Electronic Supplementary Material (ESI) for Chem.Commun.

Electronic Supplementary Information for

A protein structure-guided covalent scaffold selectively targets the B1 and B2 subclass metallo-β-lactamases

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Percent inhibition of other MβLs

The percent inhibition of MβLs from the subclasses B1 (NDM-1, IMP-1), B2 (ImiS) and B3 (L1) by these compounds at 20 µM were determined, and the results are shown in Fig. S1.

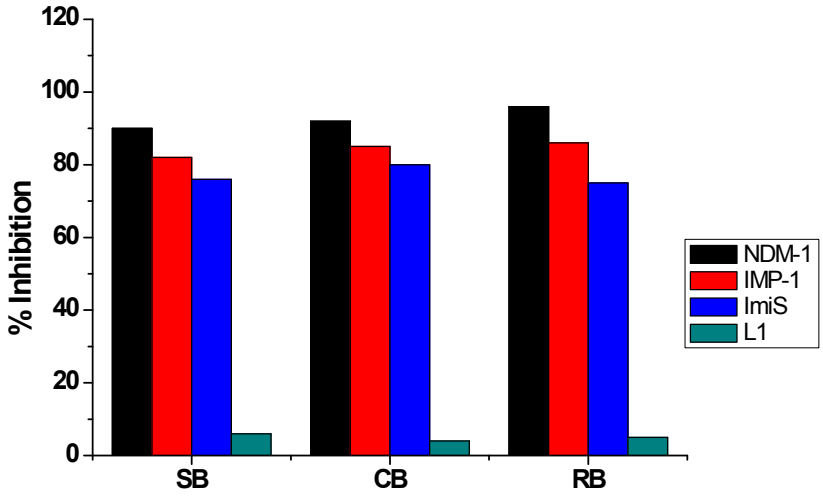


Fig. S1. Percent inhibition of compounds against MβLs NDM-1, IMP-1 from subclasses B1, ImiS from B2, andL1 from B3 using cefazolin as substrate for B1 and B3 enzymes, and imipenem for ImiS. The concentration of compounds was 20 µM.

Determination of IC_{50} values

The inhibitor concentration causing 50% decrease of enzyme activity (IC_{50}) weredeterminated at 25°C using imipenem as substrate of ImiS and cefazolin as substrate of NDM-1 and IMP-1. All compounds were dissolved in a small volume of DMSO and then diluted with 30 mM Tris, pH 8.0 for NDM-1 and pH 7.5 for IMP-1 and 50 mM Tris, pH 7.0for ImiS. The final concentrations of DMSO in inhibition experiments werebelow 0.1%; control experiments verified that the 0.1% DMSO had no inhibitory activityagainst the MβLs tested. The compounds concentrations were varied between 0 and 20 µM, andsubstrate concentrations were 50 µM. The kinetic values in this study are the means from at least three independent measurements; at least nine different concentrations of the inhibitor were used to determine the kinetic parameters (IC_{50}).The IC_{50} values for allanalyzed compounds were calculated using IC_{50} exe 1.0.0.0 software program.

Table S1. Inhibitory activity (IC_{50}, µM) of the N-substituted ebselen against four representative MβLs

Compounds	NDM-1	IMP-1	ImiS	L1
Ebselen	0.072± 0.012	1.59± 0.06	9.56± 0.34	-
SB	0.045± 0.005	0.53± 0.07	7.65± 0.21	-
CB	0.025± 0.004	0.97± 0.12	12.5± 0.4	-
RB	0.016± 0.003	0.46± 0.04	8.62± 0.32	-

-: No inhibition

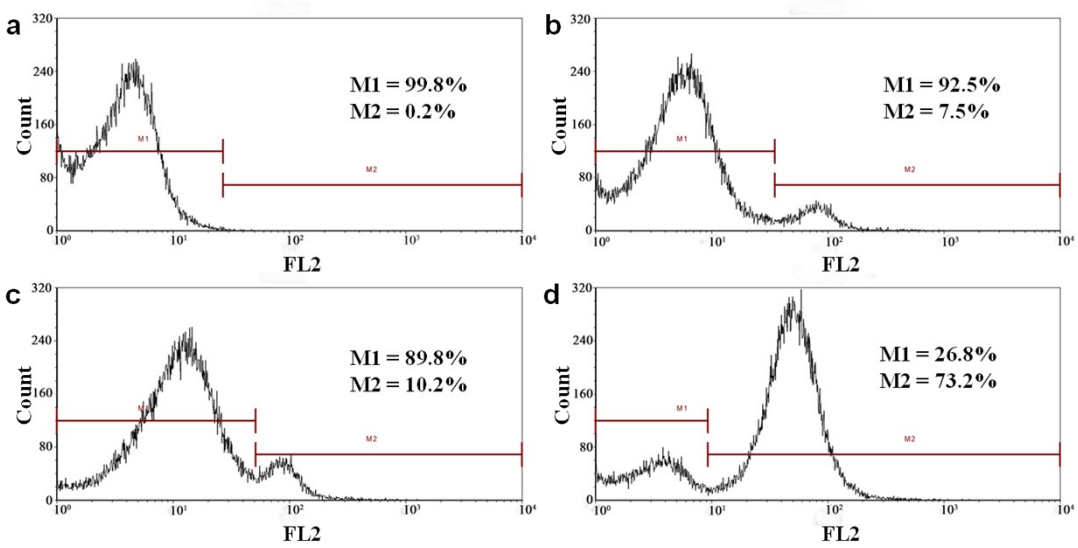


Fig. S2. Flow cytometry analysis of NDM-1 *E.coli* cells incubation with **RB** at different concentrations.NDM-1 *E.coli* cells with 0 (a), 1 (b), 5 (c), and 20 µM **RB** (d).

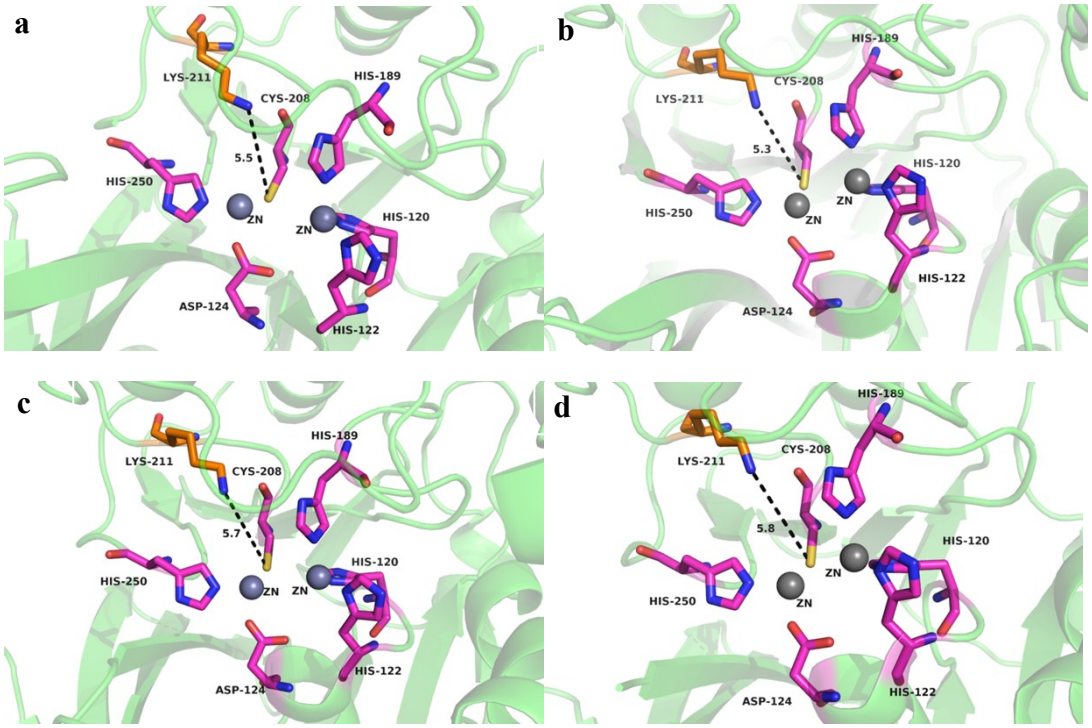


Fig. S3. The overview of the active site of NDM-1 crystal structures (Cys208 and Lys211, BBL numbering Cys221 and Lys224, respectively)[1]. PDB code: (a) 3q6x (b) 4exa (c) 4eyl (d) 4u4l.

MALDI-TOF MS analysis

A total of 20 µL **SB** stock solution (1 mM) was added to 80 µL NDM-1 solution (100 µM) in 10 mM Tris-HCl buffer (pH 7.5) at 4 °C. After incubation at 4 °Cfor 2 h, to probe further the nature of this attachment, the NDM-1-**SB** was dialyzed against 3 x 1 L of 50 mM Hepes, pH 7.5, at 4°C for 2 days. Activity assays of the resulting solution demonstrated that the dialyzed NDM-1-**SB** sample had the same activity as a control NDM-1 sample that was dialyzed but not reacted with **SB**. The samples were subsequently prepared for MALDI-TOF MS by using 3,5-Dimethoxy-4-hydroxycinnamicacid as the matrix.

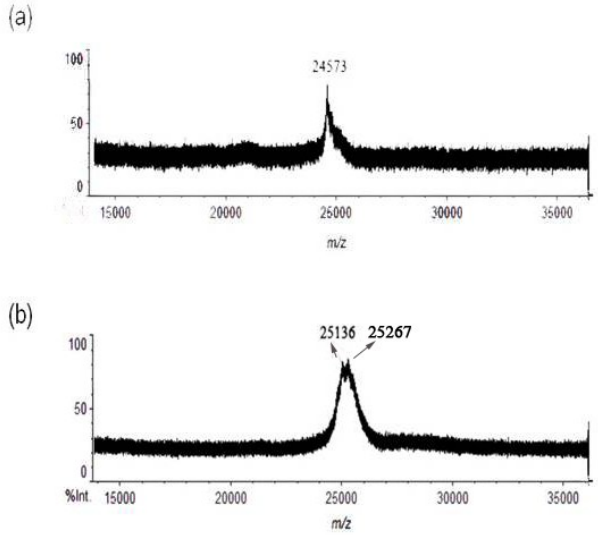
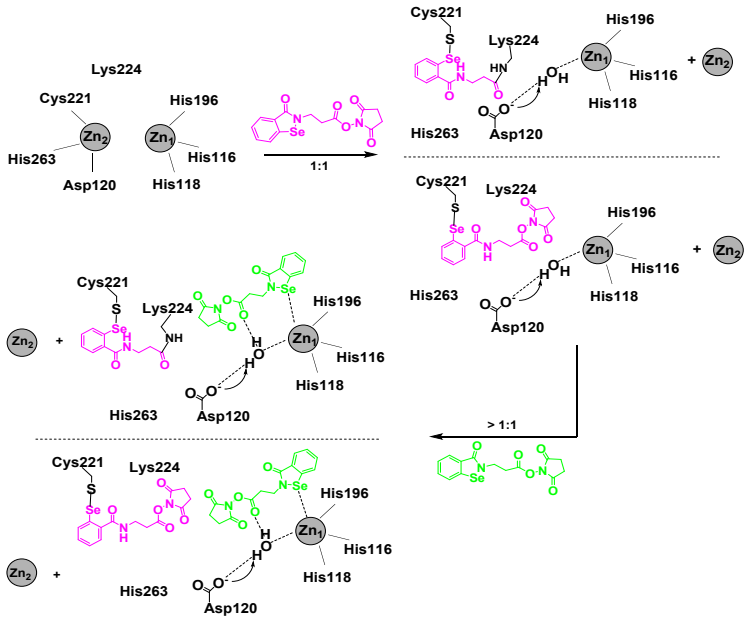


Fig. S4. Analysis of interaction between NDM-1 and **SB** by MADLI-TOF: (a) mass spertrum of recombinant NDM-1 (Enz) (b) mass spertrum of recombinant NDM-1 (Enz) after incubation with **SB**.

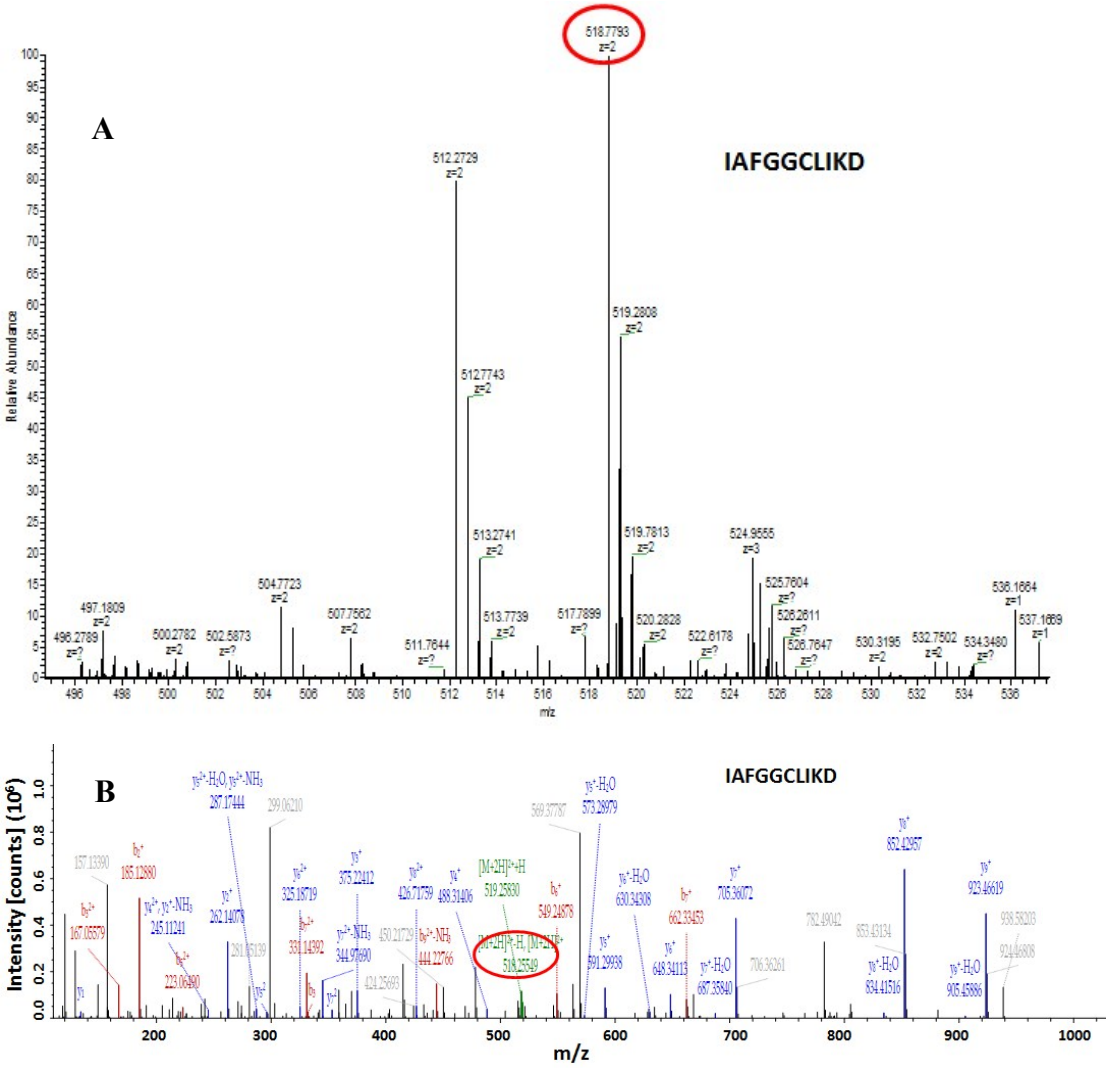


Scheme S1. Proposed possible mechanism of NDM-1 inhibition by activated ester substituted ebselen **SB**.

LC MS/MS characterization

Samples were prepared for mass spectrometry as follows: NDM-1 (0.5 mM) and labeling agent **RB** (3.0 mM) were incubated in Tris-HCl (2 mL, 50mM) at pH 7.2 for 2 h at room temperature, and then the reaction was stored at 4°C overnight. Prior to high resolution mass spectrometry analysis on digestion and bottom-up mass spectrometry analysis, after incubation of the NDM-1 protein with an labeling agent **RB**, 40 µg of the complex protein was prepared for digestion by performing a buffer exchange by using a 10 kDa molecular weight cut-off filter. The filtered protein was diluted in NH_4HCO_3 (50 mM) buffer. Firstly, for Trypsin digestion, 10 µL Trypsin (0.1 µg/µL) was added to 40 µg of buffer-exchanged protein and incubated overnight at 37°C. Following digestion, the peptides were desalted on C18 spin columns (Thermo/Pierce) and reconstituted in 1XPBS at a pH of 7.2 for second digestion. Then for Glu-C digestion, 2 µL of Glu-C (1 µg/µL) was added to the peptides and incubated overnight at 37 °C. Following digestion, the peptides were desalted on C18 spin columns (Thermo/Pierce) and reconstituted in 0.1% formic acid in water for LC MS/MS analysis. NDM-1 alone are digested as above. LC MS analysis was undertaken by using an Eksigent II nano LC system operated in a reversed-phase nano-liquid

chromatography mode at a flow rate of 300 nL/min. Separation was performed with eluent A, consisting of 0.1% formic acid in water, and eluent B, consisting of 0.1% formic acid in CH_3CN, with a 30 min linear gradient from 2–40% eluent B at a flow rate of 300 nL/min. LC MS/MS analysis was performed on an Thermo Fisher Orbitrap mass spectrometer (Onbitrap Fusion™ Lumos™ Tribrid™ mass spectrometer).



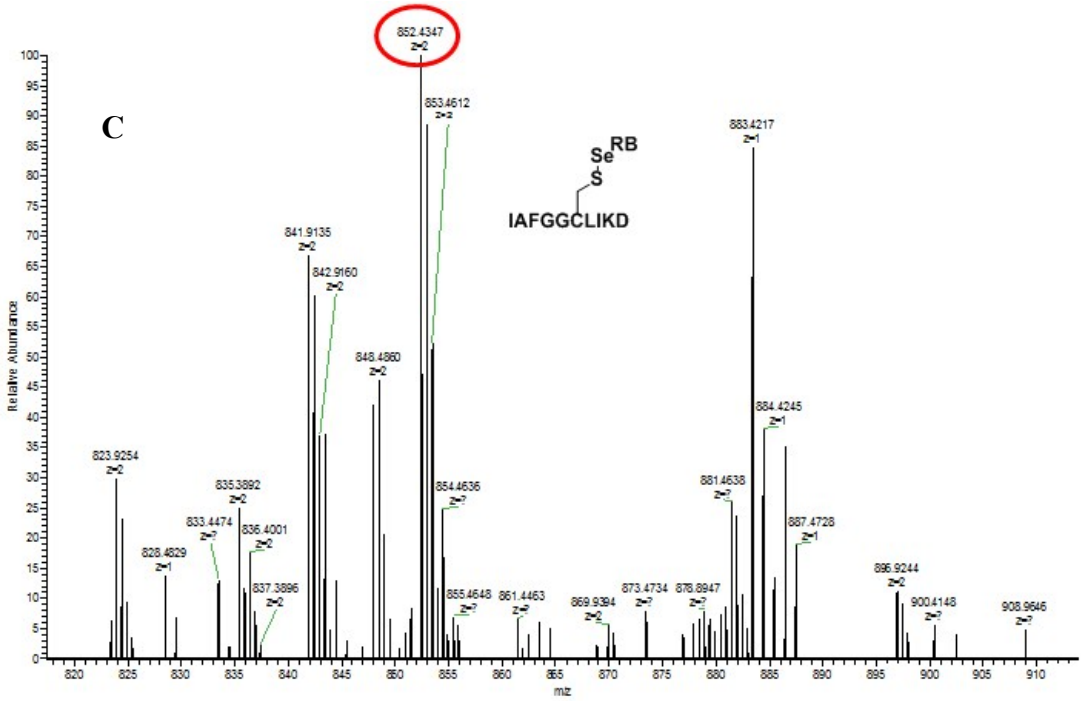


Fig. S5. MS spectra of IAFGGCLIKD (A, m/z 518.7793 (+ 2)) and IAFGGCLIKD-**RB** (C, m/z 852.4347 (+ 2)) from trypsin and Glu-C digests of RB labeled NDM-1, respectively. The difference of MS indicates the location of the **RB** modification (+ 668.2022 Da, B) MS/MS spectrum of the peptide **IAFGGCLIKD**.

Fluorescence characterization

Fluorescent assay was performed on a RF-5301PC spectrofluorometer. Enzyme assays for the quantification of NDM-1 were performed in PBS (pH 7.4) at 25 °C. A total of 50 µL purified enzyme (100 µM) was added to 950 µL of PBS containing **CB** (5 µM). The mechanism of fluorescent probe **CB** recognition is showed in Fig.S5a. The samples were excited at 365 nm, and the fluorescence intensity enhancement was monitored at 480 nm.

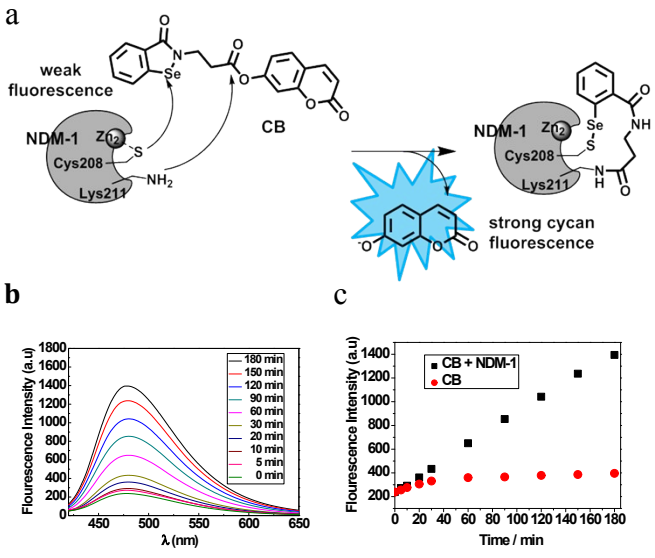


Fig.S6. Dual covalent binding mechanism of fluorescent probe **CB** (a),time-dependent emission spectra (λ_{ex} = 365 nm) of **CB** (5 µM) in the presence (b) and absence (c) of NDM-1 in PBS buffer, pH 7.5, containing 0.1% DMSO at 25 °C.

Identification of labeled protein by SDS-PAGE

NDM-1 (5 or 20 μM) was added to a solution of **RB** (10 or 20 μM) in 10 mM Tris-HCl buffer (pH 7.5) at 25 °C. After 1h, labeled protein was solubilized in 2 × SDS gel loading buffer (100 mM Tris-HCl buffer (pH 6.8), 2.5% SDS, 20% glycerol or 100 mM Tris-HCl buffer (pH 6.8), 2.5% SDS, 20% glycerol and 10% mercaptoethanol) and resolved by SDS-PAGE. The images of the gels were then captured using a Huawei P10or irradiating the gel with UV light at 365 nm. The gels were stained with Coomassie Brilliant Blue, and images of the stained gels were captured

.

Sample preparation for cell imaging with 3D-SIM super-resolution microscopy

Super-resolution fluorescence imaging experiments were performed at 25°C. *E. coli*BL21(DH3) (NDM-1) cells (OD_{600} = 0.5,prepared as described for the measurement of MHB) were incubated with**RB**(5–20 μM) in tubes at 37 °C for 2h. After incubation, the cells were repeatedly washed with PBS for five times (10,000 rpm, 10 min), to remove any adsorbed **RB** probe on the cell surface，suspended in PBS (2 mL) and thentransferred to the chambered coverglass. The bacterial cells were spotted on glass slides, immobilized by the coverslips, and the cell imaging tests were conducted with a Nikon IN-SM instrument.

MIC determination

A single colony of clinical isolates EC08 (from the Health Science Center at Xi'an Jiaotong University (Xian, China))on LB agar plates was transferred to 5 mL of Mueller-Hinton (MH) liquid medium and grown at 37 °C overnight. The bacterial cells were collected by centrifugation (4,000 rpm for 10 min). After discarding the supernatant, the pelleted cells were resuspended in MH medium and diluted to an OD_{600} of 0.5. MIC values were determined by using theClinical and Laboratory Standards Institute (CLSI) macrodilution (tube) broth method. The MIC was interpreted as the lowest concentration of the drug that completely inhibited the visible growth of bacteria after incubating plates for at least 16 h at 37 °C. Each inhibitor was tested in triplicate in at least two independent experiments and the highest MIC value was reported.

Table S2. Antibacterial activities (MICs, μg/mL) of β-lactam antibiotics against EC08 strains producing NDM-1 in the presence of the **SB, CB** and **RB** at a concentration of 16 μg/mL.

Compound	Ampicillin	Cefotaxime	Imipenem
Blank	>100000	20000	156
SB	>100000	5000	19.5
CB	>100000	10000	39
RB	>100000	5000	19.5

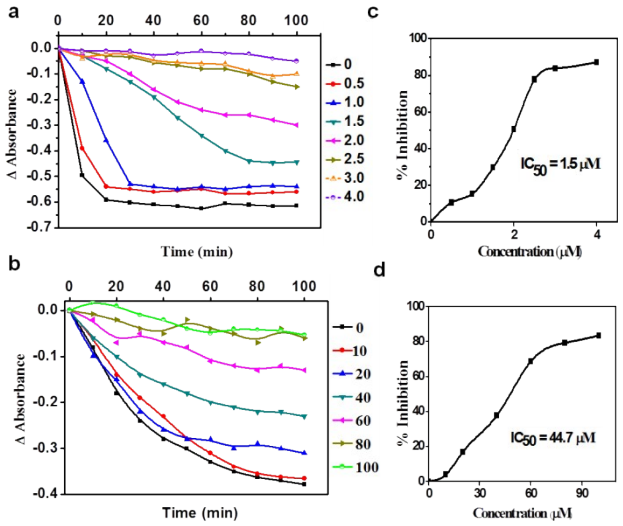


Fig. S7. Inhibition of cefazolin hydrolysis in *E. coli* BL21 cells producing NDM-1 (a) and in clinical bacterial strain *E.coli* EC08 cells harboring NDM-1 (b) by **RB** at various concentrations, and IC_{50} measurements for *E. coli* BL21 (c) and *E.coli* EC08 cells (d). For each experiment, the NDM-1 *E. coli* cells (OD_{600}=0.2) were first incubated with the inhibitor for 10 min and 100 μM cefazolin was subsequently added.

Over-expression and purification of MβLs

NDM-1 (B1): NDM-1 was overexpressed and purified as previously described[2]. *E. coli* BL21(DE3) cells were first transformed with the over-expression plasmid pET26b-NDM-1 and the cells were plated on LB-agar plates containing 25 μg/mL kanamycin. A single colony was used to inoculate 50 mL of LB containing 25 μg/mL kanamycin. After the preculture grew overnight at 37 °C, 10 mL overnight culture of these cells in LB was used to inoculate 4 × 1 L of LB containing 25 μg/mL kanamycin. The cells were allowed to grow at 37 °C with shaking until the cells reached an optical density at 600 nm of 0.6-0.8. Protein production was induced with 1 mM IPTG, and the cells were shaken at 25 °C for 3 h. The cells were collected by centrifugation (30 min at 8,275 × g) and resuspended in 25 mL of 30 mM Tris, pH 8.0, containing 500 mM NaCl. The cells were lysed by ultrasonication, and the cell debris was separated by centrifugation (30 min at 32,583 × g). The cleared supernatant was dialyzed versus 30 mM Tris, pH 8.0, containing 100 μM $ZnCl_2$ for 36 h at 4 °C, centrifuged (25 min at 32,583 × g) to remove insoluble matter, and loaded onto an equilibrated Q-Sepharose column. Bound proteins were eluted with a 0-500 mM NaCl gradient in 30 mM Tris, pH 8.0, containing 100 μM $ZnCl_2$ at 2 mL/min. Fractions (2 mL) containing NDM-1 were pooled and concentrated with an Amicon ultrafiltration cell equipped with a YM-10 membrane. The crude protein NDM-1 was run through a G75 col-umn and eluted with 30 mM Tris, pH 8.0, containing 200 mM NaCl. Protein purity was ascertained by SDS PAGE and protein concentration was determined using Beer's law and an extinction coefficient of 27,960 $M^{-1}cm^{-1}$ at 280 nm.

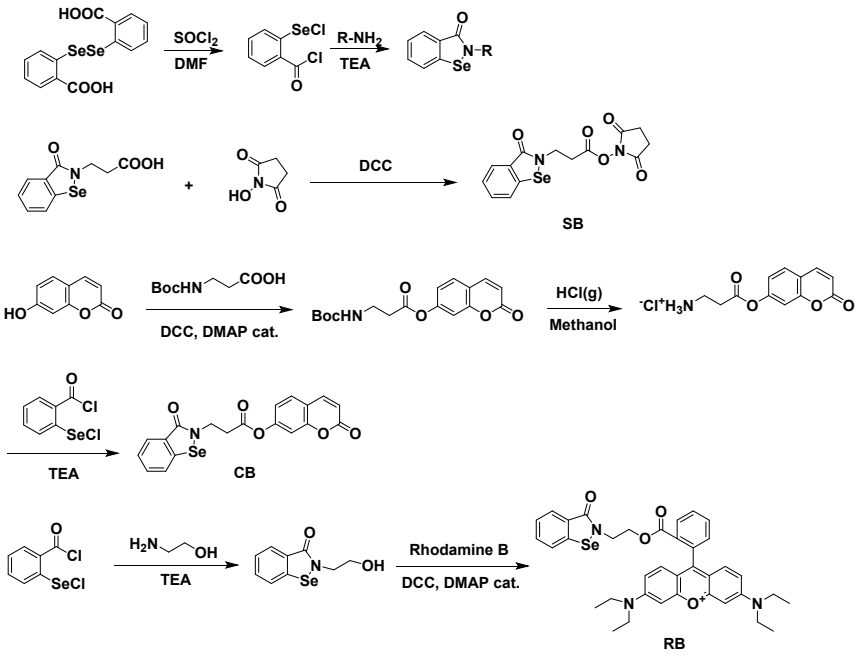
IMP-1 (B1): IMP-1 was overexpressed and purified as previously described[3]. *E. coli* BL21(DE3) cells were first transformed with the over-expression plasmid pET26b-IMP-1 and the cells were plated on LB-agar plates containing 25 μg/mL kanamycin. A single colony was used to inoculate 50 mL of LB containing 25 μg/mL kanamycin. After the preculture grew overnight at 37 °C, 10 mL overnight culture of these cells in LB was used to inoculate 4 × 1 L of LB containing 25 μg/mL kanamycin. The cells were allowed to grow at 37 °C with shaking until the cells reached an optical density at 600 nm of 0.6-0.8. Protein production was induced with 1 mM IPTG and 50 μM $ZnSO_4$, and the cultures were allowed to shake at 22° C for 20 h. The cells were collected by centrifugation (30 min at 8,275 × g) and resuspended in 25 mL of 50 mM HEPES, pH 7.5, containing 500 mM NaCl. The cells were lysed by ultrasonication, and the cell debris was separated by centrifugation (30 min at 32,583 × g). The supernatant was dialyzed versus 1 L of 50 mM HEPES, pH 7.5, overnight at 4 °C, centrifuged (25 min at 32,583 × g) to remove insoluble matter, and loaded onto an SP-Sepharose column pre-equilibrated with 50 mM HEPES, pH 7.5, at 2 mL/min. Fractions (2 mL) containing IMP-1 were pooled and concentrated with an Amicon ultrafiltration

cell equipped with a YM-10 membrane. The crude protein IMP-1 was run through a G75 column and eluted with 50 mM HEPES, pH 7.5, containing 200 mM NaCl. Protein purity was ascertained by SDS PAGE and protein concentration was determined using Beer's law and an extinction coefficient of 49,000 $M^{-1}cm^{-1}$ at 280 nm.

ImiS (B2): ImiS was overexpressed and purified as previously described[4]. *E. coli* BL21(DE3) cells were first transformed with the over-expression plasmid pET-26b-ImiS and the cells were plated on LB-agar plates containing 25 µg/mL kanamycin. A single colony was used to inoculate 50 mL of LB containing 25 µg/mL kanamycin. After the preculture grew overnight at 37 °C, 10 mL overnight culture of these cells in LB was used to inoculate 4 × 1 L of LB containing 25 µg/mL kanamycin. The cells were allowed to grow at 37 °C with shaking until the cells reached an optical density at 600 nm of 0.6-0.8. Protein production was induced with 1 mM IPTG, and the cells were shaken at 25 °C for 3 h. The cells were collected by centrifugation (30 min at 8,275 × g) and resuspended in 25 mL of 30 mM Tris, pH 7.0, containing 500 mM NaCl. The cells were lysed by ultrasonication, and the cell debris was separated by centrifugation (30 min at 32,583 × g). The cleared supernatant was dialyzed versus 30 mM Tris, pH 7.0, containing 100 µM $ZnCl_2$ for 36 h at 4 °C, cen-trifuged (25 min at 32,583 × g) to remove insoluble matter, and loaded onto an equilibrated SP-Sepharose column. Bound proteins were eluted with a 0-500 mM NaCl gradient in 30 mM Tris, pH 7, containing 100 µM $ZnCl_2$, at 2 mL/min. Fractions (2 mL) containing ImiS were pooled and concentrated with an Amicon ultrafiltration cell equipped with a YM-10 membrane. The crude protein ImiS was run through a G75 column and eluted with 30 mM Tris, pH 7.0, containing 200 mM NaCl. Protein purity was ascertained by SDS PAGE and protein concentration was determined using Beer's law and an extinction coefficient of 37,250 $M^{-1}cm^{-1}$ at 280 nm.

L1 (B3): L1 was overexpressed and purified as previously described[5]. *E. coli* BL21(DE3) cells were first transformed with the over-expression plasmid pET26b(+)-L1 and the cells were plated on LB-agar plates containing 25 µg/mL kanamycin. A single colony was used to inoculate 50 mL of LB containing 25 µg/mL kanamycin. After the preculture grew overnight at 37 °C, 10 mL overnight culture of these cells in LB was used to inoculate 4 × 1 L of LB containing 25 µg/mL kanamycin. The cells were allowed to grow at 37 °C with shaking until the cells reached an optical density at 600 nm of 0.6-0.8. Protein production was induced with 1 mM IPTG, and the cells were shaken at 37 °C for 3 h. The cells were collected by centrifugation (30 min at 8,275 × g) and resuspended in 25 mL of 30 mM Tris, pH 8.5, containing 500 mM NaCl. The cells were lysed by ultrasonication, and the cell debris was separated by centrifugation (30 min at 32,583 × g). The cleared supernatant was dialyzed versus 30 mM Tris, pH 8.5, containing 100 µM $ZnCl_2$ for 36 h at 4 °C, centrifuged (25 min at 32,583 × g) to remove insoluble matter, and loaded onto an equilibrated Q-Sepharose column. Bound proteins were eluted with a 0-500 mM NaCl gradient in 30 mM Tris, pH 8.5, containing 100 µM $ZnCl_2$ at 2 mL/min. Fractions (2 mL) containing L1 were pooled and concentrated with an Amicon ultra-filtration cell equipped with a YM-10 membrane. The crude protein L1 was run through a G75 column and eluted with 30 mM Tris, pH 8.5, containing 200 mM NaCl. Protein purity was ascertained by SDS PAGE and protein concentration was determined using Beer's law and an extinction coefficient of 54,614 $M^{-1}cm^{-1}$ at 280 nm.

Chemical experimental procedures



Scheme S2. Synthetic routesand structures of **SB**, **CB** and **RB**general chemical methods

^{1}H and ^{13}C NMR spectra were recorded on a Bruker Avance III 400-MHz spectrometer. Chemical shifts are given in parts per million (ppm) on the delta scale. The peak patterns are reported as singlet (s), doublet (d), triplet (t), quartet (q), doublet doublet (dd), and mul-tiplet (m). The spectra were recorded with TMS as internal standard. Coupling constants (*J*) were reported in Hertz (Hz). Mass spectra were obtained on a micro TOF-Q (BRUKER) mass spectrometer.The reactions were followed by thin-layer chromatography (TLC) on glasspacked precoated silica gel plates and visualized in an iodine chamber or with a UV lamp. Flash column chromatography was performed using silica gel (200–300 mesh) purchased from Qingdao Haiyang Chemical Co. Ltd. Activity evaluation of inhibitors was performed on an Agilent 8453 UV-Vis spectrometer.

A solution of 2-(chloroseleno)benzoyl chloride (1 mmol, 0.254 g) in DCM (10 mL) was added dropwise over 30 min to a stirred solution of the appropriate amine(1 mmol) and triethylamine (3.5 mmol, 0.5 mL) in DCM (10 mL) at 0°C. The reaction mixture was stirred at room temperature overnight. The solvent was removed under reduced pressure and the residue was stirred with water (20 mL) for 2 h, and extracted with DCM (3 × 10 mL). The combined organic extracts were dried over anhydrous $MgSO_4$, the solvent removed was under reduced pressure, and the crude product was purified by flash column chromatography on silica gel (eluents: 10–50% ethyl acetate in hexane gradient)[6], to get compound 3-(3-oxobenzo[d][1,2]Selenazol-2(3H)-yl)propanoic acid and 2-(2-hydroxyethyl)Benzo[d][1,2]selenazol-3(2H)-one.

2,5-Dioxopyrrolidin-1-yl 3-(3-oxobenzo[d][1,2]selenazol-2(3H)-yl)propanoate (SB)

To a stirred solution of 3-(3-oxobenzo[d][1,2]Selenazol-2(3H)-yl)propanoic acid (1.0 equiv) in CH_3CN were added at 0 °C DCC (1.5 equiv) and N-Hydroxysuccinimide (1.2 equiv). The reaction mixture was stirred for 10 minutes at 0 °C, then for 4 hours at room temperature, the reaction mixture was monitored using TLC. The solid were filtered off and from the filtrate acetonitrile was evaporated in vacuoand the crude product was purified by flash column chromatography on silica gel (ethyl acetate/petroleum ether, 1:1). Compound **SB**White solid, 59% yield.^{1}H NMR (400 MHz, DMSO-d_6) δ 7.73 (d, *J* = 8.0 Hz, 1H), 7.50 (d, *J* = 7.6 Hz, 1H), 7.30 (t, *J* = 7.4 Hz, 1H), 7.10 (t, *J* = 7.4 Hz, 1H), 3.71 (t, *J* = 6.7 Hz, 2H), 2.79 (t, *J* = 6.7 Hz, 2H), 2.19 (s, 4H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 170.54, 167.78, 167.11, 140.24, 132.07, 127.94, 127.75, 126.37, 126.21, 39.13, 31.40, 25.92. HRMS (ESI): *m/z*Calcd for: $C_{14}H_{12}N_2O_5Se$ $[M+Na]^+$390.9809; found 390.9813.

2-Oxo-2H-chromen-7-yl 3-(3-oxobenzo[d][1,2]selenazol-2(3H)-yl)propanoate (CB)

A solution of dichloride 2 (1 mmol, 0.254 g) in dry DCM (10 mL) was added dropwise over 30 min to a stirred solution of 3-oxo-3-((2-oxo-2H-chromen-7-yl)oxy)propan-1-aminium chloride (1 mmol) and triethylamine (3.5 mmol, 0.5 mL) in dry DCM (10 mL) at 0°C. The reaction mixture was monitored using TLC. When the reaction was complete (4h), the solvent was removed in vacu and extracted with DCM (3 × 10 mL). The combined organic extracts were dried over anhydrous $MgSO_4$, the solvent removed was under reduced pressure, and the crude product was purified by flash column chromatography on silica gel (ethyl acetate/petroleum ether, 1:2).Compound **CB**, gray solid, yield 54%.^{1}H NMR (400 MHz, DMSO-d_6) δ 8.05 (dd, *J* = 8.7, 6.7 Hz, 2H), 7.84 (d, *J* = 8.5 Hz, 1H), 7.77 (d, *J* = 8.5 Hz, 1H), 7.64 – 7.58 (m, 1H), 7.42 (t, *J* = 7.5 Hz, 1H), 7.29 (d, *J* = 2.1 Hz, 1H), 7.17 (dd, *J* = 8.4, 2.2 Hz, 1H), 6.48 (d, *J*= 9.6 Hz, 1H), 4.10 (t, *J* = 6.5 Hz, 2H), 2.98 (t, *J* = 6.5 Hz, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 170.13, 167.09, 160.14, 154.50, 153.18, 144.27, 140.01, 132.10, 129.83, 128.06, 127.78, 126.37, 126.30, 119.05, 117.24, 116.10, 110.54, 39.35, 35.25.HRMS (ESI): *m/z*Calcd for: $C_{19}H_{13}NO_5Se$ $[M+Na]^+$ 437.9839; found 437.9836.

3,6-Bis(diethylamino)-9-(2-((2-(3-oxobenzo[d][1,2]selenazol-2(3H)-yl)ethoxy)carbonyl)phenyl)xanthylium (RB)

To a stirred solution of 2-(2-hydroxyethyl)Benzo[d][1,2]selenazol-3(2H)-one (3.0 equiv) in DCMwere added at 0 °C DCC (1.3 equiv), DMAP (0.13 equiv) and Rhodamine B (1.0 equiv). The reaction mixture was stirred for 10 minutes at 0 °C, then for 4 hours at room temperature, the solvent was removed in vacu and extracted with DCM (3 × 10 mL). The combined organic extracts were dried over anhydrous $MgSO_4$, the solvent removed was under reduced pressure, and the crude product was purified by flash column chromatography on silica gel ($CHCl_3$/CH_3OH, 9:1).Compound **RB**. dark purple crystals with metallic glass, yield 45%.^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.36 (dd, *J* = 7.7, 1.2 Hz, 1H), 7.98 (d, *J* = 7.8 Hz, 1H), 7.79 (m, 3H), 7.67 – 7.58 (m, 1H), 7.38 (t, *J* = 7.5 Hz, 1H), 7.30 – 7.27 (m, 1H), 7.06 (d, *J* = 9.5 Hz, 2H), 6.90 (dd, *J* = 9.5, 2.4 Hz, 2H), 6.74 (d, *J* = 2.4 Hz, 2H), 4.34 (t, *J* = 5.1 Hz, 2H), 4.10 (t, *J* = 5.1 Hz, 2H), 3.61 (q, *J* = 7.1 Hz, 8H), 1.29 (t, *J* = 7.1 Hz, 12H). ^{13}C NMR (101 MHz, Chloroform-*d*)δ 165.59, 164.56, 158.68, 157.68, 155.51, 140.79, 133.89, 133.45, 132.21, 131.67, 131.31, 130.70, 130.30, 129.13, 126.40, 125.53, 123.89, 121.13, 114.39, 113.48, 63.74, 46.15, 42.67, 12.65. HRMS (ESI): *m/z*Calcd for: $C_{37}H_{38}N_3O_4Se$ $[M]^+$ 668.2022; found 668.2051.

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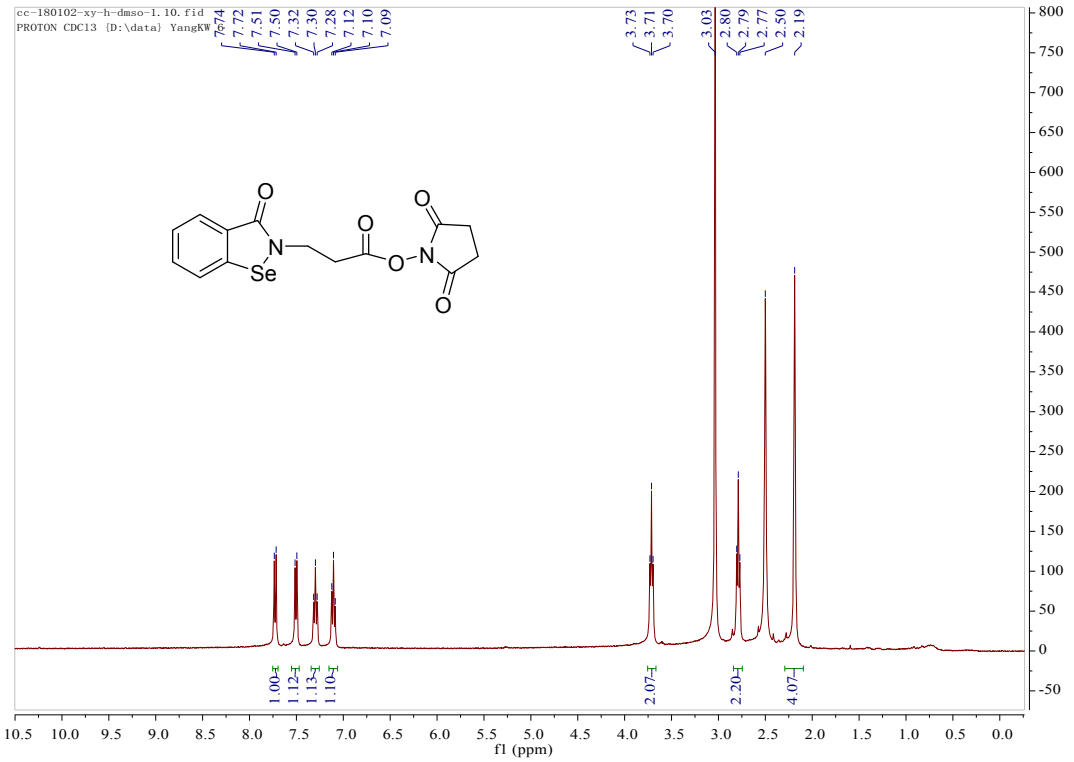
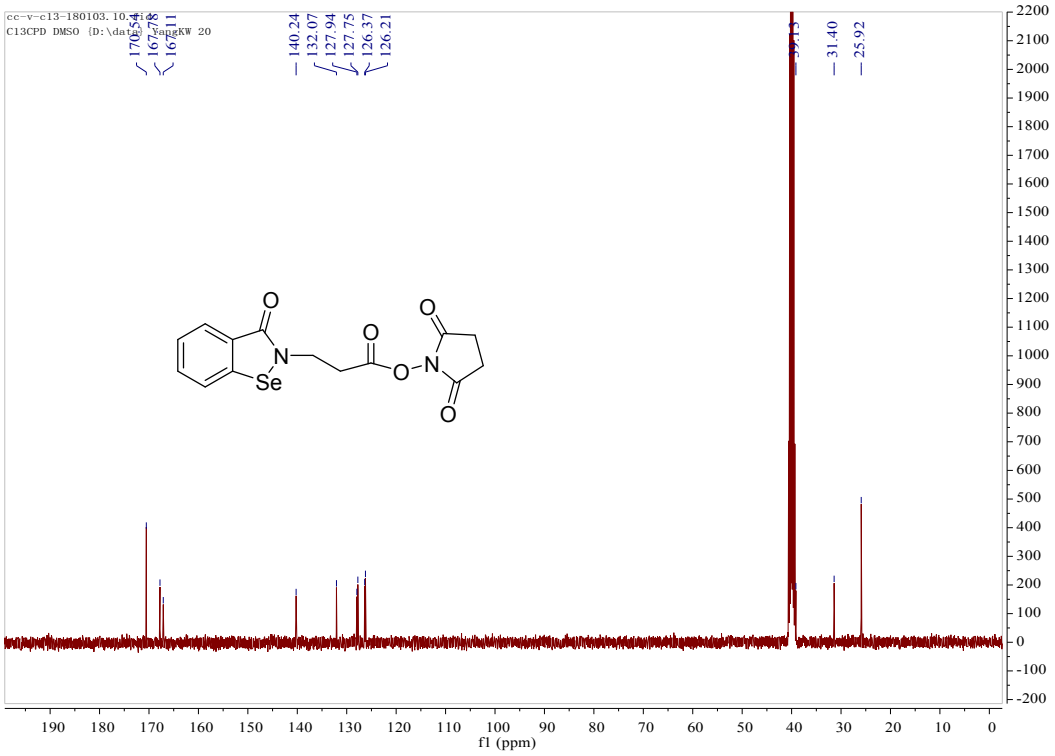
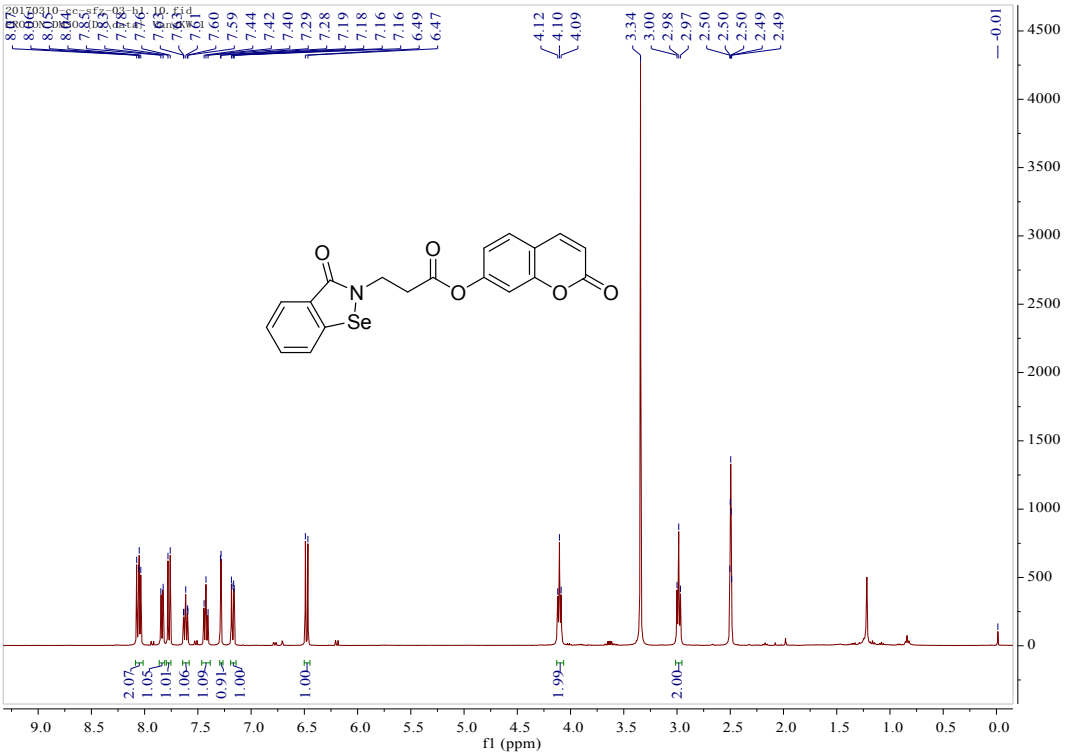
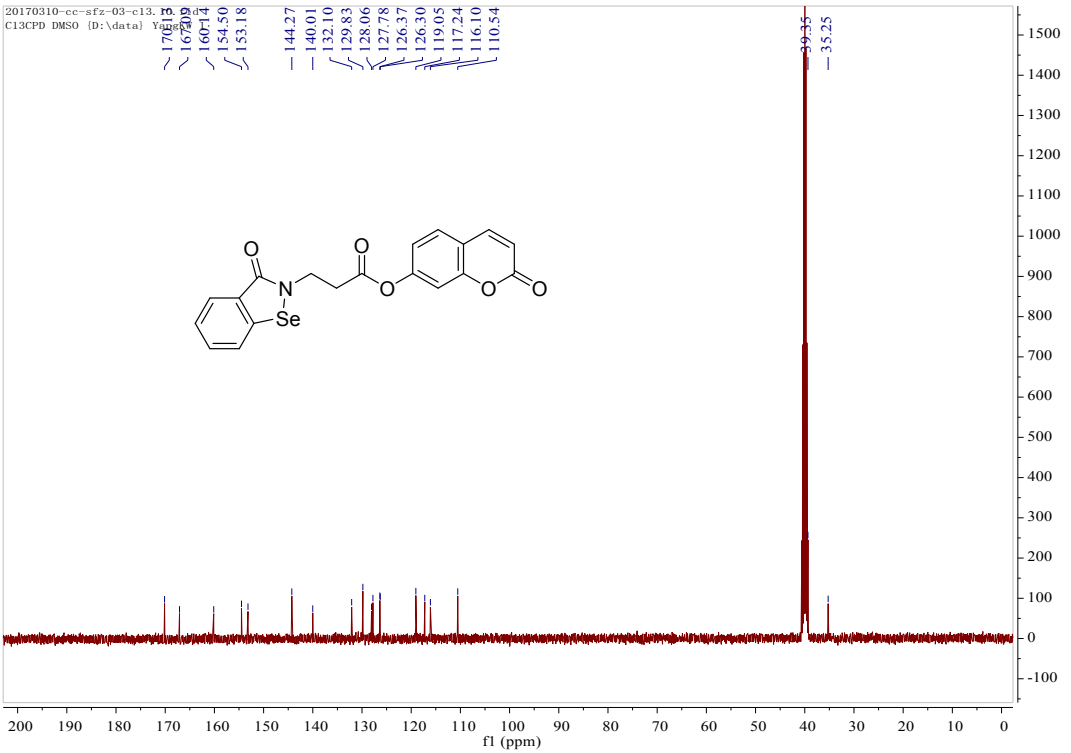
^{1}H and ^{13}C NMR spectra of compounds



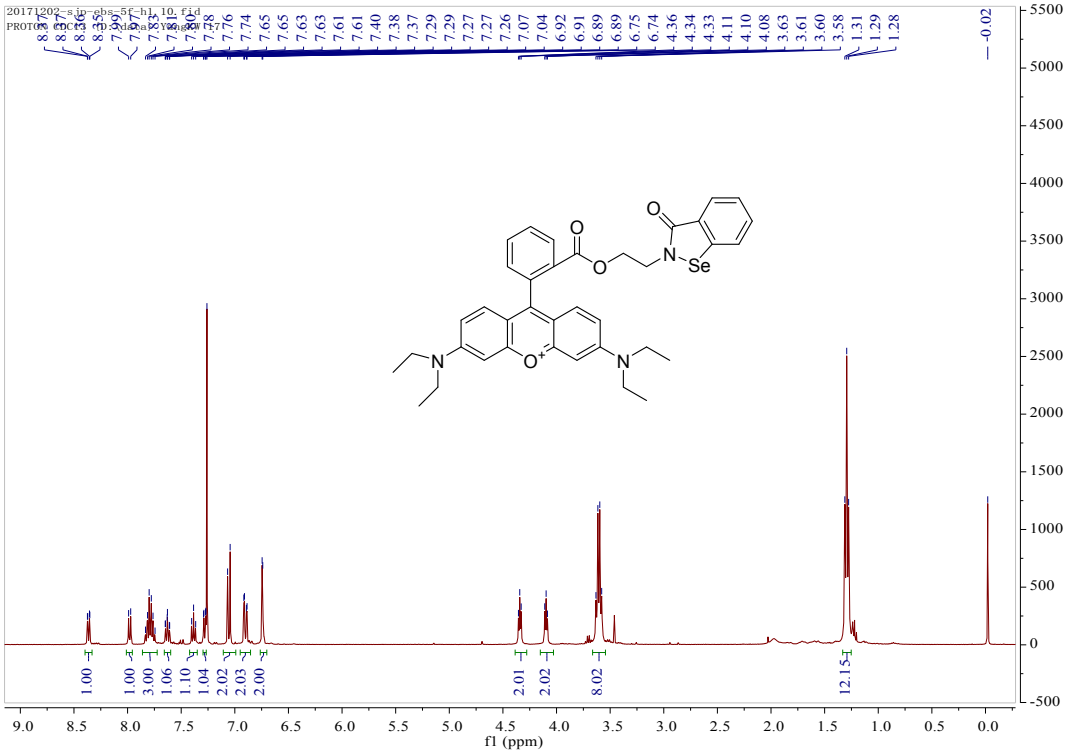


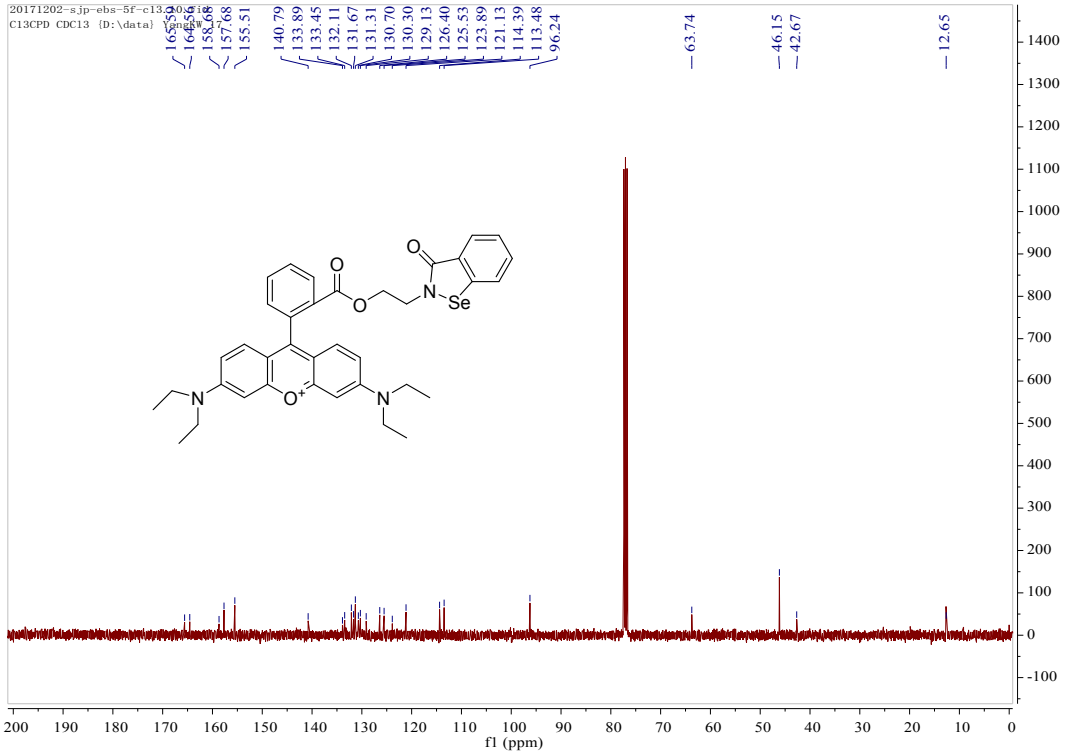
^{1}H NMR and^{13}C NMR spectra of SB





^{1}H NMR and ^{13}C NMR spectra of CB





^{1}H NMR and ^{13}C NMR spectra of RB