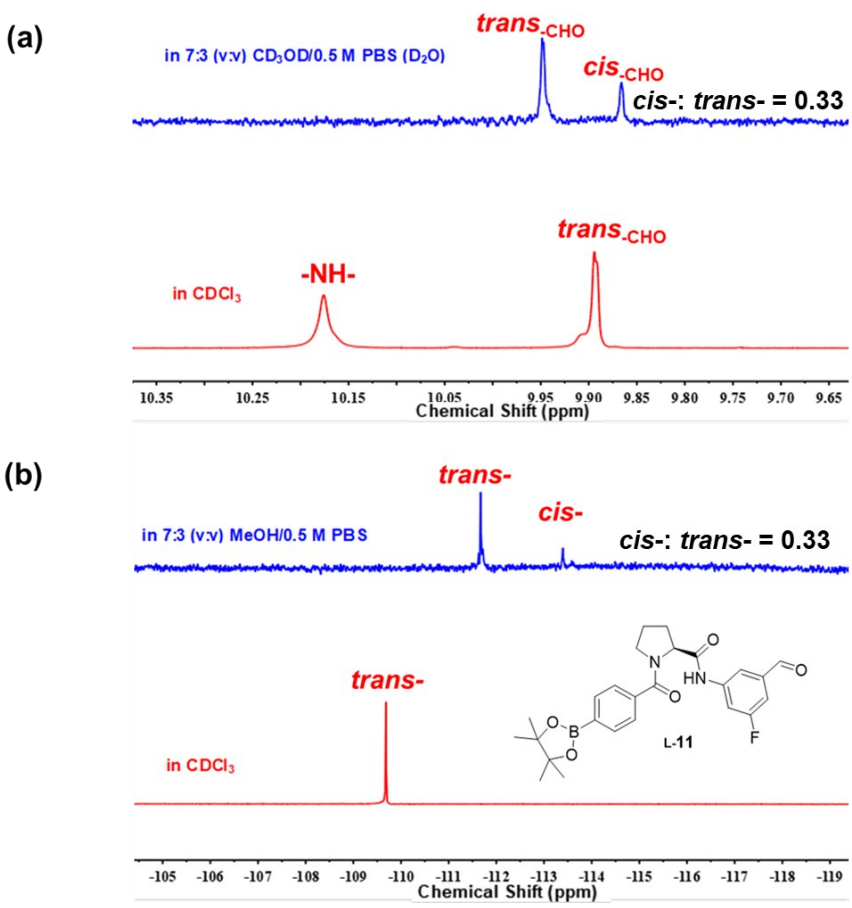


Figure S20. Partial ^{1}H NMR (a) and ^{19}F NMR (b) spectra of L-**11** in $CDCl_3$ and in 7:3 (v/v) CD_3OD/0.05 M pH 8.0 PBS buffer (PBS was dissolved in D_2O). [L-**11**] = 0.12 mM.

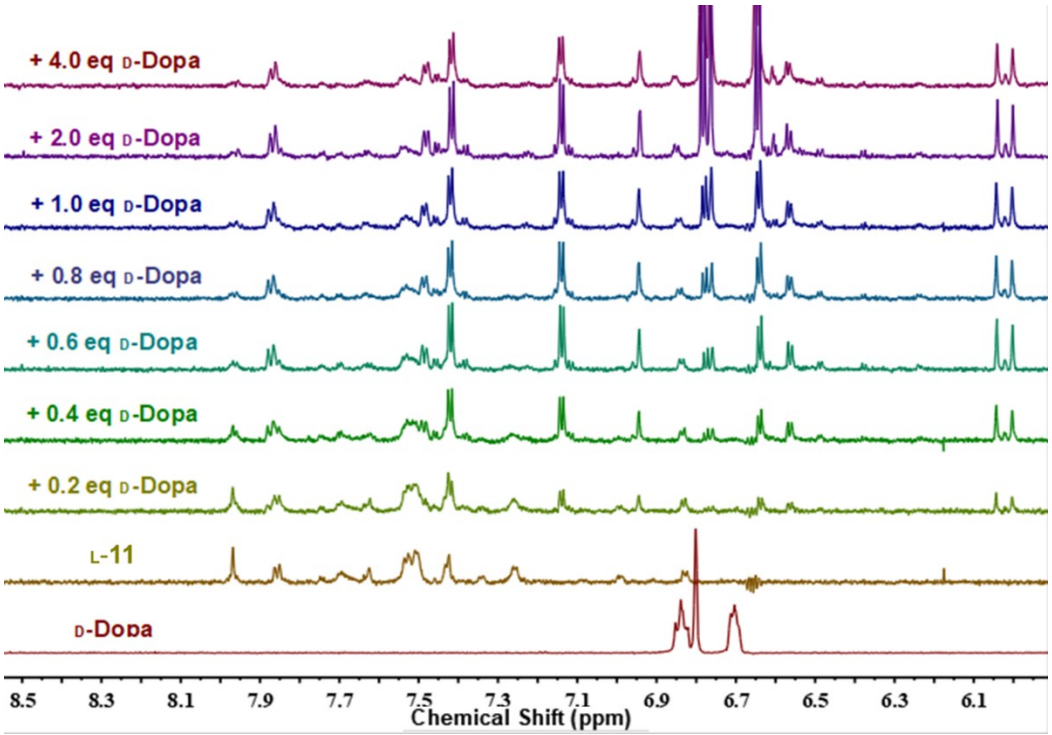


Figure S21. Partial ^{1}H NMR spectra of L-**11** in the presence of D-DOPA in 7:3 (v/v) CD_3OD/0.05 M pH 8.0 PBS buffer. PBS was dissolved in D_2O. [L-**11**] = 0.12 mM. [D-DOPA] = 0 – 0.48 mM.

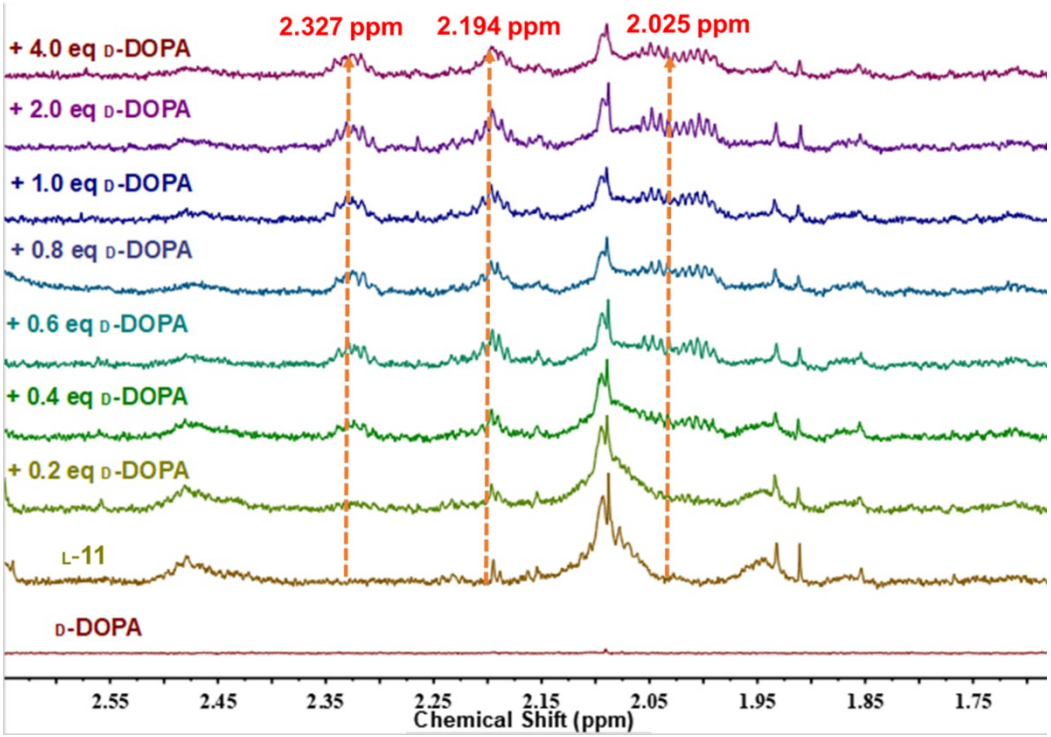


Figure S22. Partial ^{1}H NMR spectra of L-**11** in the presence of D-DOPA in 7:3 (v/v) CD_3OD/0.05 M pH 8.0 PBS buffer. PBS was dissolved in D_2O. [L-**11**] = 0.12 mM. [D-DOPA] = 0 – 0.48 mM.

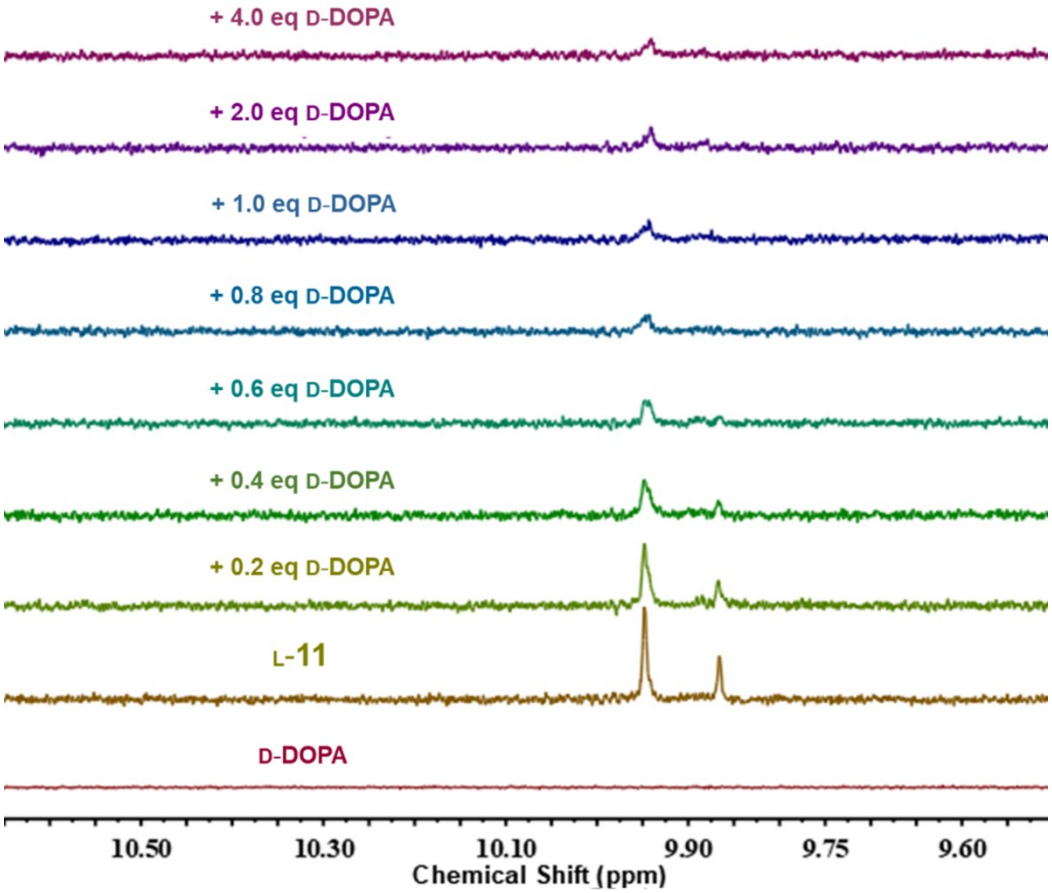


Figure S23. Partial ^{1}H NMR spectra of L-**11** in the presence of D-DOPA in 7:3 (v/v) CD_3OD/0.05 M pH 8.0 PBS buffer. PBS was dissolved in D_2O. [L-**11**] = 0.12 mM. [D-DOPA] = 0 – 0.48 mM.

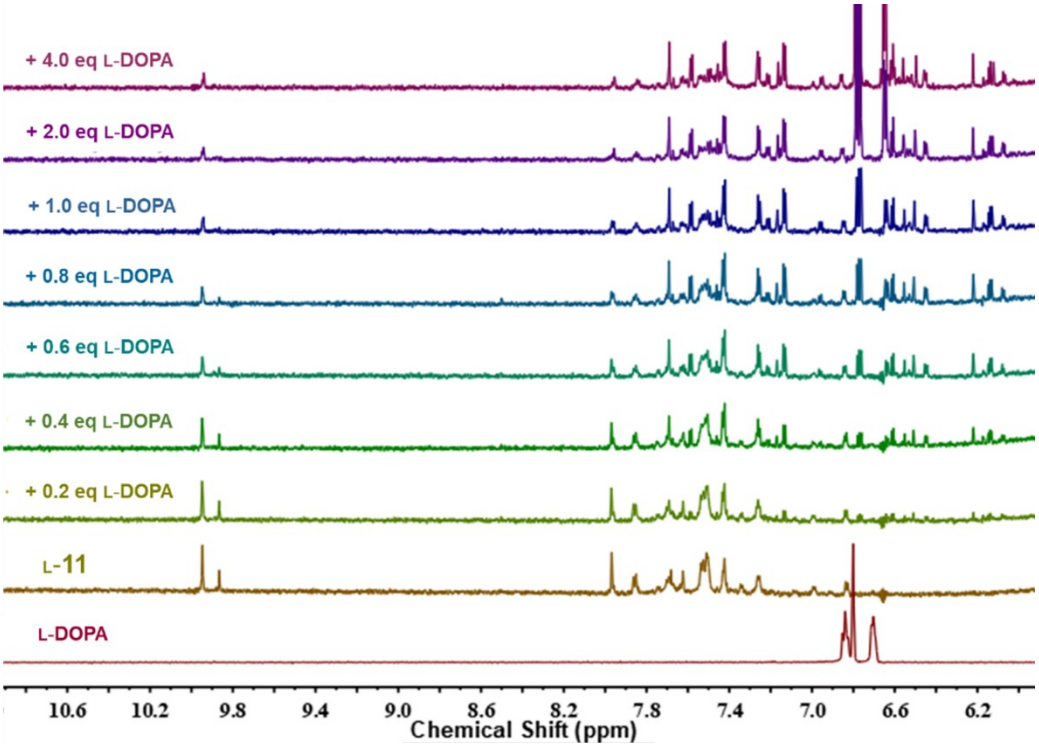


Figure S24. Partial ^{1}H NMR spectra of L-**11** in the presence of L-DOPA in 7:3 (v/v) CD_3OD/0.05 M pH 8.0 PBS buffer. PBS was dissolved in D_2O. [L-**11**] = 0.12 mM. [L-DOPA] = 0 – 0.48 mM.

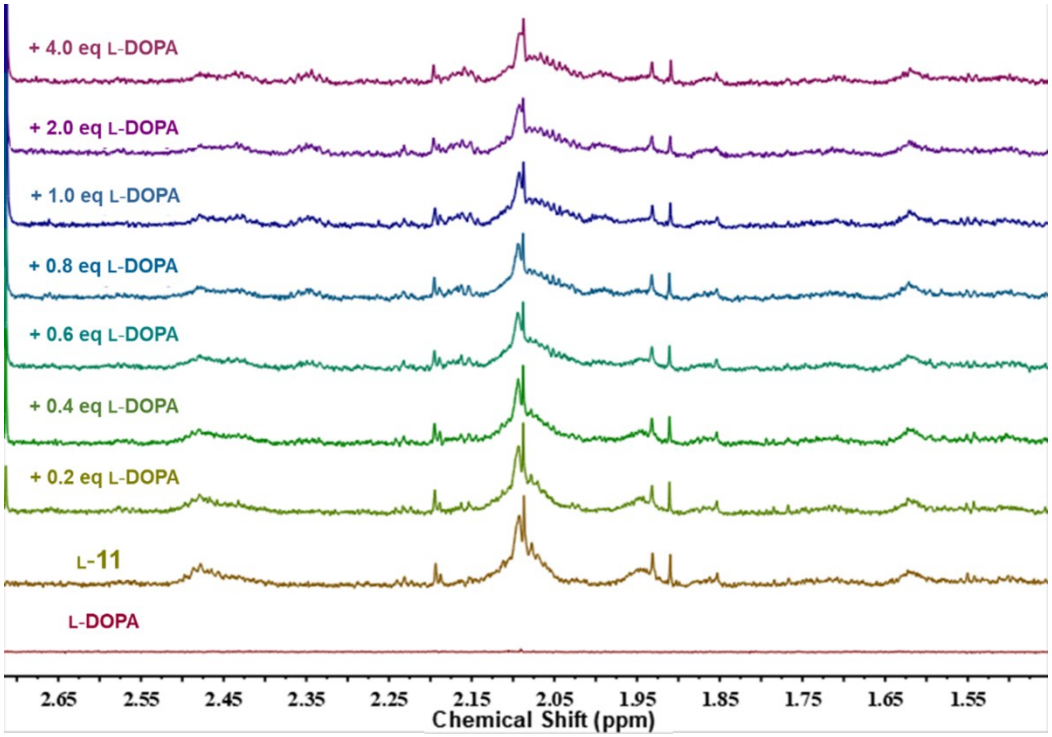


Figure S25. Partial ^{1}H NMR spectra of L-**11** in the presence of L-DOPA in 7:3 (v/v) CD_3OD/0.05 M pH 8.0 PBS buffer. PBS was dissolved in D_2O. [L-**11**] = 0.12 mM. [L-DOPA] = 0 – 0.48 mM.

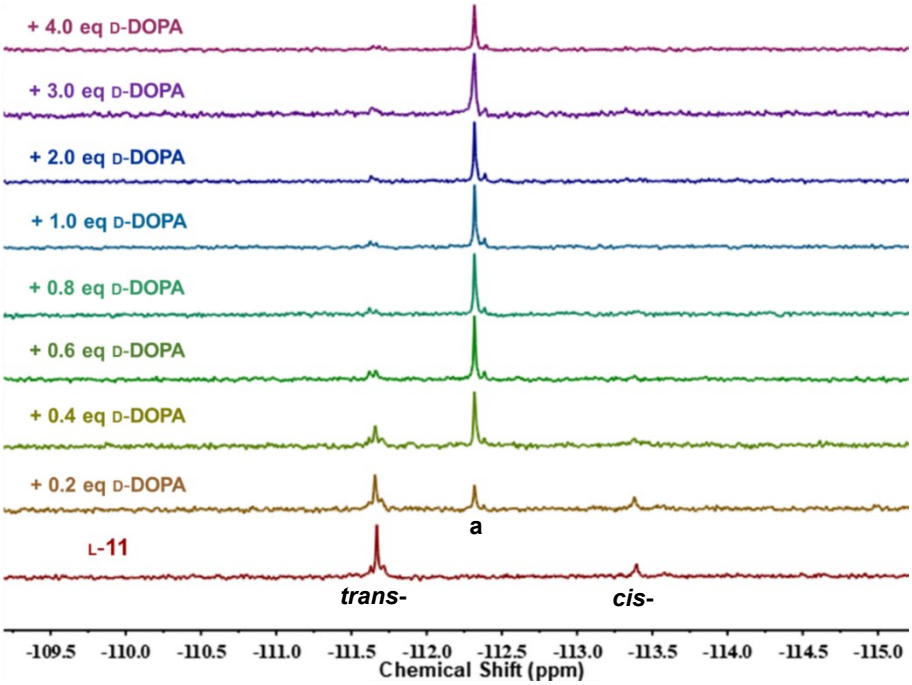


Figure S26. ^{19}F NMR spectra of L-**11** in the presence of D-DOPA of increasing equivalent in 7:3 (v/v) CD_3OD/0.05 M pH 8.0 PBS buffer, PBS was dissolved in D_2O. [L-**11**] = 0.12 mM.

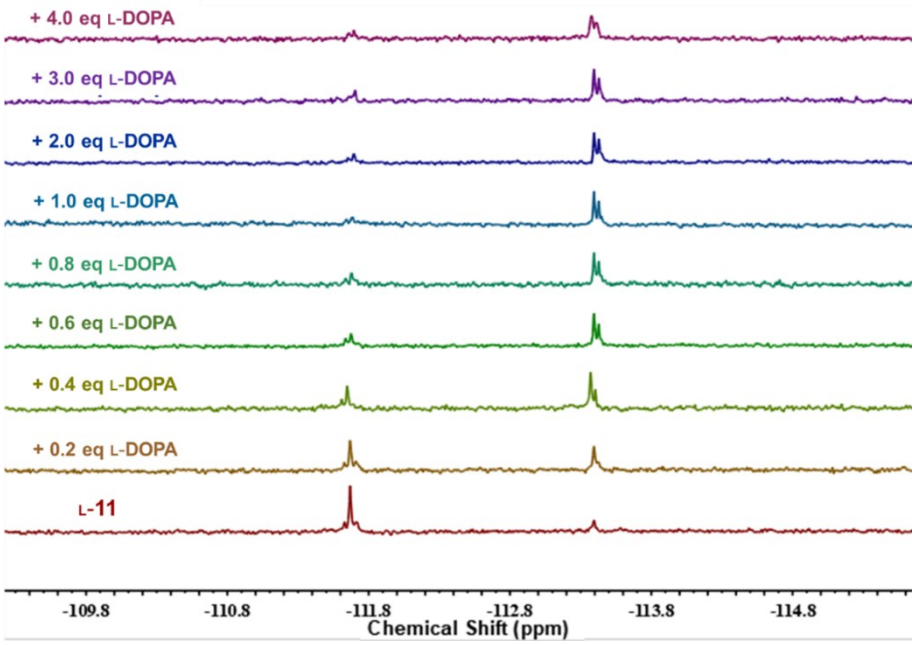


Figure S27. ^{19}F NMR spectra of L-**11** in the presence of L-DOPA of increasing equivalent in 7:3 (v/v) CD_3OD/0.05 M pH 8.0 PBS buffer. PBS was dissolved in D_2O. [L-**11**] = 0.12 mM.

Table S1. Binding constants of L-**11** with D-/L-DOPA from ^{19}F NMR titrations [a]

DOPA, μM	K_a, M^{-1}	
	D-DOPA	L-DOPA
24	2.07×10^6	1.36×10^5
48	0.90×10^6	1.10×10^5
72	1.09×10^6	0.94×10^5
96	2.58×10^6	1.66×10^5
120	1.20×10^6	1.69×10^5
Average	1.57×10^6	1.35×10^5

[a] L-**11** at 0.12 mM in 7:3 (v/v) CD_3OD/0.05 M pH 8.0 PBS buffer. Binding constants (K_a's) were calculated by mass balance equations [FS] + [F] = C_F and [FS] + [S] = C_S, that [FS] / [F]*[S] = K_a. "F" represents L-**11**, "S" represents DOPA, and "FS" represents complex of L-**11** with DOPA. T = 298 K.

Table S2 Relative peak area of *cis*- and *trans*-conformers of L-**11** in the presence of D-DOPA deduced from ^{19}F NMR spectra

D-Dopa (equiv)	Peak Area (*cis*-)	Peak Area (*trans*-)	Peak Area (**a**)
0	0.250	0.750	0
0.2	0.193	0.608	0.199
0.4	0.143	0.463	0.394
0.6	0.085	0.326	0.589
0.8	0.030	0.182	0.788
1.0	0	0.080	0.920
2.0	0	0.070	0.930
4.0	0	0.070	0.930

[a] Peak "**a**" represents the ^{19}F signal peak of L-**11**/D-DOPA complex, as shown in Figure S26.

6. DFT calculations

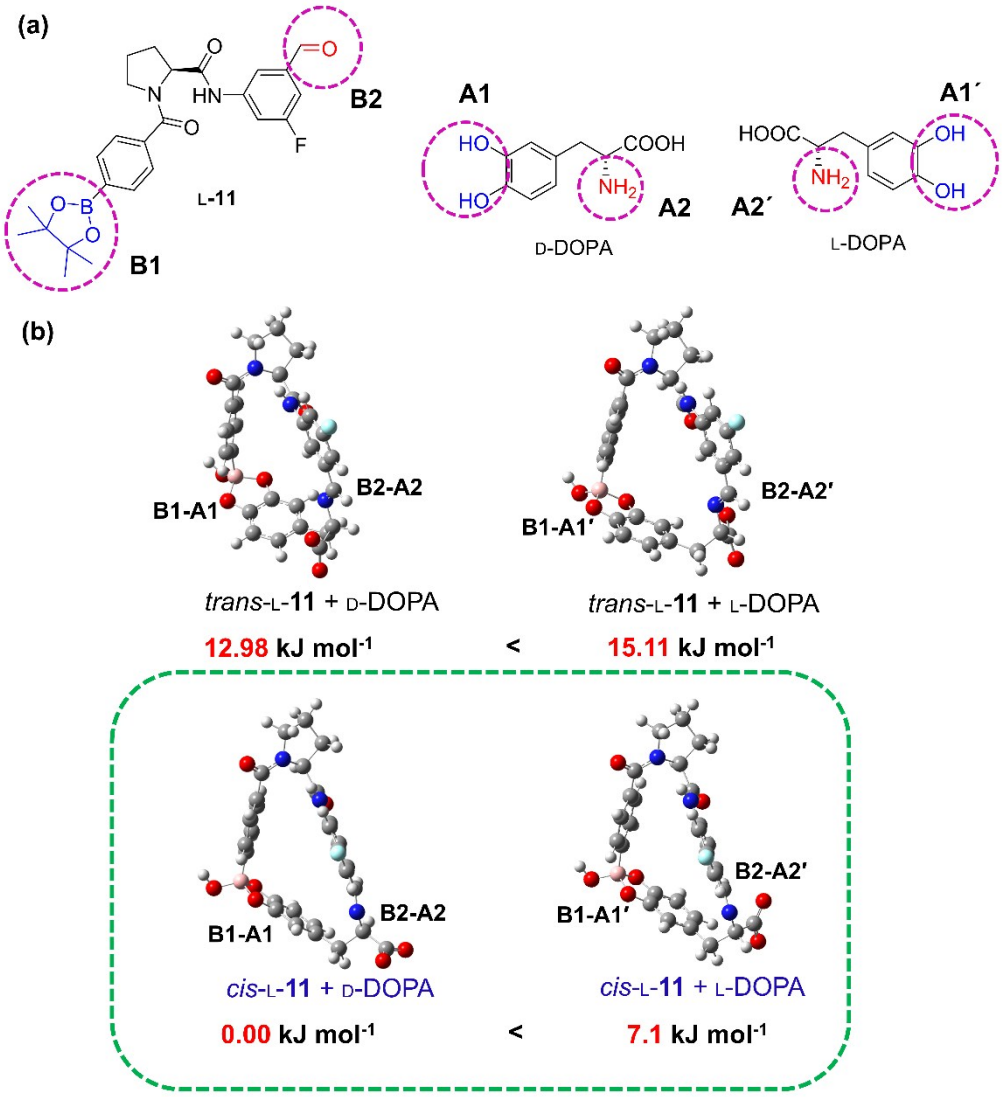


Figure S28. DFT calculation results. (a) Chemical structures of L-**11**, L-DOPA and D-DOPA with labeled binding sites. (b) Calculated relative energies of complexs of L-**11** with L-DOPA and D-DOPA in H_2O at B3LYP/6-31G* level.

7. Spectral titrations of L-1 and L-5 by DOPA in MeOH/buffer mixture of varying composition

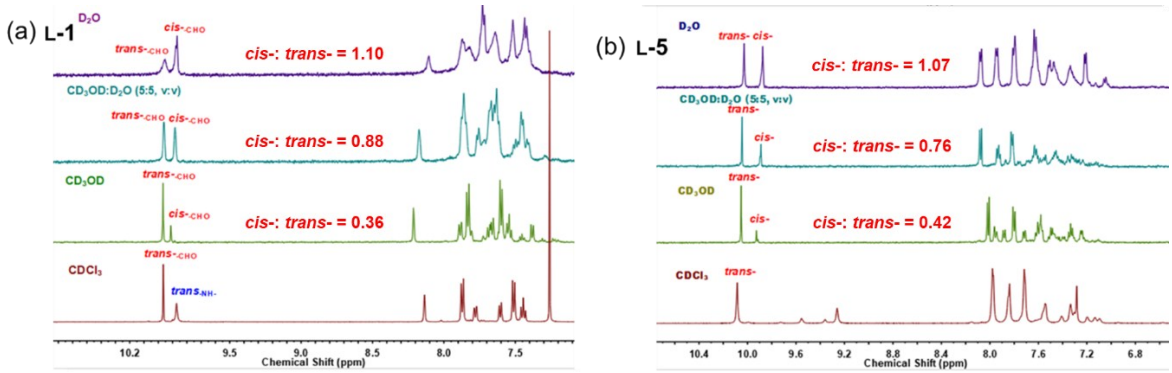


Figure S29. Partial ^{1}H NMR spectra of L-**1** (a) and L-**5** (b) in $CDCl_3$, CD_3OD, CD_3OD/D_2O (5:5, v/v) and D_2O.

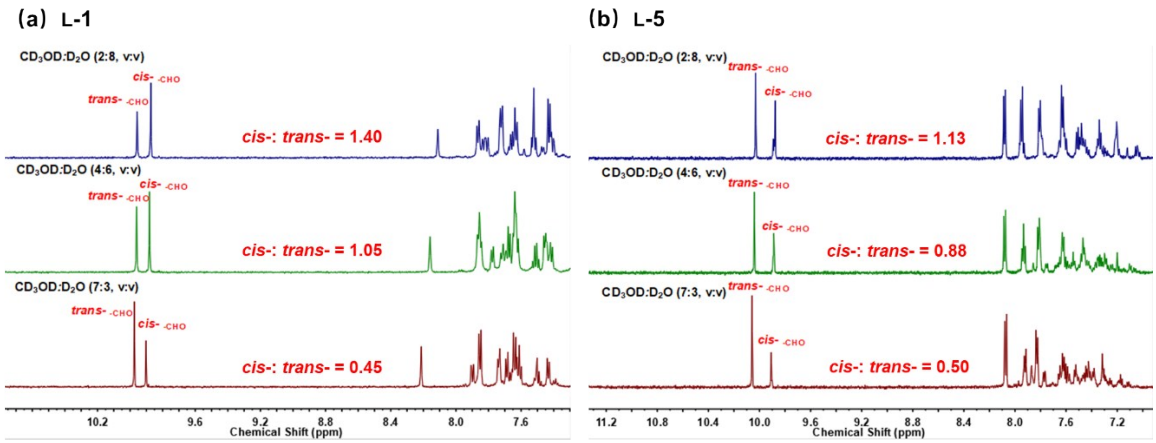


Figure S30. Partial ^{1}H NMR spectra of L-**1** (a) and L-**5** (b) in 7:3 (v/v), 4:6 (v/v) and 2:8 (v/v) CD_3OD/D_2O solutions.

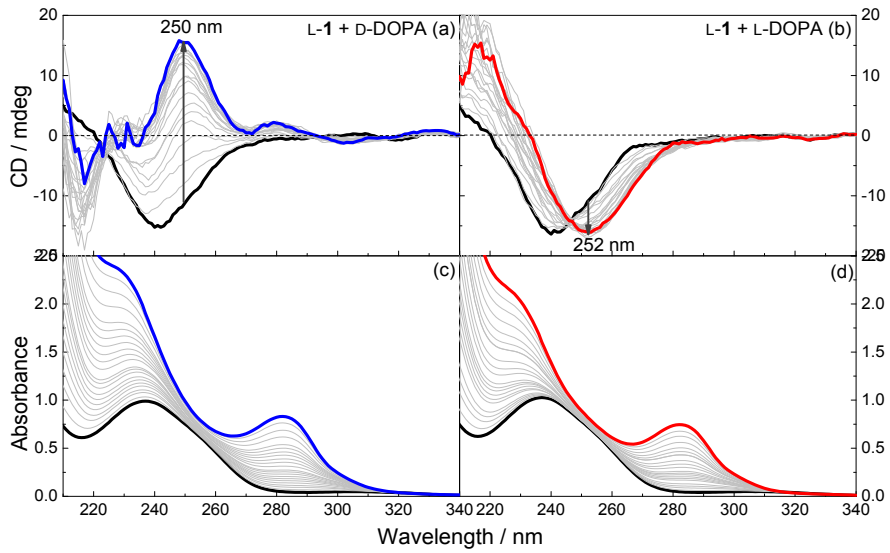


Figure S31. CD (a, b) and absorption (c, d) spectra of L-**1** in the presence of D- (a, c) or L-DOPA (b, d) in 4:6 (v/v) MeOH/0.05M pH 8.0 PBS buffer. [L-**1**] = 40 μM. [L-DOPA] = [D-DOPA] = 0 - 250 μM.

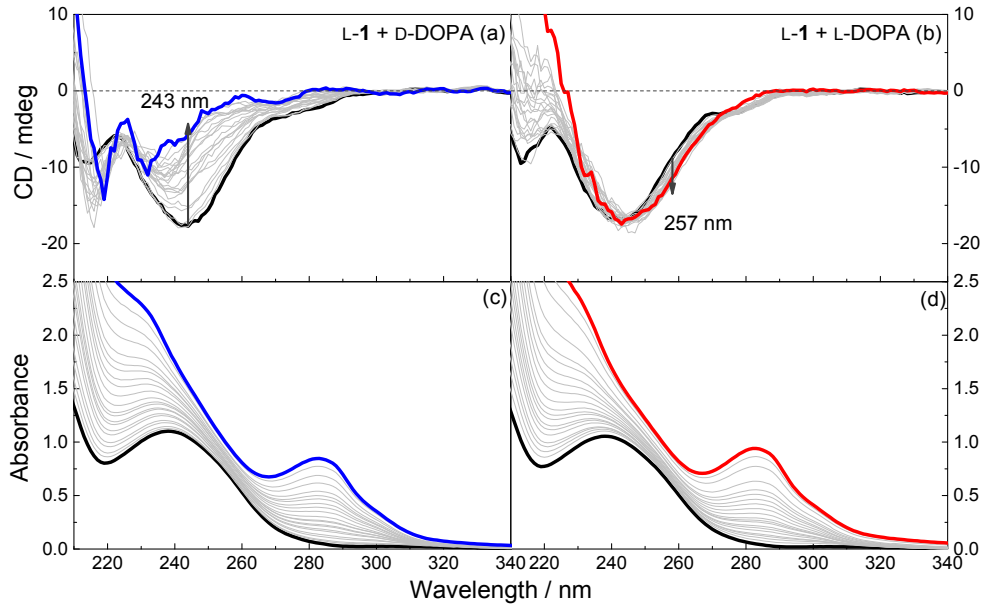


Figure S32. CD (a, b) and absorption (c, d) spectra of L-**1** in the presence of D- (a, c) or L-DOPA (b, d) in 2:8 (v/v) MeOH/0.05M pH 8.0 PBS buffer. [L-**1**] = 40 μM. [L-DOPA] = [D-DOPA] = 0 - 250 μM.

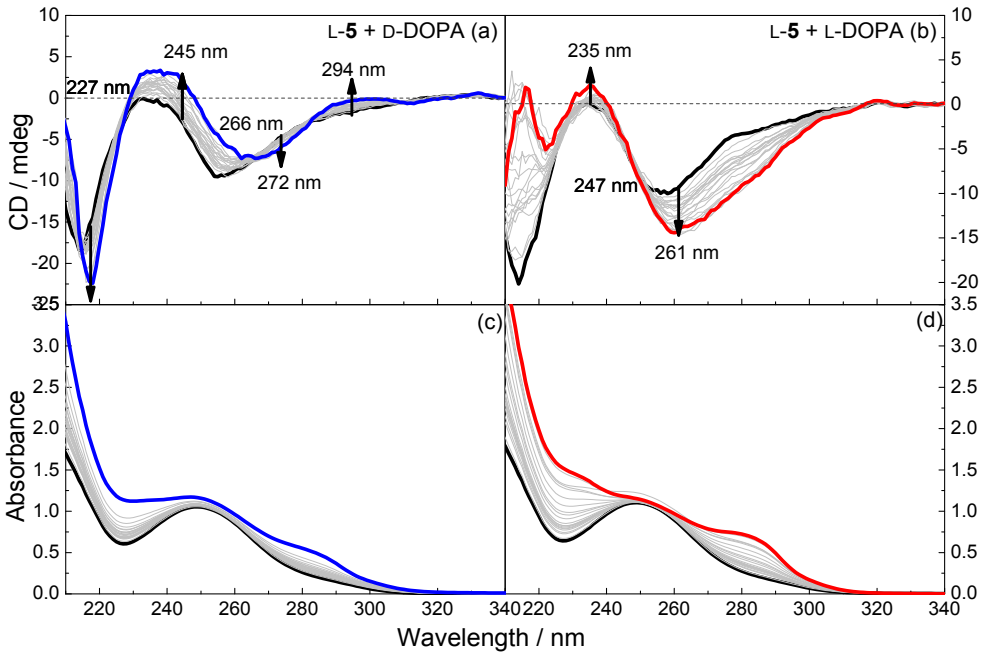


Figure S33. CD (a, b) and absorption (c, d) spectra of L-**5** in the presence of D- (a, c) or L-DOPA (b, d) in 4:6 (v/v) MeOH/0.05M pH 8.0 PBS buffer. [L-**5**] = 40 μM. [L-DOPA] = [D-DOPA] = 0 - 250 μM.

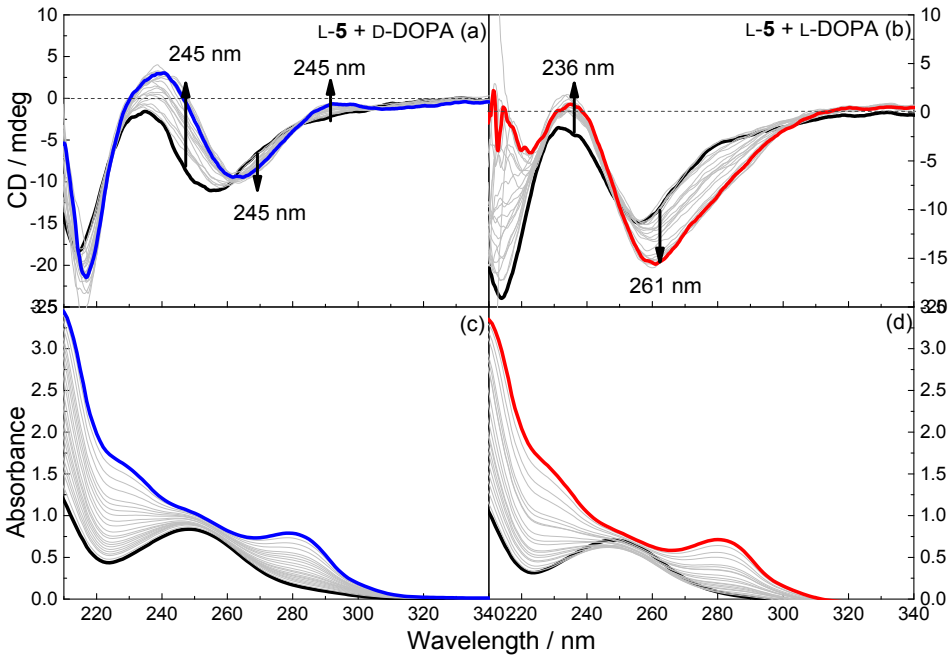


Figure S34. CD (a, b) and absorption (c, d) spectra of L-**5** in the presence of D- (a, c) or L-DOPA (b, d) in 2:8 (v/v) MeOH/0.05M pH 8.0 PBS buffer. [L-**5**] = 40 μM. [L-DOPA] = [D-DOPA] = 0 - 250 μM.

8. Job plots

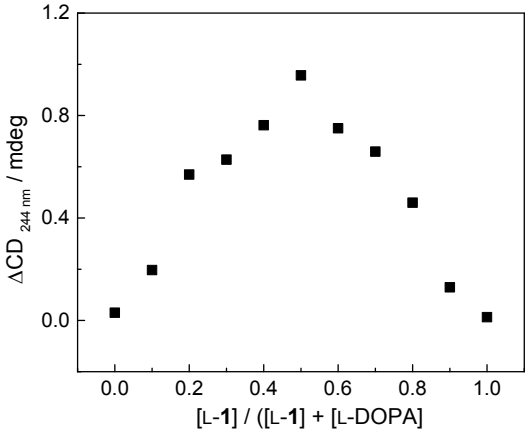


Figure S35. Job plot for the interaction of L-**1** with L-DOPA revealing a 1:1 stoichiometry. [L-**1**] + [L-DOPA] = 40 μM.

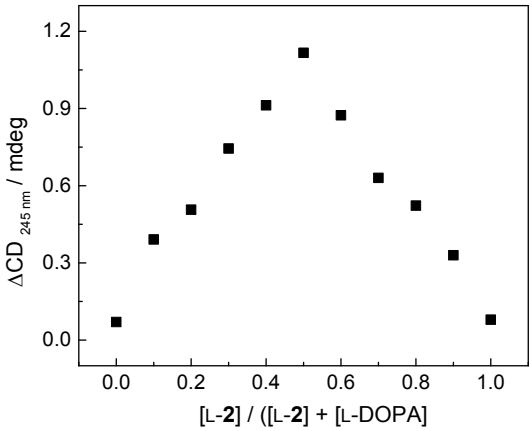


Figure S36. Job plot for the interaction of L-**2** with L-DOPA revealing a 1:1 stoichiometry. [L-**2**] + [L-DOPA] = 40 μM.

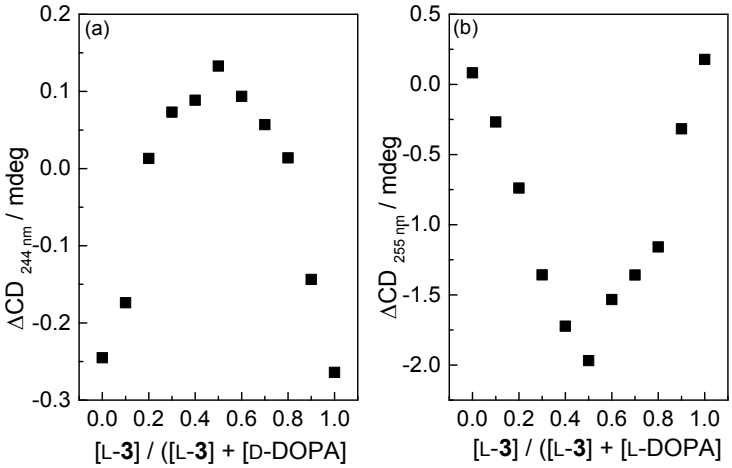


Figure S37. Job plots for the interactions of L-**3** with D-DOPA (a) and L-DOPA (b) revealing a 1:1 stoichiometry. [L-**3**] + [D-DOPA] = 40 μM, [L-**3**] + [L-DOPA] = 40 μM.

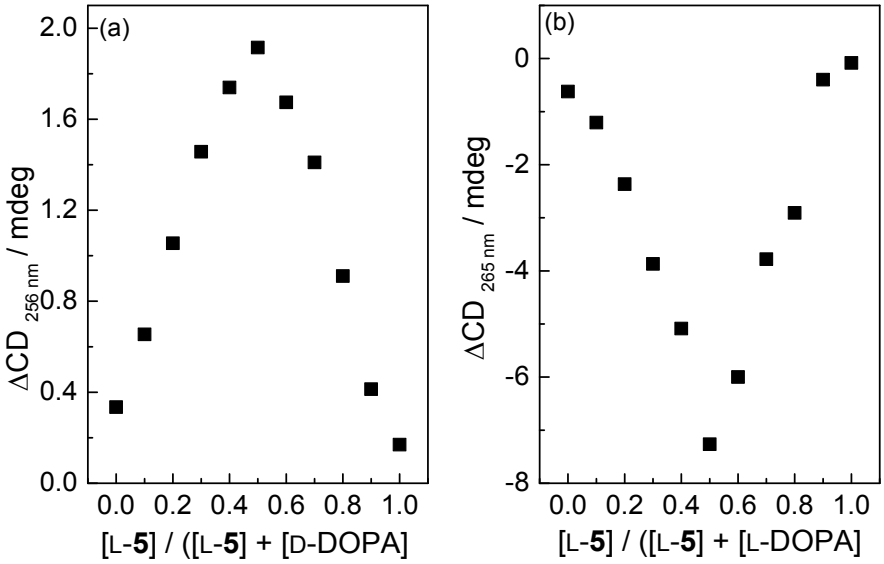


Figure S38. Job plots for the interactions of L-**5** with D-DOPA (a) and L-DOPA (b) revealing a 1:1 stoichiometry. [L-**5**] + [D-DOPA] = 40 μM, [L-**5**] + [L-DOPA] = 40 μM.

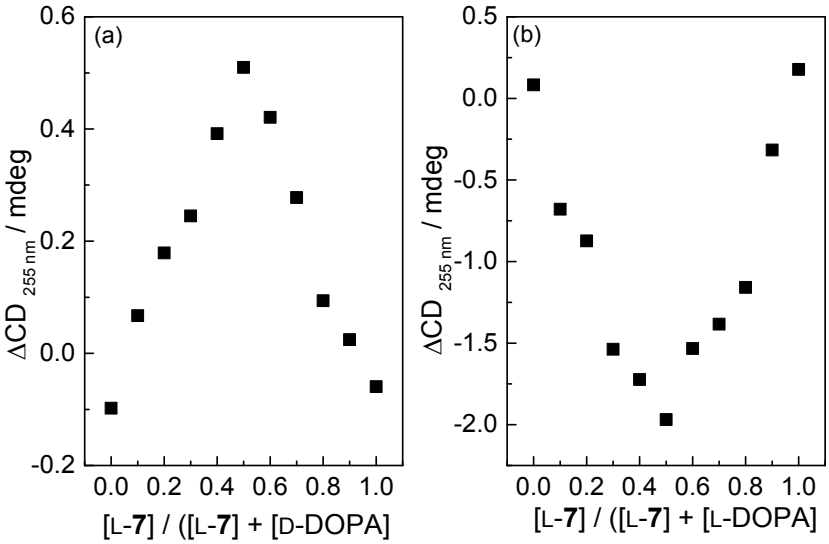


Figure S39. Job plots for the interactions of L-**7** with D-DOPA (a) and L-DOPA (b) revealing a 1:1 stoichiometry. [L-**7**] + [D-DOPA] = 40 μM, [L-**7**] + [L-DOPA] = 40 μM.

9. Titration curves and fitted binding isotherms

$$y = y_0 + \frac{a}{2c}\left[x + c + \frac{1}{K} - \sqrt{\left(x + c + \frac{1}{K}\right)^2 - 4cx}\right] \qquad \textbf{(Formula 1)}$$

Formula 1 - Nonlinear fitting equation assuming a 1:1 stoichiometry.

y_0 - CD intensity of receptor solution without chiral guest, x;

c - Total concentration of receptor molecule;

x - Molar concentration of chiral species x;

a - Fitting parameters;

K – Binding constant.

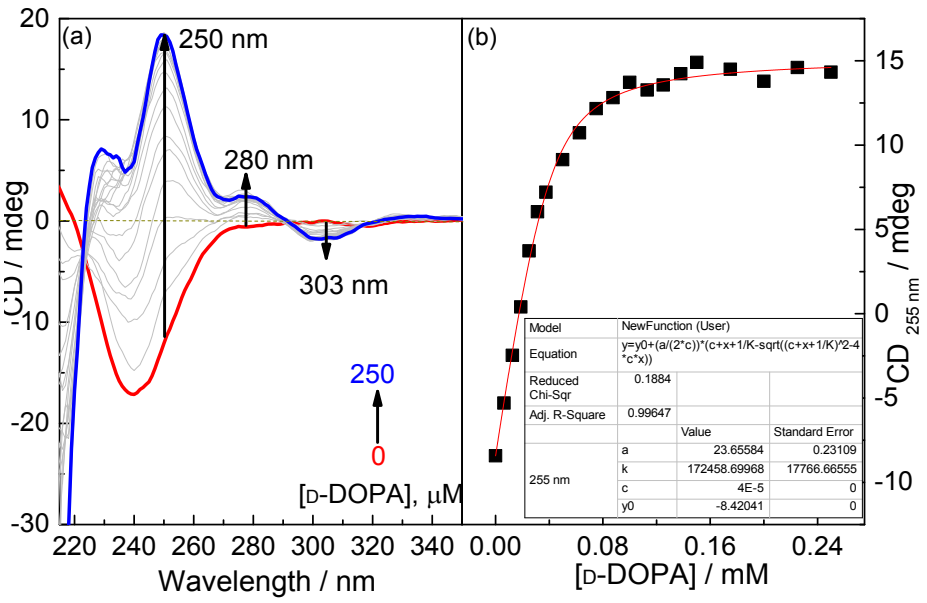


Figure S40. CD spectra (a) and CD intensities at 255 nm (b) of L-**1** in the presence of D-DOPA in 7:3 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. Red line through data points in (b) is the curve fitted by Formula 1. [L-**1**] = 40 μM, [D-DOPA] = 0 - 250 μM.

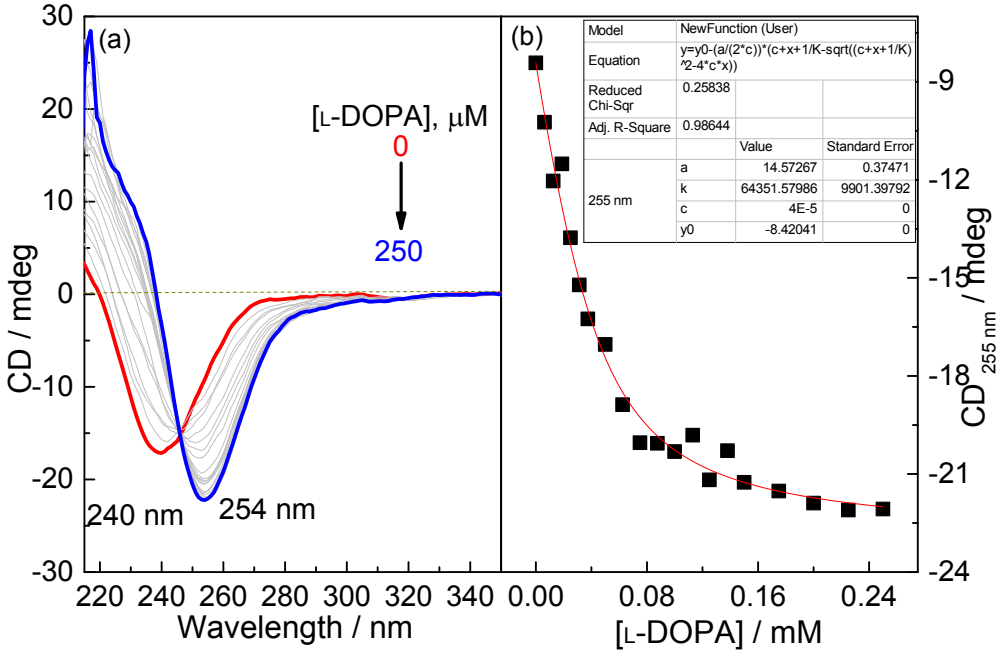


Figure S41. CD spectra (a) and CD intensities at 255 nm (b) of L-**1** in the presence of L-DOPA in 7:3 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. Red line through data points in (b) is the curve fitted by Formula 1. [L-**1**] = 40 μM, [L-DOPA] = 0 - 250 μM.

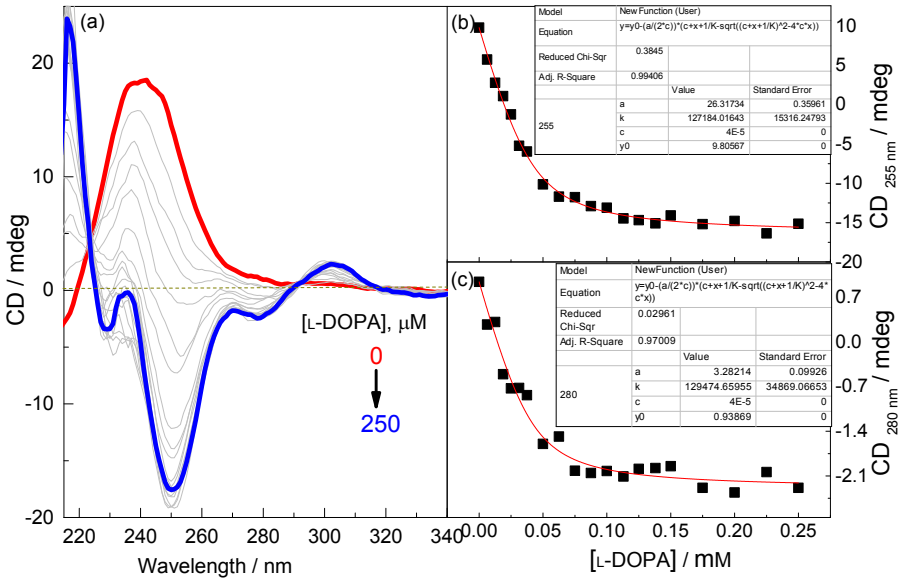


Figure S42. CD spectra (a) and CD intensities at 255 nm (b) or 280 nm (c) of D-**1** in the presence of L-DOPA in 7:3 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. Red line through data points in (b) is the curve fitted by Formula 1. [D-**1**] = 40 μM, [L-DOPA] = 0 - 250 μM.

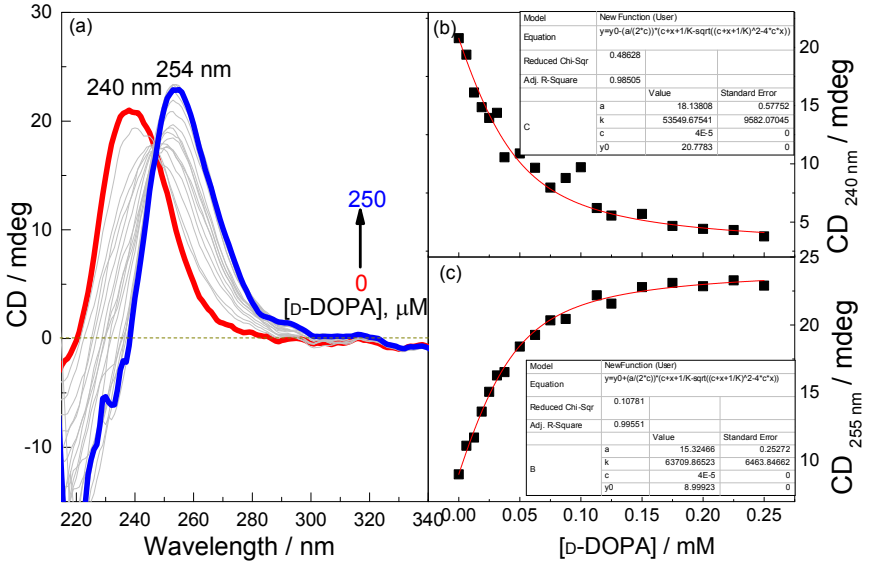


Figure S43. CD spectra (a) and CD intensities at 240 nm (b) or 255 nm (c) of D-**1** in the presence of D-DOPA in 7:3 (v/v) MeOH / 0.05 M pH 8.0 PBS buffer. Red lines through data points in (b) and (c) are the curves fitted by Formula 1. [D-**1**] = 40 μM, [D-DOPA] = 0 - 250 μM.

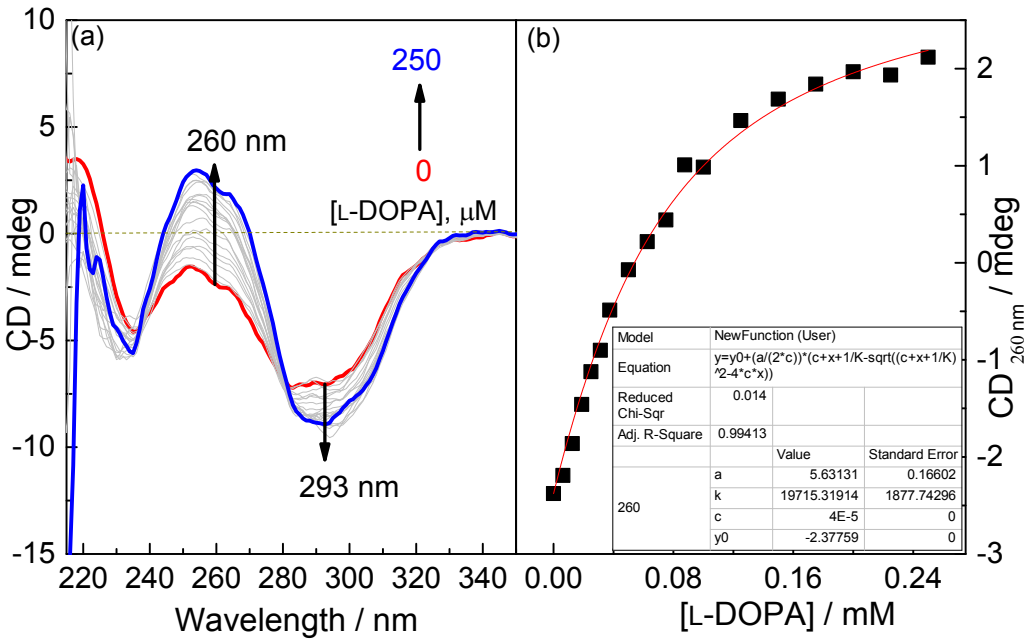


Figure S44. CD spectra (a) and CD intensities at 260 nm of L-**2** in the presence of L-DOPA in 7:3 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. Red line through data points in (b) is the curve fitted by Formula 1. [L-**2**] = 40 μM, [L-DOPA] = 0 - 250 μM.

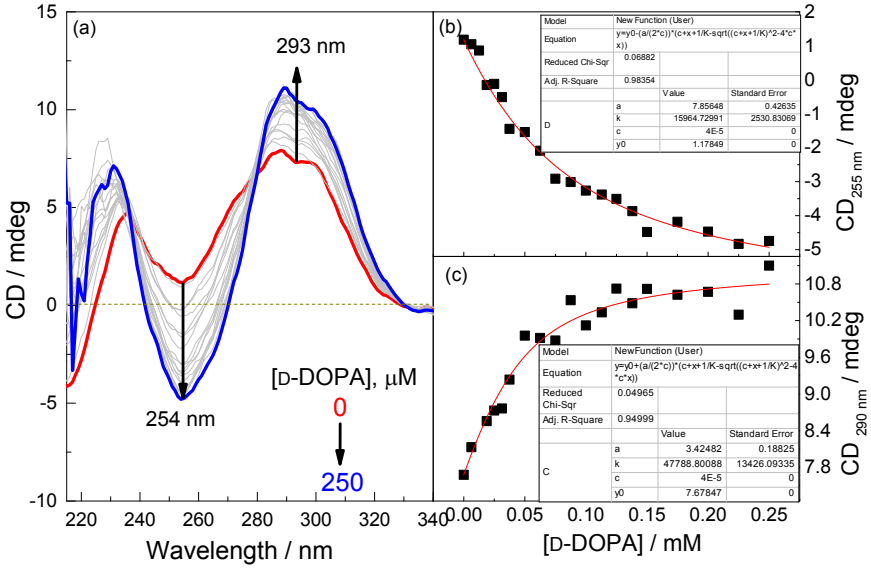


Figure S45. CD spectra (a) and CD intensities at 255 nm (b) or 290 nm (c) of D-**2** in the presence of D-DOPA in 7:3 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. Red lines through data points in (b) and (c) are the curves fitted by Formula 1. [D-**2**] = 40 μM, [D-DOPA] = 0 - 250 μM.

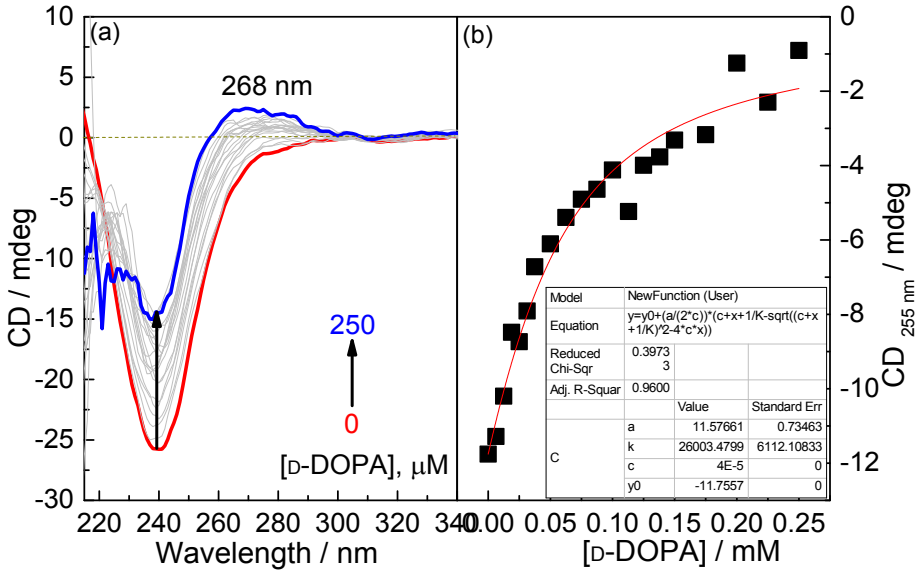


Figure S46. CD spectra (a) and CD intensities at 255 nm (b) of L-**3** in the presence of D-DOPA in 7:3 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. Red line through data points in (b) is the curve fitted by Formula 1. [L-**3**] = 40 μM, [D-DOPA] = 0 - 250 μM.

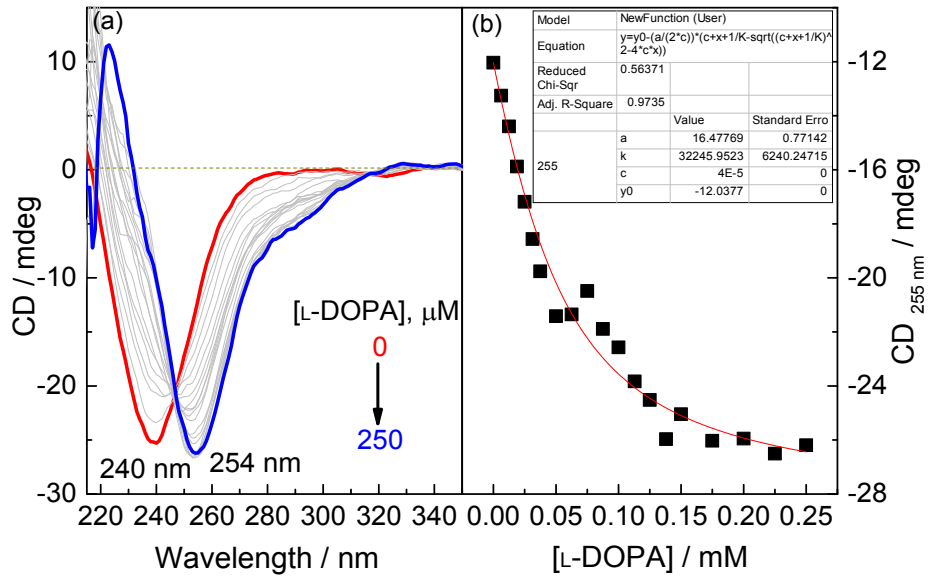


Figure S47. CD spectra (a) and CD intensities at 255 nm (b) of L-**3** in the presence of L-DOPA in 7:3 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. Red line through data points in (b) is the curve fitted by Formula 1. [L-**3**] = 40 μM, [L-DOPA] = 0 - 250 μM.

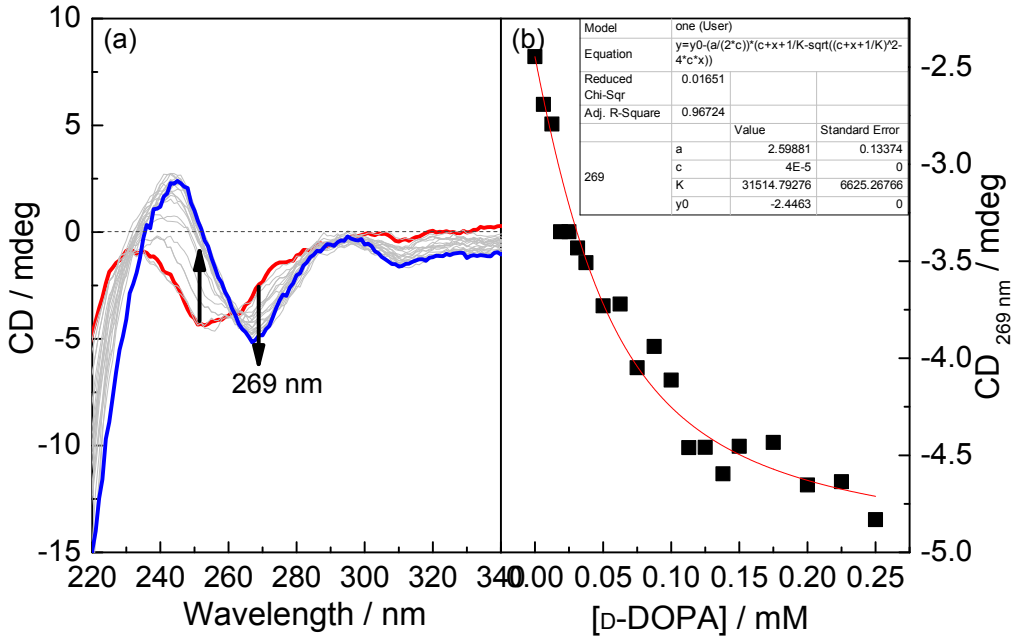


Figure S48. CD spectra (a) and CD intensities at 269 nm (b) of L-**5** in the presence of D-DOPA in 7:3 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. Red line through data points in (b) is the curve fitted by Formula 1. [L-**5**] = 40 μM, [D-DOPA] = 0 - 250 μM.

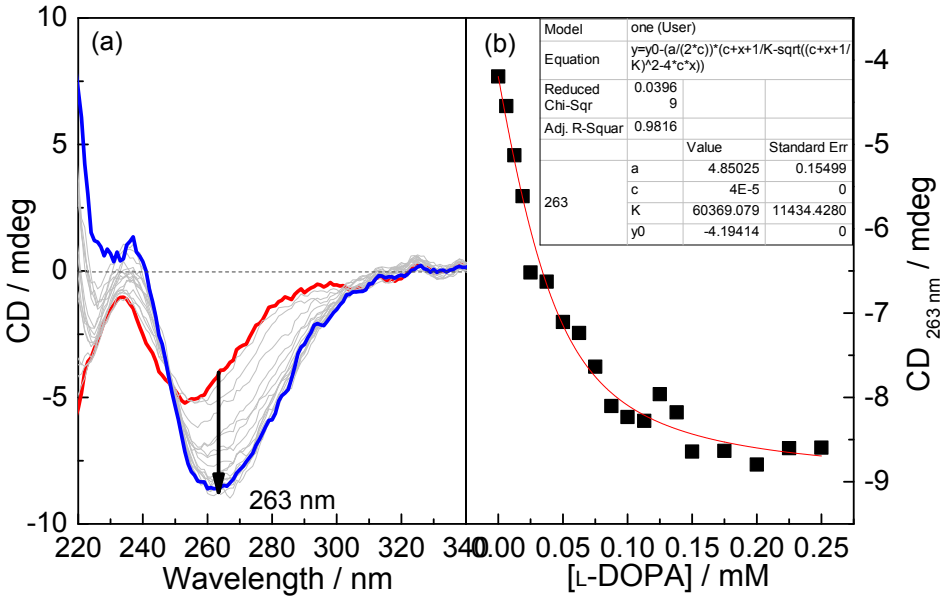


Figure S49. CD spectra (a) and CD intensities at 263 nm (b) of L-**5** in the presence of L-DOPA in 7:3 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. Red line through data points in (b) is the curve fitted by Formula 1. [L-**5**] = 40 μM, [L-DOPA] = 0 - 250 μM.

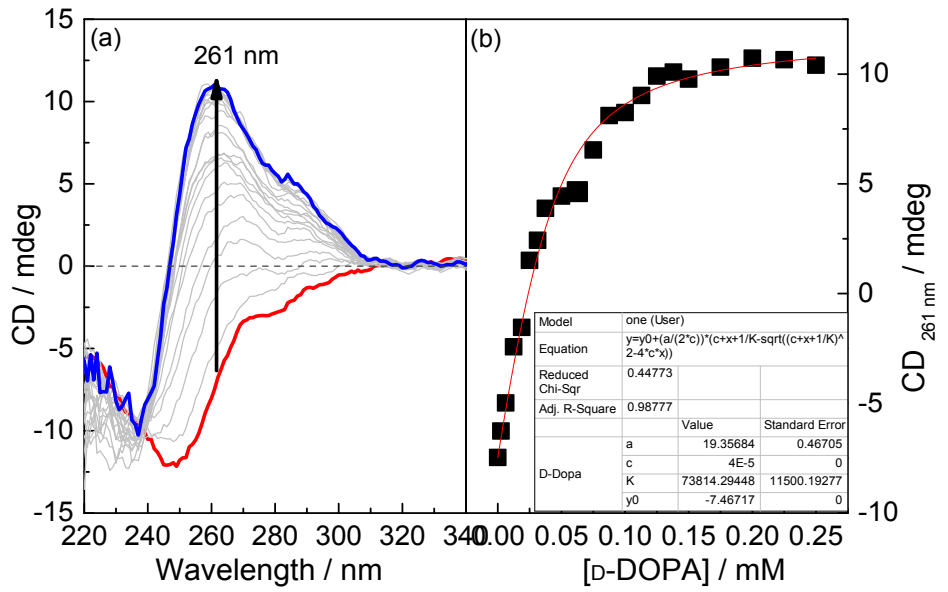


Figure S50. CD spectra (a) and CD intensities at 261 nm (b) of L-**7** in the presence of D-DOPA in 7:3 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. Red line through data points in (b) is the curve fitted by Formula 1. [L-**7**] = 40 μM, [D-DOPA] = 0 - 250 μM.

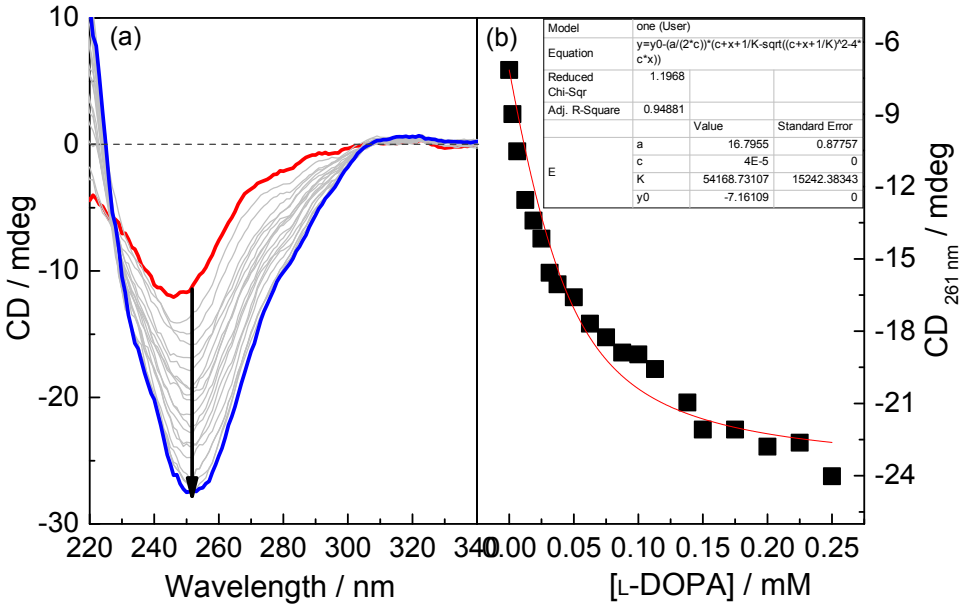


Figure S51. CD spectra (a) and CD intensities at 261 nm (b) of L-**7** in the presence of L-DOPA in 7:3 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. Red line through data points in (b) is the curve fitted by Formula 1. [L-**7**] = 40 μM, [L-DOPA] = 0 - 250 μM.

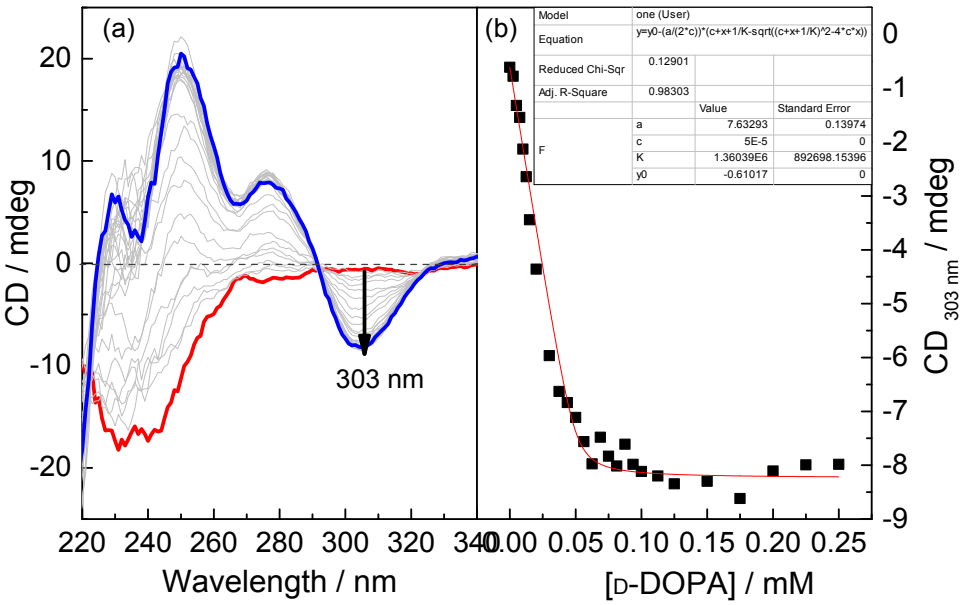


Figure S52. CD spectra (a) and CD intensities at 303 nm (b) of L-**11** in the presence of D-DOPA in 7:3 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. Red line through data points in (b) is the curve fitted by Formula 1. [L-**11**] = 50 μM, [D-DOPA] = 0 - 250 μM.

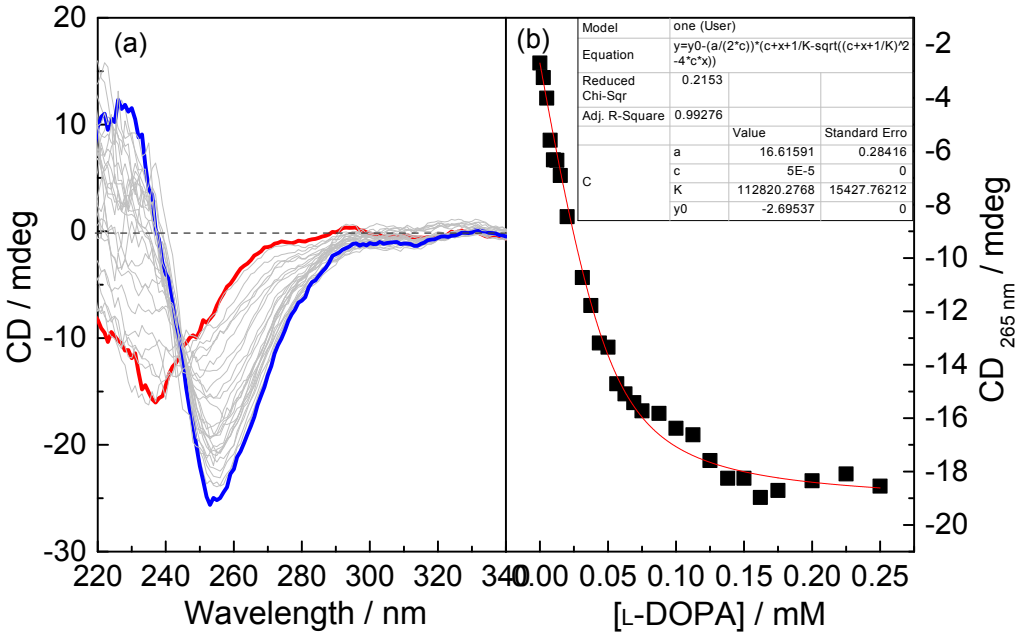


Figure S53. CD spectra (a) and CD intensities at 265 nm (b) of L-**11** in the presence of L-DOPA in 7:3 (v/v) MeOH / 0.05 M pH 8.0 PBS buffer. Red line through data points in (b) is the curve fitted by Formula 1. [L-**11**] = 50 μM, [L-DOPA] = 0 - 250 μM.

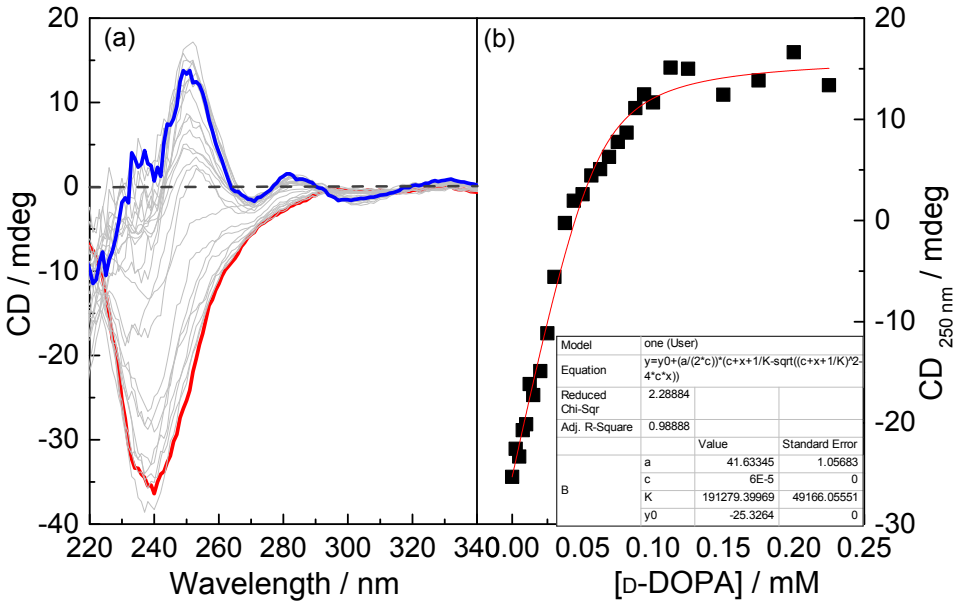


Figure S54. CD spectra (a) and CD intensities at 250 nm (b) of L-**12** in the presence of D-DOPA in 7:3 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. Red line through data points in (b) is the curve fitted by Formula 1. [L-**12**] = 60 μM, [D-DOPA] = 0 - 250 μM.

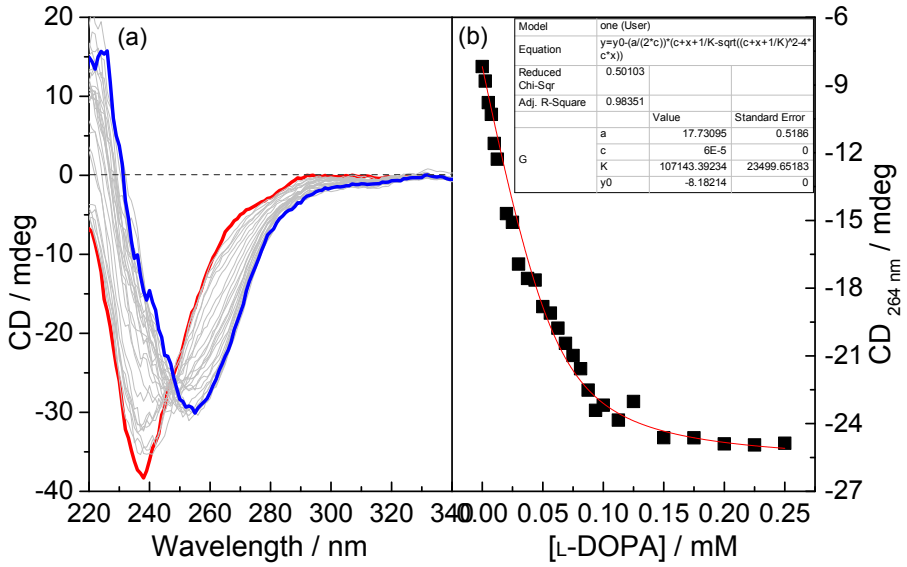


Figure S55. CD spectra (a) and CD intensities at 264 nm (b) of L-**12** in the presence of L-DOPA in 7:3 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. Red line through data points in (b) is the curve fitted by Formula 1. [L-**12**] = 60 μM, [L-DOPA] = 0 - 250 μM.

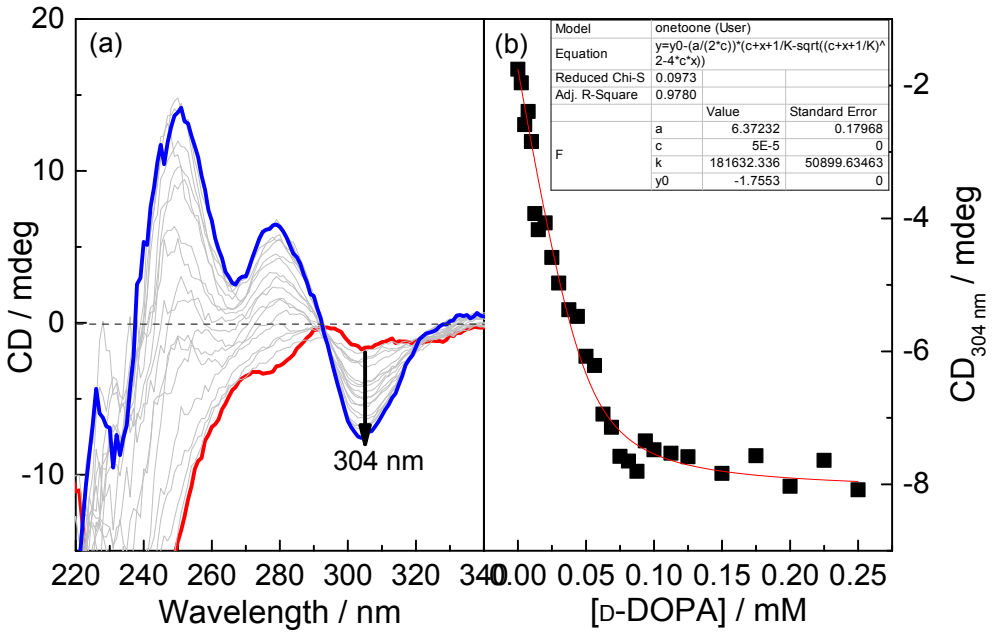


Figure S56. CD spectra (a) and CD intensities at 304 nm (b) of L-**13** in the presence of D-DOPA in 7:3 (v/v) MeOH / 0.05 M pH 8.0 PBS buffer. Red line through data points in (b) is the curve fitted by Formula 1. [L-**13**] = 50 μM, [D-DOPA] = 0 - 250 μM.

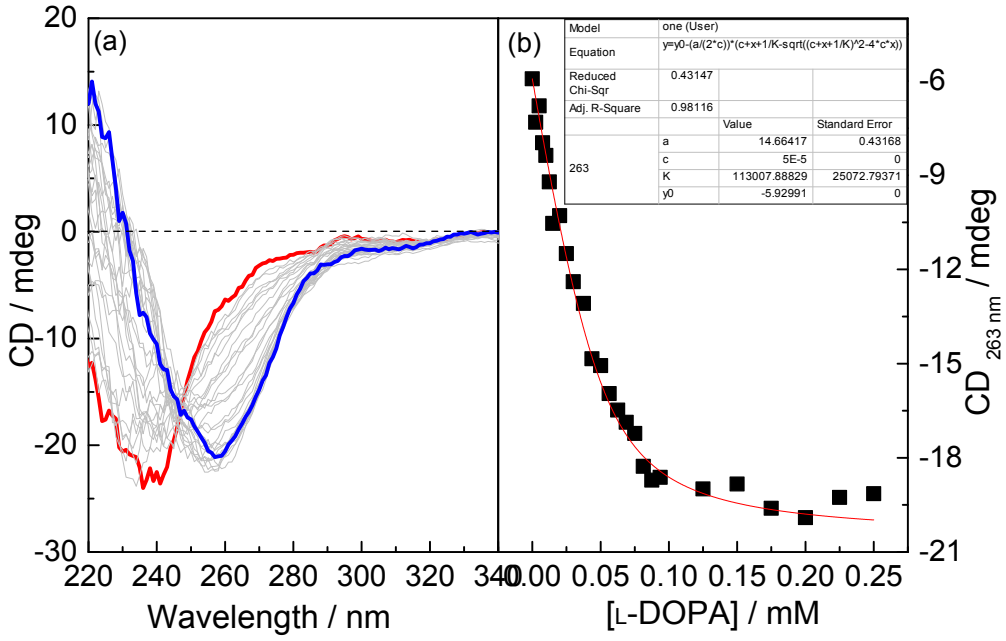


Figure S57. CD spectra (a) and CD intensities at 263 nm (b) of L-**13** in the presence of L-DOPA in 7:3 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. Red line through data points in (b) is the curve fitted by Formula 1. [L-**13**] = 50 μM, [L-DOPA] = 0 - 250 μM.

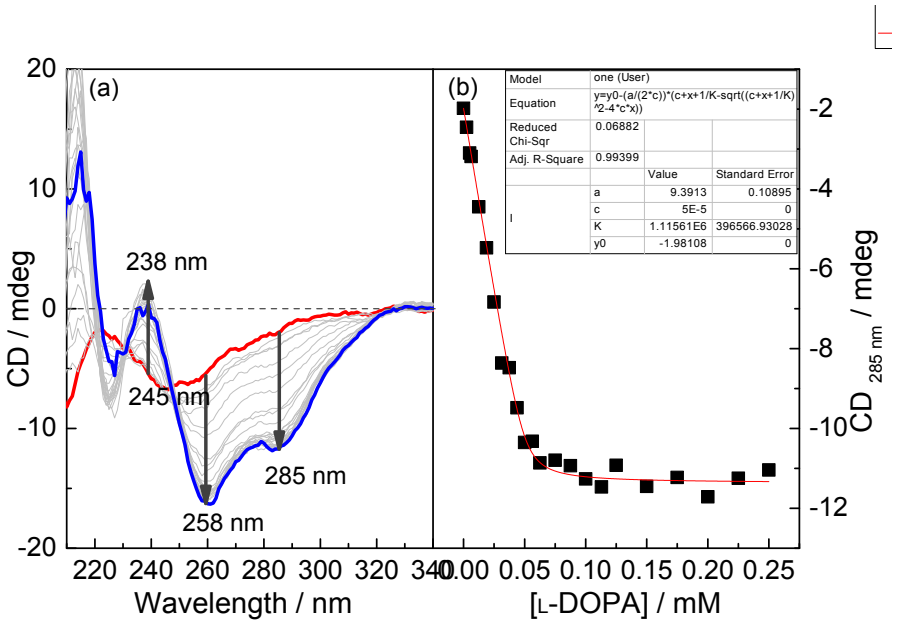


Figure S58. CD spectra (a) and CD intensities at 285 nm (b) of L-**14** in the presence of L-DOPA in 7:3 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. Red line through data points in (b) is the curve fitted by Formula 1. [L-**14**] = 50 μM, [L-DOPA] = 0 - 250 μM.

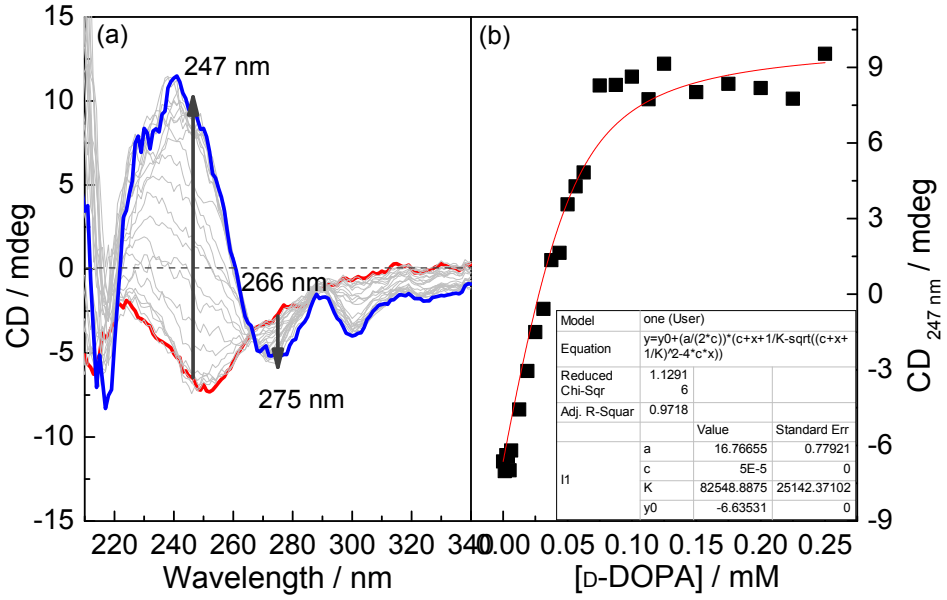


Figure S59. CD spectra (a) and CD intensities at 247 nm (b) of L-**14** in the presence of D-DOPA in 7:3 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. Red line through data points in (b) is the curve fitted by Formula 1. [L-**14**] = 50 μM, [D-DOPA] = 0 - 250 μM.

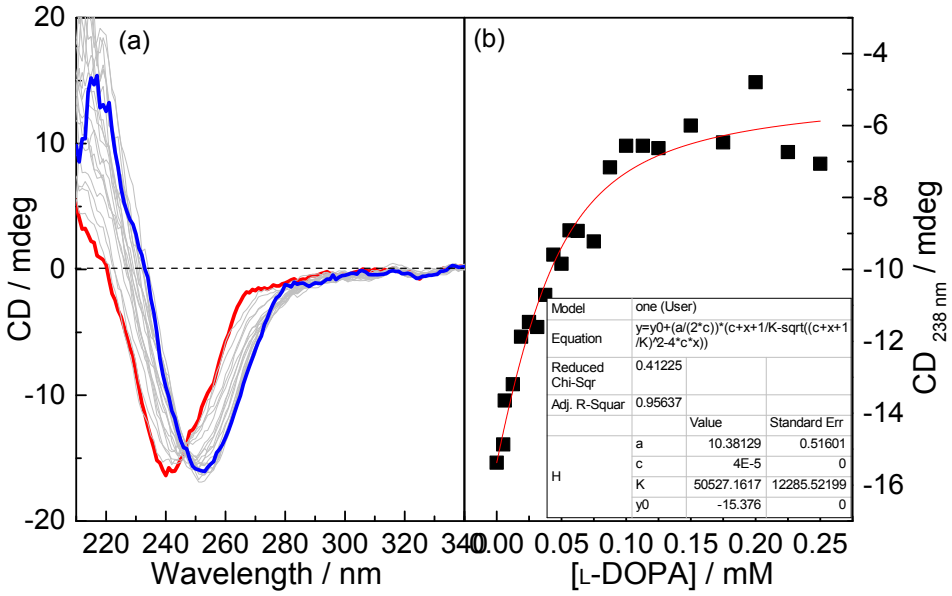


Figure S60. CD spectra (a) and CD intensities at 238 nm (b) of L-**1** in the presence of L-DOPA in 4:6 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. Red line through data points in (b) is the curve fitted by Formula 1. [L-**1**] = 40 μM, [L-DOPA] = 0 - 250 μM.

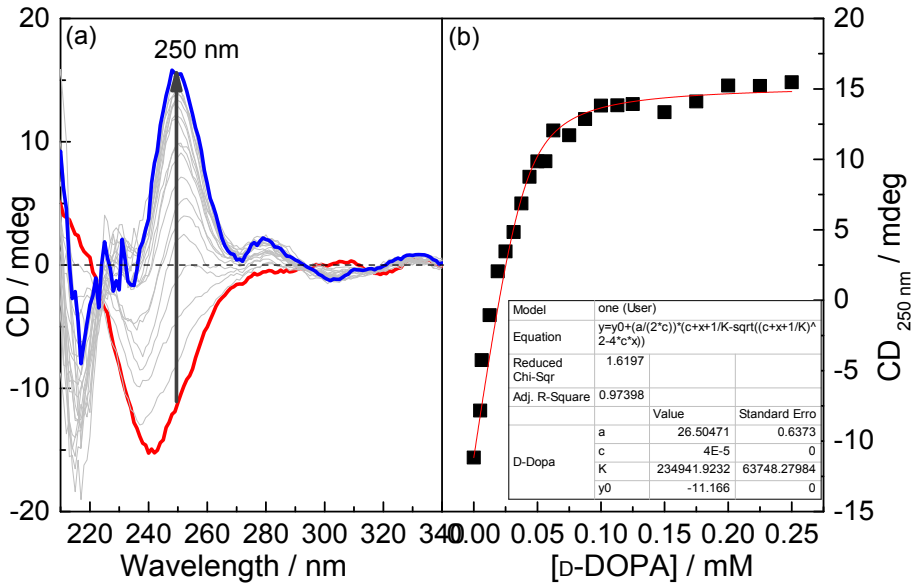


Figure S61. CD spectra (a) and CD intensities at 250 nm (b) of L-**1** in the presence of D-DOPA in 4:6 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. Red line through data points in (b) is the curve fitted by Formula 1. [L-**1**] = 40 μM, [D-DOPA] = 0 - 250 μM.

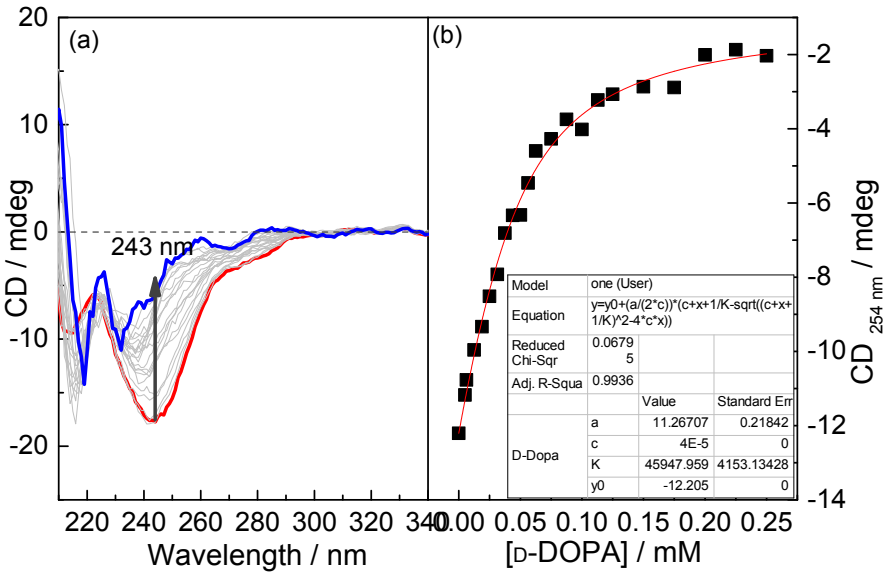


Figure S62. CD spectra (a) and CD intensities at 254 nm (b) of L-**1** in the presence of D-DOPA in 2:8 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. Red line through data points in (b) is the curve fitted by Formula 1. [L-**1**] = 40 μM, [D-DOPA] = 0 - 250 μM.

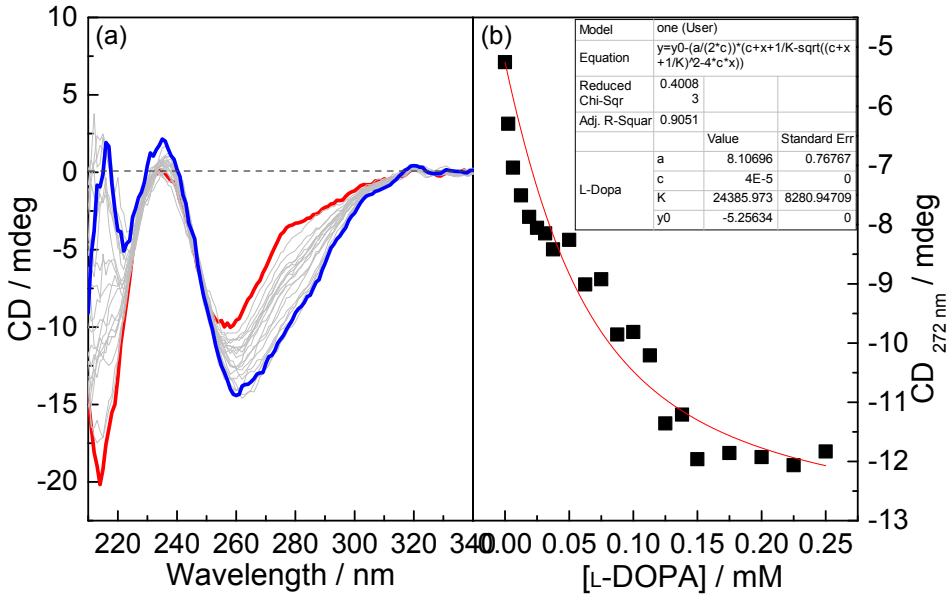


Figure S63. CD spectra (a) and CD intensities at 272 nm (b) of L-**5** in the presence of L-DOPA in 4:6 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. Red line through data points in (b) is the curve fitted by Formula 1. [L-**5**] = 40 μM, [L-DOPA] = 0 - 250 μM.

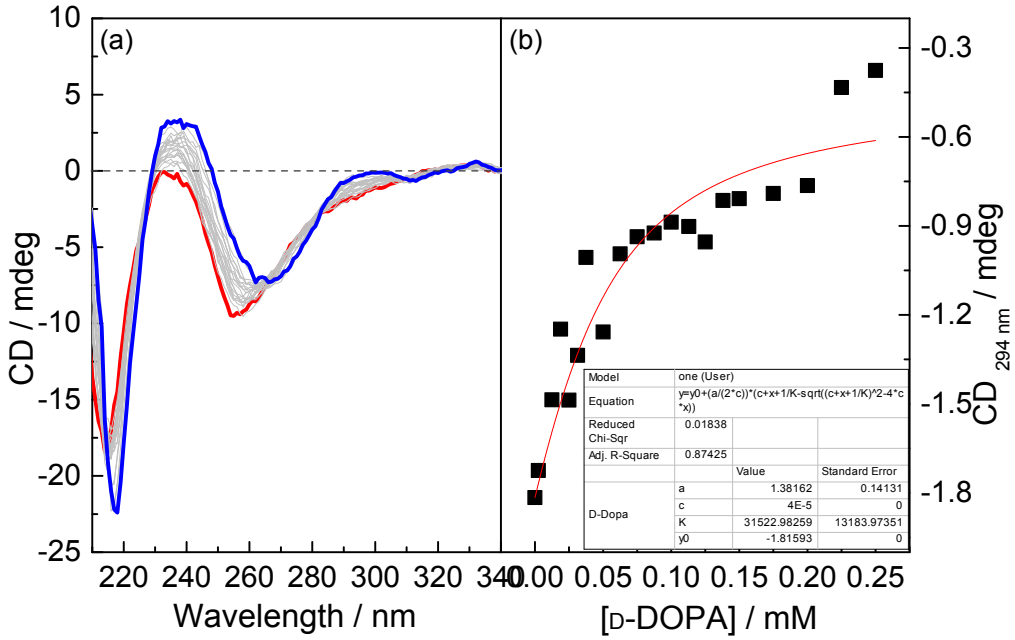


Figure S64. CD spectra (a) and CD intensities at 294 nm (b) of L-**5** in the presence of D-DOPA in 4:6 (v/v) MeOH/0.05 M pH 8.5 PBS buffer. Red line through data points in (b) is the curve fitted by Formula 1. [L-**5**] = 40 μM, [D-DOPA] = 0 - 250 μM.

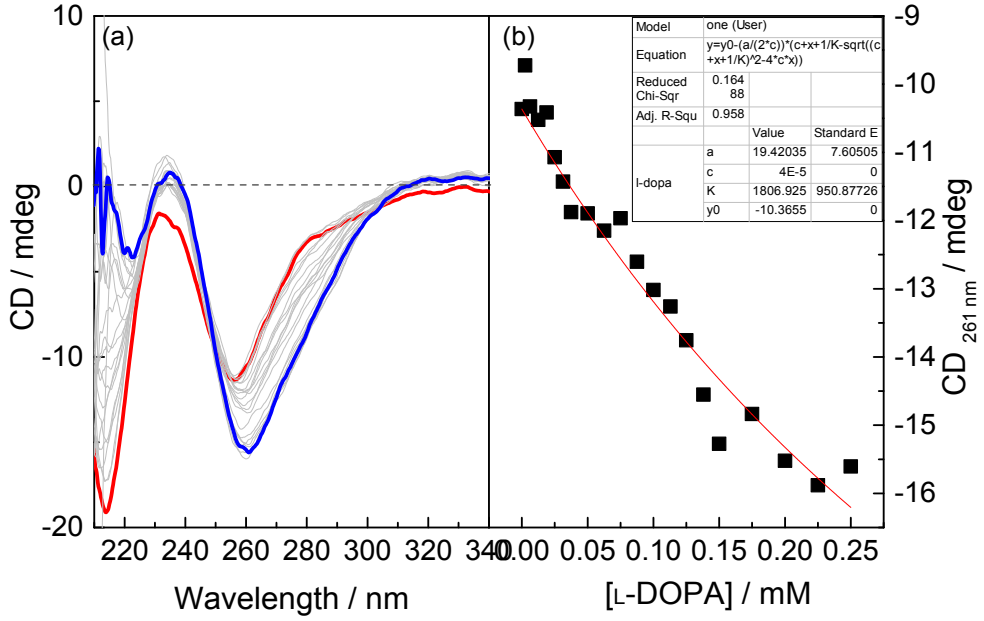


Figure S65. CD spectra (a) and CD intensities at 261 nm (b) of L-**5** in the presence of L-DOPA in 2:8 (v/v) MeOH/0.05 M pH 8.0 PBS buffer. Red line through data points in (b) is the curve fitted by Formula 1. [L-**5**] = 40 μM, [L-DOPA] = 0 - 250 μM.

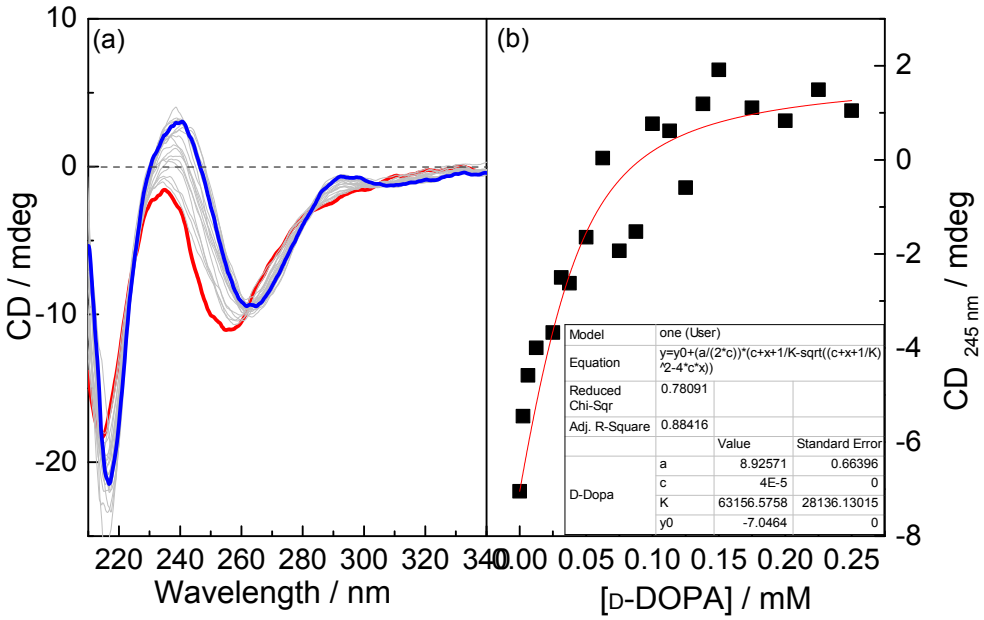


Figure S66. CD spectra (a) and CD intensities at 245 nm (b) of L-**5** in the presence of D-DOPA in 2:8 (v/v) MeOH/0.05 M pH 8.5 PBS buffer. Red line through data points in (b) is the curve fitted by Formula 1. [L-**5**] = 40 μM, [D-DOPA] = 0 - 250 μM.

10. ^{1}H NMR and ^{13}C NMR spectra of a, c, and D-/L-1 to 14

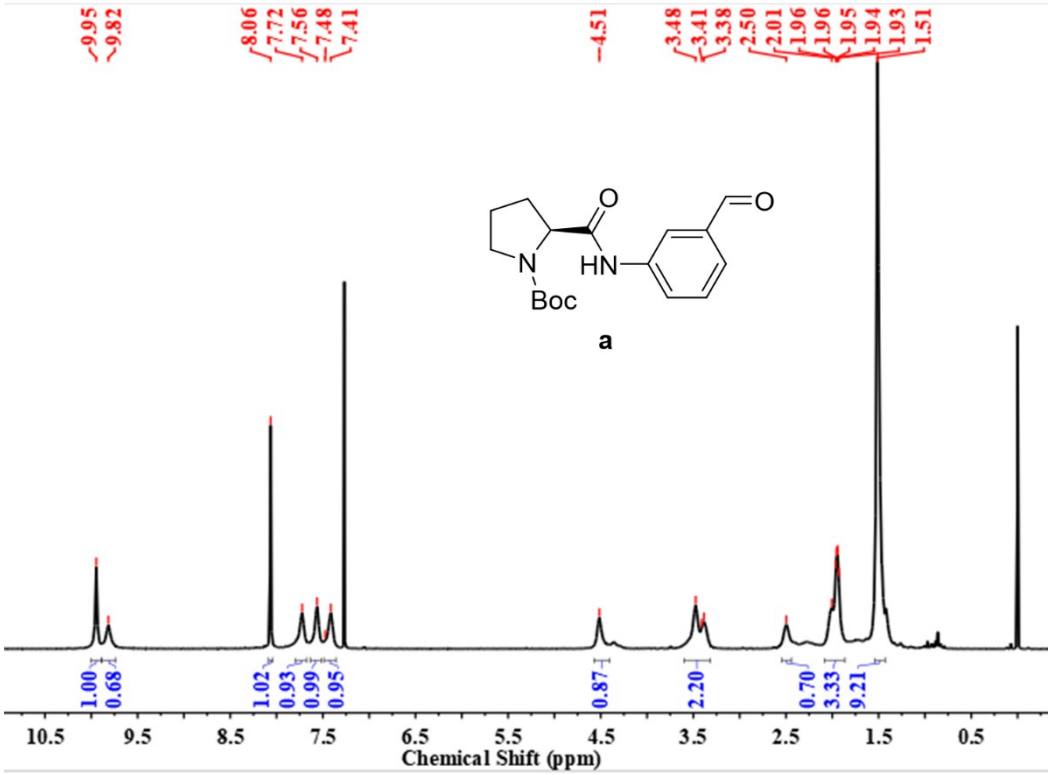


Figure S67. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of isolated product **a**.

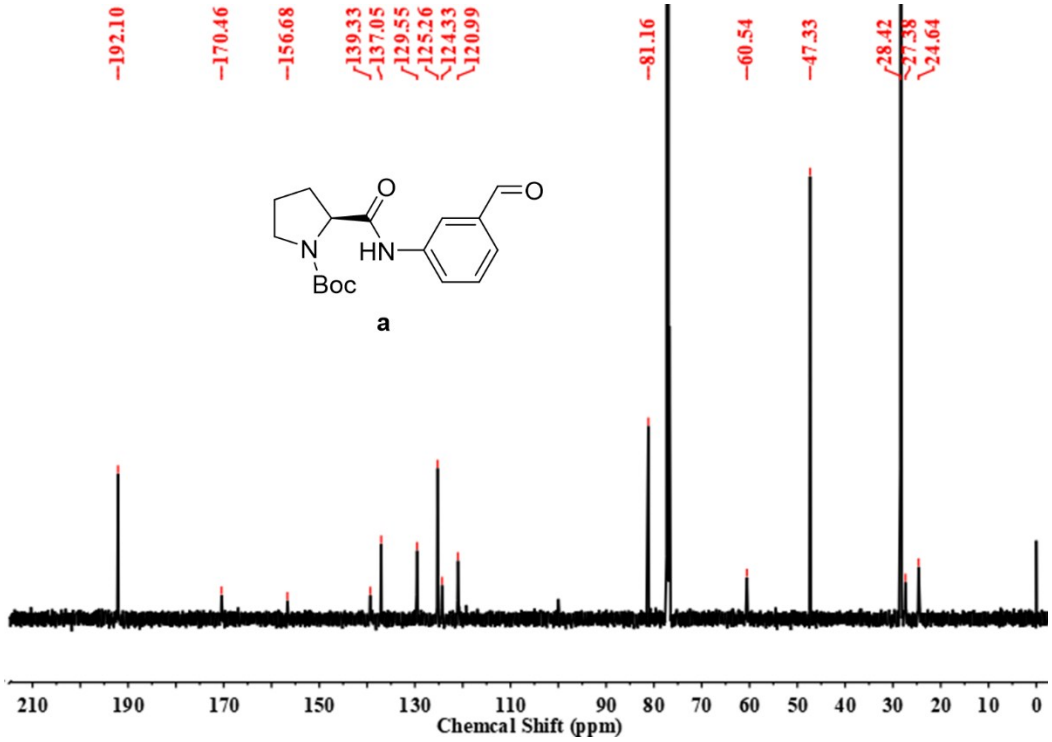


Figure S68. $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$) spectrum of isolated product **a**.

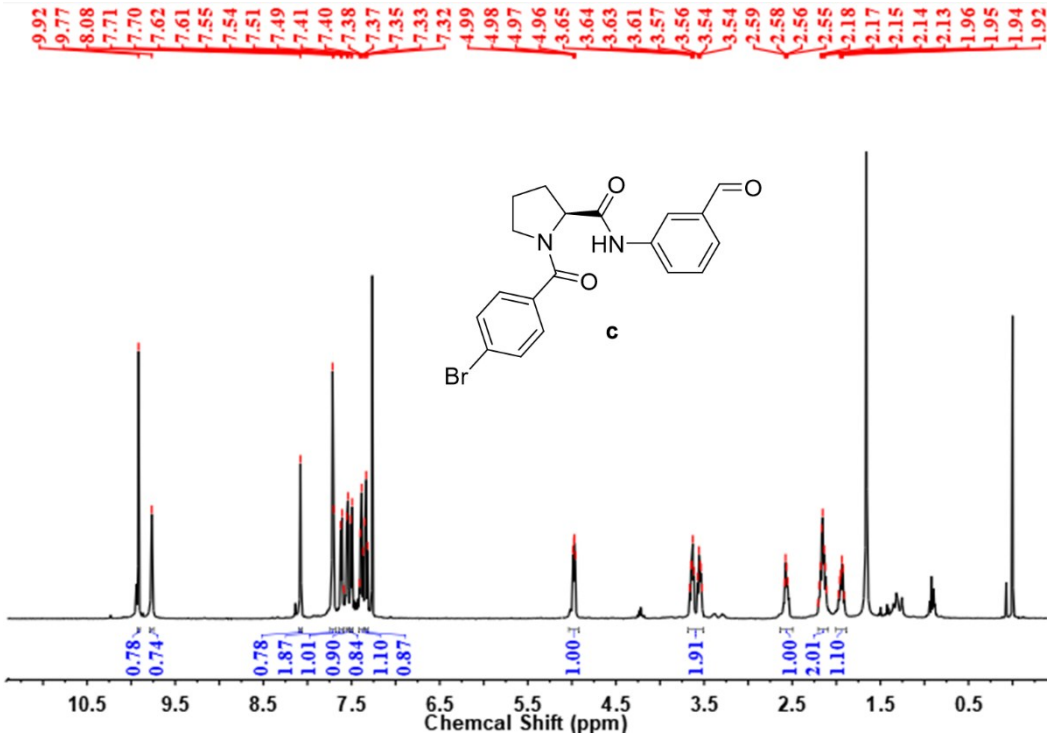


Figure S69. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of isolated product **c**.

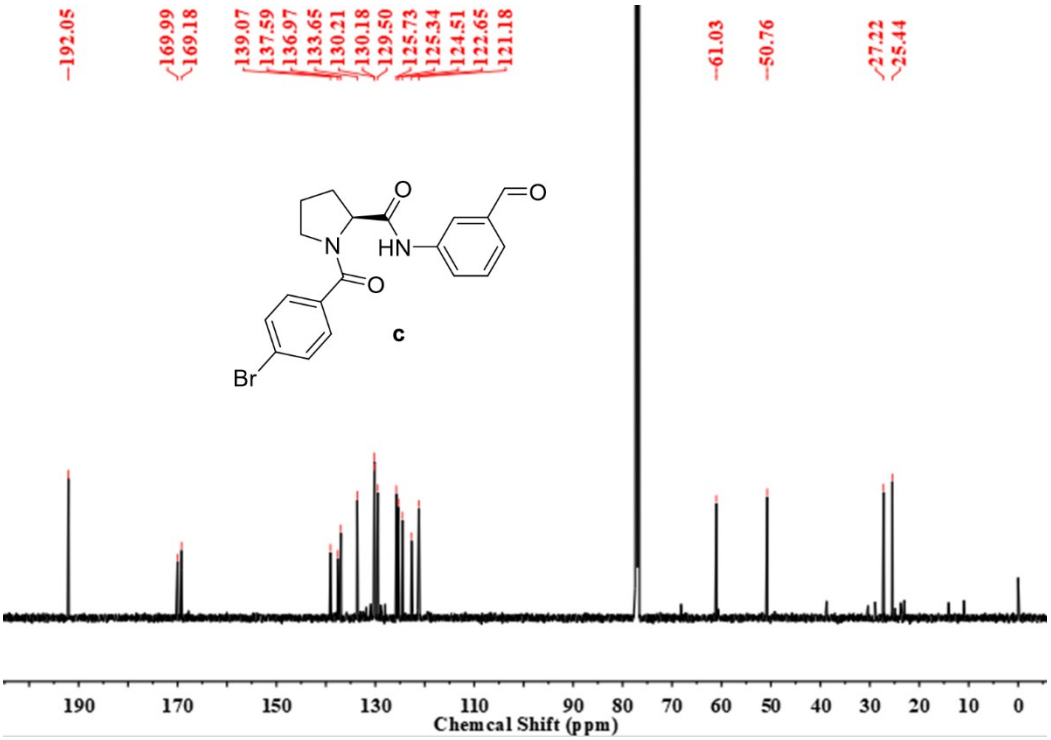


Figure S70. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of isolated product **c**.

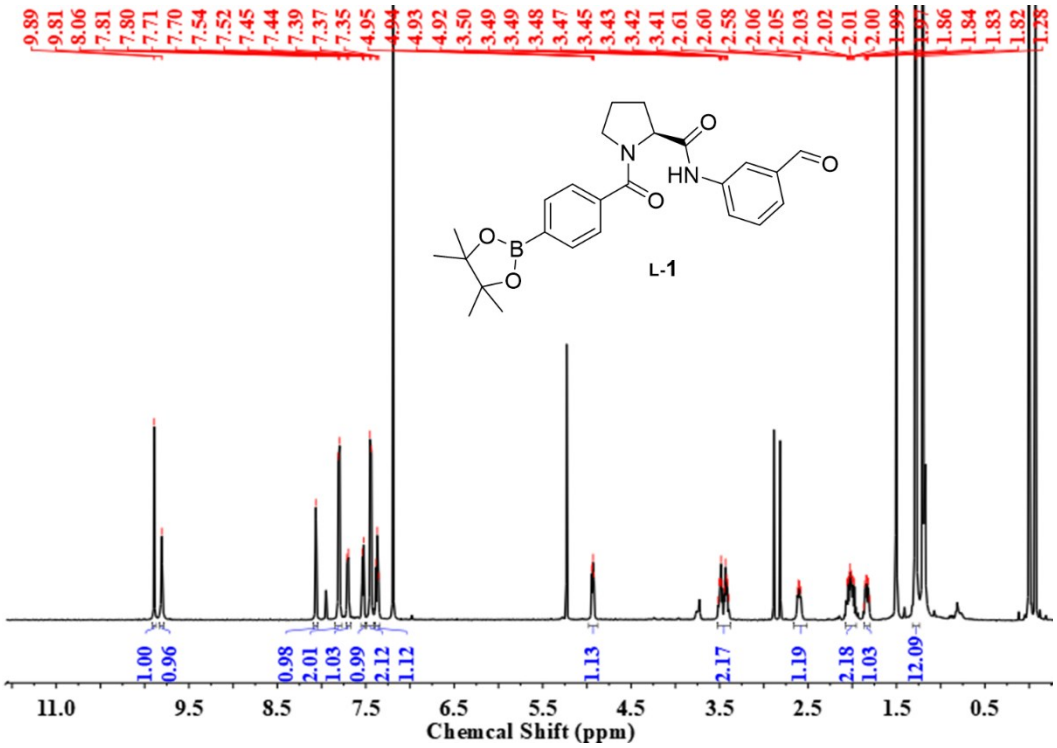


Figure S71. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of isolated product L-**1**.

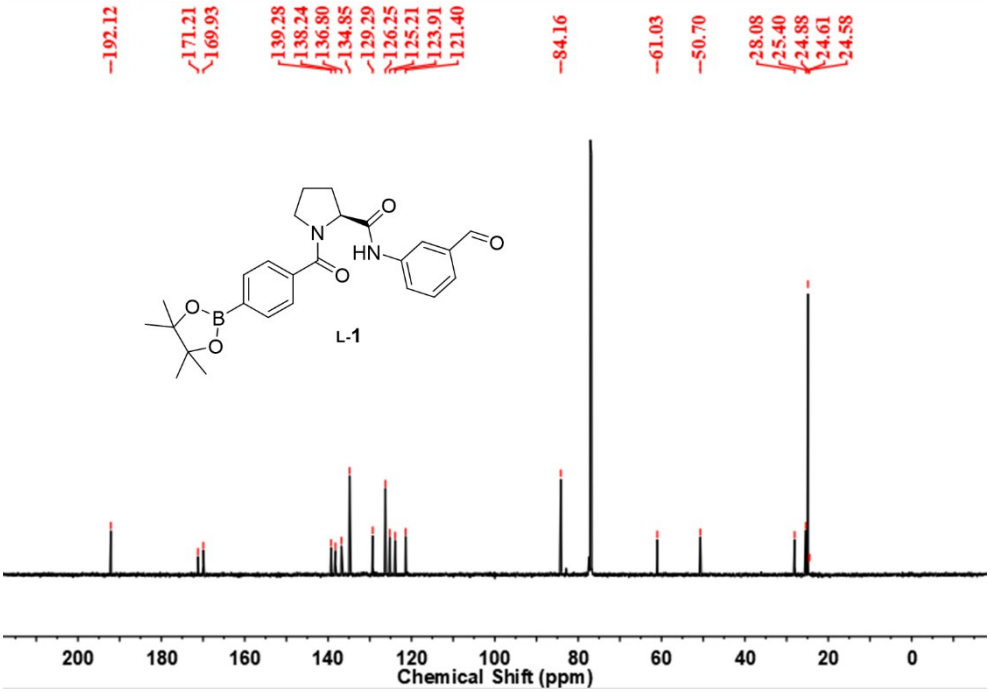


Figure S72. ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) spectrum of isolated product L-**1**.

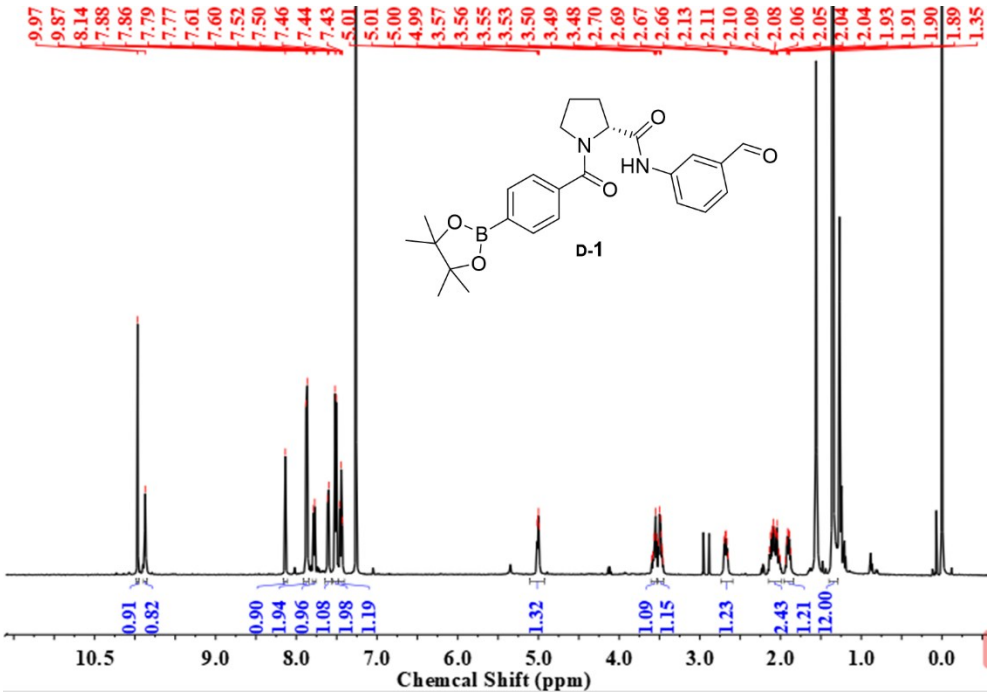


Figure S73. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of isolated product D-**1**.

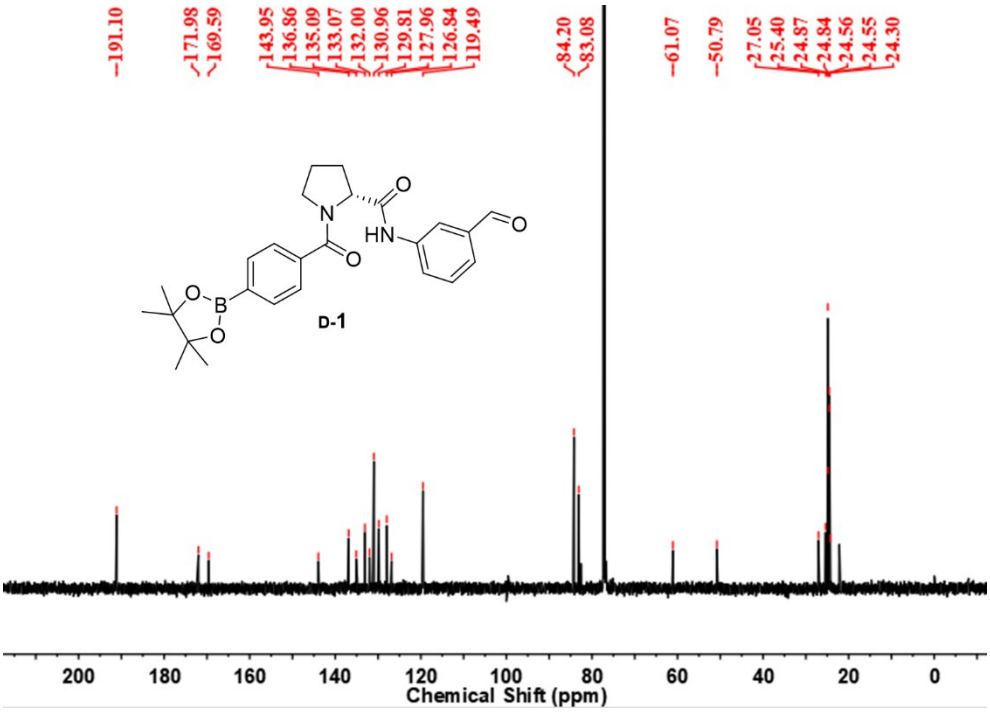


Figure S74. ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) spectrum of isolated product D-**1**.

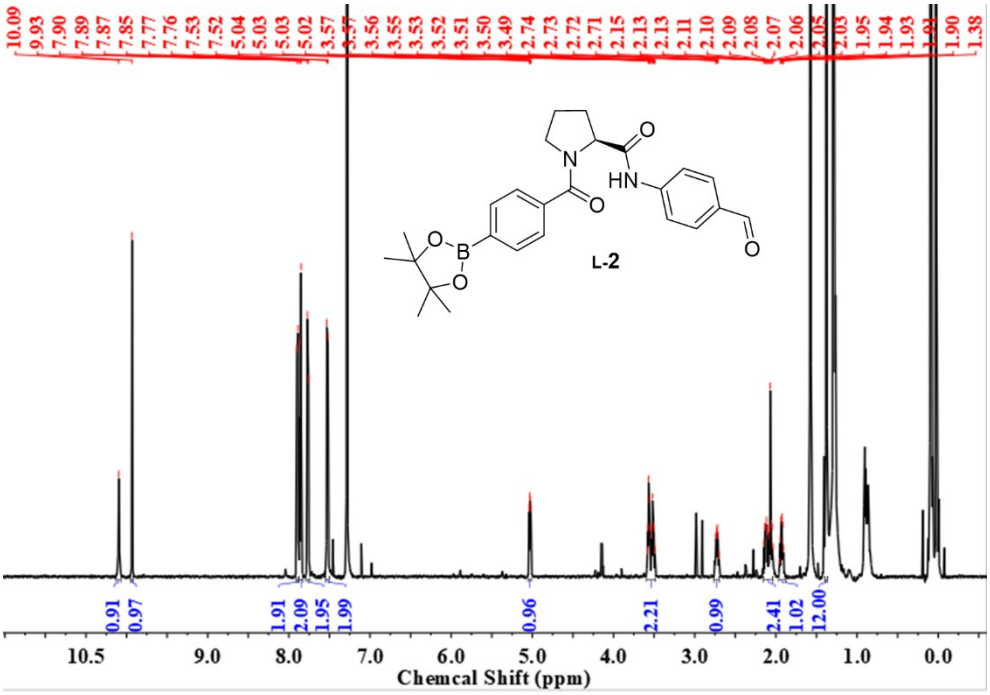


Figure S75. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of isolated product L-**2**.

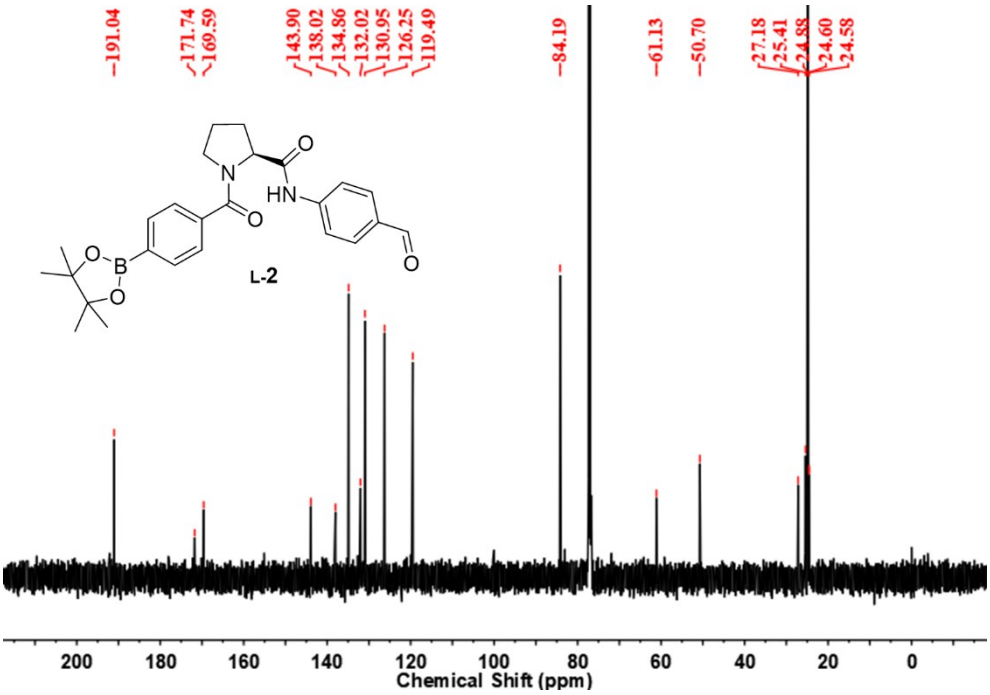


Figure S76. ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) spectrum of isolated product L-**2**.

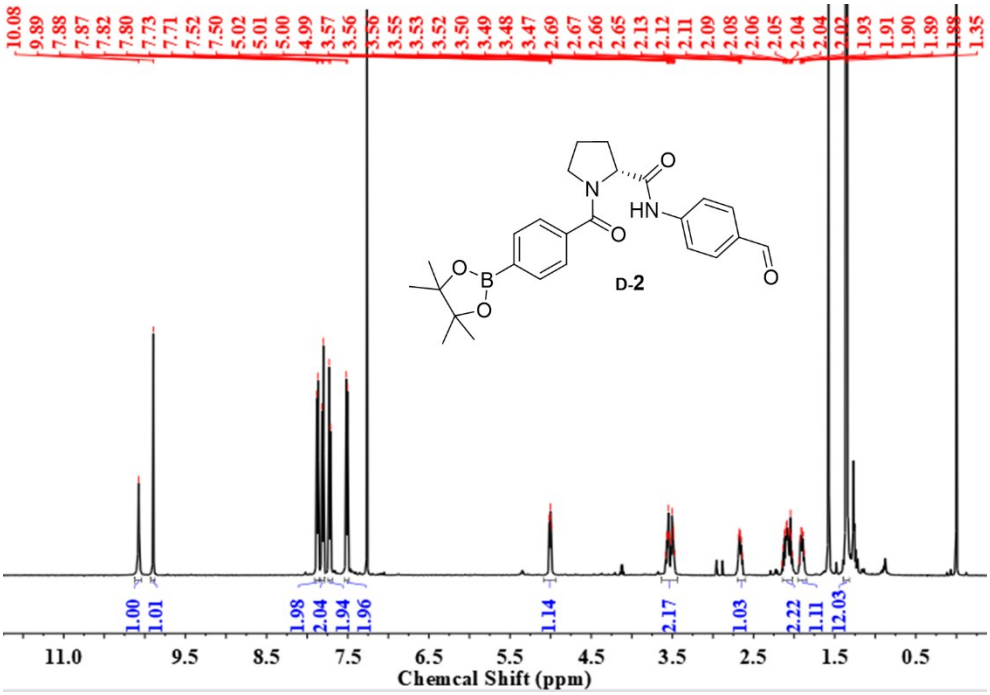


Figure S77. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of isolated product D-**2**.

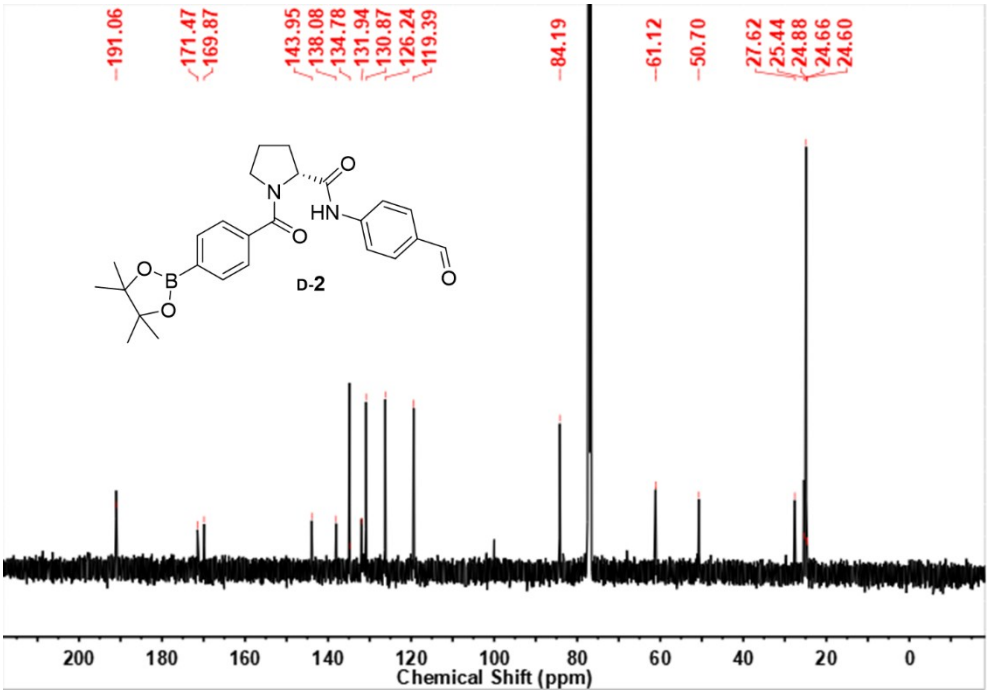


Figure S78. ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) spectrum of isolated product D-**2**.

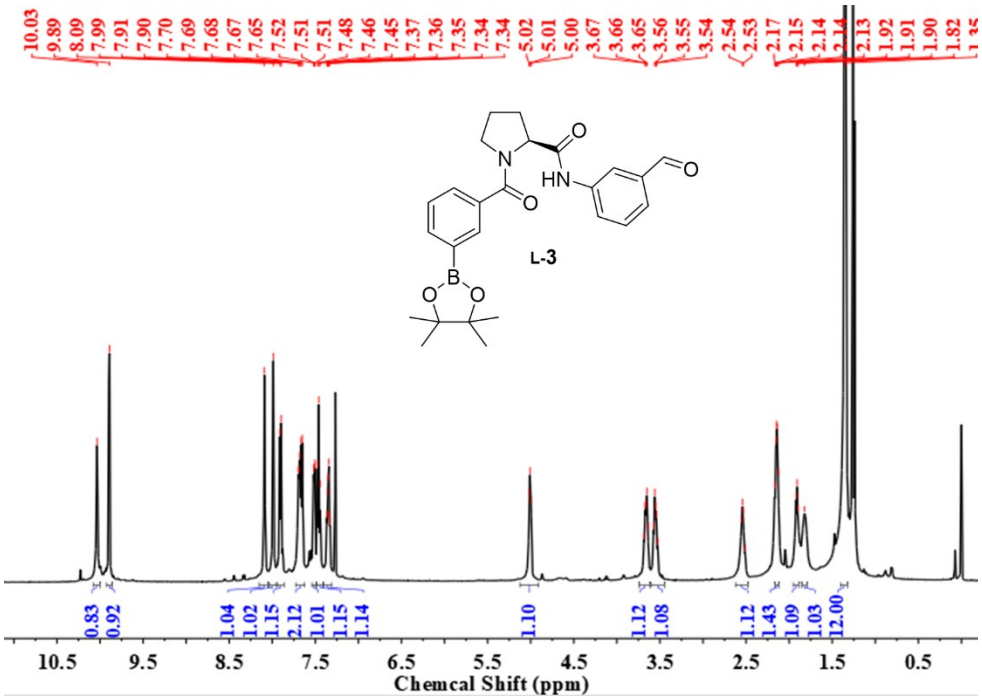


Figure S79. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of isolated product L-**3**.

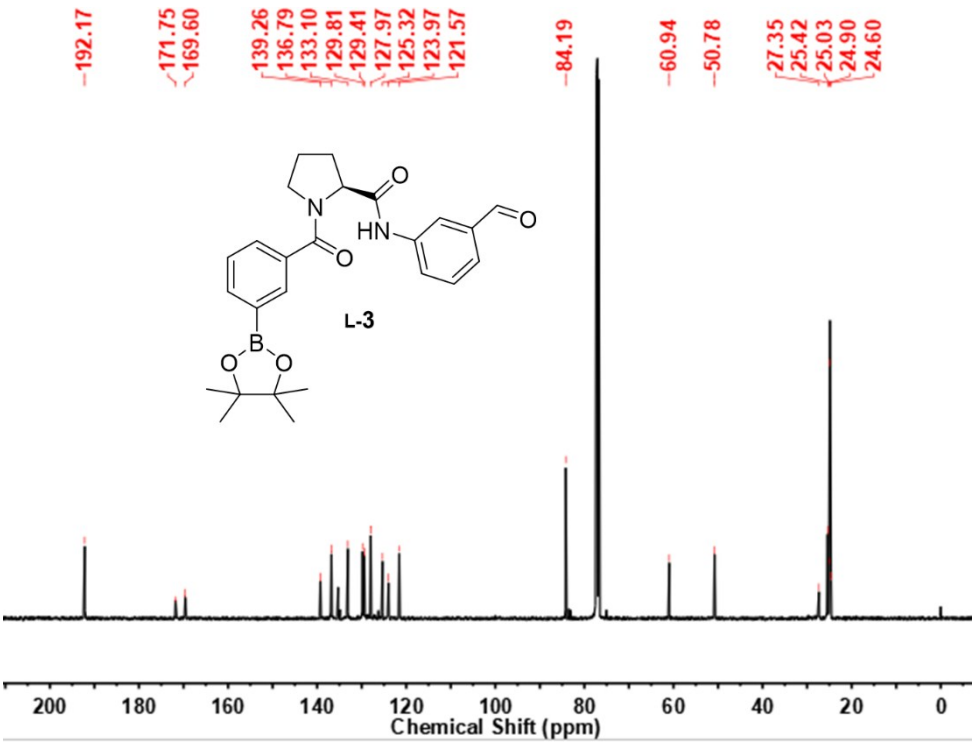


Figure S80. ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) spectrum of isolated product L-**3**.

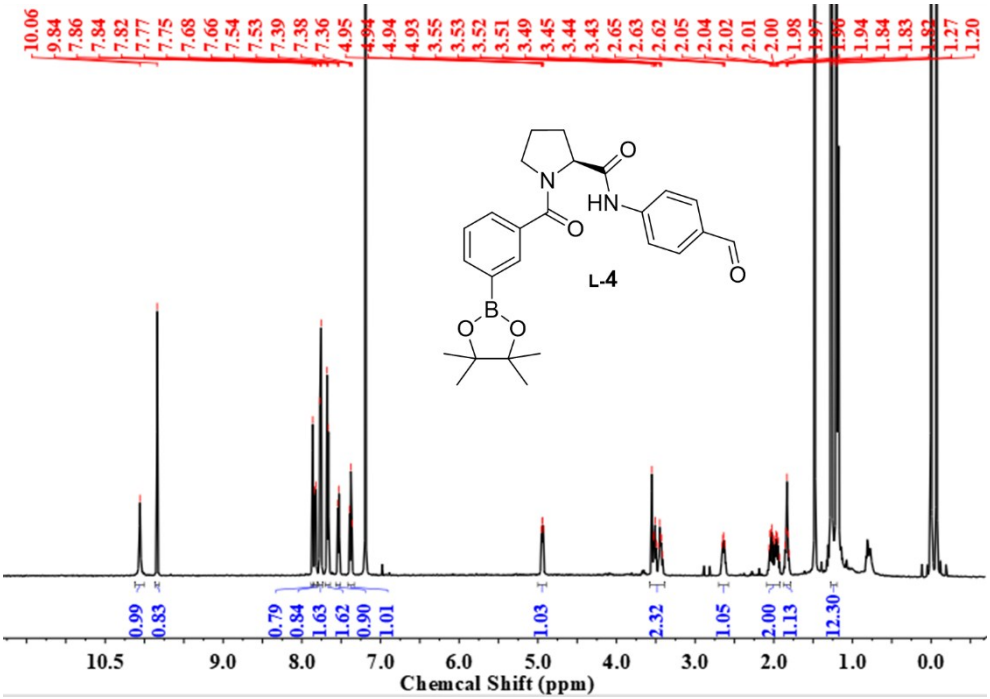


Figure S81. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of isolated product L-**4**.

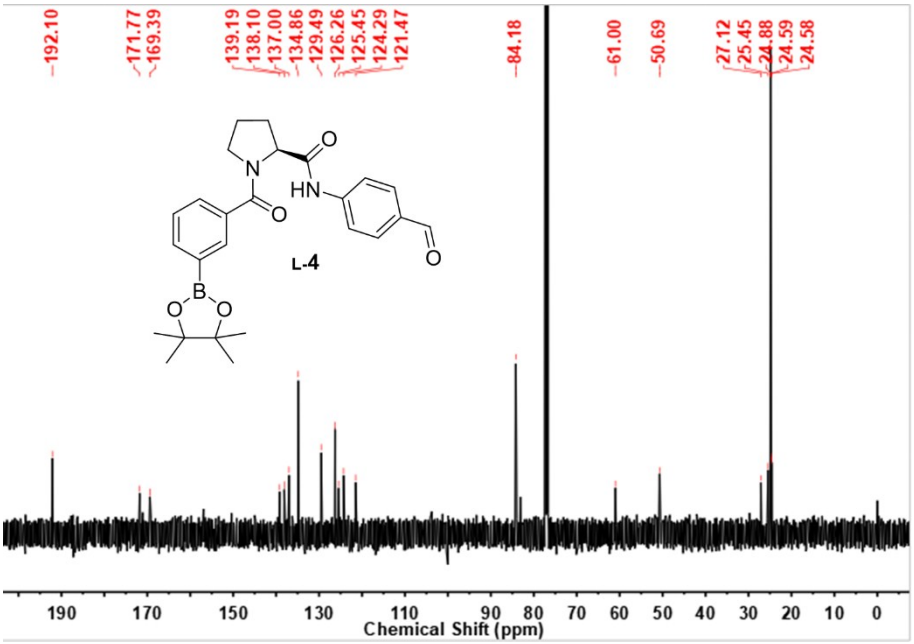


Figure S82. ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) spectrum of isolated product L-**4**.

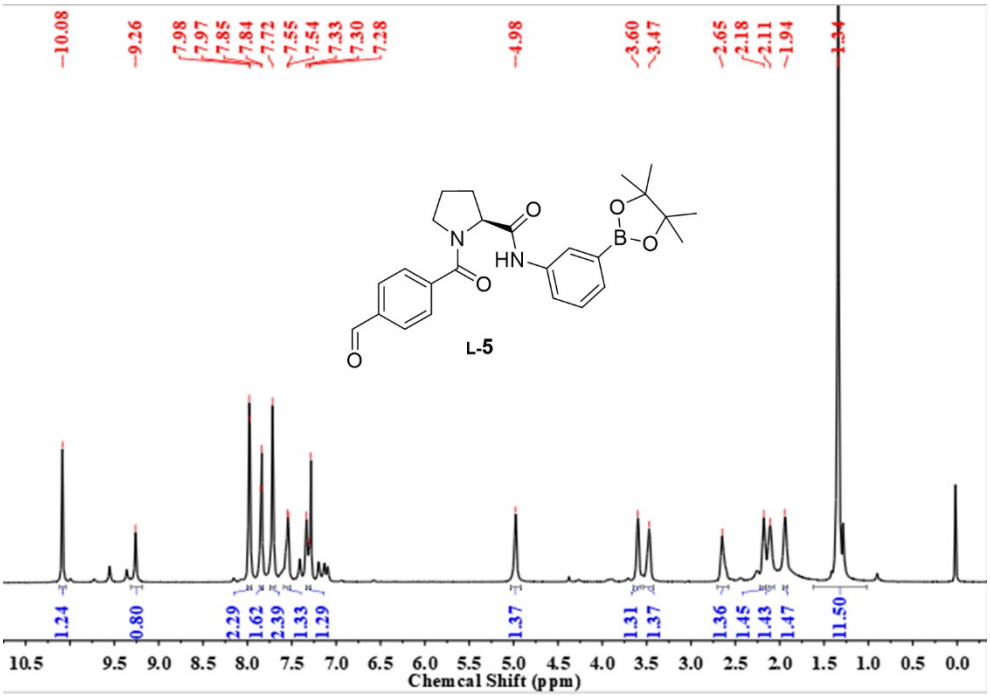


Figure S83. ^{1}H NMR (850 MHz, $CDCl_3$) spectrum of isolated product L-**5**.

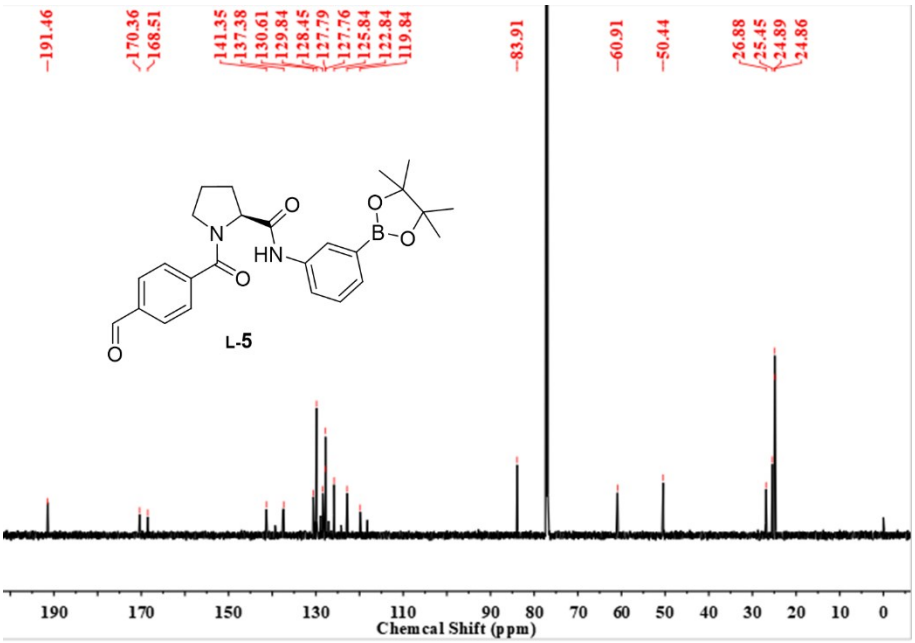


Figure S84. ^{13}C{^{1}H} NMR (214 MHz, $CDCl_3$) spectrum of isolated product L-**5**.

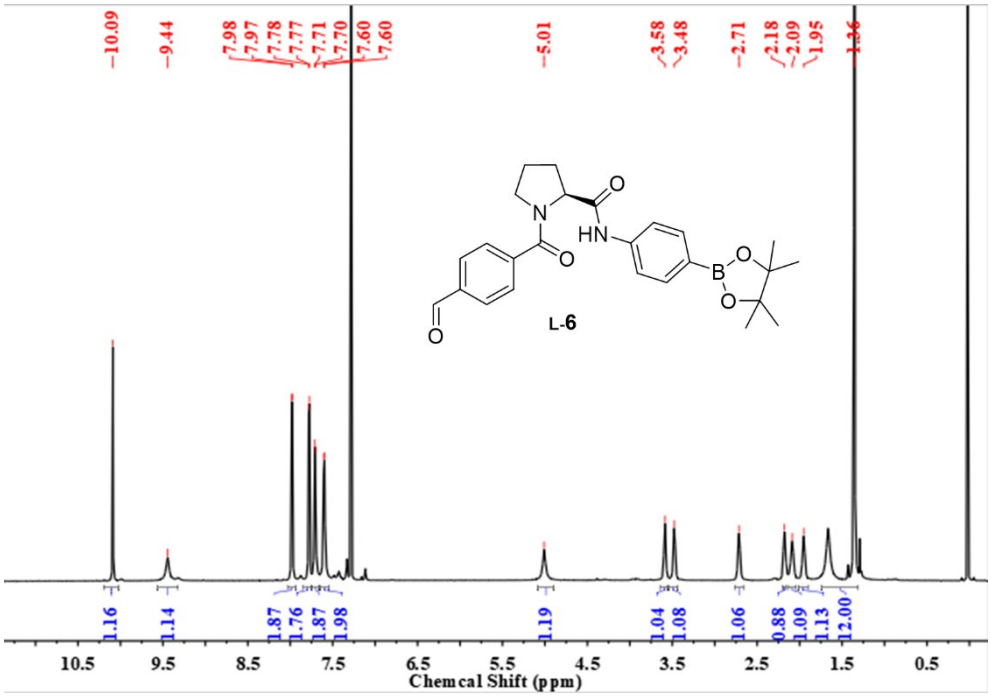


Figure S85. ^{1}H NMR (850 MHz, $CDCl_3$) spectrum of isolated product L-**6**.

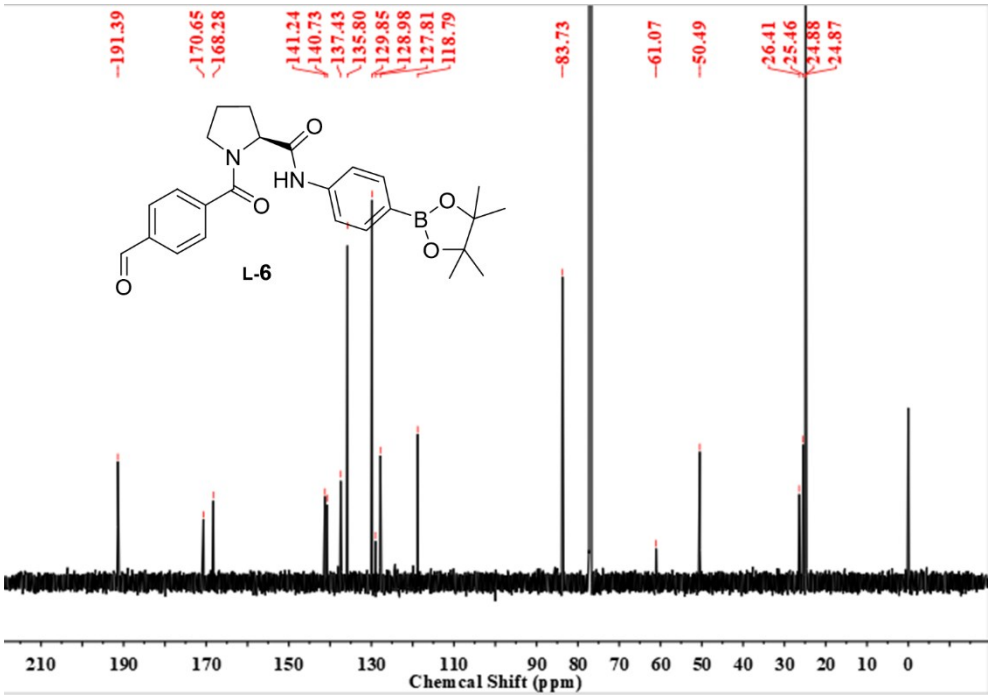


Figure S86. ^{13}C{^{1}H} NMR (214 MHz, $CDCl_3$) spectrum of isolated product L-**6**.

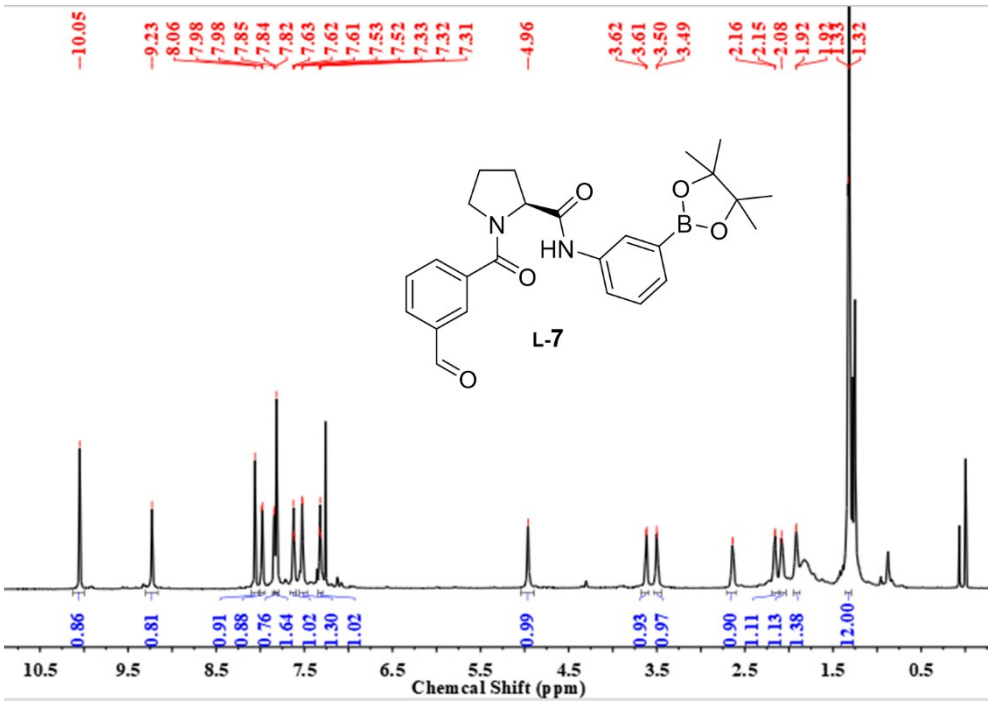


Figure S87. ^{1}H NMR (850 MHz, $CDCl_3$) spectrum of isolated product L-**7**.

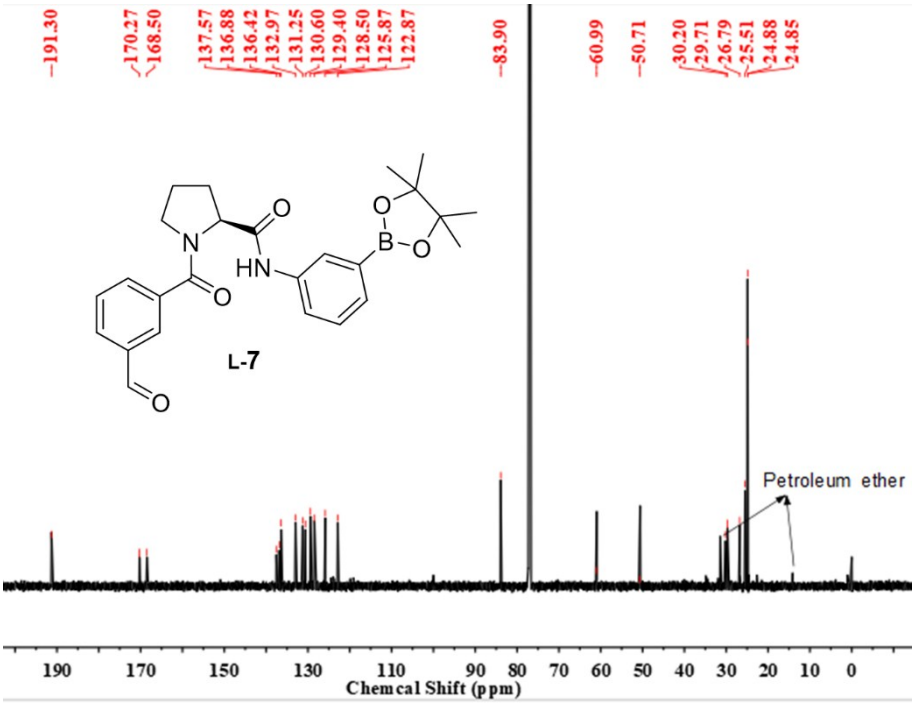


Figure S88. ^{13}C{^{1}H} NMR (214 MHz, $CDCl_3$) spectrum of isolated product L-**7**.

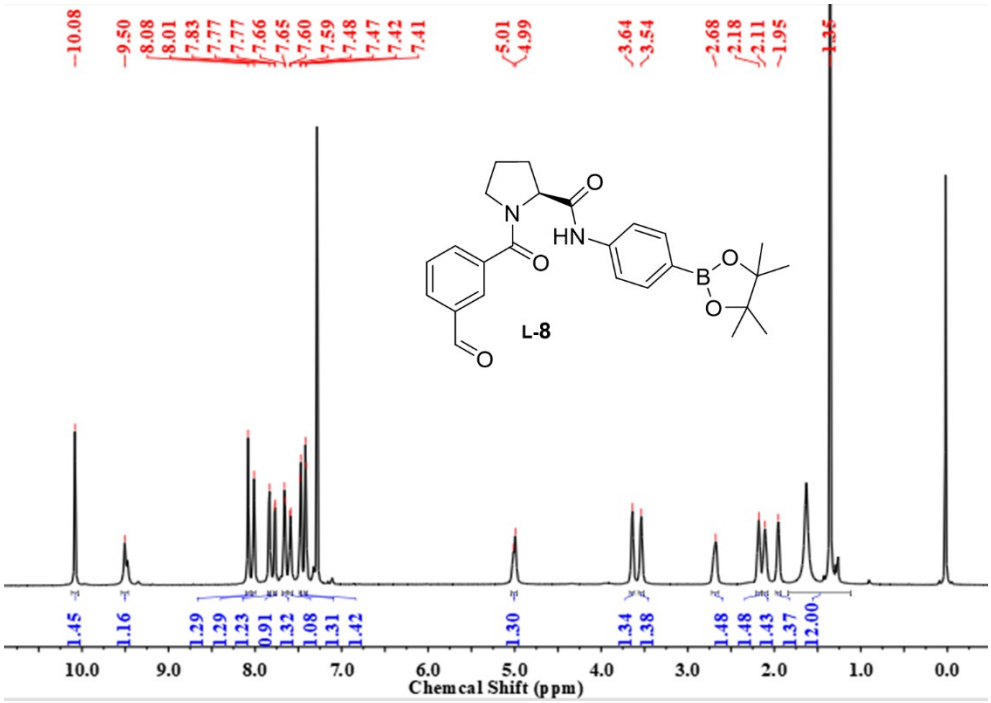


Figure S89. ^{1}H NMR (850 MHz, $CDCl_3$) spectrum of isolated product L-**8**.

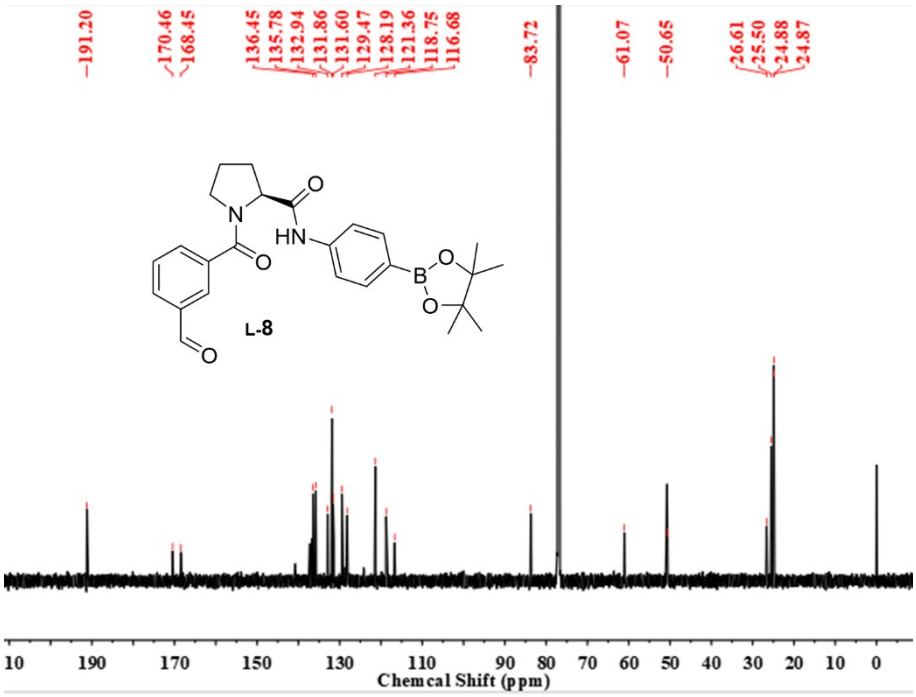


Figure S90. ^{13}C{^{1}H} NMR (214 MHz, $CDCl_3$) spectrum of isolated product L-**8**.

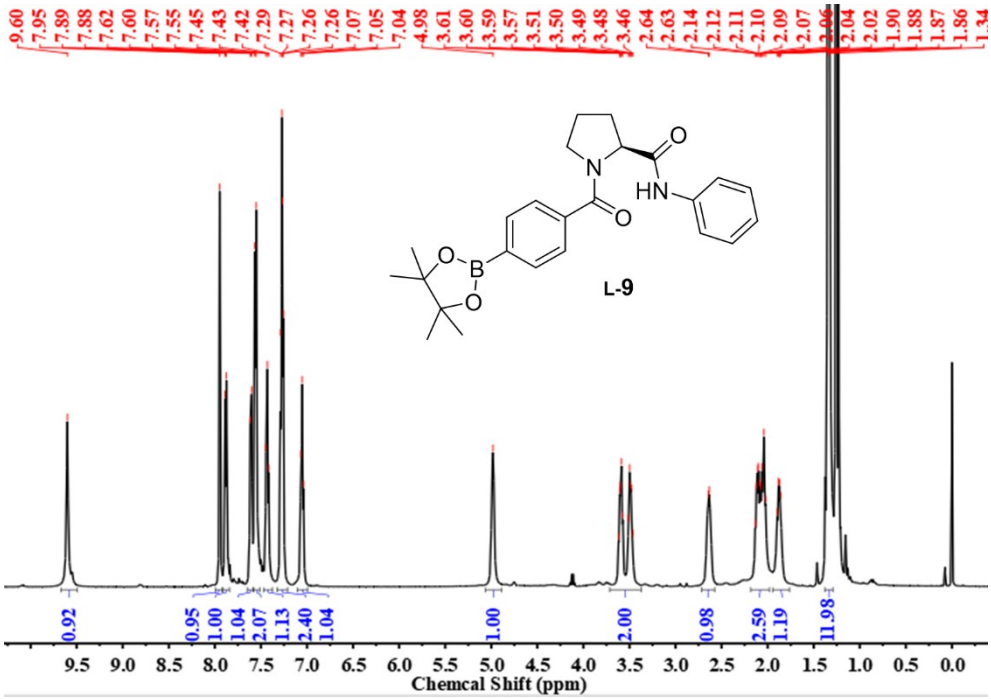


Figure S91. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of isolated product L-**9**.

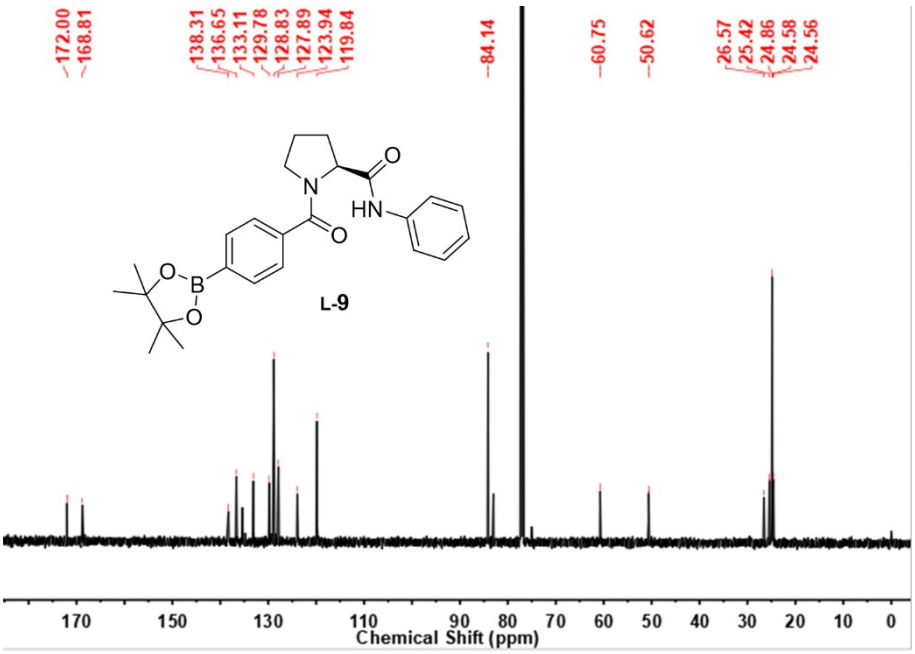


Figure S92. ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) spectrum of isolated product L-**9**.

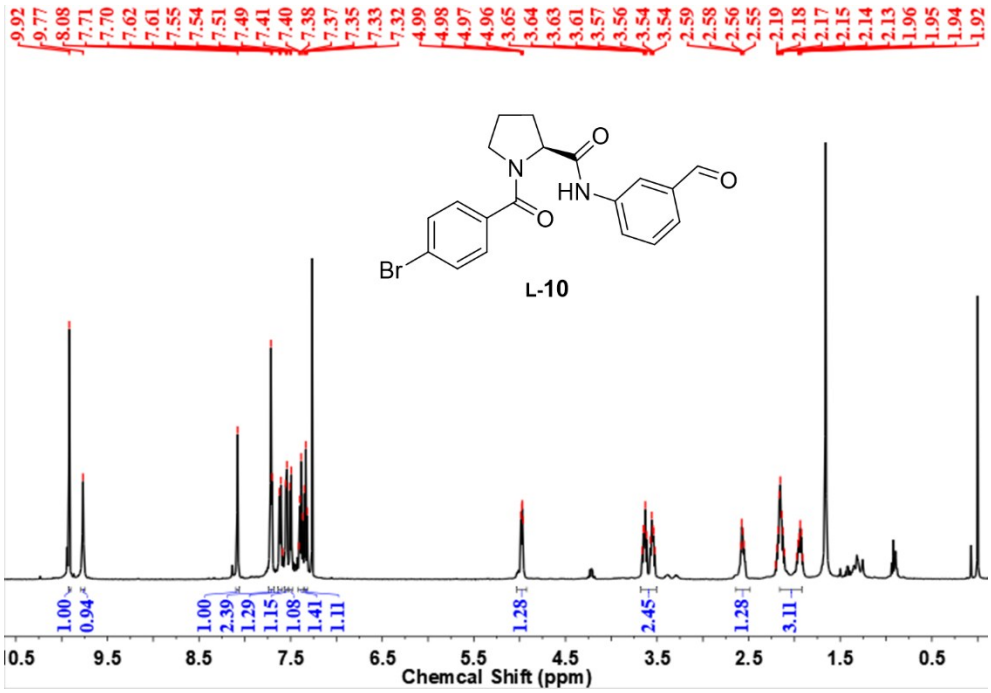


Figure S93. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of isolated product L-**10**.

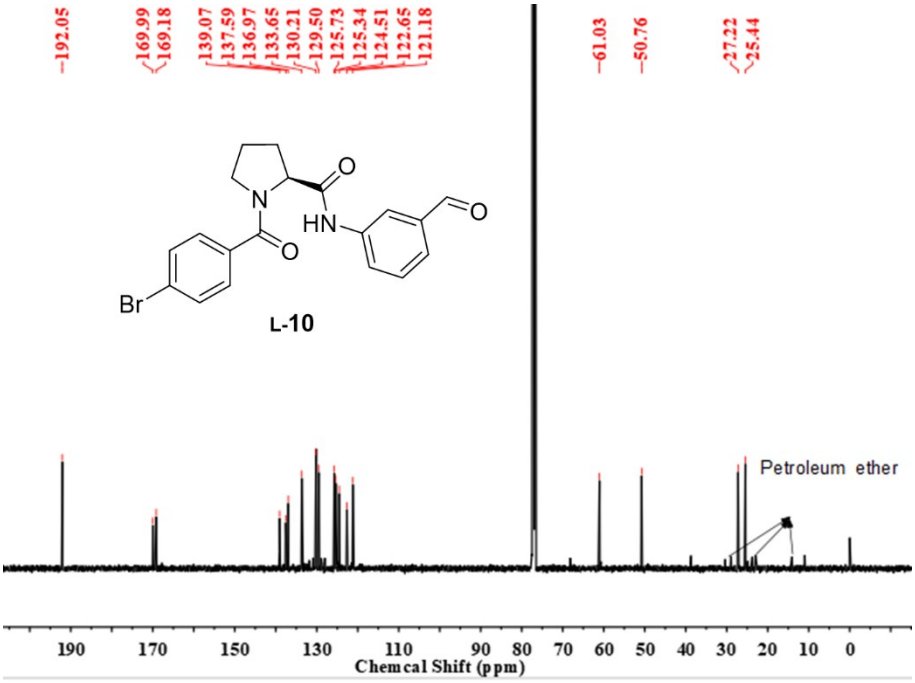


Figure S94. ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) spectrum of isolated product L-**10**.

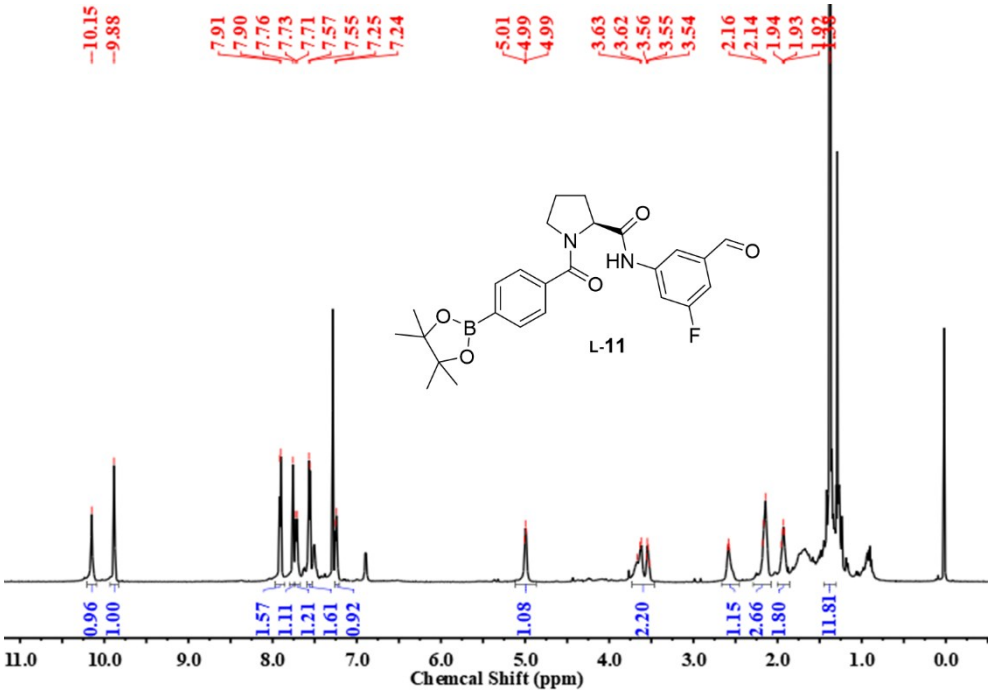


Figure S95. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of isolated product L-**11**.

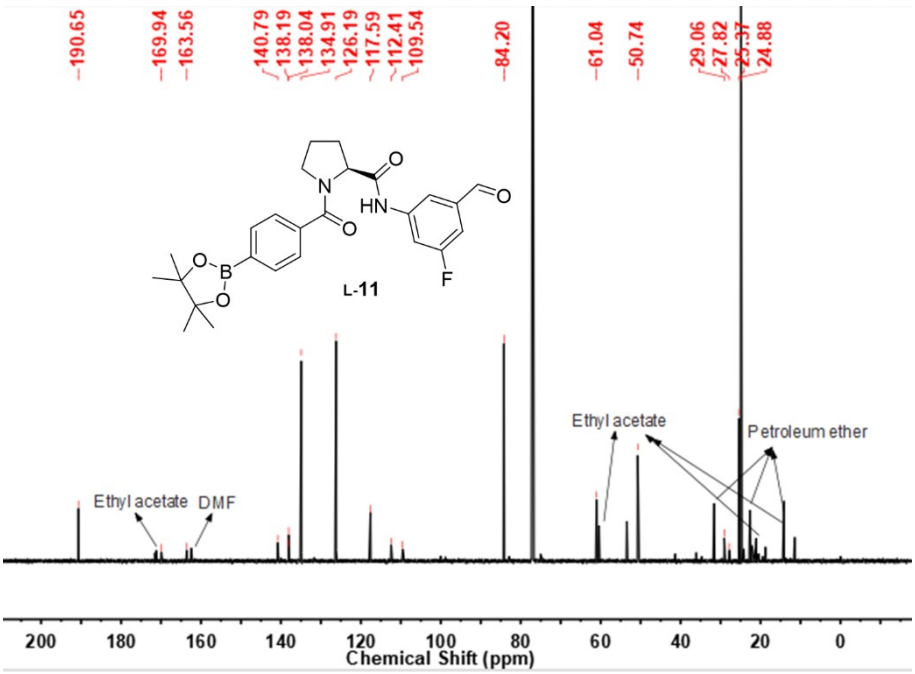


Figure S96. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of isolated product L-**11**.

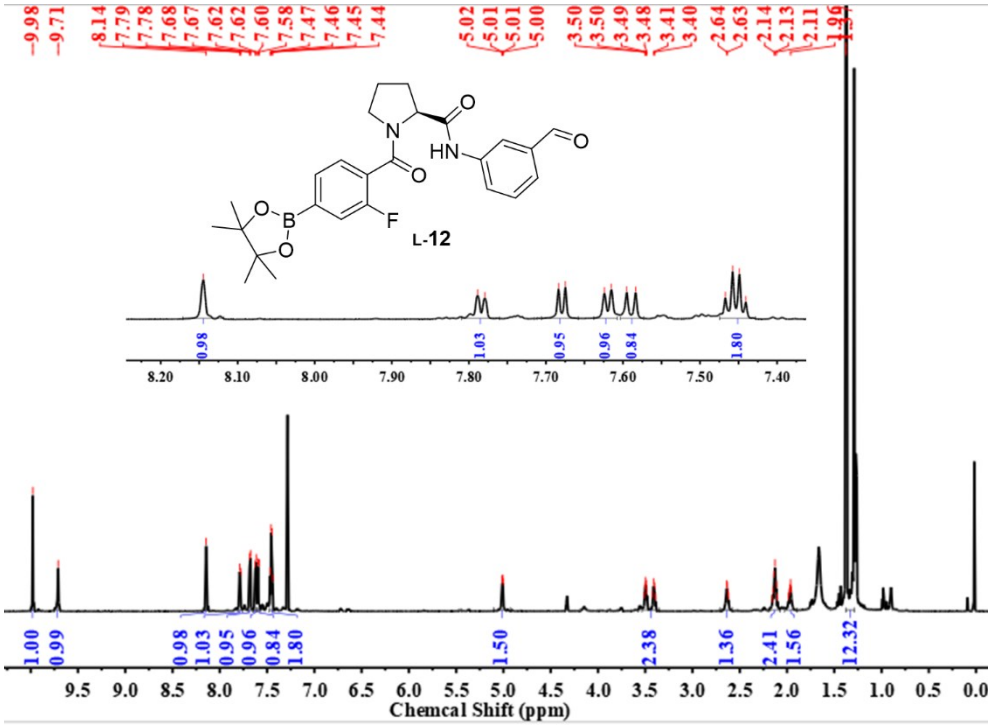


Figure S97. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of isolated product L-**12**.

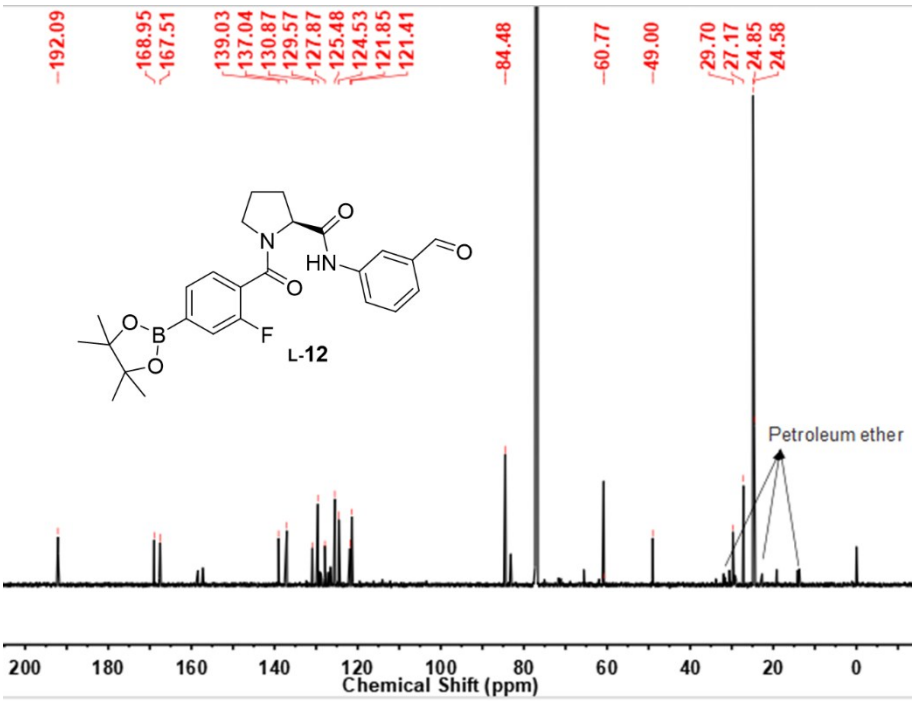


Figure S98. ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) spectrum of isolated product L-**12**.

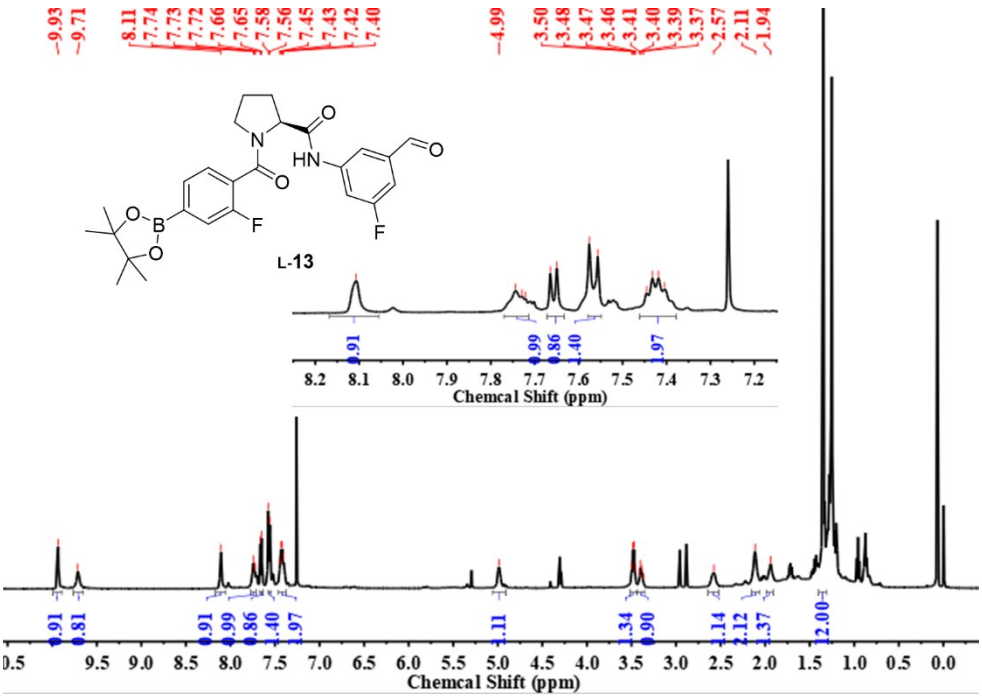


Figure S99. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of isolated product L-**13**.

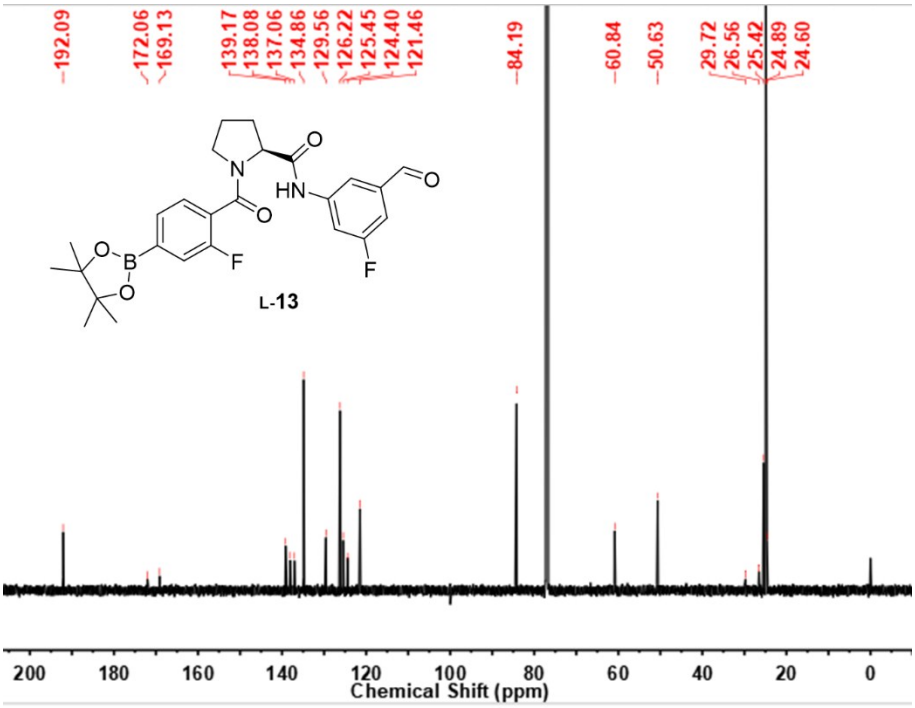


Figure S100. ^{13}C NMR (214 MHz, $CDCl_3$) spectrum of isolated product L-**13**.

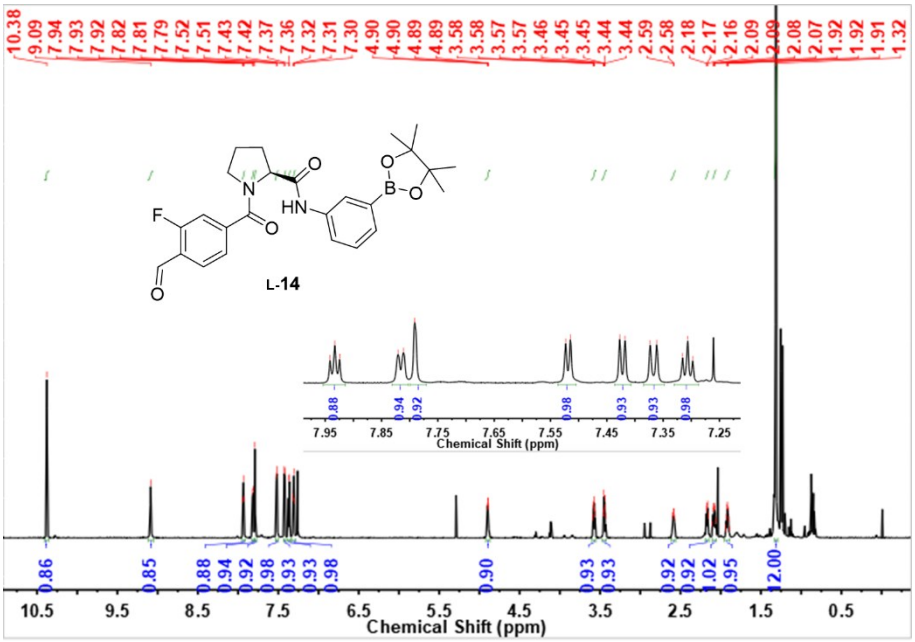


Figure S101. ^{1}H NMR (850 MHz, $CDCl_3$) spectrum of isolated product L-**14**.

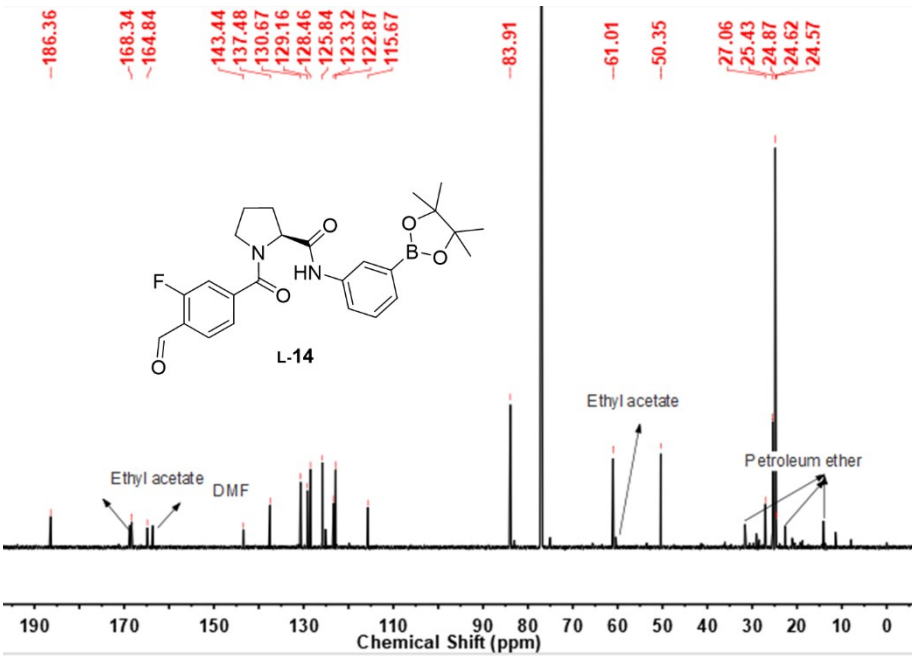


Figure S102. ^{13}C NMR (214 MHz, $CDCl_3$) spectrum of isolated product L-**14**.

11. Computational data

All calculations were performed with Gaussian 16 program package, by which structural optimizations were carried out at B3LYP/6-31G* level in water.

trans-L-**1**:

C	3.42067400	0.04942500	0.27122600
C	2.43771800	-0.95445700	0.35327800
C	1.09101900	-0.63441600	0.49617800
C	0.68204800	0.70743000	0.53373900
C	1.65021200	1.71888400	0.46015400
C	2.99920600	1.38866200	0.33631200
H	2.73671400	-1.99842400	0.31211500
H	0.34267300	-1.41629600	0.57964700
H	1.35780900	2.76205800	0.52485000
H	3.73850100	2.18382900	0.29122600
B	4.92985300	-0.31244600	0.12448500
O	5.93186100	0.62492100	0.11701000
O	5.38573900	-1.59991800	-0.00741600
C	7.17116600	-0.06073800	-0.25296800
C	6.84446800	-1.56247100	0.10940800
C	7.37015700	0.17726700	-1.75500100
H	7.39893900	1.25495200	-1.94415600
H	8.31078400	-0.25745200	-2.10739500
H	6.54950500	-0.24878600	-2.34094100
C	8.31975700	0.56275300	0.53629900
H	8.13404700	0.53674800	1.61249200
H	9.25925700	0.03830200	0.33137400
H	8.44537400	1.60845100	0.23717800
C	7.17517000	-1.92825400	1.56172900
H	6.74631200	-2.90947000	1.78821400
H	8.25617400	-1.98138900	1.72447900
H	6.75323300	-1.20271400	2.26448900
C	7.43048900	-2.60247700	-0.84240900
H	8.52519800	-2.56711900	-0.82744300
H	7.12141400	-3.60422700	-0.52664400
H	7.09116300	-2.44978200	-1.86948100
C	-0.77884300	0.98323700	0.75385300
O	-1.42198600	0.30801800	1.57043300
N	-1.38200100	1.97993800	0.05034600
C	-2.80743100	2.22870600	0.28443100
C	-0.86880000	2.70836600	-1.12983300
C	-3.12755400	3.39505800	-0.68059600

C	-2.14485900	3.17556800	-1.84091500
H	-0.26565100	3.56880700	-0.81771100
H	-2.92212600	4.34426000	-0.17405900
H	-1.97701000	4.07879700	-2.43362800
H	-0.24453700	2.05613300	-1.74458300
H	-2.51481400	2.38716200	-2.50246700
H	-4.17555700	3.40074800	-0.99234300
C	-3.65021800	0.98603900	-0.06454500
O	-3.39309100	0.28189800	-1.03593400
N	-4.73739600	0.81036700	0.75242100
H	-4.81055000	1.44133900	1.54078900
C	-5.76236800	-0.15224900	0.66643300
C	-6.75977000	-0.12103600	1.66166900
C	-5.83612900	-1.11662400	-0.34285400
C	-7.81041300	-1.03356600	1.64917400
H	-6.70608200	0.62716000	2.44867700
C	-6.89945100	-2.03221100	-0.34712000
H	-5.08335300	-1.16377700	-1.11591300
C	-7.88835000	-1.99707500	0.64333600
H	-8.56634600	-0.98858500	2.42711700
H	-8.70452800	-2.71438600	0.62431800
C	-6.98298400	-3.05367300	-1.41178200
H	-7.85669100	-3.73328300	-1.33251100
O	-6.18189200	-3.17999900	-2.32483700
H	-2.96788100	2.50479700	1.33130500

Total energy: -3885989.85 kJ mol^{-1}

cis-L-**1**:

C	-1.89291300	-1.15398200	-0.36682500
C	-1.15179100	-0.79082200	-1.50677300
C	0.14683600	-1.25272500	-1.69976700
C	0.75674300	-2.06985300	-0.73598500
C	0.02892500	-2.44751200	0.40123700
C	-1.27995300	-1.99824200	0.57448100
H	-1.60417400	-0.14380700	-2.25347700
H	0.69969700	-0.98325000	-2.59473100
H	0.46794100	-3.11597100	1.13572600
H	-1.83650500	-2.31088400	1.45378600
B	-3.35211300	-0.64573000	-0.15981000
O	-4.08842700	-0.90969100	0.96735000
O	-4.02501900	0.10787500	-1.08798200
C	-5.46045000	-0.47024400	0.70747600
C	-5.26251000	0.57420100	-0.46021900

C	-6.24568100	-1.71874700	0.28680900
H	-6.17315100	-2.46892500	1.08053300
H	-7.30412800	-1.49065200	0.12707700
H	-5.84218400	-2.15611400	-0.63199600
C	-6.03534900	0.10333800	2.00030600
H	-5.40971200	0.90307800	2.40319900
H	-7.04290100	0.49909900	1.83298800
H	-6.10478200	-0.68784300	2.75391600
C	-4.99068700	2.00072300	0.03327800
H	-4.67503300	2.61657700	-0.81469200
H	-5.88847800	2.45112800	0.46809900
H	-4.19359900	2.02107100	0.78329000
C	-6.36438100	0.58329900	-1.51700300
H	-7.32329300	0.87209400	-1.07324200
H	-6.11992400	1.31318200	-2.29563400
H	-6.48035400	-0.39400500	-1.99112900
C	2.12993300	-2.61339400	-1.03292600
O	2.34774500	-3.17926200	-2.10900100
N	3.12435800	-2.45912900	-0.10564100
C	3.06029200	-1.73625400	1.17898500
C	4.40386800	-3.18139200	-0.27985400
C	4.48615400	-1.92220100	1.76473800
C	4.96800400	-3.23929300	1.14184700
H	4.21055800	-4.16061500	-0.72183700
H	4.46450600	-1.93052100	2.85662300
H	4.54158100	-4.09330100	1.67982300
H	5.06570400	-2.62995400	-0.95940100
H	6.05676000	-3.33705300	1.15385100
H	5.13196900	-1.09637000	1.44506400
C	2.69999400	-0.24539700	1.09898800
O	2.17838300	0.30478100	2.06425000
N	3.07273200	0.38533800	-0.05630000
H	3.48078300	-0.20996300	-0.76748400
C	2.93438100	1.74302600	-0.40712800
C	3.34418600	2.11839400	-1.70183300
C	2.42126800	2.71449100	0.45663400
C	3.24435300	3.44015100	-2.12599200
H	3.74231500	1.36488200	-2.37673600
C	2.32324100	4.04408200	0.01918500
H	2.09937500	2.45166200	1.45374900
C	2.73236400	4.41351900	-1.26779700
H	3.56683300	3.70564100	-3.12802400
H	2.64967100	5.44811800	-1.58983200
C	1.78186300	5.07659200	0.92769400

H	1.74479400	6.09854400	0.49687300
O	1.39484100	4.87132600	2.06749800
H	2.32433600	-2.18145600	1.85199800

Total energy: -3885980.81 kJ mol^{-1}

trans-L-**11**:

C	-3.68937500	0.02994400	-0.28348100
C	-2.69145800	-0.96235300	-0.29412900
C	-1.34595900	-0.62974100	-0.41730200
C	-0.95375700	0.71470900	-0.50774900
C	-1.93698500	1.71427500	-0.50651400
C	-3.28417000	1.37061300	-0.40058600
H	-2.97753900	-2.00749700	-0.21181100
H	-0.58513200	-1.40341000	-0.44480000
H	-1.65774100	2.75747200	-0.61335600
H	-4.03478500	2.15632000	-0.41098100
B	-5.19676900	-0.34663500	-0.15612900
O	-6.21018100	0.57750900	-0.19728200
O	-5.63923800	-1.63520800	0.00695200
C	-7.44760700	-0.11235300	0.17124500
C	-7.09570200	-1.62008900	-0.13878600
C	-7.67692500	0.16888400	1.66141300
H	-7.72181700	1.25139000	1.81689400
H	-8.61867200	-0.26642000	2.01002400
H	-6.86223100	-0.22907200	2.27475400
C	-8.58932300	0.47150600	-0.65728200
H	-8.38355900	0.41523900	-1.72865000
H	-9.52553400	-0.05916100	-0.45325100
H	-8.73399300	1.52400400	-0.39264800
C	-7.39401400	-2.03358900	-1.58527800
H	-6.94964200	-3.01594200	-1.77374400
H	-8.47105900	-2.10447400	-1.76646600
H	-6.96715200	-1.32447400	-2.30169500
C	-7.68758900	-2.63814700	0.83289200
H	-8.78213300	-2.61709700	0.79554000
H	-7.36027900	-3.64499700	0.55386100
H	-7.37048700	-2.45019600	1.86122200
C	0.50918700	0.99813500	-0.70163700
O	1.18571200	0.28304300	-1.45512700
N	1.08082700	2.04352900	-0.04348600
C	2.50989500	2.29348300	-0.25313600
C	0.52652400	2.84274500	1.07019500
C	2.79475200	3.51578200	0.65203400

C	1.77708200	3.35898100	1.79217800
H	-0.06663800	3.67977800	0.68383200
H	2.60152600	4.43233800	0.08431100
H	1.58670800	4.29465000	2.32466000
H	-0.11726900	2.22830000	1.70331900
H	2.12923400	2.61329400	2.51054900
H	3.83242500	3.54602100	0.99516900
C	3.35252400	1.08074300	0.18766000
O	3.08824200	0.44023000	1.19906800
N	4.45190400	0.85709200	-0.60468600
H	4.52880800	1.43304200	-1.43357200
C	5.47326800	-0.09533400	-0.44527000
C	6.47050000	-0.13354000	-1.43832900
C	5.54335100	-0.98457900	0.63389100
C	7.50500100	-1.04990900	-1.33032600
H	6.44564300	0.54136900	-2.28823000
C	6.60509400	-1.89637600	0.70833300
H	4.78809300	-0.97520400	1.40519300
C	7.60249100	-1.94330400	-0.27285400
H	8.42605600	-2.64805100	-0.21928900
C	6.68545700	-2.83860500	1.84830400
H	7.55845100	-3.52219300	1.82391900
O	5.87910100	-2.89247700	2.76179500
H	2.69718000	2.51170000	-1.30912000
F	8.44929200	-1.06710700	-2.29488500

Total energy: -4146401.82 kJ mol^{-1}

cis-L-**11**:

C	-2.12111300	-1.08526400	-0.45054900
C	-1.29739400	-0.64923700	-1.50494000
C	-0.02818900	-1.18726700	-1.69858700
C	0.46824000	-2.15887300	-0.81706900
C	-0.34316700	-2.61042300	0.23353200
C	-1.62229500	-2.08241400	0.40495100
H	-1.66136000	0.11639900	-2.18475200
H	0.58857600	-0.85755400	-2.52938300
H	0.00831100	-3.39372600	0.89866800
H	-2.24521800	-2.45183600	1.21498200
B	-3.54632900	-0.48885000	-0.24162900
O	-4.36155700	-0.83877100	0.80490600
O	-4.10707800	0.43615500	-1.08544100
C	-5.67900600	-0.25416900	0.54902800
C	-5.33709900	0.91698400	-0.45364000

C	-6.53517900	-1.36359500	-0.07407300
H	-6.56513000	-2.21726300	0.61029700
H	-7.56212200	-1.02651200	-0.24627200
H	-6.11756300	-1.70593100	-1.02627500
C	-6.27671200	0.18649100	1.88306000
H	-5.61449300	0.87067600	2.41849500
H	-7.24118600	0.68244600	1.72976100
H	-6.44570800	-0.69018800	2.51678300
C	-4.98252100	2.23618500	0.24350600
H	-4.57478800	2.93179800	-0.49665900
H	-5.86496800	2.69771000	0.69752500
H	-4.22797900	2.08824600	1.02263800
C	-6.37517700	1.16079900	-1.54632700
H	-7.33135500	1.46890100	-1.10975900
H	-6.03148800	1.96433000	-2.20582500
H	-6.54140300	0.26896600	-2.15491100
C	1.81019200	-2.77513700	-1.11377600
O	2.03914200	-3.24737400	-2.23139600
N	2.76295200	-2.79488500	-0.13142700
C	2.68737800	-2.18581800	1.21002300
C	3.98637900	-3.60683400	-0.31201800
C	4.05593100	-2.55245700	1.84595800
C	4.45989900	-3.84498600	1.12390600
H	3.73840700	-4.52024800	-0.85587700
H	3.96998900	-2.65869900	2.92945200
H	3.93201200	-4.70284200	1.55505600
H	4.72992000	-3.05566600	-0.90130800
H	5.53392900	-4.04043200	1.18111400
H	4.78728700	-1.76261200	1.64009000
C	2.46468300	-0.66688300	1.24600800
O	1.92286900	-0.15227800	2.21820700
N	2.97881300	0.02199000	0.17847700
H	3.38737700	-0.54783900	-0.55271000
C	3.00167200	1.40956000	-0.04734200
C	3.59425400	1.85093200	-1.24532700
C	2.47326900	2.34748900	0.84706500
C	3.64340700	3.20899200	-1.51940200
H	4.01478600	1.14928900	-1.95903300
C	2.54135100	3.71195900	0.53429300
H	2.01529000	2.03053700	1.77200400
C	3.12744700	4.16347200	-0.65400100
H	3.18303100	5.21890900	-0.90052600
C	1.98374200	4.71010900	1.47621100
H	2.08057100	5.76430400	1.14583200

O	1.45277000	4.43806400	2.53989000
H	1.87655300	-2.61664200	1.80105900
F	4.21654400	3.60954700	-2.67377000

Total energy: -4146392.50 kJ mol^{-1}

trans-L-**11** + D-DOPA:

C	6.23505800	-0.71019000	-1.23013000
C	5.85659100	-0.53366600	0.24276400
N	4.53421100	0.11766600	0.16671400
C	3.88451400	-0.07700400	-1.14317600
C	4.88486800	-0.98808000	-1.90791900
C	2.48598000	-0.71858700	-1.09544500
C	4.07846500	0.89087200	1.20408000
O	1.64066000	-0.43236200	-1.93556700
N	2.31979500	-1.66579700	-0.11796300
C	1.25895800	-2.59380800	0.00787400
C	-0.06196200	-2.28685600	-0.33370600
C	-1.06844400	-3.25685400	-0.18478100
C	-0.74694500	-4.53261000	0.30182600
C	0.56827600	-4.79796300	0.65425800
C	1.58121800	-3.86250300	0.51999500
C	2.88782600	1.76796300	0.94695800
O	4.63725300	0.86503800	2.30598900
C	2.90274500	2.74745200	-0.05801900
C	1.78284900	3.55034300	-0.26883900
C	0.60203400	3.40658100	0.48462300
C	0.63659000	2.45905400	1.52414000
C	1.75579100	1.66017400	1.76530900
B	-0.76650300	4.17374700	0.02601200
F	0.88201300	-6.02207500	1.13991900
C	-2.48710500	-2.96684700	-0.48510400
N	-2.92057200	-1.78827300	-0.70856300
C	-4.35028500	-1.61617200	-0.87825300
C	-4.67539200	-0.23969900	-1.50423900
O	-1.87826300	3.96482700	1.05532400
O	-1.31112200	3.43367800	-1.19431900
C	-2.98726400	1.64943700	-1.44228600
C	-4.03441300	0.94532200	-0.80404100
C	-4.41981800	1.32983100	0.48597100
C	-3.75279600	2.35864800	1.18395600
C	-2.69233400	3.00299100	0.56227700
C	-2.33669700	2.66890100	-0.76198600
O	-0.58179400	5.56562200	-0.31130700

C	-5.17771700	-1.88600800	0.46649500
O	-6.34420100	-1.41211400	0.46324100
O	-4.63232400	-2.59040300	1.34635900
H	6.67145200	0.21766200	-1.61653800
H	6.95664100	-1.51718100	-1.38359500
H	5.79075300	-1.49845000	0.76334000
H	6.54221200	0.10179200	0.80682200
H	3.75642800	0.86933500	-1.67087800
H	4.87704000	-0.77068700	-2.97838900
H	4.61046500	-2.04105500	-1.77752100
H	3.12647600	-1.84012000	0.46923000
H	-0.32085300	-1.30741500	-0.71008800
H	-1.50676800	-5.29783400	0.42515000
H	2.59957300	-4.12402200	0.78859100
H	3.79224600	2.88468200	-0.66879500
H	1.81809600	4.29629200	-1.06149700
H	-0.24501200	2.33300600	2.14784800
H	1.74920300	0.92985600	2.57105600
H	-3.14924600	-3.84289000	-0.46757900
H	-4.74361200	-2.39095600	-1.56145200
H	-5.76647400	-0.15613100	-1.49679200
H	-4.35334100	-0.24528400	-2.55397300
H	-2.67379200	1.37838900	-2.44842100
H	-5.23558700	0.79878700	0.96688500
H	-4.04737000	2.62781900	2.19600100
H	0.20660000	5.90055600	0.13658100

Total energy: -4977668.93 kJ mol^{-1}

trans-L-**11** + L-DOPA:

C	6.12539500	-0.48587500	-1.76824800
C	5.91205200	-0.04517300	-0.31782200
N	4.51652300	0.43996900	-0.31595800
C	3.75296100	-0.04051200	-1.48202900
C	4.74334400	-1.01064100	-2.18188400
C	2.42513900	-0.74894100	-1.16729800
C	4.09968900	1.31569600	0.65403000
O	1.49267500	-0.68535600	-1.96098300
N	2.42076500	-1.49418900	-0.01689000
C	1.42558800	-2.38830900	0.43513600
C	0.08610100	-2.29232300	0.04511300
C	-0.85433900	-3.21829900	0.52442200
C	-0.45706700	-4.24481800	1.39172100

C	0.87510300	-4.29913000	1.77922400
C	1.82708800	-3.39990200	1.32566700
C	2.76610700	1.98693700	0.49788800
O	4.80815000	1.53493800	1.64375300
C	2.41492800	2.72567200	-0.64268700
C	1.17651500	3.36551700	-0.70959100
C	0.23137700	3.28929200	0.33123500
C	0.62741400	2.57792900	1.47938700
C	1.86861100	1.94950400	1.57428800
B	-1.28038400	3.89020800	0.14740500
F	1.26849500	-5.27596300	2.62991000
C	-2.28063200	-3.10659500	0.14302000
N	-2.75005700	-2.05986400	-0.40776300
C	-4.15869800	-2.00303100	-0.74524700
C	-4.91648900	-1.00938800	0.18486900
O	-2.06924800	3.72254100	1.44792400
O	-2.04727800	2.98319000	-0.81157200
C	-3.51101900	1.04209000	-0.44546600
C	-4.21855800	0.29657400	0.52876500
C	-4.25297000	0.76423600	1.84587300
C	-3.57976400	1.93987000	2.24310400
C	-2.84963000	2.63025300	1.28816600
C	-2.82926500	2.18360300	-0.05272100
O	-1.31920500	5.24459000	-0.35012200
C	-4.40010300	-1.65613900	-2.26440200
O	-5.61114600	-1.70973500	-2.60689300
O	-3.40721700	-1.37779100	-2.98254300
H	6.40521800	0.37604300	-2.38428600
H	6.90893900	-1.24241900	-1.86398300
H	6.03366800	-0.88060600	0.38397800
H	6.57745300	0.75830900	0.00456200
H	3.49458700	0.77725400	-2.15745600
H	4.58209400	-1.02740300	-3.26212400
H	4.60078800	-2.02962400	-1.80418000
H	3.28011300	-1.48371200	0.51914500
H	-0.23689000	-1.51391200	-0.62949600
H	-1.16485600	-4.97441600	1.77230300
H	2.85928700	-3.49938800	1.64602300
H	3.11519100	2.81882300	-1.46904300
H	0.93308200	3.93247400	-1.60713200
H	-0.06273000	2.51147100	2.31640500
H	2.14765100	1.41117500	2.47674700
H	-2.90945500	-3.97949900	0.38700500
H	-4.64026600	-2.98597100	-0.59408100

H	-5.88049700	-0.83402300	-0.31143300
H	-5.14292800	-1.52433800	1.12751500
H	-3.43326100	0.67846000	-1.46537700
H	-4.79295400	0.19138800	2.59768700
H	-3.59973100	2.27398600	3.27786900
H	-0.46676900	5.66955300	-0.18617900

Total energy: -4977666.80 kJ mol^{-1}

cis-L-**11** + D-DOPA:

C	6.33417500	-1.82199800	-1.76547400
C	6.20031300	-1.26852600	-0.34423400
N	4.91245000	-0.53891400	-0.37187200
C	4.12689100	-0.85061400	-1.58072600
C	4.87972500	-2.06212100	-2.18737600
C	2.64026200	-1.17476200	-1.37802100
O	1.84306700	-0.93011000	-2.27881600
N	2.32690200	-1.79952800	-0.20148300
C	1.05500600	-2.12708700	0.30972800
C	-0.13967800	-1.85131600	-0.37230600
C	-1.37550600	-2.12461000	0.22984600
C	-1.43163700	-2.71254300	1.50268200
C	-0.23524700	-3.00598000	2.13442000
C	1.00669600	-2.72552400	1.57792200
F	-0.26501300	-3.58566500	3.35789400
C	-2.60185900	-1.72738300	-0.49109000
C	4.65805000	0.38499700	0.61225200
O	5.42425300	0.47585400	1.58013800
C	3.42296200	1.23515400	0.54515400
N	-3.74702500	-1.66758600	0.06815000
C	-4.86341900	-1.19121700	-0.72709500
C	-5.26984800	0.23300800	-0.24746200
O	-0.93837800	3.83835500	-0.73136300
O	-1.38219900	2.89529500	1.40815800
C	-3.34579100	1.59900200	0.68926000
C	-4.17870600	1.27090100	-0.40657000
C	-3.93045500	1.86426700	-1.64889300
C	-2.85594800	2.75744100	-1.84537100
C	-2.03020900	3.04287900	-0.76745700
C	-2.28645000	2.47613600	0.50097200
C	3.01261900	1.95000600	-0.58922700
C	1.85966400	2.73883000	-0.54506400
C	1.06156700	2.84060100	0.60746400

C	1.51124300	2.13421500	1.74115200
C	2.67058300	1.36384400	1.72449600
B	-0.32141600	3.70796000	0.65168600
O	-0.15971400	5.02600900	1.22825400
C	-6.09668600	-2.15828800	-0.58710500
O	-6.55089300	-2.60649800	-1.67244200
O	-6.52241300	-2.36132700	0.57859100
H	6.79927500	-1.07524600	-2.41886500
H	6.94079100	-2.73082500	-1.80197100
H	6.16437600	-2.06901700	0.40527200
H	7.00342300	-0.58512000	-0.06070400
H	4.14572900	-0.02137000	-2.29313400
H	4.73323600	-2.11709200	-3.26852300
H	4.50570800	-2.99307000	-1.74521600
H	3.10000700	-1.92963000	0.44039500
H	-0.10015800	-1.39658200	-1.35188700
H	-2.38225100	-2.92566400	1.97697600
H	1.90975600	-2.96412100	2.13082200
H	-2.45192800	-1.44067500	-1.54348600
H	-4.59513600	-1.13274900	-1.79415100
H	-5.58056400	0.14835400	0.79902400
H	-6.15658300	0.52063800	-0.82848300
H	-3.51878500	1.15126300	1.66504800
H	-4.57258200	1.61916600	-2.49296600
H	-2.66986200	3.20347000	-2.81946900
H	3.59790200	1.91142800	-1.50358500
H	1.55930600	3.27492700	-1.44285200
H	0.92523100	2.17595800	2.65738200
H	2.99618900	0.83469600	2.61601900
H	0.69314600	5.07813100	1.67990000

Total energy: -4977681.91 kJ mol^{-1}

cis-L-**11** + L-DOPA:

C	6.18595100	-1.52162800	-1.95692700
C	6.12798900	-0.90402800	-0.55701300
N	4.80307700	-0.24553700	-0.51995900
C	3.94621900	-0.66162100	-1.64614900
C	4.71967600	-1.85994000	-2.25282400
C	2.50046300	-1.05334300	-1.30800700
O	1.61902000	-0.88452000	-2.14530800
N	2.31926900	-1.64941000	-0.08987200
C	1.11778600	-2.08713900	0.50512300

C	-0.14787700	-1.80781600	-0.03253700
C	-1.30895800	-2.22962800	0.62955200
C	-1.21617300	-2.94939200	1.83076500
C	0.04557400	-3.21741500	2.33213800
C	1.21626000	-2.80521000	1.70601500
F	0.15827200	-3.91138000	3.49050800
C	-2.61525800	-1.86875700	0.03551800
C	4.56914000	0.71680800	0.43128300
O	5.39461400	0.90174600	1.33481300
C	3.28572100	1.49390400	0.40458400
N	-3.72460400	-2.16800500	0.59431800
C	-4.96118700	-1.70506000	-0.02637300
C	-5.30339900	-0.25055400	0.43437200
O	-1.34542200	3.62196100	-0.73928500
O	-1.54807400	2.85765000	1.50549200
C	-3.42028200	1.32448000	1.06072100
C	-4.29638900	0.82049400	0.07030100
C	-4.19371300	1.30850300	-1.23829700
C	-3.22193200	2.26563800	-1.59743500
C	-2.35317700	2.72915600	-0.61842800
C	-2.46526000	2.26940000	0.71151700
C	2.77031700	2.12737600	-0.73522900
C	1.56847800	2.83654300	-0.66307100
C	0.82425500	2.93481600	0.52525100
C	1.38302100	2.32053000	1.66393900
C	2.59126800	1.63052900	1.61764000
B	-0.62527700	3.68284500	0.59956500
O	-0.54930100	5.05954600	1.04193400
C	-5.12145200	-1.86602200	-1.59134400
O	-6.21856100	-1.42899400	-2.03602100
O	-4.20890300	-2.43644800	-2.23875600
H	6.55755800	-0.78548100	-2.67864900
H	6.83876600	-2.39765100	-1.99814700
H	6.19376200	-1.66587600	0.22988100
H	6.91018600	-0.16556000	-0.36903000
H	3.86168300	0.12909400	-2.39630600
H	4.49623400	-1.97706200	-3.31572300
H	4.43449800	-2.78667500	-1.74126200
H	3.15005000	-1.73568900	0.48369100
H	-0.22362300	-1.25496300	-0.95809800
H	-2.10911900	-3.27746400	2.34983800
H	2.17681600	-3.04287000	2.15190100
H	-2.55732400	-1.33048600	-0.91234900
H	-5.76576500	-2.32516400	0.39717700

H	-6.27770200	-0.03565200	-0.01451300
H	-5.43532900	-0.26124100	1.52373200
H	-3.48484400	0.96652600	2.08601800
H	-4.87137200	0.92366000	-1.99530600
H	-3.14755300	2.62925000	-2.61974800
H	3.30862600	2.08302500	-1.67778900
H	1.18398300	3.30443000	-1.56692400
H	0.84153800	2.36472500	2.60685300
H	2.99811100	1.16608100	2.51196900
H	0.32921100	5.23263200	1.40551600

Total energy: -4977674.81 kJ mol^{-1}