Supplementary Information

Chalcogen Bonding Mediated Chiral Recognition and Enantioenrichment of Organoselenocyanates

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Content

A.Experimental Procedures

Materials. Reagents were obtained from commercial sources and used without further purification. Binaphthol, 2,9-Dichloro-1,10-phenanthroline, pyrene, N-Bromosuccinimide were purchased from Bide pharm. And other reagents were purchased from Shanghai Xiensi Biotechnology Co., Ltd. All solvents were reagent grade. All water used in this work was deionized (DI) water.

Instrumentation. ^{1}H NMR spectra, ^{13}C NMR, ^{77}Se NMR spectra were obtained by BRUKER AVANCE III HD 400. High-Resolution Mass Spectra (HR-MS) were performed on an Agilent Q-TOF 6510. Circularly polarized luminescence (CPL), Circular dichroism (CD), temperature-variable CD were measured with an Applied Photophysics ChirascanV100 model. UV-Visible absorption spectra at room temperature were recorded on UV-1900 Shimadzu spectrophotometer. X-ray photoelectron spectroscopy (XPS) measurements were performed using a Thermo Fisher ESCALAB XI+ instrument, equipped with an Al Kα source (spot size: 500

μm). Fluorescence spectra were made on a RF-6000 Shimadzu fluorophotometer. Scanning electron microscope (SEM) images were measured by a Zeiss scanning electron microscope (Germany). Grazing incidence wide-angle X-ray scattering (GIWAXS) measurements were conducted at a Xeuss 3.0 SAXS/WAXS laboratory beamline at Vacuum Interconnected Nanotech Workstation (Nano-X) in China with Kα X-ray of Cu source (operated at 50kV, 0.06 mA, 1.542 Å). GIWAXS patterns were recorded by a two-dimensional X-ray detector (Eiger2 R 1M, Dectris). The incident angle was set to 0.18 degree. High-performance liquid chromatography (HPLC) was carried out on an Agilent 1260 Infinity system using a Daicel IC chiral column. The mobile phase consisted of isopropanol/n-hexane in a 1:9 volume ratio. Infrared (IR) spectra were recorded using a Bruker ALPHA II spectrometer.

Assembly methods. The solvent used for the NMR measurements was deuterated chloroform ($CDCl_3$), with concentration of 1 mM. Unless otherwise specified, all solution-phase measurements were conducted in a chloroform/methylcyclohexane mixture (v/v = 1/39) at a concentration of 0.05 mM. For the preparation of the assembled structures, the concentration was increased to 0.125 mM.

Quantum mechanical calculation. Structural information was first obtained from the crystal structures, followed by geometry optimization at the B3LYP-D3(BJ)/6-311G(d,p) level of theory. For guest molecules without available crystal structures, the structures were derived from related crystal models and subsequently optimized. The binding energies of the complexes were then calculated with correction for basis set superposition error (BSSE). Electrostatic potential (ESP) maps were generated using Gaussian 16, while reduced density gradient (RDG) analyses were carried out with Multiwfn.[S1,S2] Energy decomposition analysis was performed using Psi4 at the SAPT0 level with the jun-cc-pVDZ basis set.

Solution-phase experimental methods The solvent system consisted of chloroform and methylcyclohexane with a volume ratio of 1:39. The host concentration was fixed at 0.05 mM, and solutions were prepared by adding different equivalents of the guest. Solutions with varying host–guest ratios were then measured individually to obtain the corresponding data. Taking the titration experiment of ^{R}Pyr with ^{R}MBA as an

example to illustrate the experimental details, 10.4 mg of ^{R}Pyr was first weighed and dissolved in 1 mL of chloroform to prepare a 10 mM stock solution. Similarly, 10.7 mg of ^{R}MBA was weighed and dissolved in 4 mL of chloroform to prepare a 10 mM stock solution. Eleven small glass vials were prepared and labeled. To each vial, 10 μL of the ^{R}Pyr stock solution was added. Subsequently, 0, 5, 10, 15, 20, 25, 30, 35, 40, 45, and 50 μL of the ^{R}MBA stock solution were added to vials 1-11, respectively. After allowing the solvent to evaporate naturally, 50 μL of chloroform was added to each vial to ensure complete dissolution, followed by the addition of 1950 μL of methylcyclohexane. Solutions in vials 1-11 were then measured sequentially to obtain the data required to complete the titration experiment.

Assembly-state experimental methods. The solvent system consisted of chloroform and methylcyclohexane with a volume ratio of 1:39. The host concentration was fixed at 0.125 mM, and solutions were prepared by adding different equivalents of the guest. After aging for a certain period followed by centrifugation, assembly-state solids were obtained and used for XPS, IR, CD, and CPL measurements.

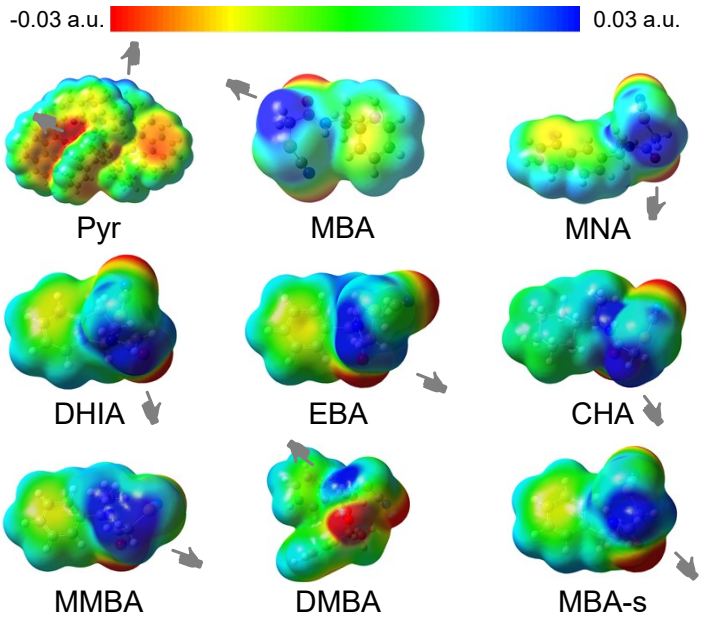
NMR experimental methods. $CDCl_3$ was used as the solvent, and the concentration was set to 1 mM. Taking the titration experiment of ^{R}Pyr with ^{R}MBA as an example to illustrate the experimental details, 10.4 mg of ^{R}Pyr was first weighed and dissolved in 1 mL of chloroform to prepare a 10 mM stock solution, while 10.7 mg of ^{R}MBA was weighed and dissolved in 4 mL of chloroform to prepare a 10 mM stock solution. Eleven NMR tubes were prepared and labeled, and 50 μL of the ^{R}MBA stock solution was added to each tube. Subsequently, 0, 5, 10, 15, 20, 25, 30, 35, 40, 45, and 50 μL of the ^{R}Pyr stock solution were added to tubes 1-11, respectively. After allowing the solvent to evaporate naturally, 500 μL of $CDCl_3$ was added to each tube to ensure complete dissolution. The solutions in tubes 1-11 were then measured sequentially to obtain the data required to complete the titration experiment.

B. Additional experimental data

Table S1. Energy decomposition of the interactions within the complex was performed using symmetry-adapted perturbation theory (SAPT).

EDA (kcal/mol)	^{R}Pyr-^{R}MBA	^{R}Pyr-^{R}DHIA	^{R}Pyr-^{R}EBA	^{R}Pyr-^{R}MNA
Dispersion	-43.2	-61.4	-60.4	-60.8
Electrostatics	-18.3	-33.7	-33.8	-35.1
Induction	-6.7	-12.0	-12.4	-12.4
Exchange	39.2	62.9	62.5	61.4
Total Energy	-29.1	-44.2	-44.0	-46.9

EDA (kcal/mol)	^{R}Pyr-^{S}MBA	^{R}Pyr-^{S}DHIA	^{R}Pyr-^{S}EBA	^{R}Pyr-^{S}MNA
Dispersion	-62.4	-32.5	-41.4	-48.6
Electrostatics	-34.4	-15.3	-18.4	-20.4
Induction	-11.9	-6.2	-6.8	-7.4
Exchange	63.3	28.7	37.6	43.1
Total Energy	-45.4	-25.3	-29.0	-33.3



Entry	$V_{s,max,1}$/ kcal · mol^{-1}	$V_{s,max,2}$ / kcal · mol^{-1}
MBA	41.8	23.8
MNA	42.0	23.5
DHIA	42.1	23.8
EBA	41.8	24.3
CHA	42.0	23.6
MMBA	40.4	21.6
DMBA	34.2	18.6
MBA-s	35.4	20.8

Entry	$V_{s,min}$/ kcal · mol^{-1}	$V_{s,max}$ / kcal · mol^{-1}
Pyr	-42.2	22.1

Figure S1. The electrostatic potential maps (ESP) of each molecule.

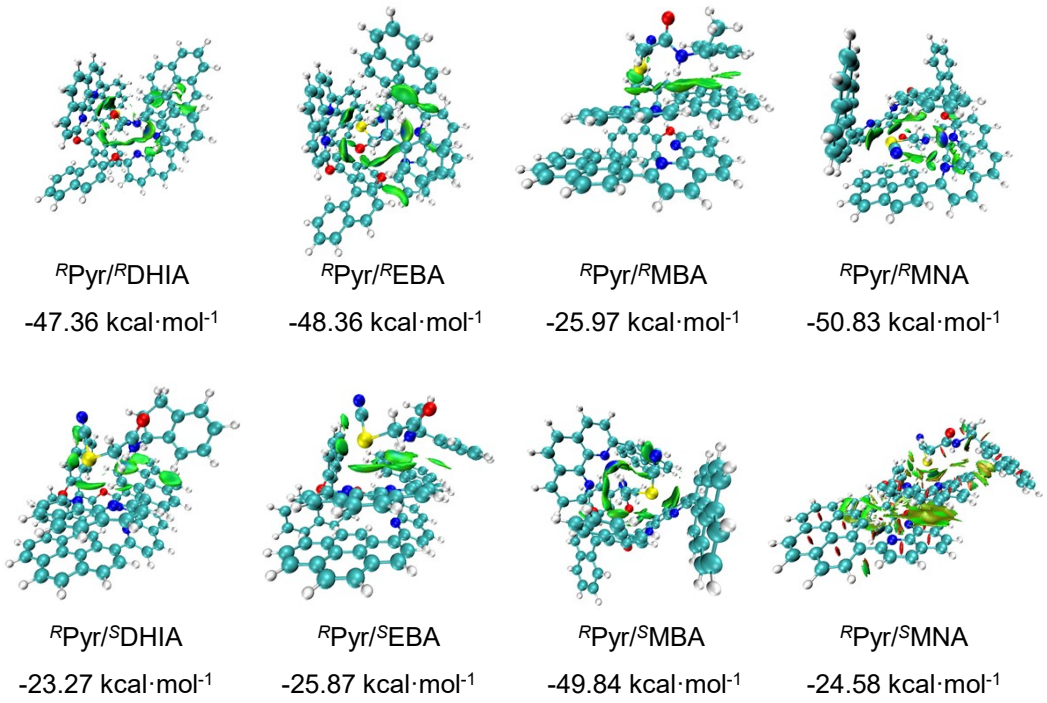


Figure S2. Investigating intermolecular binding energy and weak interactions via Independent Gradient Model (IGM). Blue represents attraction, and red represents repulsion.

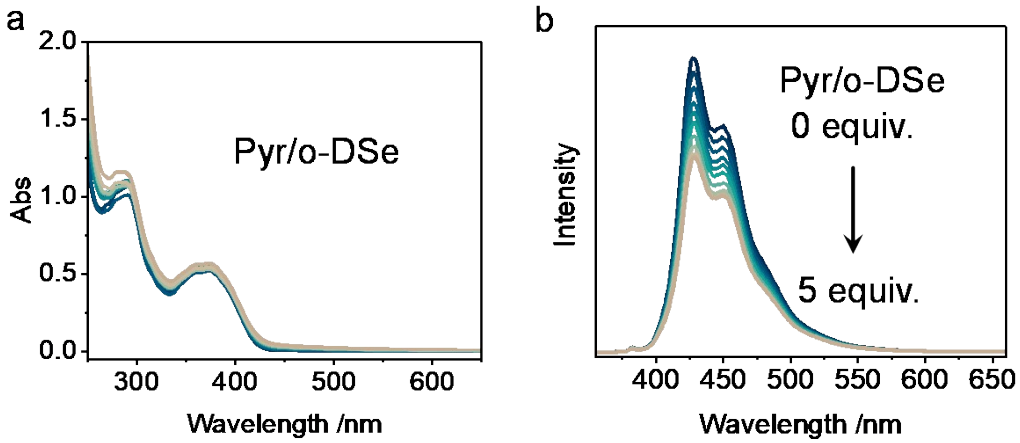


Figure S3. UV-visible absorption (a) and fluorescence intensity (b) titration spectra of Pyr/*o*-DSe. (0.05 mM, $CHCl_3$/methylcyclohexane (MCH), v/v = 1: 39)

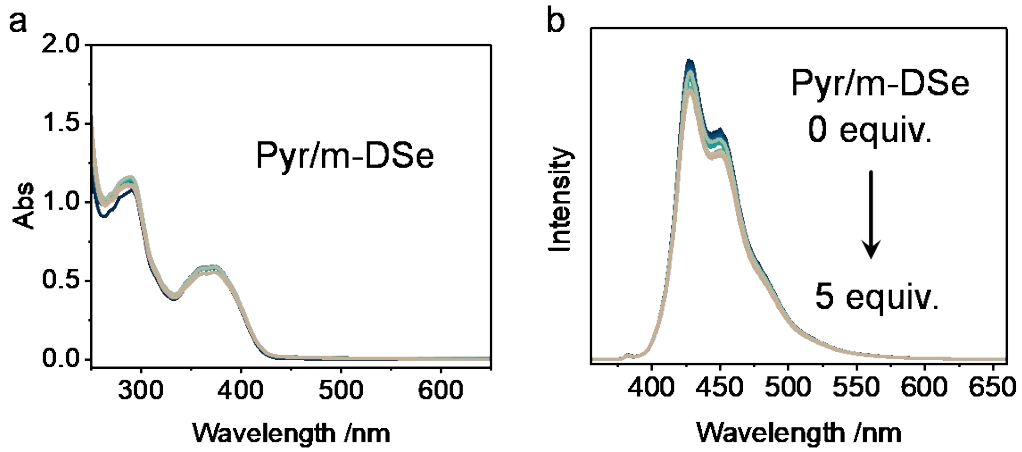


Figure S4. UV-visible absorption (a) and fluorescence intensity (b) titration spectra of Pyr/*m*-DSe. (0.05 mM, $CHCl_3$/ MCH, v/v = 1: 39)

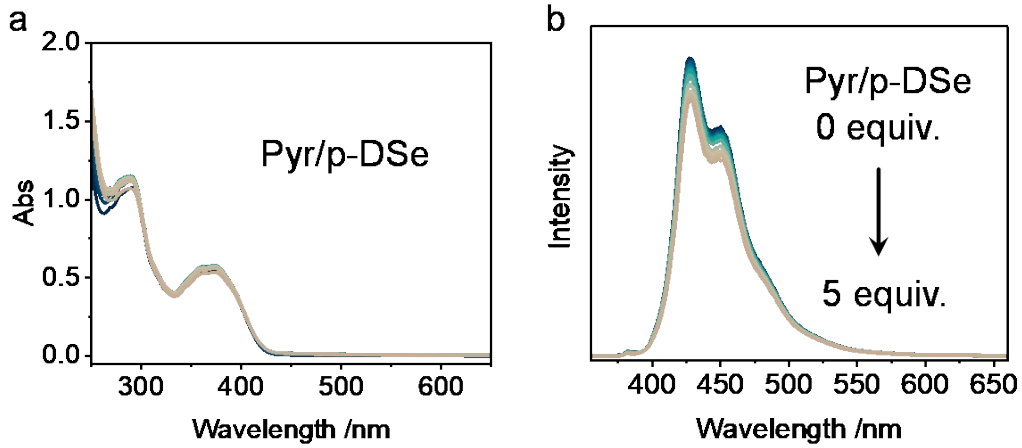


Figure S5. UV-visible absorption (a) and fluorescence intensity (b) titration spectra of Pyr/*p*-DSe. (0.05 mM, $CHCl_3$/ MCH, v/v = 1: 39)

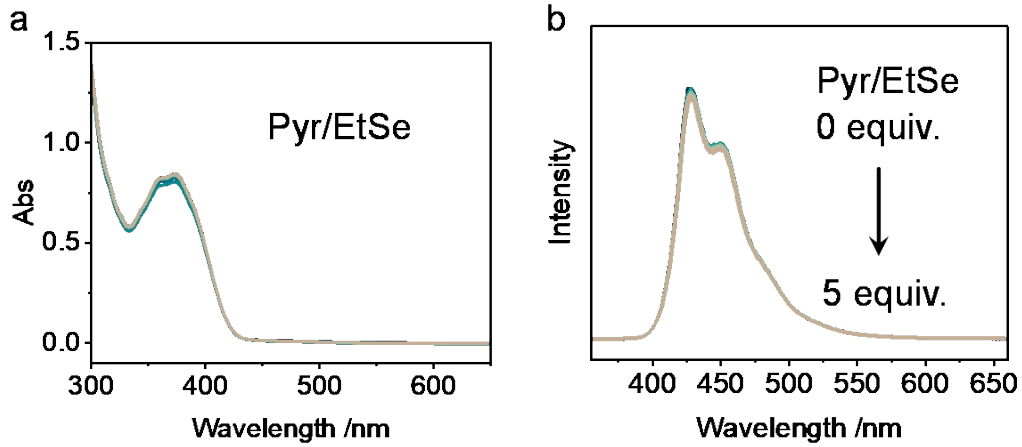


Figure S6. UV-visible absorption (a) and fluorescence intensity (b) titration spectra of Pyr/EtSe. (0.05 mM, $CHCl_3$/ MCH, v/v = 1: 39)

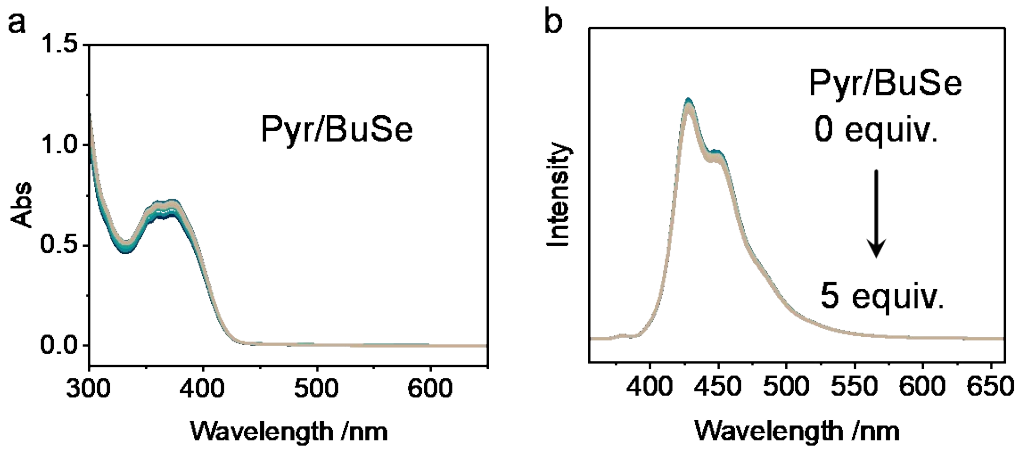


Figure S7. UV-visible absorption (a) and fluorescence intensity (b) titration spectra of Pyr/BuSe. (0.05 mM, $CHCl_3$/ MCH, v/v = 1: 39)

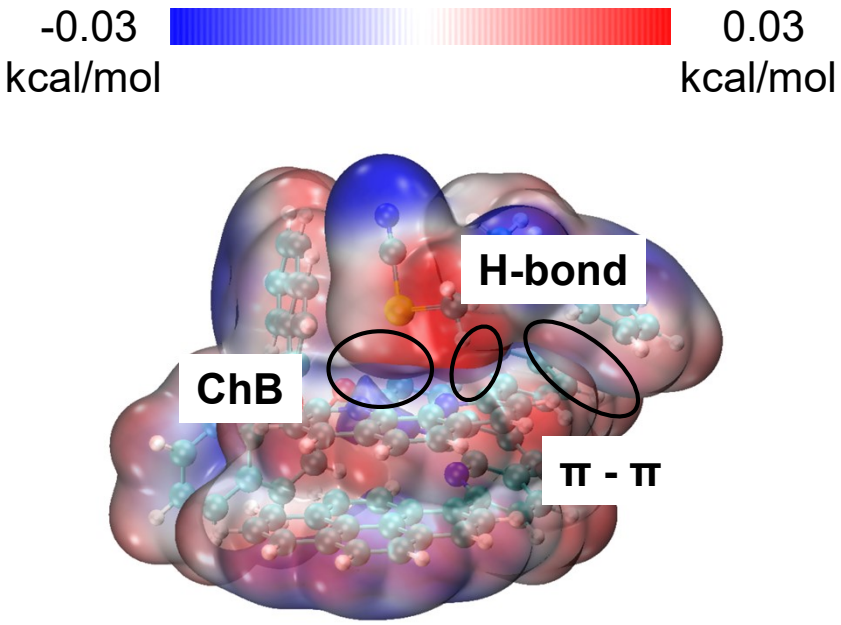


Figure S8. MESP between ^{R}Pyr and ^{R}MBA.

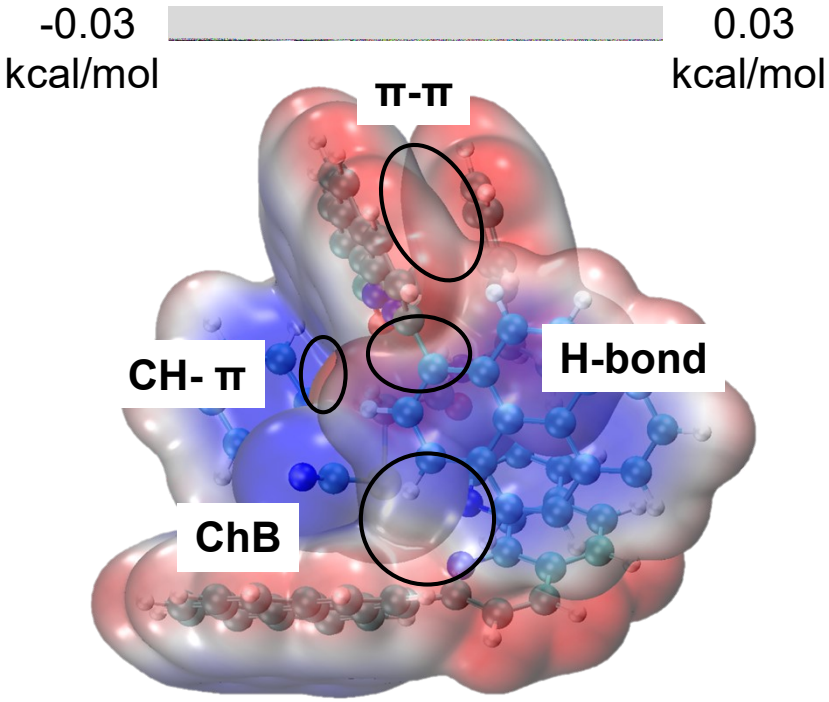


Figure S9. MESP between ^{R}Pyr and ^{S}MBA.

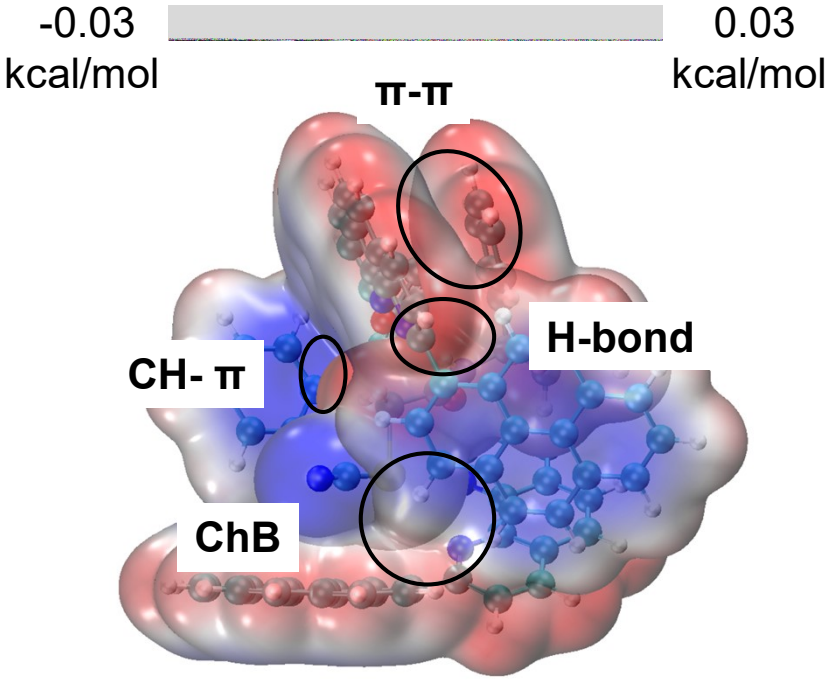


Figure S10. MESP between ^{R}Pyr and ^{R}EBA.

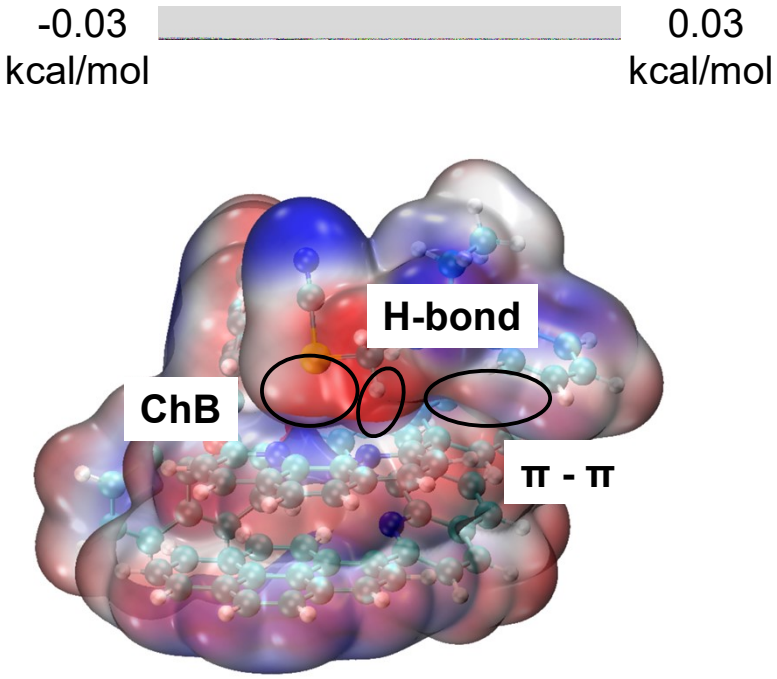


Figure S11. MESP between ^{R}Pyr and ^{S}EBA.

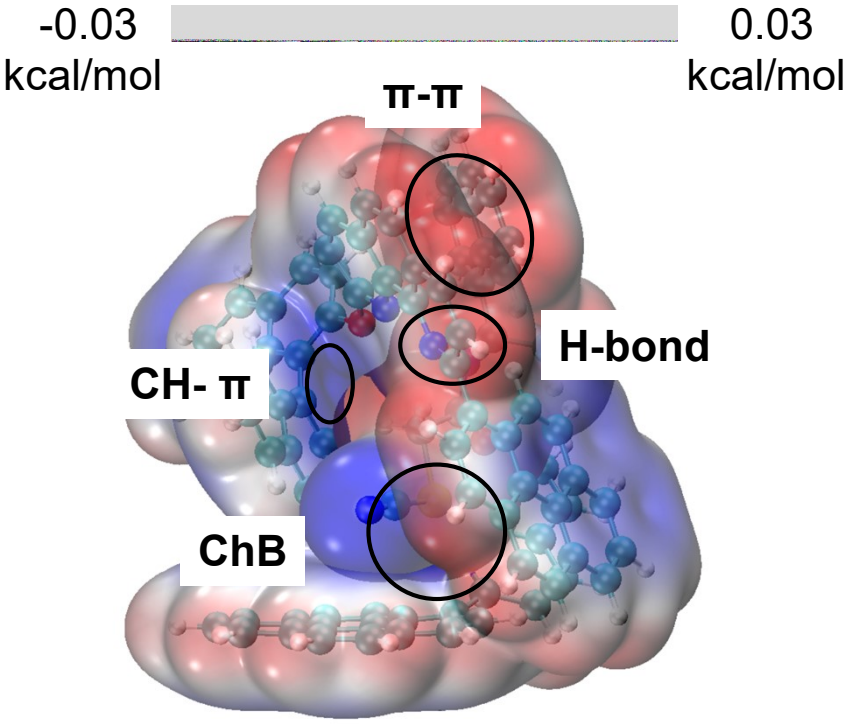


Figure S12. MESP between ^{R}Pyr and ^{R}MNA.

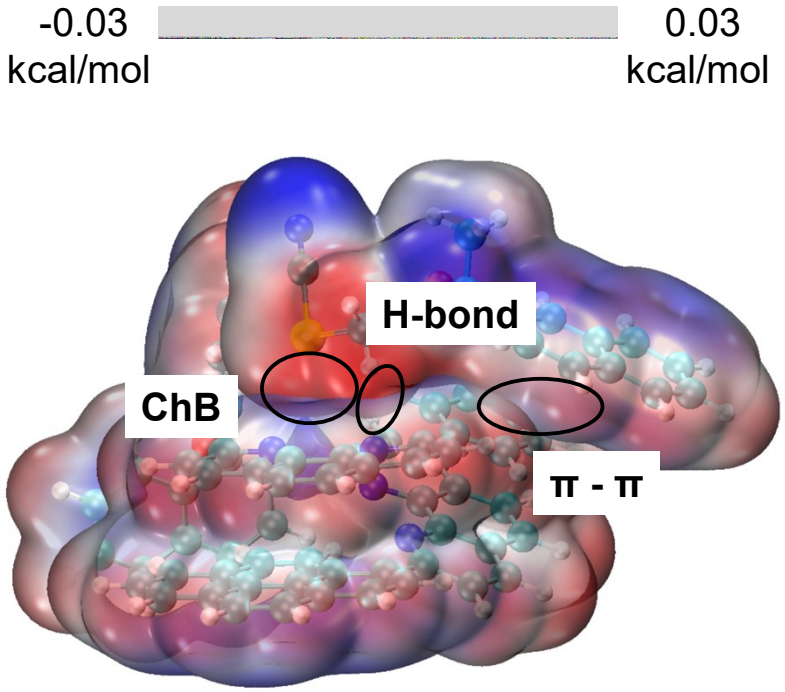


Figure S13. MESP between ^{R}Pyr and ^{S}MNA.

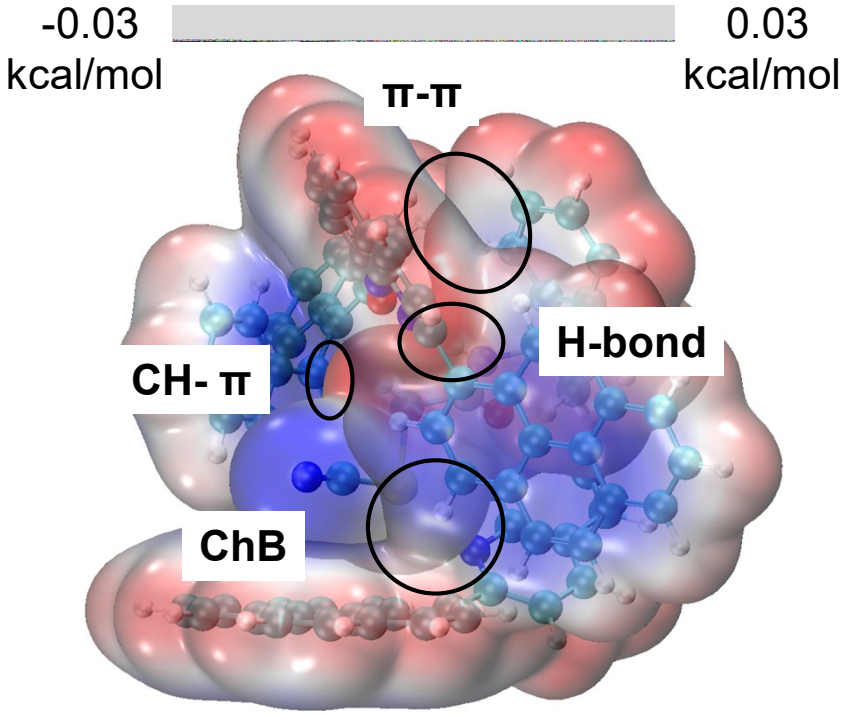


Figure S14. MESP between ^{R}Pyr and ^{R}DHIA.

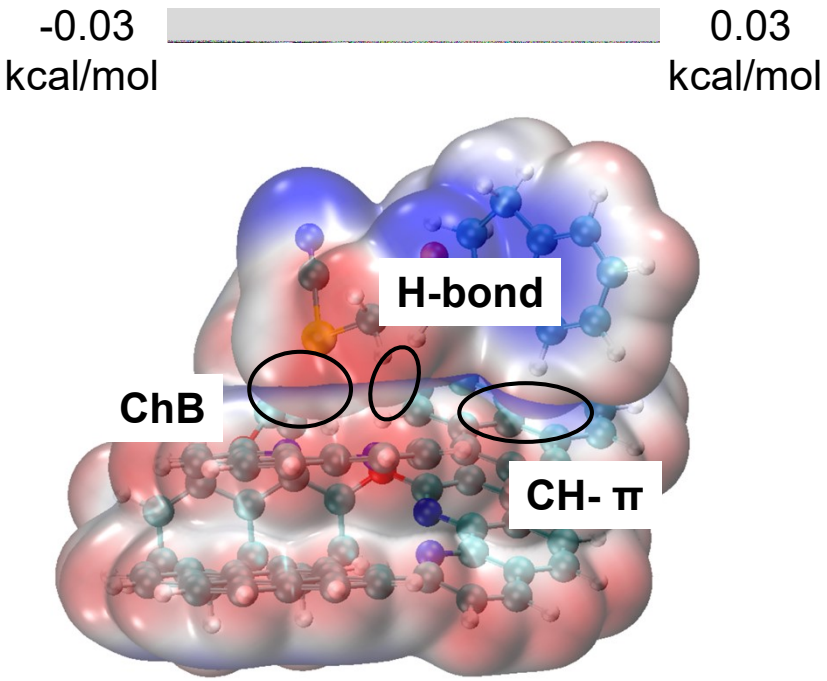


Figure S15. MESP between ^{R}Pyr and ^{S}DHIA.

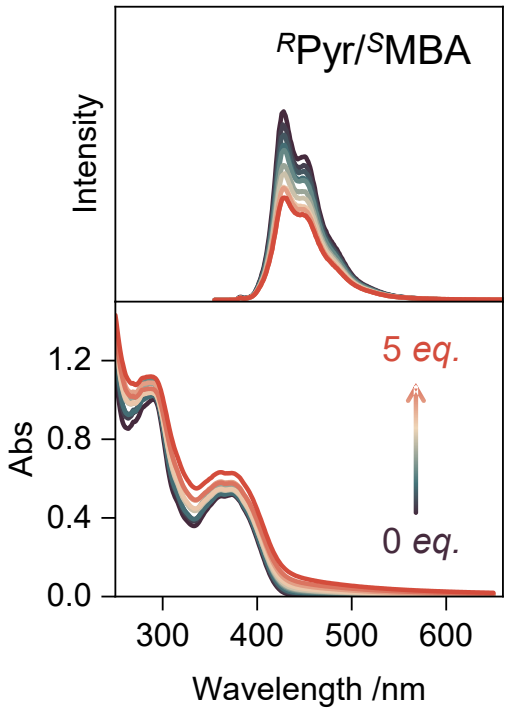


Figure S16. UV-visible absorption and fluorescence intensity titration spectra of ^{R}Pyr/^{S}MBA. (0.05 mM, $CHCl_3$/ MCH, v/v = 1: 39)

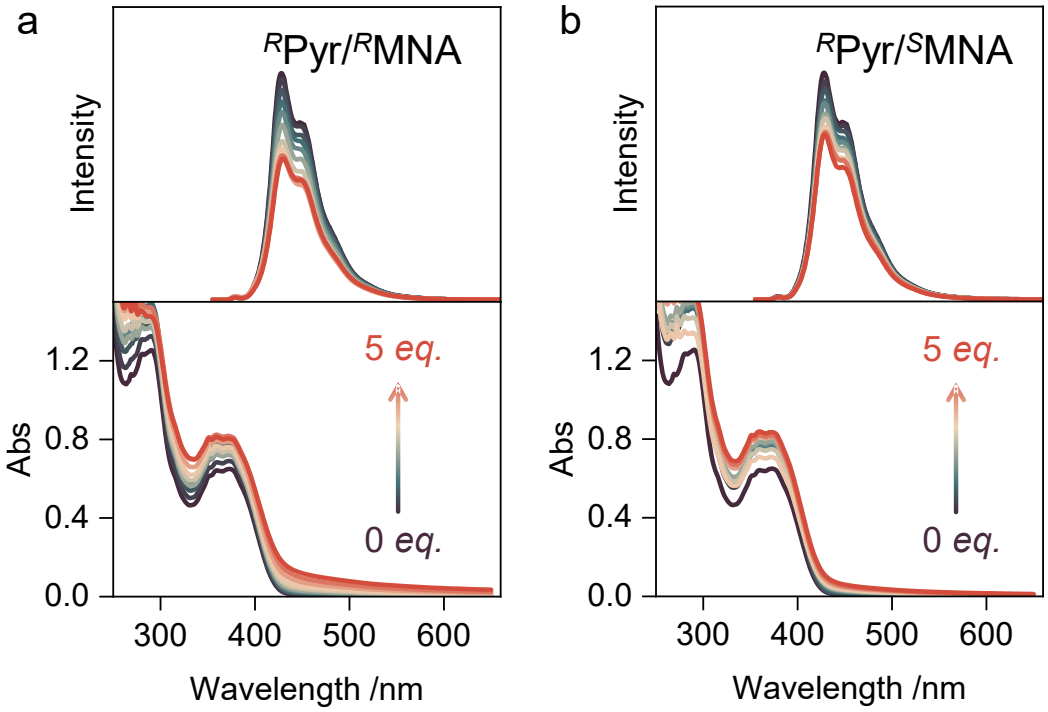


Figure S17. UV-visible absorption and fluorescence intensity titration spectra of ^{R}Pyr/^{R}MNA (a) and ^{R}Pyr/^{S}MNA (b). (0.05 mM, $CHCl_3$/ MCH, v/v = 1: 39)

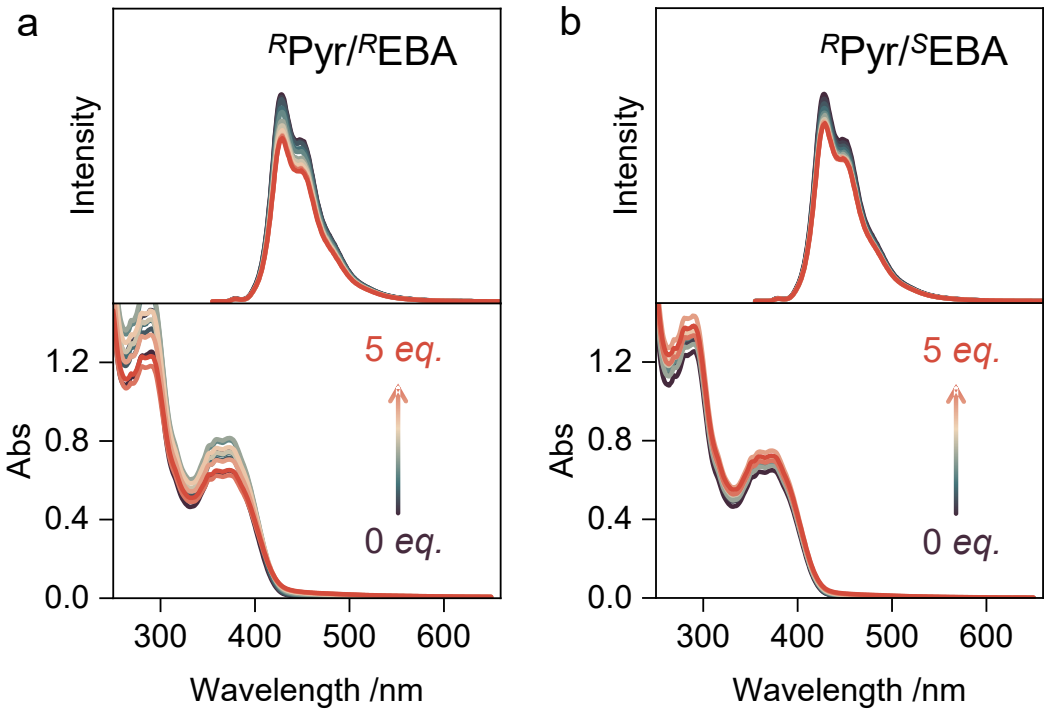


Figure S18. UV-visible absorption and fluorescence intensity titration spectra of ^{R}Pyr/^{R}EBA (a) and ^{R}Pyr/^{S}EBA (b). (0.05 mM, $CHCl_3$/ MCH, v/v = 1: 39)

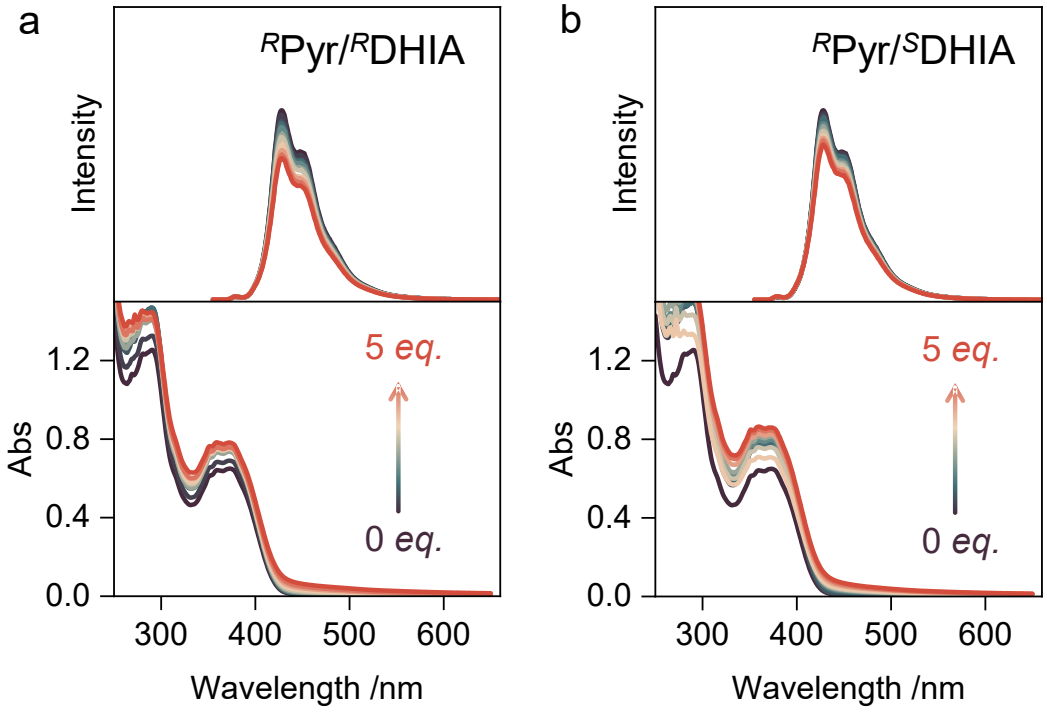


Figure S19. UV-visible absorption and fluorescence intensity titration spectra of ^{R}Pyr/^{R}DHIA (a) and ^{R}Pyr/^{S}DHIA (b). (0.05 mM, $CHCl_3$/ MCH, v/v = 1: 39)

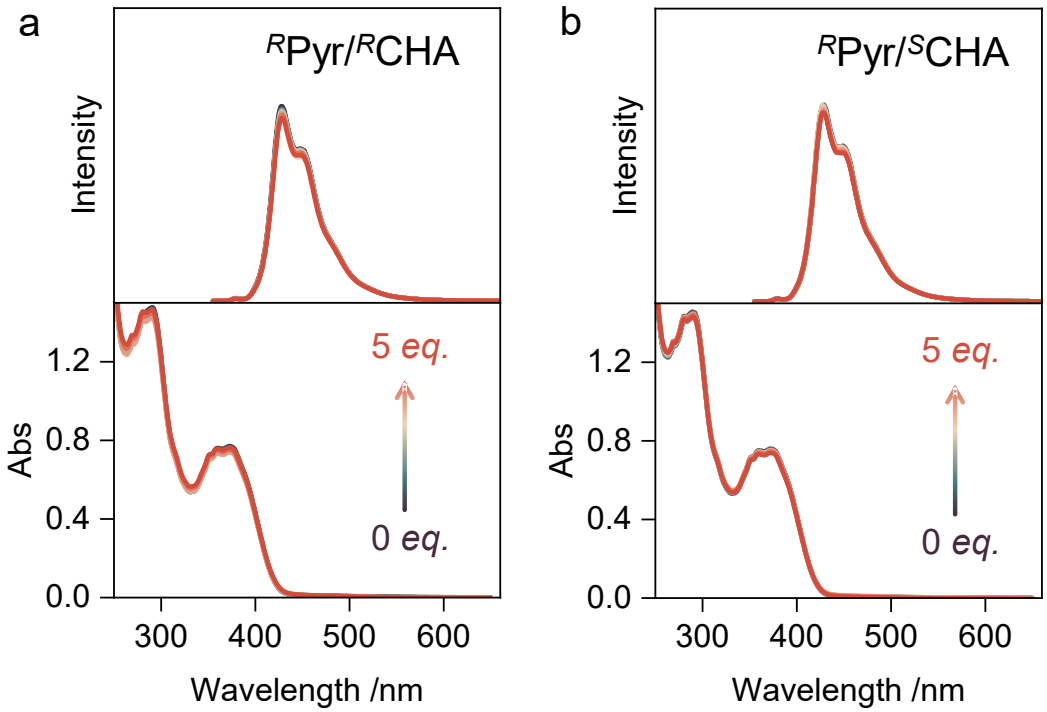


Figure S20. UV-visible absorption and fluorescence intensity titration spectra of ^{R}Pyr/^{R}CHA (a) and ^{R}Pyr/^{S}CHA (b). (0.05 mM, $CHCl_3$/ MCH, v/v = 1: 39)

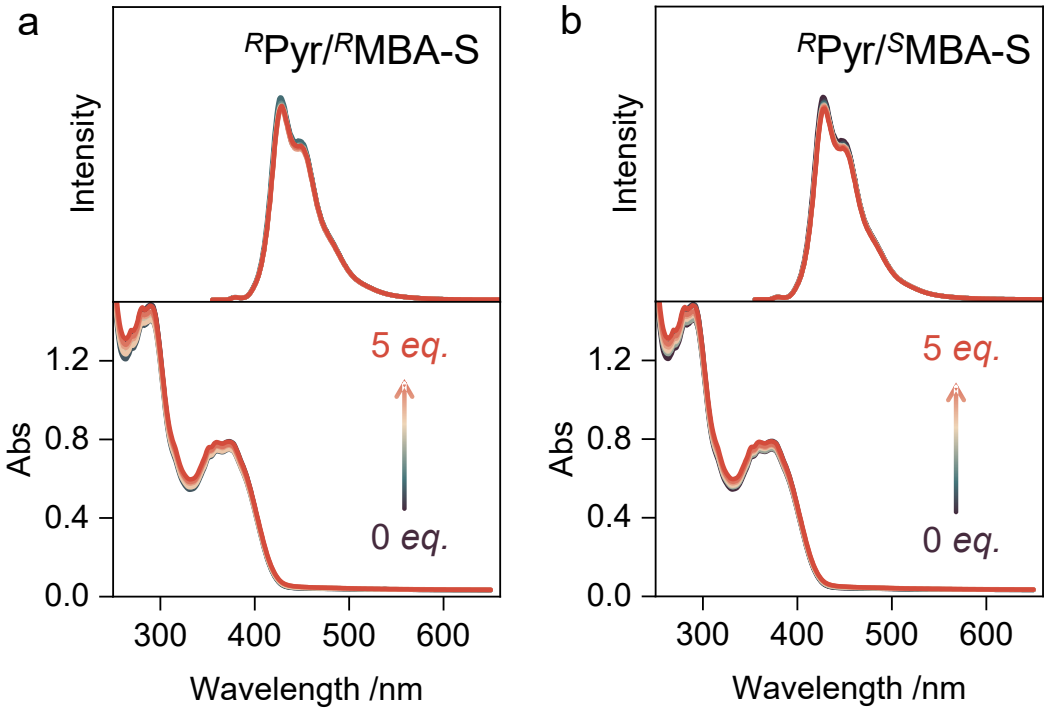


Figure S21. UV-visible absorption and fluorescence intensity titration spectra of ^{R}Pyr/^{R}MBA-S (a) and ^{R}Pyr/^{S}MBA-S (b). (0.05 mM, $CHCl_3$/ MCH, v/v = 1: 39)

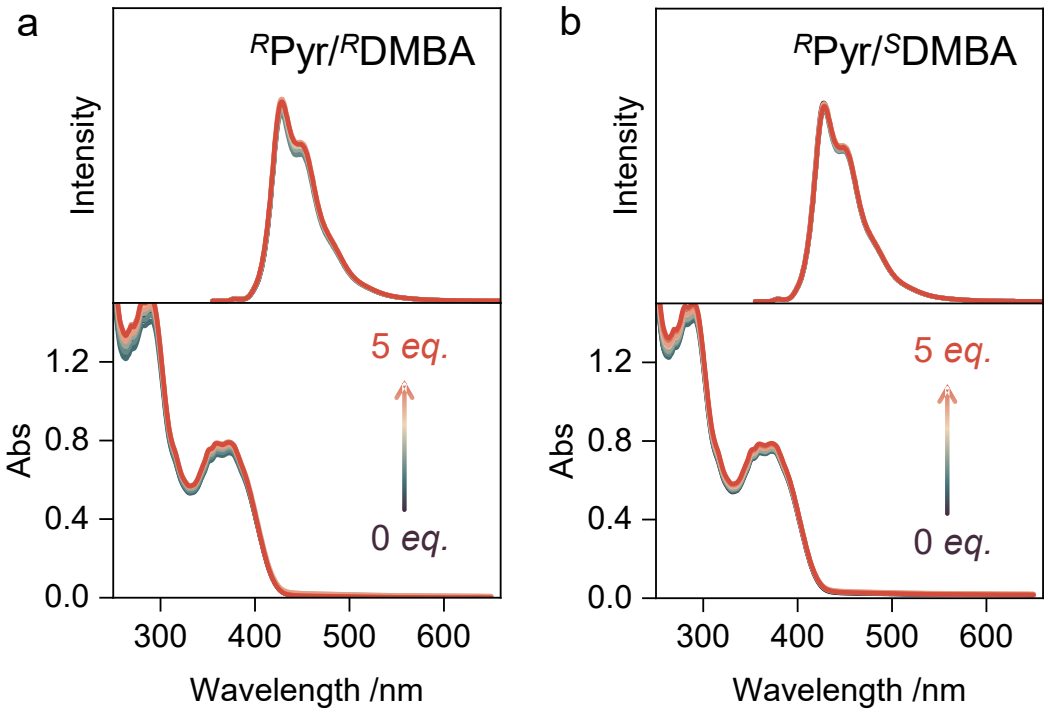


Figure S22. UV-visible absorption and fluorescence intensity titration spectra of ^{R}Pyr/^{R}DMBA (a) and ^{R}Pyr/^{S}DMBA (b). (0.05 mM, $CHCl_3$/ MCH, v/v = 1: 39)

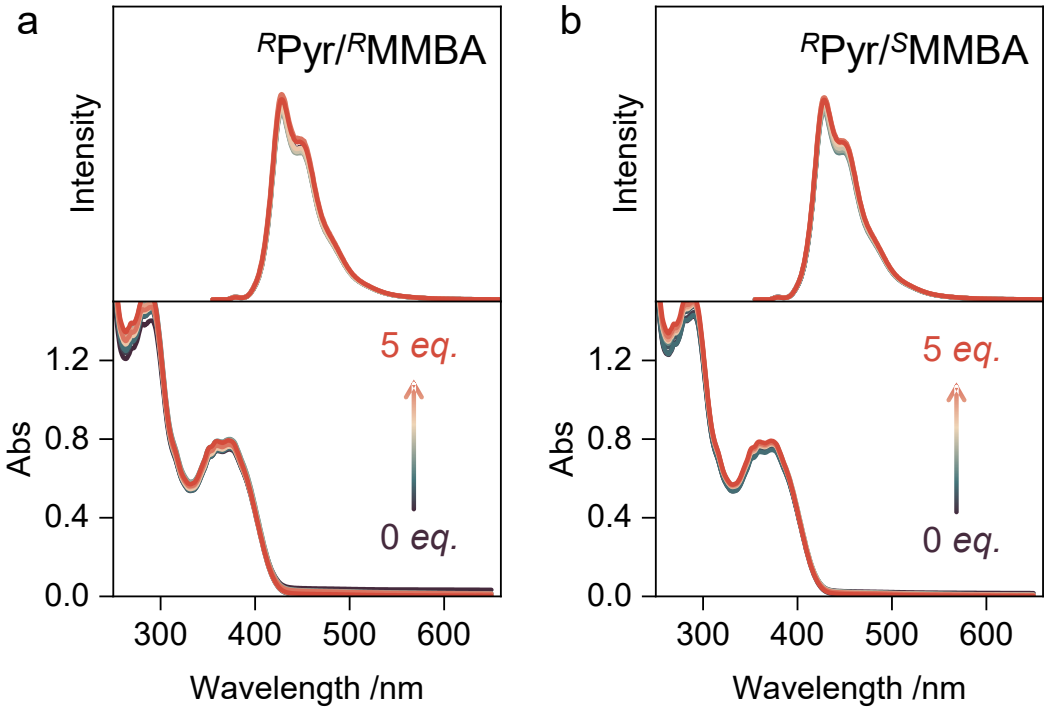


Figure S23. UV-visible absorption and fluorescence intensity titration spectra of ^{R}Pyr/^{R}MMBA (a) and ^{R}Pyr/^{S}MMBA (b). (0.05 mM, $CHCl_3$/ MCH, v/v = 1: 39)

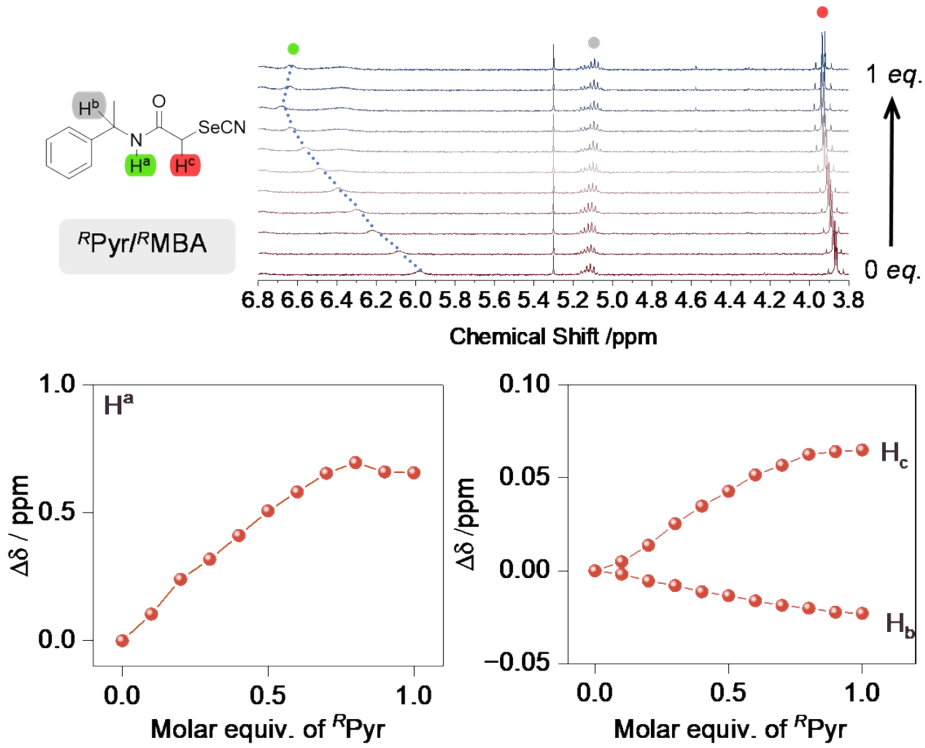


Figure S24. ^{1}H NMR titration spectra of ^{R}MBA (1 mM in $CDCl_3$) with increasing ^{R}Pyr from 0 to 1 equiv. and chemical shift curves of H_a, H_b and H_c.

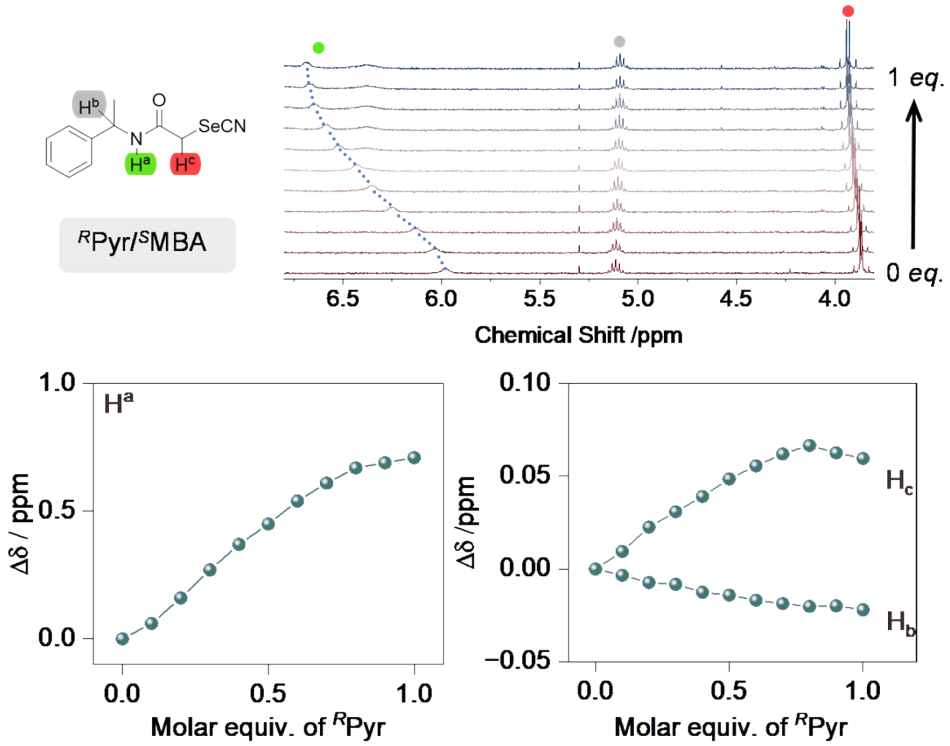


Figure S25. ^{1}H NMR titration spectra of ^{S}MBA (1 mM in $CDCl_3$) with increasing ^{R}Pyr from 0 to 1 equiv. and chemical shift curves of H_a, H_b and H_c.

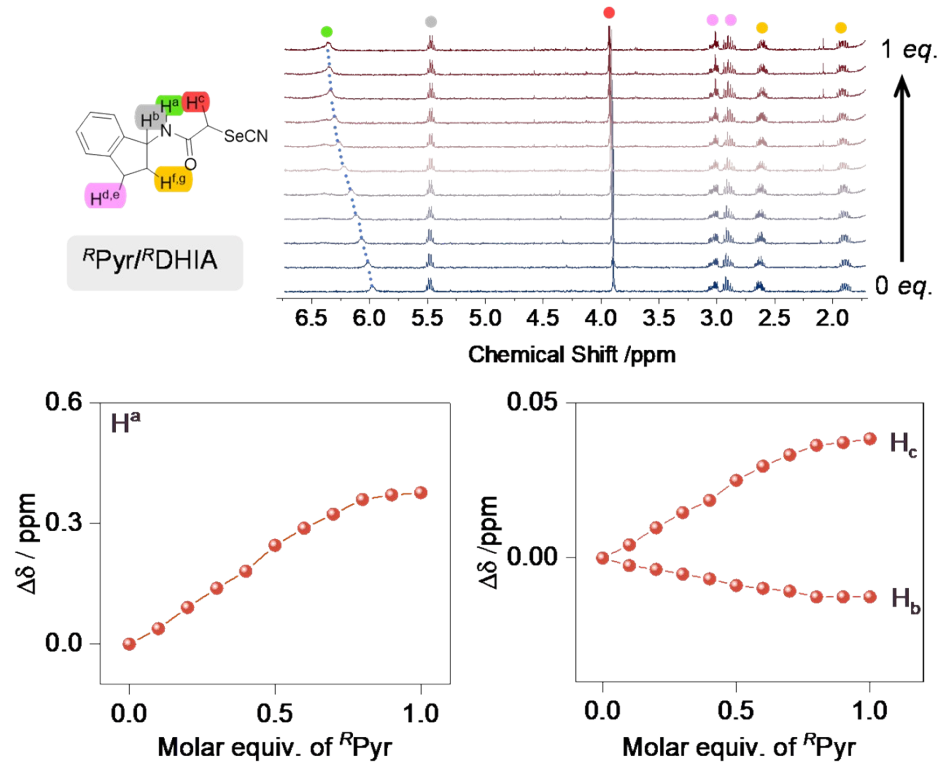


Figure S26. ^{1}H NMR titration spectra of ^{R}DHIA (1 mM in $CDCl_3$) with increasing ^{R}Pyr from 0 to 1 equiv. and chemical shift curves of H_a, H_b and H_c.

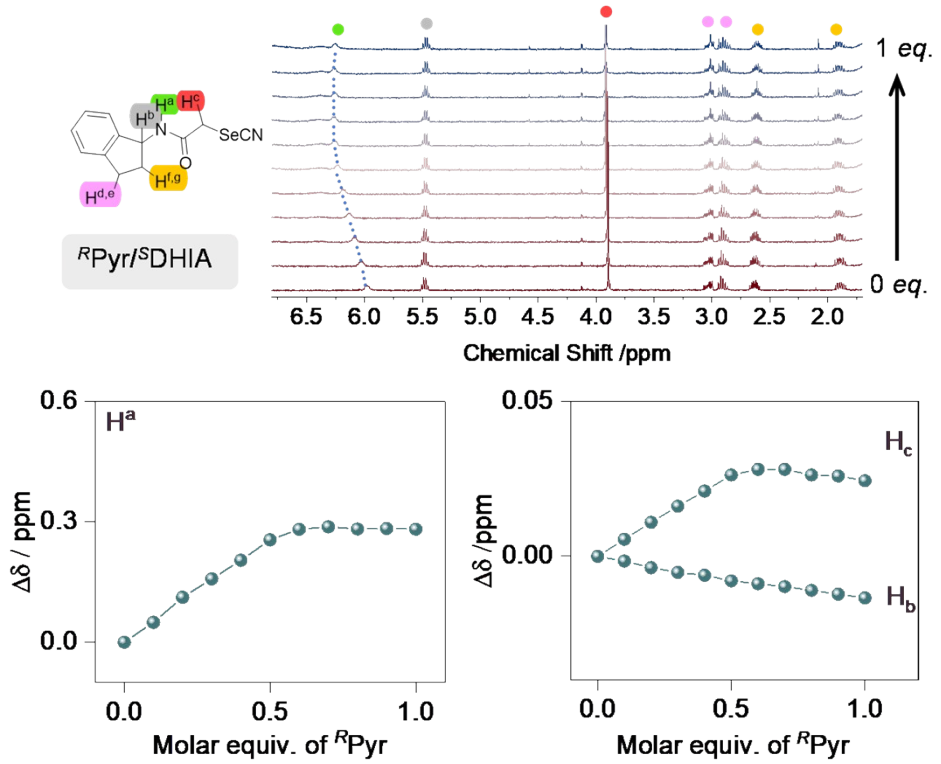


Figure S27. ^{1}H NMR titration spectra of ^{S}DHIA (1 mM in $CDCl_3$) with increasing ^{R}Pyr from 0 to 1 equiv. and chemical shift curves of H_a, H_b and H_c.

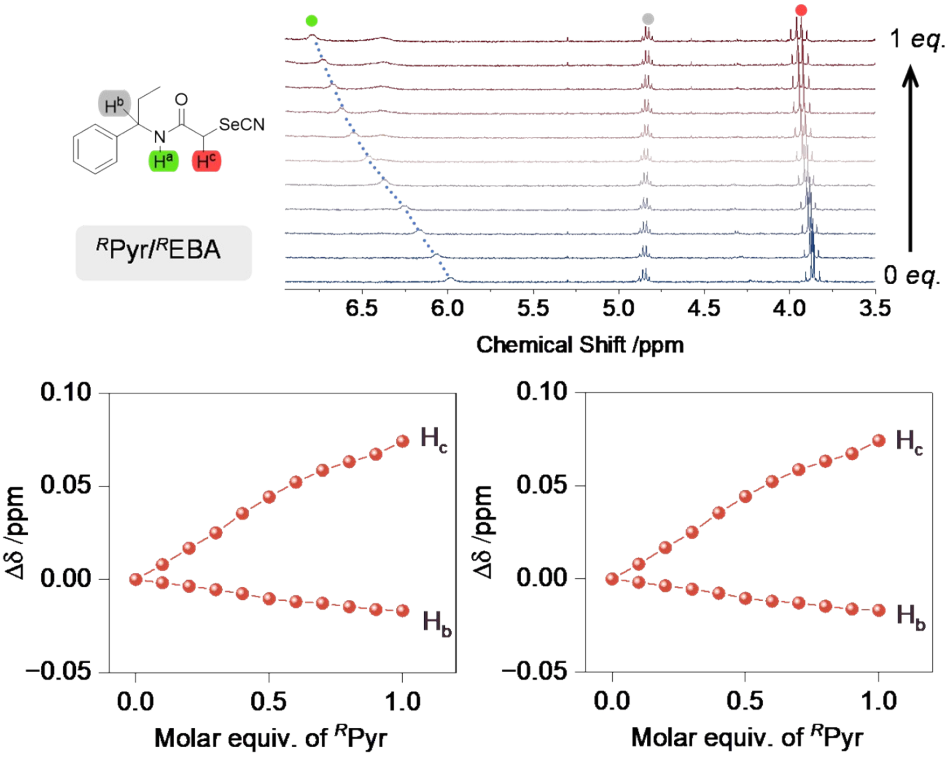


Figure S28. ^{1}H NMR titration spectra of ^{R}EBA (1 mM in $CDCl_3$) with increasing ^{R}Pyr from 0 to 1 equiv. and chemical shift curves of H_a, H_b and H_c.

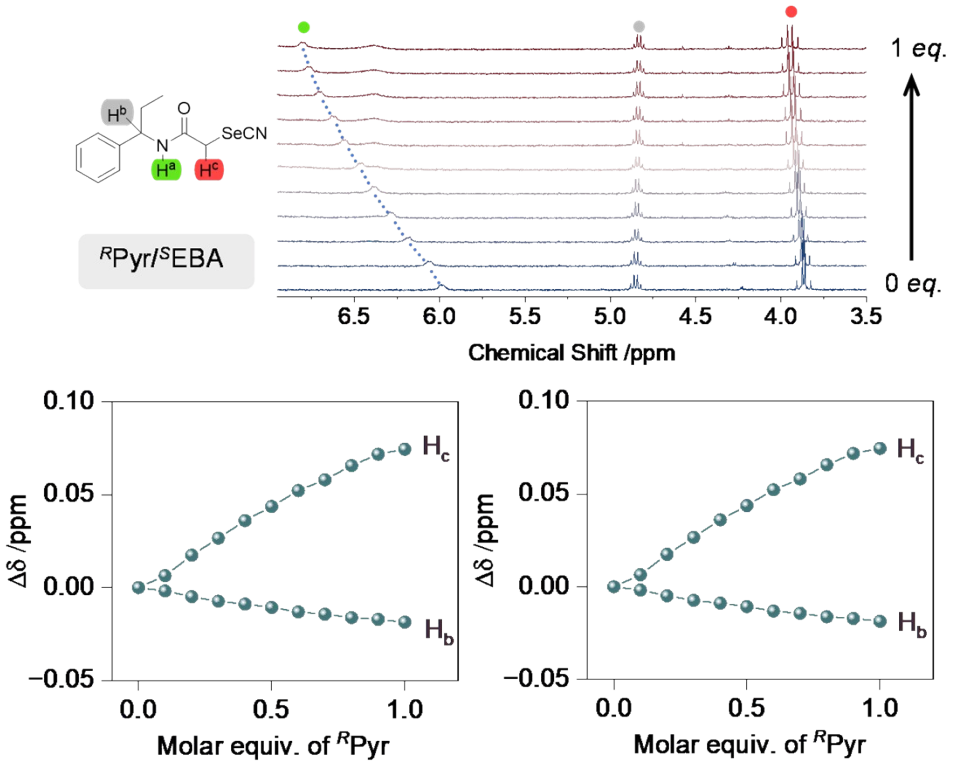


Figure S29. ^{1}H NMR titration spectra of ^{S}EBA (1 mM in $CDCl_3$) with increasing ^{R}Pyr from 0 to 1 equiv. and chemical shift curves of H_a, H_b and H_c.

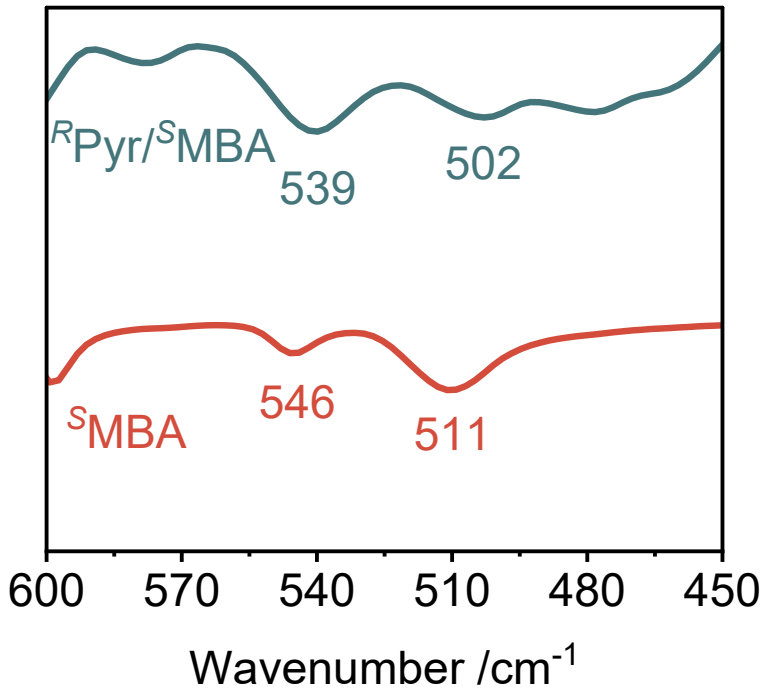


Figure S30. Infrared (IR) spectra of self-assembled ^{S}MBA and ^{R}Pyr/ ^{S}MBA.

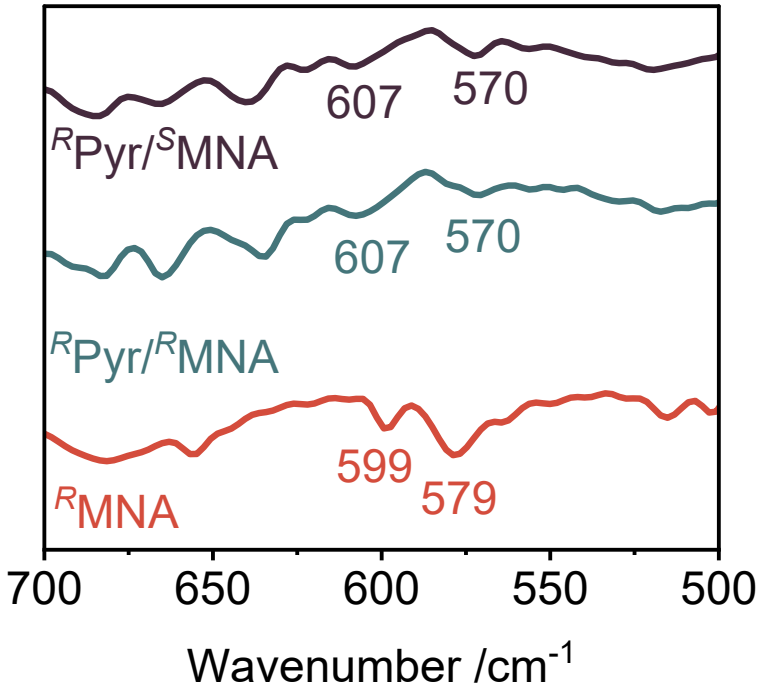


Figure S31. IR spectra of self-assembled ^{R}MNA, ^{R}Pyr/ ^{R}MNA and ^{R}Pyr/ ^{S}MNA.

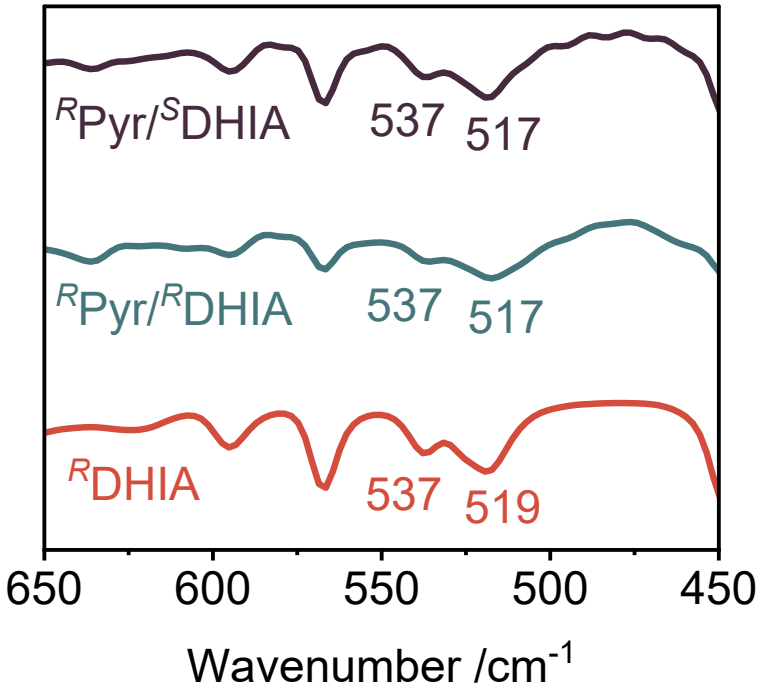


Figure S32. IR spectra of self-assembled ^{R}DHIA, ^{R}Pyr/ ^{R}DHIA and ^{R}Pyr/ ^{S}DHIA.

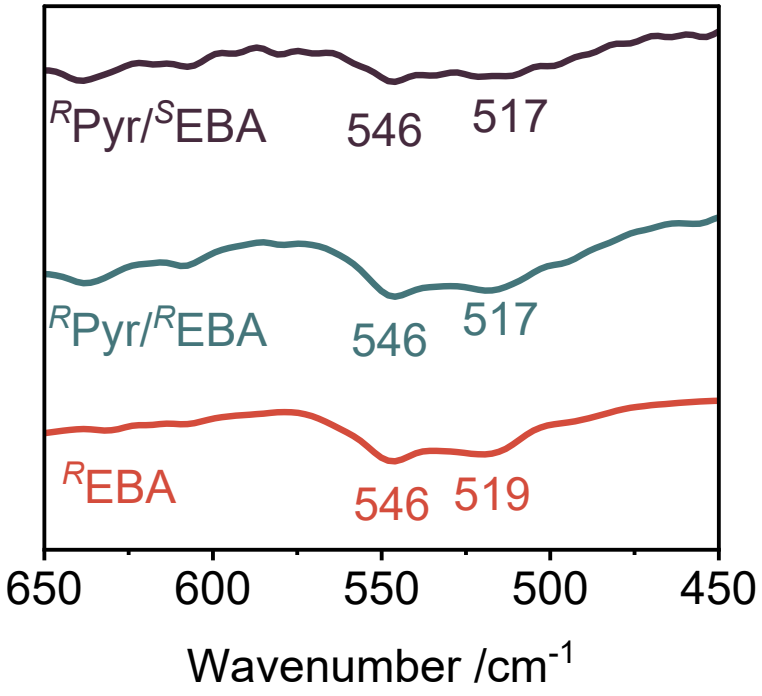


Figure S33. IR spectra of self-assembled ^{R}EBA, ^{R}Pyr/ ^{R}EBA and ^{R}Pyr/ ^{S}EBA.

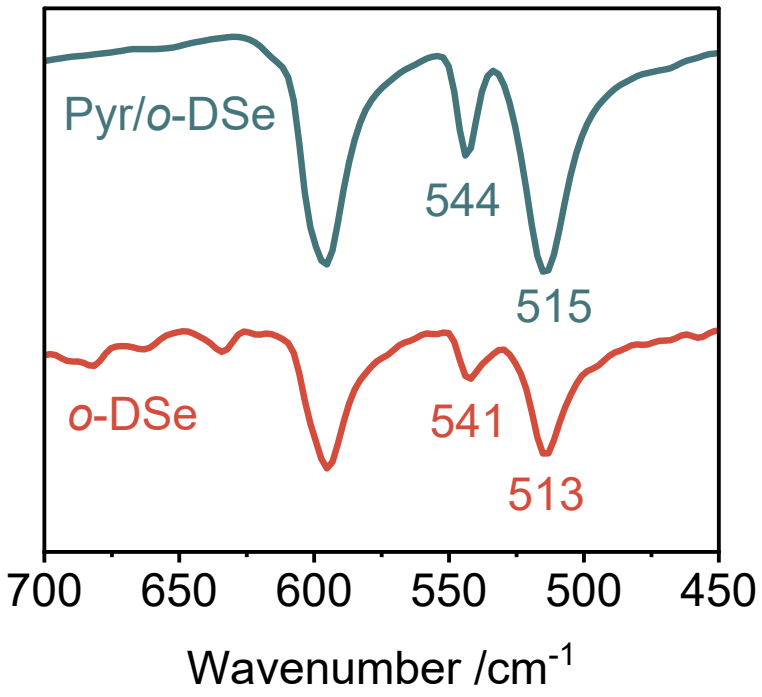


Figure S34. IR spectra of self-assembled *o*-DSe and Pyr/ *o*-DSe.

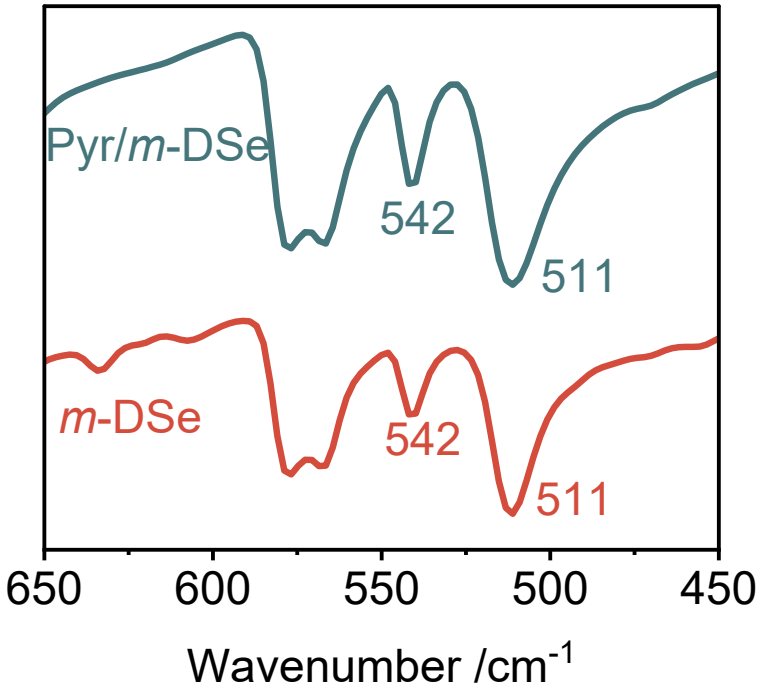


Figure S35. IR spectra of self-assembled *m*-DSe and Pyr/ *m*-DSe.

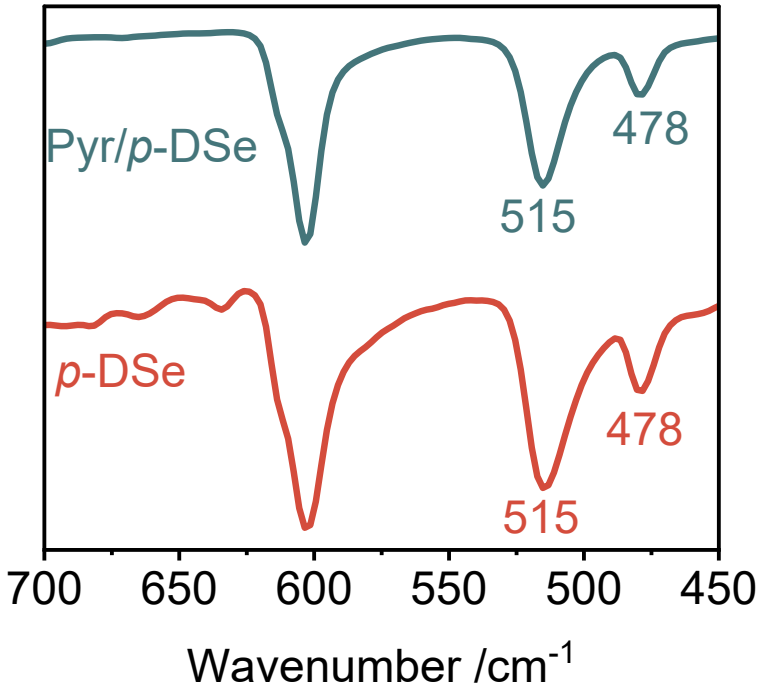


Figure S36. IR spectra of self-assembled *p*-DSe and Pyr/ *p*-DSe.

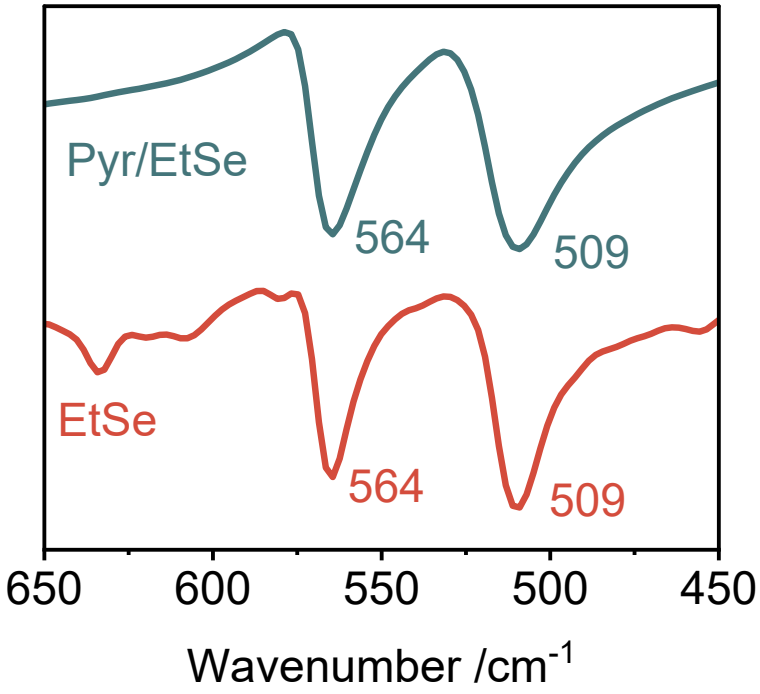


Figure S37. IR spectra of self-assembled EtSe and Pyr/ EtSe.

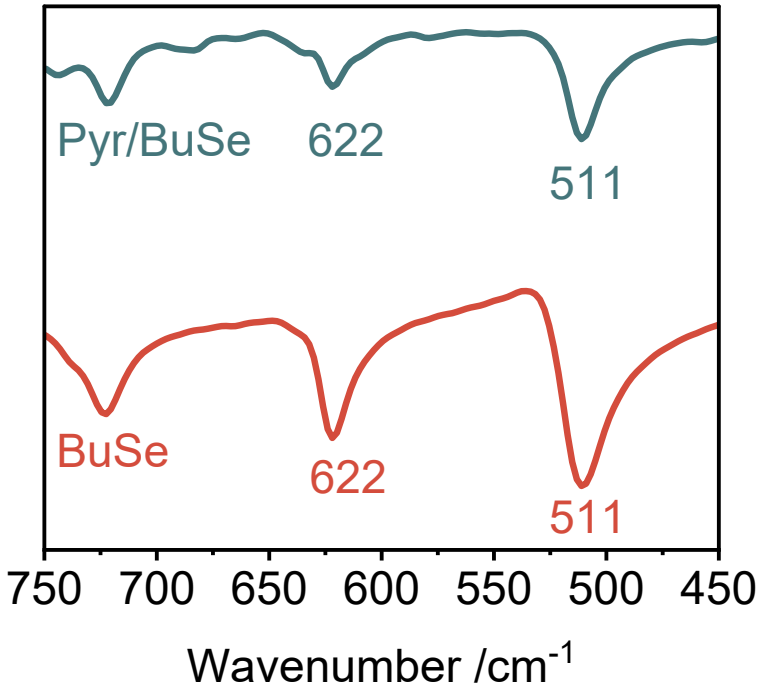


Figure S38. IR spectra of self-assembled BuSe and Pyr/ BuSe.

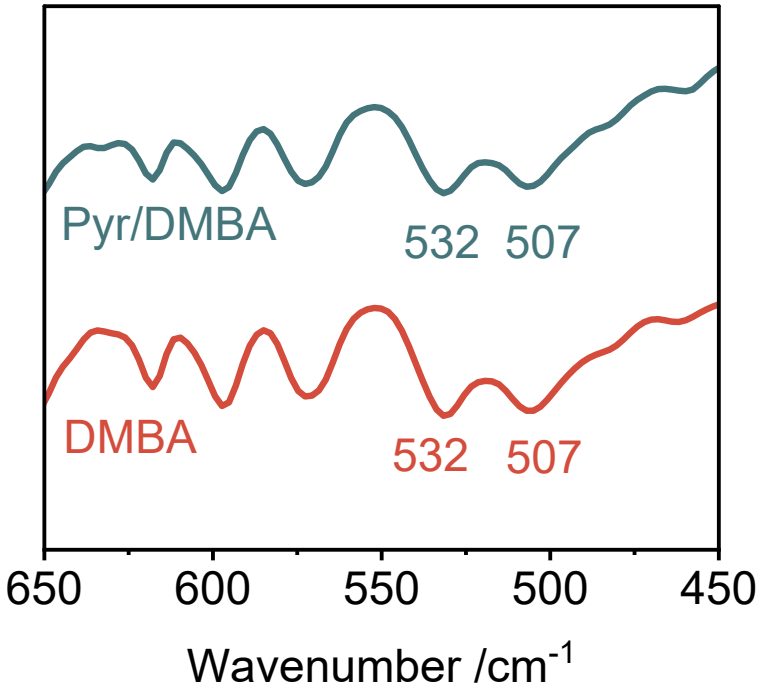


Figure S39. IR spectra of self-assembled DMBA and Pyr/ DMBA.

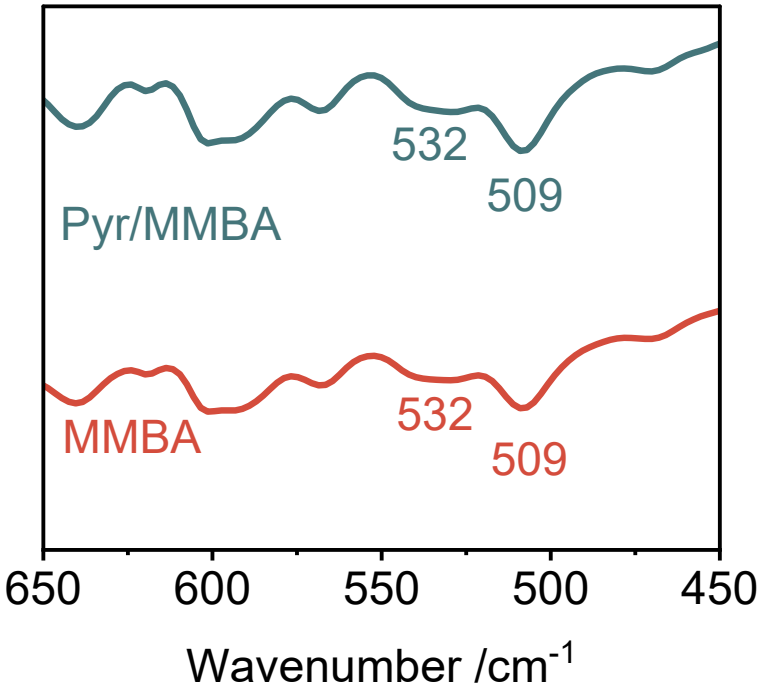


Figure S40. IR spectra of self-assembled MMBA and Pyr/ MMBA.

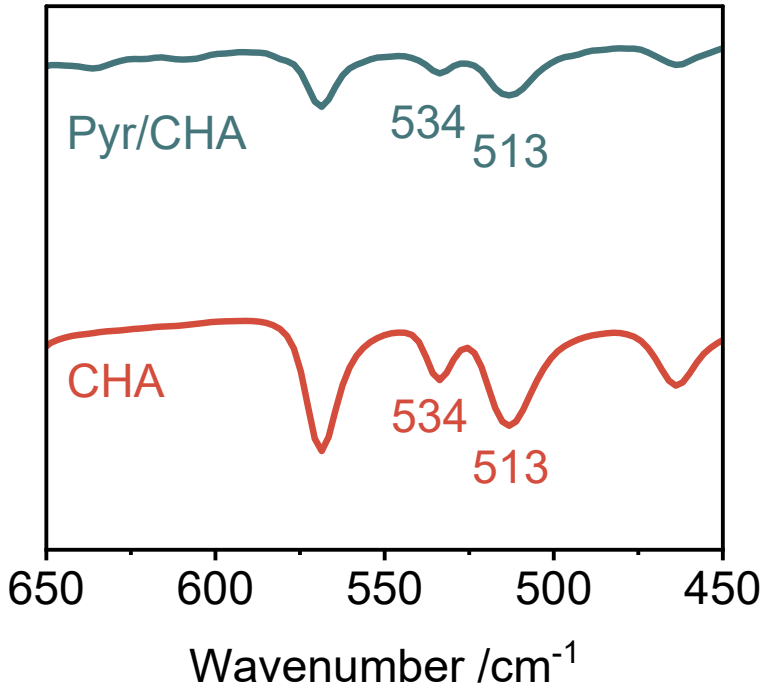


Figure S41. IR spectra of self-assembled CHA and Pyr/ CHA.

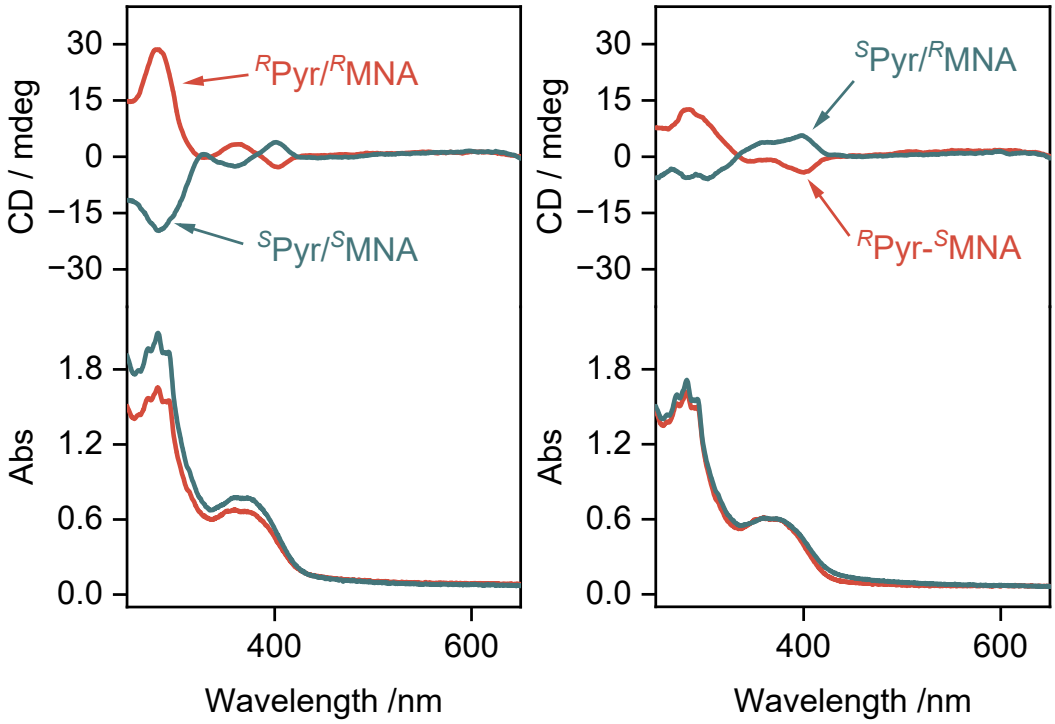


Figure S42. Circular dichroism spectra of the combination of Pyr/MNA.

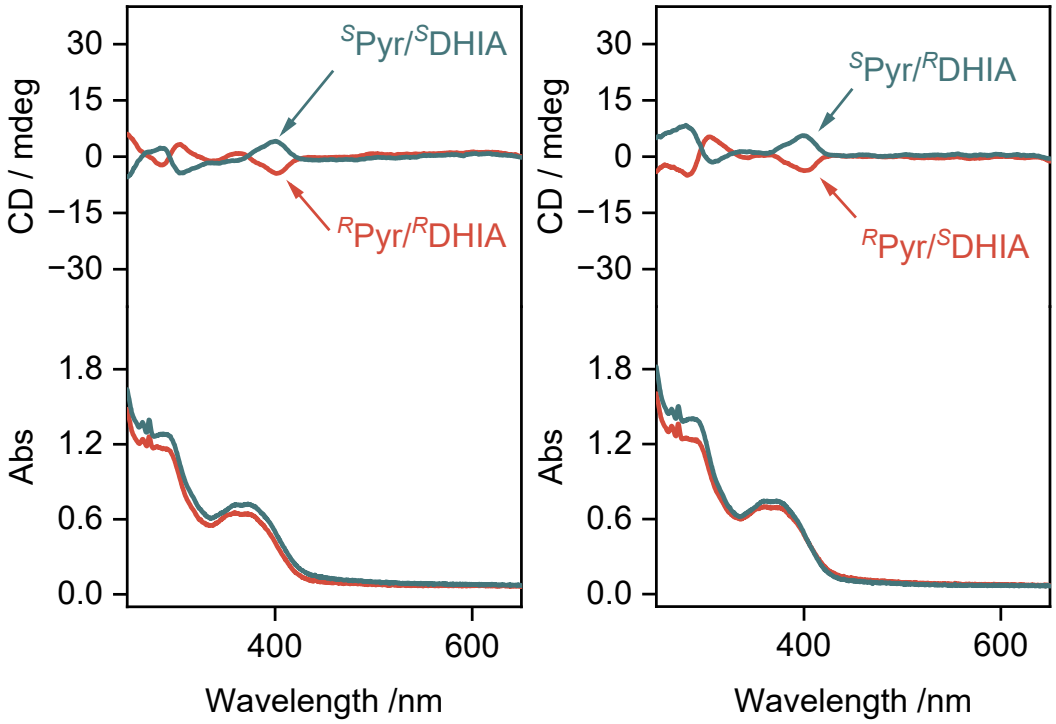


Figure S43. Circular dichroism spectra of the combination of Pyr/DHIA.

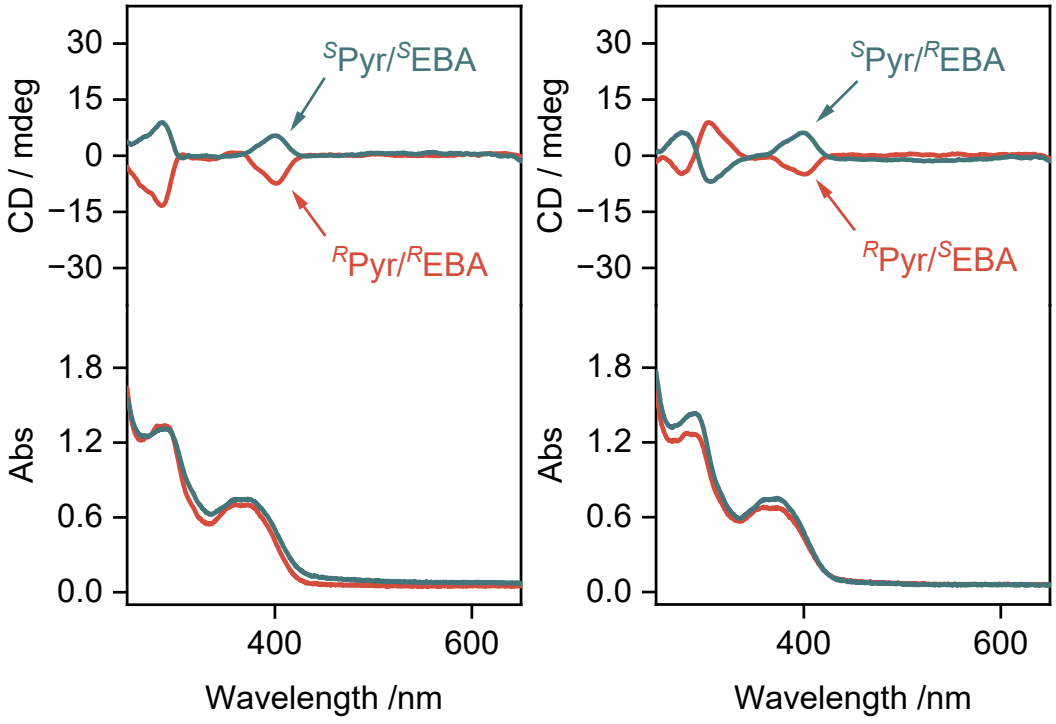


Figure S44. Circular dichroism spectra of the combination of Pyr/EBA.

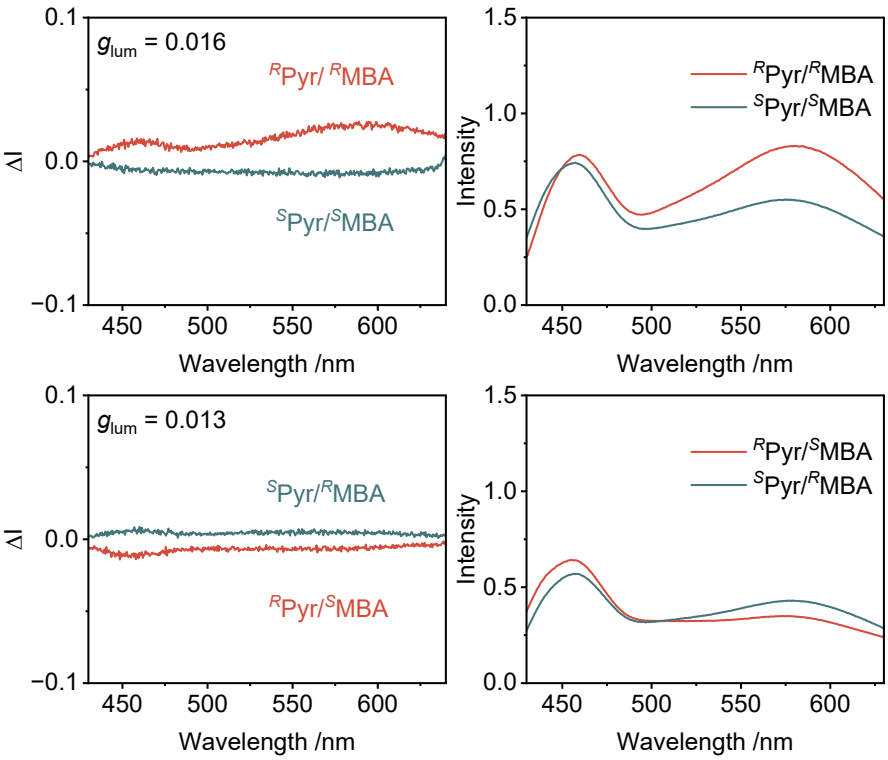


Figure S45. Circularly polarized luminescence of the combination of Pyr/MBA.

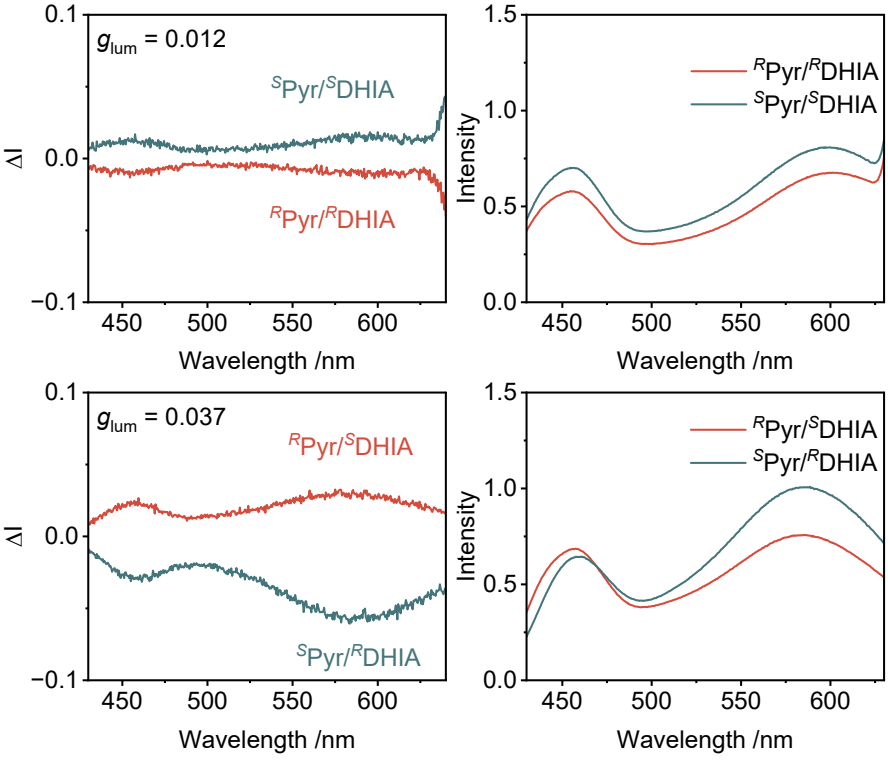


Figure S46. Circularly polarized luminescence of the combination of Pyr/DHIA.

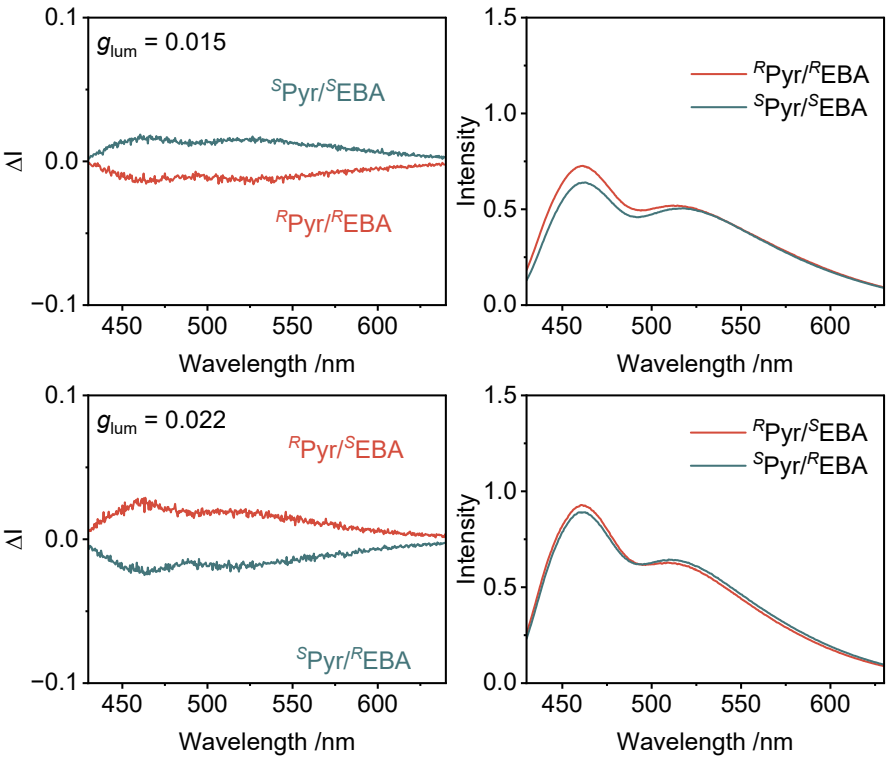


Figure S47. Circularly polarized luminescence of the combination of Pyr/EBA.

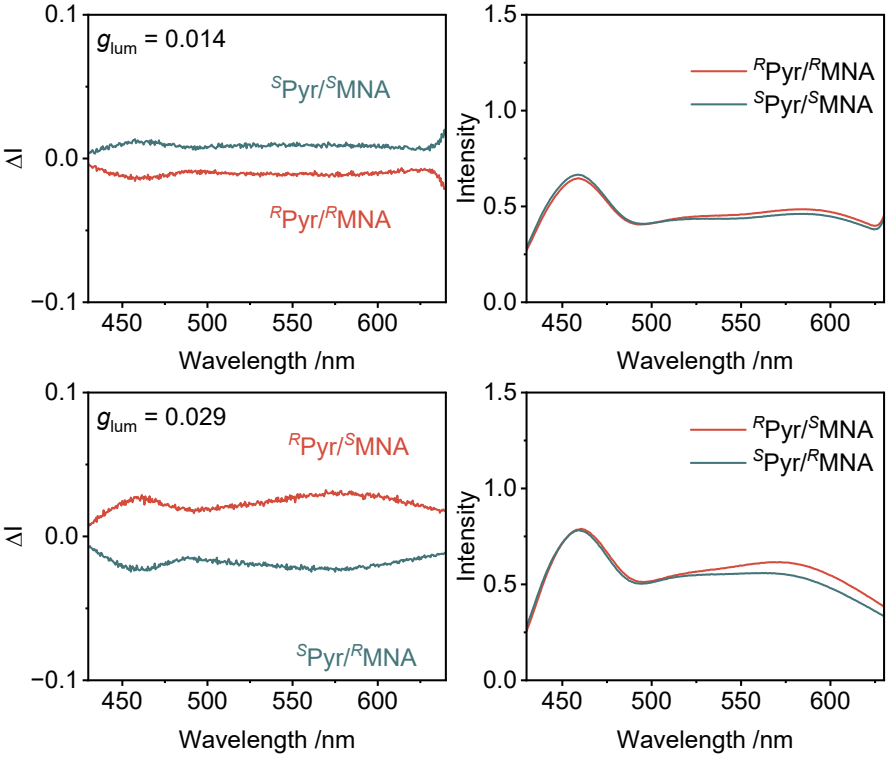


Figure S48. Circularly polarized luminescence of the combination of Pyr/MNA.

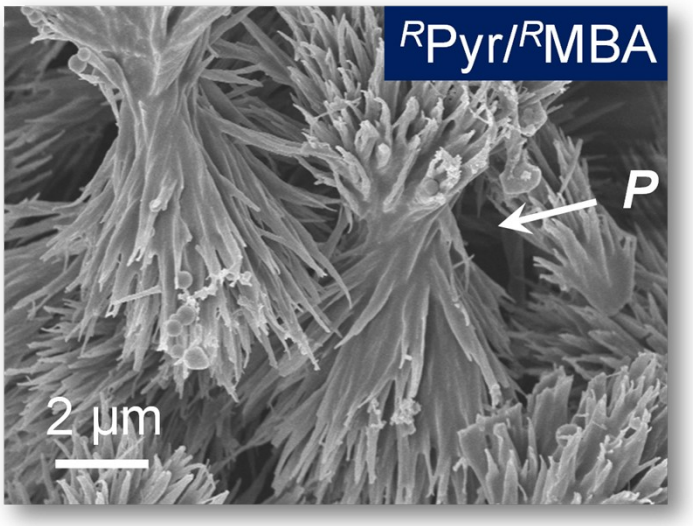


Figure S49. Morphologies of ^{R}Pyr/^{R}MBA captured by scanning electron microscopy (SEM).

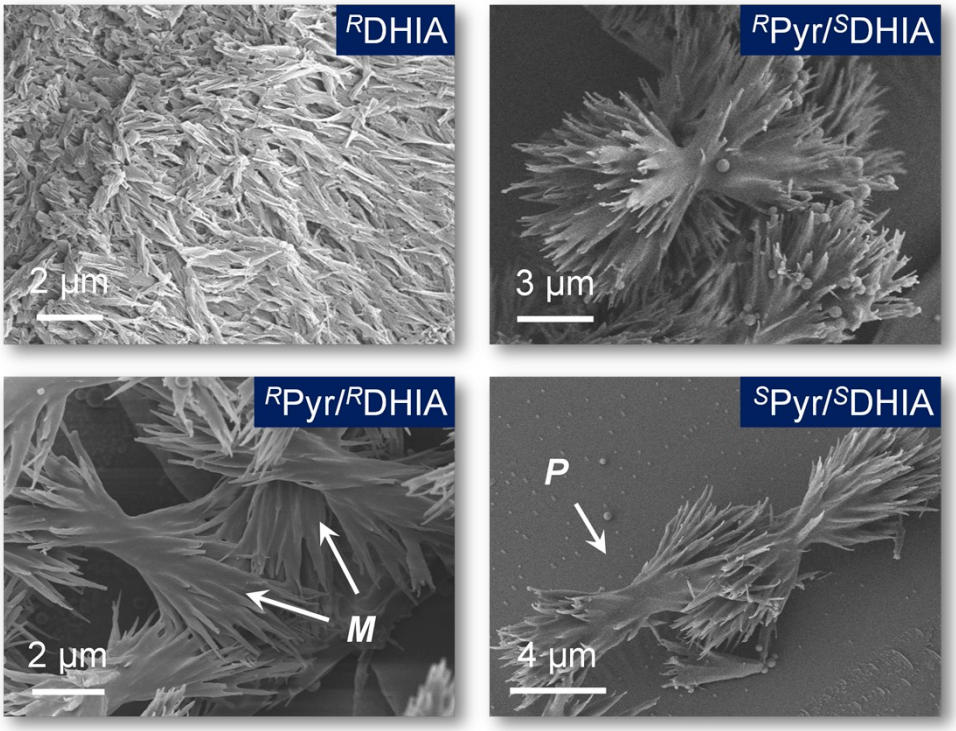


Figure S50. Morphologies of combination of Pyr/DHIA captured by SEM.

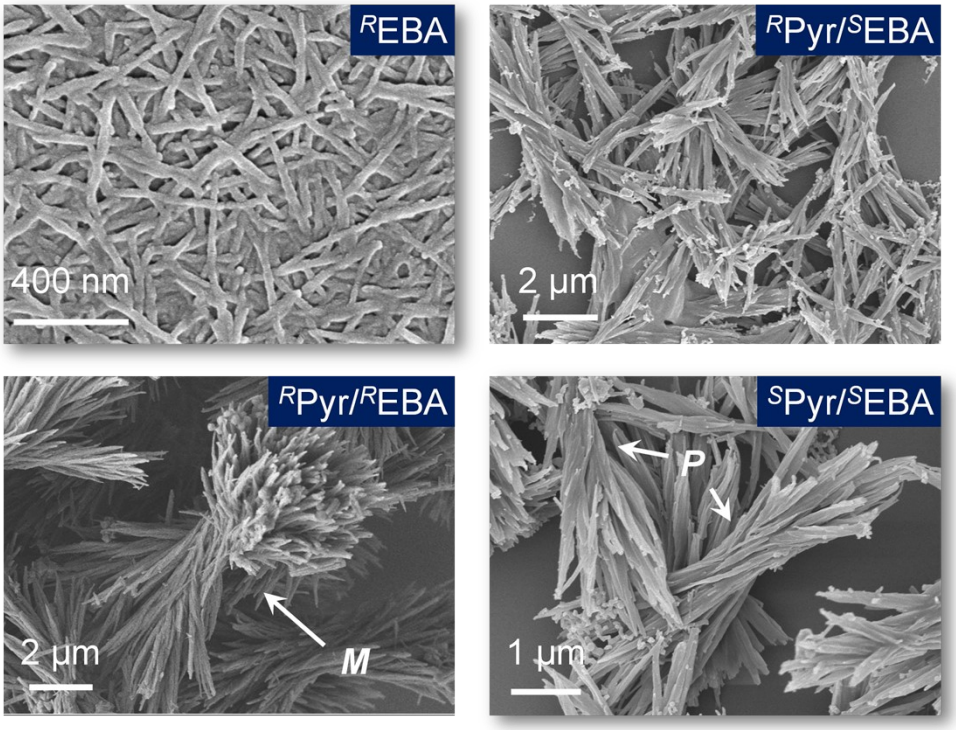


Figure S51. Morphologies of combination of Pyr/EBA captured by SEM.

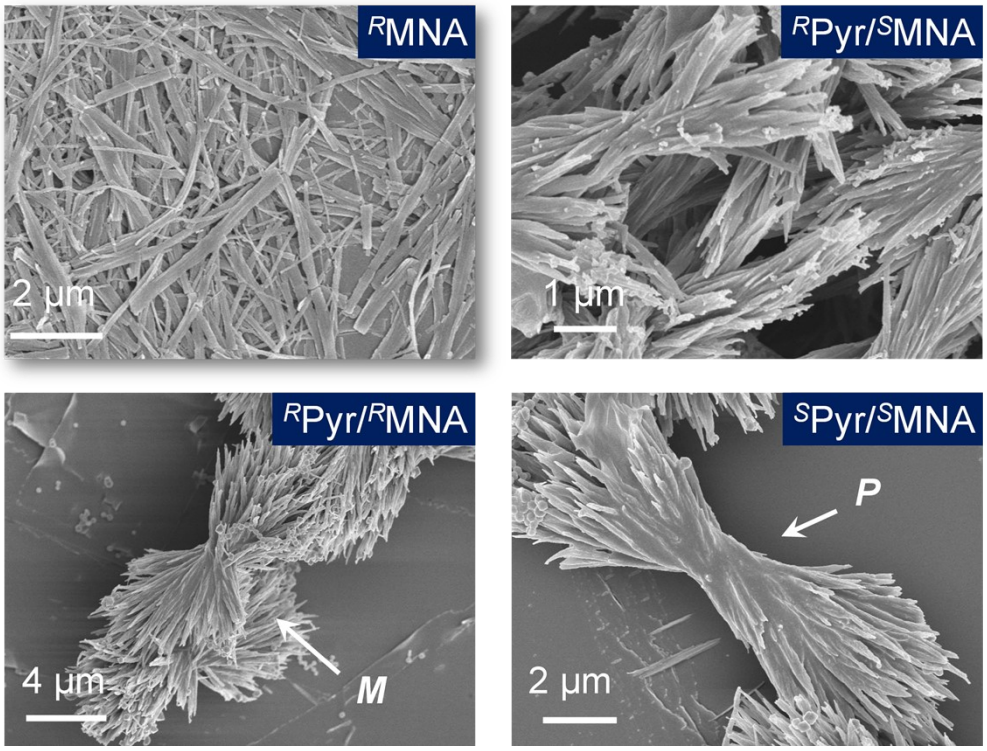


Figure S52. Morphologies of combination of Pyr/MNA captured by SEM.

C.Synthesis and Characterization

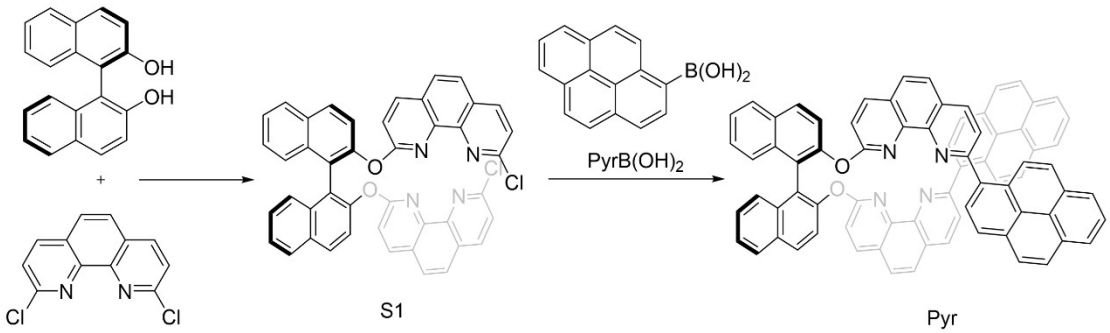


Figure S53. Synthetic route of Pyr.

Synthesis of S1. A solution of Binol (1.15 g, 4.0 mmol), 2,9-dichloro-1,10-phenanthroline (2.24 g, 9.0 mmol) in dry DMF (100 mL) was purged with N_2. After addition of potassium carbonate (0.69 g, 5.0 mmol), the mixture was stirred 24 h at 160 °C under N_2. After the solution is cooled, add 100 mL of ethyl acetate and then wash three times with deionized water, using 100 mL each time. The organic phase was collected and dried over anhydrous Na_2SO_4. The solution was then filtered. After removing the solvent under vacuum, the product was purified by column chromatography to obtain pure S1 as a white powder. Yield: 1.44 g (51%).

Synthesis of Pyr. A solution of S1 (0.71 g, 1.0 mmol), $PyrB(OH)_2$ (0.74 g, 3 mmol) in toluene (50 mL) was purged with N_2 and stirred 15 min at 80 °C with N_2 bubbling. After addition of degassed aqueous potassium carbonate 2 M solution (0.5 mL, 1 mmol), of $Pd(PPh_3)_4$ (40 mg, 0.03 mmol), the mixture was stirred 24 h at 100 °C under N_2. After washing the solution three times with 100 mL of water, the organic phase was collected and dried over anhydrous Na_2SO_4. The solution was then filtered. After removing the solvent under vacuum, the product was purified by column chromatography to obtain pure Pyr as a yellow powder. Yield: 0.55 g (53%).

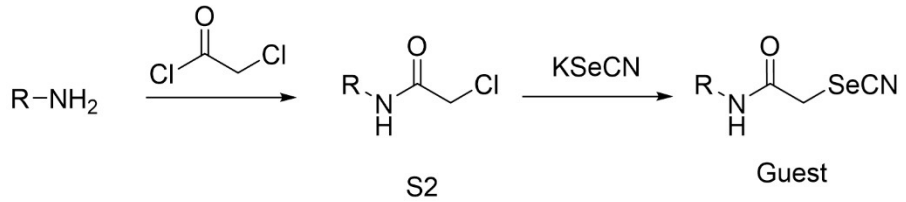


Figure S54. Synthetic route of Guest.

Synthesis of S2. Take MBA as an example. Methylbenzylamine (1.21 g, 10 mmol) was dissolved in 50 mL of anhydrous dichloromethane, and add 2 mL of

triethylamine. Then chloroacetyl chloride (1.36 g, 12 mmol) was added to the amine solution at 0 °C. After the addition is complete, stir at room temperature for 0.5 h. Then, the product was washed three times with 50 mL of deionized water, and the organic phase was dried with anhydrous sodium sulfate, and the liquid phase solvent was removed under reduced pressure. Then, the product was separated by column chromatography to obtain the pure S2 as a white powder. Yield: 1.97 g (100%). The synthesis methods of other guests are similar, except that methylbenzylamine is replaced by the corresponding amine.

Synthesis of guest molecules. Take MBA as an example. S2 (1.97 g, 10 mmol) and potassium selenocyanate (2.16 g, 15 mmol) were dissolved in MeCN and stirred overnight at 80°C under N_2. The solvent was then removed under reduced pressure and the pure guest molecule was separated by column chromatography as a white powder. Yield: 2.40 g (90%). The synthesis methods of other guests are similar, but MBA-S needs to replace KSeCN with KSCN.

Characterization of Pyr. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.93 (d, J = 9.4 Hz, 2H), 8.52 (d, J = 8.4 Hz, 2H), 8.32 – 8.18 (m, 10H), 8.11 (d, J = 8.3 Hz, 2H), 8.03 (t, J = 7.6 Hz, 2H), 7.96 (d, J = 7.6 Hz, 2H), 7.84 (d, J = 9.0 Hz, 2H), 7.72 (d, J = 8.8 Hz, 2H), 7.62 (d, J = 9.0 Hz, 3H), 7.55 (d, J = 8.1 Hz, 3H), 7.42 (dd, J = 12.0, 9.0 Hz, 4H), 7.25 (dd, J = 17.3, 8.6 Hz, 4H), 7.16 (d, J = 8.6 Hz, 2H), 7.08 (t, J = 7.6 Hz, 2H), 6.74 (t, J = 7.7 Hz, 2H). ^{13}C NMR (101 MHz, DMSO) δ 162.17, 158.23, 151.15, 144.36, 144.04, 139.91, 137.24, 135.20, 133.53, 132.53, 132.01, 131.91, 131.47, 131.25, 130.92, 130.59, 129.84, 129.30, 129.18, 128.96, 128.88, 128.52, 128.20, 128.07, 127.68, 127.36, 126.61, 126.37, 126.15, 125.96, 125.84, 125.73, 125.67, 125.59, 125.21, 125.12, 124.67, 124.51, 124.24, 123.10, 122.54, 114.32. HRMS m/z $[M+H]^+$, calculated for $C_{76}H_{43}N_4O_2^+$, 1043.3381; found 1043.3269.

Characterization of MBA. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.42 – 7.27 (m, 5H), 6.20 – 6.11 (m, 1H), 5.09 (p, J = 7.0 Hz, 1H), 3.91 – 3.79 (m, 2H), 1.54 (d, J = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.35, 142.12, 129.40, 128.88, 127.83, 126.20, 102.09, 77.38, 77.06, 76.74, 53.47, 50.18, 42.63, 31.87, 31.63, 31.39, 29.71, 21.60, 0.02. ^{77}Se NMR (76 MHz, DMSO-d_6) δ 203.58 (t, J = 12.3 Hz). HRMS m/z $[M+H]^+$, calculated for $C_{11}H_{13}N_2OSe^+$, 269.0188; found 269.0188.

Characterization of DHIA. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.67 (d, J = 8.1 Hz, 1H), 7.31 – 7.14 (m, 4H), 5.26 (q, J = 7.8 Hz, 1H), 3.91 – 3.76 (m, 2H), 2.99 – 2.72 (m, 2H), 2.41 (dtd, J = 12.7, 7.8, 3.7 Hz, 1H), 1.79 (dq, J = 12.6, 8.4 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 167.23, 143.69, 143.50, 128.11, 126.87, 125.03, 124.56, 104.66, 54.78, 33.51, 31.38, 30.20. ^{77}Se NMR (76 MHz, DMSO-d_6) δ 209.78 (t, J = 12.8 Hz). HRMS m/z $[M+H]^+$, calculated for $C_{12}H_{13}N_2OSe^+$, 281.0188; found 281.0192.

Characterization of MNA. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.90 (d, J = 7.8 Hz, 1H), 8.10 (d, J = 8.2 Hz, 1H), 7.95 (dd, J = 7.7, 1.8 Hz, 1H), 7.85 (d, J = 8.1 Hz, 1H), 7.64 – 7.46 (m, 4H), 5.69 (p, J = 7.0 Hz, 1H), 3.92 – 3.76 (m, 2H), 1.51 (d, J = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 166.50, 139.93, 133.83, 130.72, 129.16, 127.94, 126.80, 126.16, 125.93, 123.53, 122.89, 45.36, 31.35, 22.05. ^{77}Se NMR (76 MHz, DMSO-d_6) δ 206.14 (t, J = 12.6 Hz). HRMS m/z $[M+H]^+$, calculated for $C_{15}H_{15}N_2OSe^+$, 319.0345; found 319.0343.

Characterization of EBA. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.39 – 7.26 (m, 5H), 6.20 (d, J = 8.1 Hz, 1H), 4.83 (q, J = 7.6 Hz, 1H), 3.93 – 3.78 (m, 2H), 1.94 – 1.80 (m, 2H), 0.91 (t, J = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-d) δ 165.34, 140.90, 128.88, 127.86, 126.66, 101.91, 56.35, 31.68, 28.93, 10.73. ^{77}Se NMR (76 MHz, Chloroform-d) δ 191.45. HRMS m/z $[M+H]^+$, calculated for $C_{12}H_{15}N_2OSe^+$, 283.0345; found 283.0345.

Characterization of MBA-S. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.40 – 7.28 (m, 5H), 6.55 (d, J = 7.6 Hz, 1H), 5.08 (p, J = 7.1 Hz, 1H), 3.70 – 3.54 (m, 2H), 1.53 (d, J = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-d) δ 163.95, 142.04, 128.89, 127.85, 126.23, 111.51, 50.06, 36.91, 21.56. HRMS m/z $[M+H]^+$, calculated for $C_{11}H_{13}N_2OS^+$, 221.0744; found 221.0743.

Characterization of CHA. ^{1}H NMR (400 MHz, Chloroform-d) δ 5.78 (d, J = 8.7 Hz, 1H), 3.88 (s, 2H), 1.76 (tdt, J = 10.3, 5.5, 2.5 Hz, 3H), 1.70 – 1.61 (m, 2H), 1.42 – 0.89 (m, 10H). ^{13}C NMR (101 MHz, Chloroform-d) δ 165.30, 101.98, 50.93, 42.92, 31.95, 28.99, 28.95, 26.28, 26.09, 26.06, 17.76. ^{77}Se NMR (76 MHz, Chloroform-d) δ 190.57. HRMS m/z $[M+H]^+$, calculated for $C_{11}H_{19}N_2OSe^+$, 275.0658; found 275.0661.

Characterization of MMBA. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.45 – 7.24 (m, 5H), 5.69 (q, J = 7.1 Hz, 1H), 4.78 (s, 1H), 4.70 – 4.54 (m, 1H), 2.73 (s, 2H), 2.52 (s, 1H), 1.56 (d, J = 6.8 Hz, 1H), 1.45 (d, J = 7.1 Hz, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 167.61, 167.14, 140.51, 140.05, 129.01, 128.93, 128.06, 127.77, 127.54, 127.40, 104.97, 104.76, 55.81, 51.60, 34.17, 30.26, 28.18, 17.26, 16.33. ^{77}Se NMR (76 MHz, DMSO-d_6) δ 150.17, 145.39. ^{77}Se NMR (76 MHz, Chloroform-d) δ 151.26. HRMS m/z $[M+H]^+$, calculated for $C_{12}H_{15}N_2OSe^+$, 283.0345; found 283.0352.

Characterization of DMBA. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.53 – 7.38 (m, 2H), 7.37 – 7.24 (m, 3H), 7.02 (dd, J = 5.1, 2.0 Hz, 3H), 6.74 (dd, J = 6.6, 2.9 Hz, 2H), 5.22 (q, J = 6.9 Hz, 1H), 5.01 (d, J = 13.9 Hz, 1H), 4.73 – 4.54 (m, 2H), 1.72 (d, J = 6.9 Hz, 3H), 1.65 (d, J = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-d) δ 166.51, 139.58, 139.05, 128.94, 128.40, 128.27, 128.11, 127.91, 126.83, 103.65, 53.93, 53.69, 53.46, 35.88, 19.00, 17.65. ^{77}Se NMR (76 MHz, Chloroform-d) δ 151.23. HRMS m/z $[M+H]^+$, calculated for $C_{19}H_{21}N_2OSe^+$, 373.0814; found 373.0818.

Characterization of EtSe. ^{1}H NMR (400 MHz, Chloroform-d) δ 3.52 (s, 6H), 3.56 – 3.47 (m, 1H). ^{13}C NMR (101 MHz, Chloroform-d) δ 99.80, 28.09. ^{77}Se NMR (76 MHz, Chloroform-d) δ 262.36 (t, J = 12.2 Hz). HRMS m/z $[M+H]^+$, calculated for $C_4H_5N_2Se_2^+$, 240.8778; found 240.8781.

Characterization of BuSe. ^{1}H NMR (400 MHz, Chloroform-d) δ 3.16 – 3.02 (m, 1H), 2.19 – 2.02 (m, 1H). ^{13}C NMR (101 MHz, Chloroform-d) δ 101.03, 30.28, 28.39, 28.13, 27.87. ^{77}Se NMR (76 MHz, Chloroform-d) δ 216.40 (t, J = 18.8 Hz). HRMS m/z $[M+H]^+$, calculated for $C_6H_9N_2Se_2^+$, 268.9091; found 268.9095.

Characterization of *o*-DSe. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.47 – 7.33 (m, 4H), 4.43 (s, 4H). ^{13}C NMR (101 MHz, Chloroform-d) δ 133.69, 131.60, 129.95, 101.21, 29.71, 29.48, 29.24. ^{77}Se NMR (76 MHz, DMSO-d_6) δ 313.81 (t, J = 18.3 Hz). HRMS m/z $[M+H]^+$, calculated for $C_{10}H_9N_2Se_2^+$, 316.9091; found 316.9098.

Characterization of *m*-DSe. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.47 – 7.31 (m, 4H), 4.28 (s, 4H). ^{13}C NMR (101 MHz, Chloroform-d) δ 136.69, 130.02, 129.44, 129.29, 101.51, 53.45, 32.37, 32.12, 31.89. ^{77}Se NMR (76 MHz, DMSO-d_6) δ 318.73

(t, J = 18.1 Hz). HRMS m/z $[M+H]^+$, calculated for $C_{10}H_9N_2Se_2^+$, 316.9091; found 316.9091.

Characterization of *p*-DSe. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.38 (s, 1H), 4.28 (s, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 136.16, 129.78, 101.50, 32.09. ^{77}Se NMR (76 MHz, DMSO-d_6) δ 320.76 (t, J = 18.3 Hz). HRMS m/z $[M+H]^+$, calculated for $C_{10}H_9N_2Se_2^+$, 316.9091; found 316.9093.

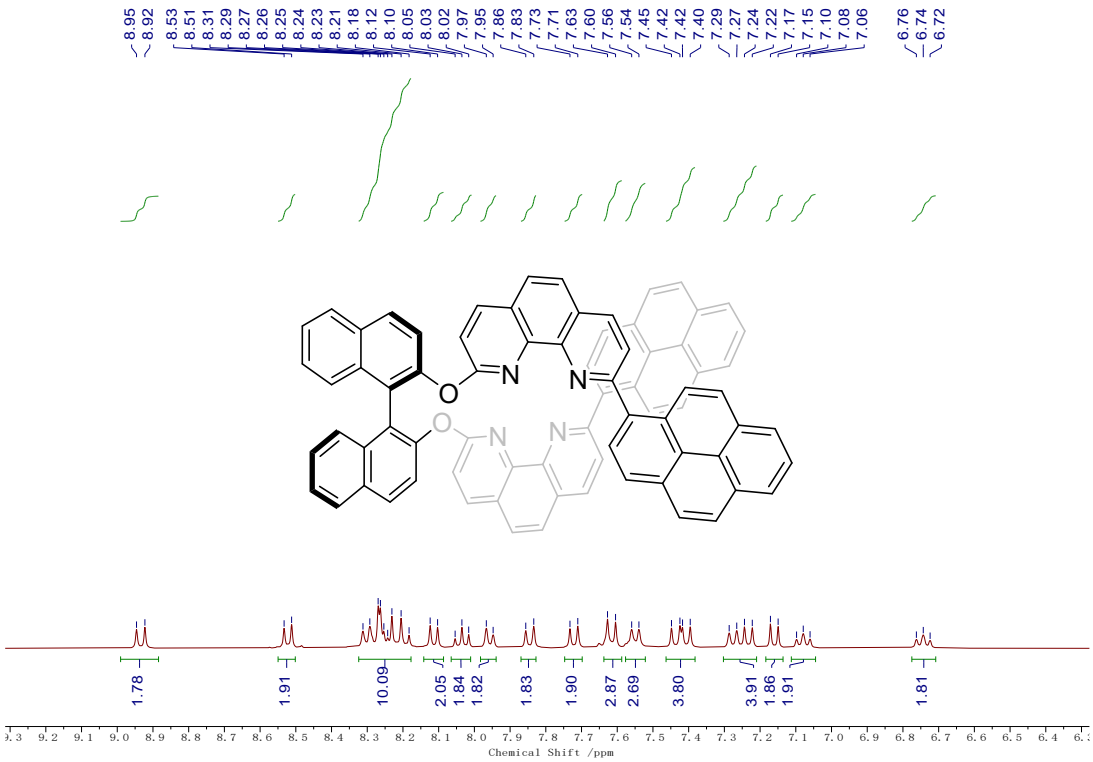


Figure S55. ^{1}H NMR spectra of Pyr.

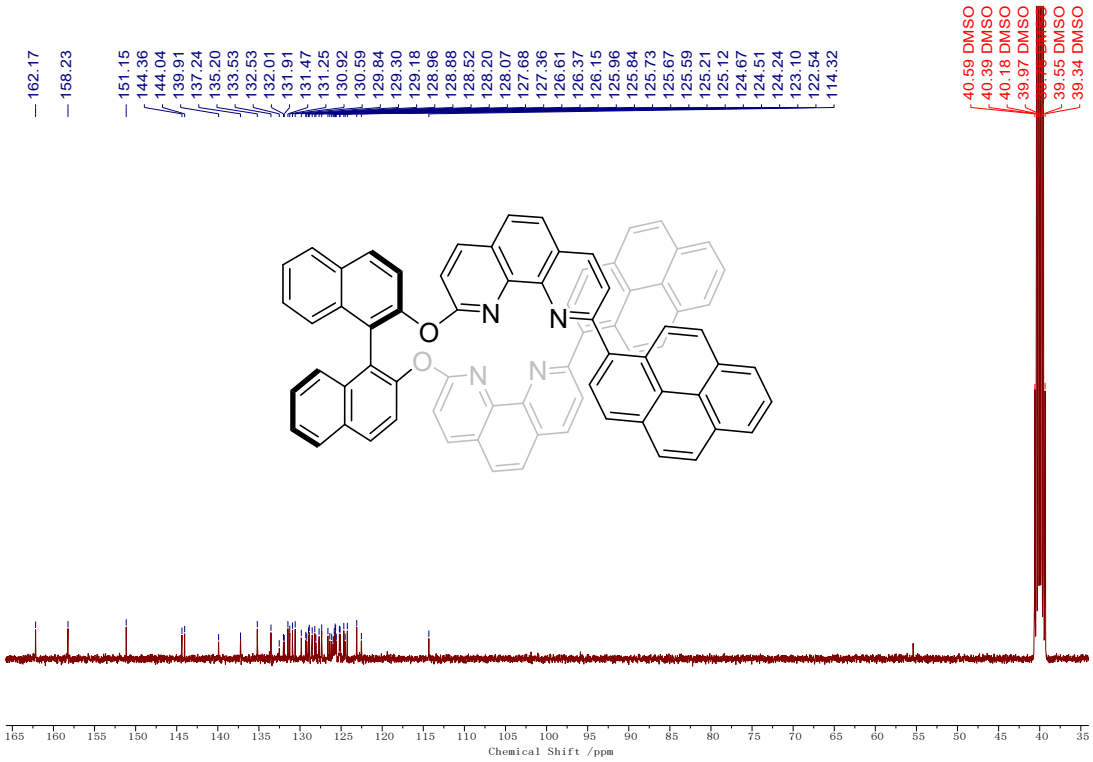


Figure S56. ^{13}C NMR spectra of Pyr.

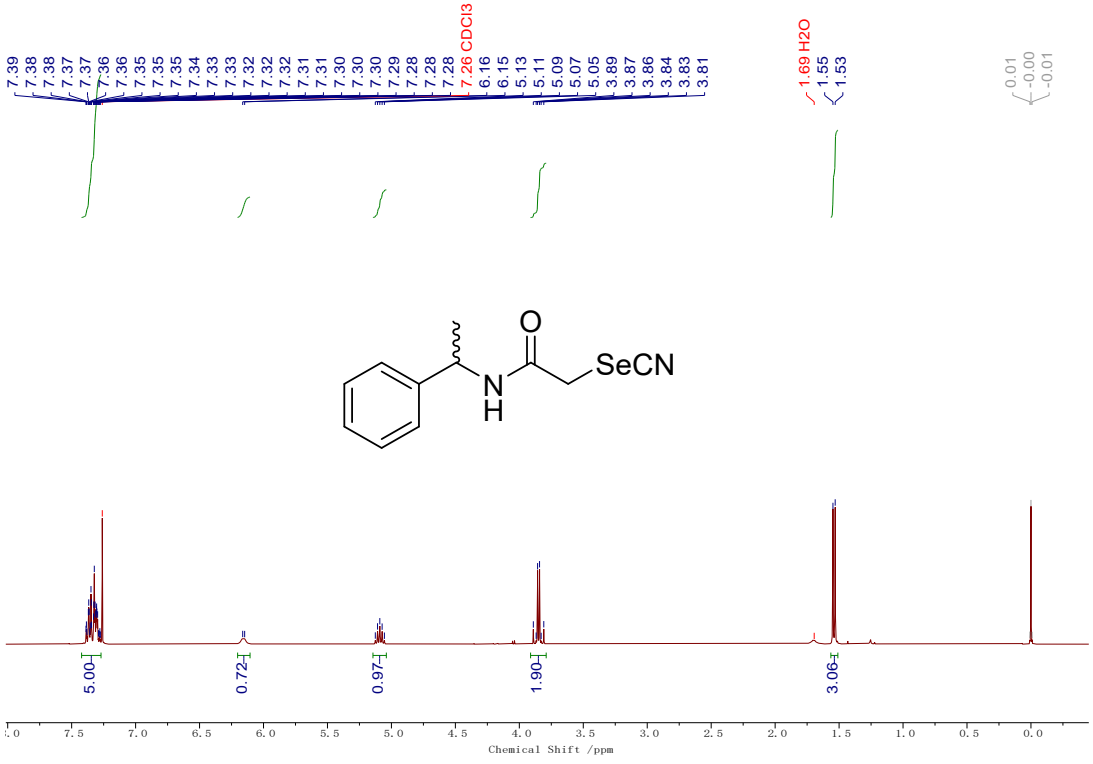


Figure S57. ^{1}H NMR spectra of MBA.

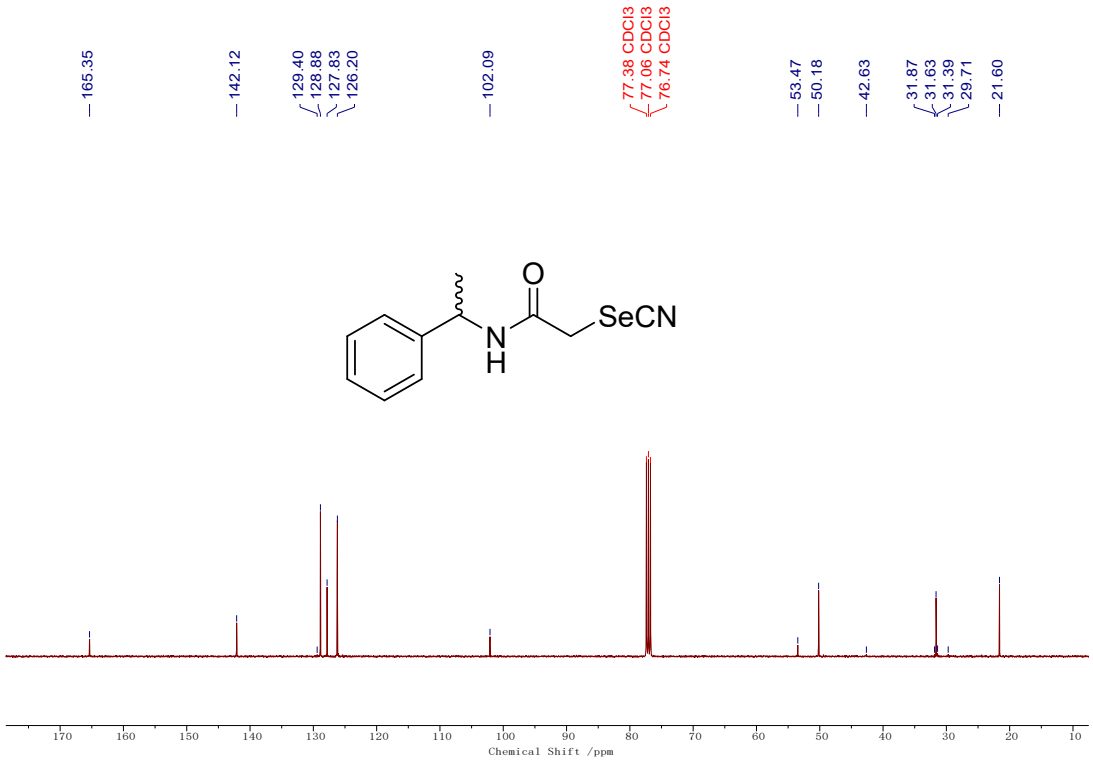


Figure S58. ^{13}C NMR spectra of MBA.

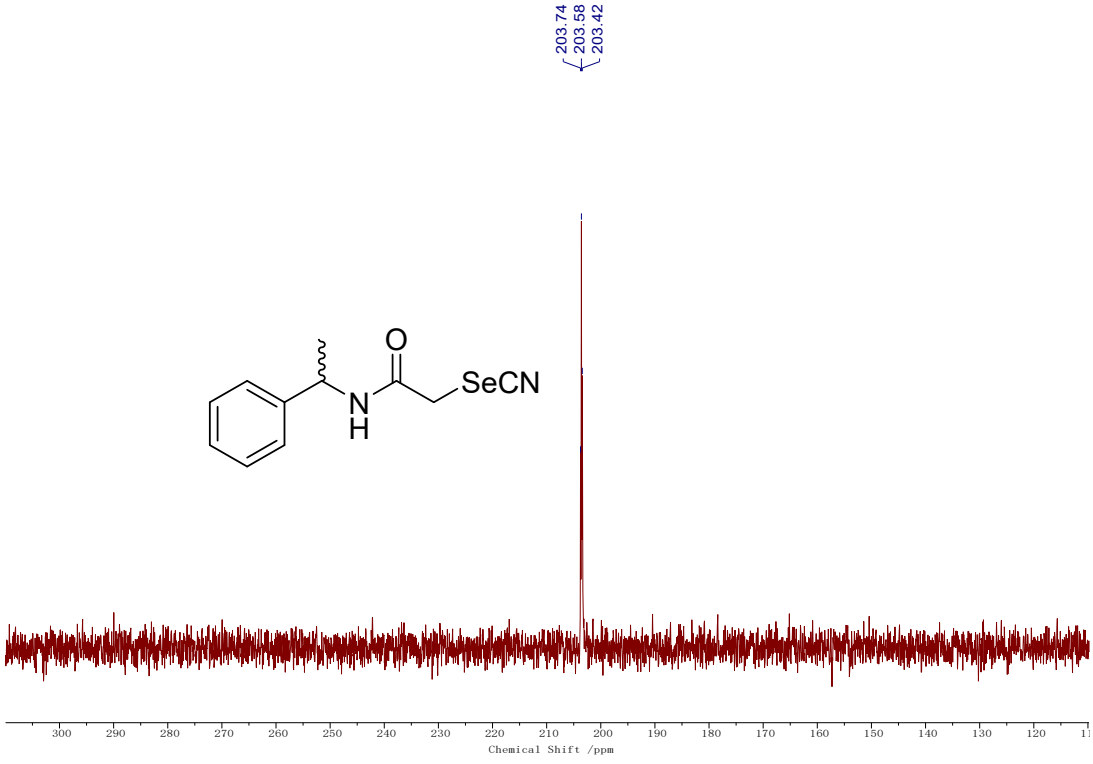


Figure S59. ^{77}Se NMR spectra of MBA.

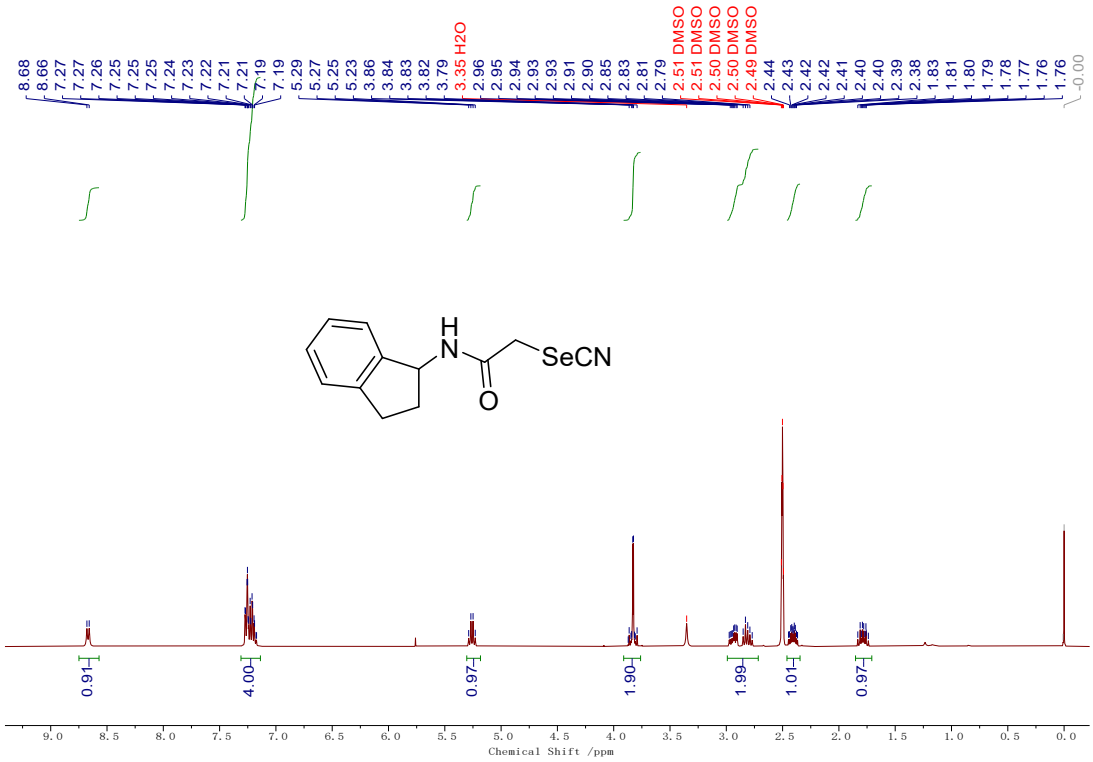


Figure S60. ^{1}H NMR spectra of DHIA.

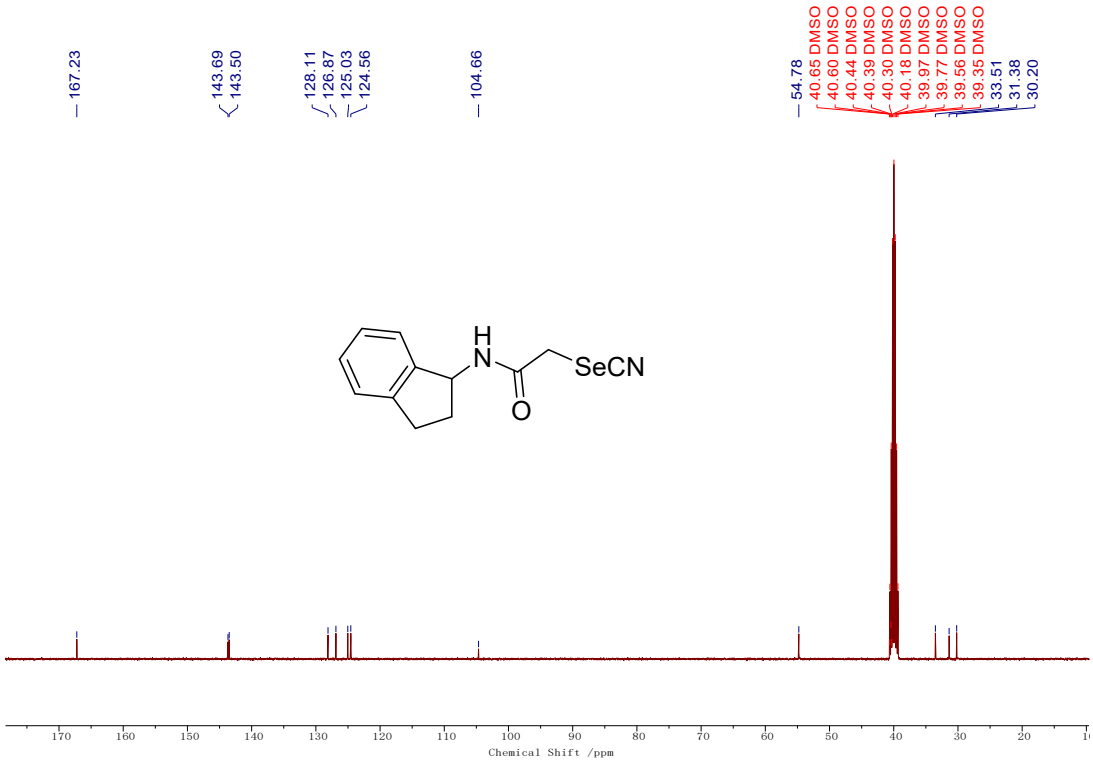


Figure S61. ^{13}C NMR spectra of DHIA.

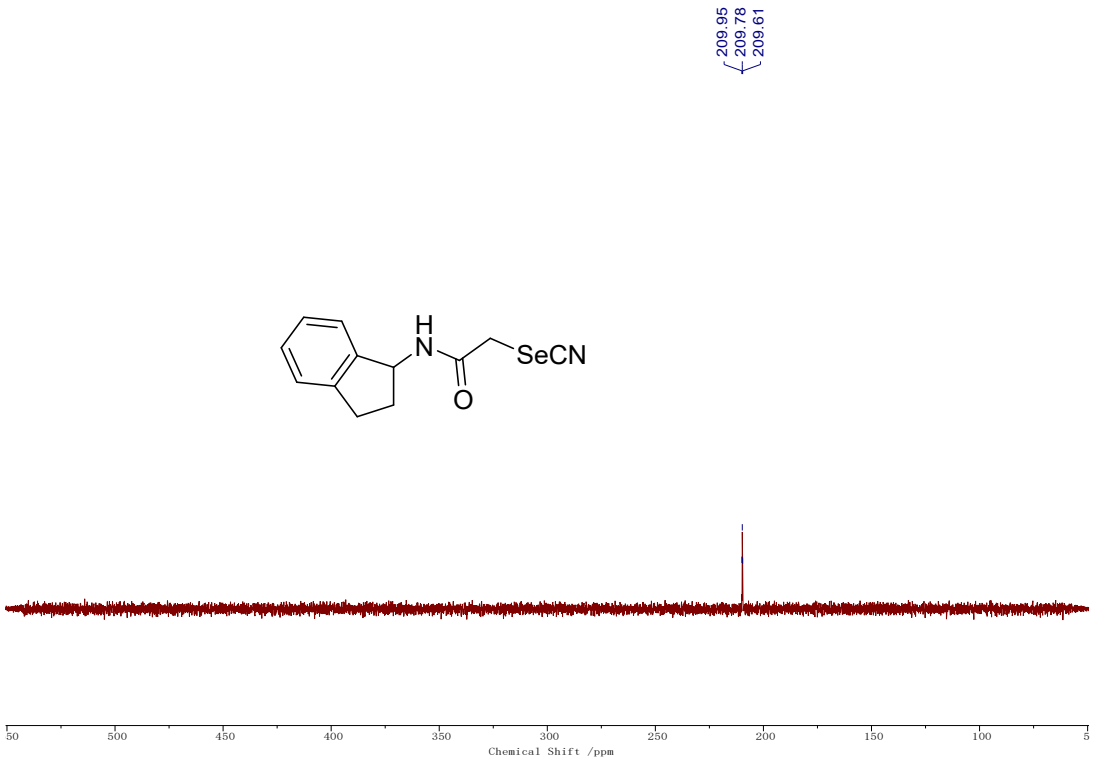


Figure S62. ^{77}Se NMR spectra of DHIA.

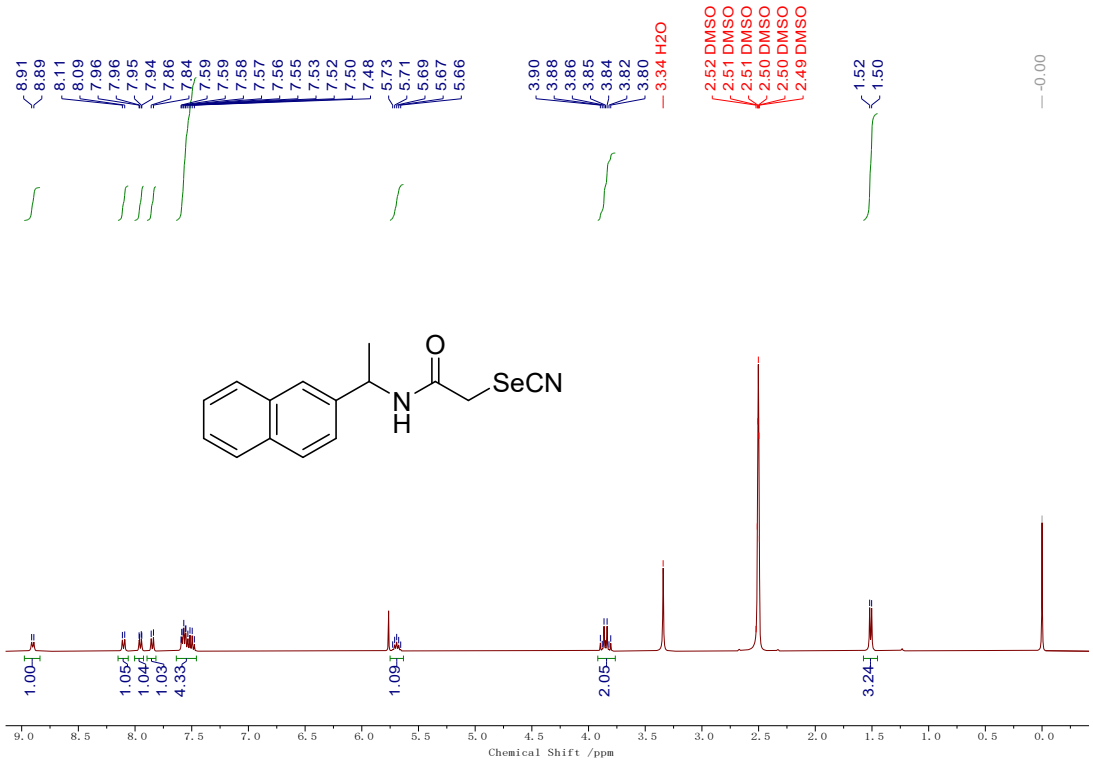


Figure S63. ^{1}H NMR spectra of MNA.

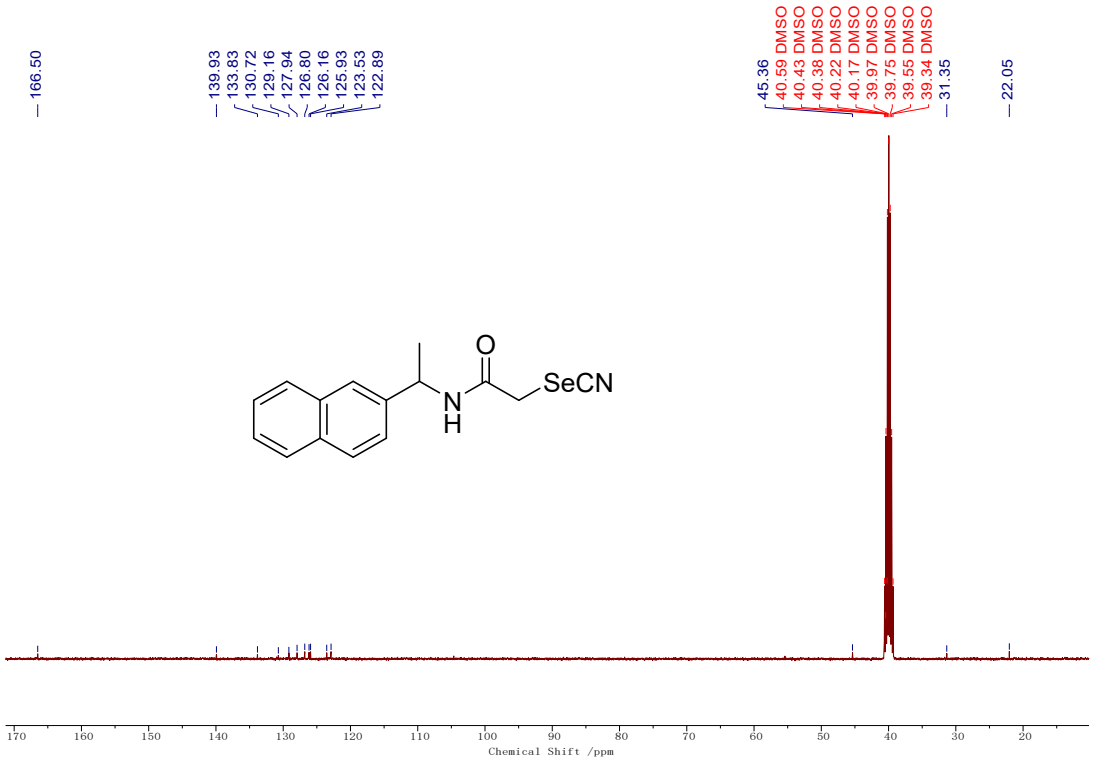


Figure S64. ^{13}C NMR spectra of MNA.

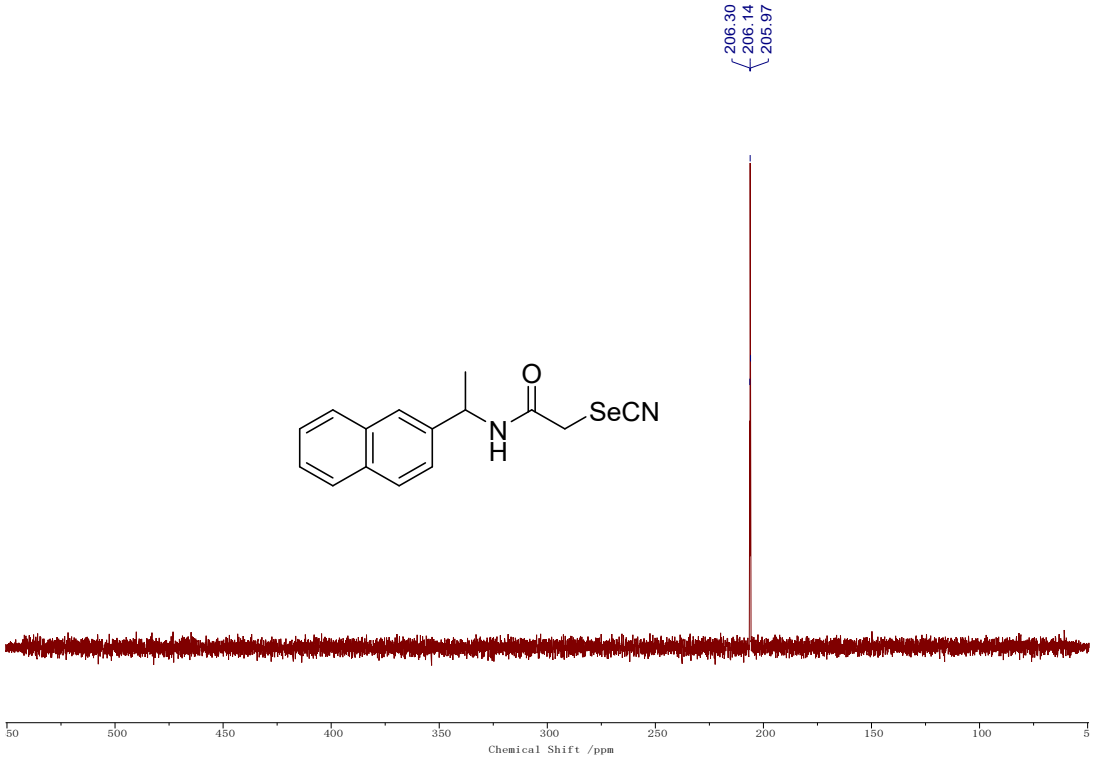


Figure S65. ^{77}Se NMR spectra of MNA.

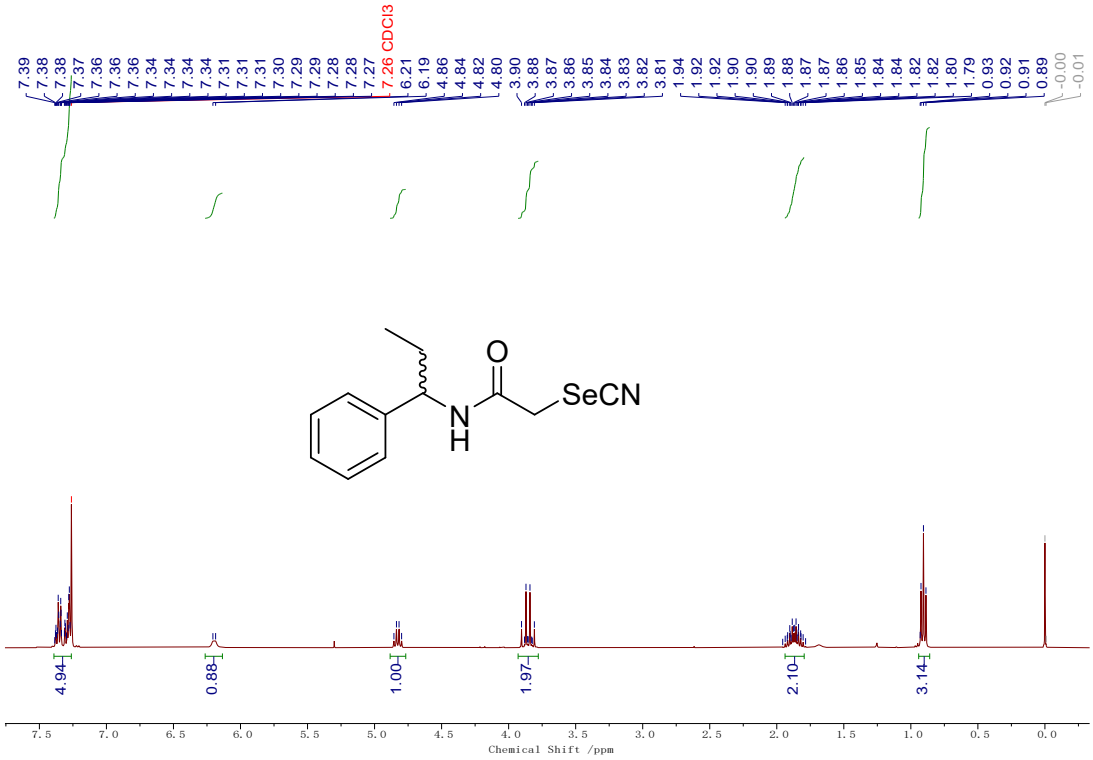


Figure S66. ^{1}H NMR spectra of EBA.

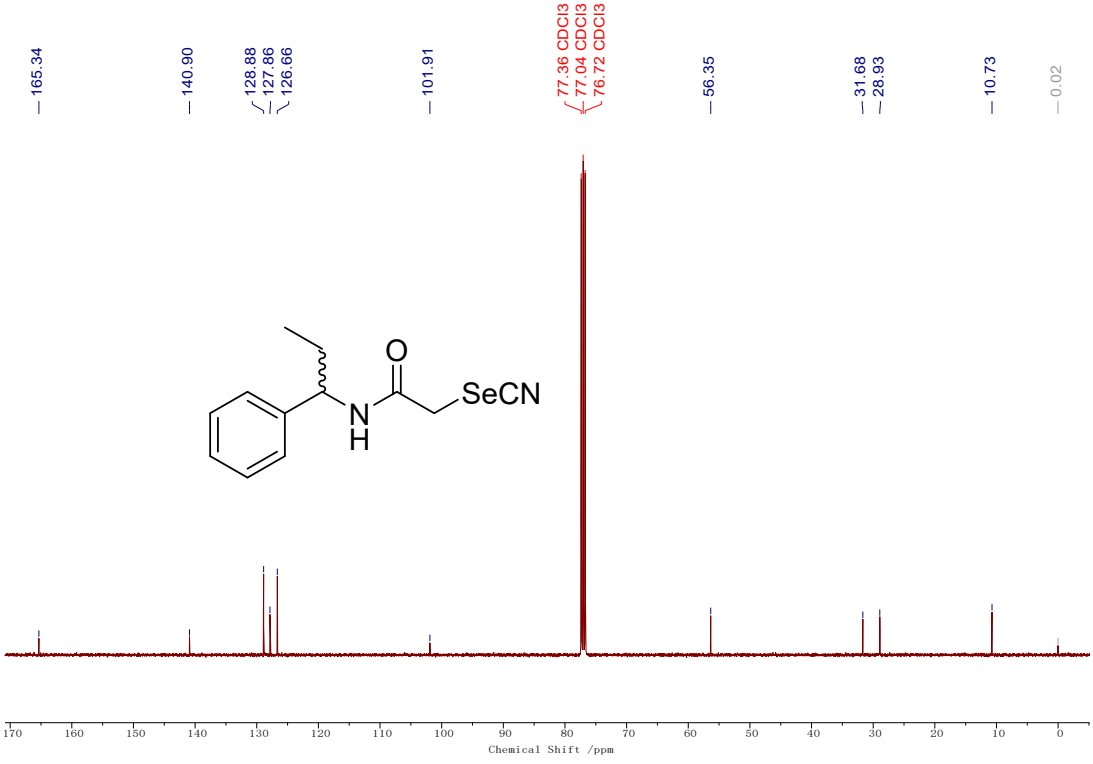


Figure S67. ^{13}C NMR spectra of EBA.

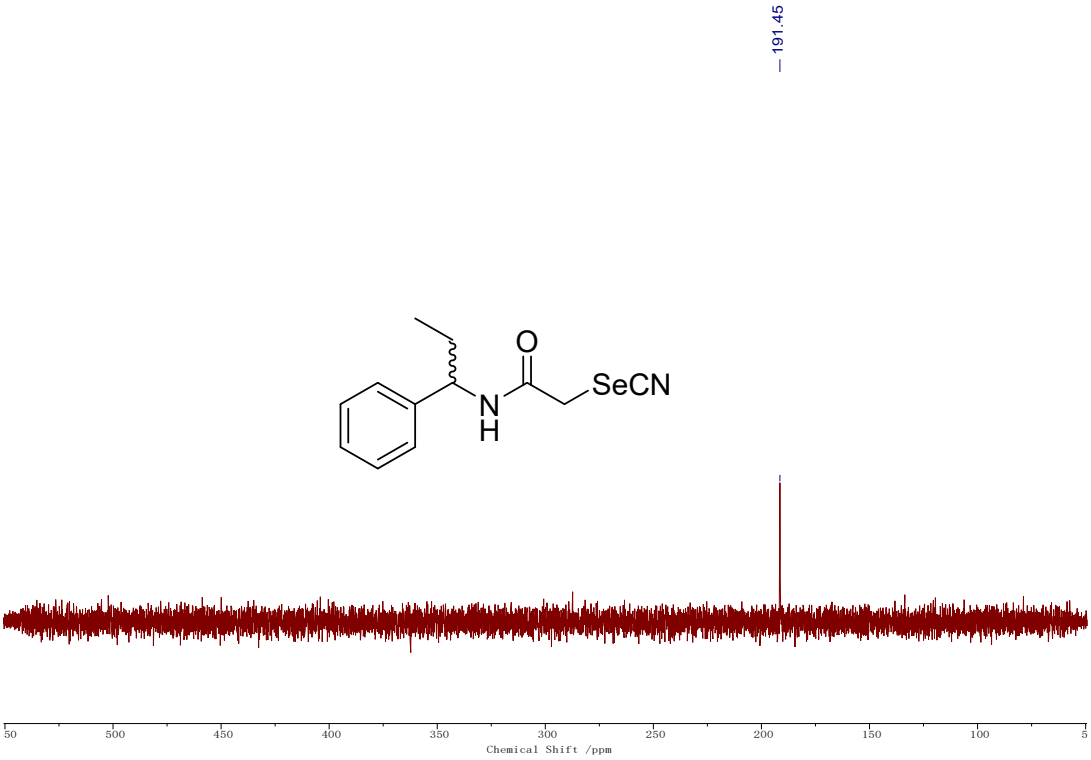


Figure S68. ^{77}Se NMR spectra of EBA.

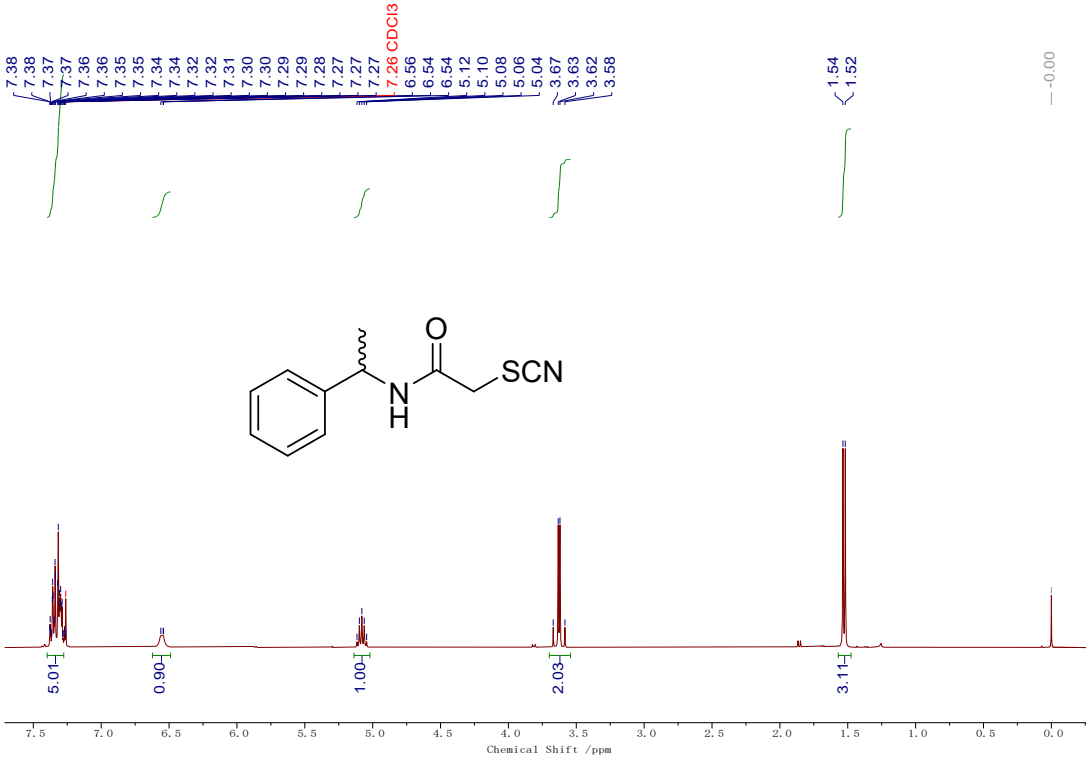


Figure S69. ^{1}H NMR spectra of MBA-S.

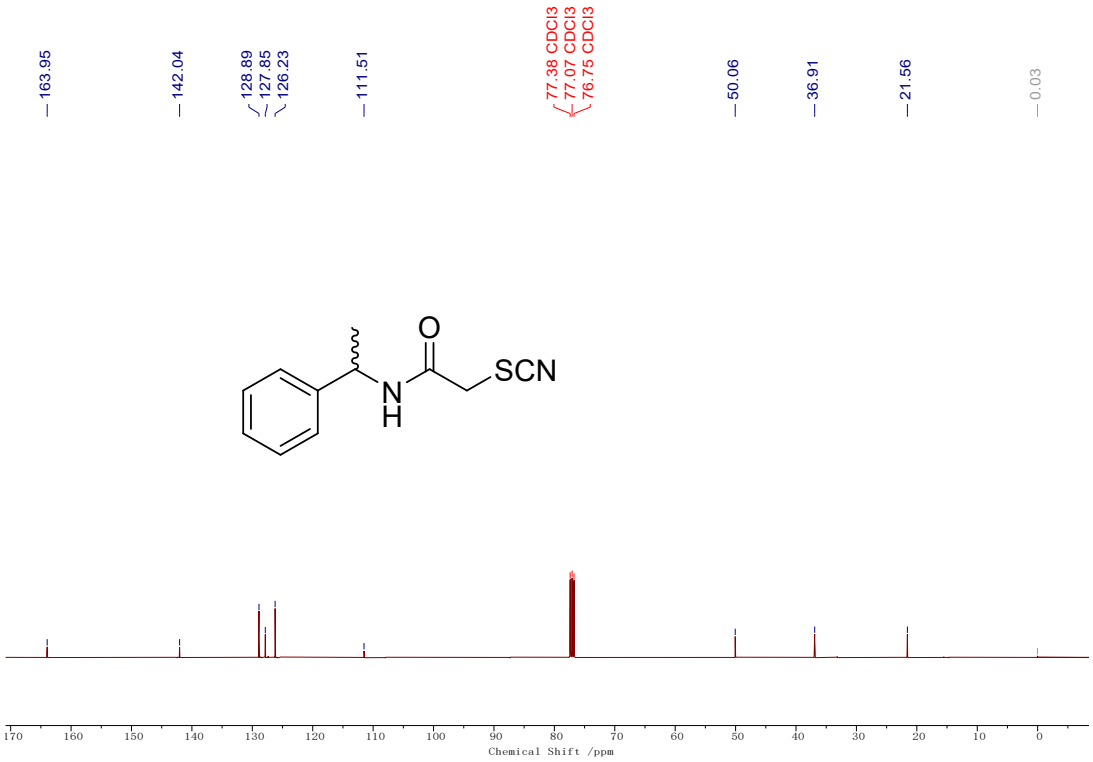


Figure S70. ^{13}C NMR spectra of MBA-S.

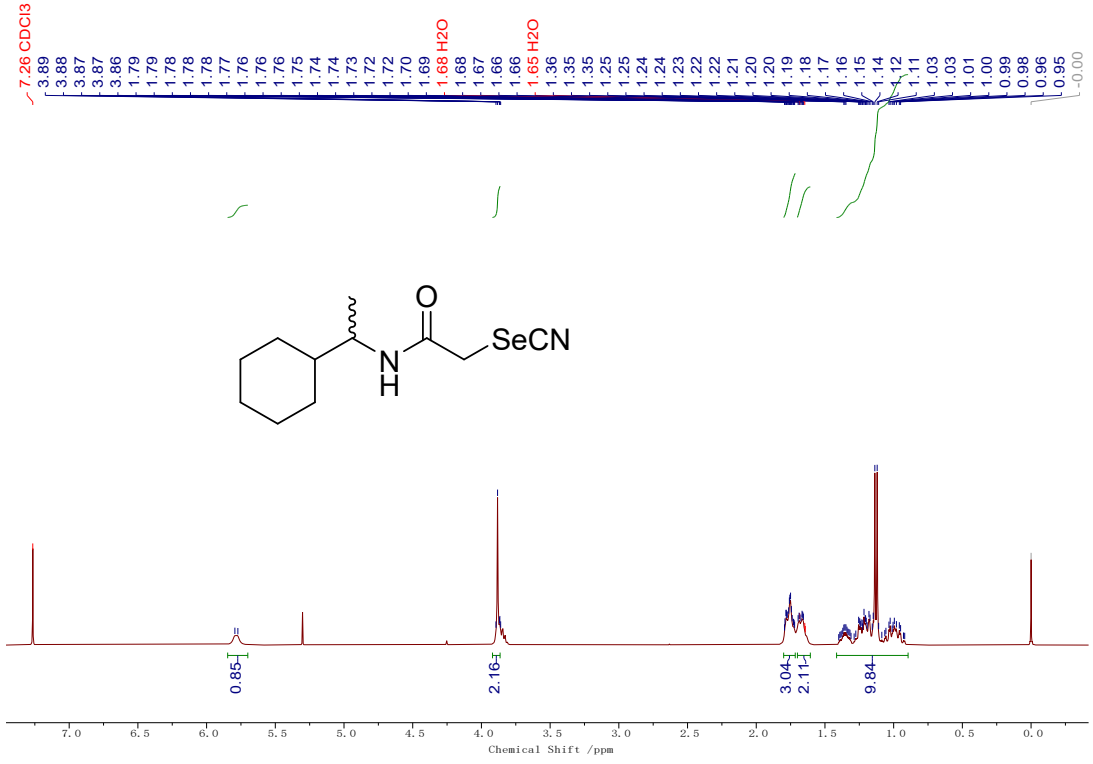


Figure S71. ^{1}H NMR spectra of CHA.

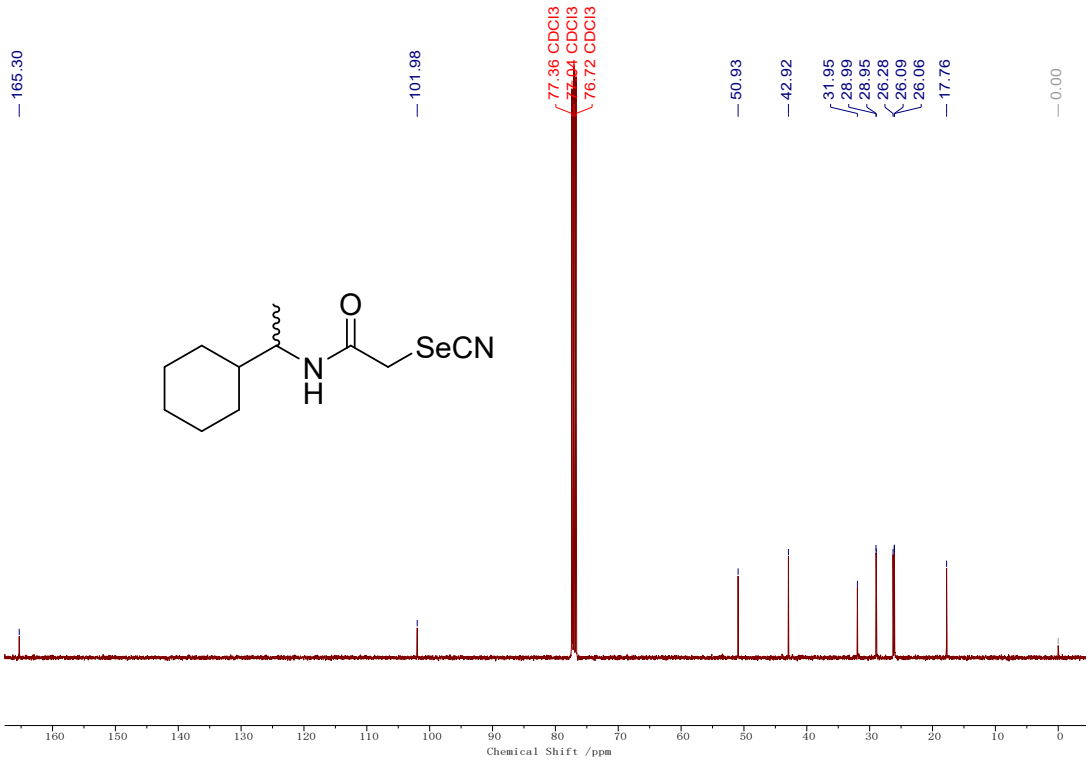


Figure S72. ^{13}C NMR spectra of CHA.

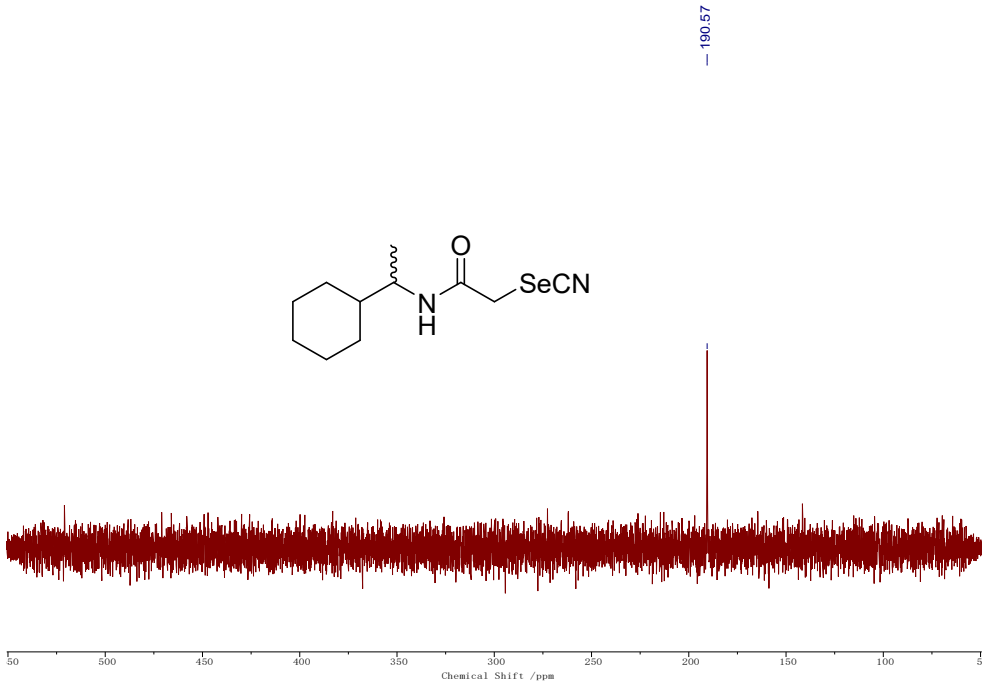


Figure S73. ^{77}Se NMR spectra of CHA.

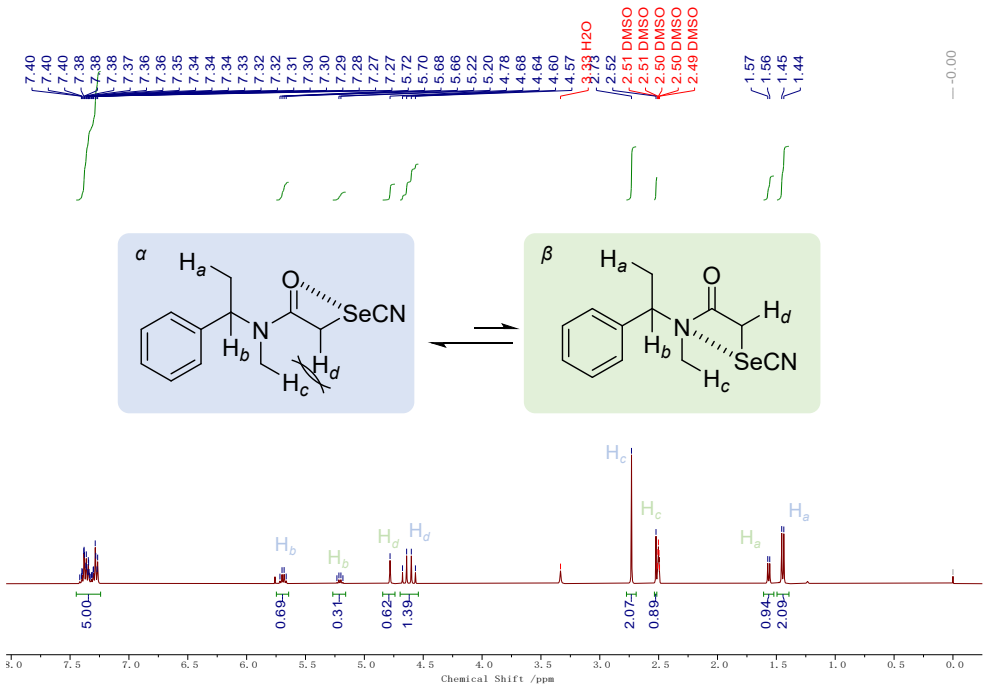


Figure S74. ^{1}H NMR spectra of MMBA. MMBA is an interesting molecule that exists as two dynamically equilibrated conformations in DMSO. In the α-form, the carbonyl group interacts with selenium through chalcogen bonding, bringing H_d and H_c into proximity and causing H_d to appear as a quartet. In the β-form, the amide nitrogen instead interacts with selenium, separating H_d and H_c and resulting in a singlet for H_d. In DMSO, the α/β ratio is approximately 2:1.

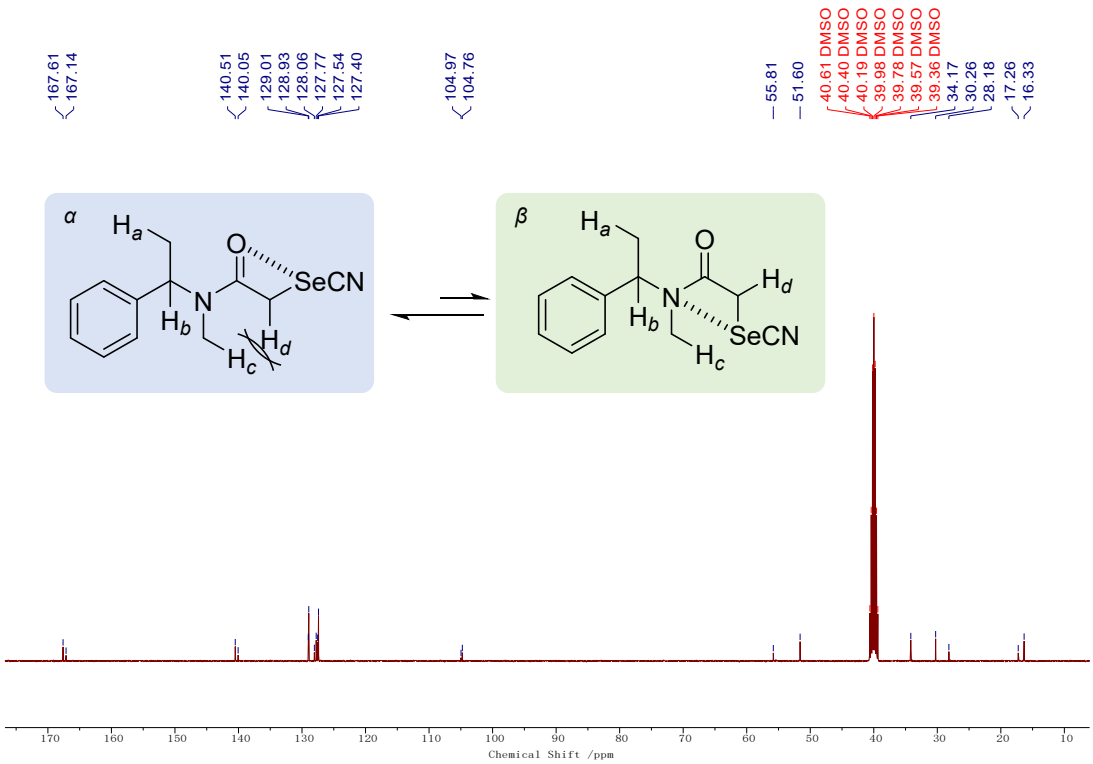


Figure S75. ^{13}C NMR spectra of MMBA.

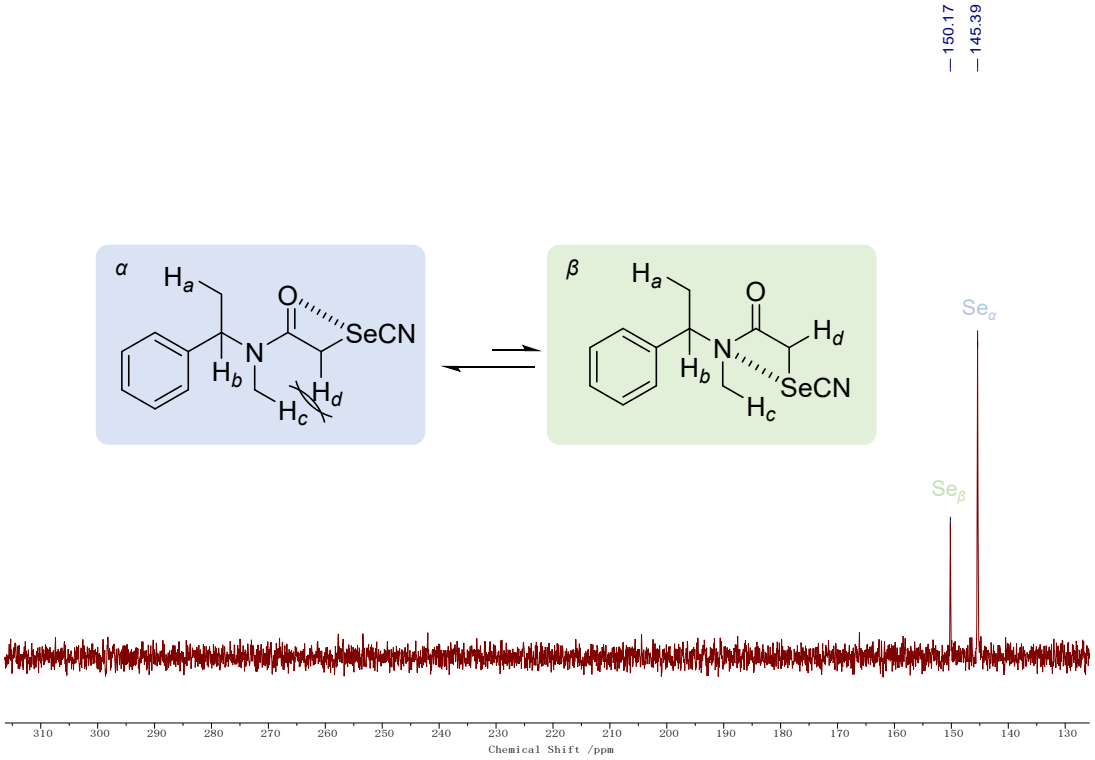


Figure S76. ^{77}Se NMR spectra of MMBA.

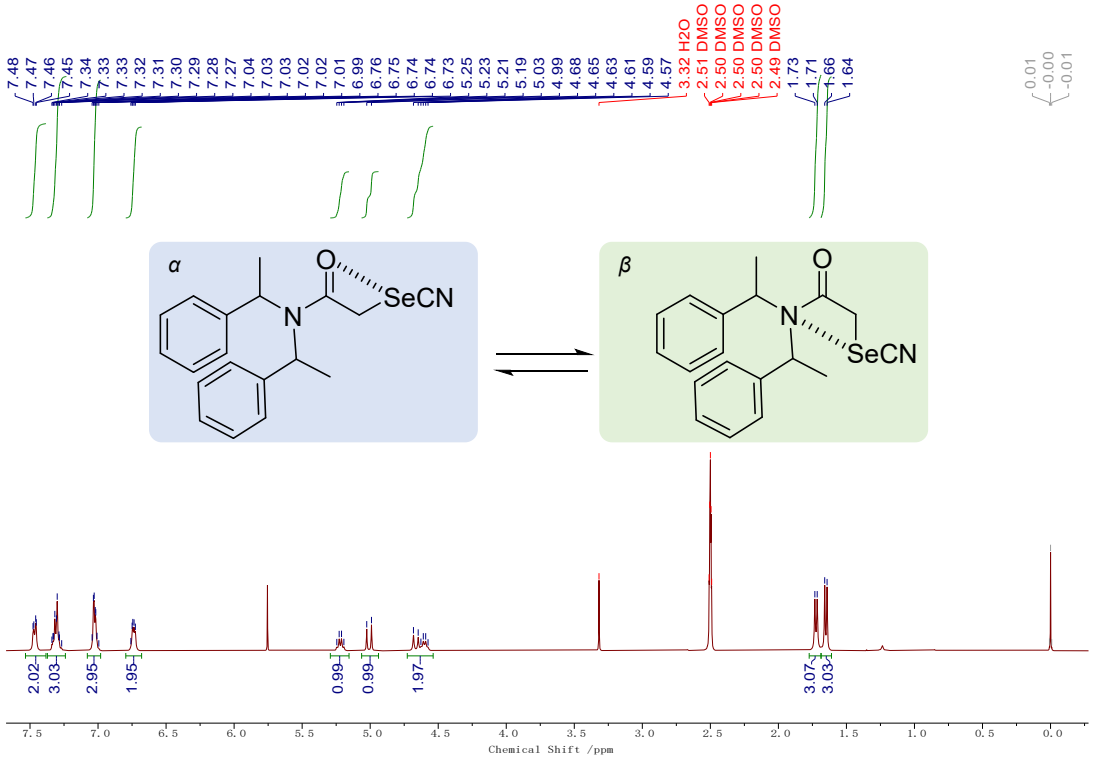


Figure S77. ^{1}H NMR spectra of DMBA.

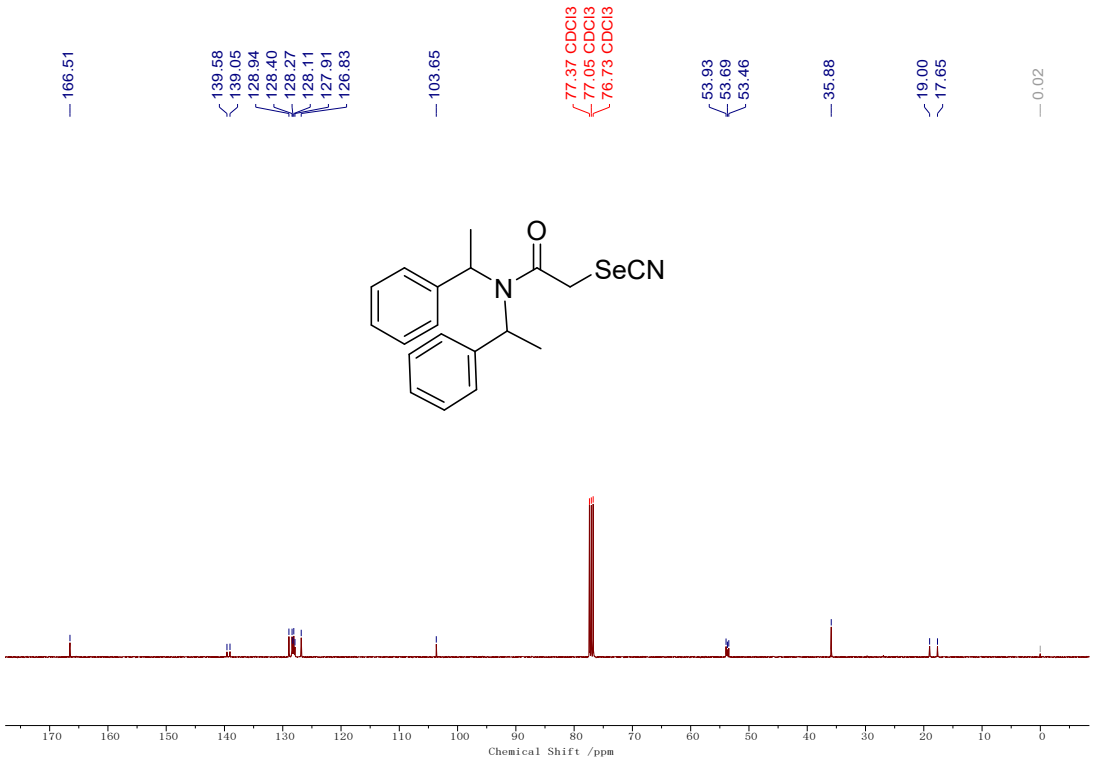


Figure S78. ^{13}C NMR spectra of DMBA.

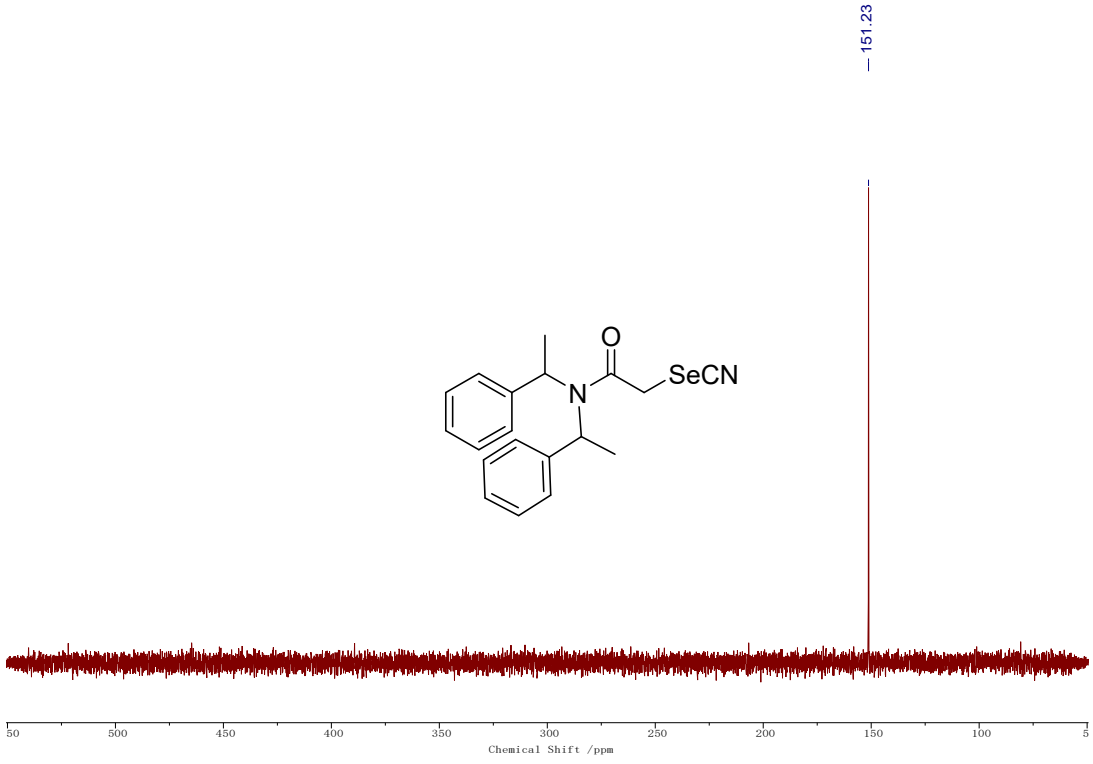


Figure S79. ^{77}Se NMR spectra of DMBA.

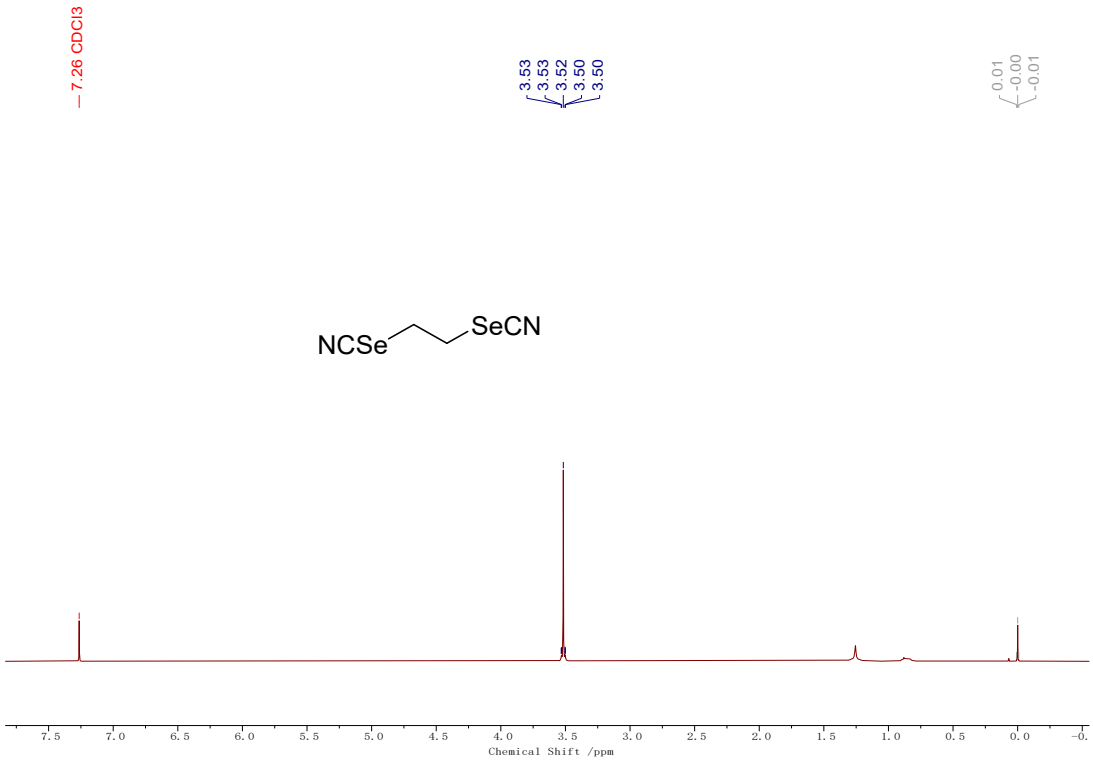


Figure S80. ^{1}H NMR spectra of EtSe.

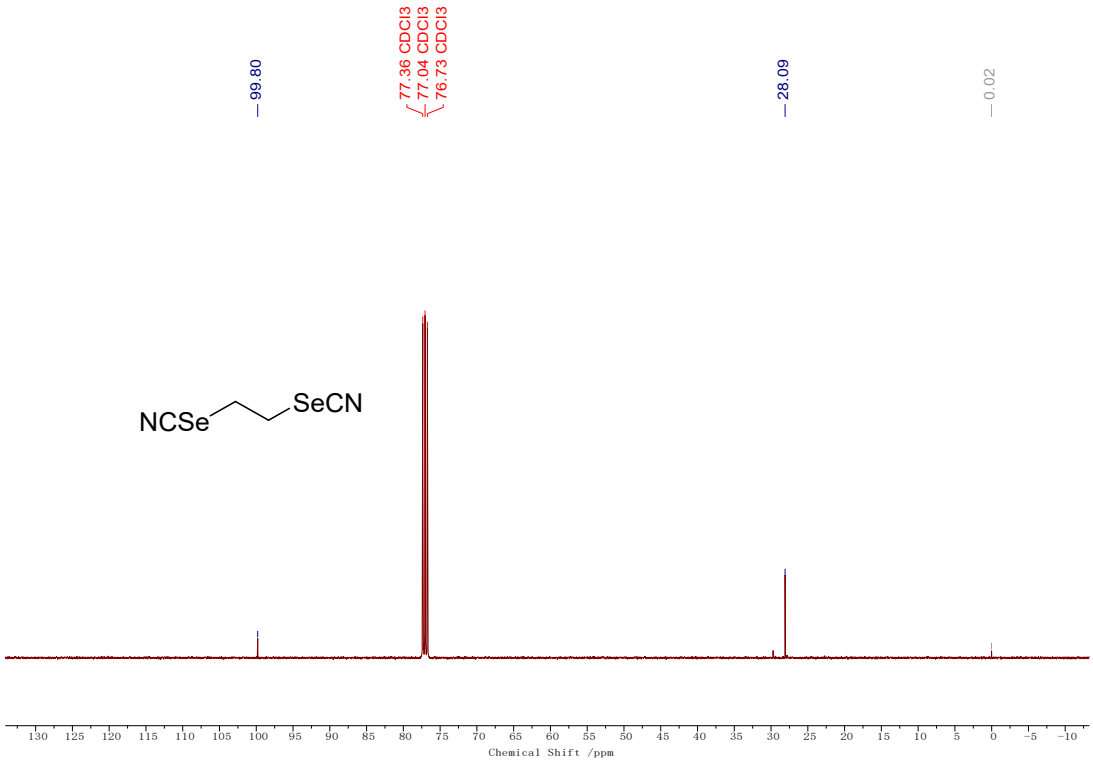


Figure S81. ^{13}C NMR spectra of EtSe.

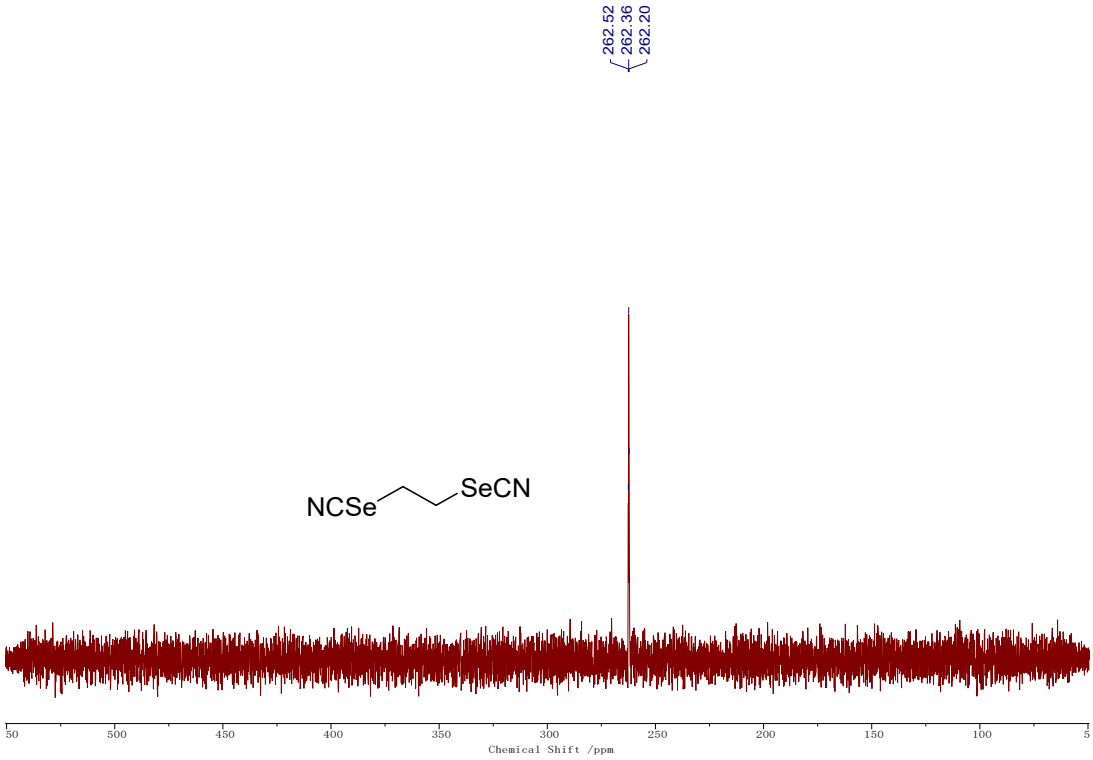


Figure S82. ^{77}Se NMR spectra of EtSe.

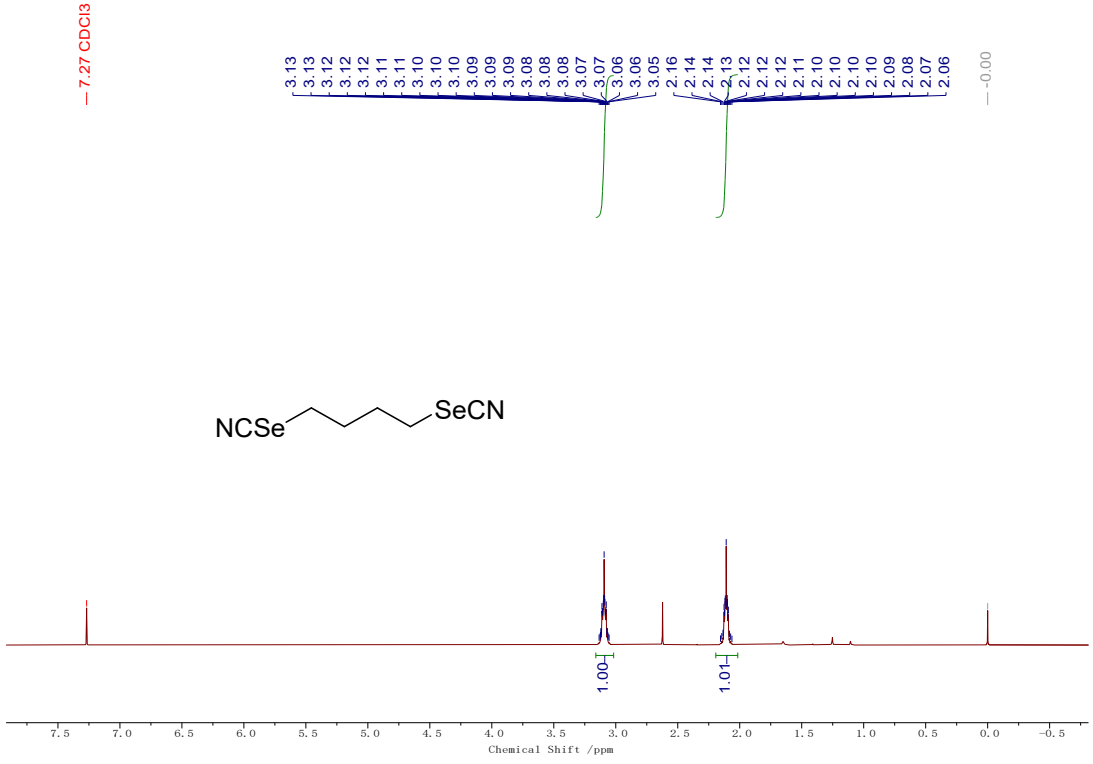


Figure S83. ^{1}H NMR spectra of BuSe.

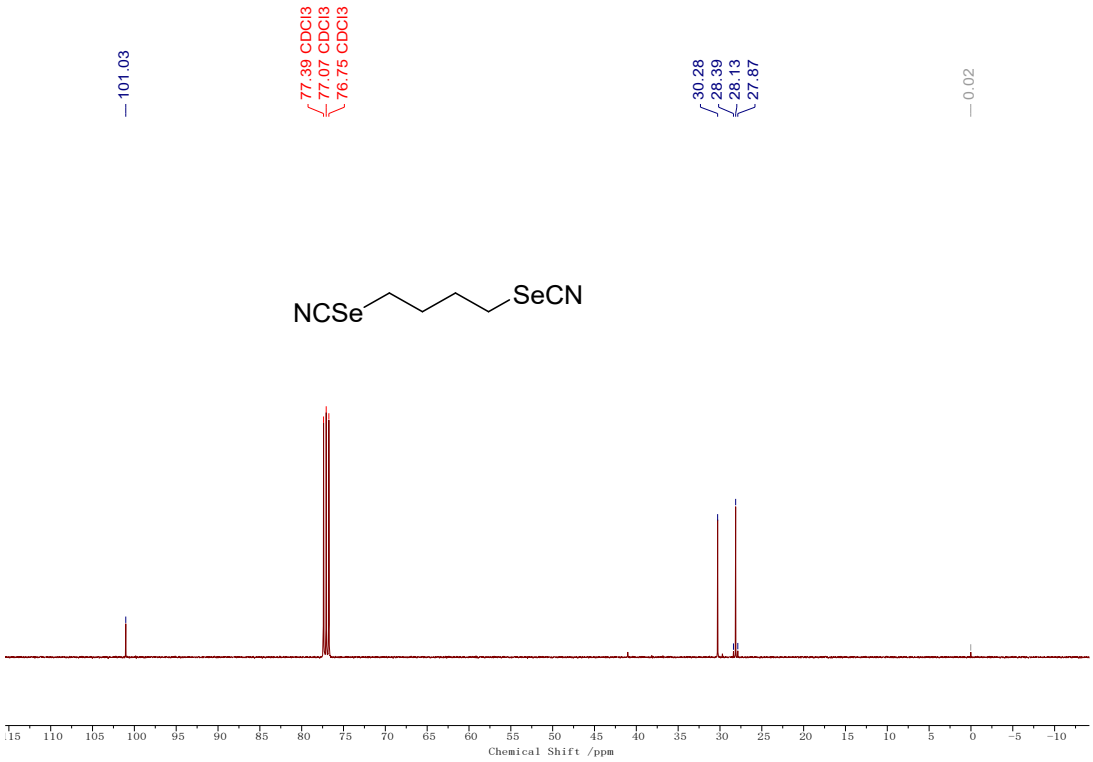


Figure S84. ^{13}C NMR spectra of BuSe.

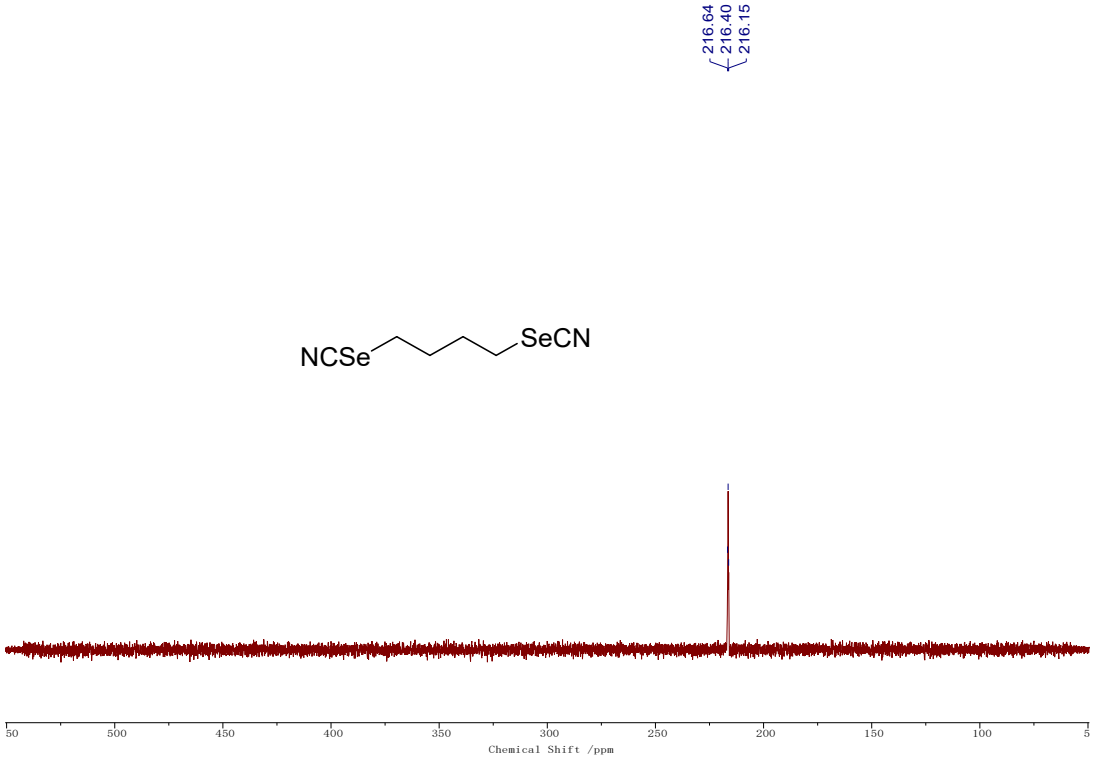


Figure S85. ^{77}Se NMR spectra of BuSe.

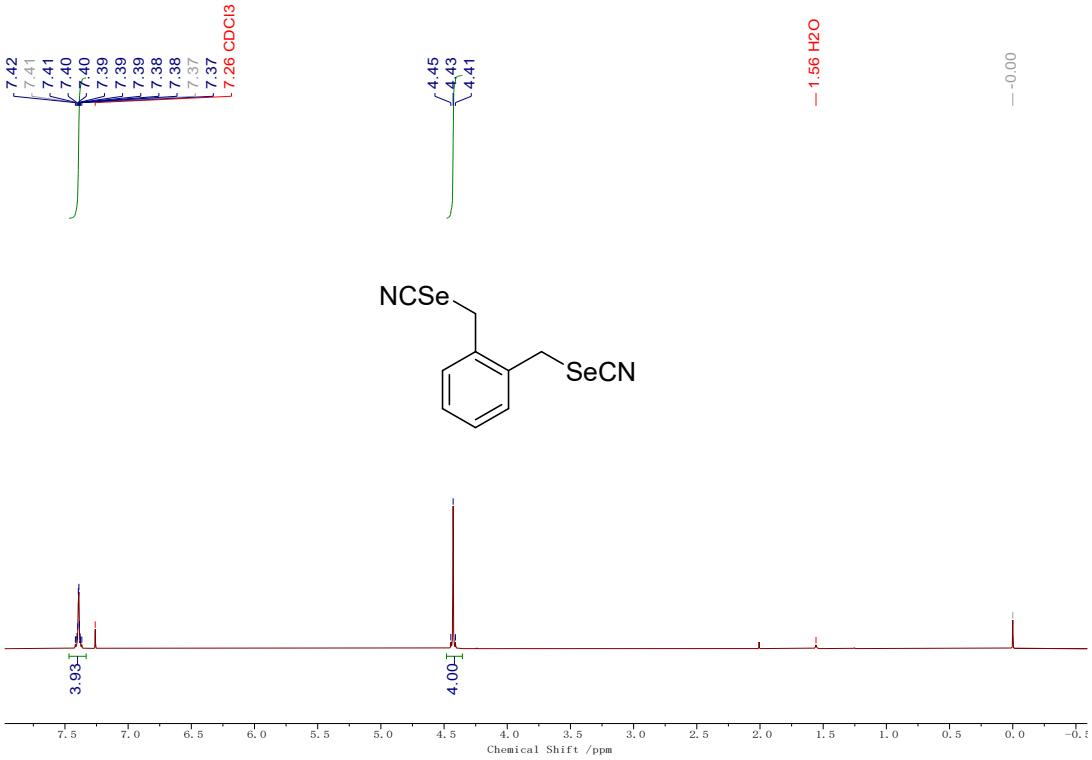


Figure S86. ^{1}H NMR spectra of *o*-DSe.

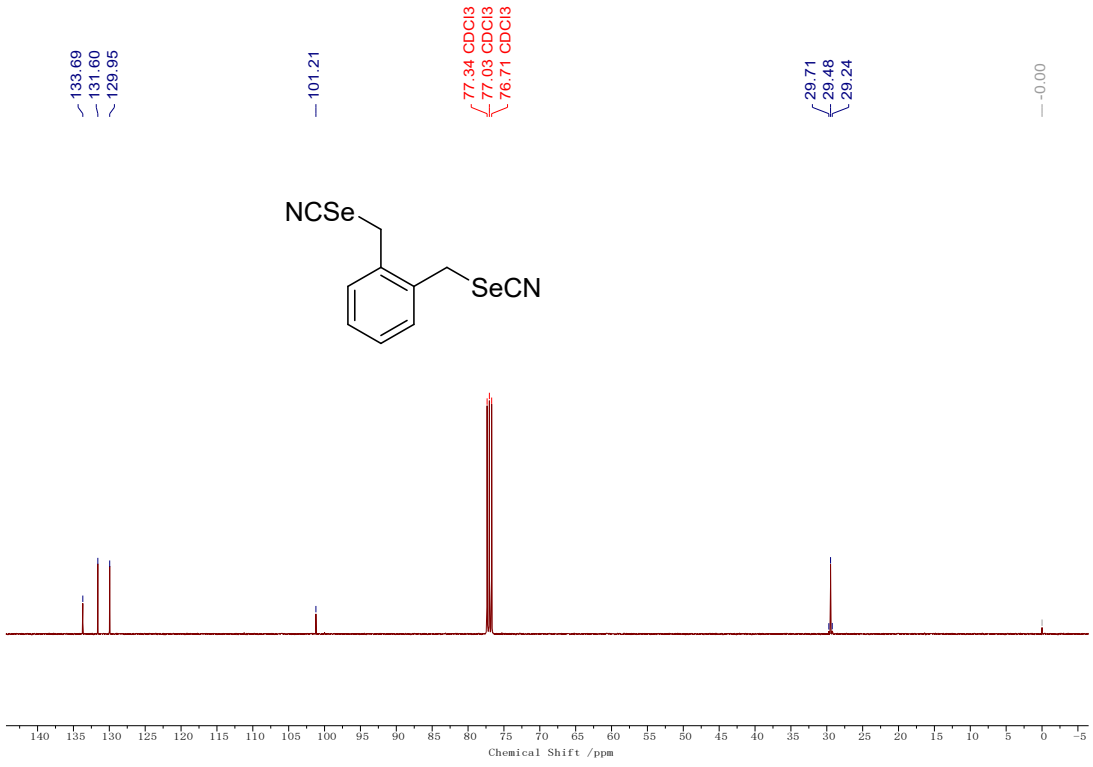


Figure S87. ^{13}C NMR spectra of *o*-DSe.

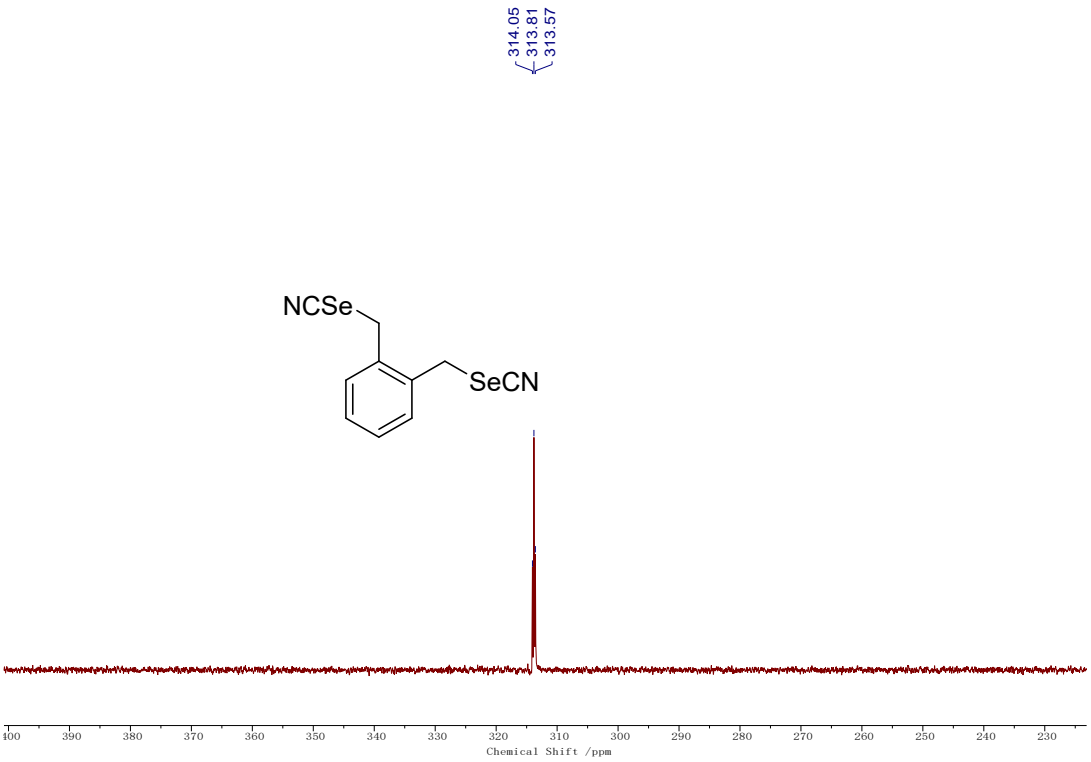


Figure S88. ^{77}Se NMR spectra of *o*-DSe.

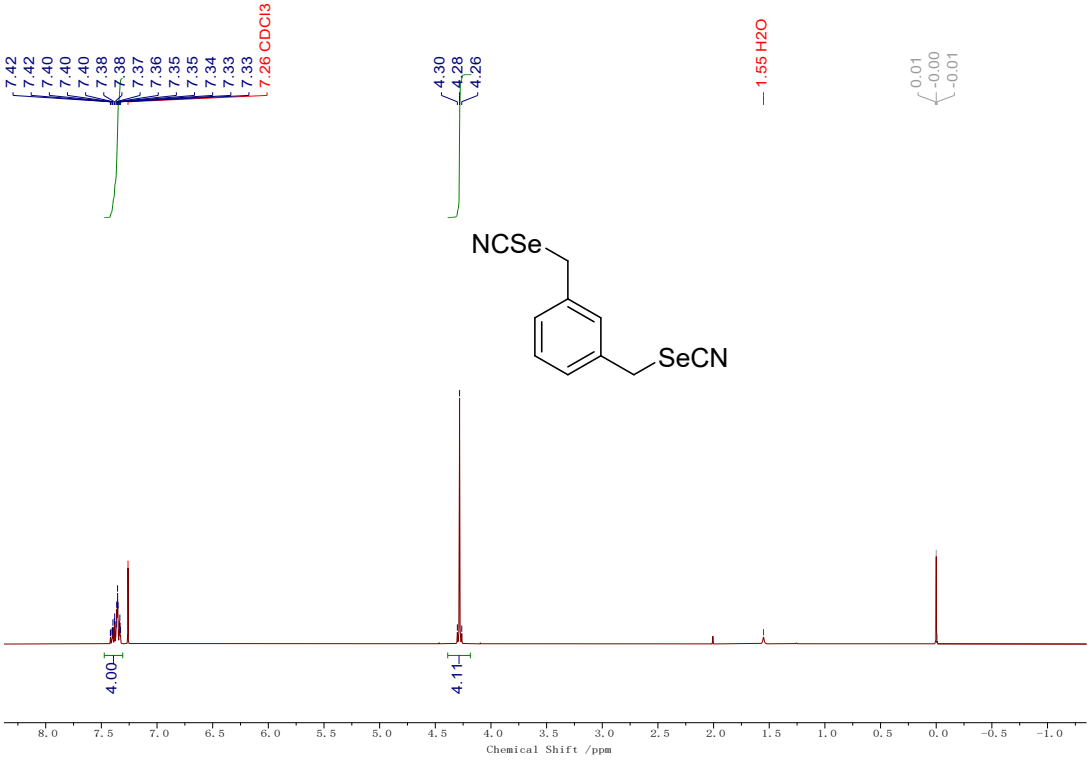


Figure S89. ^{1}H NMR spectra of *m*-DSe.

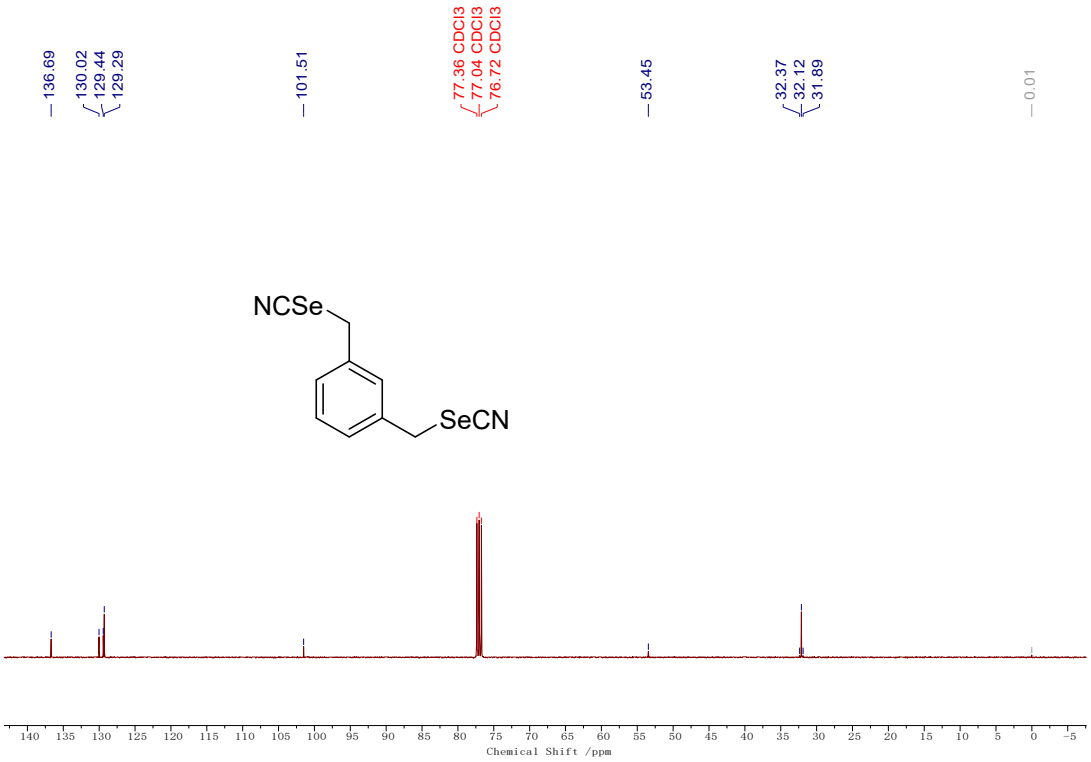


Figure S90. ^{13}C NMR spectra of *m*-DSe.

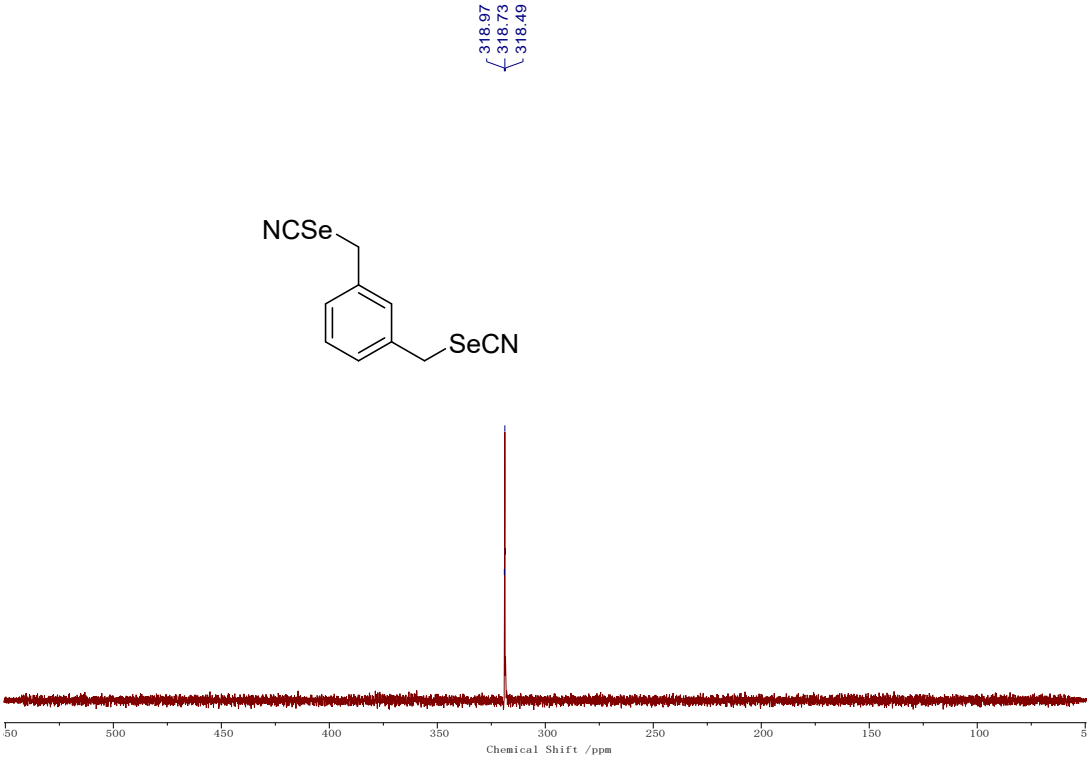


Figure S91. ^{77}Se NMR spectra of *m*-DSe.

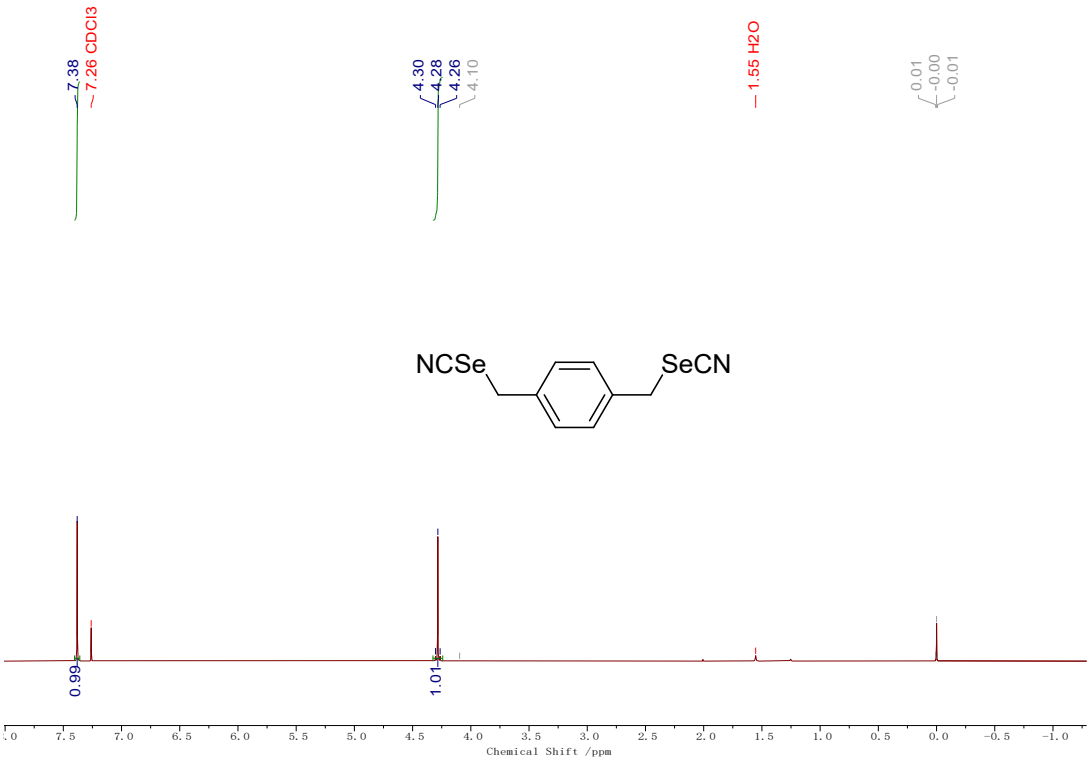


Figure S92. ^{1}H NMR spectra of *p*-DSe.

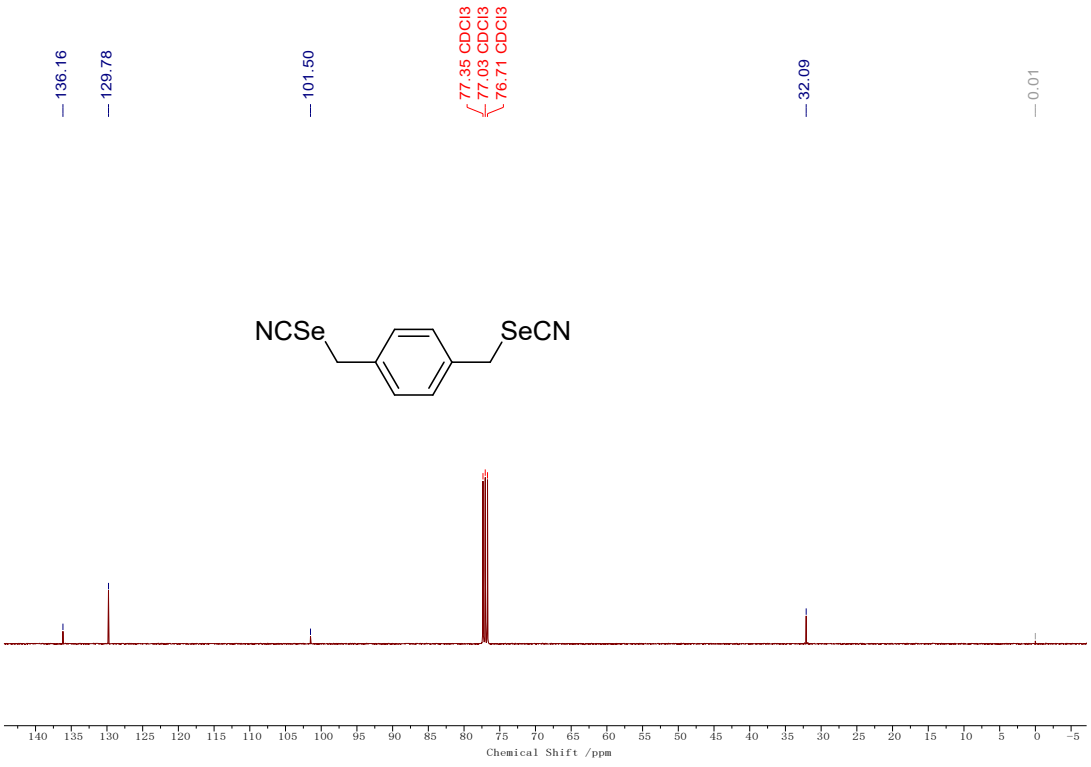


Figure S93. ^{13}C NMR spectra of *p*-DSe.

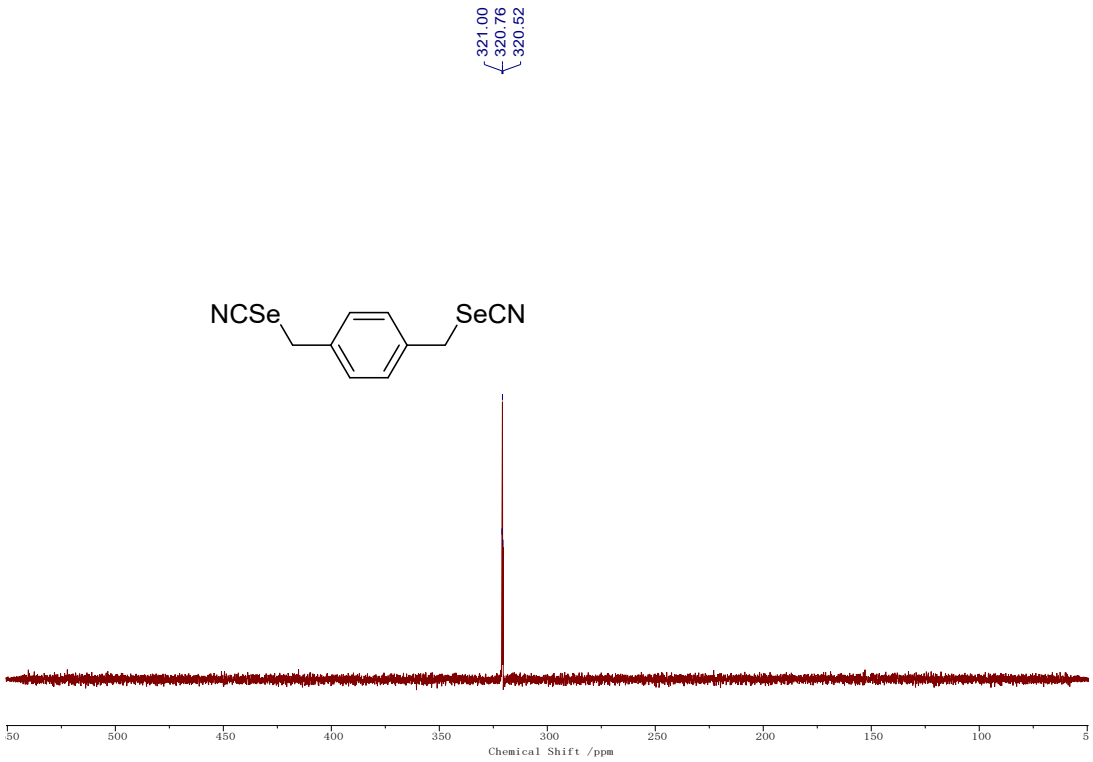


Figure S94. ^{77}Se NMR spectra of *p*-DSe.

Table S2. Atomic coordinates of the optimized structure of Pyr.

Symbol	X	Y	Z
O	0.5852000	-0.6429000	1.6469000
O	-0.5851000	-0.6433000	-1.6474000
N	-0.7072000	1.2612000	1.5065000
N	0.7073000	1.2608000	-1.5069000
N	3.1561000	2.4174000	-1.1841000
N	-3.1562000	2.4176000	1.1838000
C	-0.4558000	0.7116000	-1.7204000
C	-0.3263000	3.4375000	-1.7811000
C	0.4559000	0.7119000	1.7200000
C	0.5405000	-1.4530000	-1.5237000
C	-0.5404000	-1.4526000	1.5235000
C	0.5452000	-2.3788000	-0.5061000
C	-0.5452000	-2.3786000	0.5061000
C	0.7980000	2.6084000	-1.5531000
C	5.3968000	0.7038000	-0.2037000
C	1.6063000	-3.3341000	-0.4495000
C	-0.7981000	2.6087000	1.5528000
C	2.6489000	-3.2836000	-1.4254000
C	-1.6409000	1.4274000	-2.0079000
H	-2.5637000	0.8946000	-2.1803000
C	4.3478000	2.9304000	-0.9178000
C	5.5038000	2.0136000	-0.7516000
C	-2.0906000	3.2211000	1.3372000

C	1.5731000	-1.3861000	-2.4839000
H	1.5390000	-0.6193000	-3.2443000
C	2.0905000	3.2208000	-1.3374000
C	2.1812000	4.6358000	-1.2853000
C	-5.5038000	2.0136000	0.7516000
C	-1.6063000	-3.3339000	0.4496000
C	2.6062000	-2.2801000	-2.4259000
H	3.4098000	-2.2294000	-3.1515000
C	-1.5655000	2.7938000	-2.0154000
H	-2.4529000	3.3910000	-2.1924000
C	-4.3479000	2.9305000	0.9178000
C	3.6957000	-4.2354000	-1.3665000
H	4.4918000	-4.1769000	-2.1003000
C	6.5959000	-0.0450000	0.0276000
C	-5.3967000	0.7038000	0.2037000
C	-2.1814000	4.6361000	1.2853000
C	0.3262000	3.4379000	1.7809000
C	4.0997000	-1.1156000	0.7853000
H	3.1395000	-1.5385000	1.0546000
C	5.2852000	-1.8602000	1.0737000
C	4.1484000	0.0929000	0.1667000
H	3.2356000	0.6005000	-0.0960000
C	-6.5958000	-0.0451000	-0.0275000
C	6.5366000	-1.3225000	0.6617000
C	1.0233000	5.4380000	-1.5165000
H	1.1212000	6.5174000	-1.4793000
C	-4.1483000	0.0930000	-0.1668000
H	-3.2356000	0.6007000	0.0958000
C	1.6606000	-4.3394000	0.5498000
H	0.8776000	-4.3784000	1.2958000
C	-6.5365000	-1.3227000	-0.6616000
C	1.6409000	1.4278000	2.0075000
H	2.5638000	0.8951000	2.1798000
C	-1.5730000	-1.3855000	2.4837000
H	-1.5390000	-0.6186000	3.2439000
C	-0.1826000	4.8585000	-1.7637000
H	-1.0642000	5.4669000	-1.9300000
C	3.4504000	5.1727000	-0.9791000
H	3.5662000	6.2478000	-0.8897000
C	7.8655000	0.4769000	-0.3581000
C	6.7702000	2.4894000	-1.1231000
H	6.8480000	3.4654000	-1.5858000
C	-4.0996000	-1.1155000	-0.7854000
H	-3.1394000	-1.5384000	-1.0547000
C	7.9214000	1.7428000	-0.9517000
H	8.8791000	2.1395000	-1.2697000
C	7.7306000	-2.0660000	0.9008000
C	4.5206000	4.3368000	-0.7774000

H	5.4840000	4.7416000	-0.4987000
C	-6.7703000	2.4893000	1.1232000
H	-6.8481000	3.4652000	1.5859000
C	3.7108000	-5.2087000	-0.3989000
H	4.5200000	-5.9280000	-0.3623000
C	5.2490000	-3.0992000	1.7262000
H	4.2910000	-3.5003000	2.0308000
C	1.5655000	2.7941000	2.0151000
H	2.4528000	3.3914000	2.1921000
C	-2.6489000	-3.2832000	1.4255000
C	-7.8654000	0.4766000	0.3583000
C	-5.2850000	-1.8602000	-1.0737000
C	-1.0236000	5.4383000	1.5166000
H	-1.1215000	6.5177000	1.4795000
C	-2.6062000	-2.2795000	2.4259000
H	-3.4097000	-2.2287000	3.1514000
C	6.4181000	-3.8127000	1.9594000
H	6.3720000	-4.7723000	2.4615000
C	2.6819000	-5.2593000	0.5666000
H	2.7026000	-6.0265000	1.3323000
C	0.1824000	4.8589000	1.7637000
H	1.0640000	5.4673000	1.9300000
C	-4.5208000	4.3369000	0.7776000
H	-5.4843000	4.7416000	0.4990000
C	-3.4507000	5.1729000	0.9793000
H	-3.5666000	6.2480000	0.8900000
C	-7.9214000	1.7425000	0.9518000
H	-8.8791000	2.1392000	1.2699000
C	-7.7304000	-2.0663000	-0.9006000
C	9.0466000	-0.3007000	-0.1259000
H	10.0001000	0.1112000	-0.4383000
C	-9.0465000	-0.3011000	0.1262000
H	-10.0000000	0.1108000	0.4386000
C	-8.9837000	-1.5157000	-0.4765000
H	-9.8862000	-2.0907000	-0.6534000
C	8.9839000	-1.5153000	0.4767000
H	9.8864000	-2.0903000	0.6538000
C	-1.6608000	-4.3394000	-0.5495000
H	-0.8777000	-4.3786000	-1.2955000
C	-5.2488000	-3.0992000	-1.7262000
H	-4.2907000	-3.5003000	-2.0308000
C	7.6463000	-3.3065000	1.5474000
H	8.5565000	-3.8680000	1.7278000
C	-6.4178000	-3.8128000	-1.9593000
H	-6.3717000	-4.7724000	-2.4614000
C	-7.6460000	-3.3068000	-1.5471000
H	-8.5562000	-3.8683000	-1.7275000
C	-3.6958000	-4.2349000	1.3668000

H	-4.4919000	-4.1763000	2.1006000
C	-2.6821000	-5.2592000	-0.5662000
H	-2.7028000	-6.0265000	-1.3317000
C	-3.7110000	-5.2084000	0.3994000
H	-4.5202000	-5.9276000	0.3628000

Table S3. Atomic coordinates of the optimized structure of MBA.

Symbol	X	Y	Z
Se	-2.6063090	-1.0178070	0.5918430
O	-1.2922990	2.9018430	0.1115230
C	-1.2462130	1.6927830	0.2652190
N	-0.1290810	0.9467270	0.1905550
H	-0.1798240	-0.0374290	0.4025110
C	-2.5685170	0.9737110	0.5532890
H	-3.2986890	1.3088560	-0.1793890
H	-2.9216410	1.2567980	1.5463790
N	-1.5433940	-1.4732370	-2.1824510
C	2.1156220	-0.8071420	-0.6365760
H	1.2822470	-0.9857100	-1.3081580
C	3.0738230	-1.7994670	-0.4549680
H	2.9761290	-2.7424370	-0.9801780
C	1.1862700	1.4976350	-0.1700420
H	1.3943330	2.3293630	0.5084830
C	2.2257760	0.4159050	0.0357400
C	-1.9804600	-1.2786850	-1.1279190
C	3.3120810	0.6251820	0.8846250
H	3.4022980	1.5688300	1.4117350
C	1.1834350	2.0304780	-1.6095970
H	0.9459270	1.2294260	-2.3125560
H	2.1704350	2.4277200	-1.8556100
H	0.4447410	2.8249130	-1.7118200
C	4.2768110	-0.3645460	1.0602500
H	5.1167390	-0.1871500	1.7219060
C	4.1582920	-1.5799740	0.3924330
H	4.9060080	-2.3521900	0.5303850

Table S4. Atomic coordinates of the optimized structure of EBA.

Symbol	X	Y	Z
Se	-2.7286140	-1.1405810	-0.6793330
O	-0.1290980	-0.4082390	2.4799470
C	-0.5758530	-0.4037810	1.3444760
N	-0.0652460	0.3004160	0.3155600
H	-0.4509000	0.1642680	-0.6077520
C	-1.8101890	-1.2689100	1.0817810
H	-2.5435680	-1.0648090	1.8580120
H	-1.5216580	-2.3194190	1.1486900
N	-3.6246500	1.7142650	-0.3949930
C	2.8809270	0.3656610	-1.2734600
H	2.4389790	1.0227940	-2.0126290

C	3.9730490	-0.4227080	-1.6307890
H	4.3651590	-0.3723180	-2.6401790
C	1.1446530	1.1229340	0.4463010
H	1.2310010	1.3236820	1.5157140
C	2.3654550	0.3194140	0.0233130
C	-3.2876930	0.6104520	-0.4861640
C	2.9626020	-0.5348250	0.9565440
H	2.5543950	-0.5840620	1.9595780
C	0.9491110	2.4529560	-0.2881570
H	0.7291050	2.2636750	-1.3453630
H	1.9013530	2.9905410	-0.2646590
C	4.0523820	-1.3227970	0.6007520
H	4.5069460	-1.9766580	1.3362160
C	4.5618440	-1.2684830	-0.6953070
H	5.4133600	-1.8789230	-0.9727170
C	-0.1600380	3.3113460	0.3214710
H	-1.1301520	2.8142270	0.2681000
H	0.0499110	3.5285980	1.3726480
H	-0.2465220	4.2637480	-0.2064420

Table S5. Atomic coordinates of the optimized structure of DHIA.

Symbol	X	Y	Z
Se	-2.6908560	1.1283120	-0.4152460
O	-1.4211430	-2.7997140	-0.3695690
C	-1.3588530	-1.5925890	-0.5259170
N	-0.2130400	-0.8825250	-0.5352360
H	-0.2503890	0.1214140	-0.6260050
C	-2.6701280	-0.8344900	-0.7543740
H	-3.4351900	-1.2948740	-0.1353950
H	-2.9671430	-0.9176360	-1.8019210
N	-1.6122120	1.0006920	2.3876580
C	-2.0492410	1.0352050	1.3160950
C	1.0817050	-1.4933910	-0.2011690
C	1.2137460	-1.7925070	1.3129010
H	1.1853110	-2.3962530	-0.8040850
C	1.7940620	-0.4997230	1.9300080
H	1.9262400	-2.6123960	1.4362700
H	0.2655220	-2.1048230	1.7474540
H	2.4304570	-0.6985600	2.7950880
H	0.9946600	0.1697710	2.2646120
C	2.1676220	-0.4670090	-0.4357860
C	2.5531610	0.1151190	0.7758490
C	3.5097350	1.1252810	0.7857740
C	2.7190740	-0.0509190	-1.6419960
H	2.4111570	-0.5068470	-2.5767610
C	3.6824670	0.9575860	-1.6283500
C	4.0727220	1.5402560	-0.4214990
H	4.8248580	2.3209580	-0.4228050
H	4.1339370	1.2874580	-2.5567170

H	3.8191640	1.5828100	1.7190140

Table S6. Atomic coordinates of the optimized structure of MNA.

Symbol	X	Y	Z
Se	3.3140290	1.4163030	0.6524740
O	2.6665740	-2.6489960	0.2614710
C	2.4036400	-1.4639020	0.3723380
N	1.2111410	-0.9119450	0.0665190
H	1.0968610	0.0887060	0.1328460
C	3.4910630	-0.5457190	0.9364730
H	4.4461300	-0.8628590	0.5268110
H	3.5248620	-0.6485980	2.0230300
N	3.2368630	1.3143750	-2.3509660
C	-2.0471330	-0.4457650	-0.9791990
C	-3.2719320	0.1055580	-0.5187100
C	0.1366170	-1.6830700	-0.5743660
H	0.2243680	-2.6945660	-0.1691460
C	-1.1909260	-1.1001220	-0.1271330
C	3.2866970	1.3425320	-1.1947370
C	-1.5433390	-1.2221980	1.2446820
C	0.3586610	-1.7526590	-2.0852470
H	0.3870640	-0.7554780	-2.5302550
H	-0.4300730	-2.3347460	-2.5669430
H	1.3152880	-2.2373800	-2.2824610
C	-2.7165440	-0.7030020	1.7230160
C	-3.6165830	-0.0233140	0.8609560
C	-4.1644600	0.7826280	-1.3867260
C	-4.8389900	0.5275440	1.3183370
C	-5.3425300	1.3075070	-0.9134620
C	-5.6833990	1.1785830	0.4519470
H	-3.9010300	0.8800300	-2.4343590
H	-6.0169560	1.8230940	-1.5870870
H	-6.6160450	1.5964340	0.8125720
H	-5.0978670	0.4263450	2.3667590
H	-2.9762110	-0.8093210	2.7707970
H	-0.8631320	-1.7388010	1.9129880
H	-1.8039040	-0.3398130	-2.0293460

Table S7. Atomic coordinates of the optimized structure of CHA.

Symbol	X	Y	Z
Se	-3.1620250	-0.6485950	-0.7401540
O	-0.3765130	-0.6955600	2.3223880
C	-0.8264760	-0.5281030	1.2018840
N	-0.2443070	0.2071780	0.2329700
H	-0.7188340	0.2985550	-0.6534120
C	-2.1417630	-1.2363790	0.8658650
H	-2.7972140	-1.1576650	1.7289800
H	-1.9441360	-2.2929450	0.6739270
N	-3.5384420	2.2060770	0.1234530

C	0.9585490	1.0136460	0.4567730
H	1.1382030	0.9616620	1.5331640
C	-3.4028140	1.0999470	-0.1898730
C	0.6540660	2.4587400	0.0545250
H	0.5145390	2.5411110	-1.0288970
H	1.4645000	3.1298950	0.3395650
H	-0.2609320	2.8009770	0.5409150
C	2.1762680	0.4037510	-0.2682460
C	3.4590660	1.2049710	0.0122580
C	2.3782090	-1.0715920	0.1156680
H	1.9779430	0.4507620	-1.3503860
C	4.6896010	0.5861000	-0.6622360
H	3.6190830	1.2387780	1.0982130
H	3.3456490	2.2391410	-0.3211950
C	3.6046490	-1.6866830	-0.5660850
H	2.4881400	-1.1404580	1.2045570
H	1.4840280	-1.6449520	-0.1400740
C	4.8735710	-0.8822860	-0.2687960
H	5.5820330	1.1656030	-0.4072340
H	4.5731380	0.6546020	-1.7513350
H	3.7267790	-2.7254850	-0.2446590
H	3.4414940	-1.7118610	-1.6513610
H	5.7318660	-1.3124720	-0.7938320
H	5.0963790	-0.9440030	0.8038120

Table S8. Atomic coordinates of the optimized structure of MMBA.

Symbol	X	Y	Z
Se	-3.3344480	-0.3988390	-0.5574020
O	-0.4663250	-1.0362140	1.9030240
C	-0.6625430	-0.8256360	0.7148460
N	0.0864100	0.0251020	-0.0359970
C	-1.8158170	-1.5657760	0.0436200
H	-2.2199340	-2.2501840	0.7810540
H	-1.5204900	-2.1049150	-0.8563710
N	-2.6610800	2.0700630	1.0081120
C	3.4046720	1.0527300	-0.5170870
H	3.1513760	2.0568440	-0.8333660
C	4.6425680	0.5171420	-0.8758340
H	5.3308450	1.1070470	-1.4703280
C	1.1295240	0.8270920	0.6483280
H	0.9880420	0.6054320	1.7050270
C	2.5046090	0.3118660	0.2482800
C	-2.9122360	1.0982500	0.4308380
C	2.8696510	-0.9779520	0.6544440
H	2.1773760	-1.5528660	1.2597700
C	0.8930390	2.3212120	0.4365480
H	0.9803550	2.6170910	-0.6115250
H	1.6258930	2.8945300	1.0079670
H	-0.1054550	2.5878030	0.7841270

C	4.1016270	-1.5125500	0.2994950
H	4.3716930	-2.5096340	0.6282140
C	4.9935190	-0.7654270	-0.4708480
H	5.9559350	-1.1805100	-0.7467230
C	-0.0493610	0.2106560	-1.4733100
H	-0.4791390	-0.6694270	-1.9454060
H	-0.6724690	1.0751560	-1.7170310
H	0.9449840	0.3580710	-1.8986750

Table S9. Atomic coordinates of the optimized structure of DMBA.

Symbol	X	Y	Z
Se	3.6376830	-0.0958500	0.7804490
O	0.7113670	-1.2591320	1.8538100
C	0.7736610	-0.5101460	0.8897320
N	0.0310770	-0.6791590	-0.2447040
C	1.7795850	0.6302120	0.9099370
H	1.7659670	1.0854380	1.8987020
H	1.6627860	1.3879240	0.1479190
N	3.1246510	-2.1400190	-1.3582240
C	-3.2018080	-1.4071430	-0.9644610
H	-2.9573250	-1.5092610	-2.0148650
C	-4.5005130	-1.0528090	-0.6012690
H	-5.2435150	-0.8729060	-1.3697060
C	-0.7759010	-1.9279970	-0.3311770
H	-0.3767150	-2.5529960	0.4644710
C	-2.2277790	-1.6365860	0.0084530
C	3.3147020	-1.3431200	-0.5396740
C	-2.5860450	-1.5264240	1.3580100
H	-1.8276850	-1.6956170	2.1135940
C	-0.5429170	-2.6515940	-1.6563060
H	-0.8648770	-2.0746470	-2.5259220
H	-1.1039650	-3.5885860	-1.6565060
H	0.5178760	-2.8780810	-1.7706980
C	-3.8823850	-1.1788260	1.7219390
H	-4.1441820	-1.0995920	2.7709310
C	-4.8435360	-0.9342200	0.7415360
H	-5.8535100	-0.6605340	1.0237220
C	-0.1741340	0.3452510	-1.2944980
H	-1.0656290	-0.0012730	-1.8215320
C	0.9579900	0.3764240	-2.3269860
H	0.6536130	0.9525270	-3.2034590
H	1.8735290	0.8201640	-1.9321220
H	1.1993330	-0.6349450	-2.6455730
C	-0.5621990	1.7077490	-0.7200840
C	-0.0577870	2.8999020	-1.2451750
C	-1.4818780	1.7793680	0.3328190
C	-0.4504450	4.1322940	-0.7236850
H	0.6513920	2.8800080	-2.0621810
C	-1.8745740	3.0074950	0.8515730

H	-1.8937660	0.8694940	0.7475000
C	-1.3578050	4.1914350	0.3280100
H	-0.0423320	5.0447560	-1.1429630
H	-2.5887900	3.0380750	1.6663110
H	-1.6618190	5.1486700	0.7349690

Table S10. Atomic coordinates of the optimized structure of MBA-S.

Symbol	X	Y	Z
O	2.0091460	2.5067280	-0.0398620
C	1.8030750	1.3323660	-0.2927250
N	0.6055520	0.7219470	-0.2196670
H	0.5211480	-0.2343170	-0.5258980
C	3.0059020	0.4776140	-0.7143720
H	3.8002780	0.6418070	0.0112020
H	3.3583140	0.8240540	-1.6875560
N	1.9691440	-2.1006640	1.6876660
C	-1.7916000	-0.8244430	0.5548740
H	-0.9476880	-1.1686360	1.1439280
C	-2.8743770	-1.6734790	0.3485010
H	-2.8627360	-2.6710520	0.7718560
C	-0.6158430	1.3934870	0.2500790
H	-0.7471490	2.2993700	-0.3479410
C	-1.7893120	0.4663600	0.0129710
C	2.3207390	-1.7745210	0.6333510
C	-2.8904700	0.8888830	-0.7309290
H	-2.8946490	1.8862730	-1.1570990
C	-0.4889440	1.7964620	1.7258140
H	-0.3290120	0.9143770	2.3493130
H	-1.4071740	2.2896830	2.0514080
H	0.3481550	2.4818380	1.8551750
C	-3.9790890	0.0427240	-0.9306220
H	-4.8286120	0.3851710	-1.5100400
C	-3.9722170	-1.2411870	-0.3931500
H	-4.8166040	-1.9019190	-0.5506100
S	2.7714060	-1.3409410	-0.9464740

Table S11. Atomic coordinates of the optimized structure of ^{R}Pyr/^{R}MBA.

Symbol	X	Y	Z
O	0.3442820	2.1223550	-2.1771010
O	-2.1412480	2.7918590	1.4012660
N	-0.0810720	-0.1025960	-2.6360710
N	-1.6725400	0.5222210	1.3712810
N	-0.1242100	-1.6412910	0.5699470
N	-1.6066100	-2.3458870	-2.2624330
C	-2.4489190	1.5072900	1.7338510
C	-3.2917070	-0.9999350	2.3525370
C	0.7055770	0.9329550	-2.7500970
C	-0.8408910	3.2262240	1.2063600
C	-0.9510010	2.5889900	-2.2253840

C	-0.4642910	3.6739860	-0.0409380
C	-1.3515510	3.4423540	-1.2141600
C	-2.0816110	-0.7396510	1.6590180
C	2.5772200	-1.1187770	-0.6057140
C	0.7749320	4.3820940	-0.1558630
C	0.3218230	-1.2680400	-3.1901950
C	1.5998150	4.5568050	1.0004970
C	-3.6678050	1.3712090	2.4337200
H	-4.2403820	2.2530660	2.6812530
C	0.6418980	-2.6491460	0.1706340
C	1.9031600	-2.3782160	-0.5740610
C	-0.5108960	-2.4431690	-3.0285760
C	-0.0155780	3.3605680	2.3425480
H	-0.3751170	2.9867920	3.2929190
C	-1.2720410	-1.8684740	1.2360150
C	-1.7216400	-3.1804340	1.5433880
C	-3.6468830	-3.1942940	-1.2766500
C	-2.6291230	4.0777050	-1.3193530
C	1.1902880	4.0000740	2.2385810
H	1.8320920	4.0995470	3.1056930
C	-4.0802550	0.1069040	2.7413600
H	-5.0170100	-0.0608450	3.2587470
C	-2.4361950	-3.3684320	-2.1215700
C	2.8004260	5.3029560	0.8913670
H	3.4125950	5.4288500	1.7775390
C	3.8376240	-1.0236770	-1.2841250
C	-4.2157310	-1.9258620	-0.9517920
C	-0.1402960	-3.6473580	-3.6796990
C	1.5312920	-1.3850060	-3.9198190
C	2.7555810	1.2454270	-0.0243970
H	2.3324870	2.1234650	0.4431030
C	4.0044580	1.3671140	-0.6999740
C	2.0656300	0.0765520	0.0032610
H	1.0881770	0.0427530	0.4496220
C	-5.4096100	-1.8885870	-0.1570500
C	4.5369740	0.2170660	-1.3412830
C	-2.9460190	-3.3930860	2.2389580
H	-3.2650320	-4.4098850	2.4332710
C	-3.6607880	-0.6643650	-1.3667260
H	-2.7298110	-0.6621760	-1.9066510
C	1.2038610	4.9572450	-1.3788610
H	0.5874140	4.8315070	-2.2585170
C	-6.0047930	-0.6398680	0.1978370
C	1.9568680	0.9287880	-3.4008460
H	2.5597150	1.8255720	-3.4075780
C	-1.7797400	2.3042020	-3.3343980
H	-1.4327760	1.6181030	-4.0933380
C	-3.7054510	-2.3368040	2.6273310

H	-4.6509740	-2.4881110	3.1343890
C	-0.8888250	-4.2446260	1.1441430
H	-1.1769610	-5.2621330	1.3849080
C	4.3995880	-2.1551480	-1.9411800
C	2.4856340	-3.4562780	-1.2609270
H	1.9574990	-4.3957690	-1.3198080
C	-4.2435970	0.5162250	-1.0369930
H	-3.7821750	1.4422980	-1.3490600
C	3.6944950	-3.3606630	-1.9192420
H	4.0906540	-4.2202260	-2.4476960
C	5.7623280	0.3267220	-2.0617340
C	0.2802770	-3.9923900	0.4799630
H	0.9316850	-4.8144910	0.2280050
C	-4.2657790	-4.3515080	-0.7781780
H	-3.8165420	-5.3157230	-0.9735990
C	3.1781520	5.8578860	-0.3062040
H	4.0946470	6.4319480	-0.3773200
C	4.6917510	2.5856230	-0.7828650
H	4.2727340	3.4550850	-0.2951730
C	2.3580150	-0.2406190	-3.9917940
H	3.3124880	-0.3013240	-4.5016160
C	-3.4737200	3.7869420	-2.4361300
C	-6.0054260	-3.0914680	0.3211990
C	-5.4344680	0.5808290	-0.2561360
C	1.0643410	-3.7110040	-4.4428680
H	1.3271380	-4.6451170	-4.9271790
C	-3.0126230	2.8881130	-3.4297170
H	-3.6558560	2.6619470	-4.2723860
C	5.8833690	2.6810660	-1.4888540
H	6.4017670	3.6314910	-1.5443750
C	2.3718660	5.6763800	-1.4515650
H	2.6764630	6.1138040	-2.3951680
C	1.8775790	-2.6244150	-4.5409390
H	2.8083590	-2.6783870	-5.0939960
C	-2.1703080	-4.6010840	-2.7846690
H	-2.8690420	-5.4231490	-2.7262250
C	-1.0285800	-4.7348750	-3.5343020
H	-0.8110280	-5.6698410	-4.0400240
C	-5.4100600	-4.3130800	-0.0056220
H	-5.8432550	-5.2337650	0.3694760
C	-7.1554540	-0.5977330	1.0404840
C	5.6437810	-2.0270660	-2.6389570
H	6.0514790	-2.9076030	-3.1238110
C	-7.1680050	-3.0228970	1.1555590
H	-7.5999740	-3.9533830	1.5080580
C	-7.7162840	-1.8314690	1.5065840
H	-8.5931950	-1.7932820	2.1438560
C	6.2946670	-0.8378310	-2.7025660

H	7.2337510	-0.7497500	-3.2382920
C	-3.0985810	5.0020820	-0.3504000
H	-2.4633590	5.2480400	0.4891230
C	-6.0160810	1.8021200	0.1113050
H	-5.5670470	2.7242000	-0.2386290
C	6.4157630	1.5637710	-2.1230390
H	7.3492560	1.6381910	-2.6702180
C	-7.1366910	1.8296990	0.9319040
H	-7.5737530	2.7805610	1.2147420
C	-7.6989230	0.6445080	1.3972180
H	-8.5723440	0.6704260	2.0397840
C	-4.7517350	4.3933930	-2.5210980
H	-5.3850660	4.1495670	-3.3669480
C	-4.3402120	5.5781240	-0.4638370
H	-4.6769540	6.2803340	0.2900790
C	-5.1828310	5.2676990	-1.5546510
H	-6.1626190	5.7247470	-1.6280490
Se	0.8055820	0.2331510	3.3916460
O	3.4383380	-2.1623170	4.8476790
C	2.6846520	-2.0028800	3.9040650
N	2.9869990	-2.2236230	2.5990210
H	2.3211620	-1.8882410	1.9204240
C	1.2460380	-1.5525610	4.1538820
H	1.0695550	-1.5290100	5.2240950
H	0.5184120	-2.1995580	3.6593420
N	2.8831180	1.9309930	4.7404340
C	5.0108290	-0.1674940	2.4611500
H	4.1728550	-0.0250440	3.1254060
C	5.8758830	0.8992830	2.2298330
H	5.6812970	1.8496840	2.7127800
C	4.2971380	-2.5917470	2.0539380
H	4.0723350	-2.9908290	1.0616960
C	5.2232200	-1.3991760	1.8479730
C	2.1007380	1.2136350	4.2753950
C	6.3236810	-1.5449870	0.9981290
H	6.4866830	-2.4885250	0.4883530
C	4.9647860	-3.7165910	2.8570900
H	5.2422270	-3.3735400	3.8504250
H	5.8587120	-4.0525820	2.3285430
H	4.2801860	-4.5628260	2.9567720
C	7.1919710	-0.4846510	0.7699920
H	8.0290350	-0.6116320	0.0936890
C	6.9688200	0.7457860	1.3844790
H	7.6321290	1.5799220	1.1903010

Table S12. Atomic coordinates of the optimized structure of *R*Pyr/*S*MBA.

Symbol	X	Y	Z
O	1.2931550	3.0387680	0.4743260
O	-1.3892150	2.7733770	-2.6691050

N	2.2773880	1.8977260	2.1092200
N	-1.4758430	0.4971050	-3.1349960
N	-2.2577510	-2.0332400	-2.4041450
N	2.8274560	-0.5935730	3.0584320
C	-0.9811790	1.6777290	-3.3749460
C	0.0525020	-0.4208630	-4.7770940
C	1.9884460	3.0849470	1.6405350
C	-1.8780980	2.6873180	-1.3756380
C	1.1225130	4.1442910	-0.3380470
C	-1.2900750	3.5225890	-0.4425940
C	-0.1440610	4.3913690	-0.8274510
C	-0.9473980	-0.5613990	-3.7824960
C	-4.4793360	-2.3492140	-0.5057580
C	-1.7805630	3.5033640	0.8984970
C	2.9039180	1.7938510	3.2933300
C	-2.8404900	2.6072750	1.2447870
C	0.0018440	1.9509160	-4.3540510
H	0.3412490	2.9680390	-4.4956570
C	-2.6507860	-3.2432860	-2.0279070
C	-3.4975640	-3.3234810	-0.8143620
C	3.1858590	0.4687410	3.8052360
C	-2.9646320	1.8484440	-1.0539850
H	-3.3766140	1.2052370	-1.8133760
C	-1.3798530	-1.8961790	-3.4140230
C	-0.8287680	-3.0141780	-4.0972450
C	2.5600700	-2.8825380	2.5759610
C	-0.3193550	5.4984320	-1.7168430
C	-3.4234660	1.8068570	0.2350160
H	-4.2281630	1.1354100	0.4996480
C	0.5032940	0.8907700	-5.0604610
H	1.2702690	1.0400770	-5.8124020
C	3.0327780	-1.8214250	3.5138600
C	-3.2711230	2.5244630	2.5928090
H	-4.0604670	1.8227450	2.8387430
C	-5.0650910	-2.3469930	0.7969460
C	3.3911210	-3.3070570	1.5222320
C	3.8108570	0.3265520	5.0698970
C	3.2788520	2.9208900	4.0629770
C	-5.8333740	-0.4115810	-1.1034250
H	-6.1502440	0.3260310	-1.8326470
C	-6.3774720	-0.3358980	0.2193200
C	-4.9202760	-1.3559210	-1.4453050
H	-4.4955180	-1.3596270	-2.4364540
C	2.8177740	-4.0532990	0.4520100
C	-5.9862380	-1.3232670	1.1672600
C	0.1567600	-2.8234440	-5.1128800
H	0.5665090	-3.6949580	-5.6111630
C	4.7831150	-2.9608980	1.4483620

H	5.2217030	-2.3981890	2.2632350
C	-1.2369070	4.3220180	1.9221110
H	-0.4680870	5.0382410	1.6657100
C	3.6112350	-4.4022190	-0.6775360
C	2.3090540	4.2871870	2.3175740
H	2.0417890	5.2469660	1.9002020
C	2.2454580	4.9072730	-0.7224160
H	3.2224300	4.6209640	-0.3585920
C	0.5843640	-1.5728790	-5.4342890
H	1.3481490	-1.4288140	-6.1906140
C	-1.2952440	-4.2896900	-3.7155340
H	-0.9286730	-5.1666100	-4.2384490
C	-4.7009830	-3.3371450	1.7546880
C	-3.2057340	-4.3182950	0.1284430
H	-2.4509100	-5.0580130	-0.1072980
C	5.5449480	-3.3174720	0.3814780
H	6.5937880	-3.0443910	0.3424840
C	-3.7907230	-4.3330250	1.3826560
H	-3.5051400	-5.0866750	2.1070970
C	-6.5031990	-1.2692410	2.4947820
C	-2.2044400	-4.4123250	-2.6941880
H	-2.5834550	-5.3826470	-2.3998960
C	1.2180100	-3.2568980	2.6095380
H	0.5825010	-2.9083000	3.4135150
C	-2.6944140	3.3031300	3.5649800
H	-3.0213520	3.2229100	4.5949620
C	-7.2581230	0.6811620	0.6117030
H	-7.5467650	1.4356720	-0.1114400
C	2.9568650	4.1877690	3.5246900
H	3.2115320	5.0838690	4.0798910
C	0.8095110	6.2908550	-2.0962420
C	1.4317960	-4.3844060	0.4764230
C	4.9867870	-4.0339510	-0.7281190
C	4.1816380	1.4936950	5.8127910
H	4.6638240	1.3652430	6.7752190
C	2.0880940	5.9596920	-1.5826740
H	2.9479200	6.5433820	-1.8922090
C	-7.7465770	0.7334840	1.9123220
H	-8.4203930	1.5313680	2.2021840
C	-1.6753840	4.2190980	3.2195940
H	-1.2360260	4.8465910	3.9867450
C	3.9283430	2.7387030	5.3251350
H	4.2078920	3.6181120	5.8949230
C	3.6344700	-2.0645560	4.7649580
H	3.7815880	-3.0829510	5.1008730
C	4.0269910	-0.9890940	5.5324590
H	4.4976580	-1.1423590	6.4976060
C	0.6607490	-4.0025530	1.5798270

H	-0.3956210	-4.2402650	1.6048350
C	3.0189560	-5.0768980	-1.7850600
C	-5.2444620	-3.2652560	3.0777180
H	-4.9327610	-4.0109440	3.7994920
C	0.8654510	-5.0616690	-0.6531260
H	-0.1946470	-5.2819990	-0.6391440
C	1.6208200	-5.3919050	-1.7310030
H	1.1712710	-5.8862170	-2.5846560
C	-6.1007690	-2.2750840	3.4339490
H	-6.4900490	-2.2215760	4.4445560
C	-1.5930460	5.8550450	-2.2292910
H	-2.4539040	5.2687600	-1.9382560
C	5.7390230	-4.3565550	-1.8654730
H	6.7849500	-4.0732180	-1.9039340
C	-7.3763550	-0.2300120	2.8444650
H	-7.7604800	-0.1842570	3.8574920
C	5.1542700	-5.0203900	-2.9380110
H	5.7493070	-5.2572210	-3.8123630
C	3.8099330	-5.3752700	-2.9016380
H	3.3575700	-5.8819660	-3.7470050
C	0.6249010	7.3833040	-2.9808260
H	1.4905150	7.9718840	-3.2655090
C	-1.7394470	6.9237790	-3.0788120
H	-2.7223490	7.1791320	-3.4574840
C	-0.6206940	7.6949240	-3.4652610
H	-0.7506460	8.5327430	-4.1403430
Se	-1.5921170	-1.0498330	0.7439800
O	0.4464750	0.5186770	-1.1805210
C	0.8253760	0.1062550	-0.0896850
N	1.9923210	-0.5265620	0.1313200
H	2.3017630	-0.5658320	1.1014200
C	-0.0786250	0.2037950	1.1211070
H	-0.4991740	1.1995060	1.2014610
H	0.3934680	-0.1077910	2.0459860
N	-1.9059940	-2.0790910	3.5507360
C	4.8730860	0.9456460	-0.5912740
H	5.2751030	0.2739710	0.1603850
C	5.5287390	2.1414450	-0.8766190
H	6.4415240	2.3974770	-0.3498760
C	3.7011580	0.5903070	-1.2618980
C	-1.7753860	-1.6520040	2.4799720
C	3.1839350	1.4671310	-2.2202490
H	2.2529010	1.2277870	-2.7117550
C	3.8393900	2.6584000	-2.5122900
H	3.4206290	3.3318110	-3.2512680
C	5.0160130	2.9991550	-1.8465470
H	5.5263780	3.9272710	-2.0799710
C	3.0128200	-0.7204930	-0.9052570

H	3.7641220	-1.3469910	-0.4257310
C	2.4699280	-1.4936590	-2.1095410
H	3.2966860	-1.7917670	-2.7580250
H	1.9577600	-2.3927500	-1.7686110
H	1.7616880	-0.9027910	-2.6815970

Table S13. Atomic coordinates of the optimized structure of ^{R}Pyr/^{R}EBA.

Symbol	X	Y	Z
O	-0.1350080	3.4465900	-0.2818840
O	2.4084560	2.0642830	2.7330370
N	-1.6667290	2.7094370	-1.7205240
N	1.9531010	-0.2097130	2.9702860
N	2.0614220	-2.7867800	2.0240910
N	-3.0142480	0.5049480	-2.6259850
C	1.8144540	1.0215540	3.3773460
C	0.4580330	-0.9073300	4.7509350
C	-1.0374070	3.7569550	-1.2531300
C	2.8208760	2.0317190	1.4139810
C	0.2714100	4.3239750	0.7016670
C	2.4457970	3.1110670	0.6292750
C	1.5577270	4.1684810	1.1831580
C	1.2696990	-1.1771270	3.6217700
C	3.9340830	-3.4151900	-0.1491440
C	2.8928000	3.1624070	-0.7254240
C	-2.5932200	2.8740240	-2.6792420
C	3.6852260	2.0899770	-1.2431560
C	1.0583700	1.4122760	4.5075560
H	1.0116730	2.4592930	4.7734290
C	2.1125490	-4.0122380	1.5197940
C	2.7816410	-4.1609540	0.2056850
C	-3.3099960	1.7082330	-3.1567060
C	3.6495660	1.0028520	0.9239060
H	3.8955680	0.1732730	1.5659010
C	1.3424050	-2.5410610	3.1324450
C	0.6194440	-3.5629520	3.8068140
C	-3.3185680	-1.8150980	-2.2803860
C	1.9975830	5.0326020	2.2335400
C	4.0568730	1.0318410	-0.3832590
H	4.6510420	0.2206270	-0.7799680
C	0.3852810	0.4372950	5.1891470
H	-0.2238160	0.6843440	6.0517880
C	-3.6985640	-0.5687650	-3.0004420
C	4.0736770	2.1040930	-2.6072520
H	4.6579890	1.2720060	-2.9845690
C	4.3744070	-3.4281920	-1.5075570
C	-4.1976320	-2.4218400	-1.3578220
C	-4.3305160	1.8753960	-4.1264620
C	-2.9159340	4.1466510	-3.2111940
C	5.7801590	-1.9276800	0.4212730

H	6.3402800	-1.3631290	1.1587440
C	6.1950250	-1.8556820	-0.9478130
C	4.6977560	-2.6533010	0.8003020
H	4.3842310	-2.6527090	1.8320520
C	-3.6788790	-3.4101890	-0.4669380
C	5.4806270	-2.6233870	-1.9102720
C	-0.1757280	-3.2454280	4.9489600
H	-0.7219370	-4.0414660	5.4425610
C	-5.5705620	-2.0264740	-1.2027240
H	-5.9785690	-1.2811890	-1.8724090
C	2.5639020	4.2323930	-1.5988180
H	1.9986470	5.0696770	-1.2108630
C	-4.4975240	-3.9367940	0.5735190
C	-1.2291350	5.0681160	-1.7444960
H	-0.6470550	5.8941290	-1.3614640
C	-0.6297820	5.2580220	1.2582890
H	-1.6405210	5.3084090	0.8800980
C	-0.2538370	-1.9634250	5.3987410
H	-0.8663080	-1.7190170	6.2599020
C	0.7280160	-4.8707390	3.2877530
H	0.2193340	-5.6848230	3.7930770
C	3.6907510	-4.2115330	-2.4813160
C	2.1663870	-4.9652270	-0.7633080
H	1.2853020	-5.5335450	-0.4922700
C	-6.3579380	-2.5526370	-0.2287980
H	-7.3888500	-2.2311090	-0.1288450
C	2.6057460	-4.9962440	-2.0753640
H	2.0770730	-5.5909160	-2.8109780
C	5.8658900	-2.5684870	-3.2816190
C	1.4687390	-5.1039370	2.1547520
H	1.5696880	-6.1033910	1.7512310
C	-1.9993220	-2.2597110	-2.3859670
H	-1.3376380	-1.7941930	-3.1045890
C	3.7122080	3.1404870	-3.4302430
H	4.0058850	3.1387090	-4.4733320
C	7.2583080	-1.0452310	-1.3681950
H	7.7939700	-0.4556170	-0.6326460
C	-2.1792370	5.2472170	-2.7204970
H	-2.3670240	6.2363410	-3.1234950
C	1.0960420	5.9929940	2.7907030
C	-2.3179040	-3.8180610	-0.5658030
C	-5.8511720	-3.5129780	0.7055420
C	-4.6261250	3.1792120	-4.6373970
H	-5.4074160	3.2791600	-5.3824460
C	-0.2231520	6.0704540	2.2828370
H	-0.9157090	6.7810250	2.7200740
C	7.6156050	-0.9844670	-2.7105390
H	8.4346580	-0.3460200	-3.0207770

C	2.9585290	4.2193520	-2.9137530
H	2.6904550	5.0445260	-3.5638560
C	-3.9437210	4.2703840	-4.1975380
H	-4.1715490	5.2561440	-4.5879670
C	-4.7180120	-0.5022740	-3.9754750
H	-5.2357170	-1.4052610	-4.2726750
C	-5.0254370	0.7169630	-4.5339560
H	-5.8019620	0.8001610	-5.2867500
C	-1.5111430	-3.2631030	-1.5650090
H	-0.4825580	-3.5837020	-1.6637050
C	-3.9531390	-4.8583020	1.5163790
C	4.1082410	-4.1479350	-3.8495160
H	3.5580410	-4.7302950	-4.5792120
C	-1.8000340	-4.7484580	0.3930680
H	-0.7546220	-5.0206190	0.3260250
C	-2.5771960	-5.2425870	1.3893430
H	-2.1627850	-5.9278620	2.1204450
C	5.1422160	-3.3585440	-4.2342020
H	5.4352520	-3.3045500	-5.2767570
C	3.3220660	4.9845070	2.7407130
H	4.0161940	4.2718140	2.3170020
C	-6.6312070	-4.0225440	1.7521320
H	-7.6608210	-3.6967340	1.8495550
C	6.9306220	-1.7380950	-3.6577800
H	7.2150060	-1.6885150	-4.7030270
C	-6.0937090	-4.9262880	2.6615610
H	-6.7089010	-5.3084280	3.4678830
C	-4.7702090	-5.3383610	2.5484240
H	-4.3544760	-6.0363000	3.2668530
C	1.5401640	6.8402440	3.8373370
H	0.8423790	7.5583920	4.2545900
C	3.7239830	5.8245040	3.7492370
H	4.7412630	5.7713560	4.1194980
C	2.8252450	6.7592410	4.3109480
H	3.1557930	7.4119490	5.1104390
Se	1.3684400	-1.1966100	-0.6021780
O	-0.1261790	0.9693560	1.4608040
C	-0.6112130	0.6093340	0.3945190
N	-1.9173530	0.2998060	0.2268070
H	-2.2553200	0.2783850	-0.7345230
C	0.2419960	0.4411530	-0.8443260
H	0.9187220	1.2816430	-0.9391260
H	-0.3472540	0.3085710	-1.7447510
N	1.3660900	-1.9765880	-3.5058960
C	-4.8631950	1.4391900	-0.1006010
H	-5.1198130	0.4135080	-0.3295890
C	-5.5799900	2.4745610	-0.6934800
H	-6.3861150	2.2465230	-1.3815820

C	-2.8927510	0.6037790	1.2775910
H	-2.3055630	0.9951450	2.1100480
C	-3.8001300	1.7090070	0.7637510
C	1.3698400	-1.6426760	-2.3948840
C	-3.4979230	3.0406940	1.0551420
H	-2.6725200	3.2566320	1.7238440
C	-3.6070410	-0.6690340	1.7422740
H	-4.1719820	-1.0951710	0.9146450
H	-2.8350310	-1.4017210	1.9920610
C	-4.2177100	4.0789880	0.4714320
H	-3.9704810	5.1089470	0.7044630
C	-5.2535210	3.7997100	-0.4175540
H	-5.8032440	4.6066140	-0.8877190
C	-4.5308900	-0.4436970	2.9371110
H	-5.3245520	0.2688940	2.6973420
H	-5.0010880	-1.3819780	3.2413600
H	-3.9763300	-0.0487030	3.7941370

Table S14. Atomic coordinates of the optimized structure of *R*Pyr/*S*EBA.

Symbol	X	Y	Z
O	-0.4858980	3.6715390	-0.9288280
O	-3.3300110	1.0751310	1.4707810
N	0.2798680	1.9897530	-2.2932090
N	-2.0960450	-0.8333780	1.1093760
N	0.1486870	-1.9932570	0.1190920
N	0.1190060	-0.5994360	-3.0582400
C	-3.1988100	-0.2881960	1.5412560
C	-3.0342220	-3.0118060	1.6363890
C	0.4137330	3.2099110	-1.8570980
C	-2.3454030	1.9034190	1.9764330
C	-1.8424590	3.5143120	-1.1287770
C	-2.0690170	3.0896210	1.3185730
C	-2.6580230	3.3559410	-0.0211020
C	-2.0051520	-2.1825270	1.1291650
C	2.3845660	-0.1647850	-0.4291240
C	-1.1955930	4.0291320	1.9579100
C	1.2018440	1.5202460	-3.1601570
C	-0.5638660	3.6863640	3.1942270
C	-4.3077010	-1.0049630	2.0375470
H	-5.1898830	-0.4702110	2.3574770
C	1.3092520	-2.4783730	-0.2884450
C	2.3152790	-1.5321080	-0.8217950
C	1.0930510	0.1452590	-3.5939660
C	-1.7484090	1.5791010	3.2148070
H	-2.0242180	0.6508380	3.6982300
C	-0.7927690	-2.7965060	0.6316480
C	-0.6320460	-4.2014340	0.7257260
C	-1.1932780	-2.6046320	-2.8363880
C	-4.0771110	3.4231630	-0.2087850

C	-0.8599040	2.4399920	3.7991010
H	-0.3860310	2.1840370	4.7386790
C	-4.2115890	-2.3727560	2.0884790
H	-5.0324300	-2.9688110	2.4680410
C	-0.0689820	-1.8495150	-3.4439470
C	0.3283220	4.6044730	3.8035740
H	0.8117210	4.3161140	4.7302640
C	3.4692900	0.6318810	-0.9137410
C	-2.3677990	-1.9799580	-2.3197100
C	2.0061880	-0.3566560	-4.5522750
C	2.2683560	2.3146420	-3.6467360
C	1.6104930	1.7434400	0.8895370
H	0.8768280	2.1845940	1.5503550
C	2.6997060	2.5502730	0.4434850
C	1.4447930	0.4662960	0.4593610
H	0.5588610	-0.0756010	0.7403500
C	-3.4171770	-2.8092820	-1.8058530
C	3.6254790	1.9818300	-0.4757230
C	-1.6871020	-5.0021240	1.2586020
H	-1.5521420	-6.0768080	1.3095080
C	-2.5712120	-0.5568180	-2.2816570
H	-1.7694710	0.0865950	-2.5983130
C	-0.9400450	5.3149510	1.4152770
H	-1.4344150	5.6025280	0.4981050
C	-4.6137480	-2.2254810	-1.2889400
C	1.4504450	4.0887100	-2.2313770
H	1.4991900	5.0774410	-1.7988750
C	-2.3724100	3.6351210	-2.4333130
H	-1.6933520	3.7231770	-3.2704490
C	-2.8472490	-4.4287970	1.6827120
H	-3.6543150	-5.0411170	2.0670360
C	0.6129230	-4.7168580	0.2983240
H	0.8029210	-5.7818520	0.3793060
C	4.4090400	0.0933770	-1.8382450
C	3.2615010	-2.0238320	-1.7287540
H	3.1885830	-3.0504930	-2.0603350
C	-3.7103700	-0.0095320	-1.7877350
H	-3.8144290	1.0657070	-1.7525600
C	4.2701430	-1.2347520	-2.2445380
H	4.9771870	-1.6512510	-2.9512230
C	4.6990630	2.7807310	-0.9675230
C	1.5826010	-3.8726110	-0.1860420
H	2.5548470	-4.2591560	-0.4580320
C	-1.0898720	-4.0006430	-2.7769720
H	-0.1765430	-4.4741150	-3.1125550
C	0.5698060	5.8313500	3.2374140
H	1.2505390	6.5283310	3.7119310
C	2.8480630	3.8860410	0.8430970

H	2.1262730	4.3123300	1.5286570
C	2.3714770	3.6308540	-3.1417070
H	3.1855950	4.2671270	-3.4673260
C	-4.6158010	3.5478330	-1.5271660
C	-3.2790180	-4.2280150	-1.7830400
C	-4.7708760	-0.8117600	-1.2724440
C	3.0482590	0.4855170	-5.0479980
H	3.7446370	0.0807100	-5.7742240
C	-3.7260610	3.6349970	-2.6263590
H	-4.1329490	3.7148040	-3.6279740
C	3.8969400	4.6552040	0.3540580
H	3.9998570	5.6869150	0.6705410
C	-0.0839890	6.1903850	2.0372790
H	0.0911740	7.1685560	1.6042410
C	3.1814910	1.7649020	-4.6013890
H	3.9913440	2.3904810	-4.9580030
C	0.7790020	-2.4335580	-4.4274940
H	0.6013810	-3.4415240	-4.7769030
C	1.8077340	-1.6938840	-4.9594110
H	2.4651300	-2.1259310	-5.7065860
C	-2.0959150	-4.7975310	-2.2618460
H	-1.9679380	-5.8732900	-2.2174200
C	-5.6525710	-3.0479680	-0.7625660
C	5.4755430	0.9186260	-2.3186790
H	6.1755060	0.4852350	-3.0241000
C	-4.3408350	-5.0309320	-1.2538480
H	-4.2109780	-6.1077250	-1.2464070
C	-5.4777100	-4.4702960	-0.7696360
H	-6.2739240	-5.0912100	-0.3728470
C	5.6201910	2.2012870	-1.9012610
H	6.4363360	2.8138650	-2.2694160
C	-4.9863740	3.3882400	0.8800540
H	-4.5947700	3.3250670	1.8856540
C	-5.9360620	-0.2486000	-0.7317800
H	-6.0356690	0.8296170	-0.7072410
C	4.8144590	4.1104380	-0.5388860
H	5.6333900	4.7140380	-0.9154730
C	-6.9432040	-1.0615340	-0.2255740
H	-7.8398260	-0.6126020	0.1867360
C	-6.8062940	-2.4456510	-0.2408270
H	-7.5950540	-3.0769030	0.1544490
C	-6.0212260	3.5835900	-1.7077890
H	-6.4114630	3.6621080	-2.7165930
C	-6.3432820	3.4385580	0.6748150
H	-7.0160560	3.4142100	1.5243370
C	-6.8721190	3.5255220	-0.6323240
H	-7.9451090	3.5556780	-0.7809190
Se	0.1265370	-1.3326670	3.5667820

O	3.7250130	-3.2392560	3.8216110
C	2.8826550	-2.5052210	3.3276520
N	3.1333970	-1.4425620	2.5361930
H	2.3424410	-0.9113850	2.2000970
C	1.4116420	-2.8453740	3.5719080
H	1.3418420	-3.3696110	4.5201100
H	1.0404580	-3.4914140	2.7745760
N	1.4242300	0.3015950	5.7318990
C	4.4482640	-0.8353810	2.2960580
H	4.2127930	0.1382930	1.8607160
C	0.9460490	-0.3712400	4.9191630
C	5.2055360	-0.5911150	3.6112660
H	6.1193150	-0.0300220	3.4076360
H	4.5818270	-0.0138580	4.2977940
H	5.4679160	-1.5371670	4.0812910
C	5.3035870	-1.5763060	1.2800100
C	6.2880710	-0.8565900	0.5996310
C	5.1730730	-2.9410140	1.0202410
C	7.1329650	-1.4823600	-0.3104430
H	6.3809560	0.2111380	0.7682060
C	6.0124220	-3.5682660	0.1030660
H	4.4332240	-3.5198560	1.5530750
C	6.9966220	-2.8441930	-0.5646350
H	7.8836030	-0.9005720	-0.8329860
H	5.9015080	-4.6310770	-0.0825370
H	7.6511240	-3.3364000	-1.2750970

Table S15. Atomic coordinates of the optimized structure of ^{R}Pyr/^{R}DHIA.

Symbol	X	Y	Z
O	-2.3572810	-2.7582710	0.2476610
O	-4.7239620	0.3714350	1.5930420
N	-0.5710370	-3.2921360	-0.9926100
N	-2.8940310	1.5025390	2.4789730
N	-0.8256050	3.3296180	2.2441690
N	1.9969360	-2.6001720	-1.7013730
C	-3.8587380	0.6366700	2.6234470
C	-2.2877940	1.1076780	4.7934700
C	-1.7856490	-3.6263700	-0.6373470
C	-4.3022620	0.3574930	0.2724120
C	-3.6383100	-2.9906770	0.7323140
C	-4.3240660	-0.8680050	-0.3693070
C	-4.6358980	-2.0896960	0.4235200
C	-2.0990350	1.7531420	3.5461020
C	-0.6381160	4.9035580	-0.2063330
C	-3.9634190	-0.9258590	-1.7471910
C	0.0927310	-4.0699690	-1.8719630
C	-3.5233770	0.2667840	-2.4028400
C	-4.1402100	-0.0750610	3.8098980
H	-4.9527550	-0.7885940	3.8203240

C	0.1389530	4.2332170	2.1134830
C	0.4007270	4.7269990	0.7410780
C	1.4480290	-3.7082920	-2.2408460
C	-3.9261160	1.5454970	-0.3813040
H	-3.8889150	2.4651990	0.1814470
C	-1.0323550	2.7298540	3.4287360
C	-0.2328630	3.0200880	4.5675000
C	3.7774850	-1.0249190	-1.4075230
C	-5.9435440	-2.3220750	0.9559850
C	-3.5303850	1.4912570	-1.6924490
H	-3.1898710	2.3876900	-2.1931130
C	-3.3400690	0.1692610	4.8929820
H	-3.4993840	-0.3545050	5.8291110
C	3.2499000	-2.2773200	-1.9987480
C	-3.0720850	0.1925580	-3.7450390
H	-2.6895240	1.0921140	-4.2111100
C	-0.2990950	5.0180940	-1.5884500
C	5.0376260	-0.9505120	-0.7704170
C	2.1587140	-4.5485010	-3.1366480
C	-0.4786870	-5.2427840	-2.4272860
C	-3.0014730	5.0204290	-0.7878760
H	-4.0440810	5.0521400	-0.4905960
C	-2.6940140	5.0324170	-2.1868060
C	-2.0278620	4.9415580	0.1543100
H	-2.2919660	4.8843080	1.1984480
C	5.4736580	0.3091430	-0.2564490
C	-1.3254700	5.0416960	-2.5774610
C	-0.4527810	2.3345890	5.8001190
H	0.1833540	2.5678020	6.6467230
C	5.8793290	-2.0929760	-0.5535940
H	5.5252040	-3.0684010	-0.8537240
C	-4.0032800	-2.1303760	-2.4938300
H	-4.3898980	-3.0240940	-2.0236420
C	6.7310440	0.4184580	0.4059220
C	-2.4602340	-4.7693180	-1.1300090
H	-3.4662900	-5.0008350	-0.8139520
C	-3.8457890	-4.0810910	1.6042720
H	-3.0060820	-4.7194790	1.8492360
C	-1.4409280	1.4084390	5.9043870
H	-1.6103160	0.8834510	6.8381290
C	0.7647200	4.0064090	4.4201240
H	1.3761280	4.2732440	5.2755520
C	1.0662700	5.0438670	-1.9969440
C	1.7324550	4.8275650	0.3190680
H	2.5223780	4.6817940	1.0458190
C	7.0817260	-1.9844370	0.0676830
H	7.6898650	-2.8677680	0.2288110
C	2.0636670	4.9981840	-1.0147430

H	3.1040390	5.0365930	-1.3178910
C	-0.9867800	5.0416290	-3.9612320
C	0.9514500	4.6201660	3.2068230
H	1.7014410	5.3902910	3.0809170
C	2.9760070	0.1159700	-1.5006020
H	2.0196120	0.0383200	-1.9975180
C	-3.0800020	-1.0001670	-4.4234930
H	-2.7140280	-1.0485220	-5.4420780
C	-3.6881410	5.0164680	-3.1746780
H	-4.7297730	5.0038900	-2.8736940
C	-1.7929360	-5.5651220	-2.0249110
H	-2.2723470	-6.4491860	-2.4306670
C	-6.1706670	-3.4398650	1.8180820
C	4.6428210	1.4610940	-0.3806120
C	7.5604050	-0.7293710	0.5624180
C	1.5399040	-5.7159640	-3.6815670
H	2.1089880	-6.3301120	-4.3703140
C	-5.0881600	-4.2984570	2.1364930
H	-5.2557460	-5.1287850	2.8131500
C	-3.3478990	4.9983790	-4.5227740
H	-4.1286120	4.9729540	-5.2741000
C	-3.5673620	-2.1682920	-3.7952130
H	-3.5924950	-3.1028160	-4.3440500
C	0.2673640	-6.0497850	-3.3405040
H	-0.2017690	-6.9369480	-3.7512130
C	4.0278210	-3.0510290	-2.8944230
H	5.0309890	-2.7320990	-3.1426040
C	3.4809140	-4.1757240	-3.4567010
H	4.0500780	-4.7799020	-4.1547730
C	3.3957470	1.3380480	-1.0045380
H	2.7513940	2.2032920	-1.0927020
C	7.1622720	1.6742280	0.9268700
C	1.3767470	5.0743280	-3.3946990
H	2.4204900	5.0798680	-3.6880070
C	5.1037250	2.7099480	0.1518440
H	4.4599350	3.5743270	0.0469060
C	6.3057050	2.8142680	0.7737300
H	6.6394380	3.7661550	1.1723790
C	0.3970750	5.0588010	-4.3332280
H	0.6462930	5.0493920	-5.3881720
C	-7.0373260	-1.4750460	0.6464700
H	-6.8718110	-0.6308750	-0.0093490
C	8.7920070	-0.6009390	1.2192900
H	9.4193370	-1.4774430	1.3385710
C	-2.0134590	5.0113870	-4.9141700
H	-1.7538020	4.9930760	-5.9666400
C	9.2065470	0.6291570	1.7164600
H	10.1619250	0.7112230	2.2216620

C	8.4023370	1.7549460	1.5741050
H	8.7293660	2.7110870	1.9675650
C	-7.4694480	-3.6559630	2.3443670
H	-7.6287640	-4.5036580	3.0019910
C	-8.2851050	-1.7162160	1.1660040
H	-9.1090450	-1.0584120	0.9153320
C	-8.5057660	-2.8138840	2.0275930
H	-9.4948960	-2.9886640	2.4343720
Se	-0.3318670	1.7326360	-0.3867950
O	-0.1080690	-0.0879310	2.3288910
C	0.1231940	-0.5640560	1.2202780
N	1.1276500	-1.4273150	0.9757660
H	1.2628250	-1.8014540	0.0368940
C	-0.7026620	-0.1851540	0.0103390
H	-1.7564870	-0.2373080	0.2528030
H	-0.4837060	-0.7757500	-0.8723190
N	0.0538840	1.5110440	-3.3609830
C	-0.0926500	1.5454470	-2.2103300
C	2.0249650	-1.8463670	2.0348640
C	3.1726320	-0.8459930	2.3387790
H	1.4159040	-1.9828530	2.9352290
C	2.7583610	-3.1240460	1.6975360
C	4.3809580	-1.7173780	2.7542810
H	2.8791240	-0.1139790	3.0903510
H	3.4008350	-0.3063900	1.4205850
C	4.0885720	-3.0544300	2.1118730
C	2.2627880	-4.2598520	1.0675930
H	4.4330880	-1.8272200	3.8440480
H	5.3345750	-1.2966640	2.4286560
C	4.9389610	-4.1360670	1.9050170
H	1.2307070	-4.2942420	0.7420570
C	3.1216540	-5.3334890	0.8382200
C	4.4518420	-5.2730110	1.2596520
H	5.9753650	-4.0872360	2.2202390
H	2.7560010	-6.2178040	0.3285860
H	5.1118330	-6.1143130	1.0787240

Table S16. Atomic coordinates of the optimized structure of ^{R}Pyr/^{S}DHIA.

Symbol	X	Y	Z
O	0.5412770	3.7110120	0.7670560
O	3.0924690	1.0490790	-1.8710110
N	0.0923760	2.0928550	2.3358050
N	2.0560510	-0.8890280	-1.1906920
N	0.0711680	-2.0850600	0.2127680
N	0.5151170	-0.4273210	3.2277760
C	3.0397090	-0.3202370	-1.8303350
C	3.0322390	-3.0483320	-1.7259910
C	-0.1744860	3.2729980	1.8525750
C	1.9905600	1.7862370	-2.2628020

C	1.9192430	3.6248800	0.7496840
C	1.7662440	3.0137060	-1.6628000
C	2.5510080	3.4131830	-0.4638730
C	2.0482630	-2.2381730	-1.1113380
C	-2.1494210	-0.3236550	0.9735670
C	0.7537240	3.8624340	-2.2175650
C	-0.6616440	1.6408170	3.3605840
C	-0.0534830	3.3921270	-3.3003760
C	4.0991560	-1.0129400	-2.4527020
H	4.8842050	-0.4579150	-2.9448410
C	-0.9814180	-2.5938490	0.8291610
C	-1.9502700	-1.6548760	1.4434900
C	-0.4099610	0.3063930	3.8577240
C	1.2071240	1.3301530	-3.3458780
H	1.4363420	0.3692790	-3.7876440
C	0.9661020	-2.8755460	-0.3932660
C	0.8729420	-4.2892530	-0.3782320
C	1.8944370	-2.3783670	2.9367350
C	3.9754870	3.5565330	-0.5202400
C	0.1942900	2.1057200	-3.8399700
H	-0.4165700	1.7469940	-4.6591790
C	4.0821590	-2.3841960	-2.4006350
H	4.8679060	-2.9629380	-2.8704940
C	0.8329670	-1.6352110	3.6604260
C	-1.0740680	4.2245120	-3.8256400
H	-1.6849470	3.8423710	-4.6358060
C	-3.1924300	0.4616390	1.5602390
C	2.9372640	-1.7383080	2.2024120
C	-1.1394670	-0.1696380	4.9739540
C	-1.6889140	2.4145210	3.9535690
C	-1.6578740	1.5238010	-0.5505800
H	-1.0467890	1.9475270	-1.3351680
C	-2.7134230	2.3142230	-0.0053860
C	-1.3749330	0.2832550	-0.0772640
H	-0.5147680	-0.2426040	-0.4534560
C	3.9401010	-2.5527770	1.5826320
C	-3.4732650	1.7724810	1.0683990
C	1.8771900	-5.0722070	-1.0241890
H	1.7984600	-6.1531120	-0.9911000
C	3.0502920	-0.3137280	2.0416690
H	2.2725420	0.3131280	2.4405680
C	0.5261020	5.1795280	-1.7412930
H	1.1466870	5.5606810	-0.9424960
C	5.0054100	-1.9527670	0.8446170
C	-1.1905360	4.1264530	2.3292600
H	-1.3570990	5.0814340	1.8525450
C	2.6459560	3.8718170	1.9360240
H	2.1075640	3.9971810	2.8657170

C	2.9227730	-4.4728090	-1.6581210
H	3.6941330	-5.0700010	-2.1297440
C	-0.2536700	-4.8321390	0.2794290
H	-0.3899940	-5.9081330	0.2995380
C	-3.9622570	-0.0462220	2.6470640
C	-2.7174580	-2.1119420	2.5230280
H	-2.5262630	-3.0990390	2.9224490
C	4.0648670	0.2489610	1.3379660
H	4.0998330	1.3225420	1.2176260
C	-3.6849040	-1.3294790	3.1265140
H	-4.2429920	-1.7122700	3.9731610
C	-4.5088960	2.5567020	1.6540730
C	-1.1809820	-4.0035300	0.8654510
H	-2.0683980	-4.4202770	1.3218420
C	1.8644640	-3.7784040	2.9855210
H	1.0431260	-4.2688030	3.4913170
C	-1.2792890	5.4866370	-3.3264340
H	-2.0590190	6.1172830	-3.7371160
C	-2.9865070	3.6091510	-0.4675710
H	-2.3903630	4.0159540	-1.2746330
C	-1.9394970	3.6879860	3.3934700
H	-2.7304540	4.3059910	3.8010840
C	4.7134050	3.8109430	0.6775470
C	3.8818790	-3.9743670	1.6729420
C	5.0758140	-0.5382640	0.7117240
C	-2.1459030	0.6525220	5.5669820
H	-2.7020010	0.2666790	6.4143880
C	4.0109680	3.9463320	1.9006410
H	4.5702510	4.1238640	2.8121430
C	-3.9995270	4.3637570	0.1117440
H	-4.2017410	5.3634070	-0.2554840
C	-0.4601090	5.9686210	-2.2807170
H	-0.6106630	6.9732220	-1.9023590
C	-2.4188910	1.8889320	5.0662000
H	-3.2027720	2.4978320	5.5011280
C	0.1790420	-2.1860710	4.7992200
H	0.4683170	-3.1548490	5.1831420
C	-0.8018710	-1.4616590	5.4325080
H	-1.3126000	-1.8692840	6.2986270
C	2.8226590	-4.5625190	2.3696770
H	2.7517140	-5.6434550	2.4154310
C	5.9942510	-2.7619310	0.2119990
C	-4.9962620	0.7636740	3.2168100
H	-5.5694180	0.3537520	4.0407960
C	4.8921330	-4.7631580	1.0331410
H	4.8247030	-5.8425250	1.1153610
C	5.9049660	-4.1865640	0.3382170
H	6.6634460	-4.7967040	-0.1406880

C	-5.2626680	2.0059260	2.7413500
H	-6.0542410	2.6056400	3.1773880
C	4.6954450	3.4730230	-1.7401270
H	4.1490140	3.3102720	-2.6585910
C	6.1066180	0.0377410	-0.0449940
H	6.1389610	1.1146660	-0.1547500
C	-4.7535880	3.8454510	1.1595260
H	-5.5456190	4.4368810	1.6061010
C	7.0665870	-0.7618890	-0.6536650
H	7.8592460	-0.3026930	-1.2335520
C	7.0143790	-2.1460340	-0.5269050
H	7.7659490	-2.7668480	-1.0028960
C	6.1251110	3.9241850	0.6178920
H	6.6694970	4.1015050	1.5389440
C	6.0624520	3.6005900	-1.7683820
H	6.5882720	3.5371730	-2.7140930
C	6.7911120	3.8175460	-0.5775690
H	7.8704100	3.9080030	-0.6127950
Se	-0.4874080	-1.8768930	-3.2464260
O	-4.3357380	-2.9621890	-3.3106660
C	-3.3727990	-2.4350860	-2.7802700
N	-3.4107250	-1.2952390	-2.0596060
H	-2.5454610	-0.9013840	-1.7193560
C	-2.0047410	-3.1108690	-2.8885540
H	-2.0513880	-3.8542820	-3.6777920
H	-1.7227950	-3.5822450	-1.9446870
N	-1.7174440	-0.3808990	-5.5453660
C	-1.2720410	-1.0029910	-4.6754340
C	-4.6230980	-0.5039700	-1.8387760
C	-5.3036990	0.0215100	-3.1365240
H	-4.2919030	0.3292600	-1.2195460
C	-5.7248750	-1.2798400	-1.1478600
C	-6.5909800	-0.8144370	-3.3310350
H	-5.5609930	1.0725890	-2.9847130
H	-4.6251210	-0.0339000	-3.9874410
C	-6.8419090	-1.4156820	-1.9700210
C	-5.6986140	-1.8305900	0.1264420
H	-7.4291450	-0.2094010	-3.6867540
H	-6.4216750	-1.6194540	-4.0504730
C	-7.9672110	-2.0897200	-1.5051700
H	-4.8183690	-1.7403450	0.7470620
C	-6.8260210	-2.5042460	0.5924190
C	-7.9560630	-2.6276470	-0.2182310
H	-8.8410460	-2.2050180	-2.1376930
H	-6.8257300	-2.9313430	1.5892310
H	-8.8300850	-3.1512010	0.1533960

Table S17. Atomic coordinates of the optimized structure of ^{R}Pyr/^{R}MNA.

Symbol	X	Y	Z

O	-3.3815570	0.7731400	-0.2555360
O	-1.2331410	3.8582550	0.9435310
N	-3.0764290	-1.2685710	-1.1072930
N	0.4357700	2.8957010	2.2224910
N	2.9454090	1.8615880	2.3586930
N	-1.2542570	-3.3365780	-1.5820630
C	-0.7915810	3.3173500	2.1233870
C	-0.0064260	2.2487340	4.5123420
C	-3.8800460	-0.2340720	-1.0244740
C	-0.8508190	3.3028500	-0.2742540
C	-4.0065630	2.0135020	-0.1936390
C	-1.8889670	2.9287340	-1.1063340
C	-3.2853910	3.1034440	-0.6246510
C	0.8429970	2.3507190	3.3855350
C	4.6369230	2.1860260	0.0273370
C	-1.5897190	2.3266660	-2.3620310
C	-3.4605680	-2.3529840	-1.8132670
C	-0.2207830	2.1119980	-2.7202320
C	-1.7368430	3.2728060	3.1727070
H	-2.7402810	3.6403070	3.0044190
C	4.1569740	1.3224300	2.3653040
C	4.8270690	1.2202750	1.0480090
C	-2.5324540	-3.4548770	-2.0092540
C	0.5006230	3.1563410	-0.6485340
H	1.2778990	3.4479240	0.0368320
C	2.1873600	1.8207790	3.4631270
C	2.6290620	1.2290830	4.6731220
C	1.0481030	-4.1621830	-1.5077700
C	-3.8830520	4.3977550	-0.5264910
C	0.7997500	2.5670930	-1.8506890
H	1.8333490	2.4175020	-2.1324730
C	-1.3255720	2.7389900	4.3698520
H	-2.0120880	2.6725760	5.2072720
C	-0.3942160	-4.3168830	-1.8374340
C	0.0809050	1.4242540	-3.9234370
H	1.1194530	1.2243250	-4.1574790
C	4.9938910	1.8522850	-1.3130200
C	1.5264520	-3.8571960	-0.2164040
C	-3.0016220	-4.6083630	-2.6962450
C	-4.7505920	-2.4345710	-2.3976410
C	3.8371450	4.3570540	-0.7421590
H	3.4137470	5.3327520	-0.5299780
C	4.0941250	4.0106180	-2.1071880
C	4.0823170	3.4874650	0.2715130
H	3.8385760	3.7625750	1.2854480
C	2.9366240	-3.7978770	0.0032200
C	4.6917570	2.7479060	-2.3807740
C	1.7468710	1.1608690	5.7964860

H	2.1058310	0.7046390	6.7128120
C	0.6566550	-3.6277210	0.8994250
H	-0.4088050	-3.6730050	0.7335940
C	-2.6005860	1.8886620	-3.2560760
H	-3.6375940	2.0795470	-3.0107220
C	3.4462130	-3.4841050	1.2954270
C	-5.1439320	-0.1721590	-1.6508860
H	-5.7516070	0.7173830	-1.5972290
C	-5.2850460	2.1355540	0.3913970
H	-5.7822760	1.2480560	0.7550460
C	0.4781230	1.6478150	5.7170980
H	-0.1905120	1.5825720	6.5687070
C	3.9428650	0.7136220	4.6832890
H	4.3349290	0.2737880	5.5942080
C	5.5995430	0.5958690	-1.6066740
C	5.4737740	0.0178080	0.7385920
H	5.5811530	-0.7335340	1.5091200
C	1.1449690	-3.3003990	2.1220050
H	0.4694900	-3.0934570	2.9406730
C	5.8629870	-0.2879710	-0.5552120
H	6.3072030	-1.2511490	-0.7694180
C	4.9544840	2.3699870	-3.7301450
C	4.7066860	0.7541510	3.5421420
H	5.7099530	0.3493740	3.5315930
C	1.9619500	-4.3825600	-2.5453600
H	1.5844070	-4.5783320	-3.5416620
C	-0.9233050	0.9821420	-4.7477440
H	-0.6821940	0.4404380	-5.6546700
C	3.7633340	4.8580470	-3.1732770
H	3.3001310	5.8150410	-2.9605430
C	-5.5751400	-1.2942090	-2.3073300
H	-6.5537470	-1.3102650	-2.7740960
C	-5.1889340	4.5323700	0.0397660
C	3.8427570	-4.0368500	-1.0681490
C	2.5516150	-3.2006090	2.3650980
C	-4.3402730	-4.6808140	-3.1892040
H	-4.6576540	-5.5872930	-3.6922900
C	-5.8612060	3.3735090	0.5032730
H	-6.8423770	3.4788850	0.9529780
C	4.0092930	4.4747760	-4.4863710
H	3.7370220	5.1368060	-5.3002710
C	-2.2749270	1.2288860	-4.4154110
H	-3.0611700	0.8881870	-5.0796480
C	-5.1791730	-3.6222660	-3.0623730
H	-6.1854710	-3.6568000	-3.4644400
C	-0.7913500	-5.5198660	-2.4754230
H	-0.0643370	-6.3079220	-2.6199040
C	-2.0882720	-5.6625060	-2.8922920

H	-2.4197420	-6.5700680	-3.3853370
C	3.3282730	-4.3126940	-2.3394500
H	4.0096010	-4.4583370	-3.1693960
C	4.8522500	-3.4345690	1.5210770
C	5.8753850	0.2538440	-2.9695460
H	6.3157260	-0.7153910	-3.1735280
C	5.2521670	-3.9904310	-0.8114860
H	5.9290970	-4.1840990	-1.6364820
C	5.7355500	-3.7140190	0.4268230
H	6.8049300	-3.6844430	0.6071420
C	5.5599210	1.0956210	-3.9849240
H	5.7468660	0.8113620	-5.0143640
C	-3.2186380	5.5638610	-0.9828730
H	-2.2317000	5.4643730	-1.4148780
C	3.0694720	-2.8366950	3.6141750
H	2.3833310	-2.5859830	4.4146480
C	4.5994300	3.2461440	-4.7643520
H	4.7864060	2.9511250	-5.7909620
C	4.4426920	-2.7896100	3.8249130
H	4.8275860	-2.5103460	4.7986480
C	5.3267290	-3.0961250	2.7962370
H	6.3973080	-3.0640300	2.9686700
C	-5.7721860	5.8210830	0.1335720
H	-6.7617240	5.9135940	0.5681230
C	-3.8137450	6.7972610	-0.8825860
H	-3.2921570	7.6777410	-1.2391330
C	-5.1014250	6.9306040	-0.3167580
H	-5.5565780	7.9111910	-0.2408360
Se	2.0764880	-0.2767220	-0.0734650
O	0.3590300	-0.1913070	2.2233570
C	-0.3450010	-0.5705630	1.2922200
N	-1.5856990	-1.0807600	1.4371310
H	-2.0970070	-1.2315300	0.5674030
C	0.1153660	-0.4916740	-0.1478650
H	-0.3125740	0.3914420	-0.6188160
H	-0.1585910	-1.3737870	-0.7235970
N	2.5763500	-0.8990210	-2.9751430
C	-2.3576870	-0.9246660	2.6750960
H	-2.3046300	0.1308260	2.9618870
C	2.3513170	-0.6803070	-1.8587920
C	-1.7807450	-1.7292810	3.8506330
H	-1.8047480	-2.8028390	3.6590740
H	-2.3752200	-1.5330230	4.7461080
H	-0.7543900	-1.4121820	4.0304380
C	-3.8173540	-1.2455010	2.4047890
C	-4.2375070	-2.4601200	1.7694470
C	-4.7679070	-0.3250670	2.7823250
C	-3.3432330	-3.5006590	1.4027010

C	-5.6267540	-2.6383280	1.4672720
C	-6.1438630	-0.5331110	2.5422620
H	-4.4471580	0.5976350	3.2524840
C	-3.7819420	-4.6247620	0.7483240
H	-2.2931510	-3.3915110	1.6202660
C	-6.0438040	-3.8036040	0.7749660
C	-6.5624530	-1.6539940	1.8742830
H	-6.8610280	0.2116860	2.8684810
C	-5.1446340	-4.7757630	0.4168130
H	-3.0714210	-5.3936250	0.4693280
H	-7.0962130	-3.9130670	0.5361760
H	-7.6132660	-1.8106430	1.6564330
H	-5.4748630	-5.6559950	-0.1209700

Table S18. Atomic coordinates of the optimized structure of ^{R}Pyr/^{S}MNA.

Symbol	X	Y	Z
O	-2.2205920	1.2667160	1.7119990
O	-1.3072000	1.2575980	-1.9123570
N	-0.6111240	-0.2818170	1.0727810
N	-1.8724120	-0.9829210	-1.9415000
N	-3.7101710	-2.9555770	-1.4980510
N	1.9028920	-0.9443160	0.0925820
C	-1.0218170	-0.0367230	-2.2343960
C	-0.3090350	-2.6026990	-2.8457920
C	-1.7782600	-0.0143400	1.5963930
C	-2.6144490	1.6681100	-1.6868760
C	-1.4217100	2.3493510	1.3550520
C	-2.8247200	2.5919670	-0.6882910
C	-1.7226330	3.0417250	0.2061400
C	-1.5483690	-2.2570440	-2.2552350
C	-6.2292100	-2.1683190	-0.1304680
C	-4.1282010	3.1648000	-0.5406100
C	-0.2803790	-1.5879290	0.9013680
C	-5.1817450	2.7552020	-1.4138700
C	0.2253620	-0.2507700	-2.8644000
H	0.8659510	0.5894540	-3.0862710
C	-4.5964740	-3.8780510	-1.1498520
C	-5.9438210	-3.4478520	-0.6949310
C	1.0022730	-1.9259300	0.3179170
C	-3.6564010	1.2497200	-2.5474990
H	-3.4546970	0.5053660	-3.3030060
C	-2.5017370	-3.3071470	-1.9624840
C	-2.1267640	-4.6570530	-2.1792850
C	4.0303170	-0.1295950	-0.7570920
C	-1.0376110	4.2700200	-0.0473560
C	-4.9075290	1.7802310	-2.4055270
H	-5.7100010	1.4556510	-3.0576130
C	0.5771660	-1.5428780	-3.1509810
H	1.5341720	-1.7616170	-3.6101240

C	3.0486560	-1.2141930	-0.5217890
C	-6.4663750	3.3317250	-1.2682220
H	-7.2612820	2.9998430	-1.9265810
C	-7.5619520	-1.8978770	0.3268610
C	3.6735560	1.2103460	-1.0687430
C	1.2777010	-3.2837330	0.0073950
C	-1.1641520	-2.6434930	1.2386360
C	-5.5592610	0.0599090	0.6162180
H	-4.7945040	0.8195710	0.7191800
C	-6.8699390	0.3434510	1.1042610
C	-5.2524080	-1.1248280	0.0268870
H	-4.2629450	-1.2859350	-0.3642550
C	4.7163190	2.1480630	-1.3554790
C	-7.8769350	-0.6479850	0.9410450
C	-0.8628460	-4.9659640	-2.7671950
H	-0.6091860	-6.0059840	-2.9414430
C	2.3159380	1.6790810	-1.1343680
H	1.5240010	1.0090130	-0.8435110
C	-4.4128200	4.1396550	0.4499280
H	-3.6234370	4.4523760	1.1205320
C	4.3968170	3.4835520	-1.7418330
C	-2.6996990	-0.9841690	2.0566530
H	-3.6291490	-0.6662160	2.5035670
C	-0.4518490	2.7948460	2.2732770
H	-0.2725630	2.2118950	3.1654600
C	0.0052060	-3.9730820	-3.1031220
H	0.9636210	-4.2051550	-3.5537170
C	-3.0509860	-5.6362590	-1.7583980
H	-2.7918660	-6.6861960	-1.8463340
C	-8.5954650	-2.8688270	0.1784040
C	-6.9969740	-4.3658790	-0.8386880
H	-6.8059900	-5.3153840	-1.3207150
C	2.0162080	2.9483950	-1.5153500
H	0.9812360	3.2636300	-1.5580890
C	-8.2864110	-4.0925520	-0.4244050
H	-9.0698340	-4.8283000	-0.5676590
C	-9.2005990	-0.3793660	1.4010390
C	-4.2583100	-5.2609050	-1.2236260
H	-4.9421550	-6.0137980	-0.8580130
C	5.3873250	-0.4764150	-0.6927040
H	5.6584700	-1.4860710	-0.4248690
C	-6.7066660	4.2857950	-0.3106380
H	-7.6947090	4.7179570	-0.2073700
C	-7.1886930	1.5598260	1.7228660
H	-6.4144510	2.3082560	1.8345740
C	-2.3915140	-2.2970220	1.8502610
H	-3.0863500	-3.0786650	2.1341970
C	-0.0531600	4.7330680	0.8814070

C	6.0865850	1.7607040	-1.2714770
C	3.0380300	3.8913390	-1.8501480
C	0.3446090	-4.3086510	0.3353940
H	0.5863710	-5.3331040	0.0797980
C	0.2255810	3.9605750	2.0366020
H	0.9716680	4.3074970	2.7420810
C	-8.4800230	1.8087120	2.1702500
H	-8.7124520	2.7558510	2.6433250
C	-5.6682280	4.6906220	0.5555150
H	-5.8639390	5.4395980	1.3142640
C	-0.8287980	-3.9982890	0.9455100
H	-1.5460250	-4.7715300	1.1951610
C	3.3578860	-2.5350080	-0.9475580
H	4.2760180	-2.7276530	-1.4834450
C	2.4930910	-3.5545630	-0.6544360
H	2.7220350	-4.5748160	-0.9422650
C	6.3946620	0.4407690	-0.9246240
H	7.4302540	0.1307140	-0.8518920
C	5.4343250	4.4172380	-2.0364910
C	-9.9188480	-2.5701820	0.6391090
H	-10.6875390	-3.3243080	0.5099860
C	7.1086910	2.7249110	-1.5522470
H	8.1436170	2.4107380	-1.4722070
C	6.7985320	3.9943460	-1.9188300
H	7.5816530	4.7127730	-2.1354180
C	-10.2094850	-1.3813900	1.2259970
H	-11.2144080	-1.1692040	1.5746410
C	-1.3328970	5.0713930	-1.1800170
H	-2.0752760	4.7233800	-1.8865480
C	2.7426140	5.1951520	-2.2693250
H	1.7062300	5.4920420	-2.3540660
C	-9.4772900	0.8521790	2.0100660
H	-10.4850700	1.0509990	2.3581340
C	3.7605150	6.0954300	-2.5593430
H	3.5143240	7.1014760	-2.8791070
C	5.0927660	5.7152430	-2.4387830
H	5.8846350	6.4221550	-2.6609580
C	0.5900790	5.9729820	0.6426750
H	1.3418210	6.3104830	1.3471090
C	-0.7049310	6.2789320	-1.3702400
H	-0.9538240	6.8853610	-2.2335980
C	0.2645680	6.7368640	-0.4501750
H	0.7586450	7.6867830	-0.6165060
Se	2.4071330	0.9626530	2.1952950
O	3.6211560	-2.4805680	4.1780080
C	3.6665910	-1.4418730	3.5335120
N	4.8009060	-0.9100410	3.0294000
H	4.7299690	-0.0898130	2.4409850
C	2.3632150	-0.6899570	3.2920830
H	1.9327190	-0.4372080	4.2588570
H	1.6726150	-1.3526450	2.7767900
N	3.1564630	2.8391420	4.4449270

C	7.7030020	-1.9850950	1.3531660
C	8.0479300	-2.7144070	0.1853860
C	6.1232280	-1.4834250	3.2890250
H	5.9672480	-2.1796400	4.1167560
C	6.5819400	-2.2915640	2.0847590
C	2.8915620	2.0773130	3.6124120
C	5.7722370	-3.3893560	1.6822260
C	7.0754300	-0.3763010	3.7330620
H	7.2029400	0.3772380	2.9505630
H	8.0576370	-0.7829340	3.9819540
H	6.6712960	0.1205310	4.6158580
C	6.0839920	-4.1216830	0.5681320
C	7.2174020	-3.8018140	-0.2245600
C	9.1744480	-2.3786970	-0.6066450
C	7.5462000	-4.5089230	-1.4074960
C	9.4643400	-3.0795870	-1.7523130
C	8.6422650	-4.1554460	-2.1569740
H	9.8062950	-1.5547010	-0.2922580
H	10.3270100	-2.8106600	-2.3505290
H	8.8823040	-4.7017650	-3.0615850
H	6.9155870	-5.3372820	-1.7127010
H	5.4569810	-4.9555540	0.2713340
H	4.8973600	-3.6322940	2.2735950
H	8.3369800	-1.1544180	1.6375360

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