

Supporting Information

Engineering of Electrodeposited Binder-free Organic - Nickel Hydroxide Based Nanohybrids for Energy Storage and Electrocatalytic Alkaline Water Splitting

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Materials and methods

Materials

All starting reagents and chemicals were obtained commercially and used without further treatment. 1-naphthalene methanol was purchased from Sigma Aldrich chemicals whereas 3,4-diaminobenzoic acid was purchased from Alfa Aser Pvt. Ltd. Amino acids and coupling agents such as *N,N'*-dicyclohexylcarbodiimide (DCC) were purchased from SRL chemicals. Anhydrous Na_2SO_4 and KOH and hexahydro-nickel(II) nitrate ($\text{Ni}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$) were purchased from SRL chemicals, India. Hexane, dimethyl sulfoxide (DMSO) and *N, N'*-dimethylformamide (DMF) were purchased from Merck India Ltd. 20% phosgene in toluene solution was purchased from Spectrochem Chemicals India Pvt. Ltd. Thin layer chromatography (TLC, silica gel 60 F_{254}) sheets were obtained from Merck KGaA. DMF was freshly dried and distilled for the synthesis and electrochemical studies. ITO and Carbon paper was purchased from Global Nanotech

Characterization

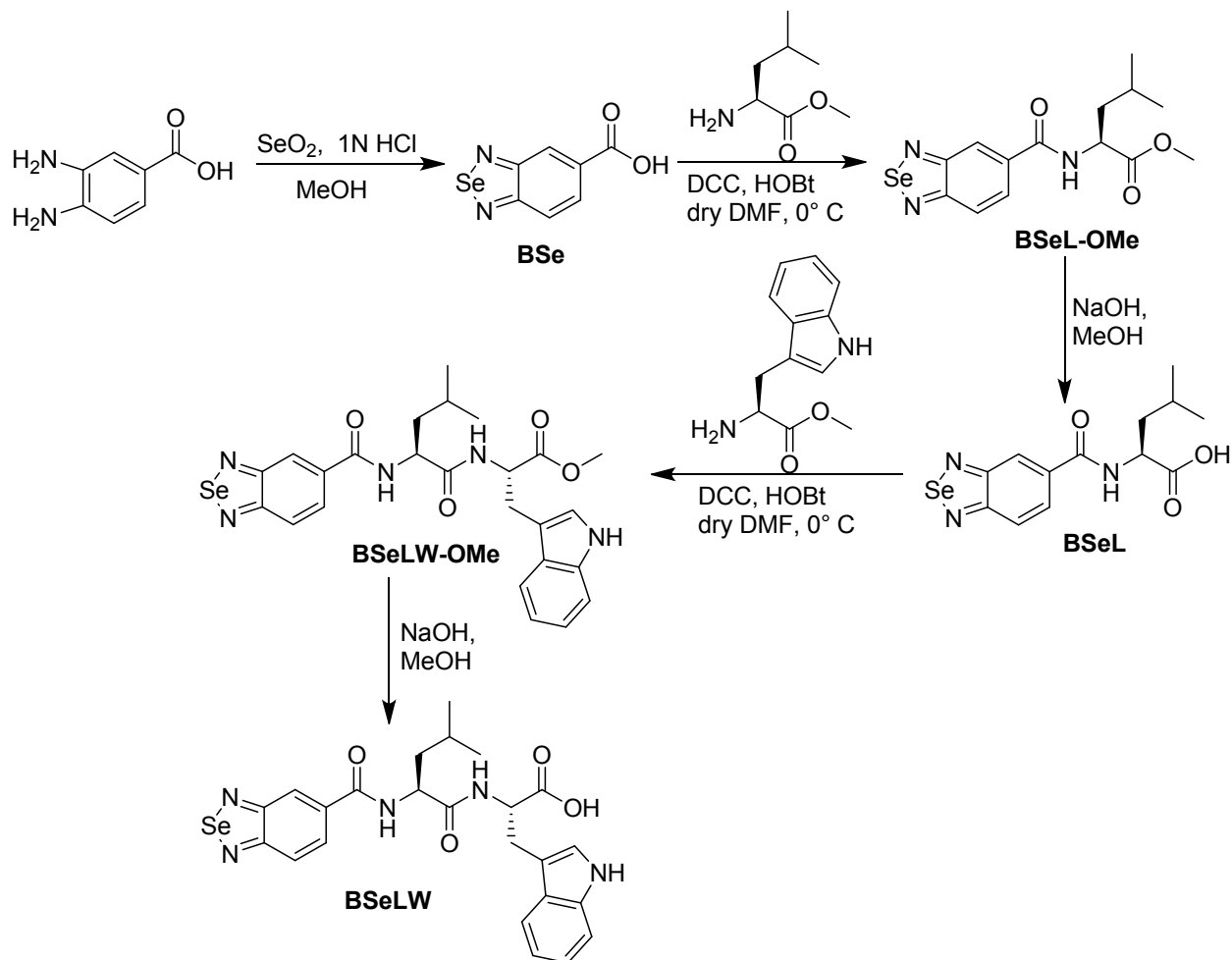
^1H NMR (400 MHz) spectra of organic compounds were recorded on a Bruker AV 400 MHz spectrometer at 300 K using tetramethylsilane as the internal standard. Compound concentrations were in the range 5-10 mmol L^{-1} in CDCl_3 and $\text{DMSO}-d_6$. For SEM measurements, thin films were coated with gold. Then, the images were recorded on a field-gun scanning electron microscope (Jeol Scanning Microscope-JSM-7600F). Transmission electron microscopy (TEM) study was performed on a TECNAI-120 KV system. X-ray Photoelectron Spectroscopy (XPS) analysis was performed on PHI 5000 Versa Probe II, FEI Inc.

Single crystal X-ray diffraction study

Crystallographic data of BSeLW were collected on a Rigaku FRX microfocus rotating anode (3 kW) at the copper $\text{K}\alpha$ edge equipped with a Dectris Pilatus 200K hybrid detector. Data for single crystal of BSeLW was processed with the CrystalClear suite version 2.1b25. All structures were solved with SHELXT and refined using SHELXL 2014 version. Full-matrix least-squares refinement were performed on F^2 for all unique reflections, minimizing $w(F_o^2 - F_c^2)^3$, with anisotropic displacement parameters for non-hydrogen atoms. All H atoms found in difference electron-density maps were refined freely, all the other were treated as riding on their parent C or

N atoms. Data statistics are reported in the **Table S1** and cif file. Crystallographic data of BSeLW has been deposited with the CCDC: 1909606

Synthetic procedure



Scheme S1. Synthetic scheme for solution phase synthesis of BSeLW.

Synthesis of benzo[2,1,3]selenadiazole-5-carboxylic acid (BSe): 2.28 g of 3,4-diamino benzoic acid (15 mmol) and 3.32 g of selenium dioxide (30 mmol) were refluxed in methanol (20 mL) and 1N HCl (10 mL) for 2 hours at 80 °C. After completion of the reaction mixture was cooled at room temperature and methanol was evaporated at reduced pressure. The product was precipitated and filtered with Milli-Q water. Final product **BSe** was obtained after dry precipitant. Yield = 86% (2.96 g, 12.98 mmol); ¹H NMR (DMSO-*d*₆, 400 MHz) δ 13.35 (s, 1H),

8.42 (s, 1H), 7.91-7.98 (dd, 2H) ppm. ^{13}C NMR (DMSO-*d*₆, 100 MHz) δ 167.33, 161.17, 159.63, 131.68, 128.32, 125.84, 123.66 ppm.

Synthesis of BSeL-OMe: In dry round bottom flask, 2.72 g of **BSe** (10 mmol) was dissolved in minimum amount of DMF at cold condition. l-Leucine methyl ester (2.17 g, 15 mmol) was added to reaction mixture followed by addition of HOBT (1.68 g, 12.5 mmol) and coupling agent N,N'-dicyclohexyl carbodiimide (2.57 g, 12.5 mmol). Reaction mixture was allowed to stir at room temperature for 12 hours. The progress of the reaction was monitored by thin layer chromatography (TLC). After completion of the reaction, the reaction mixture was diluted with ethyl acetate and washed with 1N HCl (3 \times 20 mL), saturated Na₂CO₃ solution (3 \times 20 mL) and (3 \times 20 mL) brine solution. Organic layer was separated and dried over anhydrous Na₂SO₄. Ethyl acetate was evaporated to obtained product. Product was further purified using silica gel flash column chromatography using hexane: ethyl acetate solvent system. Light yellowish coloured compound of BSeL-OMe was obtained.

Yield = 57% (2.41 g, 7.65 mmol); ^1H NMR (CDCl₃, 400 MHz) δ 8.18 (s, 1H), 7.83 (m, 2H), 6.66-6.68 (d, 1H, *J* = 8 Hz), 4.83 (m, 1H), 3.73 (s, 3H), 1.72 (m, 2H), 1.18 (s, 1H), 0.93-0.96 (t, 6H) ppm. ^{13}C NMR (DMSO-*d*₆, 100 MHz) δ 173.42, 166.37, 160.81, 159.68, 134.26, 128.22, 123.53, 123.04, 52.46, 51.68, 33.83, 24.97, 23.32, 21.67 ppm. HRMS (ESI) *m/z*: [M+K]⁺ Calcd for C₁₄H₁₇N₃O₃Se 394.007; Found: 394.005.

Synthesis of BSeL: A solution of BSeL-OMe (2.13 g, 6 mmol) in 30 mL distilled methanol was allowed to react with a solution of 4 mL (1N) NaOH solution. The reaction mixture was stirred upto 3 hours. The reaction progress was monitored by thin layer chromatography. After the completion of the reaction, excess methanol was evaporated and diluted with 40 mL milli-Q water. Water mixture washed with diethyl ether. The water mixture was acidified with 1N HCl in an ice bath. The product was extracted with ethyl acetate and dried over anhydrous Na₂SO₄. Ethyl acetate was evaporated under reduced pressure to obtained BSeL.

Yield = 96% (1.97 g, 5.81 mmol); ^1H NMR (CDCl₃, 400 MHz) δ 8.30 (s, 1H), 7.91(d, 2H), 6.76-6.78 (d, 1H, *J* = 8 Hz), 4.89-4.90 (d, 1H, *J* = 7 Hz), 1.87 (m, 2H), 1.43 (s, 1H), 1.03 (s, 6H) ppm. ^{13}C NMR (DMSO-*d*₆, 100 MHz) δ 174.51, 166.26, 160.81, 159.73, 134.55, 128.33, 123.46, 122.94, 51.62, 25.06, 23.44, 21.65 ppm. HRMS (ESI) *m/z*: [M+Na]⁺ Calcd for C₁₃H₁₅N₃O₃Se 364.017; Found 364.024.

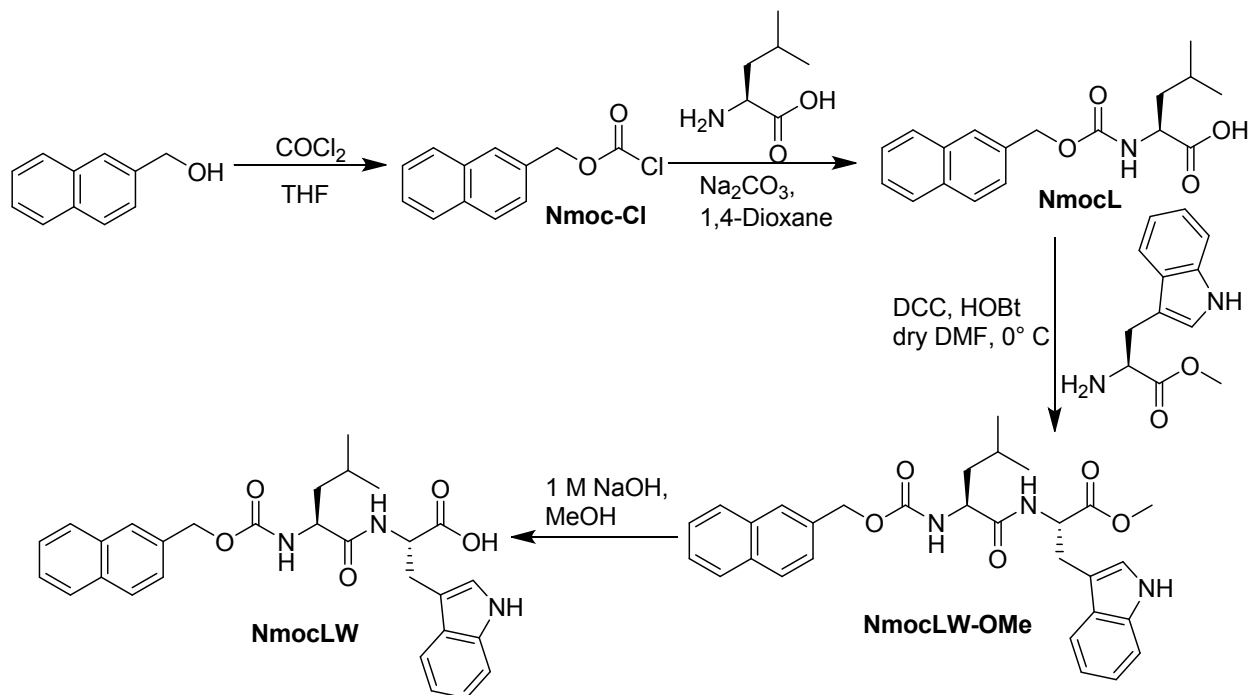
Synthesis of BSeLW-OMe: In dry round bottom flask, 1.7 g of BSeL (5 mmol) was dissolved in minimum amount of DMF at cold condition. l-Tryptophan methyl ester (1.63 g, 7.5 mmol) was added to reaction mixture followed by addition of HOBT (0.81 g, 6 mmol) and coupling agent N,N'-dicyclohexyl carbodiimide (1.23 g, 6 mmol). Reaction mixture was allowed to stir at room temperature for 12 hours. The progress of the reaction was monitored by thin layer chromatography (TLC). After completion of the reaction, the reaction mixture was diluted with ethyl acetate and washed with 1N HCl (3×20 mL), saturated Na₂CO₃ solution (3×20 mL) and (3×20 mL) brine solution. Organic layer was separated and dried over anhydrous Na₂SO₄. Ethyl acetate was evaporated to obtained product. Product was further purified using silica gel flash column chromatography using hexane: ethyl acetate solvent system. Yellow coloured compound of BSeLW-OMe was obtained.

Yield = 84% (2.27 g, 4.2 mmol): ¹H NMR (CDCl₃, 400 MHz) δ 8.18 (s, 1H), 8.00 (s, 1H), 7.66-7.68(dd, 2H), 7.40-7.42 (d, 1H, *J* = 7 Hz), 7.12-7.13 (s, 1H), 6.96 (m, 4H), 6.80-6.82 (d, 1H, *J* = 8 Hz), 4.71-4.91 (dd, 2H), 3.66 (s, 3H), 3.26 (m, 2H), 1.18 (s, 1H), 0.85 (s, 6H) ppm. ¹³C NMR (DMSO-*d*₆, 100 MHz) 172.74, 166.09, 160.80, 159.75, 136.53, 134.75, 128.51, 124.17, 123.34, 123.00, 121.42, 118.89, 118.44, 111.89, 109.83, 53.64, 52.28, 27.31, 23.57, 23.46, 21.95, 21.84 ppm. HRMS (ESI) *m/z*: [M+Na]⁺ Calcd for C₂₅H₂₇N₅O₄Se 564.112; Found 564.112.

Synthesis of BSeLW: 1 g of BSeLW-OMe (2 mmol) was dissolved in 40 mL distilled Methanol. The reaction mixture was allowed to react with 4 mL of 1N solution of NaOH. . The reaction mixture was stirred upto 3 hours. The reaction progress was monitored by thin layer chromatography. After the completion of the reaction, excess methanol was evaporated and diluted with 40 mL milli-Q water. Water mixture washed with diethyl ether. The water mixture was acidified with 1N HCl in an ice bath. The product was extracted with ethyl acetate and dried over anhydrous Na₂SO₄. Ethyl acetate was evaporated under reduced pressure to obtained orange coloured BSeLW.

Yield = 78% (0.76 g, 1.45 mmol). ¹H NMR (DMSO-*d*₆, 400 MHz,) δ 12.63 (s, 1H), 10.86 (s, 1H), 8.78-8.77 (d, 1H, *J* = 8 Hz), 8.42 (s, 1H), 8.20-8.22 (d, 1H, *J* = 7 Hz), 7.91-7.94 (dd, 2H), 7.53-7.54 (d, 1H, *J* = 8 Hz), 7.31-7.33 (d, 1H, *J* = 8 Hz), 7.19 (s, 1H), 6.96-7.04 (m, 2H), 4.49-4.61 (m, 2H), 3.13-3.23 (m, 2H), 1.56-1.59 (m, 2H), 0.89-0.94 (m, 6H) ppm. ¹³C NMR (DMSO-

*d*₆, 100 MHz) δ 173.73, 172.57, 166.10, 160.81, 159.76, 136.52, 134.79, 128.53, 124.08, 123.33, 122.99, 121.37, 118.84, 111.82, 110.22, 53.43, 52.40, 29.50, 27.37, 24.92, 23.62, 21.92 ppm. HRMS (ESI) *m/z*: [M+Na]⁺ Calcd for C₂₄H₂₅N₃O₄Se 550.097; Found 550.097.



Scheme S2. Synthetic scheme for solution phase synthesis of NmocLW.

Synthesis of Naphthalene-2-methoxychloroformate (Nmoc-Cl): To a stirred solution of naphthalene methanol (3.16 g, 20 mmol) in dry THF (30 mL), phosgene (78.5 mL, 20 mmol) was added at 0° C. The stirring was continued at ambient temperature for 24h. The reaction was monitored by thin layer chromatography (TLC). After completion of reaction, excess phosgene was removed under low vacuum and trapped with aqueous NaOH. Reaction mixture was concentrated and oily product was obtained. Then it was dissolved in hot hexane and kept overnight to yield crystalline product of Nmoc-Cl.

Yield = 81% (3.56 g, 16.2mmol). ¹H NMR (CDCl₃, 400 MHz) δ 7.85-7.87 (m, 4H), 7.49-7.53 (m, 2H), 5.44 (s, 1H).

Synthesis of NmocL: A solution of leucine (2.62 g, 20 mmol) in a mixture of 1, 4-dioxane (30 mL) and 2M sodium carbonate (30 mL) was stirred and cooled in an ice-water bath. Naphthalene-2- methoxychloroformate (3 g, 15 mmol) was added to reaction mixture and stirring was continued at room temperature for 12 h. Reaction mixture was diluted with 200 ml of water and

dioxane was evaporated under vacuum. Aqueous layer was washed with diethyl ether and the pH of aqueous layer was adjusted to 2 with 1N HCl. The aqueous phase was extracted with ethyl acetate (3 x 50 mL) and dried with Na₂SO₄ and concentrated to give NmocL as colorless oil.

Yield = 96% (4.15 g, 13.2 mmol). ¹H NMR (CDCl₃, 400 MHz) δ 7.80-7.82 (m, 4H), 7.45-7.43 (m, 2H), 5.27 (s, 2H), 1.58-1.71(m, 3H), 0.94 (s, 6H) ppm. ¹³C NMR (DMSO-*d*₆, 100 MHz) δ 174.91, 156.73, 135.18, 133.23, 132.97, 128.44, 128.19, 126.82, 16.68, 126.60, 126.18, 65.96, 52.72, 24.83, 23.37, 21.61 ppm. HRMS (ESI) *m/z*: [M+K]⁺ Calcd for C₁₈H₂₁NO₄ 354.110; Found 354.110.

Synthesis of NmocLW-OMe: In dry round bottom flask, 3.15 g of NmocL (10 mmol) was dissolved in minimum amount of DMF at cold condition. L-Tryptophan methyl ester (3.27 g, 15 mmol) was added to reaction mixture followed by addition of HOBt (1.62 g, 12 mmol) and coupling agent N,N'-dicyclohexylcarbodiimide (2.40 g, 12 mmol). Reaction mixture was allowed to stir at room temperature for 12 hours. The progress of the reaction was monitored by thin layer chromatography (TLC). After completion of the reaction, the reaction mixture was diluted with ethyl acetate and washed with 1N HCl (3×20 mL), saturated Na₂CO₃ solution (3×20 mL) and (3×20 mL) brine solution. Organic layer was separated and dried over anhydrous Na₂SO₄. Ethyl acetate was evaporated to obtain product. Product was further purified using silica gel flash column chromatography using hexane: ethyl acetate solvent system. Light yellow coloured liquid compound of NmocLW-OMe was obtained.

Yield = 75% (3.88 g, 7.54 mmol): ¹H NMR (CDCl₃, 400 MHz) δ 7.98 (s, 1H), 7.80 (m, 4H), 7.47-7.49 (dd, 3H), 7.38-7.40 (d, 1H, *J* = 8 Hz), 7.21-7.23(d, 1H, *J* = 8 Hz), 7.06-7.12 (dt, 2H), 6.89 (s, 1H), 6.66-6.67 (m, 1H), 5.14-5.26 (m, 2H), 4.88-4.89 (d, 1H, *J* = 6 Hz), 4.28 (m, 1H), 3.64 (s, 3H), 3.26-3.27 (d, 2H, *J* = 4 Hz), 1.60-1.70 (m, 3H), 1.46 (m, 1H), 0.86-0.88 (m, 6H) ppm. ¹³C NMR (DMSO-*d*₆, 100 MHz) δ 137.01, 172.71, 153.43, 136.56, 135.19, 133.23, 128.43, 128.18, 128.09, 127.60, 126.81, 126.67, 126.58, 126.19, 121.46, 118.91, 118.47, 111.90, 109.76, 76.40, 65.99, 53.55, 53.44, 52.26, 41.16, 27.41, 24.65, 21.96 ppm. HRMS (ESI) *m/z*: [M+Na]⁺ Calcd for C₃₀H₃₃N₃O₅Na 538.231; Found 538.231.

Synthesis of NmocLW: 1 g of NmocLW-OMe (1.94 mmol) was dissolved in 40 mL distilled Methanol. The reaction mixture was allowed to react with 4 mL of 1N solution of NaOH. The reaction mixture was stirred upto 4 hours. The reaction progress was monitored by thin layer

chromatography. After the completion of the reaction, excess methanol was evaporated and diluted with 40 mL milli-Q water. Water mixture washed with diethyl ether. The water mixture was acidified with 1N HCl in an ice bath. The product was extracted with ethyl acetate and dried over anhydrous Na₂SO₄. Ethyl acetate was evaporated under reduced pressure to obtained light yellow coloured NmocLW.

Yield = 86% (0.84 g, 1.68 mmol). ¹H NMR (CDCl₃, 400 MHz) δ 7.77-7.81 (m, 5H), 7.48 (m, 4H), 7.12 (m, 2H), 7.02 (m, 1H), 6.84-6.86 (d, 1H, *J* = 6 Hz), 6.77 (s, 1H), 5.36-5.38 (d, 1H, *J* = 8 Hz), 5.18 (s, 2H), 4.81-4.83 (d, 1H, *J* = 2 Hz), 4.24 (m, 1H), 3.24-3.29 (m, 2H), 1.40-1.56 (3, 4H), 1.25 (m, 1H), 0.81 (m, 6H) ppm. ¹³C NMR (DMSO-*d*₆, 100 MHz) δ 173.69, 172.80, 156.41, 136.53, 135.19, 133.22, 128.43, 128.18, 128.08, 127.74, 126.82, 126.62, 126.17, 124.09, 121.38, 118.84, 118.67, 111.80, 110.11, 79.66, 65.97, 53.54, 53.31, 27.44, 24.64, 23.56, 21.89 ppm. HRMS (ESI) *m/z*: [M+Na]⁺ Calcd for C₂₉H₃₁N₃O₅ 524.216; Found: 524.216.

Table S1. Crystal and diffraction parameters of BSeLW

| | |
|--------------------------------|--|
| Empirical Formula | C ₂₄ H ₂₅ N ₅ O ₄ Se |
| Crystal Habit | Orange Needles |
| Crystal Structure | Orthorhombic |
| Crystallizing Solvent | Water/Methanol |
| Space group | <i>P</i> 2 ₁ |
| a (Å) | 4.8659(2) |
| b (Å) | 19.7685(6) |
| c (Å) | 27.0010(8) |
| α (deg) | 90 |
| β (deg) | 90 |
| γ (deg) | 90 |
| Volume (Å ³) | 2597.27(15) |
| Z | 4 |
| Co-crystallized solvent | None |
| Molecular weight | 526.45 |
| F (000) | 1080 |
| θ Max. (°) | 71.332 |
| Reflections collected / unique | 16728 / 4953 |
| Max. and min. transmission | 1.00000 and 0.49996 |
| R _{int} | 0.0801 |
| Final R (%) / wR2 (%) | 0.0690/0.1872 |
| Goodness-of-fit (S) | 0.868 |
| λ (Å) | 1.54184 |
| CCDC | 1909606 |

Table S2. Hydrogen bond parameters of BSeLW

| Peptide | Type of hydrogen bond | D-H...A | H...A(Å) | D...A(Å) | ∠D-H...A(°) |
|---------|-----------------------|--------------|----------|----------|-------------|
| BSeLW | Intermolecular | N5-H5N...N1 | 2.346 | 3.196 | 170.04 |
| | Intermolecular | N3-H3N...O1 | 1.992 | 2.853 | 179.51 |
| | Intermolecular | N4-H4N...O2 | 2.052 | 2.900 | 169.02 |
| | Intermolecular | O4-H104...N2 | 1.977 | 2.782 | 167.31 |

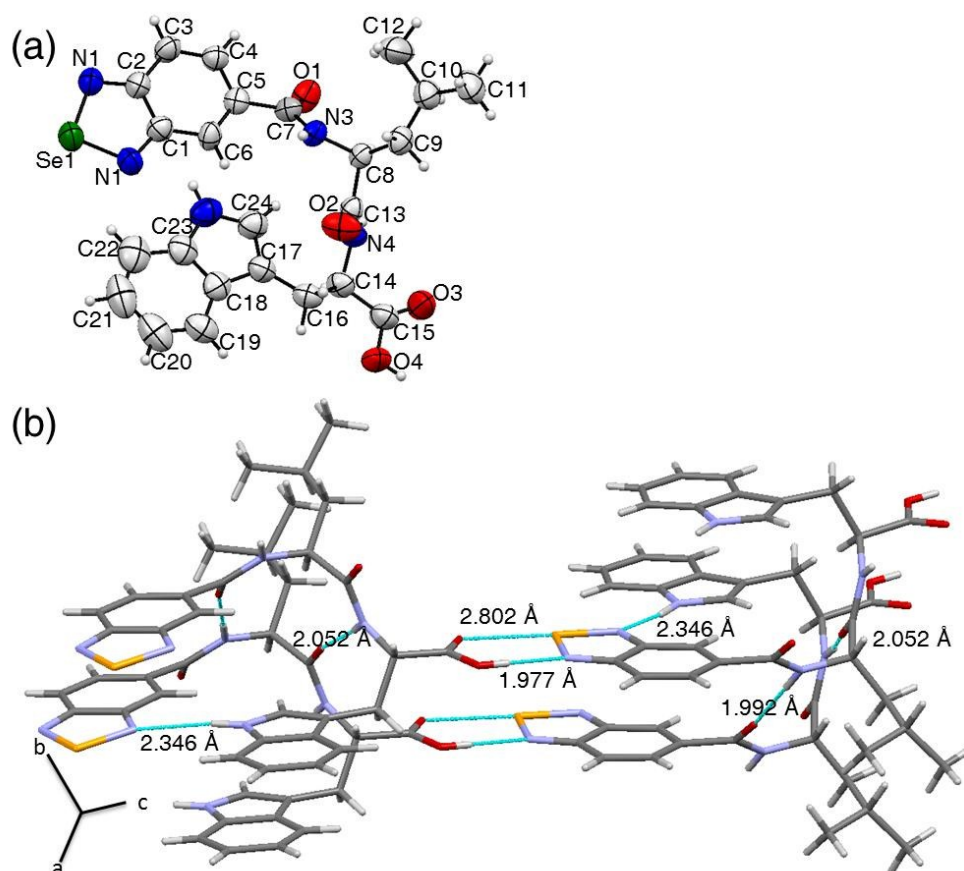


Figure S1. Solid state structure and supramolecular packing diagram in the crystal structure of BSeLW. (a) ORTEP diagram with atomic numbering, thermal ellipsoids are shown at 50% probability and hydrogen atoms are not labelled for clarity. (b) Intermolecular interactions are responsible for molecular self-assembly. (Interactions are indicated as dotted lines with distance parameters in Å).

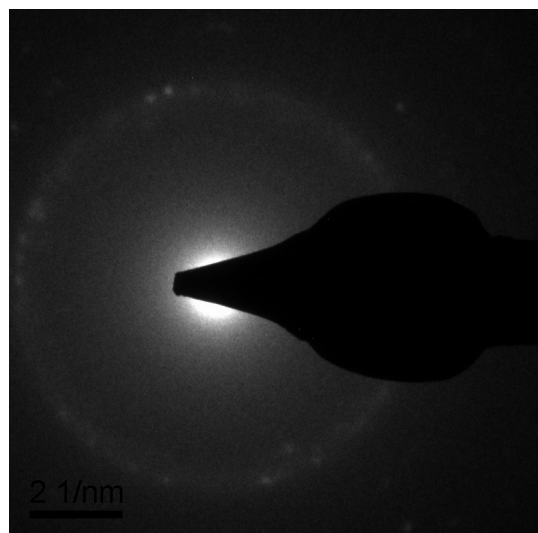


Figure S2. Selected area diffraction pattern (SAED) of BSeLW/Ni(OH)₂/CP.

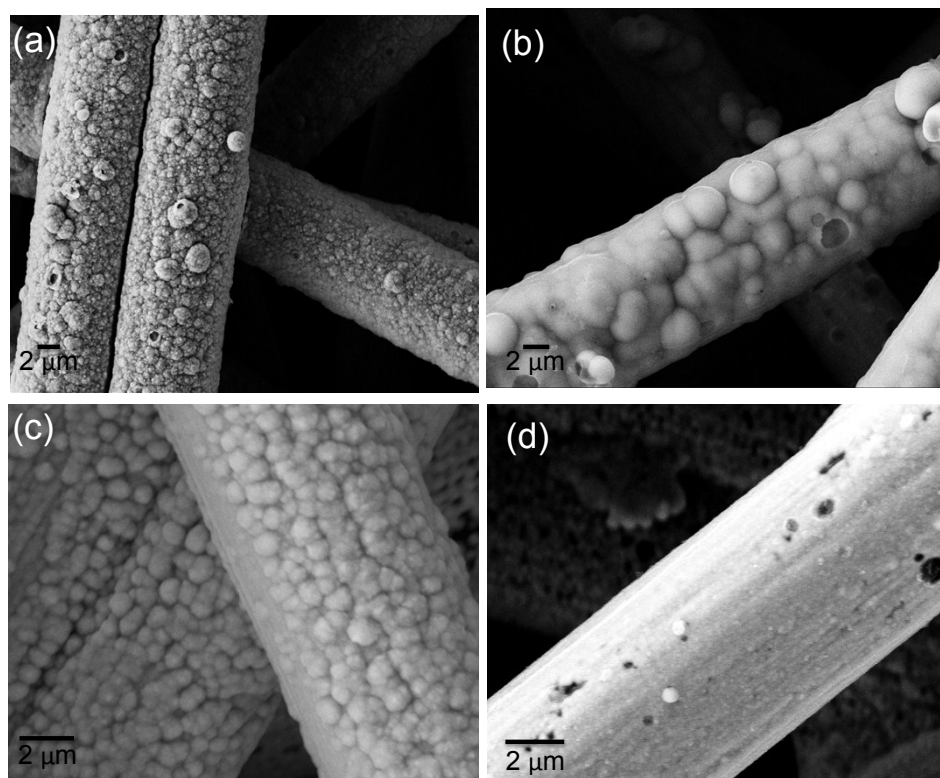


Figure S3. FE-SEM images of (a) (1:30) BSeLW/Ni(OH)₂/CP, (b) (1:40) BSeLW/Ni(OH)₂/CP, (c) Ni(OH)₂/CP and (d) (1:20) NmocLW/Ni(OH)₂/CP.

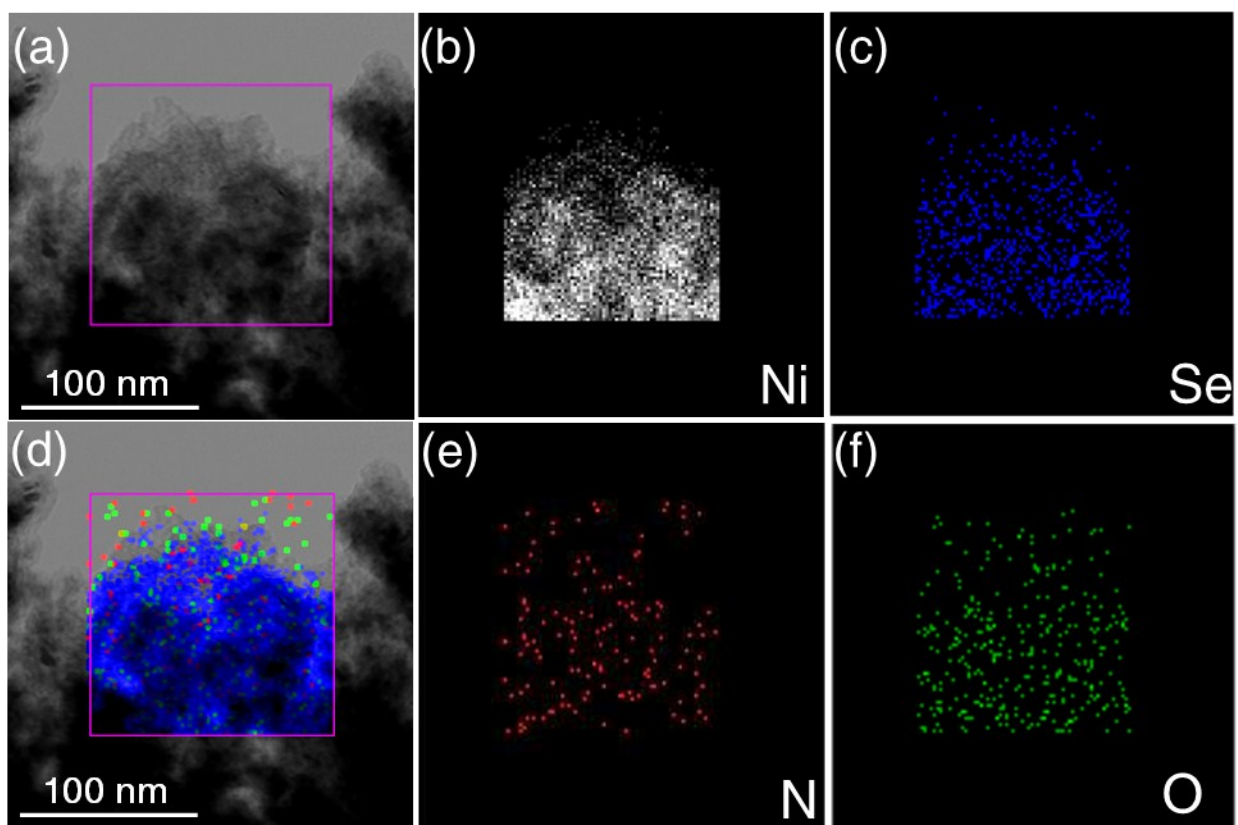


Figure S4. STEM elemental mapping images of (1:20) BSeLW/Ni(OH)₂. (a) and (d) STEM image of crosslinked sheets of (1:20) BSeLW/Ni(OH)₂ obtained from electrochemical deposition. (b) Ni mapping, (c) Se mapping, (e) N mapping and (f) O mapping.

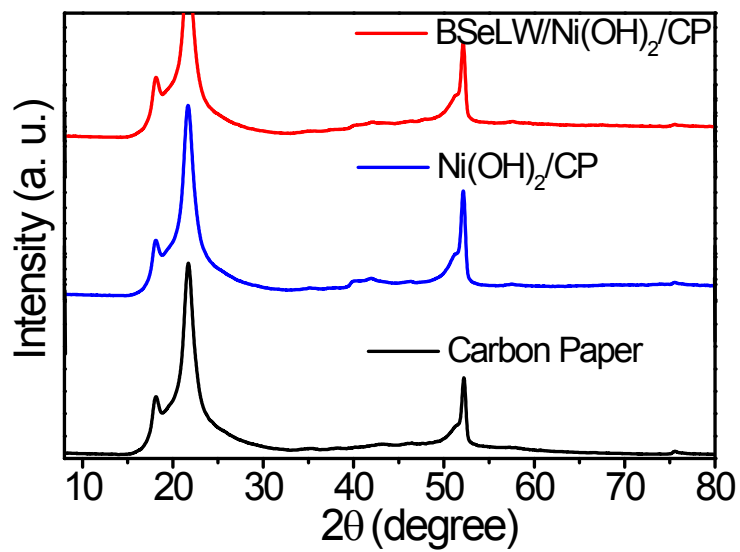


Figure S5. XRD patterns of the amorphous BSeLW/Ni(OH)₂/CP, Ni(OH)₂/CP and the bare carbon paper.

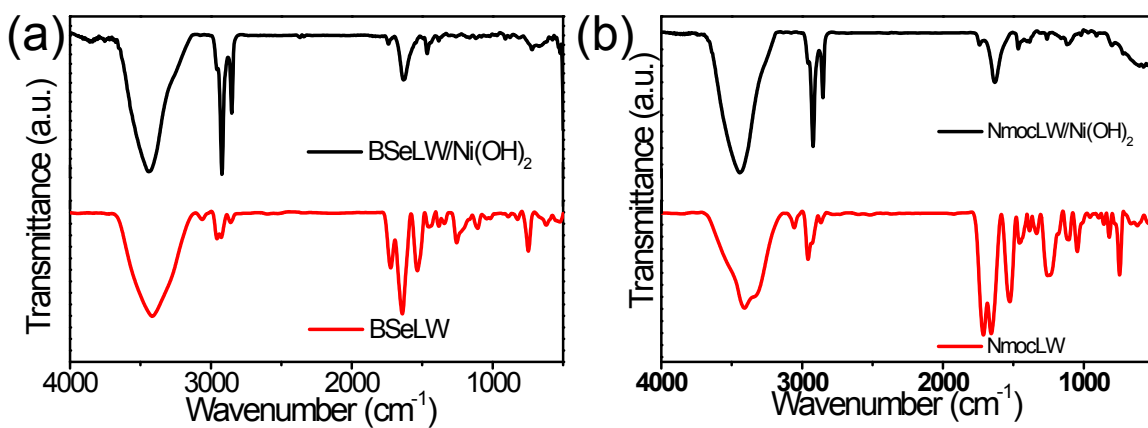


Figure S6. FT-IR spectra of (a) BSeLW/Ni(OH)₂ and BSeLW; (b) Nmoc-LW/Ni(OH)₂ and NmocLW.

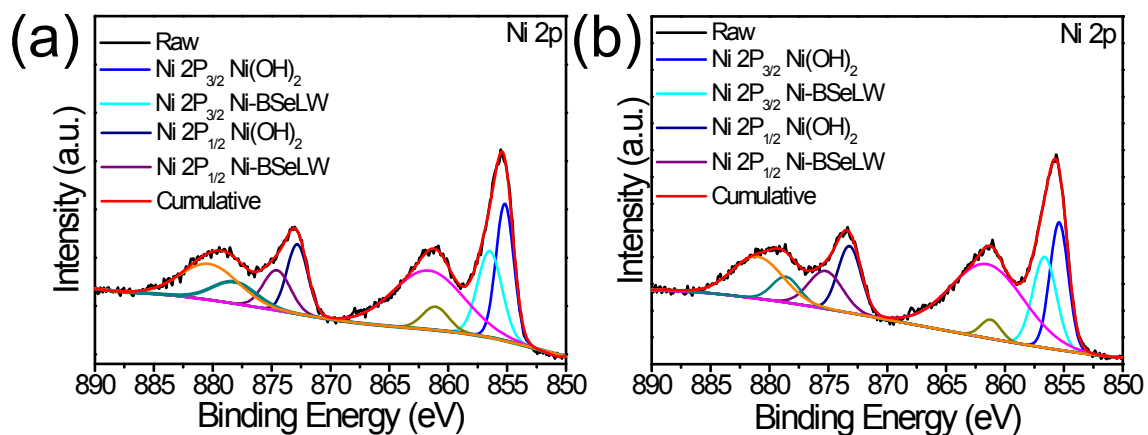


Figure S7. High resolution XPS spectra of Ni 2p of (a) (1:10) BSeLW/Ni(OH)₂ and (b) (1:30) BSeLW/Ni(OH)₂.

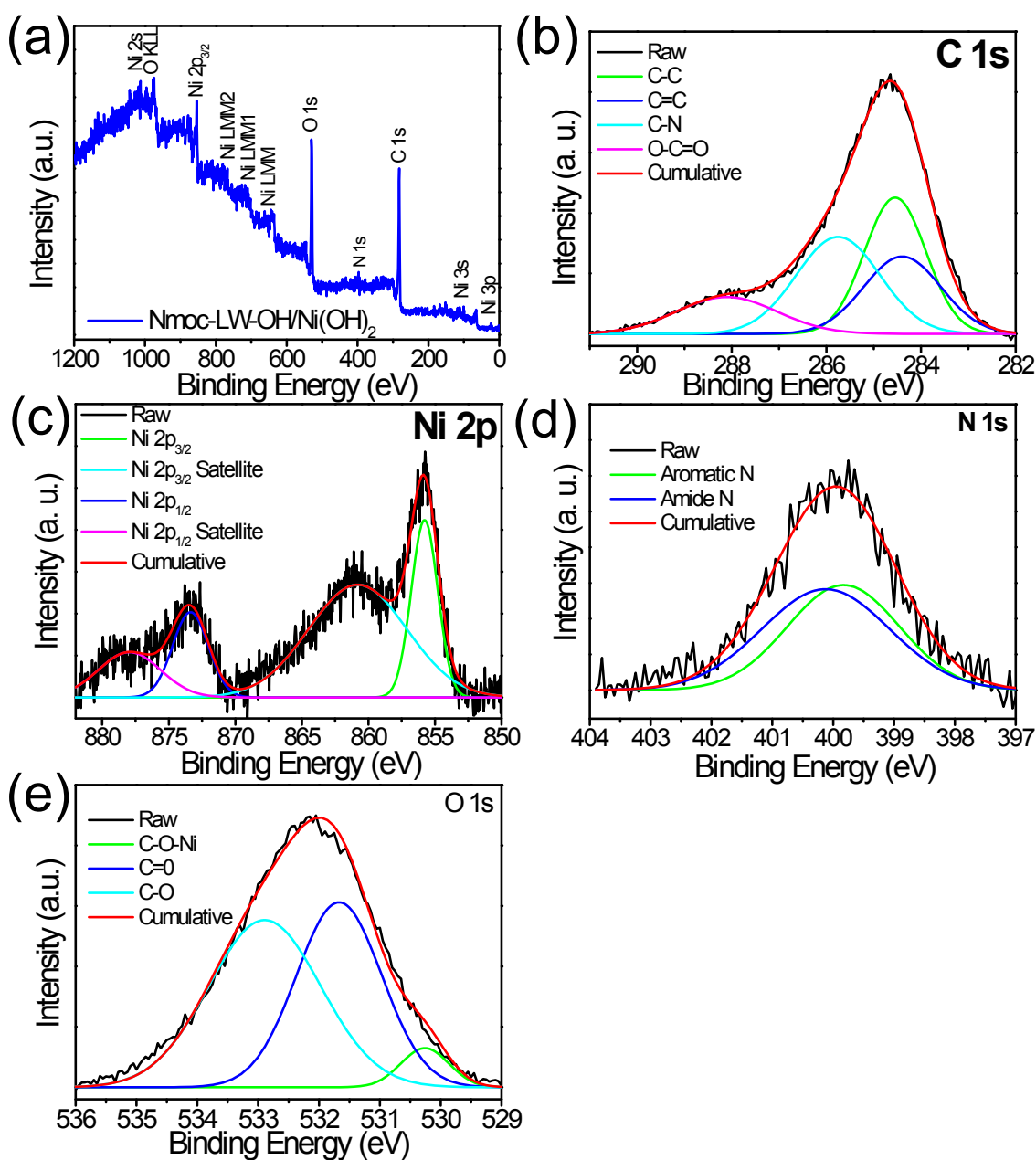
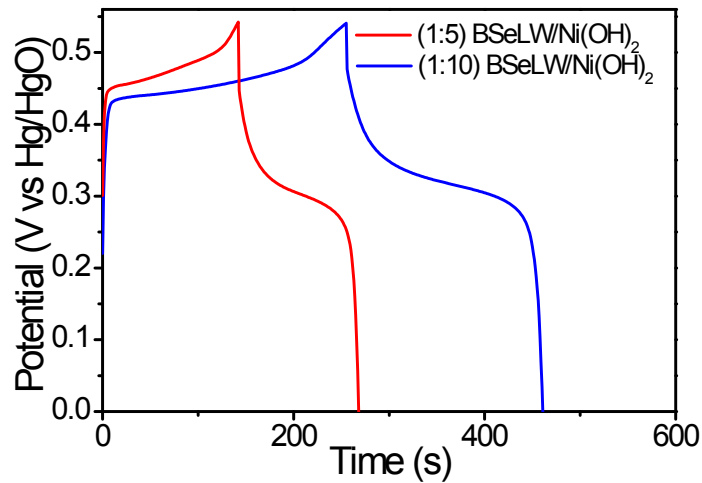


Figure S8. XPS spectra of electrochemically deposited Nmoc-LW/Ni(OH)₂ (a) Survey spectra of Nmoc-LW/Ni(OH)₂, Core level spectra of (b) C 1s, (c) Ni 2p, (d) N 1s, (e) O 1s.

Table S3. Comparative energy storage performance of Ni-based hybrid materials

| Sr. No. | Electrode Material | Synthesis Procedure | Specific Capacitance | Electrolyte | Ref. |
|---------|---|---------------------|---|--------------------------------------|-----------|
| 1. | Ni-terephthalate | Hydrothermal | 938.8 F g ⁻¹ at 1.818 A g ⁻¹ | 3 M KOH | 58 |
| 2. | Ni ₃ (HITP) ₂ | - | 111 F g ⁻¹ at 0.05 A g ⁻¹ | 1 M TEABF ₄ /CAN | 67 |
| 3. | Ni-MOF nanoflakes | Hydrothermal | 306.8 F g ⁻¹ at 0.5 A g ⁻¹ | 1 M LiOH | 68 |
| 4. | Ni-DMOF-ADC | Hydrothermal | 552 F g ⁻¹ at 1 A g ⁻¹ | 4 M KOH | 69 |
| 5. | Carbon/NiO nanosheet | - | 414 F g ⁻¹ at 5 A g ⁻¹ | 0.5 M K ₂ SO ₄ | 70 |
| 6. | Ni-MOF | Solvothermal | 634 F g ⁻¹ at 5mV s ⁻¹ | 6 M KOH | 71 |
| 7. | Ni-MOF | Hydrothermal | 1057 F g ⁻¹ at 1 A g ⁻¹ | 3 M KOH | 72 |
| 8. | Ni-MOF-1@GO-3% | Solvothermal | 590 F g ⁻¹ at 1 A g ⁻¹ | 6 M KOH | 73 |
| 9. | (1:20) BSeLW/Ni(OH) ₂ /CP | Electrodeposition | 742 F g ⁻¹ at 1.5 A g ⁻¹ | 1 M KOH | This work |

**Figure S9.** GCD profile of (1:5) BSeLW/Ni(OH)₂ and (1:10) BSeLW/Ni(OH)₂ at 1.5 A g⁻¹ in 1 M KOH.

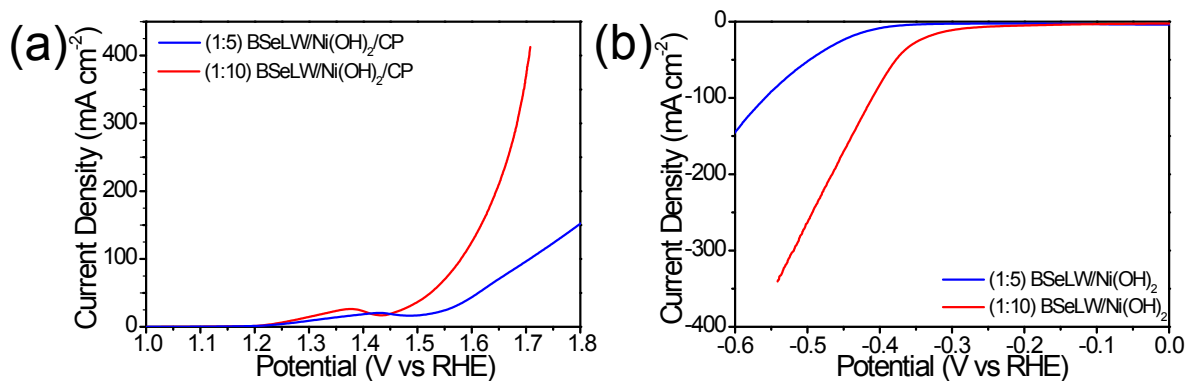


Figure S10. iR-corrected LSV profile of (1:5) BSeLW/Ni(OH)₂ and (1:10) BSeLW/Ni(OH)₂ for electrocatalytic (a) OER and (b) HER with the scan rate 5 mV s⁻¹ in 1 M KOH.

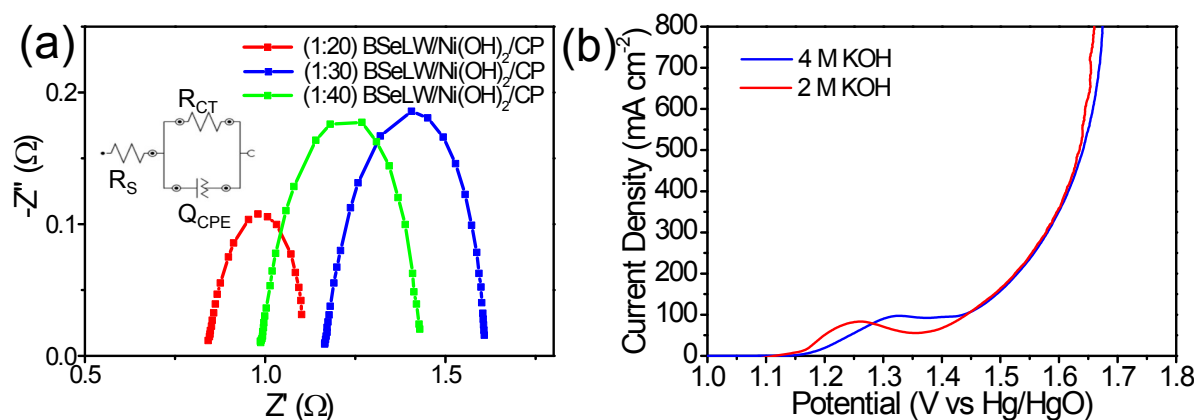


Figure S11. (a) Nyquist plots with equivalent electrochemical circuit of organic-inorganic nanohybrid electrodes measured at 1.56 V vs RHE. (b) iR-corrected LSV curve of (1:20) BSeLW/Ni(OH)₂/CP in 2 M KOH and 4 M KOH electrolyte.

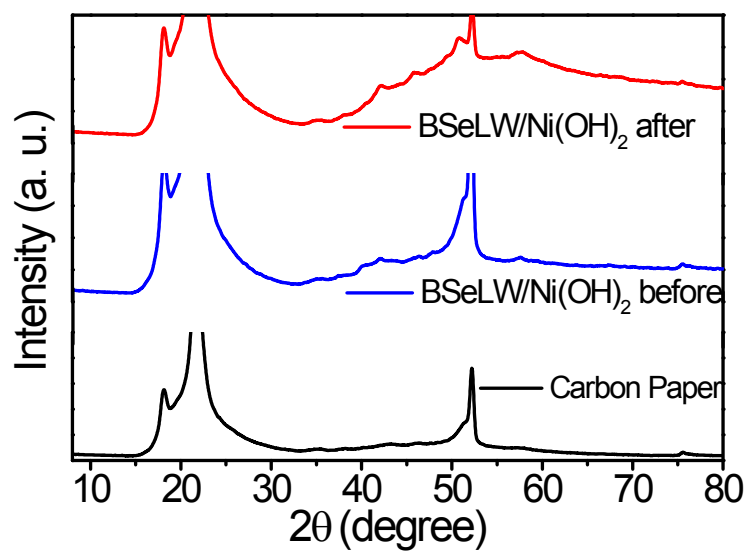


Figure S12. XRD patterns of carbon paper and BSeLW/Ni(OH)₂/CP after OER and HER.

¹H NMR data of all compounds:

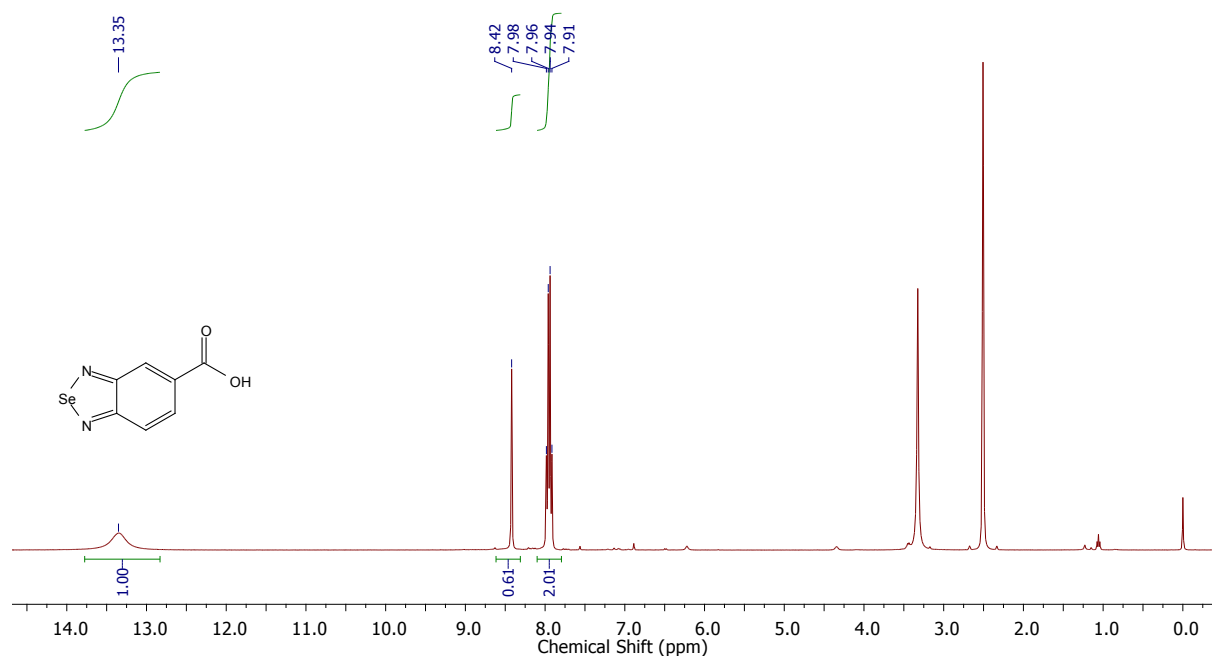


Figure S13. ¹H NMR (DMSO-*d*₆, 400 MHz) spectrum of BSe.

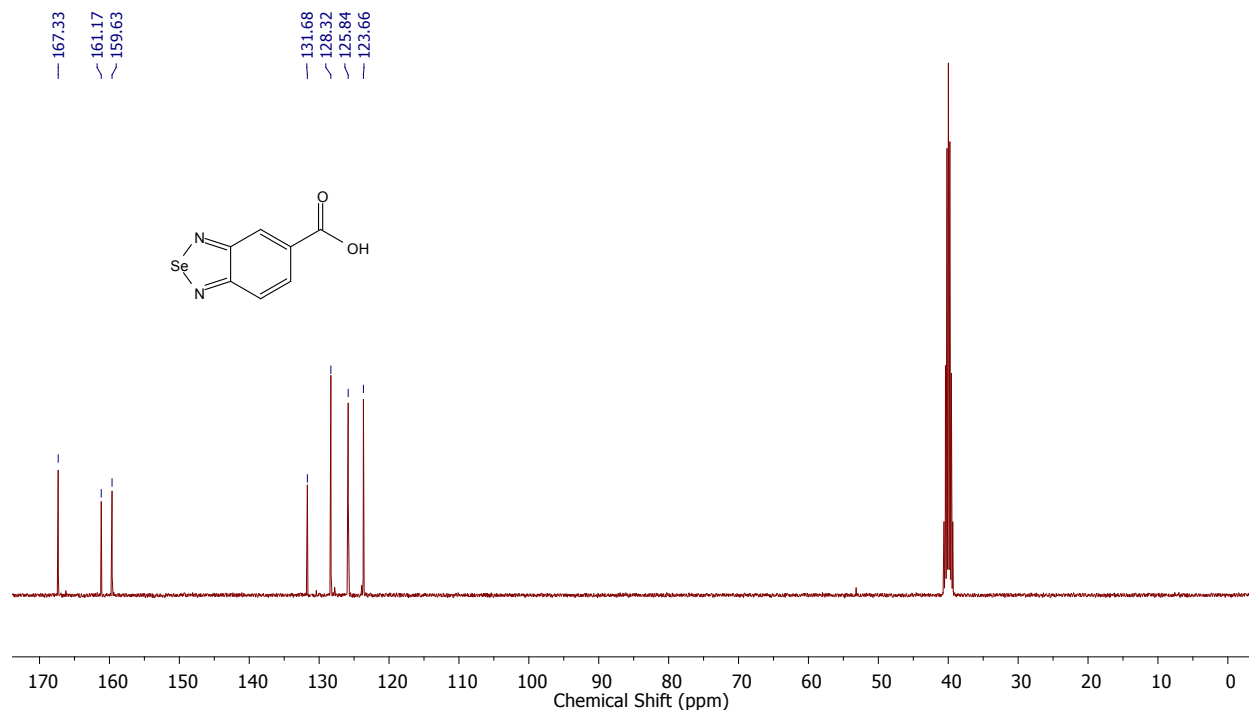


Figure S14. ¹³C NMR (DMSO-*d*₆, 100 MHz) spectrum of BSe.

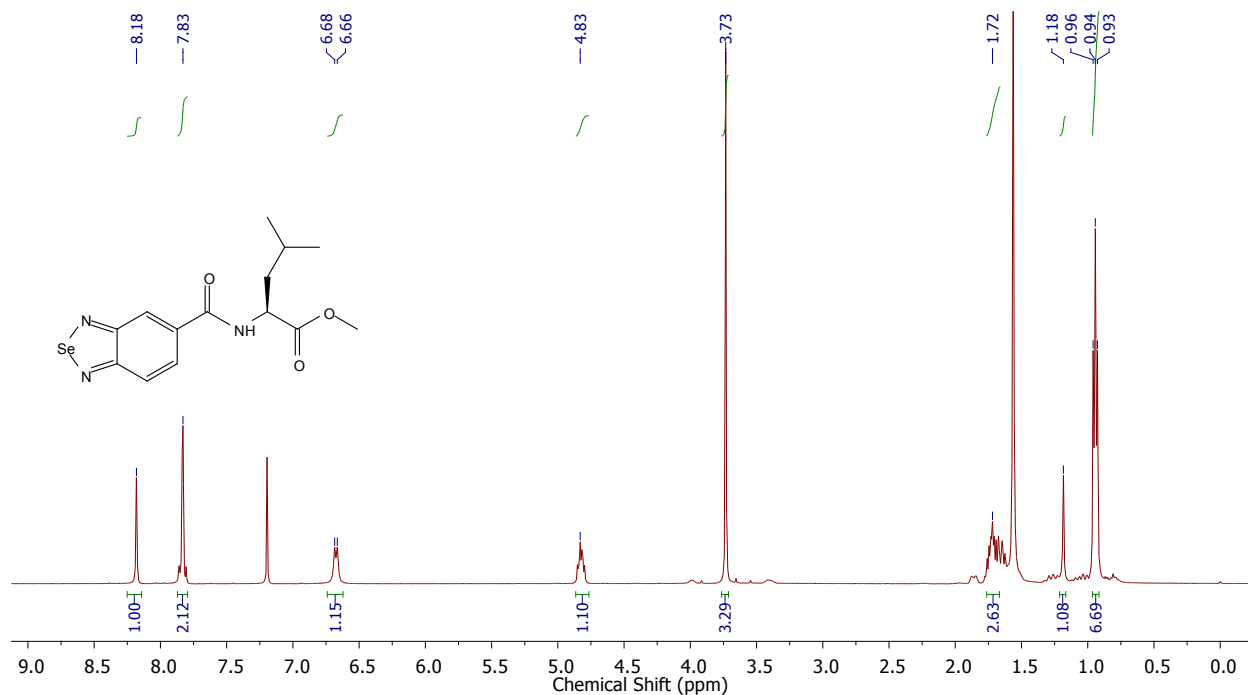


Figure S15. ^1H NMR (CDCl_3 , 400 MHz) spectrum of BSeL-OMe.

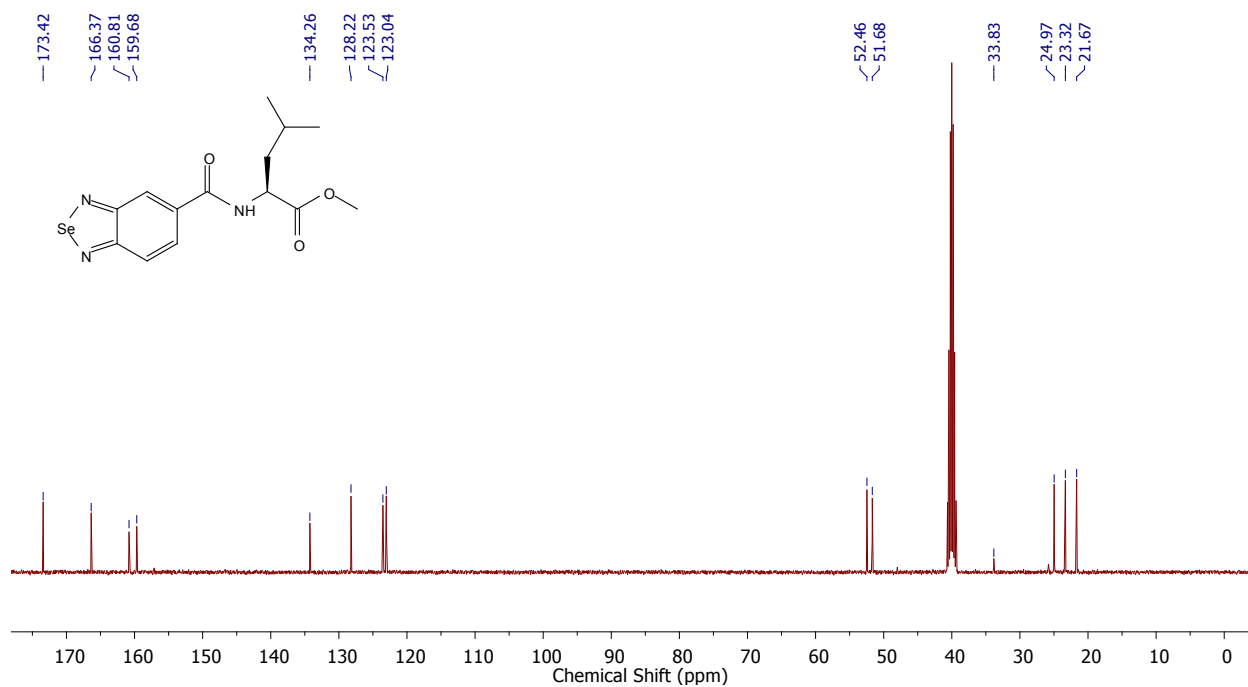


Figure S16. ^{13}C NMR ($\text{DMSO-}d_6$, 100 MHz) spectrum of BSeL-OMe.

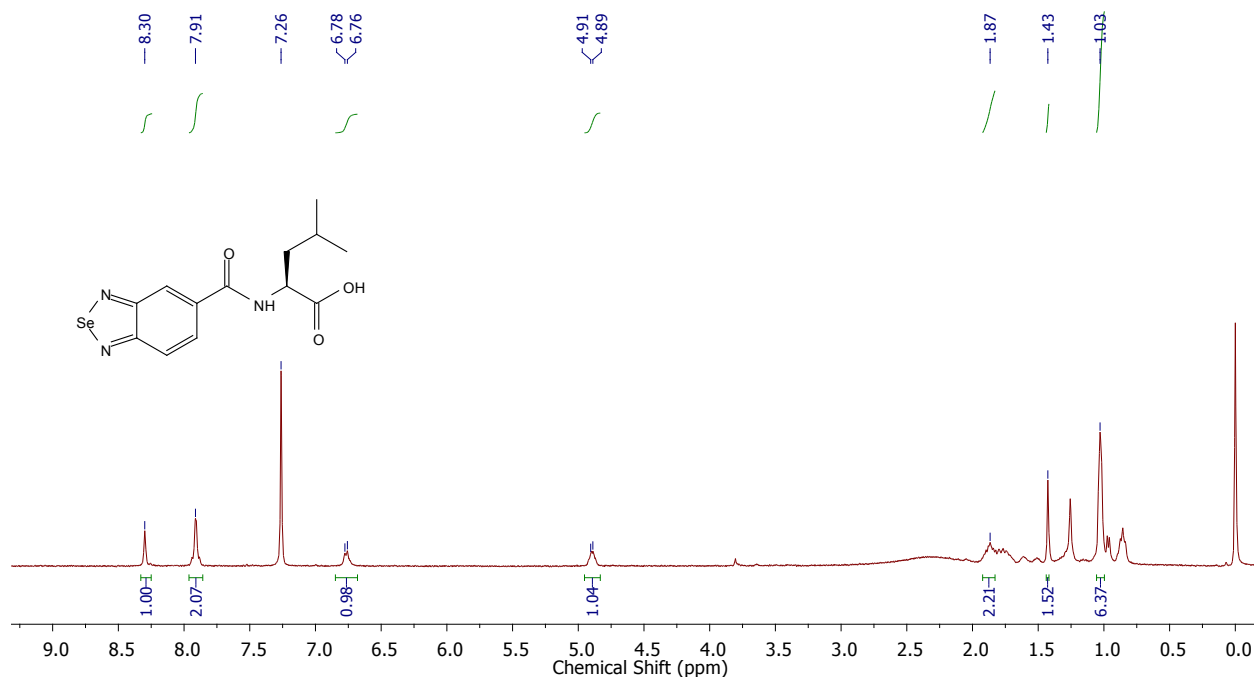


Figure S17. ^1H NMR (CDCl_3 , 400 MHz) spectrum of BSeL.

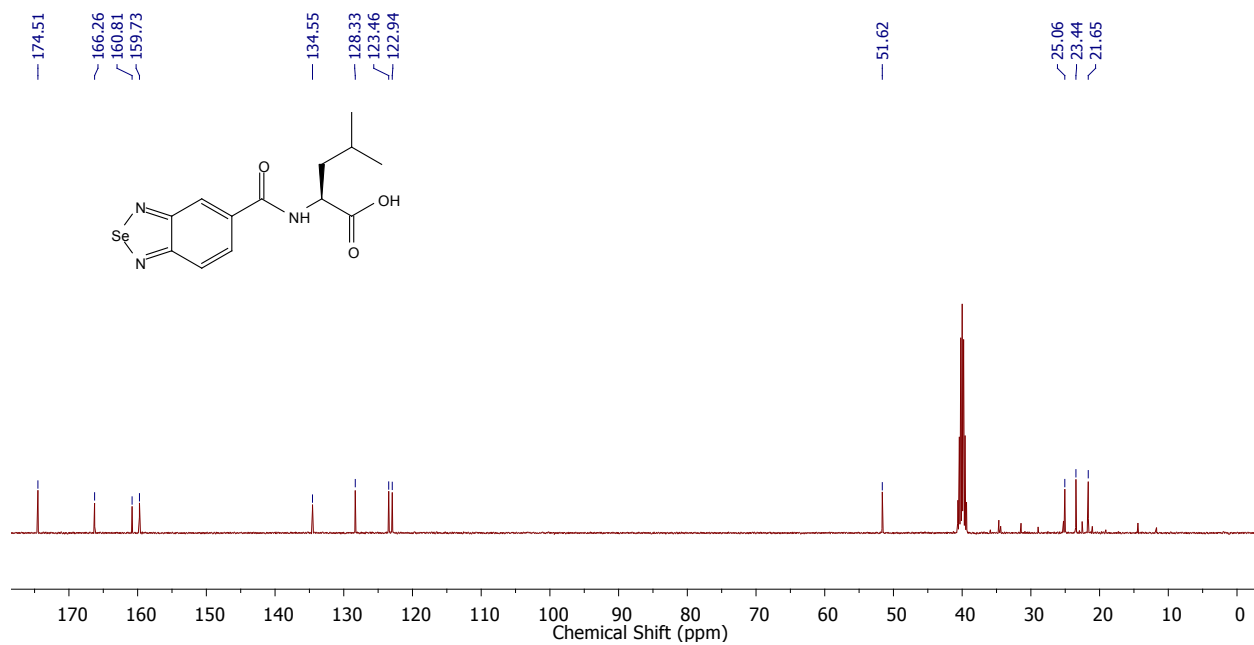


Figure S18. ^{13}C NMR ($\text{DMSO-}d_6$, 100 MHz) spectrum of BSeL.

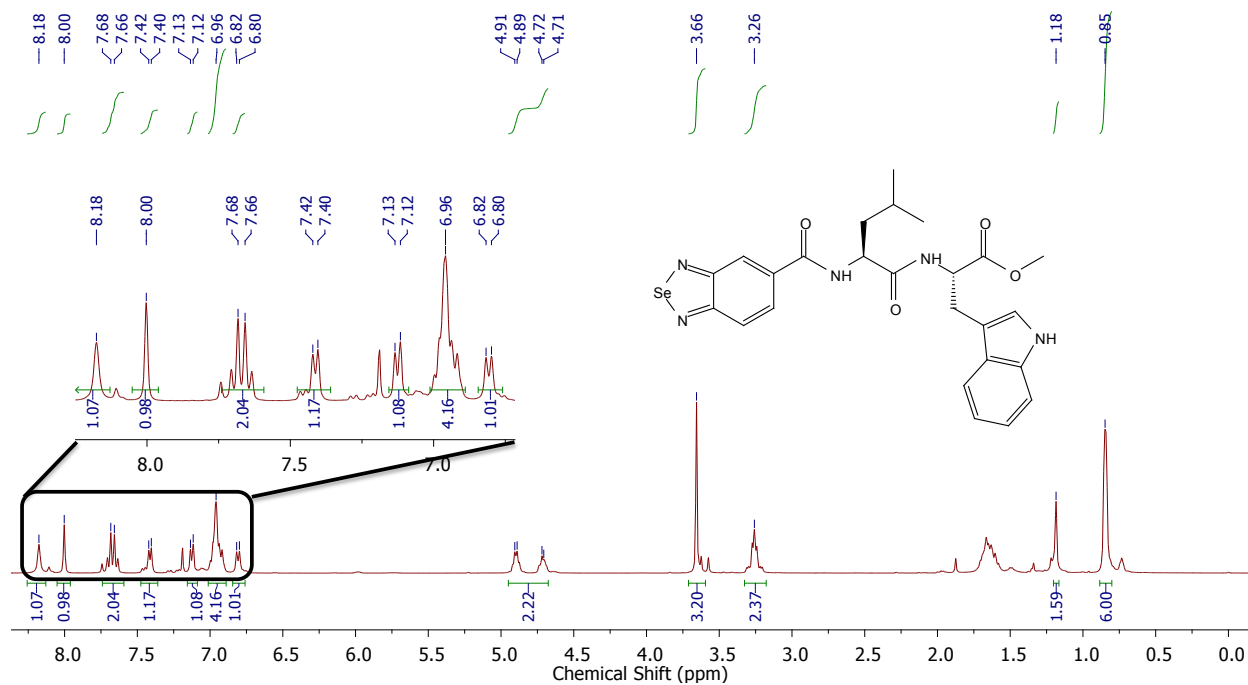


Figure S19. ¹H NMR (CDCl₃, 400 MHz) spectrum of BSeLW-OMe.

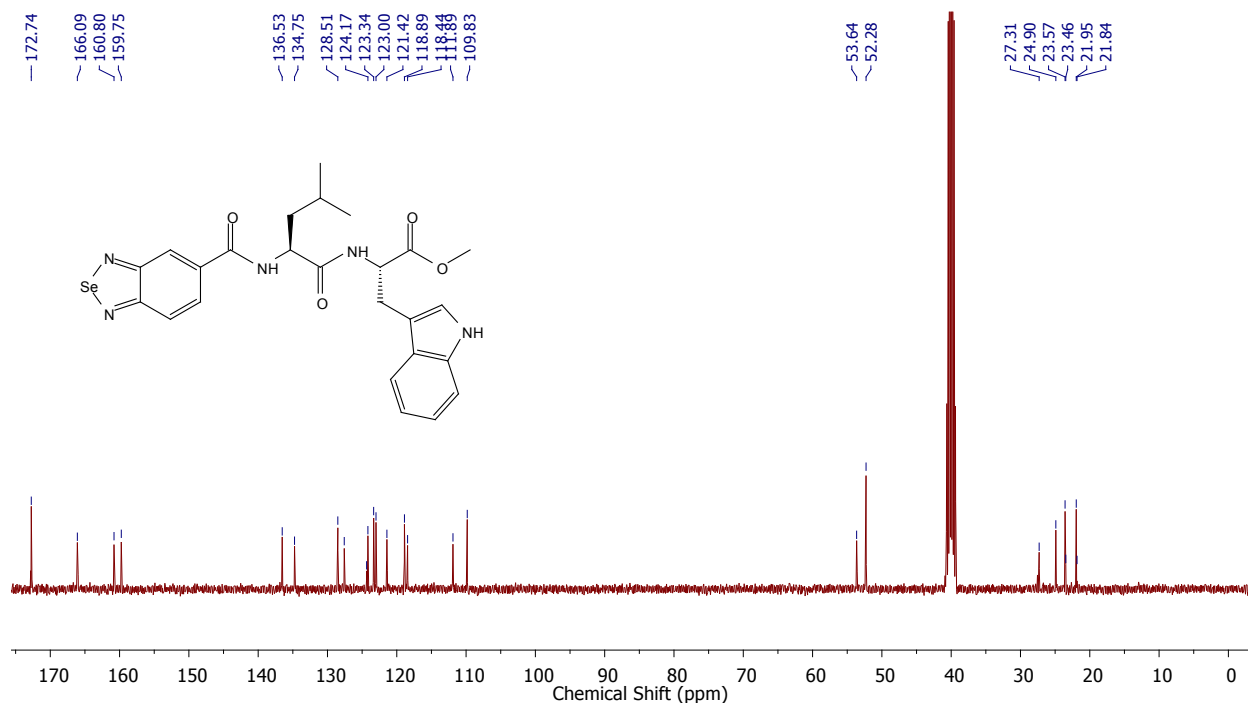


Figure S20. ¹³C NMR (DMSO-*d*₆, 100 MHz) spectrum of BSeLW-OMe.

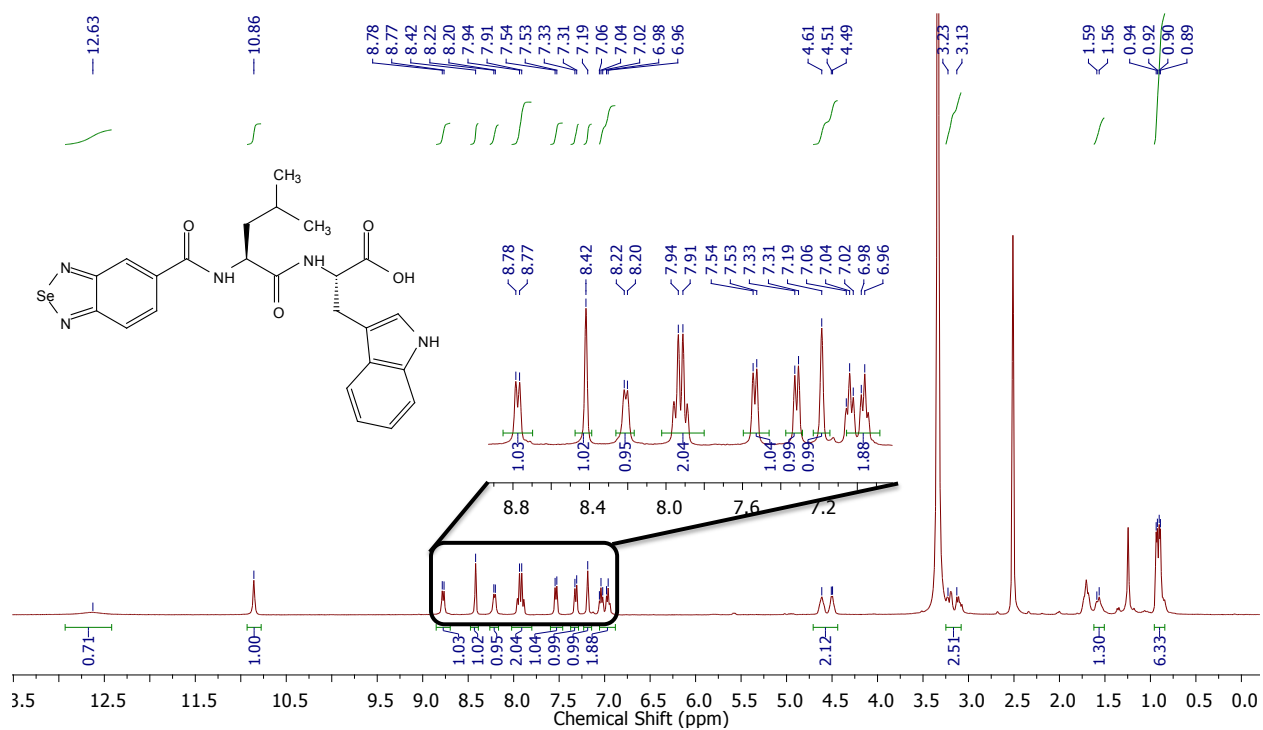


Figure S21. ^1H NMR (DMSO- d_6 , 400 MHz) spectrum of BSeLW.

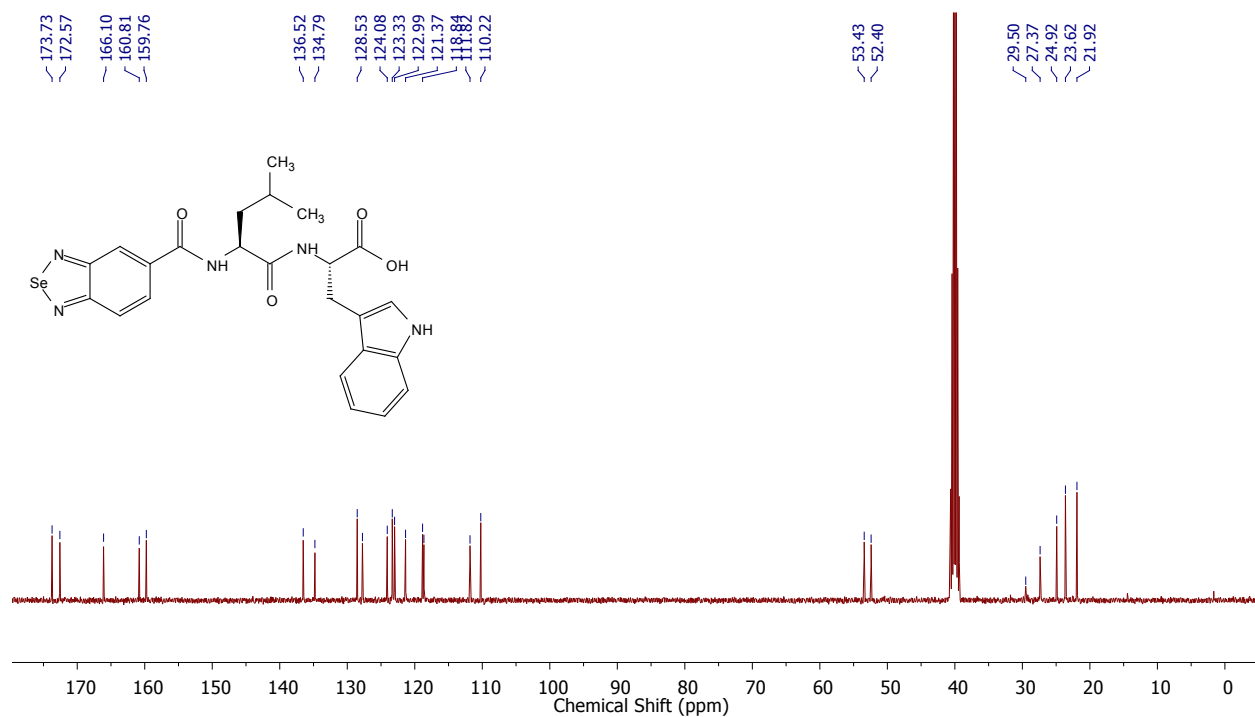


Figure S22. ^{13}C NMR (DMSO- d_6 , 100 MHz) spectrum of BSeLW.

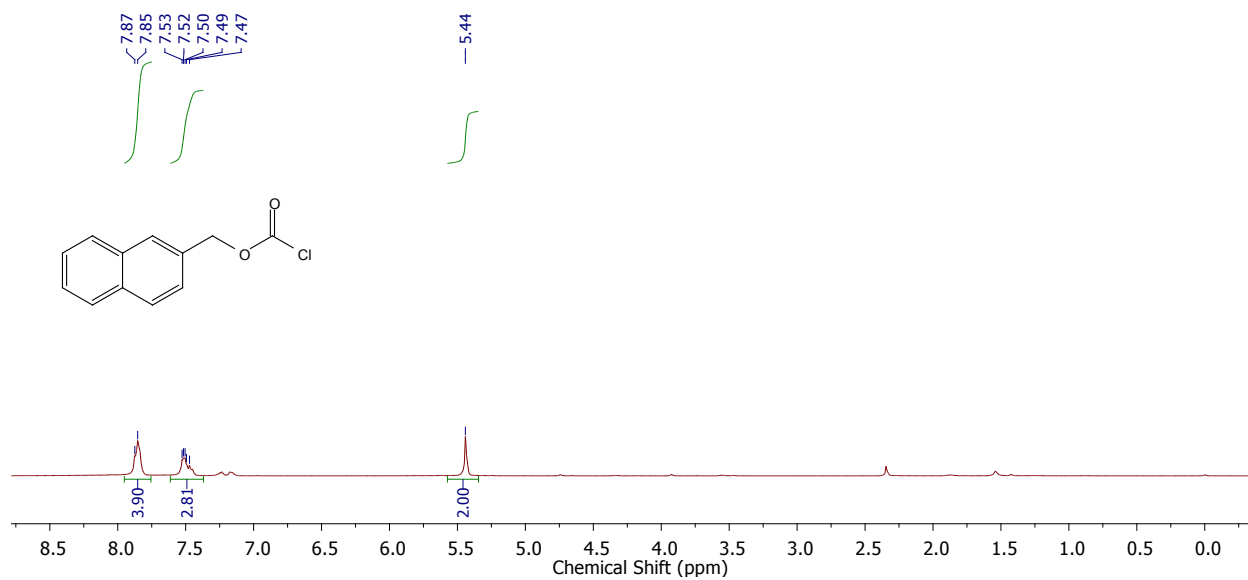


Figure S23. ¹H NMR (CDCl₃, 400 MHz) spectrum of Nmoc-Cl.

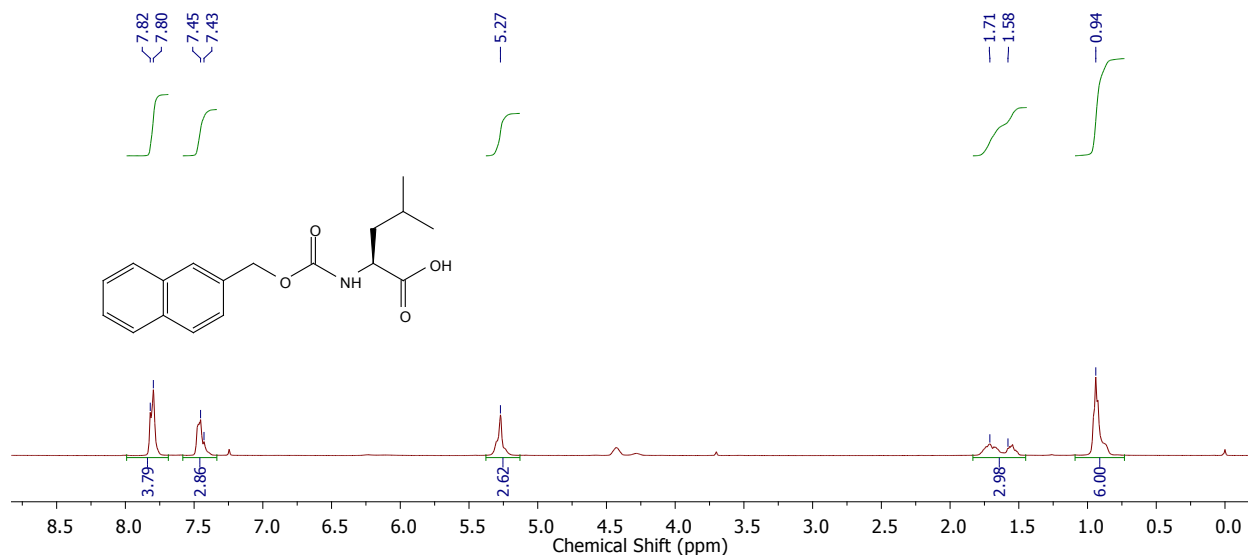


Figure S24. ¹H NMR (CDCl₃, 400 MHz) spectrum of NmocL.

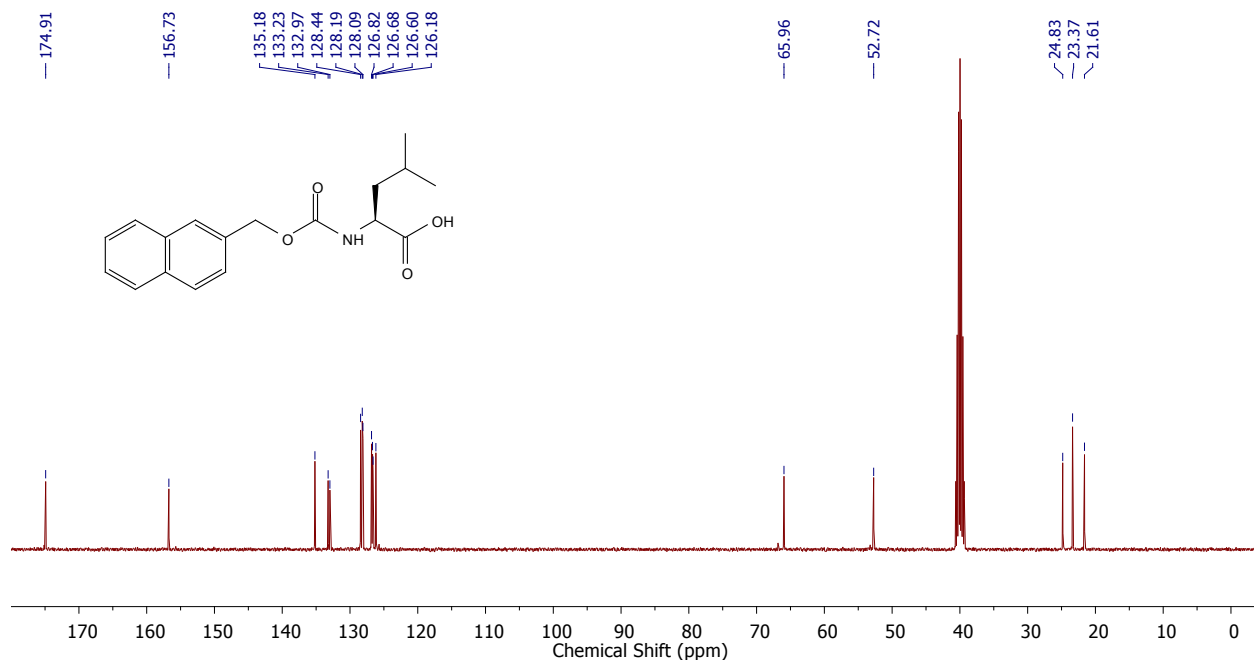


Figure S25. ¹³C NMR (DMSO-*d*₆, 100 MHz) spectrum of NmocL.

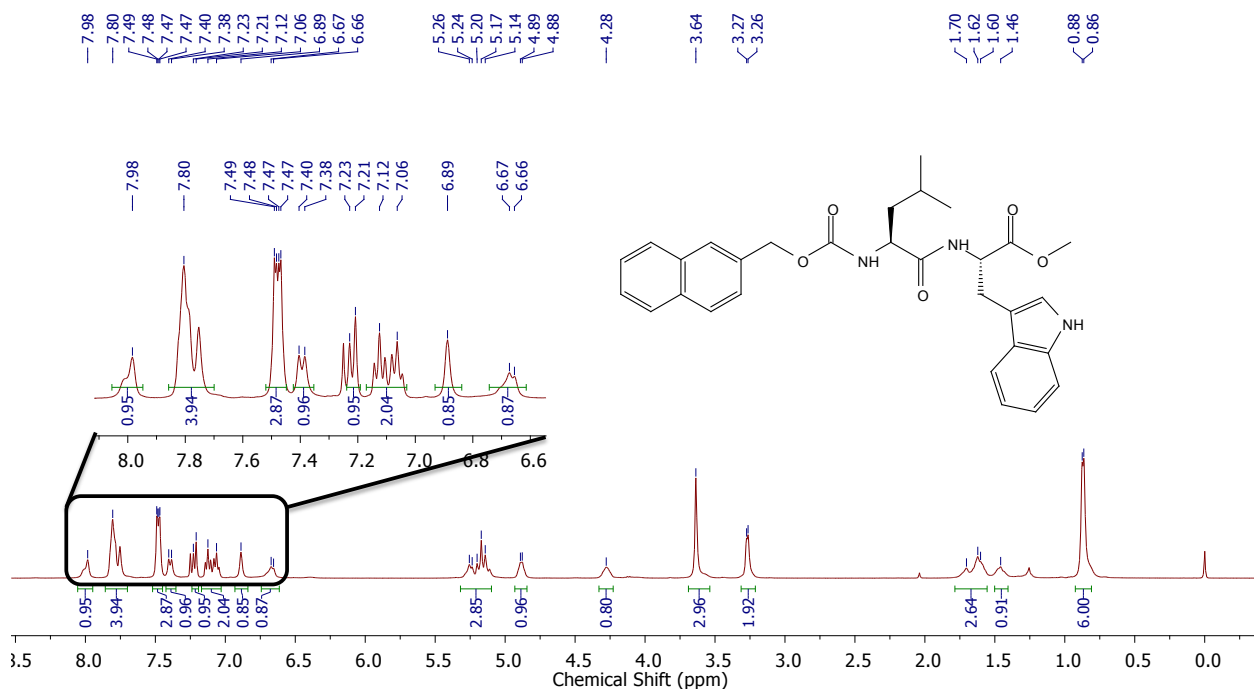


Figure S26. ¹H NMR (CDCl₃, 400 MHz) spectrum of NmocLW-OMe.

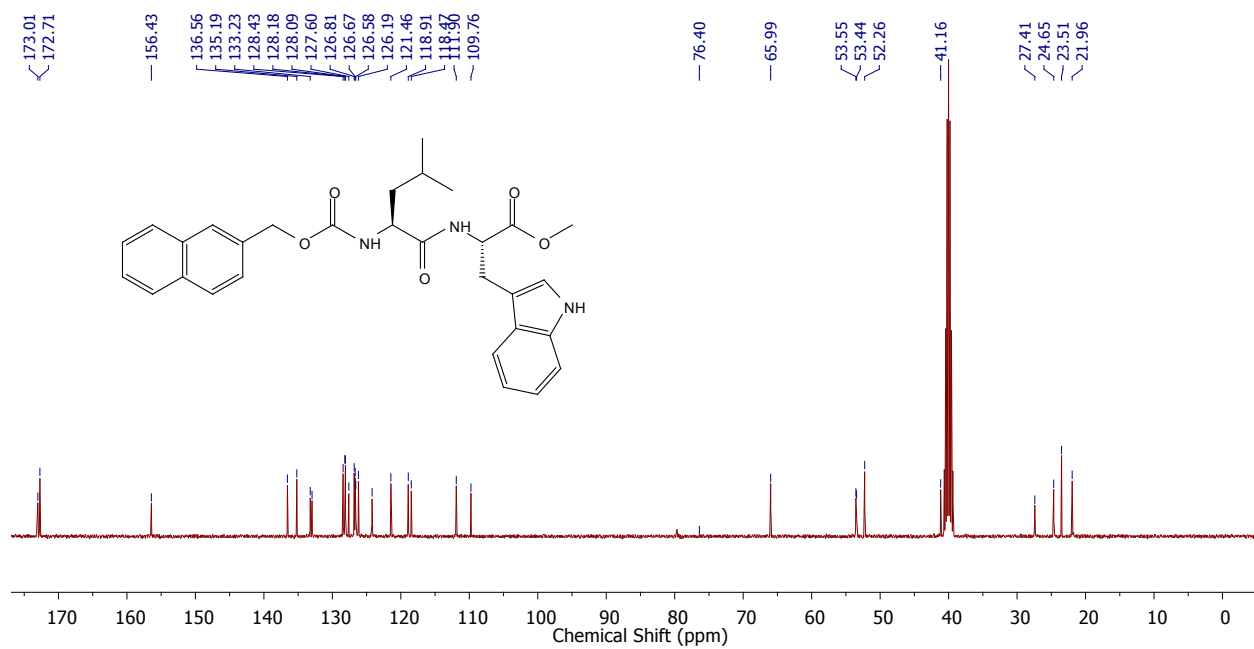


Figure S27. ¹³C NMR (DMSO-*d*₆, 100 MHz) spectrum of NmocLW-OMe.

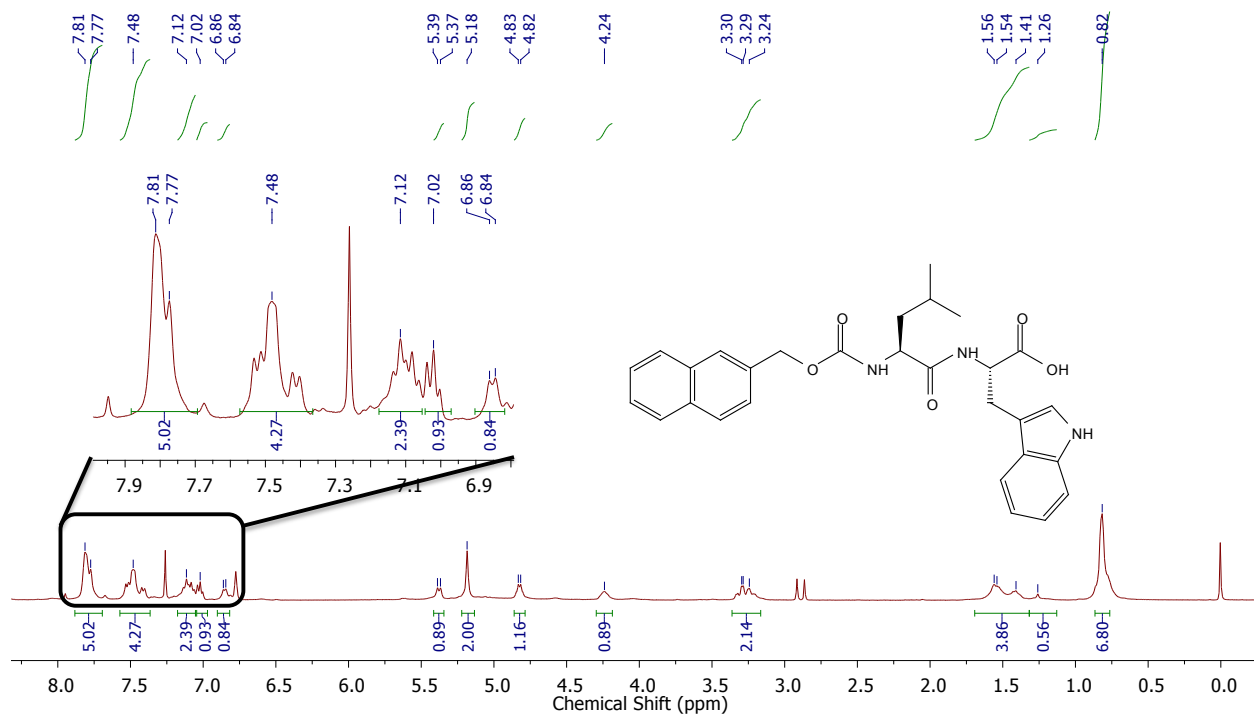


Figure S28. ¹H NMR (CDCl₃, 400 MHz) spectrum of NmocLW.

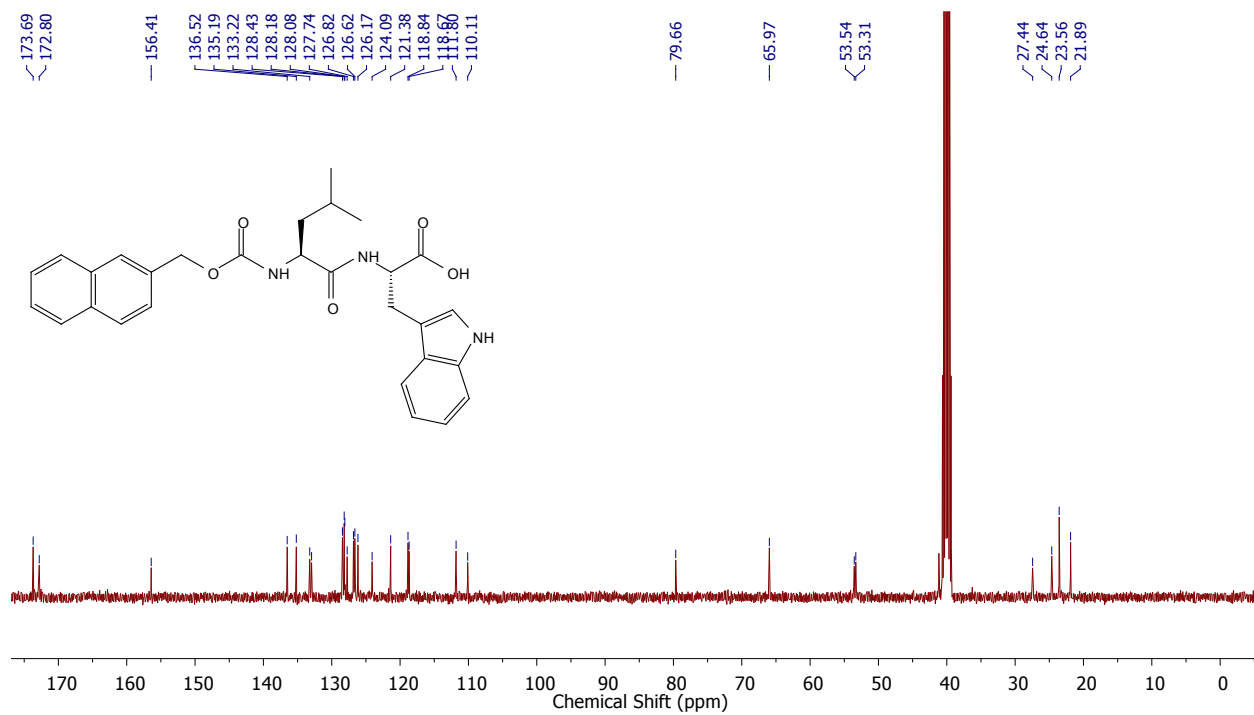


Figure S29. ¹³C NMR (DMSO-*d*₆, 400 MHz) spectrum of NmocLW.

Mass data of all compounds:

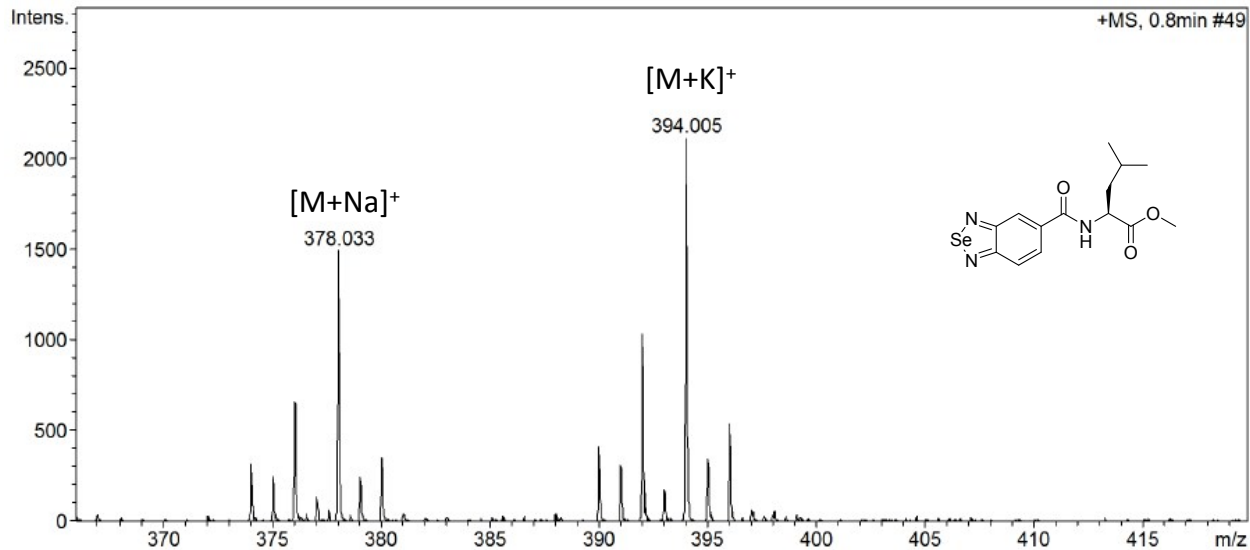


Figure S30. Mass spectrum of BSeL-OMe.

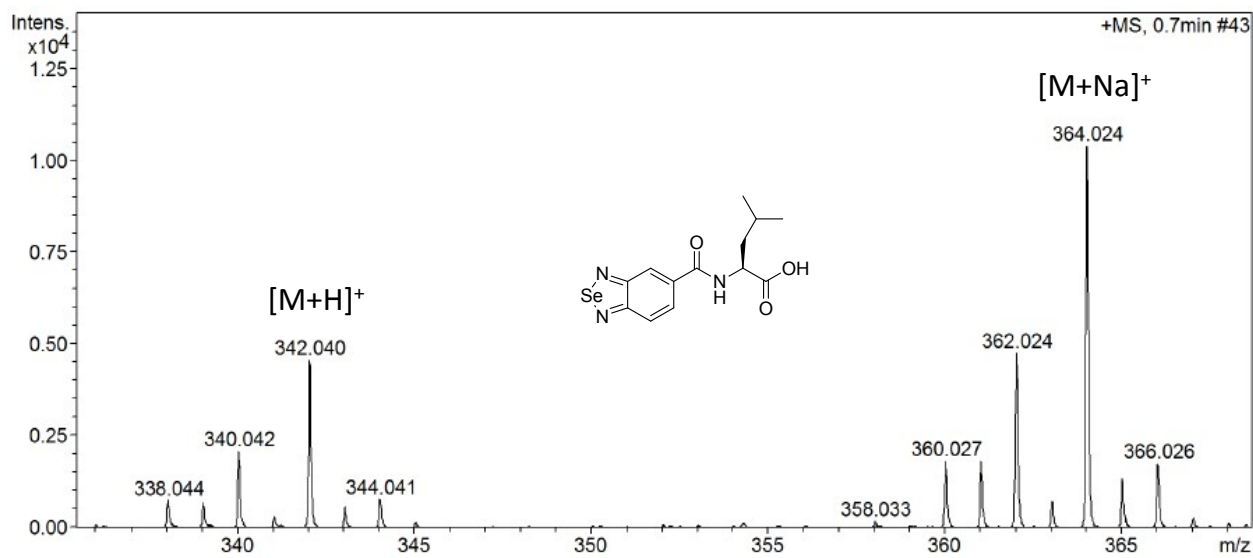


Figure S31. Mass spectrum of BSeL.

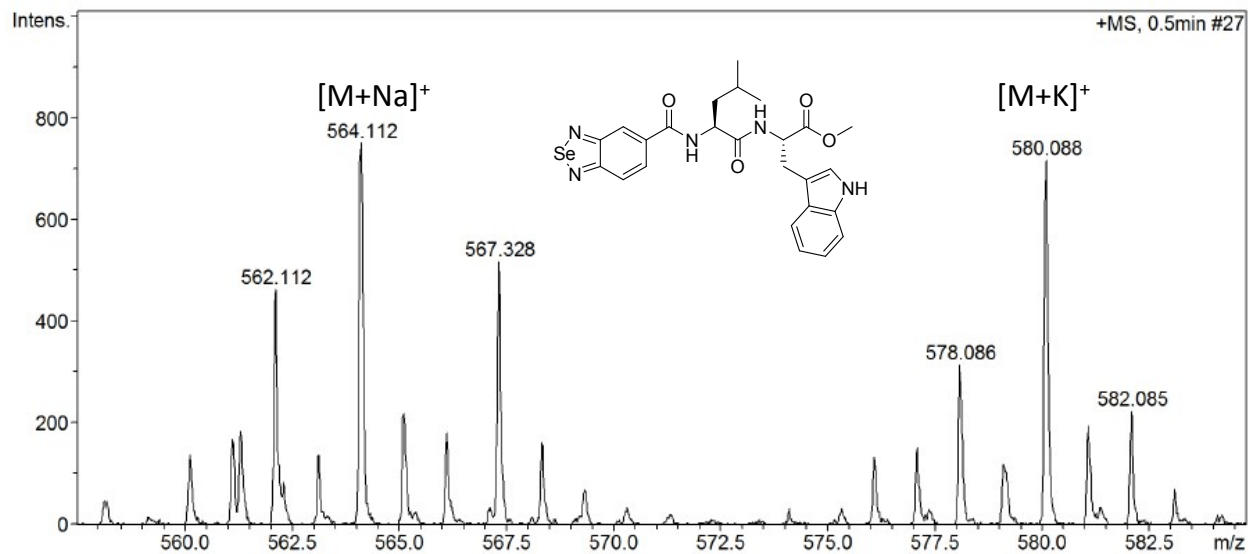


Figure S32. Mass spectrum of BSeLW-OMe.

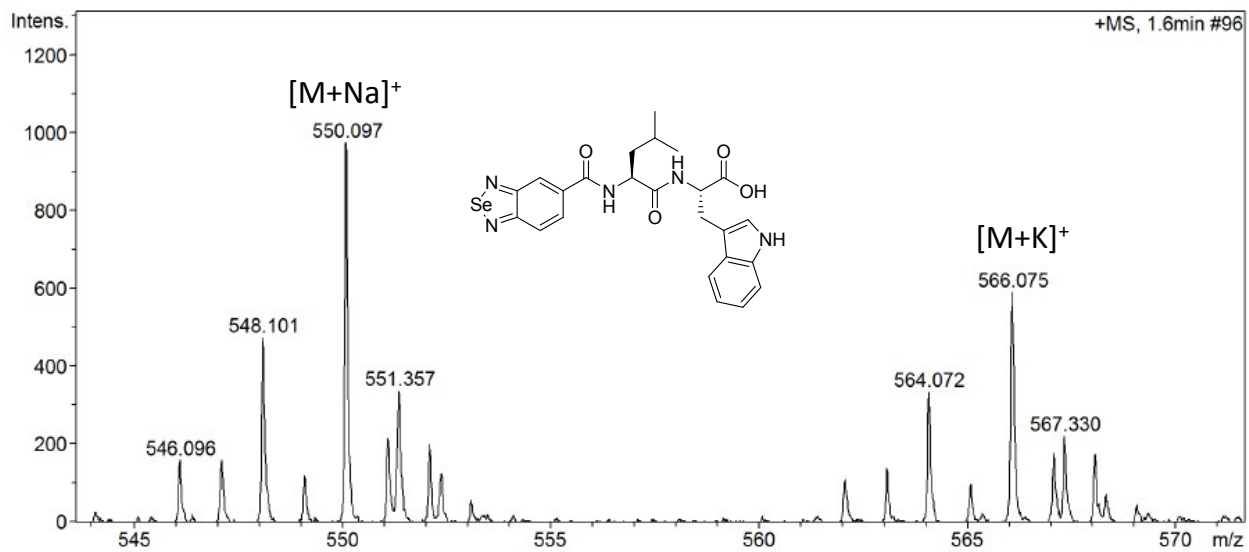


Figure S33. Mass spectrum of BSeLW.

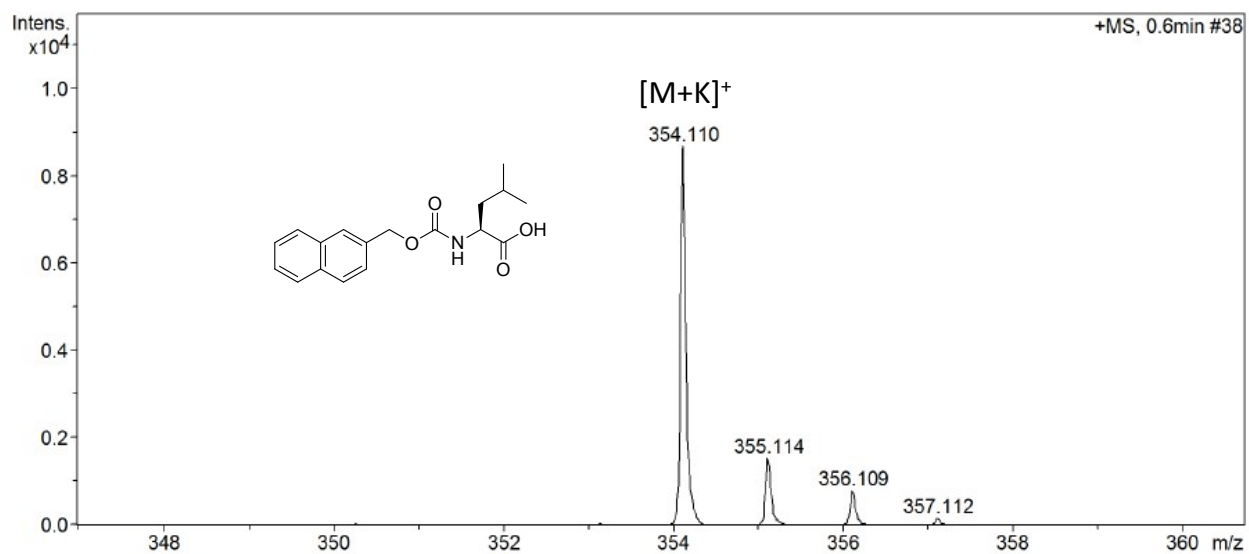


Figure S34. Mass spectrum of NmocL.

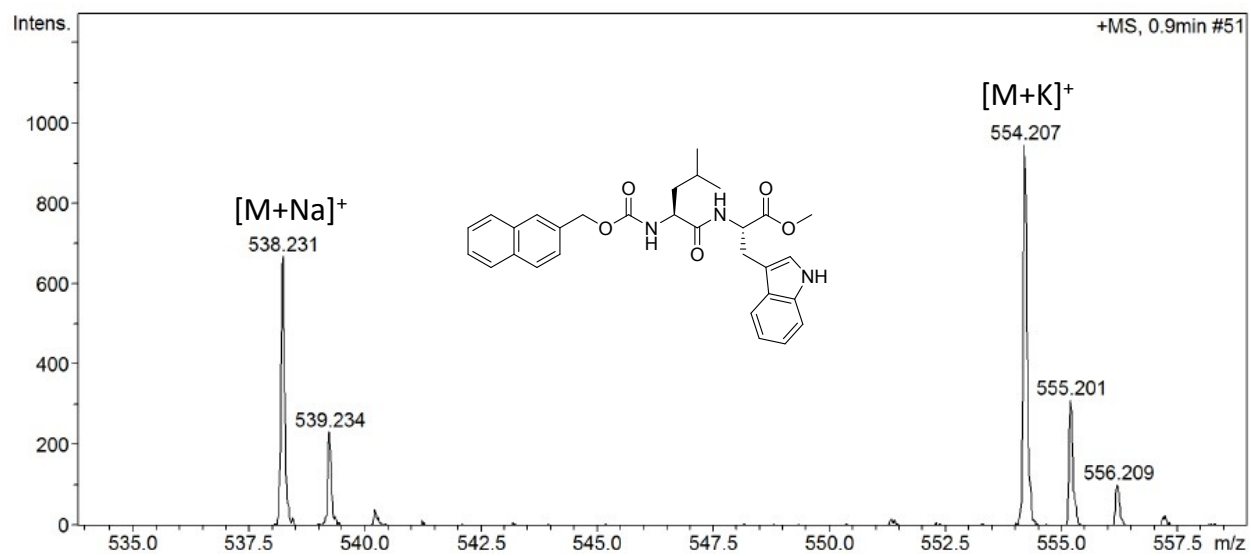


Figure S35. Mass spectrum of NmocLW-OMe.

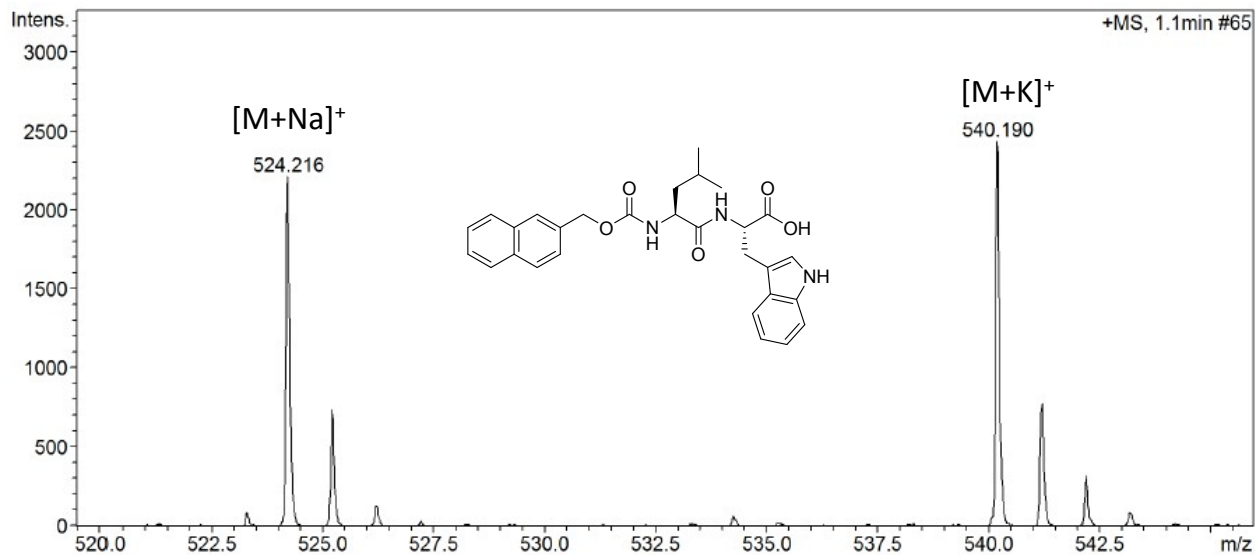


Figure S36. Mass spectrum of NmocLW.