Supporting Information

Efficient synthesis of bisulfide-bridged bicyclopeptides by intramolecular photoinduced electron transfer cycloreaction

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Contents

1. Experimental Section

1.1 General Experimental Procedures.

L-cystine(56-89-3), Boc-L-proline(15761-39-4), Boc-L-leucine(13139-15-6), Boc-Sar-OH(13734-36-6), Boc-L-Alanine(15761-38-3), L-isoleucine(73-32-5), *t*-Boc, EEDQ, N-[(trimethylsilyl)methyl]benzylamine, phthalylglycyl chloride, trifluoroacetic acid (TFA) and tetrahydrofuran (THF) were purchased from Saen Chemistry Technology (Shanghai) Co., Ltd. Dichloromethane (DCM), trimethylamine (TEA), methanol, ethyl acetate, petroleum ether, 1,4-dioxane were analytical reagent. All the solvents were distilled and purified by standard procedures. ^{1}H and ^{13}C-NMR spectra were recorded at 400 and 100 MHz, respectively, on an AMX400 spectrometer (Bruker, Bremen, Germany). Mass spectra were recorded on a JEOL JMS-700 spectrometer using the fast atom bombardment (FAB) or electron impact (EI) mode. A 450 W Hanovia medium-pressure mercury lamp surrounded by a Pyrex glass filter ($\lambda > 290$ nm) was used for electronic excitation

1.2 Synthesis of linear peptidyl-$SiMe_3$ (**1**)

The linear peptides were prepared by liquid phase method using *t*-Boc-amino acid as the starting material, EEDQ as condensing agent and TFA as deprotecting agent. Here, take the *L*-Ile-*L*-Leu-$SiMe_3$ for an example to elucidate the synthesis process. The Boc-*L*-leucine (2.31 g, 10 mmol) and *N*-[(trimethylsilyl) methyl]benzylamine (1.93 g, 10 mmol) were dissolved in 30 mL of DCM, then EEDQ(3.78 g, 15 mmol in 10 mL of DCM) was added dropwise with stirring at room temperature for 12 h. After which the reaction solution was washed thrice with 30 mL of water, and dried with anhydrous sodium sulfate. The concentrated residue was dissolved in 20 mL of DCM, followed with addition of 10 mL of TFA and stirring at room temperature for 3 h. Then the reaction solution was concentrated to remove the solvent and TFA. The residue was again dissolved in 20 mL of DCM, washed thrice with 30 mL of water, and concentrated to obtain the crude N-trimethylsilylbenzyl-Leu, which was used for further synthesis without any purification. The crude N-trimethylsilylbenzyl-Leu and *t*-Boc-*L*-Ile (1.53 g) were dissolved in 30 mL of DCM, and EEDQ (2.65 g in 10 mL of DCM) was added dropwise with stirring at room temperature for 12 h. Then the reaction solution was washed thrice with 30 mL of water, added with 10 mL of TFA and stirred at room temperature for 3 h. The reaction solution was concentrated and re-dissolved in 20 mL of DCM, then dried with anhydrous sodium sulfate and re-concentrated to obtain the crude trimethylsilyl terminal-*L*-Ile-*L*-Leu. The rest trimethylsilyl terminal peptide chains (such as Pro-Ile-Leu-$SiMe_3$, Cys-Sar-$SiMe_3$, Cys-Sar-Sar-$SiMe_3$, Sar-Sar-Sar-$SiMe_3$, Sar-Sar-Sar-Sar-$SiMe_3$, Sar-Sar-Sar-Sar-

Sar-SiMe$_3$, Ala-Sar-SiMe$_3$, Ala-Sar-Sar-SiMe$_3$, Ala-Ala-Sar-Ala-Sar-SiMe$_3$) were prepared in a similar way, and used for further reaction without purification.

1.3 Synthesis of sulfido-[peptidyl-SiMe$_3$]$_2$ (**2**)

General synthetic process: compounds **1** (6 mmol) and Boc-Cys-Cys (1.32 g, 3 mmol) was dissolved in 30 mL of THF, EEDQ (2.27 g, 9 mmol in 10 mL of DCM) was then added dropwise with stirring at room temperature for 12 h. The reaction solution was washed twice with 20 mL of water, the organic layer was dried over anhydrous sodium sulfate and concentrated. The residue was dissolved in 20 mL of DCM, added with 10 mL of TFA and stirred for 3h. The mixture was concentrated to obtain crude products sulfido-[peptidyl-SiMe$_3$]$_2$ (compounds **2**), which were used for further reaction without purification.

1.4 Synthesis of sulfido-[N-phthalimido-peptidyl-SiMe$_3$]$_2$ (**3a**~**3i**)

General synthetic process: compounds **2** (1 mmoL) and TEA (3 mL) were dissolved in DCM, then phthalimide acetyl chloride (0.41 g, 2 mmoL in 3 mL of 1,4-dioxane) was added dropwise. After stirring at room temperature for 3 h, the reaction solution washed twice with 20 mL of water. The organic layer was dried over anhydrous sodium sulphate, then concentrated and purified by silica gel column chromatography (mobile phase V_{EA}/V_{PE} = 2:1) to obtain white solid compound sulfido-[N-phthalimido-peptide-SiMe$_3$]$_2$ (**1**).

Sulfido-[N-phthalimido-Gly-*L*-Cys-Sar-SiMe$_3$]$_2$ (**3a**): white solid (yield 85%). ^{1}HNMR(CDCl$_3$) ***δ***: 0.07~0.18(m, 18H, SiMe$_3$), 2.56~2.90(m, 4H, **CH$_2$**SiMe$_3$), 3.02~3.25(m, 6H, N**CH$_3$**), 3.27~3.42(m, 4H, S**CH$_2$**CH), 4.01~4.38(m, 4H, N**CH$_2$**CO), 4.40~4.47(m, 4H, **CH$_2$**Ph), 4.49~4.56(m, 4H, N**CH$_2$**CO), 4.83~4.96(m, 1H, HN**CH**CO), 5.29~5.40(m, 1H, NH**CH**CO), 7.19~7.85(m, 18H, ArH); ^{13}CNMR(CDCl$_3$) ***δ*** : -1.5, 34.6, 35.6, 36.6, 39.1, 40.2, 49.7, 52.5, 123.4, 126.6, 127.6, 129.4, 132.5, 134.3, 136.1, 166.3, 167.3, 167.7, 169.8, 170.5. HRMS (ESI) m/z calcd for $C_{54}H_{66}N_8O_{10}S_2Si_2Na^+$ $(M+Na)^+$ 1129.37741, found 1129.37805.

Sulfido-[N-phthalimido-Gly-*L*-Cys-Sar-Sar-SiMe$_3$]$_2$ (**3b**): white solid (yield 87%). ^{1}HNMR(CDCl$_3$) ***δ***: 0.03~0.15(m, 18H, SiMe$_3$), 2.75~2.82(m, 10H, **CH$_2$**SiMe$_3$ and N**CH$_3$**), 2.95~3.35(m, 10H, N**CH$_3$** and S**CH$_2$**CH), 3.81~4.80(m, 18H, N**CH$_2$**CO, **CH$_2$**Ph and N**CH$_2$**CO), 4.85~5.15(m, 1H, HN**CH**CO), 5.19~5.40(m, 1H, NH**CH**CO), 7.17~7.79(m, 18H, ArH); ^{13}CNMR(CDCl$_3$) ***δ*** : -1.3, 35.8, 36.6, 39.0, 40.1, 41.5, 49.3, 50.2, 51.2, 52.6, 123.3, 126.1, 126.6, 127.3, 127.6, 129.0, 132.1, 133.9, 136.2, 166.2, 167.0, 167.5, 168.5, 170.2, 170.4. HRMS (ESI) m/z calcd for $C_{60}H_{76}N_{10}O_{12}S_2Si_2Na^+$ $(M+Na)^+$ 1271.45163, found 1271.45264.

Sulfido-[N-phthalimido-Gly-*L*-Cys-*L*-Ala-Sar-SiMe$_3$]$_2$ (**3c**): white solid (yield 85%). ^{1}HNMR(CDCl$_3$) ***δ***: 0.06~0.21(m, 18H, SiMe$_3$), 1.22~1.38(m, 6H, CH**CH$_3$**), 2.60~2.92(m, 4H,

$\mathbf{CH_2}SiMe_3$), 2.98~3.40(m, 10H, N$\mathbf{CH_3}$), 3.60~4.35(m, 6H, S$\mathbf{CH_2}$CH and N$\mathbf{CH_2}$CO, N$\mathbf{CH_2}$CO), 4.36~4.65(m, 6H, $\mathbf{CH_2}$Ph and N$\mathbf{CH_2}$CO), 4.67~4.85(m, 2H, HN**CH**CO), 4.86~5.28(m, 2H, NH**CH**CO), 7.21~7.84(m, 18H, ArH); ^{13}CNMR($CDCl_3$) ***δ*** : -1.6, 19.1, 20.8, 27.5, 36.0, 39.8, 42.7, 45.4, 50.1, 59.8, 123.4, 126.6, 127.6, 128.7, 132.2, 133.3, 136.4, 165.3, 166.0, 167.7, 168.7, 171.2, 173.0. HRMS (ESI) m/z calcd for $C_{60}H_{76}N_{10}O_{12}S_2Si_2Na^+$ $(M+Na)^+$ 1271.45163, found 1271.45300.

Sulfido-[N-phthalimido-Gly-*L*-Cys-Sar-Sar-Sar-$SiMe_3$]$_2$ (**3d**): white solid (yield 88%). ^{1}HNMR($CDCl_3$) ***δ***: 0.03~0.18(m, 18H, $SiMe_3$), 2.72~3.32(m, 26H, $\mathbf{CH_2}SiMe_3$, N$\mathbf{CH_3}$ and S$\mathbf{CH_2}$CH), 3.91~4.28(m, 8H, $\mathbf{CH_2}$Ph and N$\mathbf{CH_2}$CO), 4.30~4.35(m, 4H, N$\mathbf{CH_2}$CO), 4.38~4.72(m, 8H, N$\mathbf{CH_2}$CO), 4.90~5.30(m, 1H, HN**CH**CO), 5.32~5.60(m, 1H, NH**CH**CO), 7.13~7.76(m, 18H, ArH); ^{13}CNMR($CDCl_3$) ***δ*** : -1.2, 30.9, 35.8, 36.6, 37.4, 39.0, 40.1, 49.7, 50.4, 51.3, 52.8, 53.6, 123.4, 126.4, 127.4, 127.6, 128.5, 128.8, 132.1, 133.9, 136.1, 136.6, 166.4, 167.7, 168.2, 168.7, 170.4, 171.1. HRMS (ESI) m/z calcd for $C_{66}H_{86}N_{12}O_{14}S_2Si_2Na^+$ $(M+Na)^+$ 1413.52586, found 1413.52710.

Sulfido-[N-phthalimido-Gly-*L*-Cys-*L*-Ala-Sar-Sar-$SiMe_3$]$_2$ (**3e**): white solid (yield 88%). ^{1}HNMR($CDCl_3$) ***δ***: 0.01~0.24(m, 18H, $SiMe_3$), 1.32~1.56(m, 6H, CH$\mathbf{CH_3}$), 2.65~2.82(m, 4H, $\mathbf{CH_2}SiMe_3$), 2.83~2.95(m, 4H, S$\mathbf{CH_2}$CH), 3.00~3.45(m, 6H, N$\mathbf{CH_3}$), 3.60~3.81(m, 2H, N$\mathbf{CH_2}$CO), 3.82~4.05(m, 2H, N$\mathbf{CH_2}$CO), 4.06~4.31(m, 4H, $\mathbf{CH_2}$Ph), 4.32~4.65(m, 6H, N$\mathbf{CH_2}$CO), 4.70~4.80(m, 2H, HN**CH**CO), 4.82~5.00(m, 2H, NH**CH**CO), 5.01~5.25(m, 2H, NH**CH**CO), 7.14~7.84(m, 18H, ArH); ^{13}CNMR($CDCl_3$) ***δ***: -1.6, 13.4, 19.1, 21.2, 26.9, 35.3, 36.6, 39.8, 45.8, 49.6, 51.4, 61.2, 123.4, 126.3, 128.7, 131.9, 133.7, 136.4, 164.9, 166.7, 167.0, 167.7, 168.0, 171.2, 174.0. HRMS (ESI) m/z calcd for $C_{66}H_{86}N_{12}O_{14}S_2Si_2Na^+$ $(M+Na)^+$ 1413.52586, found 1413.52722.

Sulfido-[N-phthalimido-Gly-*L*-Cys-*L*-Pro-*L*-Ile-*L*-Leu-$SiMe_3$]$_2$(**3f**): white solid (yield 78%). ^{1}HNMR($CDCl_3$, 500 MHz) ***δ***: -0.28~0.30(m, 18H, $SiMe_3$), 0.55~0.96(m, 24H, $\mathbf{CH_3}$), 1.01~1.21(m, 2H, **CH**$(CH)_3)_2$), 1.23~1.41(m, 4H, $\mathbf{CH_2}CH_3$), 1.43~1.75(m, 4H, CH$\mathbf{CH_2}$CH), 1.78~2.28(m, 10H, $NCH_2\mathbf{CH_2}CH_2CH)_2$, $NCH_2\mathbf{CH_2}CH_2CH$ and **CH**CH_3), 2.78~2.95(m, 4H, $\mathbf{CH_2}SiMe_3$), 2.98~3.28(m, 4H, S$\mathbf{CH_2}$CH), 3.55~3.85(m, 4H, N$\mathbf{CH_2}CH_2CH_2CH$), 4.20~4.30(m, 2H, $NCH_2CH_2CH_2$**CH**), 4.33~4.48(m, 4H, N$\mathbf{CH_2}$CO), 4.49~4.78(m, 4H, $\mathbf{CH_2}$Ph), 4.85~5.00(m, 2H, HN**CH**CO), 5.01~5.27(m, 2H, HN**CH**CO), 5.30~5.40(m, 2H, HN**CH**CO), 7.13~7.45(m, 10H, ArH), 7.54~7.80(m, 4H, ArH), 7.81~7.91(m, 4H, ArH); ^{13}CNMR($CDCl_3$, 500 MHz) ***δ*** : 0.02, 12.7, 16.9, 22.9, 24.6, 25.8, 38.3, 39.0, 40.1, 41.4, 42.8, 44.2, 48.3, 49.2, 51.4, 51.8, 54.3, 59.2, 61.2, 61.9, 124.8, 128.0, 129.0, 129.9, 130.1, 133.3, 135.3, 167.5, 168.9, 170.1, 170.8, 171.6, 172.1. HRMS (ESI) m/z calcd for

$C_{82}H_{115}N_{12}O_{14}S_2Si_2^+$ $(M+H)^+$ 1611.76302, found 1611.76355.

Sulfido-[N-phthalimido-Gly-*L*-Cys-Sar-Sar-Sar-Sar-SiMe$_3$]$_2$(**3g**): white solid (yield 89%). ^{1}HNMR(CDCl$_3$) ***δ***: 0.08~0.15(m, 18H, SiMe$_3$), 2.59~2.98(m, 8H, **CH$_2$**SiMe$_3$ and S**CH$_2$**CH), 3.00~3.21(m, 12H, N**CH$_3$**), 3.22~3.49(m, 12H, N**CH$_3$**), 4.01~4.31(m, 16H, N**CH$_2$**CO), 4.32~4.45(m, 4H, **CH$_2$**Ph), 4.48~4.72(m, 4H, N**CH$_2$**CO), 4.93~5.16(m, 1H, HN**CH**CO), 5.28~5.36(m, 1H, NH**CH**CO), 7.19~7.83(m, 18H, ArH); ^{13}CNMR(CDCl3) ***δ***: -1.5, 14.6, 21.2, 30.0, 36.3, 37.4, 39.5, 40.2, 46.5, 49.6, 50.4, 52.8, 56.0, 60.9, 123.5, 126.3, 127.0, 128.0, 128.7, 132.2, 133.3, 135.4, 160.0, 163.8, 164.5, 166.0, 167.0, 167.7, 168.0, 170.5. HRMS (ESI) m/z calcd for $C_{72}H_{96}N_{14}O_{16}S_2Si_2Na^+$ $(M+Na)^+$ 1555.60009, found 1555.60144.

Sulfido-[N-phthalimido-Gly-*L*-Cys-Sar-Sar-Sar-Sar-Sar-SiMe$_3$]$_2$ (**3h**): white solid (yield 82%). ^{1}HNMR(CDCl$_3$) ***δ***: 0.01~0.08(m, 18H, SiMe$_3$), 2.50~2.79(m, 4H, **CH$_2$**SiMe$_3$), 2.80~2.90(m, 2H, S**CH$_2$**CH), 2.92~3.25(m, 20H, N**CH$_2$**CO), 3.26~3.35(m, 30H, N**CH$_3$**), 3.85~4.05(m, 4H, **CH$_2$**Ph), 4.10~4.32(m, 4H, N**CH$_2$**CO), 4.83~5.06(m, 1H, HN**CH**CO), 5.10~5.32(m, 1H, NH**CH**CO), 7.11~7.75(m, 18H, ArH); ^{13}CNMR(CDCl$_3$) ***δ*** :-1.37, 19.6, 22.6, 26.8, 27.7, 29.7, 31.6, 35.8, 36.8, 39.0, 40.1, 49.4, 49.7, 50.3, 52.5, 61.5, 115.3, 118.2, 123.3, 126.3, 127.7, 128.5, 128.8, 131.7, 134.1, 135.7, 166.6, 166.7, 166.9, 167.1, 167.7, 167.8, 168.4, 169.1, 169.8. HRMS (ESI) m/z calcd for $C_{78}H_{106}N_{16}O_{18}S_2Si_2Na^+$ $(M+Na)^+$ 1697.67432, found 1697.67419.

Sulfido-[N-phthalimido-Gly-*L*-Cys-*L*-Ala-*L*-Ala-Sar-*L*-Ala-Sar-SiMe$_3$]$_2$ (**3i**): white solid (yield 87%). ^{1}HNMR(CDCl$_3$) ***δ***: 0.05~0.16(m, 18H, SiMe$_3$), 1.24~1.39(m, 18H, CH**CH$_3$**), 2.72~3.08(m, 8H, **CH$_2$**SiMe$_3$ and S**CH$_2$**CH), 3.11~3.30(m, 12H, N**CH$_3$**), 3.78~4.22(m, 4H, N**CH$_2$**CO), 4.26~4.45(m, 2H, N**CH$_2$**CO), 4.46~4.55(m, 4H, **CH$_2$**Ph), 4.67~4.82(m, 4H, HN**CH**CO), 4.90~5.18(m, 4H, NH**CH**CO), 7.14~7.77(m, 18H, ArH); ^{13}CNMR(CDCl$_3$) ***δ*** : -1.5, 18.1, 18.8, 22.6, 27.2, 36.6, 38.8, 39.8, 45.1, 45.5, 48.6, 50.0, 51.4, 52.5, 60.6, 66.6, 117.1, 119.6, 126.3, 127.0, 128.0, 128.7, 132.2, 133.7, 135.0, 164.9, 166.3, 167.3, 168.4, 168.7, 169.8, 171.2, 173.0, 173.4. HRMS (ESI) m/z calcd for $C_{78}H_{106}N_{16}O_{18}S_2Si_2Na^+$ $(M+Na)^+$ 1697.67432, found 1697.67419.

1.5 Synthesis of sulfido-[isoindolone cyclopeptide]$_2$ **(4a-4i)**

0.5 g of compounds 3 in 250 mL of anhydrous methanol were placed in a reactor, then ventilated nitrogen gas flow for 20 min. Upon maintaining the ventilation of nitrogen, the solutions were irradiated by ultraviolet light (Pyrex tube filtered-light $\lambda > 290$ nm). Concentration of the photoproducts were followed by column chromatography to yield the pure products (**4a-4i**).

Sulfido-[isoindolone-cyclo-Gly-*L*-Cys-Sar]$_2$(**4a**): white solid, yield 75% (HPLC yield 83%), mobile phases V_{H2O}/V_{MeCN} = 60:40, the retention time 5.8 min, [α]D^{20} = +22.4° (c = 0.04 g/100 ml, CH_2Cl_2); ^{1}HNMR($CDCl_3$) ***δ***: 2.51~2.93(m, 4H, S**CH₂**CH), 2.95~3.30(m, 6H, N**CH₃**), 3.32~3.72(m, 4H, N**CH₂**CO), 4.01~4.52(m, 6H, **CH₂**Ph and N**CH₂**CO), 4.58~4.87(m, 6H, N**CH₂**CO), 4.93~5.45(m, 2H, HN**CH**CO), 7.14~7.50(m, 12H, ArH), 7.68~7.79(m, 6H, ArH); ^{13}CNMR($CDCl_3$) ***δ*** : 28.9, 31.5, 36.0, 39.8, 43.5, 49.2, 52.5, 89.5, 121.9, 123.8, 126.0, 127.5, 127.8, 128.6, 132.0, 134.3, 166.3, 167.7, 169.3, 171.1. HRMS (ESI) m/z calcd for $C_{48}H_{50}N_8O_{10}S_2Na^+$ $(M+Na)^+$ 985.29835, found 985.29852.

Sulfido-[isoindolone-cyclo-Gly-*L*-Cys-Sar-Sar]$_2$ (**4b**): white solid, yield 80% (HPLC yield 89%), mobile phases V_{H2O}/V_{MeCN} = 60:40, the retention time 5.2 min, [α]D^{20} = -16.67° (c = 0.06 g/100 ml, CH_2Cl_2); ^{1}HNMR($CDCl_3$) ***δ***: 2.55~3.42(m, 20H, N**CH₃,** S**CH₂**CH and N**CH₂**CO), 3.52~4.65(m, 16H, **CH₂**Ph and N**CH₂**CO), 4.75~4.92(m, 1H, HN**CH**CO), 4.95~5.33(m, 1H, NH**CH**CO), 7.16~7.30(m, 10H, ArH) , 7.62~7.79(m, 8H, ArH); ^{13}CNMR($CDCl_3$) ***δ*** : 29.6, 31.5, 36.3, 36.9, 39.1, 39.9, 49.5, 50.3, 52.4, 99.5, 123.1, 125.9, 127.0, 128.7, 131.9, 134.0, 135.4, 167.0, 167.7, 168.7, 170.5, 171.2. HRMS (ESI) m/z calcd for $C_{54}H_{60}N_{10}O_{12}S_2Na^+$ $(M+Na)^+$ 1127.37258, found 1127.37988.

Sulfido-[isoindolone-cyclo-Gly-*L*-Cys-*L*-Ala-Sar]$_2$ (**4c**): white solid, yield 51% (HPLC yield 60%), mobile phases V_{H2O}/V_{MeCN} = 40:60, the retention time 5.6 min, [α]D^{20} = -20.07° (c = 0.04 g/100 ml, CH_2Cl_2); ^{1}HNMR($CDCl_3$) ***δ***: 0.89~1.18(m, 6H, CH**CH₃**), 2.85~3.02(m, 4H, S**CH₂**CH), 3.18~3.30(m, 6H, N**CH₃**), 3.50~4.05(m, 6H, N**CH₂**CO), 4.16~4.45(m, 4H, **CH₂**Ph), 4.36~4.72(m, 6H, N**CH₂**C(OH) and N**CH₂**CO), 4.70~4.85(m, 2H, HN**CH**CO), 4.86~5.18(m, 2H, NH**CH**CO), 7.16~7.31(m, 10H, ArH) , 7.50~7.52(m, 2H, ArH) , 7.66~7.78(m, 6H, ArH); ^{13}CNMR($CDCl_3$) ***δ*** : 13.4, 23.0, 27.2, 29.2, 36.6, 46.2, 51.8, 60.2, 65.1, 99.5, 123.4, 126.3, 127.3, 128.3, 130.5, 131.9, 135.7, 139.9, 161.4, 164.2, 164.5, 168.0, 170.5. HRMS (ESI) m/z calcd for $C_{54}H_{60}N_{10}O_{12}S_2Na^+$ $(M+Na)^+$ 1127.37258, found 1127.37842.

Sulfido-[isoindolone-cyclo-Gly-*L*-Cys-*L*-Sar-Sar-Sar]$_2$ (**4d**): white solid, yield 76% (HPLC yield 88%), mobile phases V_{H2O}/V_{MeCN} = 60:40, the retention time 3.2 min, [α]D^{20} = +31.25° (c = 0.06 g/100 ml, CH_2Cl_2); HNMR($CDCl_3$) ***δ***: 2.22~3.62(m, 34H, N**CH₃**, S**CH₂**CH and N**CH₂**CO), 3.71~4.58(m, 12H, **CH₂**Ph and N**CH₂**CO), 4.60~4.71(m, 1H, HN**CH**CO), 5.01~5.25(m, 1H, NH**CH**CO), 7.15~7.78(m, 18H, ArH); ^{13}CNMR($CDCl_3$) ***δ*** : 27.5, 29.6, 31.2, 35.7, 36.4, 38.9, 40.2, 49.5, 49.7, 52.6, 53.5, 99.9, 123.4, 126.3, 127.8, 128.6, 128.8, 132.0, 134.1, 136.2, 166.4, 166.9, 167.7, 168.9, 169.6, 171.1. HRMS (ESI) m/z calcd for $C_{60}H_{70}N_{12}O_{14}S_2Na^+$ $(M+Na)^+$ 1269.44681, found 1269.44678.

Sulfido-[isoindolone-cyclo-Gly-*L*-Cys-*L*-Ala-Sar-Sar]$_2$(**4e**): white solid, yield 60% (HPLC yield 71%), mobile phases V_{H2O}/V_{MeCN} = 45:55, the retention time 4.4 min, [α]D^{20} = +33.14° (c = 0.05 g/100 ml, CH_2Cl_2); ^{1}HNMR($CDCl_3$) ***δ***: 0.89~1.18(m, 6H, CH**CH_3**), 2.65~2.72(m, 4H, S**CH_2**CH), 2.95~3.45(m, 12H, N**CH_3**), 3.59~3.81(m, 2H, N**CH_2**CO), 3.82~4.15(m, 2H, N**CH_2**CO), 4.16~4.35(m, 6H, **CH_2**Ph and N**CH_2**CO), 4.36~4.75(m, 8H, N**CH_2**C(OH) and N**CH_2**CO), 4.78~4.89(m, 2H, HN**CH**CO), 4.90~5.28(m, 4H, NH**CH**CO), 7.18~7.86(m, 18H, ArH); ^{13}CNMR($CDCl_3$) ***δ***: 18.8, 20.5, 27.5, 36.6, 39.8, 43.0, 45.8, 49.6, 51.4, 52.1, 60.2, 99.5, 120.6, 123.1, 125.9, 128.3, 132.2, 133.7, 136.1, 139.9, 164.9, 166.0, 167.3, 169.1, 171.2, 173.7. HRMS (ESI) m/z calcd for $C_{60}H_{70}N_{12}O_{14}S_2Na^+$ $(M+Na)^+$ 1269.44681, found 1269.44617.

Sulfido-[isoindolone-cyclo-Gly-*L*-Cys-*L*-Pro-*L*-Ile-*L*-Leu]$_2$(**4f**): white solid (yield 40%). ^{1}HNMR($CDCl_3$, 500 MHz) ***δ***: 0.51~0.99(m, 24H, **CH_3**), 1.15~1.30(m, 4H, **CH_2**CH_3), 1.38~1.76(m, 6H, **CH**$(CH)_3)_2$ and CH**CH_2**CH), 1.80~2.32(m, 10H, NCH_2**CH_2**CH_2CH, NCH_2CH_2**CH_2**CH and **CH**CH_3), 2.58~2.95(m, 4H, S**CH_2**CH), 2.98~3.45(m, 4H, N**CH_2**CH_2CH_2CH), 3.48~3.85(m, 4H, N**CH_2**CO), 4.18~4.28(m, 2H, $NCH_2CH_2CH_2$**CH**), 4.32~4.79(m, 8H, **CH_2**Ph and N**CH_2**C(OH)), 4.85~5.20(m, 4H, HN**CH**CO and HN**CH**CO), 5.21~5.38(m, 2H, HN**CH**CO), 6.80~7.33(m, 10H, ArH) , 7.34~7.80(m, 8H, ArH); ^{13}CNMR($CDCl_3$, 500 MHz) ***δ***: 14.1, 15.6, 22.7, 23.3, 24.9, 29.7, 31.9, 34.4, 37.2, 38.0, 41.3, 43.8, 49.0, 49.6, 51.3, 56.7, 57.7, 62.6, 97.0, 120.6, 123.5, 127.8, 128.9, 132.6, 134.1, 136.3, 138.3, 146.9, 159.6, 160.0, 161.6, 164.5, 167.7, 168.2. HRMS (ESI) m/z calcd for $C_{76}H_{99}N_{12}O_{14}S_2^+$ $(M+H)^+$ 1467.68396, found 1467.68469.

Sulfido-[isoindolone-cyclo-Gly-*L*-Cys-*L*-Sar-Sar-Sar-Sar]$_2$(**4g**): white solid, yield 78% (HPLC yield 87%), mobile phases V_{H2O}/V_{MeCN} = 60:40, the retention time 5.8 min, [α]D^{20} = -21.50° (c = 0.03 g/100 ml, CH_2Cl_2); HNMR($CDCl_3$) ***δ***: 2.80~3.19(m, 28H, S**CH_2** and N**CH_3**), 4.22~4.40(m, 16H, N**CH_2**CO), 4.48~4.81(m, 12H, **CH_2**Ph and N**CH_2**CO), 4.90~5.06(m, 1H, HN**CH**CO), 5.08~5.46(m, 1H, NH**CH**CO), 7.18~7.83(m, 18H, ArH); ^{13}CNMR($CDCl_3$) ***δ***:22.6, 24.4, 26.4, 27.0, 27.5, 28.0, 29.3, 29.9, 31.9, 32.6, 34.2, 36.0, 37.0, 39.1, 40.3, 49.3, 52.5, 99.9, 123.4, 125.6, 127.0, 128.7, 132.5, 134.0, 163.1, 165.2, 166.3, 167.0, 167.7, 168.2, 168.3, 169.0. HRMS (ESI) m/z calcd for $C_{66}H_{80}N_{14}O_{16}S_2Na^+$ $(M+Na)^+$ 1411.52104, found 1411.52258.

Sulfido-[isoindolone-cyclo-Gly-*L*-Cys-Sar-Sar-Sar-Sar-Sar]$_2$ (**4h**): white solid, yield 74% (HPLC yield 85%), mobile phases V_{H2O}/V_{MeCN} = 60:40, the retention time 4.5 min, [α]D^{20} = +26.50° (c = 0.05 g/100 ml, CH_2Cl_2); ^{1}HNMR($CDCl_3$) ***δ***: 2.82~2.92(m, 10H, S**CH_2**CH and N**CH_2**CO), 2.96~3.18(m, 14H, N**CH_2**CO), 3.26~3.39(m, 30H, N**CH_3**), 4.18~4.25(m, 4H, **CH_2**Ph), 4.26~4.39(m, 8H, N**CH_2**C(OH) and N**CH_2**CO), 4.45~4.75(m, 2H, HN**CH**CO), 7.18~7.87(m, 18H, ArH); ^{13}CNMR($CDCl_3$) $\boldsymbol{\delta}$: 20.5, 21.2, 22.6, 26.9, 29.2, 36.0, 38.8, 44.7, 49.3, 49.7, 52.8, 56.3, 57.8, 59.5, 66.9, 99.9, 118.5, 123.8, 125.9, 127.3, 128.3, 131.9, 133.7, 136.7, 164.9, 165.6, 166.3, 167.7, 168.7, 170.2, 170.5, 172.6. HRMS (ESI) m/z calcd for $C_{72}H_{90}N_{16}O_{18}S_2Na^+$ $(M+Na)^+$ 1553.59526, found 1553.59679.

Sulfido-[isoindolone-cyclo-Gly-*L*-Cys-*L*-Ala-*L*-Ala-Sar-*L*-Ala-Sar]$_2$(**4i**): white solid, while solid, yield 53% (HPLC yield 62%), mobile phases V_{H2O}/V_{MeCN} = 60:40, the retention time 3.9 min, [α]D^{20} = +13.78° (c = 0.06 g/100 ml, CH_2Cl_2); ^{1}HNMR($CDCl_3$) $\boldsymbol{\delta}$: 0.05~0.16(m, 18H, $SiMe_3$), 1.28~1.48(m, 18H, CH**CH$_3$**), 2.82~2.98(m, 4H, S**CH$_2$**CH and N**CH$_2$**CO), 3.18~3.28(m, 12H, N**CH$_3$**), 3.45~3.75(m, 4H, N**CH$_2$**CO), 3.80~4.01(m, 4H, N**CH$_2$**CO), 4.05~4.35(m, 2H, N**CH$_2$**CO), 4.38~4.52(m, 4H, **CH$_2$**Ph), 4.53~4.82(m, 6H, N**CH$_2$**C(OH) and HN**CH**CO), 4.85~5.15(m, 4H, NH**CH**CO), 7.13~7.78(m, 18H, ArH); ^{13}CNMR($CDCl_3$) $\boldsymbol{\delta}$: 8.97, 17.3, 18.4, 34.9, 36.0, 38.5, 39.5, 44.7, 45.8, 48.6, 50.4, 51.4, 52.1, 53.1, 54.6, 99.9, 117.1, 125.2, 126.3, 127.6, 128.0, 134.3, 136.1, 138.2, 163.1, 166.3, 167.0, 168.4, 170.5, 171.2, 172.9, 173.7. HRMS (ESI) m/z calcd for $C_{72}H_{90}N_{16}O_{18}S_2Na^+$ $(M+Na)^+$ 1553.59526, found 1553.59460.

2. HPLC spectra of compounds 4a~4i.

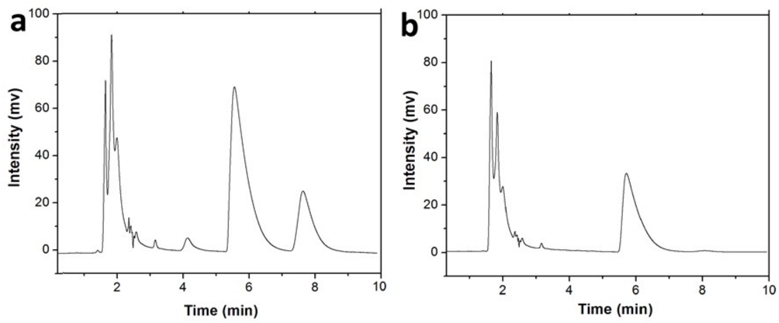


Figure S1. HPLC spectrum of compound **4a**. a) Unpurified mixture. b) Purified.

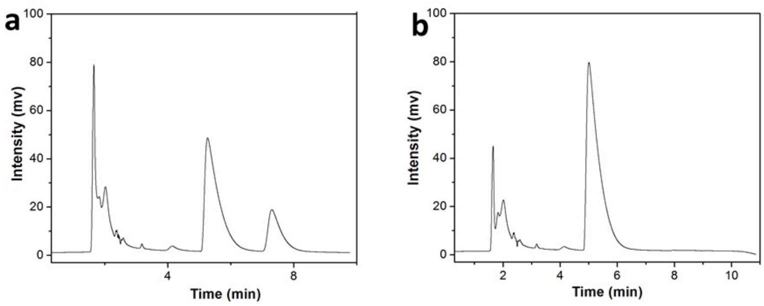


Figure S2. HPLC spectrum of compound **4b**. a) Unpurified mixture. b) Purified.

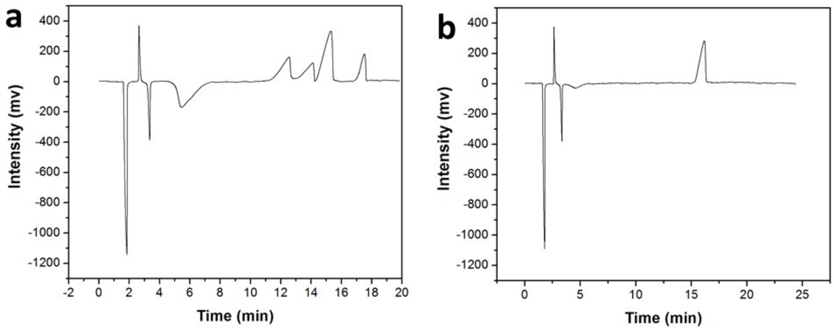


Figure S3. HPLC spectrum of compound **4c**. a) Unpurified mixture. b) Purified.

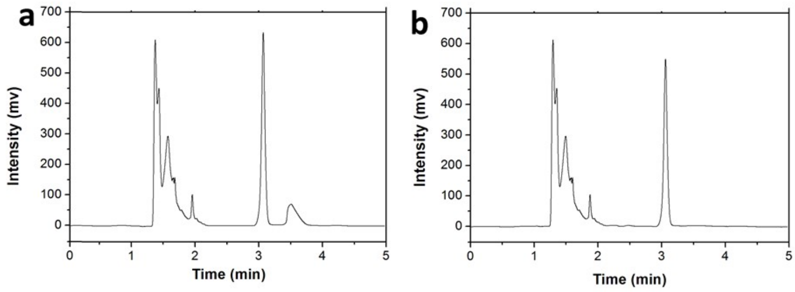


Figure S4. HPLC spectrum of compound **4d**. a) Unpurified mixture. b) Purified.

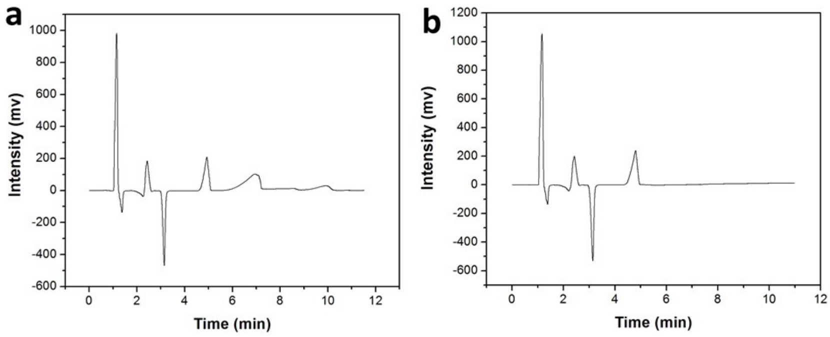


Figure S5. HPLC spectrum of compound **4e**. a) Unpurified mixture. b) Purified.

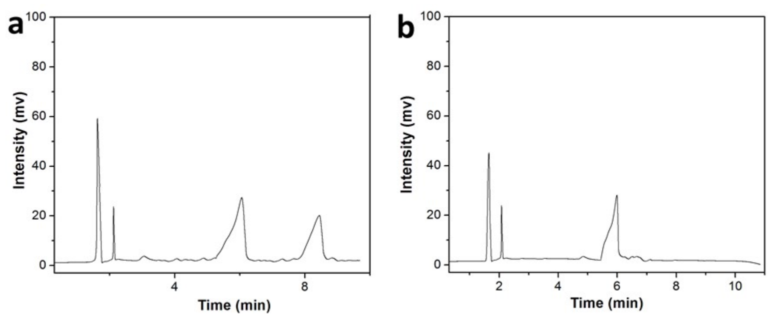


Figure S6. HPLC spectrum of compound **4g**. a) Unpurified mixture. b) Purified.

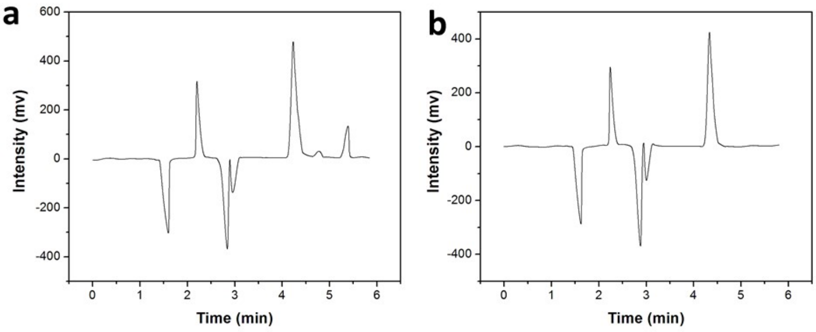


Figure S7. HPLC spectrum of compound **4h**. a) Unpurified mixture. b) Purified.

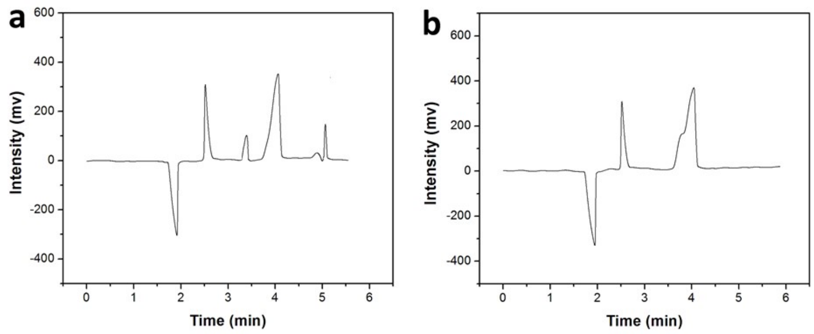


Figure S8. HPLC spectrum of compound **4i**. a) Unpurified mixture. b) Purified.

3. The mass spectra of cyclopeptide 3-hydroxy-isoindolone-cyclo-(Gly-Ile-Pro-Pro-Leu)

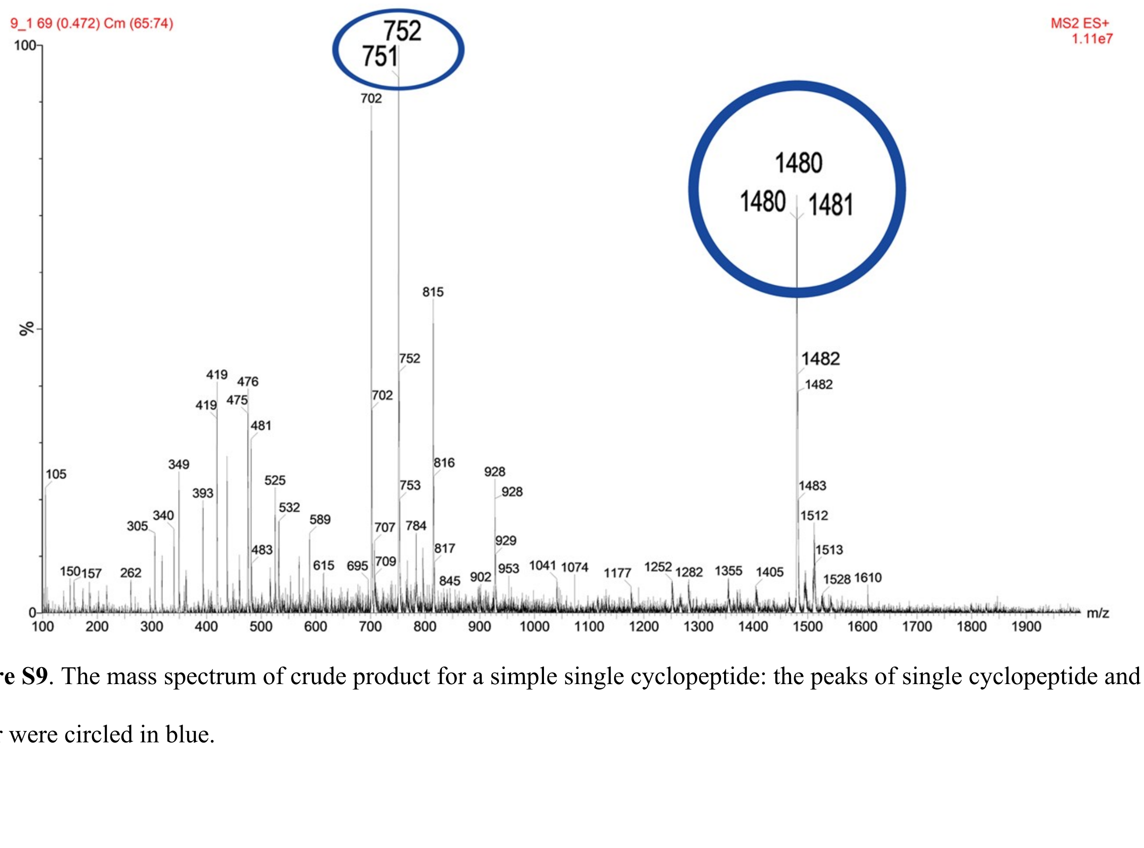


Figure S9. The mass spectrum of crude product for a simple single cyclopeptide: the peaks of single cyclopeptide and dimer were circled in blue.

4. Computational details:

There are two possible absolute configurations (ACs) for compound 2f: C-3R--C-3`R or C-3S--C-3`S isomers. In order to reduce the computational consumption, we simplify the theoretical calculation by breaking the bis-cyclic peptide 2f at the disulfur bond and simulated the ECD of half fragment of the bicyclic structure. Conformational analysis was performed by fixing the absolute configuration of C-3 for bis-cyclic peptides **2f** with the MMFF94 molecular mechanics force field. The obtained conformers were optimized at the DFT/B3LYP/6-31G(d,p) level by Gaussian 09.[1] Time-dependent DFT calculations were performed on the lowest energy conformations (>5% population) to calculate excitation energy (denoted by wavelength in nm) and rotatory strength R at the level of TDDFT/CAM-B3LYP/6-311++G(d,p) using polarizable continuum model (PCM) to consider the solvent. NMR shifts for the potential structures were simulated by the GIAO method at the level of DFT/B3LYP/6-311++G(d,p) using the optimized structures obtained from the DFT/B3LYP/6-31G(d,p) level. ECD curves were calculated based on rotatory strengths using half bandwidth of 0.30~0.40 eV by Specdis 1.71.[2] The calculated spectra were treated by UV correction to facilitate comparison to the experimental data.

References:

[1] Gaussian 09, Revision C.01; Gaussian, Inc.: Wallingford, CT, 2010.

[2] T. Bruhn, A. Schaumloffel, Y. Hemberger, G. Bringmann, *Chirality,* 2013, **25**, 243.

5. The summarized structures for 4a~4i.

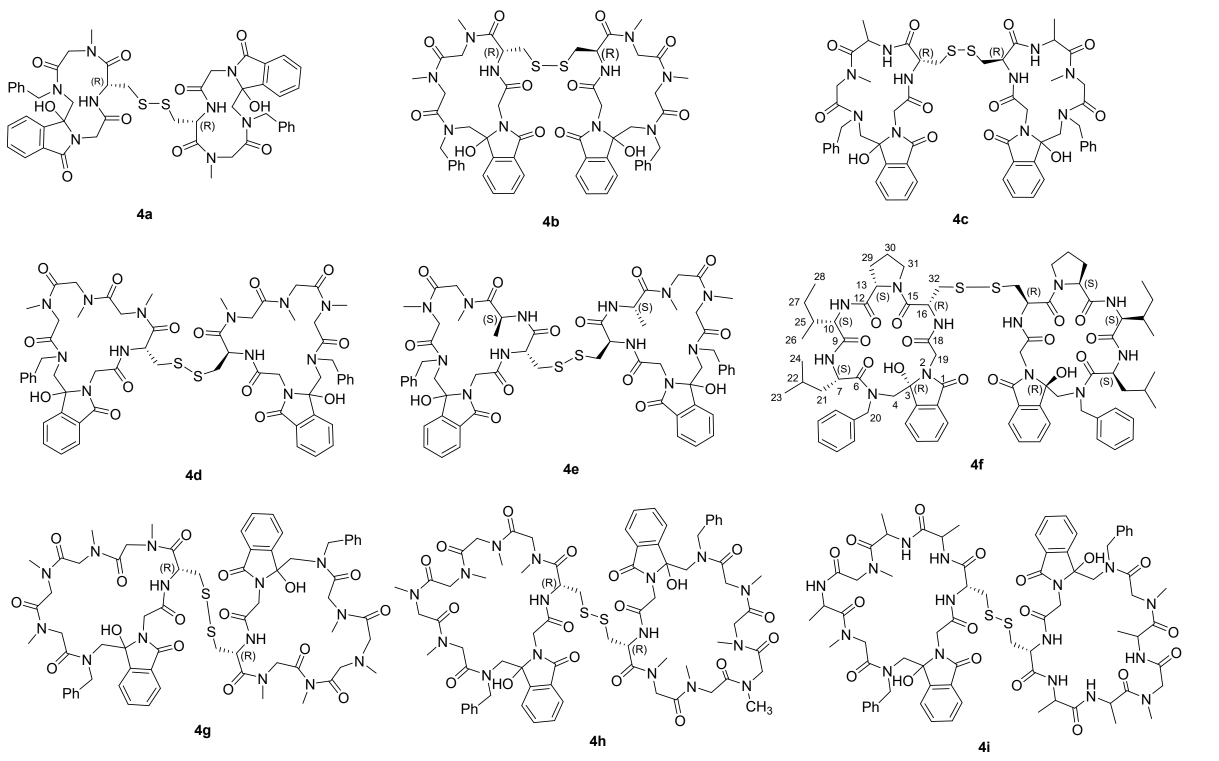


Figure S10. The structure of bicyclic peptides **4a~4i**.

6. Table S1. Experimental and theoretical ^{1}H and ^{13}C isotropic chemical shifts of 4f.

Table S1. Experimental and theoretical ^{1}H and ^{13}C isotropic chemical shifts (δ_{iso} /ppm) [a] and isotropic magnetic shielding tensors (σ_{iso} /ppm) of 4f.

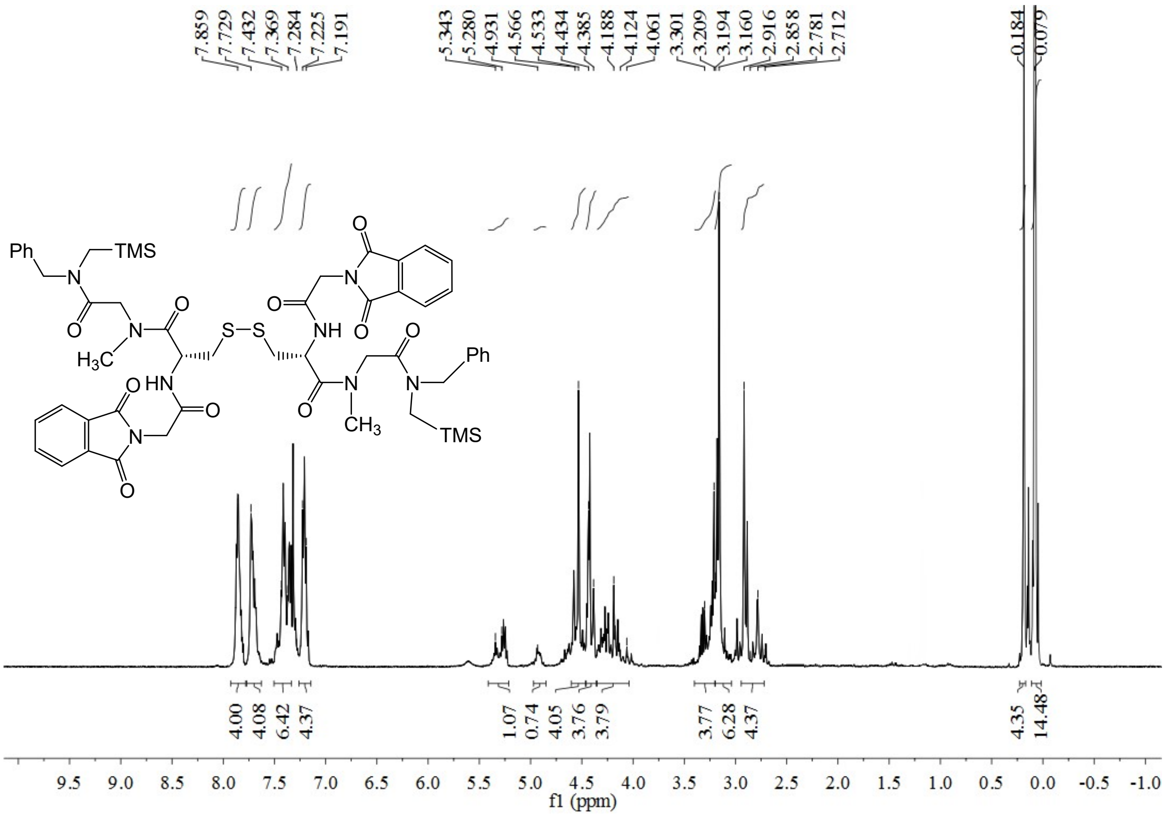
Assignments	^{1}H NMR			Assignments	^{13}C NMR		
	σ_{iso}	Calc. (δ_{iso}) [a]	Exp. (δ_{iso})		σ_{iso}	Calc. (δ_{iso}) [a]	Exp. (δ_{iso})
H23,24,26,28	31.40, 31.19, 31.09, 31.01	0.56, 0.77, 0.87, 0.96	0.51-0.99 (m,12H)	C28	176.5	7.6	14.1
H27	30.66	1.30	1.15-1.30 (m,2H)	C26	167.0	17.0	15.6
H21,22	30.26, 30.19	1.70, 1.77	1.38-1.76 (m,3H)	C23	163.1	20.9	22.7
H25,30,31	30.11, 29.96, 29.85, 29.76, 29.58	1.84, 2.01, 2.11, 2.19, 2.38	1.80-2.32 (m,5H)	C24	158.4	25.6	22.7
H32	28.91	3.05	2.58-2.95(m,2H)	C30	154.4	29.6	23.3
H29	28.71, 28.51	3.25, 3.45	2.98-3.45 (m,2H)	C22	154.1	29.9	24.9
H19	28.34	3.62	3.48-3.85(m,2H)	C27	153.6	30.4	29.7
H13	27.79	4.17	4.18-4.28(m,1H)	C32	153.4	30.6	31.9
H4,20	27.73, 27.48	4.2313, 4.4803	4.32-4.79(m,4H)	C29	151.7	32.3	34.4
H7,10	27.34, 27.03	4.62, 4.93	4.85-5.20(m,2H)	C25	145.8	38.2	37.2
H16	26.85	5.11	5.21-5.38(m,1H)	C21	140.8	43.2	38.0
ArH	25.10, 24.81, 24.60, 24.34, 24.17	6.86, 7.15, 7.36, 7.62, 7.79	6.86-7.98 (m,9H)	C19	134.1	49.9	41.3
				C31	132.2	51.8	43.8
				C20	129.1	54.9	49.0
				C7	123.3	60.7	49.6
				C16	119.0	65.1	51.3
				C4	118.4	65.6	56.7
				C10	118.2	65.9	57.7
				C13	115.1	68.9	62.6
				C3	86.9	97.1	97.0
				CPh	55.4	128.6	120.6
				CPh	52.6	131.4	123.5
				CPh	52.3	131.7	127.8
				CPh	50.3	133.7	128.9
				CPh	49.9	134.2	132.6
				CPh	47.5	136.5	134.1
				CPh	47.1	136.9	134.1
				CPh	47.1	137.0	136.3
				CPh	45.5	138.5	136.3
				CPh	43.4	140.6	138.3
				CPh	37.0	147.1	146.9
				C18	26.9	157.1	159.6
				C1	7.9	176.1	160.0
				C12	4.9	179.2	161.6
				C9	2.0	182.0	164.5
				C6	0.5	183.5	167.7
				C15	0.3	183.7	168.2

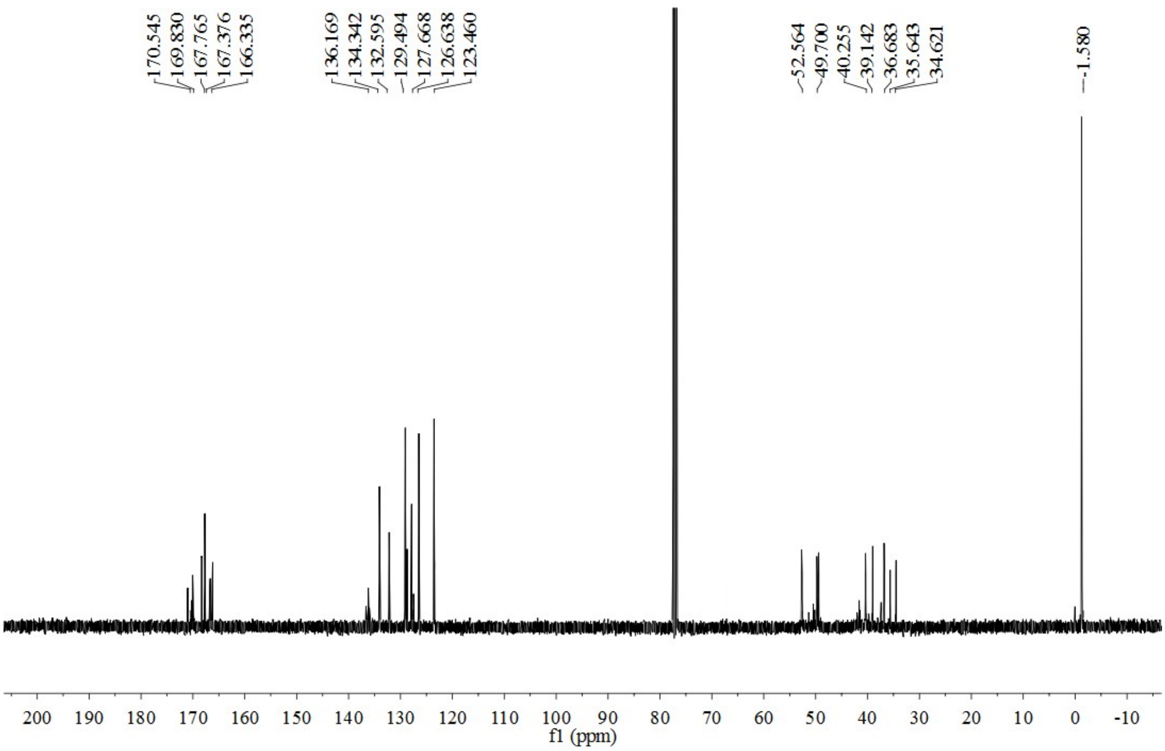
[a] δ_{isoH} and δ_{isoC} were calculated by Equations $\delta_{isoX} = \sigma_{isoTMS\text{-}X} - \sigma_{isoX}$.

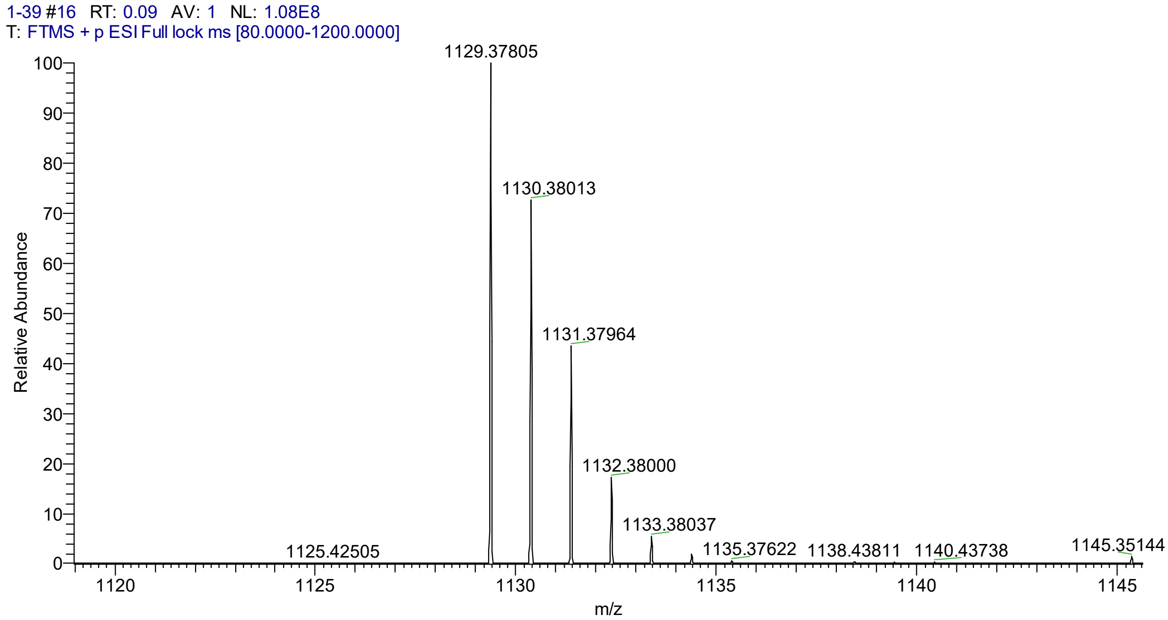
($\sigma_{isoTMS\text{-}H} = 31.9695$, $\sigma_{isoTMS\text{-}C} = 184.0330$); TMS = Tetramethylsilane

7. ^{1}H, ^{13}C-NMR and HRMS of bis-linear peptides and bis-cyclic peptides.

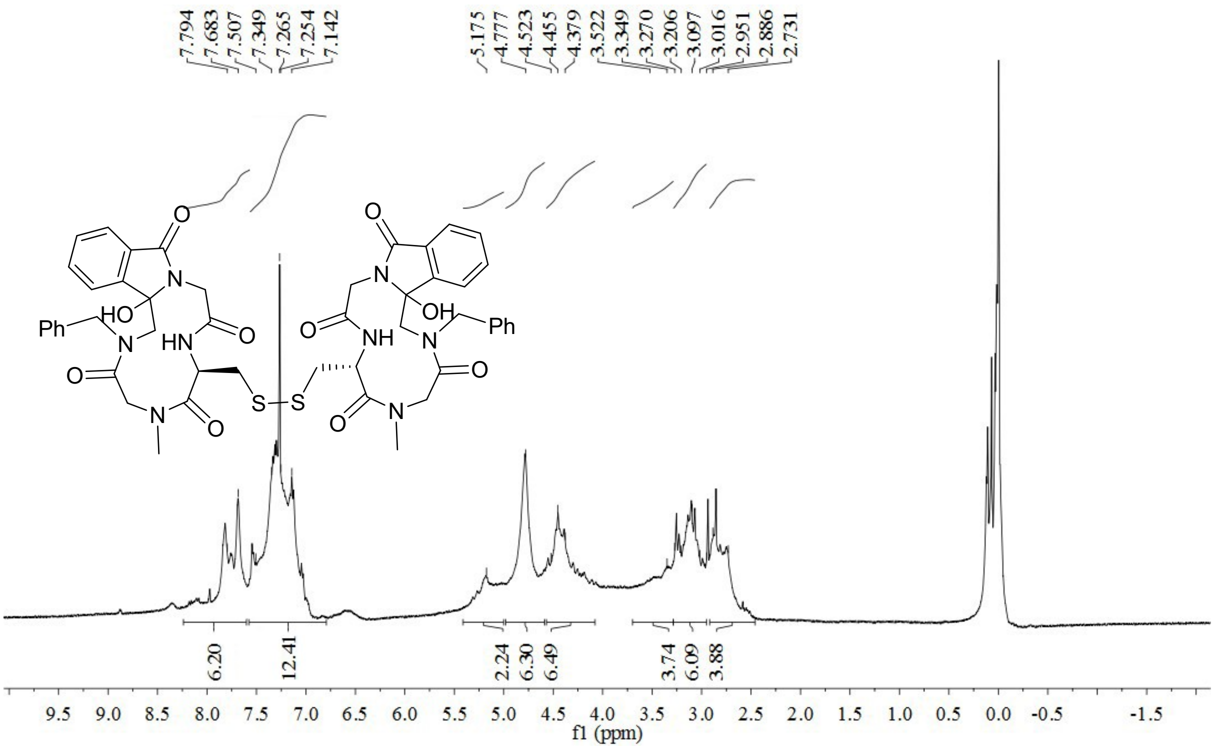
(1) ^{1}H, ^{13}C-NMR and HRMS of **3a.**

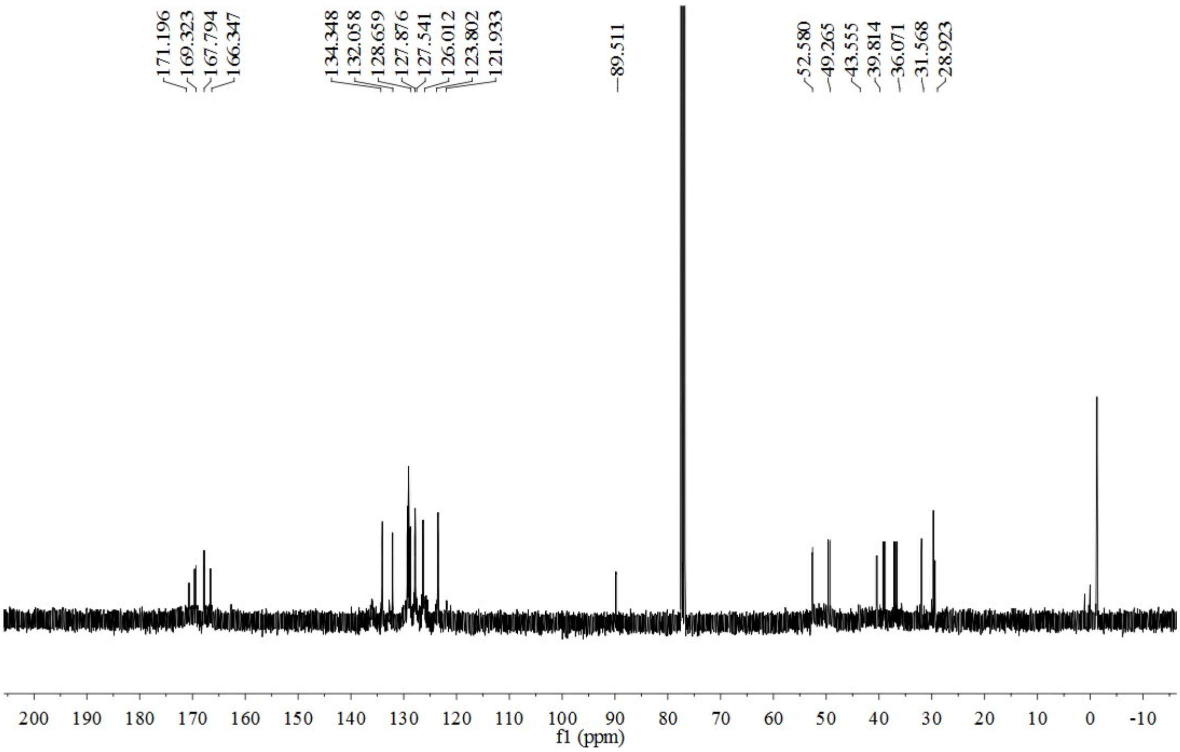






(2) [1]H, [13]C-NMR and HRMS of **4a.**

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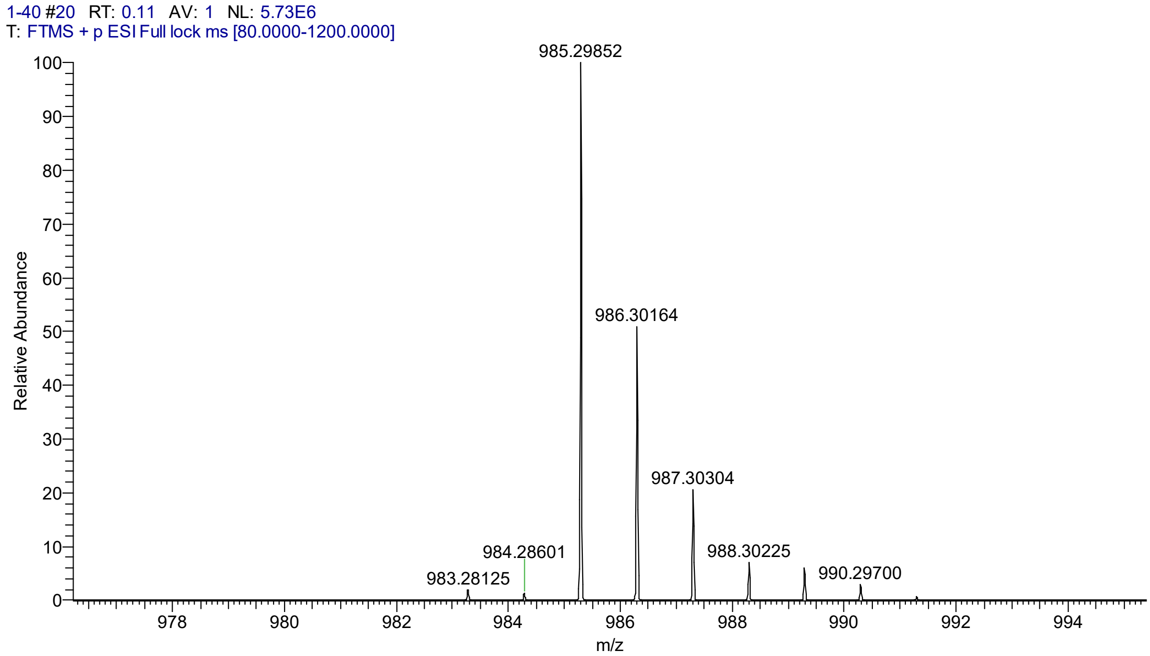
f1 (ppm)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Relative Abundance
m/z
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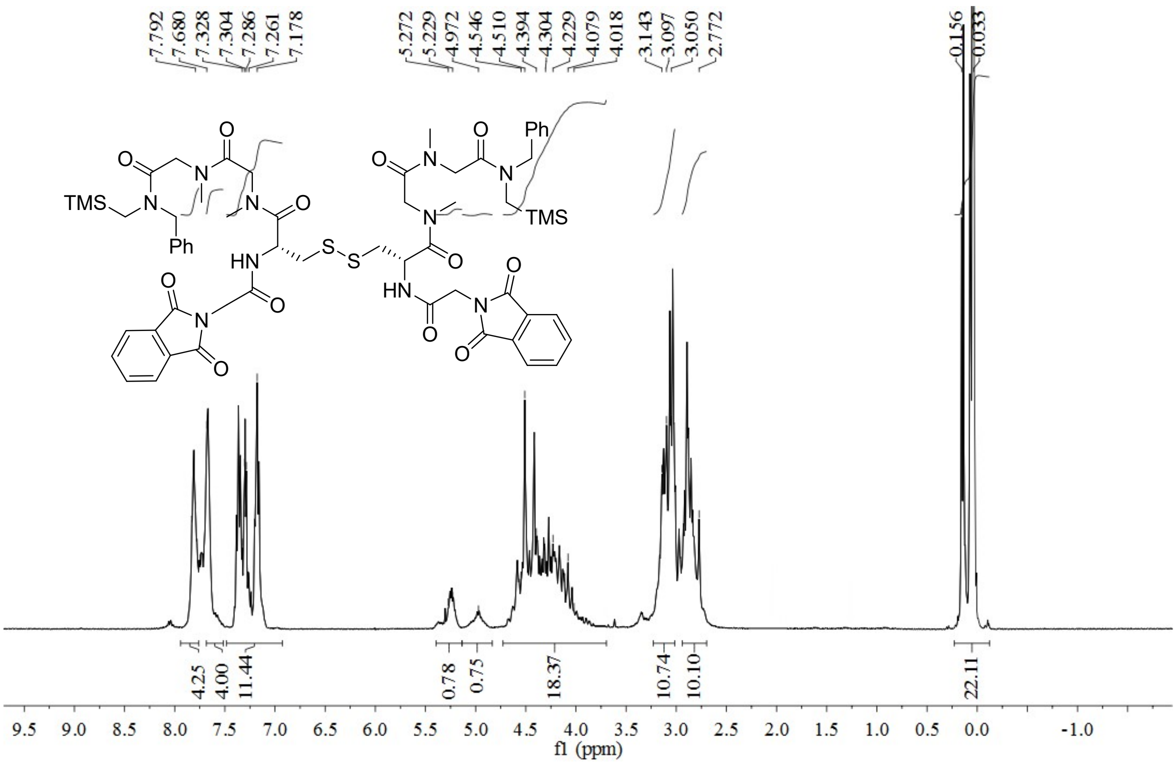
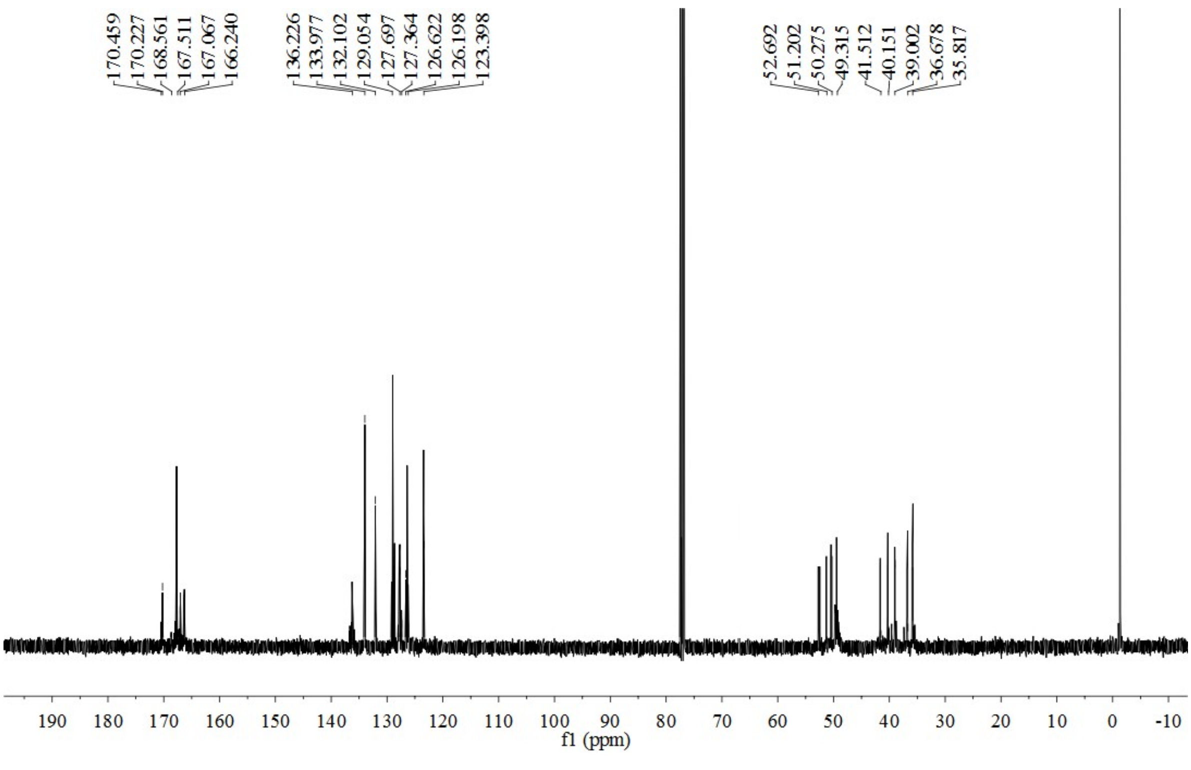
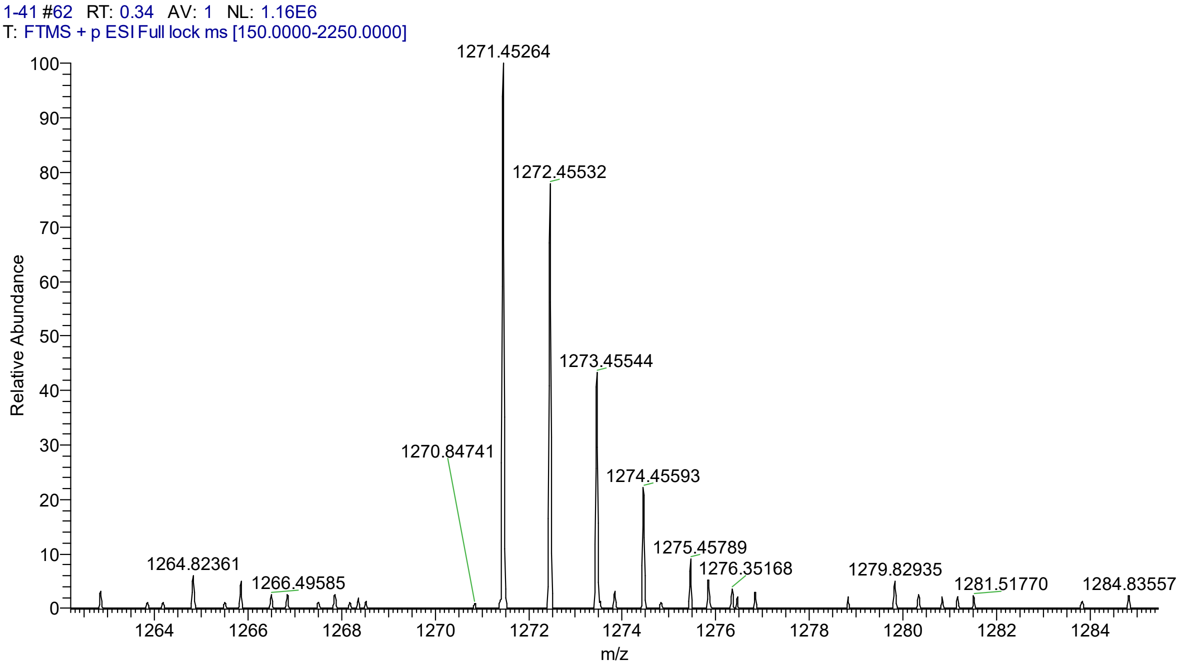
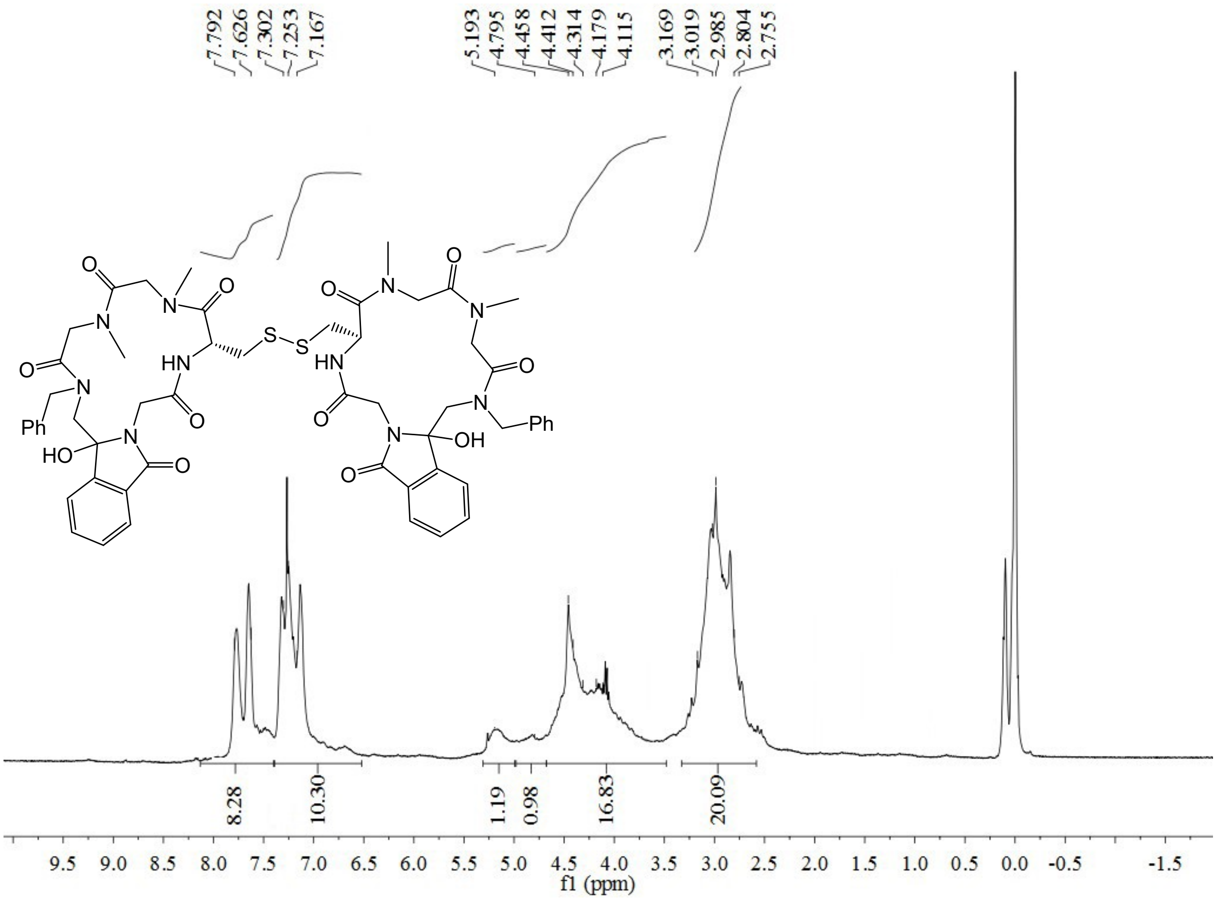
(3) ^{1}H, ^{13}C-NMR and HRMS of **3b.**

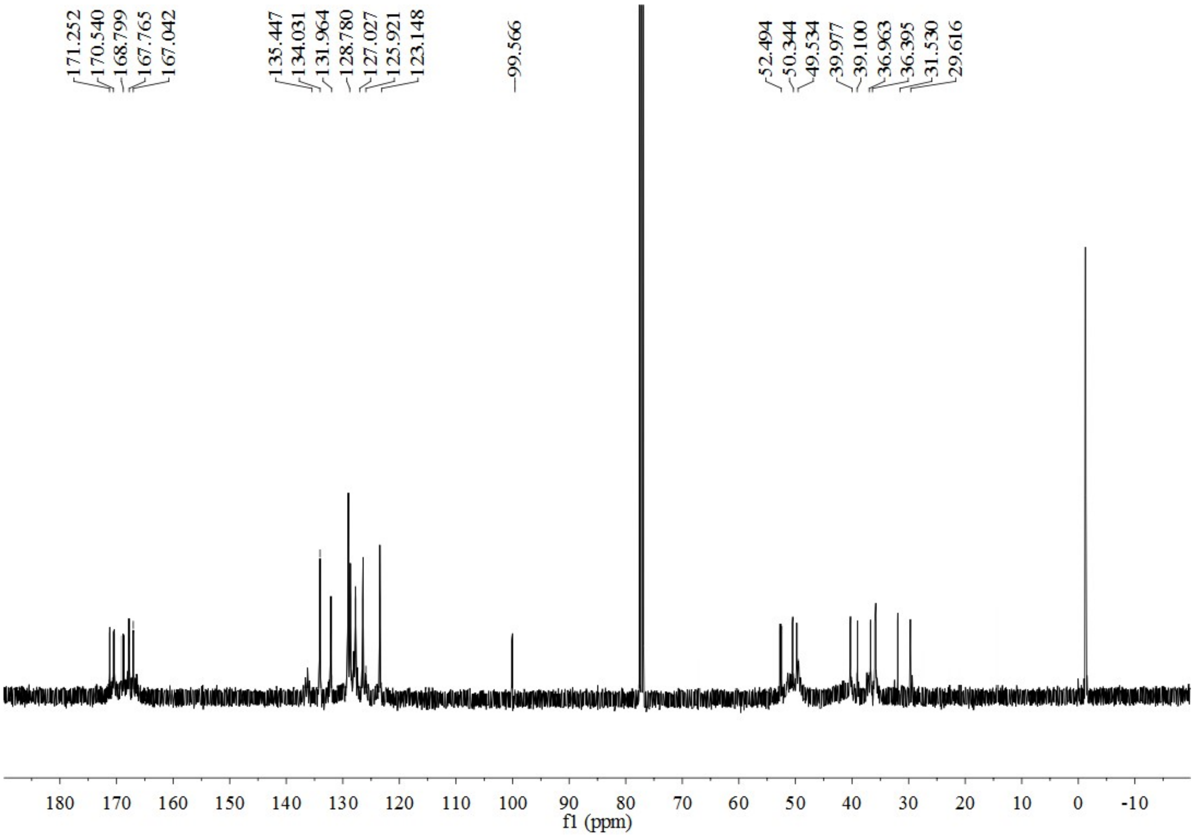






(4) ^{1}H, ^{13}C-NMR and HRMS of **4b.**





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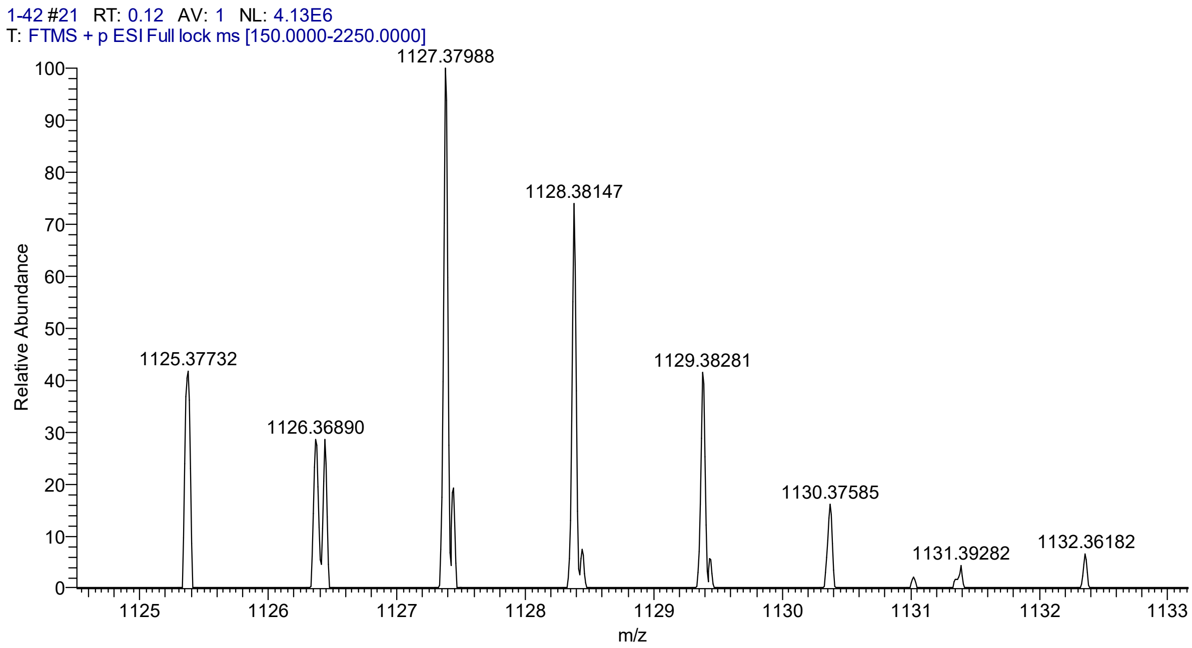

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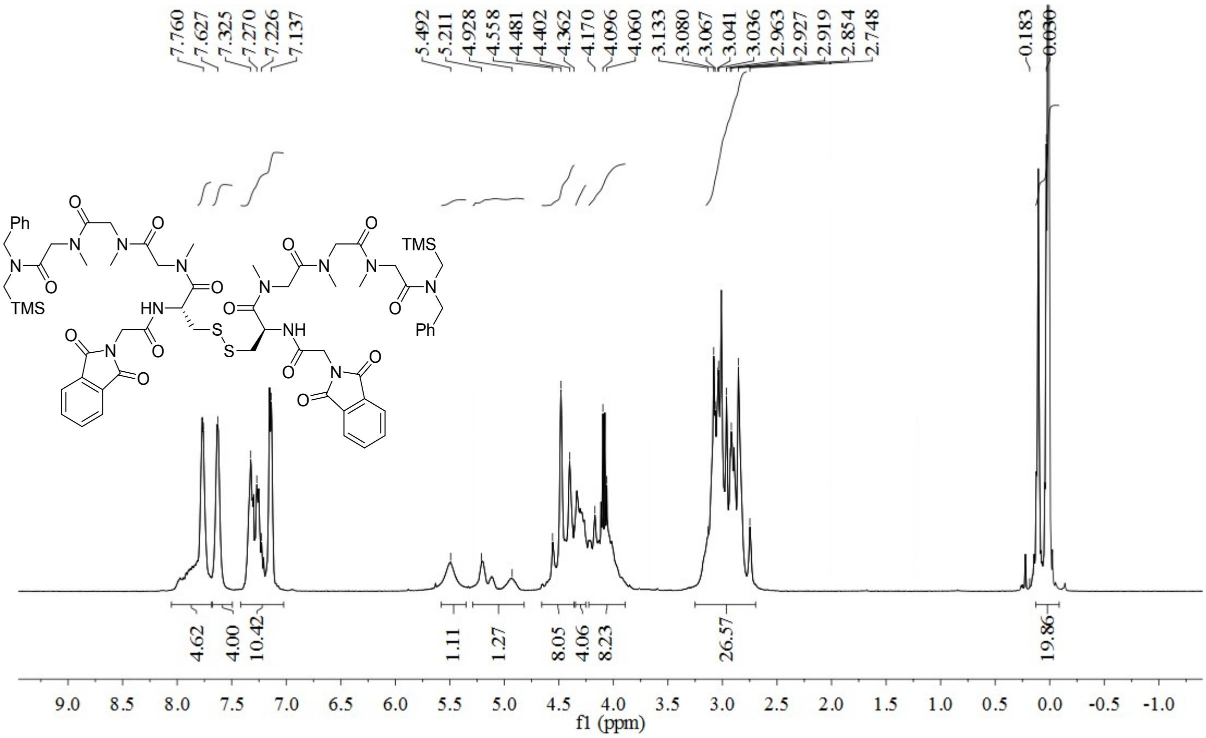
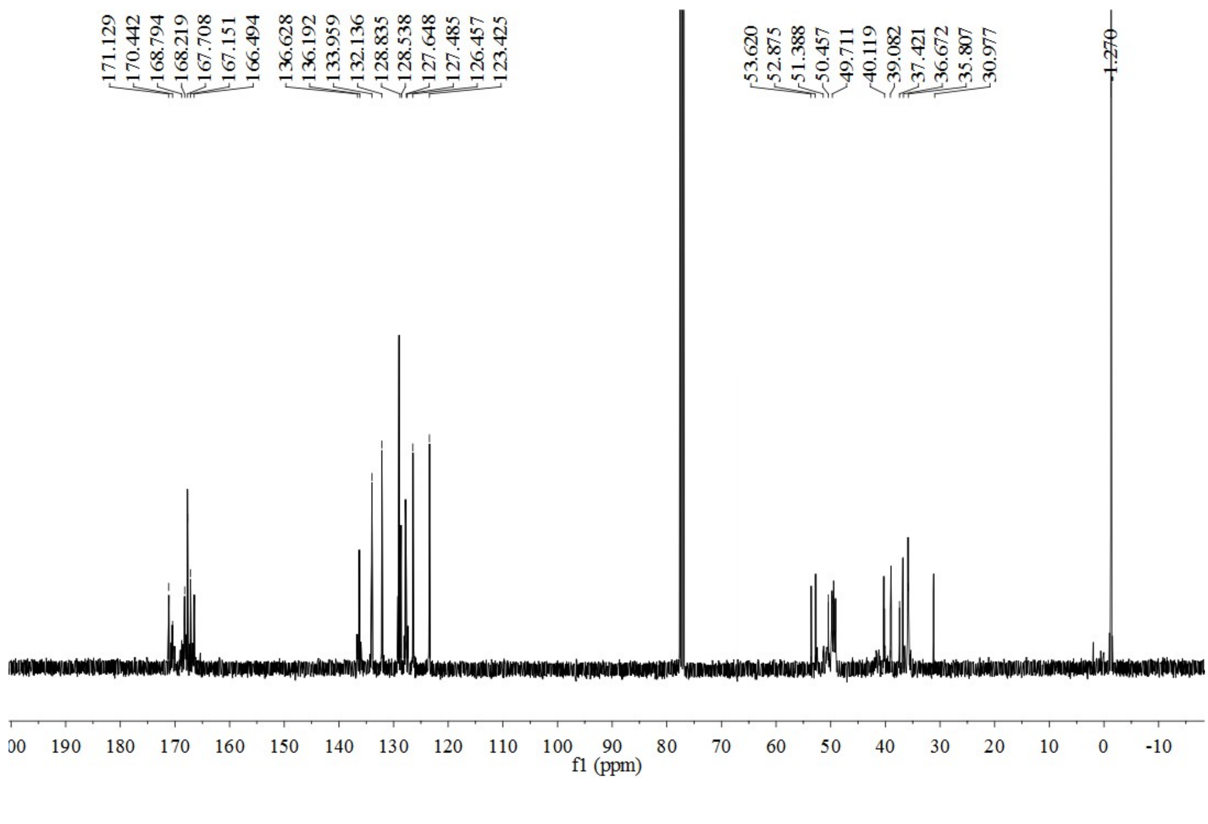
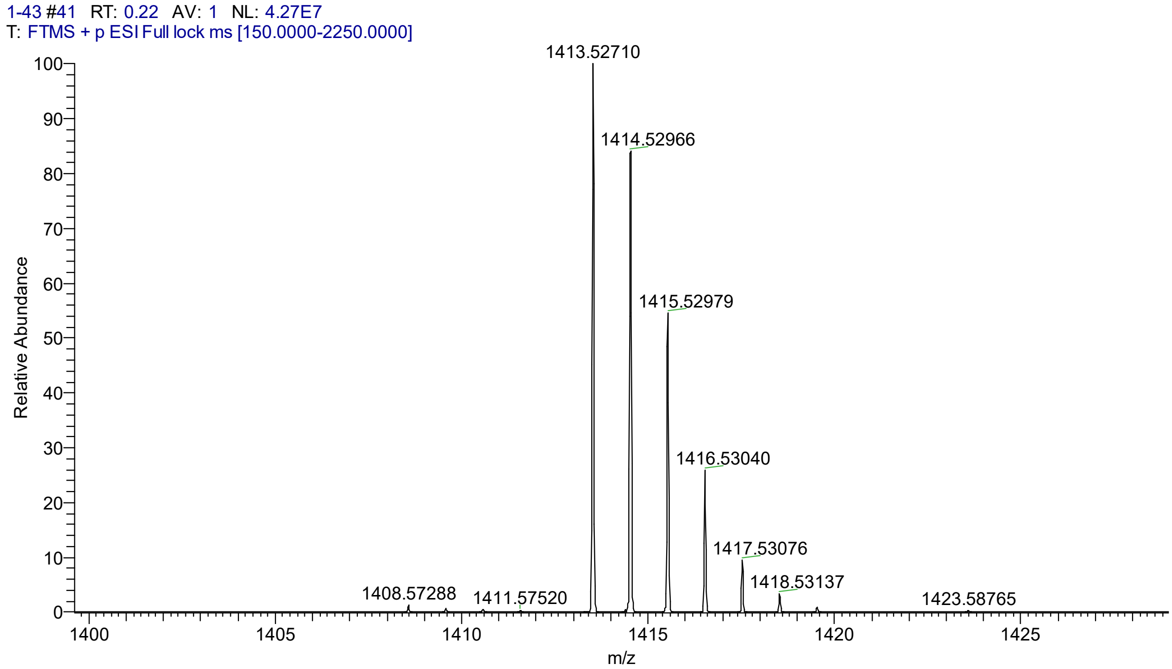
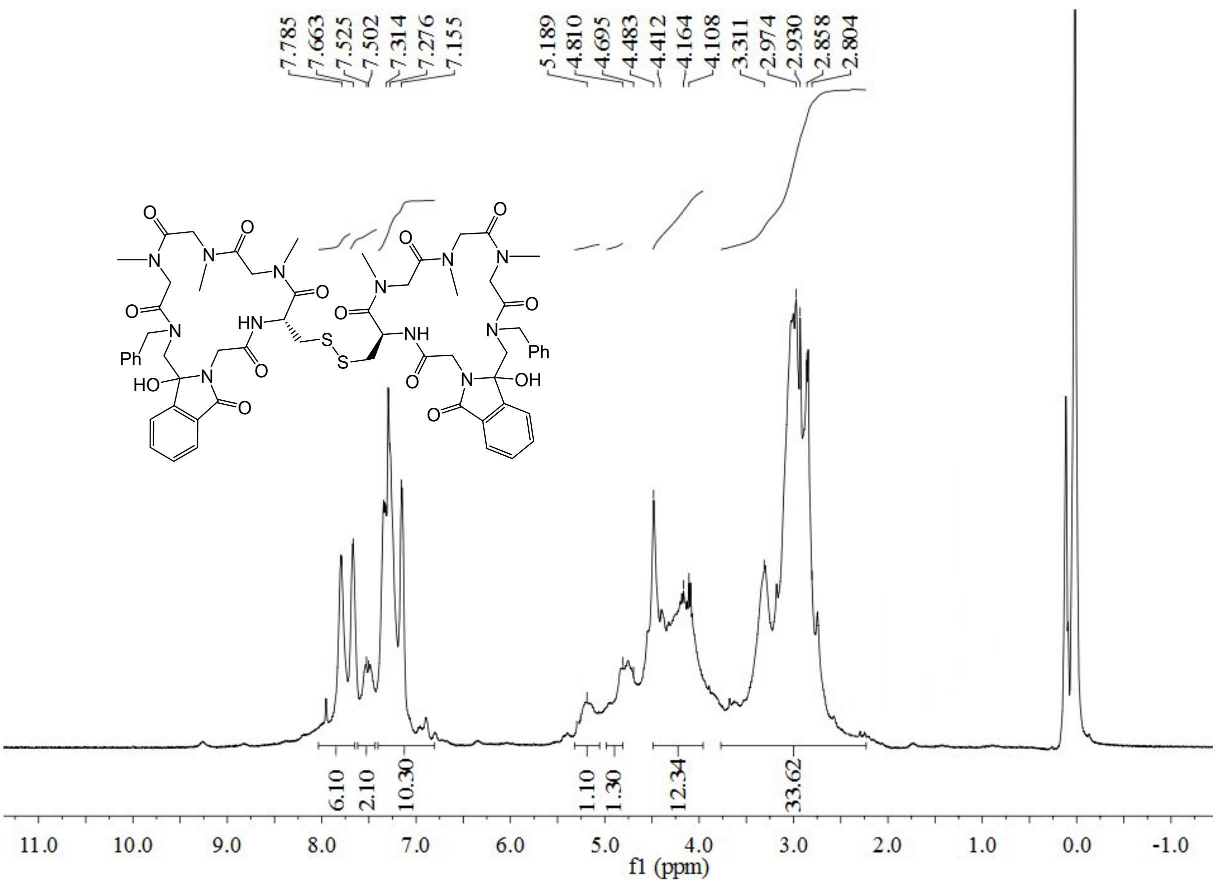
(5) ^{1}H, ^{13}C-NMR and HRMS of **3c.**

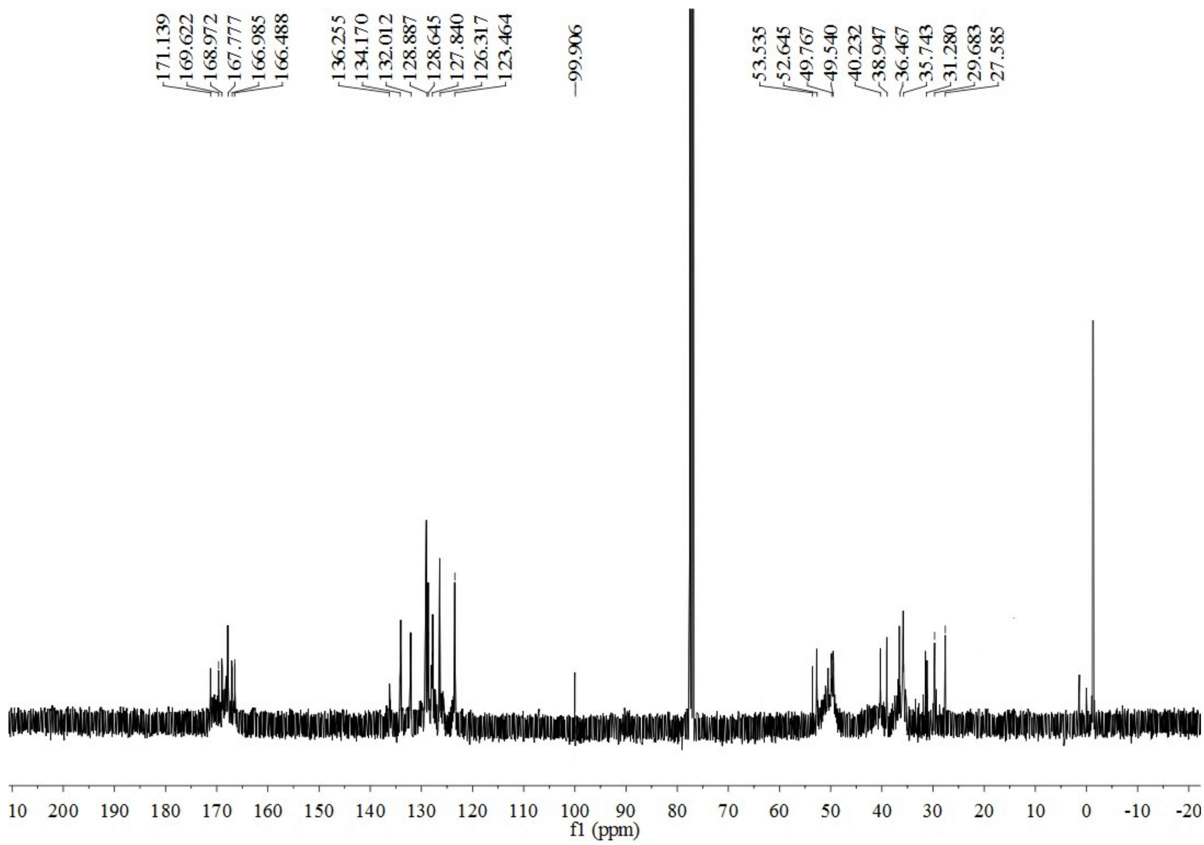




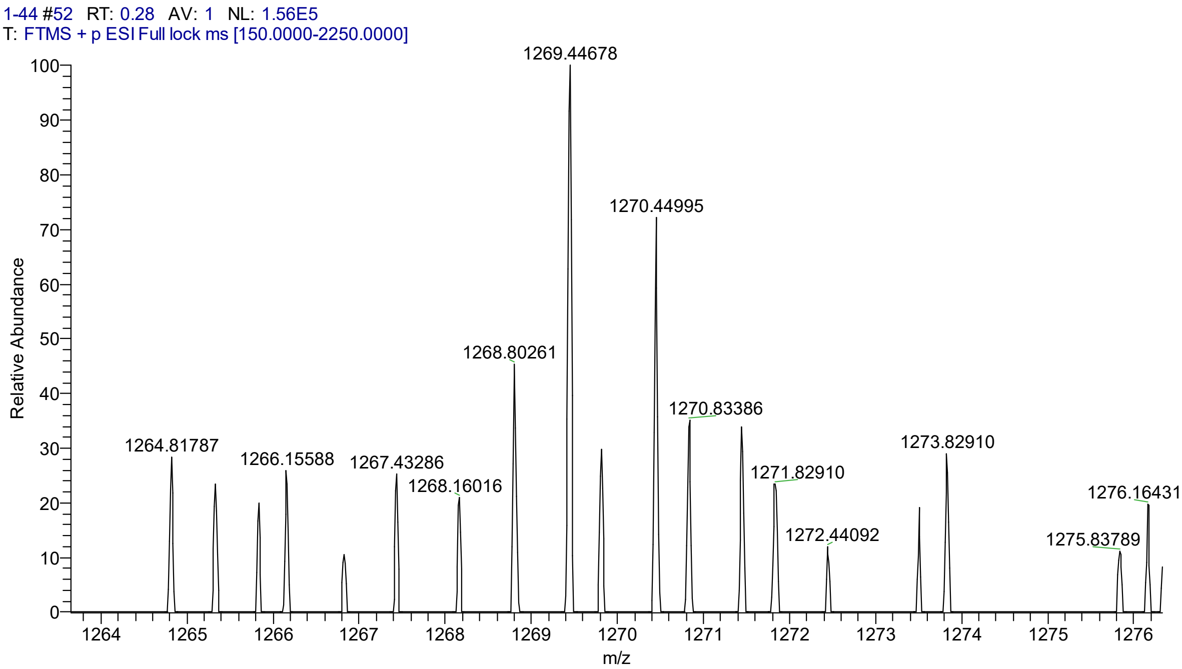


(6) ^{1}H, ^{13}C-NMR and HRMS of **4c.**



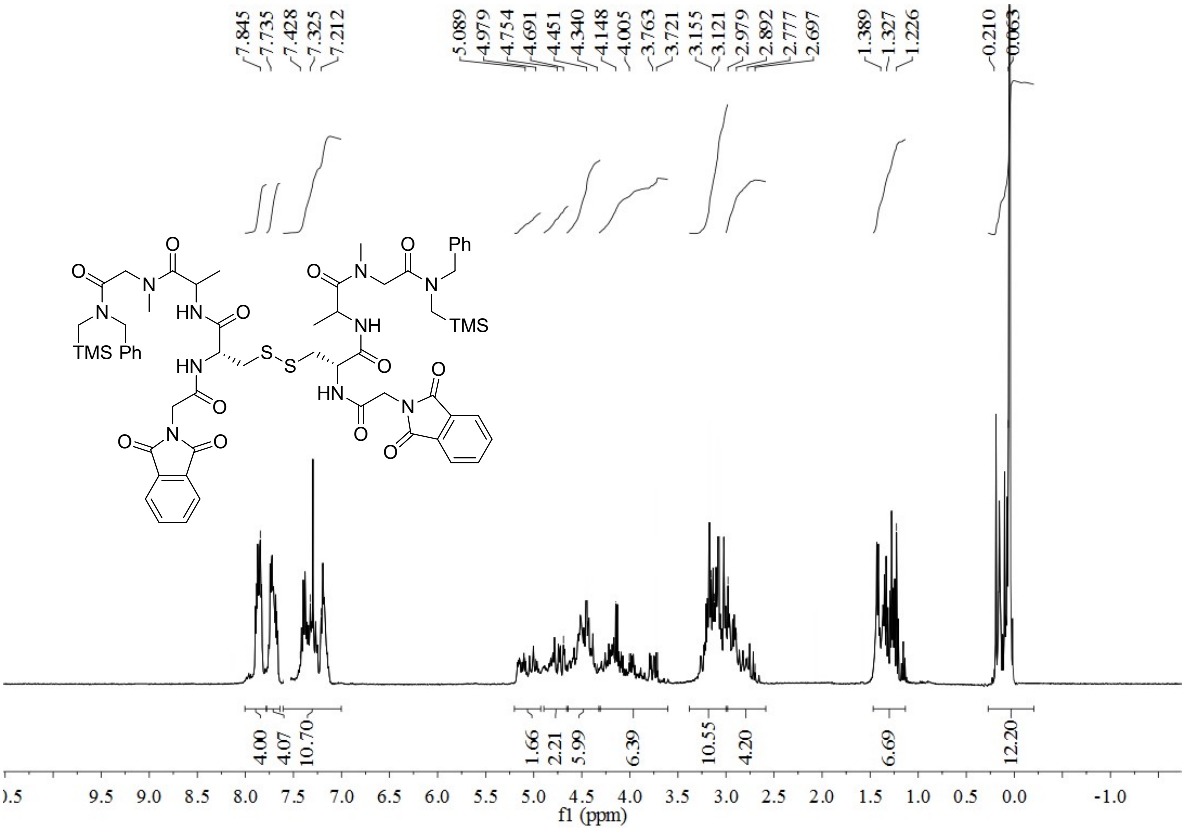


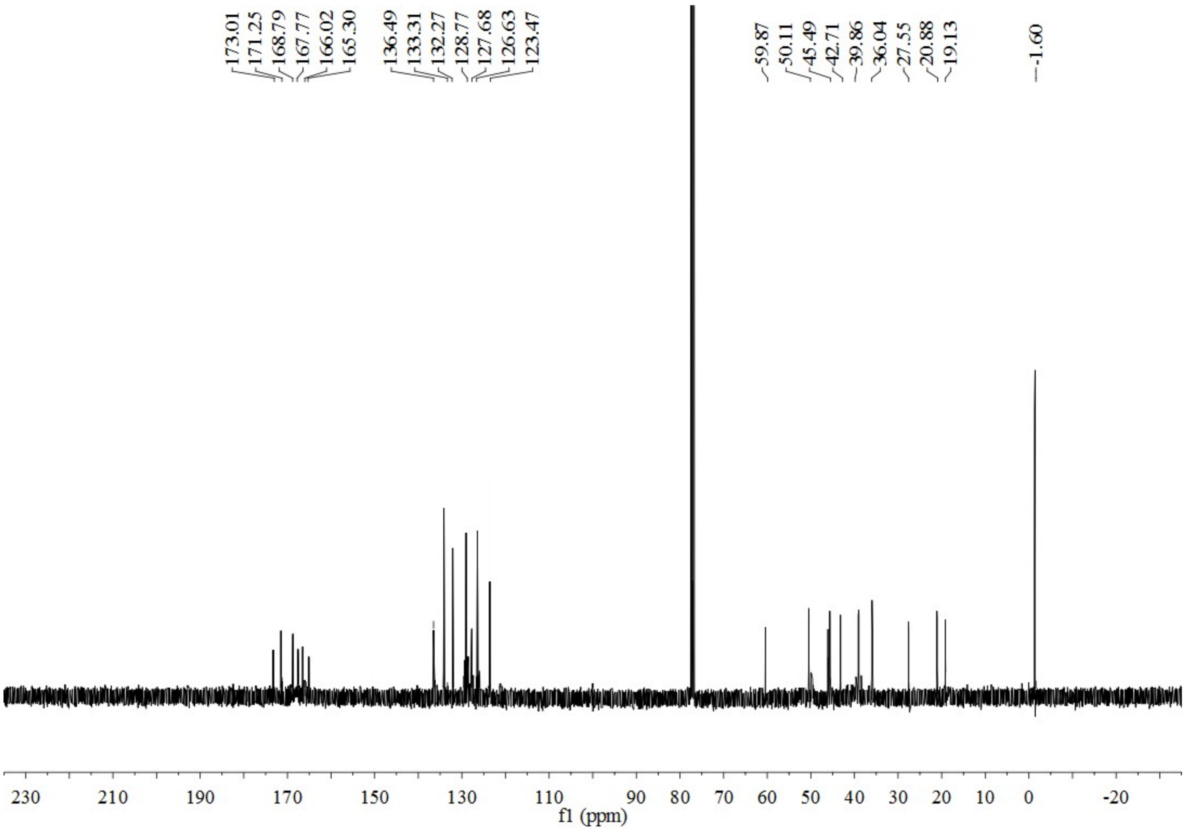
171.139
169.622
168.972
167.777
166.985
166.488
136.255
134.170
132.012
128.887
128.645
127.840
126.317
123.464
99.906
53.535
52.645
49.767
49.540
40.232
38.947
36.467
35.743
31.280
29.683
27.585
f1 (ppm)

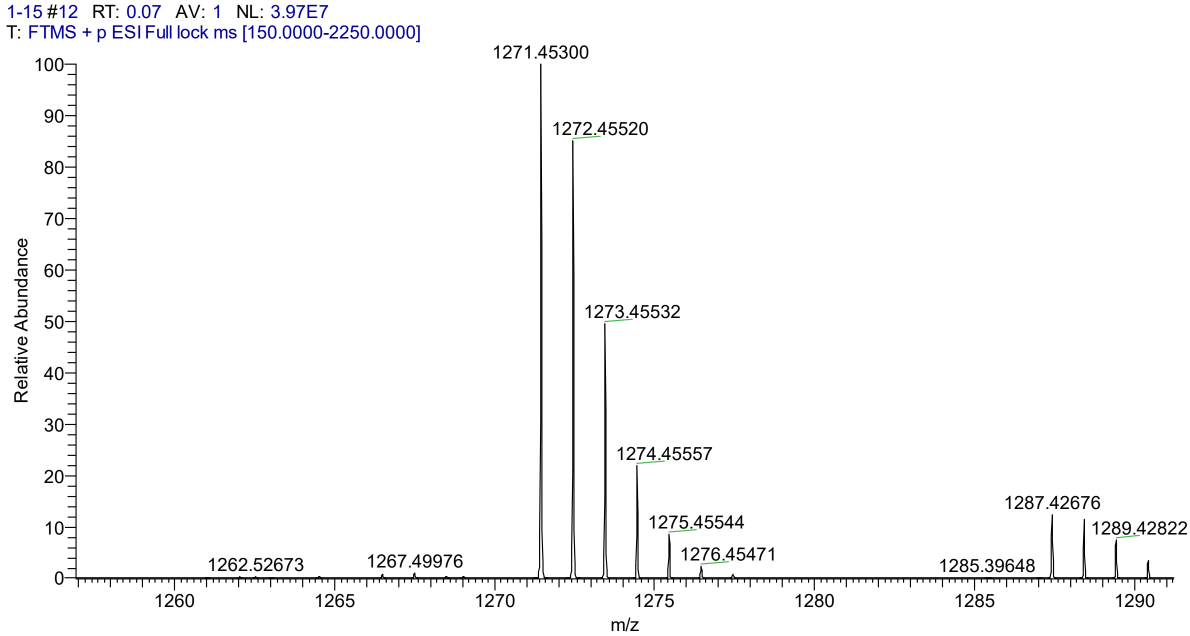


1-44 #52 RT: 0.28 AV: 1 NL: 1.56E5
T: FTMS + p ESI Full lock ms [150.0000-2250.0000]
Relative Abundance
m/z
1269.44678
1270.44995
1268.80261
1270.83386
1264.81787
1266.15588
1267.43286
1268.16016
1271.82910
1273.82910
1276.16431
1272.44092
1275.83789

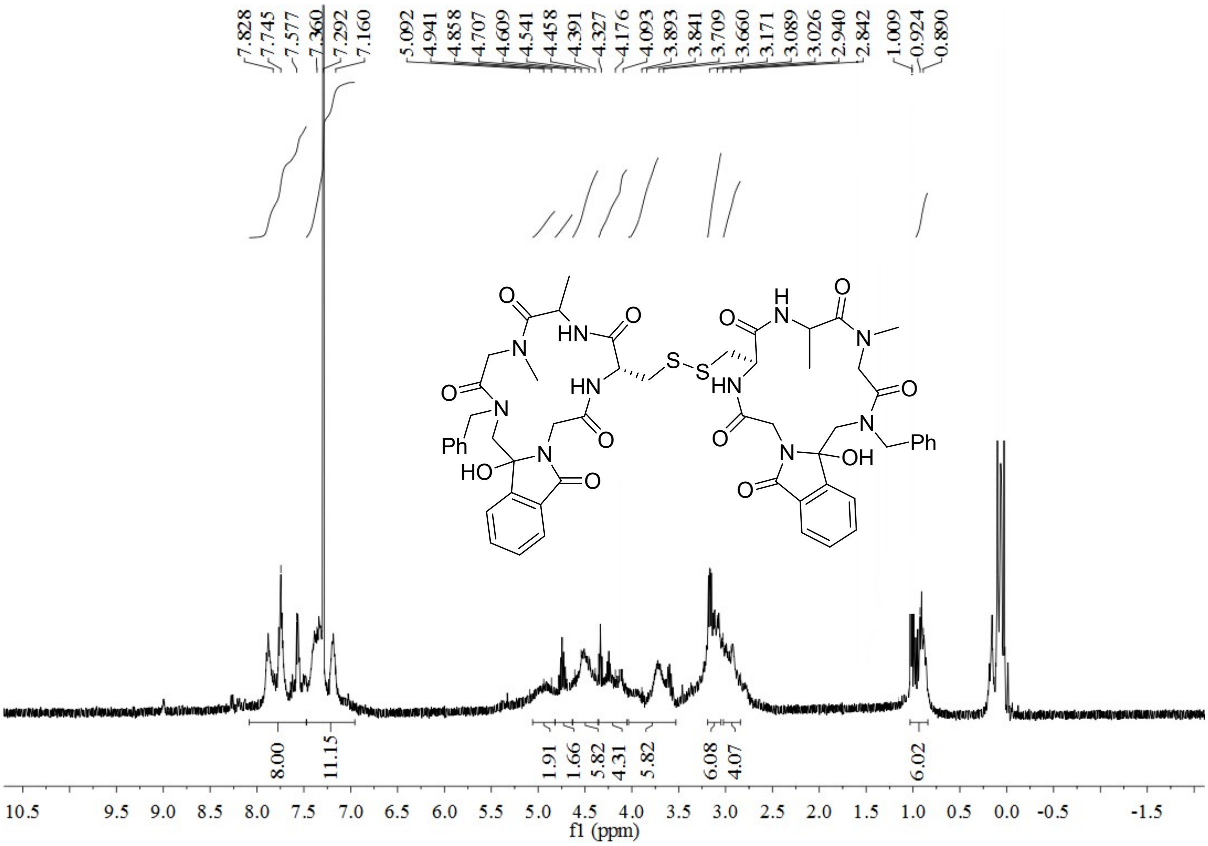
(7) [1]H, [13]C-NMR and HRMS of **3d.**

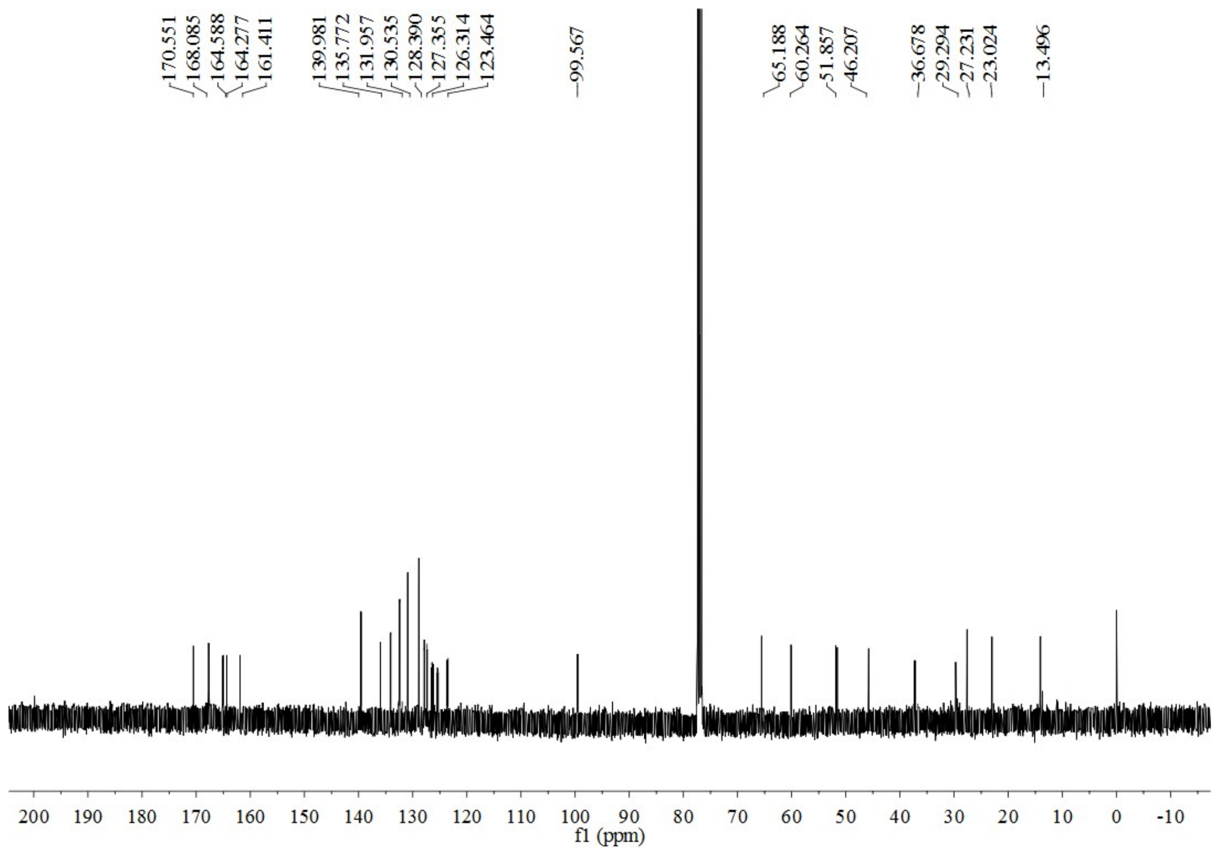


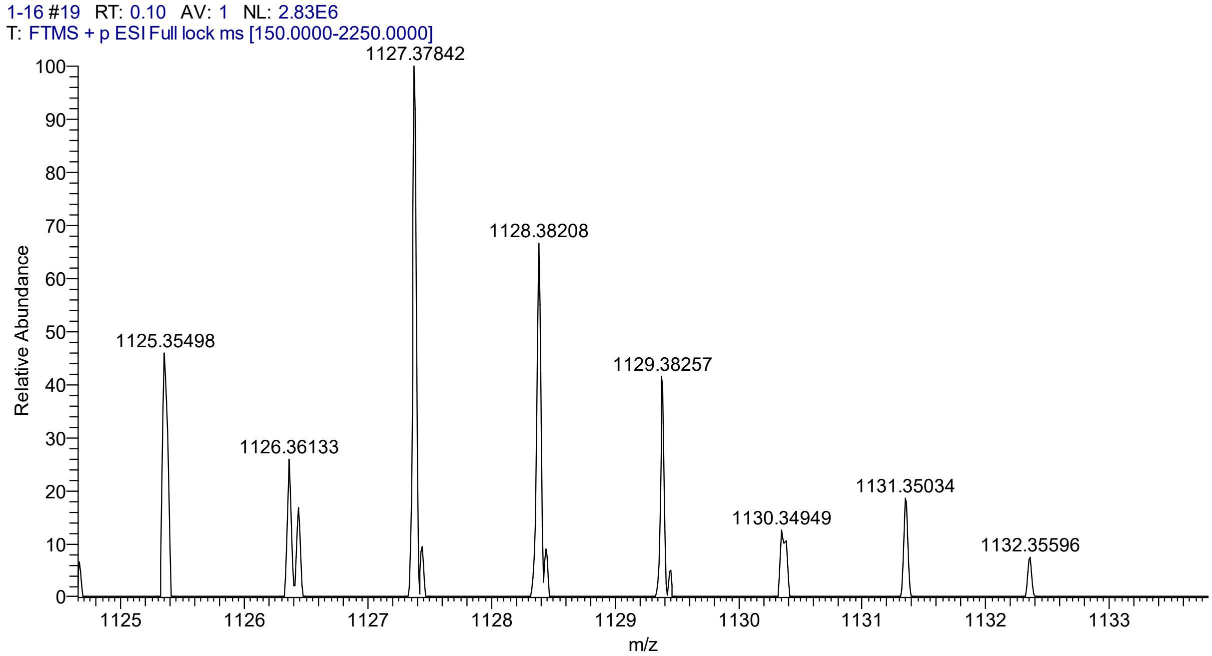




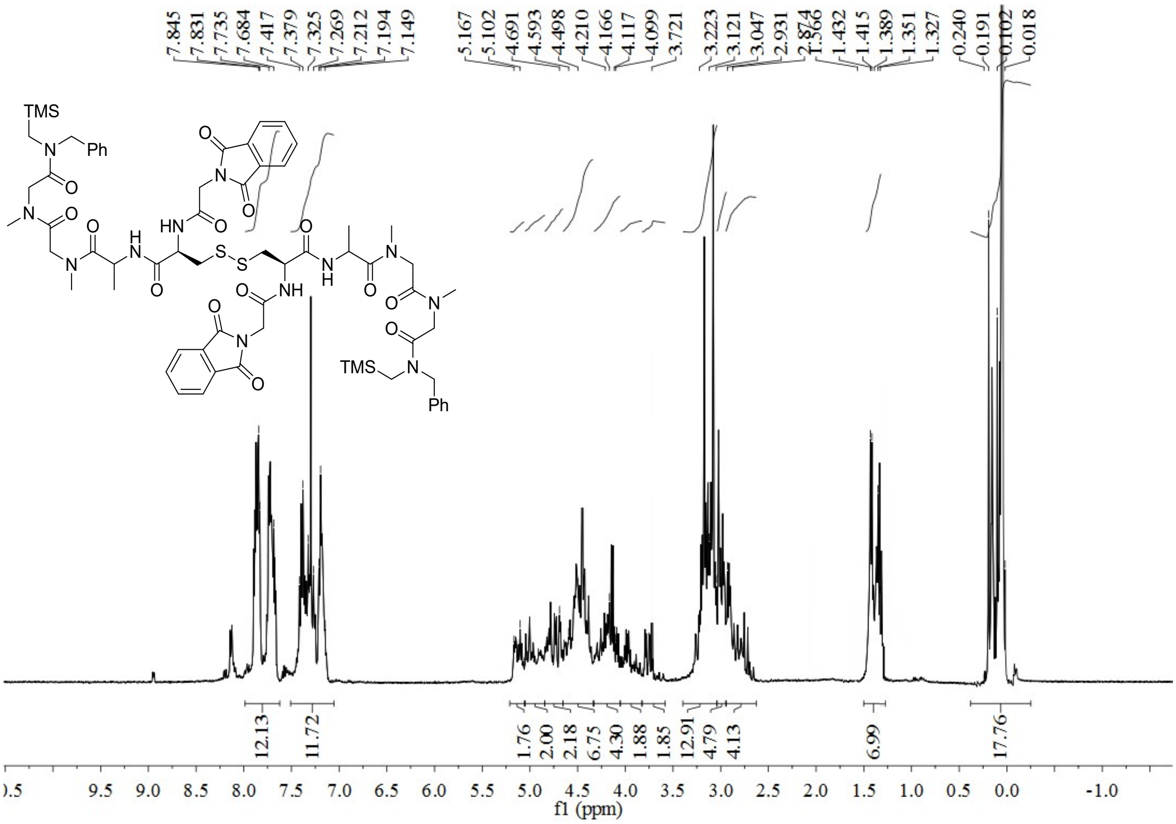
(8) ^{1}H, ^{13}C-NMR and HRMS of **4d.**

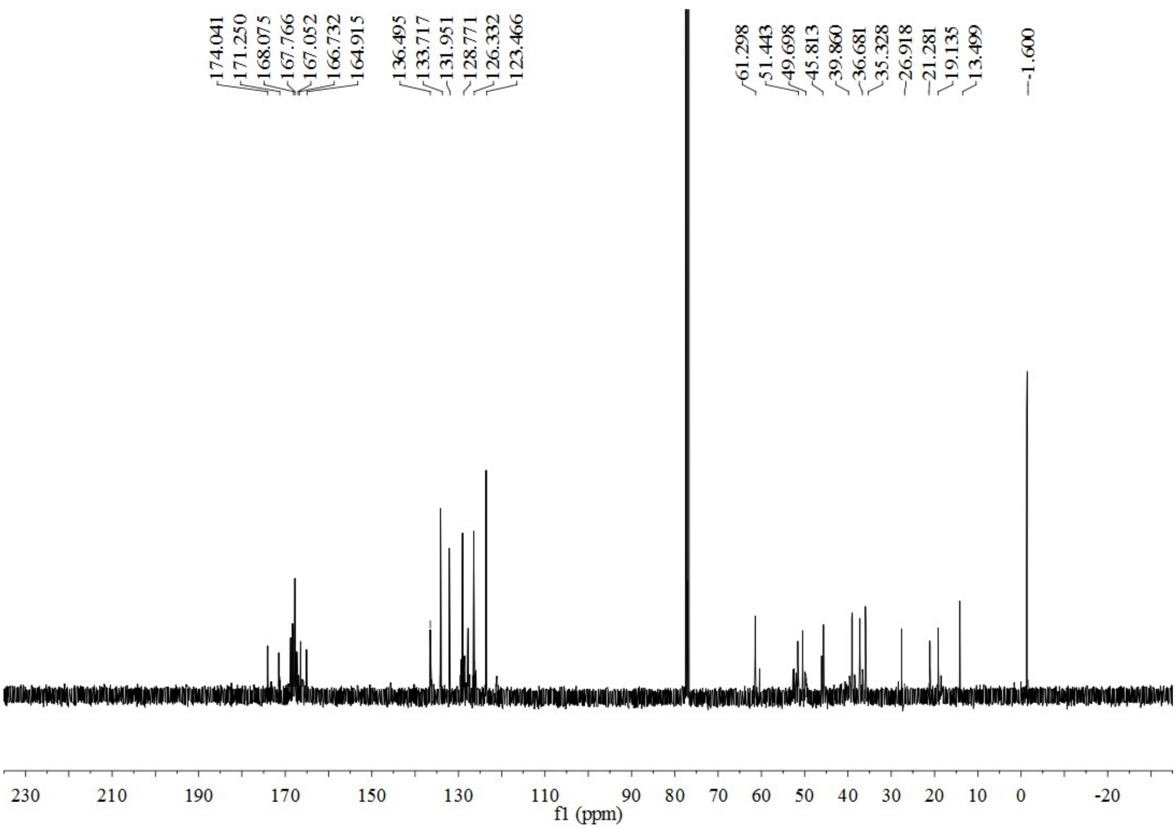


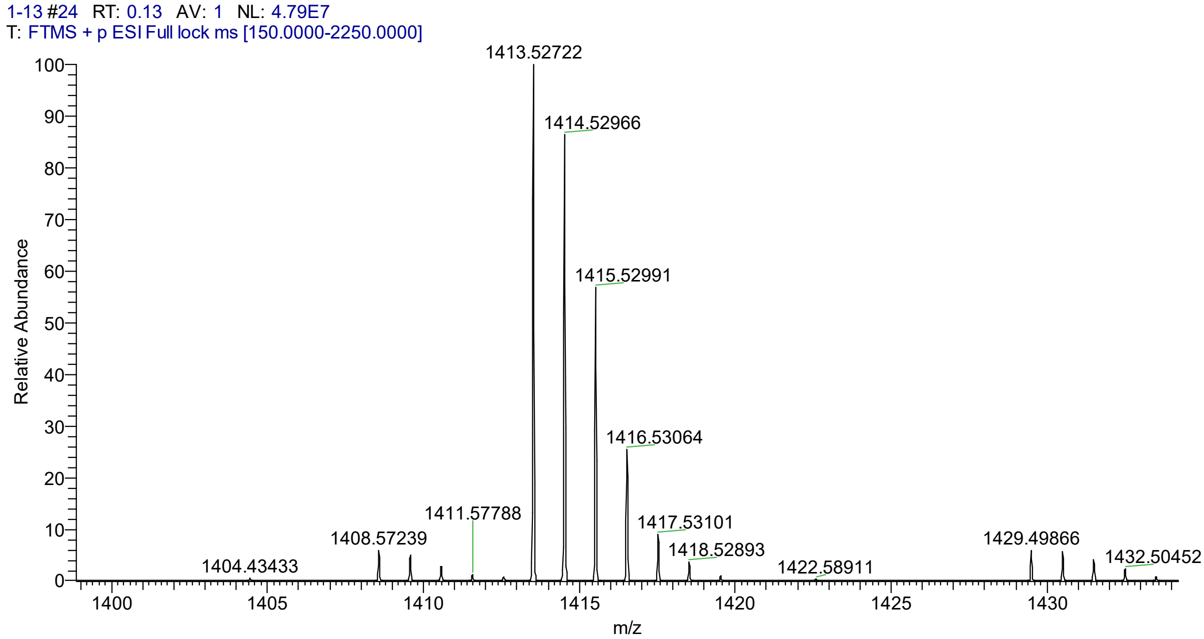

170.551
168.085
164.588
164.277
161.411
139.981
135.772
131.957
130.535
128.390
127.355
126.314
123.464
99.567
65.188
60.264
51.857
46.207
36.678
29.294
27.231
23.024
13.496
f1 (ppm)


1-16 #19 RT: 0.10 AV: 1 NL: 2.83E6
T: FTMS + p ESI Full lock ms [150.0000-2250.0000]
1127.37842
1128.38208
1125.35498
1129.38257
1126.36133
1131.35034
1130.34949
1132.35596
Relative Abundance
m/z

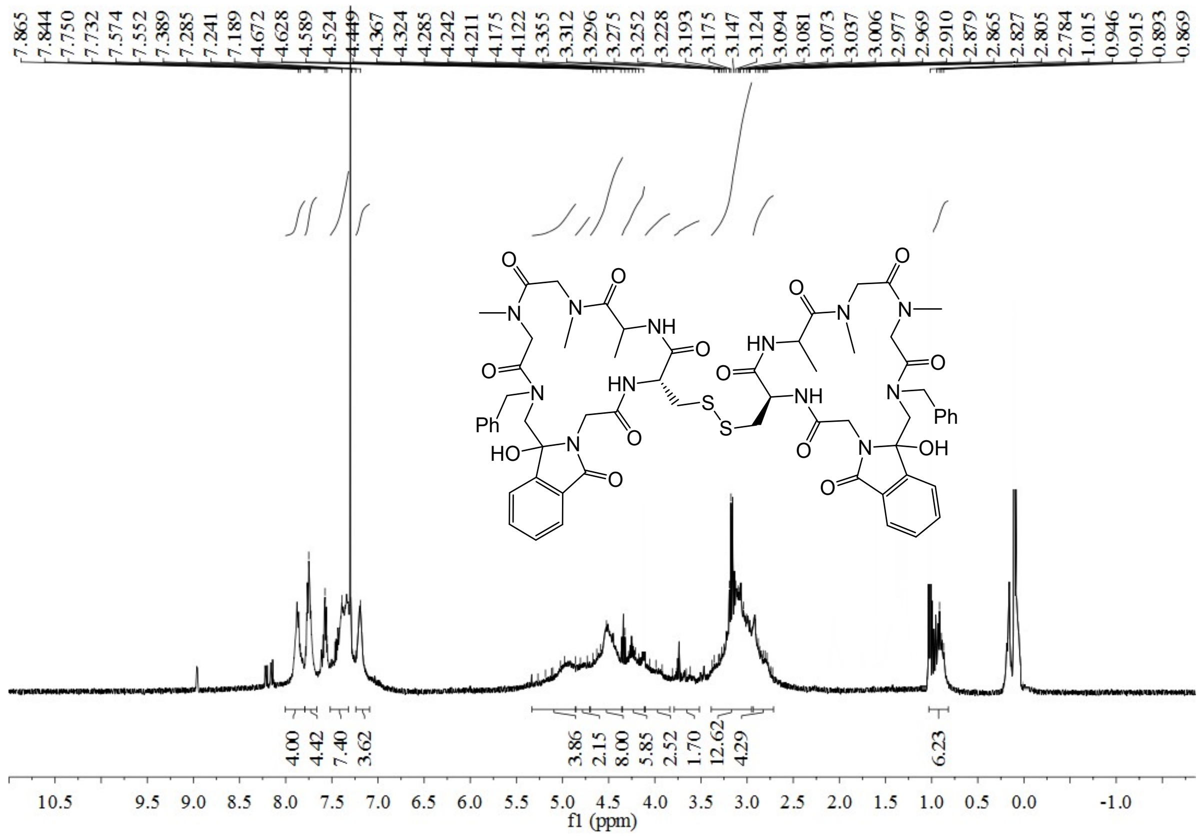
(9) ^{1}H, ^{13}C-NMR and HRMS of **3e.**

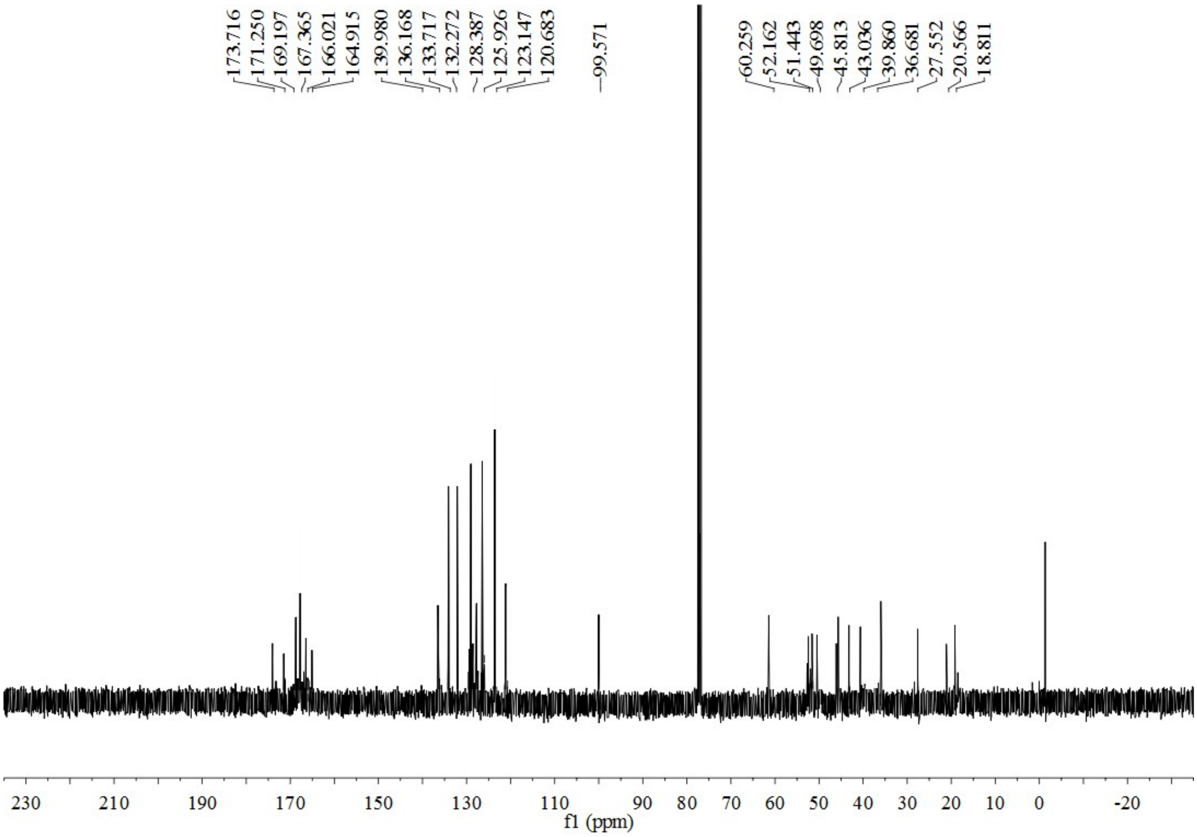


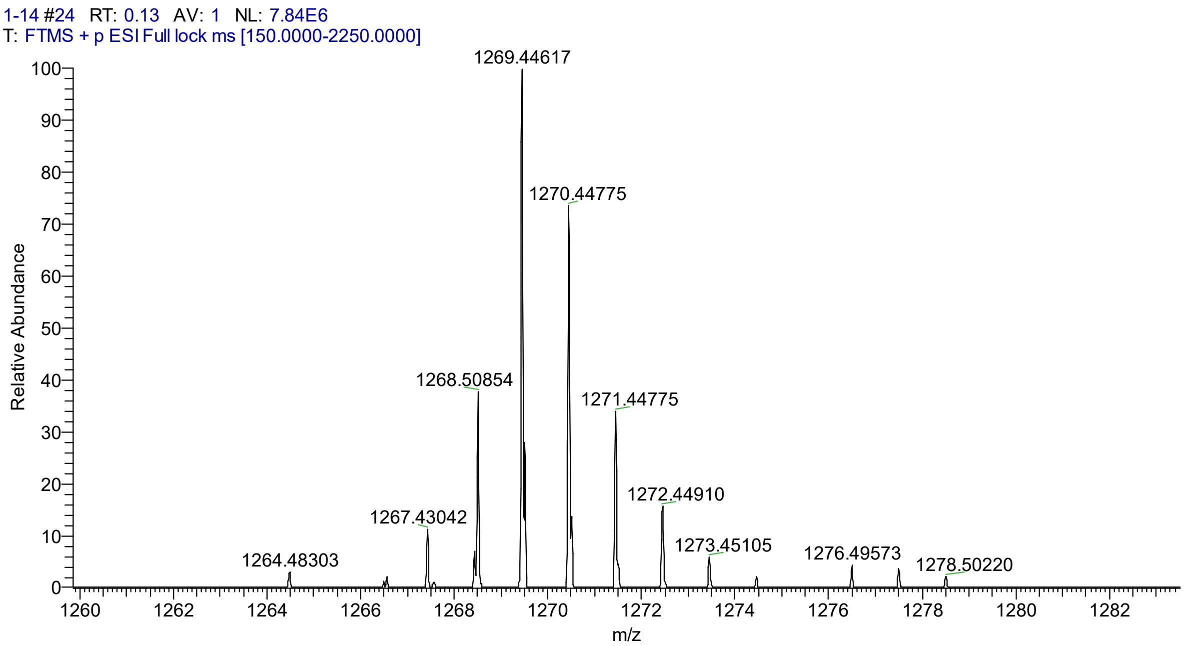




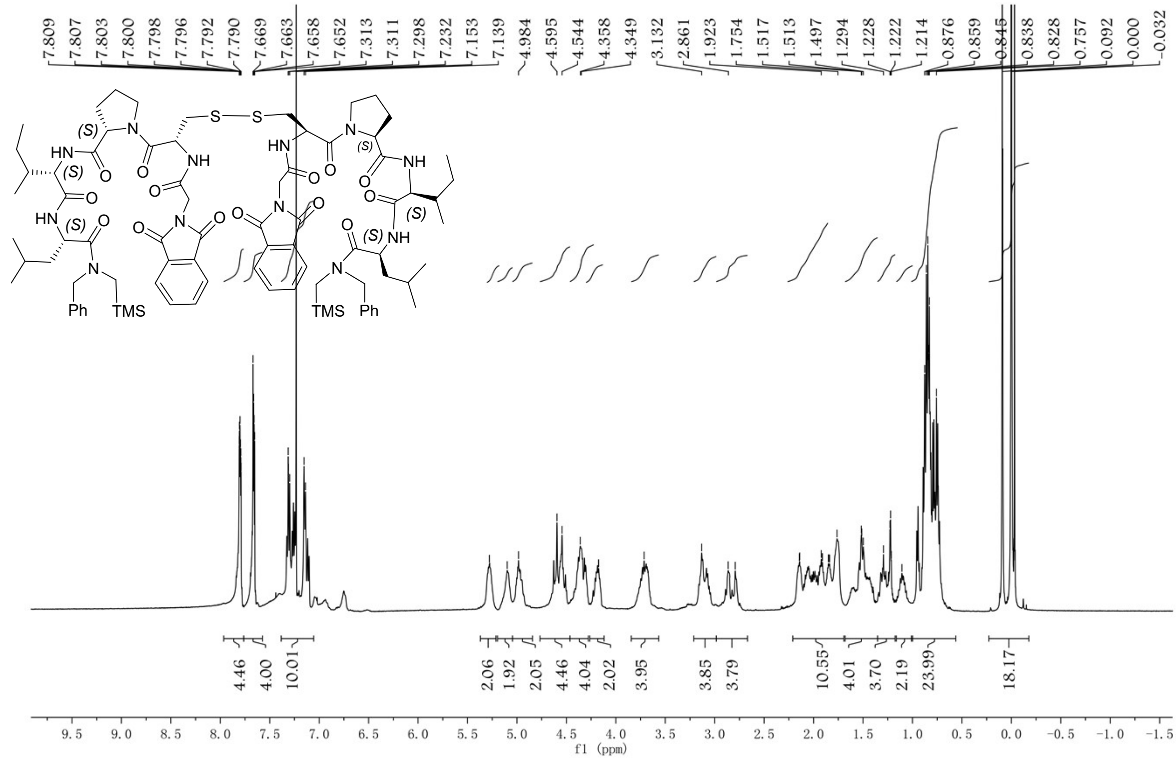
(10) ^{1}H, ^{13}C-NMR and HRMS of **4e.**

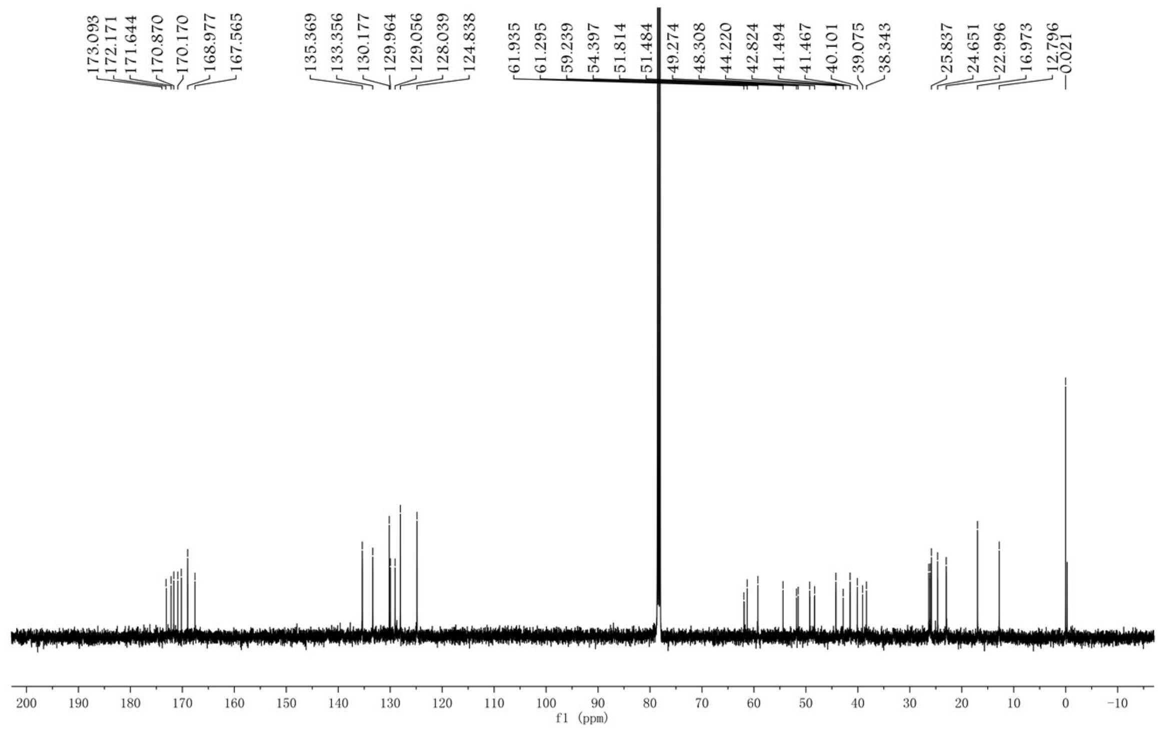


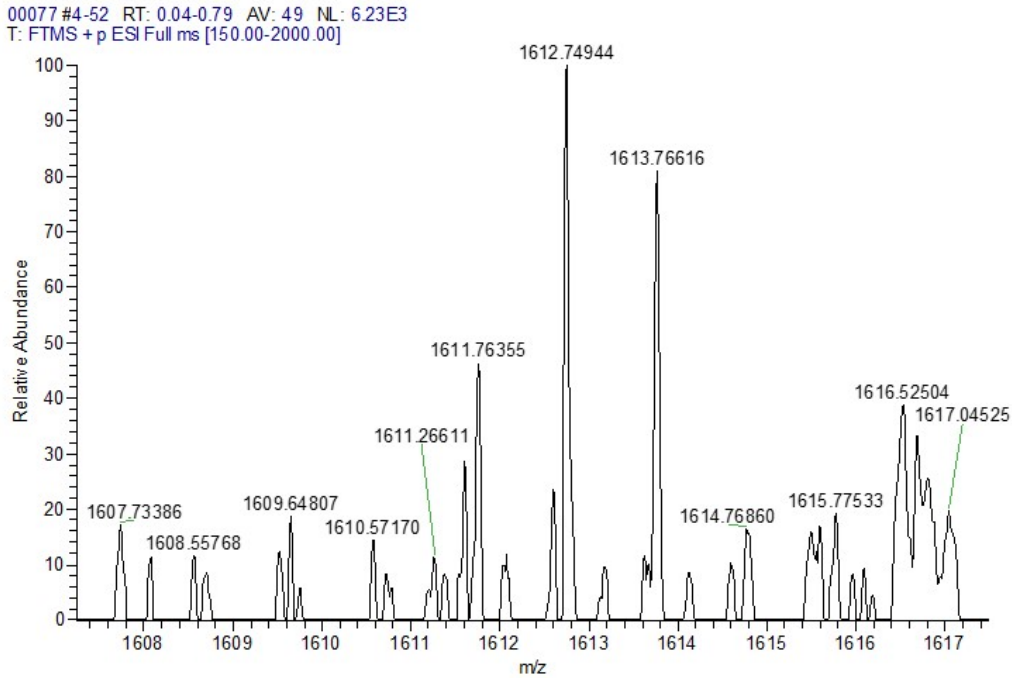

173.716
171.250
169.197
167.365
166.021
164.915
139.980
136.168
133.717
132.272
128.387
125.926
123.147
120.683
99.571
60.259
52.162
51.443
49.698
45.813
43.036
39.860
36.681
27.552
20.566
18.811
230
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-20
f1 (ppm)


1-14 #24 RT: 0.13 AV: 1 NL: 7.84E6
T: FTMS + p ESI Full lock ms [150.0000-2250.0000]
1269.44617
1270.44775
1268.50854
1271.44775
1272.44910
1267.43042
1273.45105
1276.49573
1264.48303
1278.50220
Relative Abundance
m/z

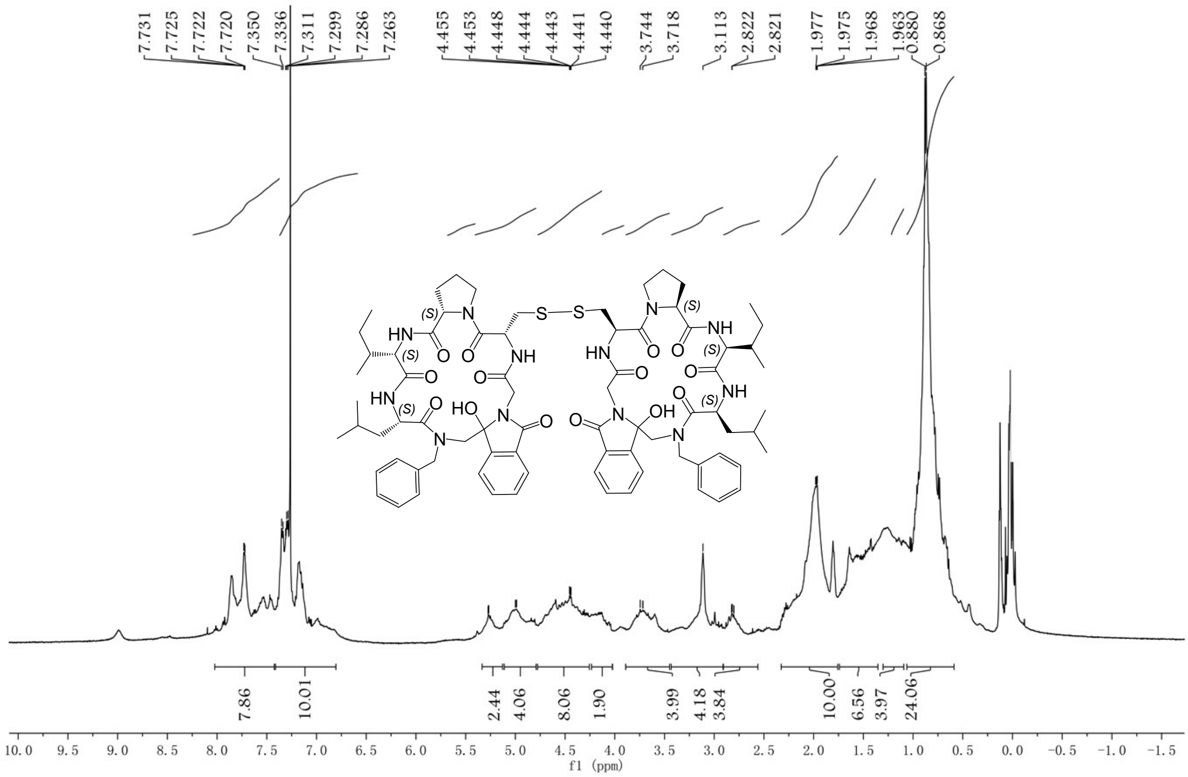
(11) ^{1}H, ^{13}C-NMR and HRMS of **3f.**

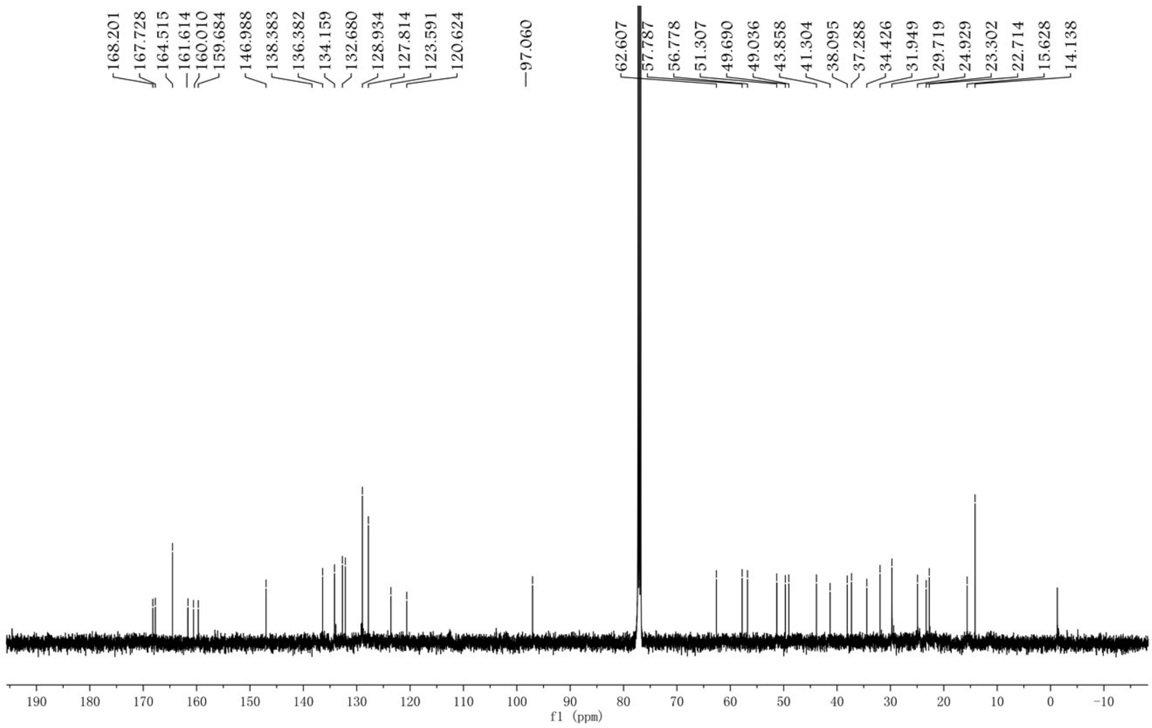


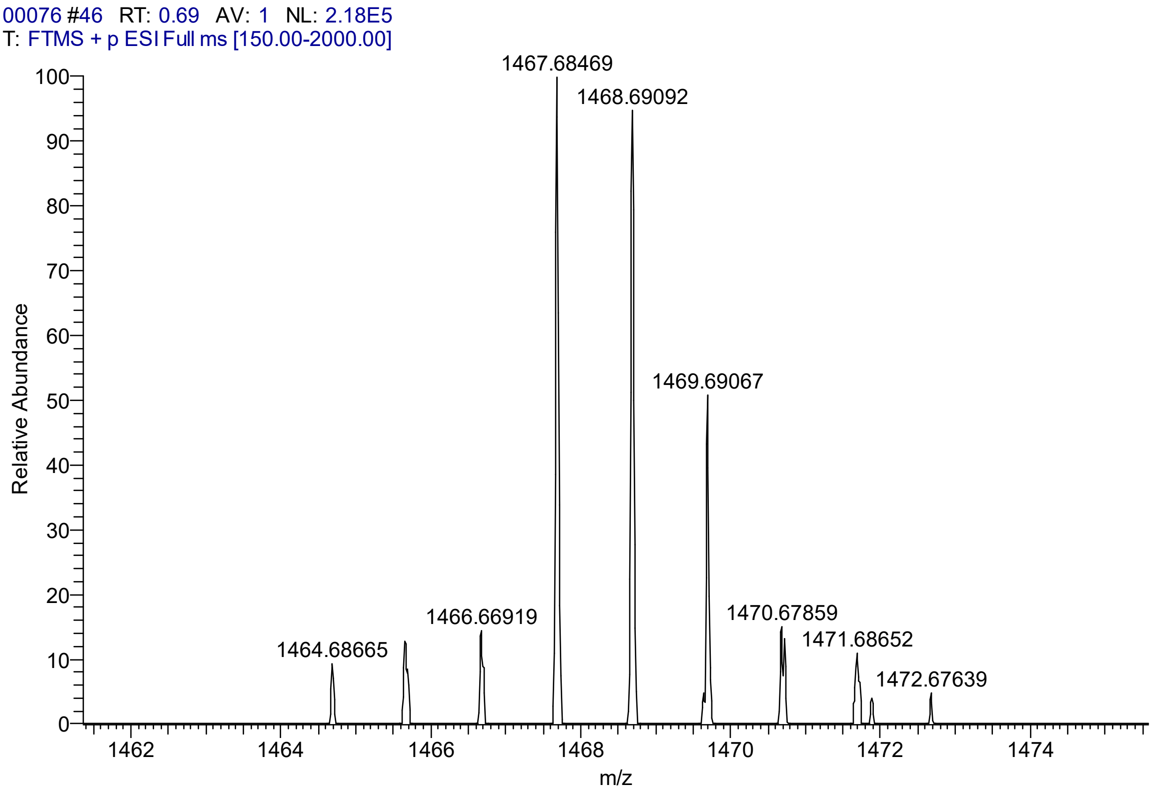




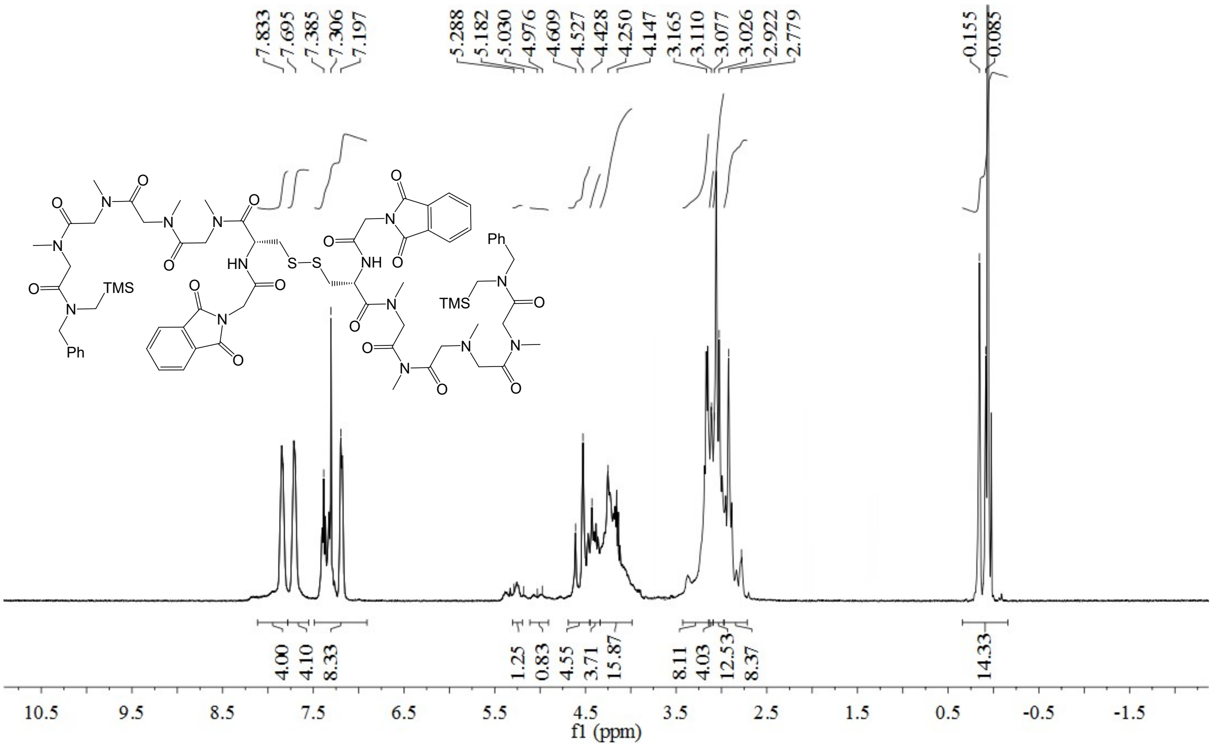
(12) ^{1}H, ^{13}C-NMR and HRMS of **4f.**

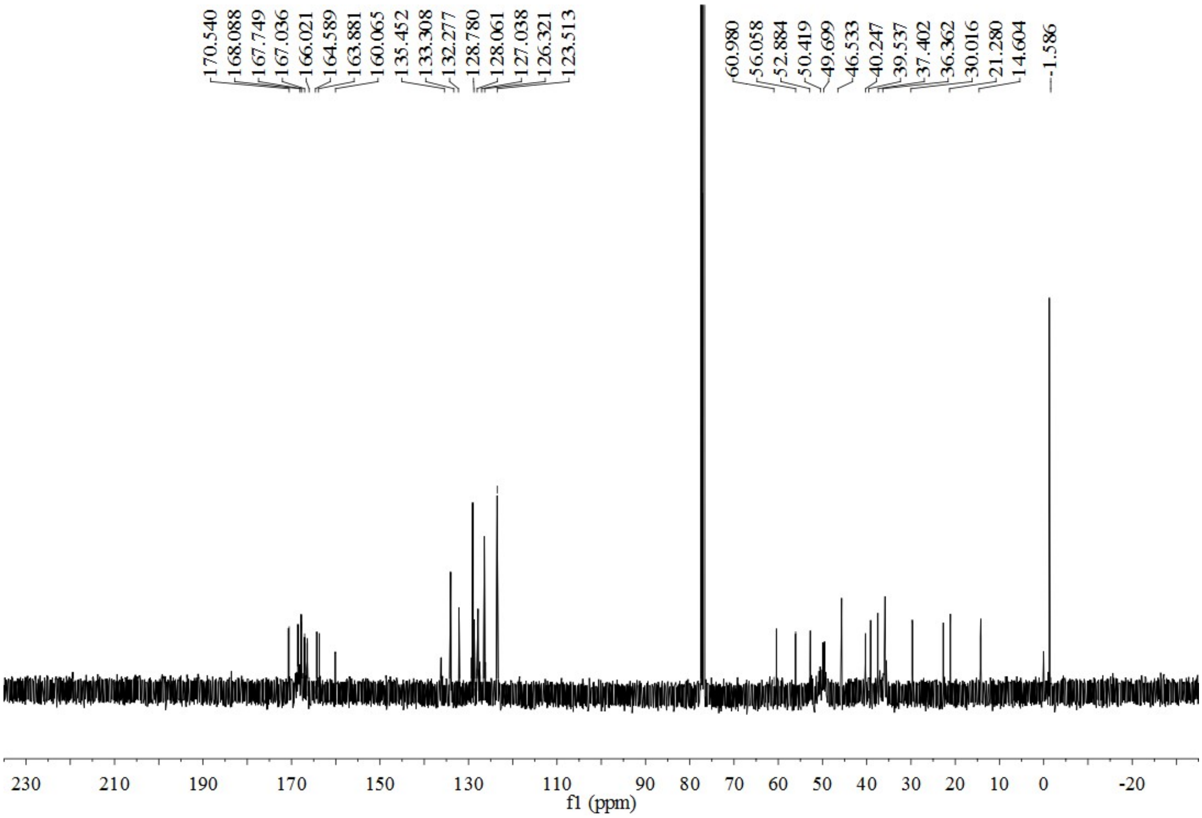


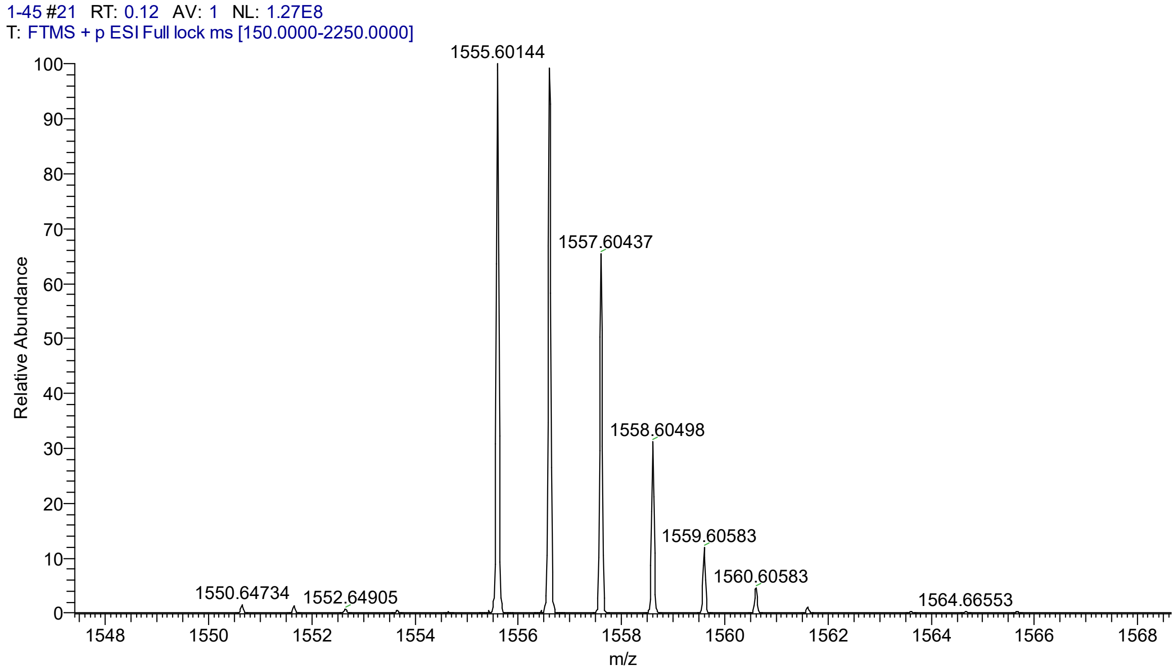

168.201
167.728
164.515
161.614
160.010
159.684
146.988
138.383
136.382
134.159
132.680
128.934
127.814
123.591
120.624
97.060
62.607
57.787
56.778
51.307
49.690
49.036
43.858
41.304
38.095
37.288
34.426
31.949
29.719
24.929
23.302
22.714
15.628
14.138
f1 (ppm)


00076 #46 RT: 0.69 AV: 1 NL: 2.18E5
T: FTMS + p ESI Full ms [150.00-2000.00]
1467.68469
1468.69092
1469.69067
1464.68665
1466.66919
1470.67859
1471.68652
1472.67639
Relative Abundance
m/z

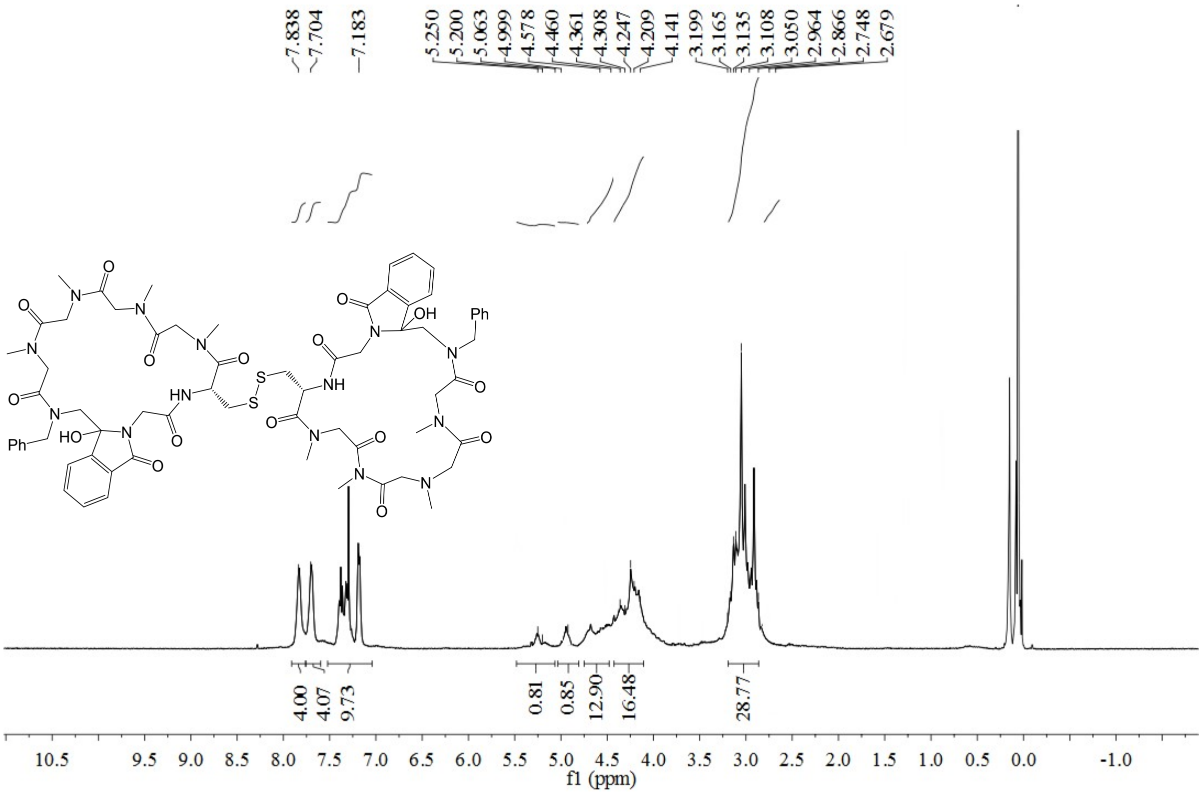
(13) [1]H, [13]C-NMR and HRMS of **3g.**

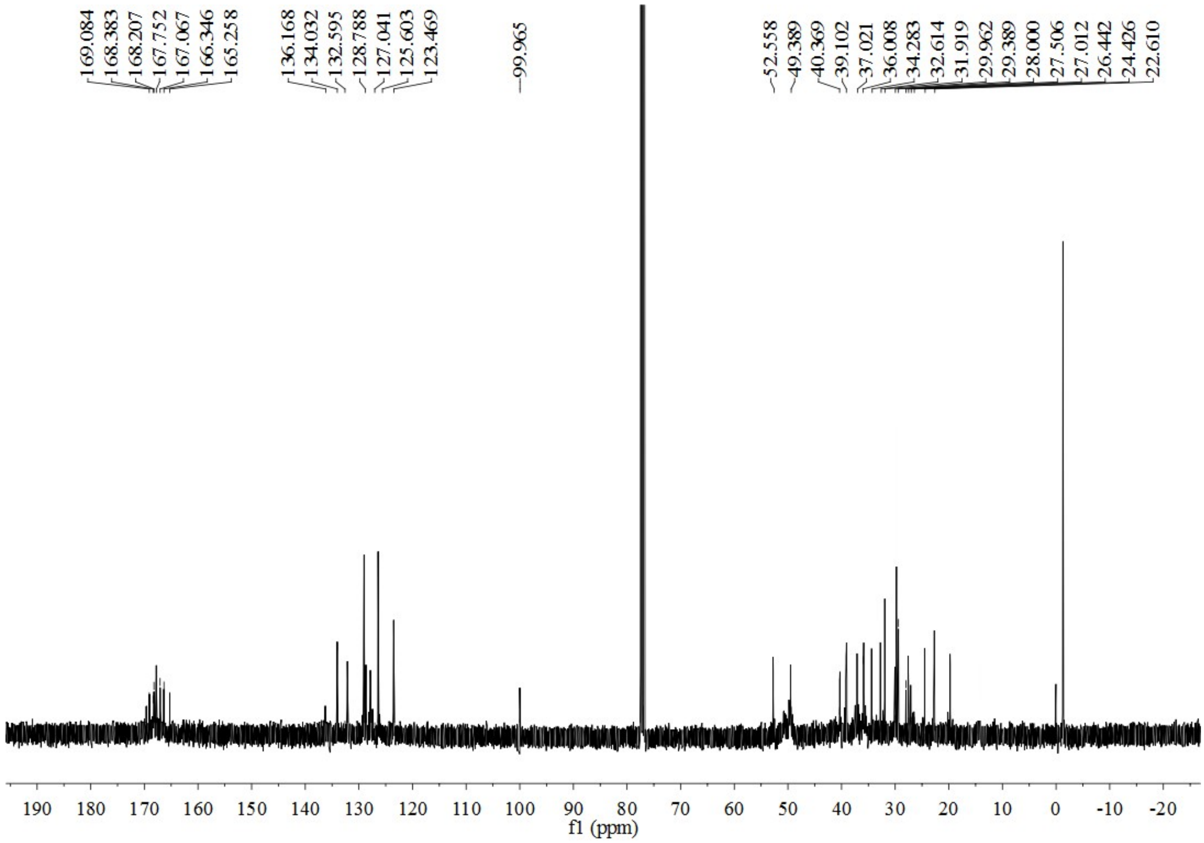


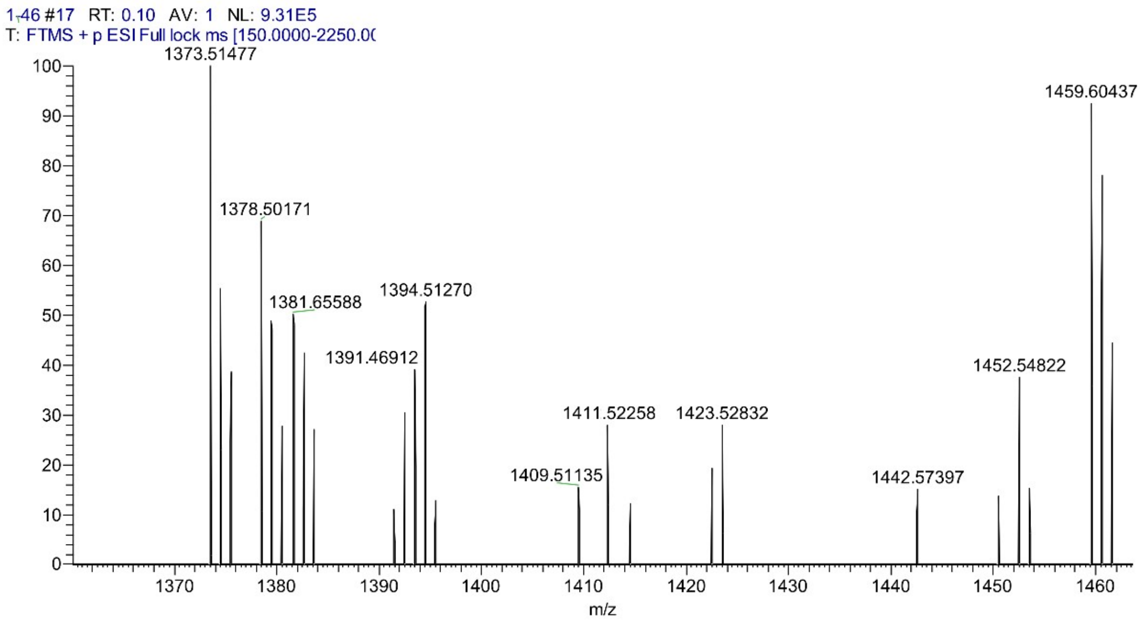




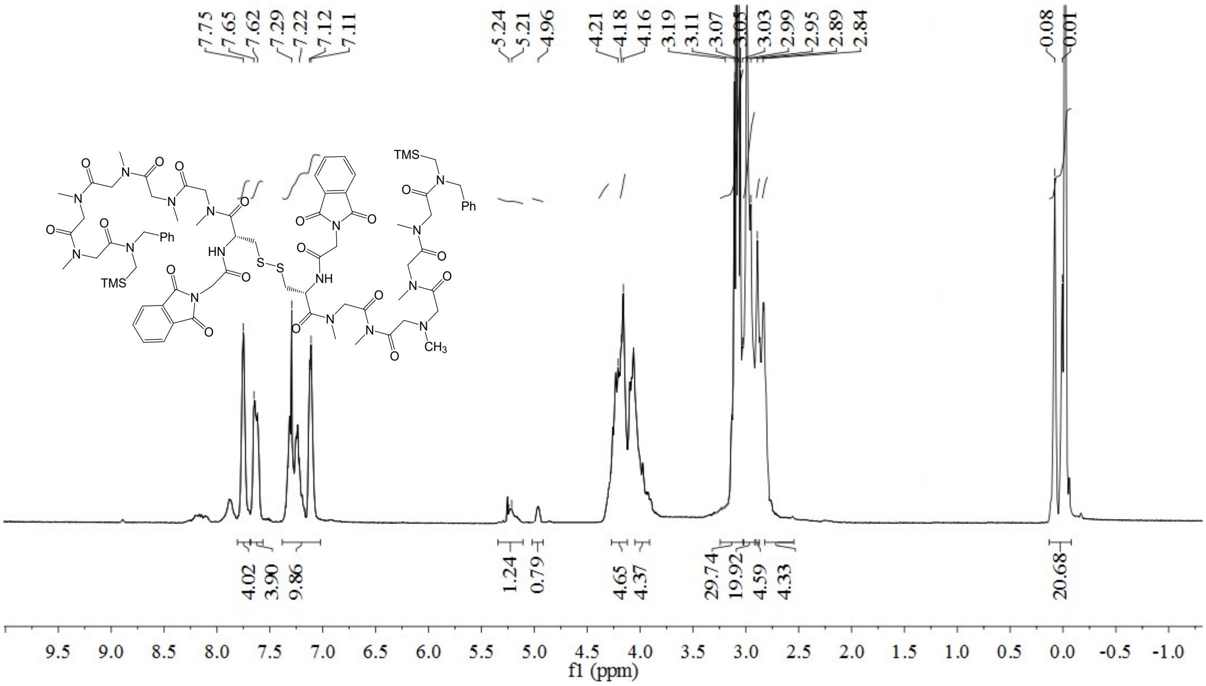
(14) ^{1}H, ^{13}C-NMR and HRMS of **4g.**

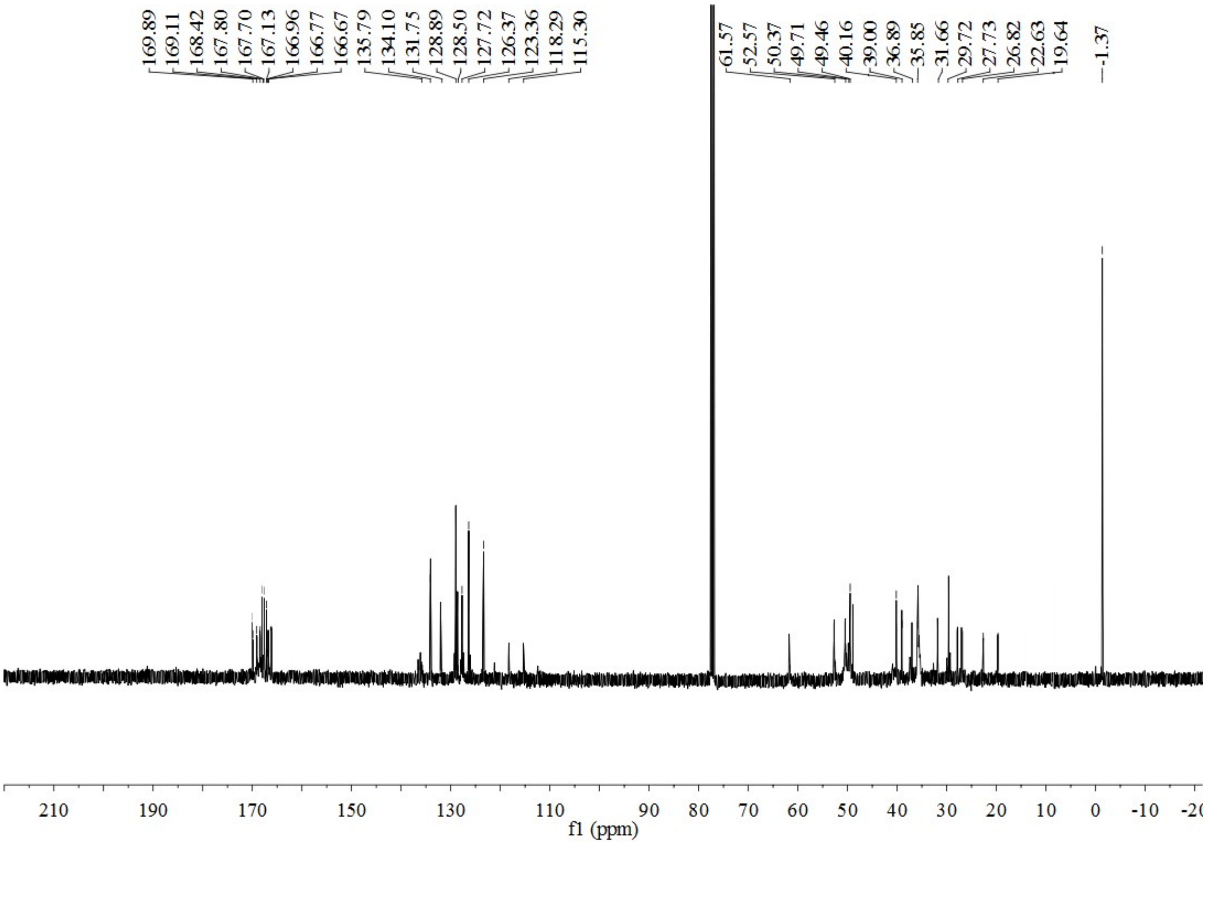


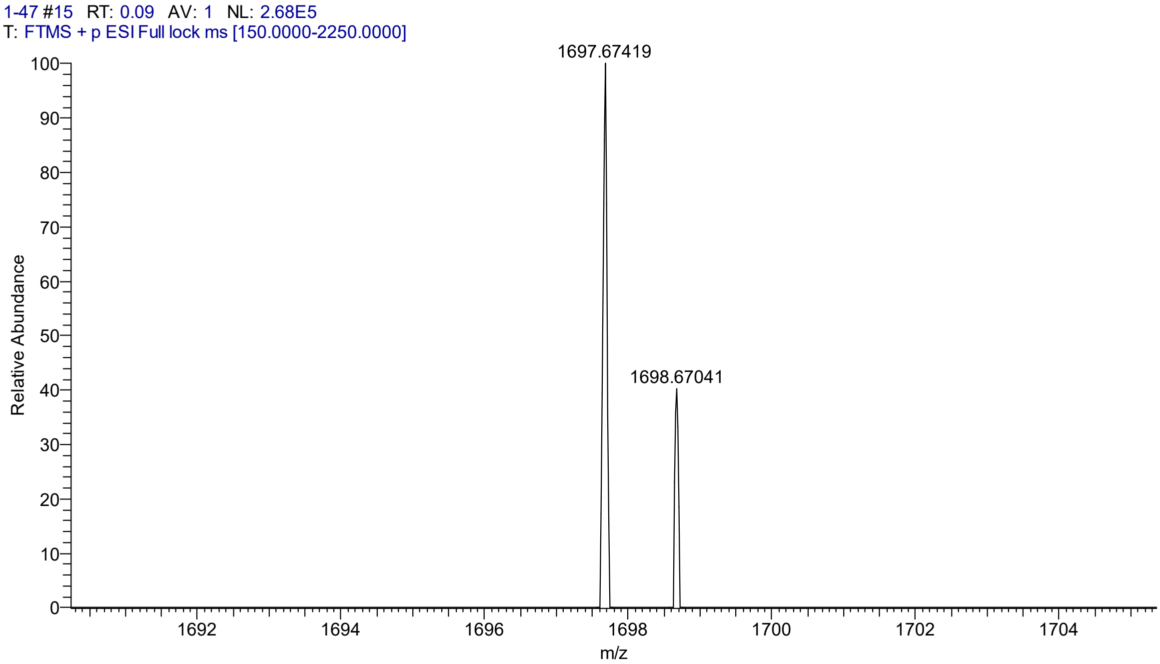

169.084
168.383
168.207
167.752
167.067
166.346
165.258
136.168
134.032
132.595
128.788
127.041
125.603
123.469
99.965
52.558
49.389
40.369
39.102
37.021
36.008
34.283
32.614
31.919
29.962
29.389
28.000
27.506
27.012
26.442
24.426
22.610
f1 (ppm)


1-46 #17 RT: 0.10 AV: 1 NL: 9.31E5
T: FTMS + p ESI Full lock ms [150.0000-2250.00
1373.51477
1459.60437
1378.50171
1381.65588
1394.51270
1391.46912
1452.54822
1411.52258
1423.52832
1409.51135
1442.57397
m/z

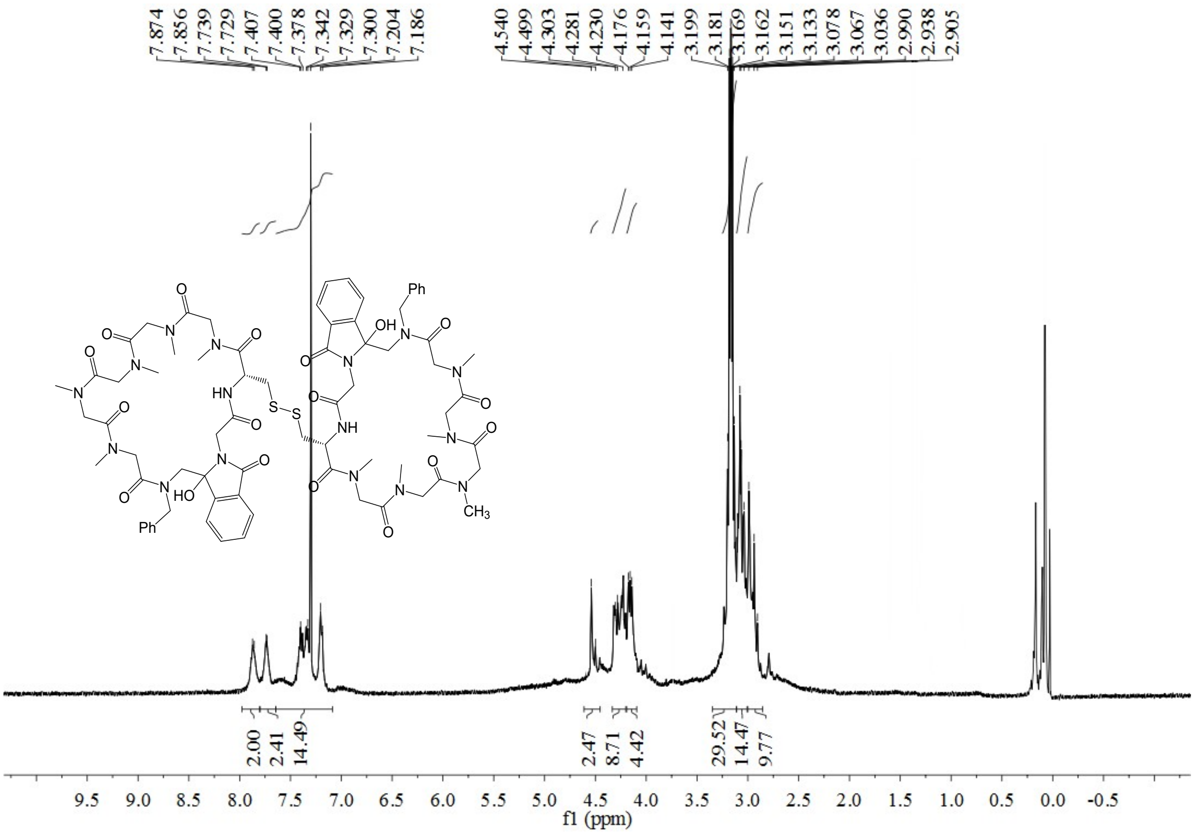
(15) ^{1}H, ^{13}C-NMR and HRMS of **3h.**

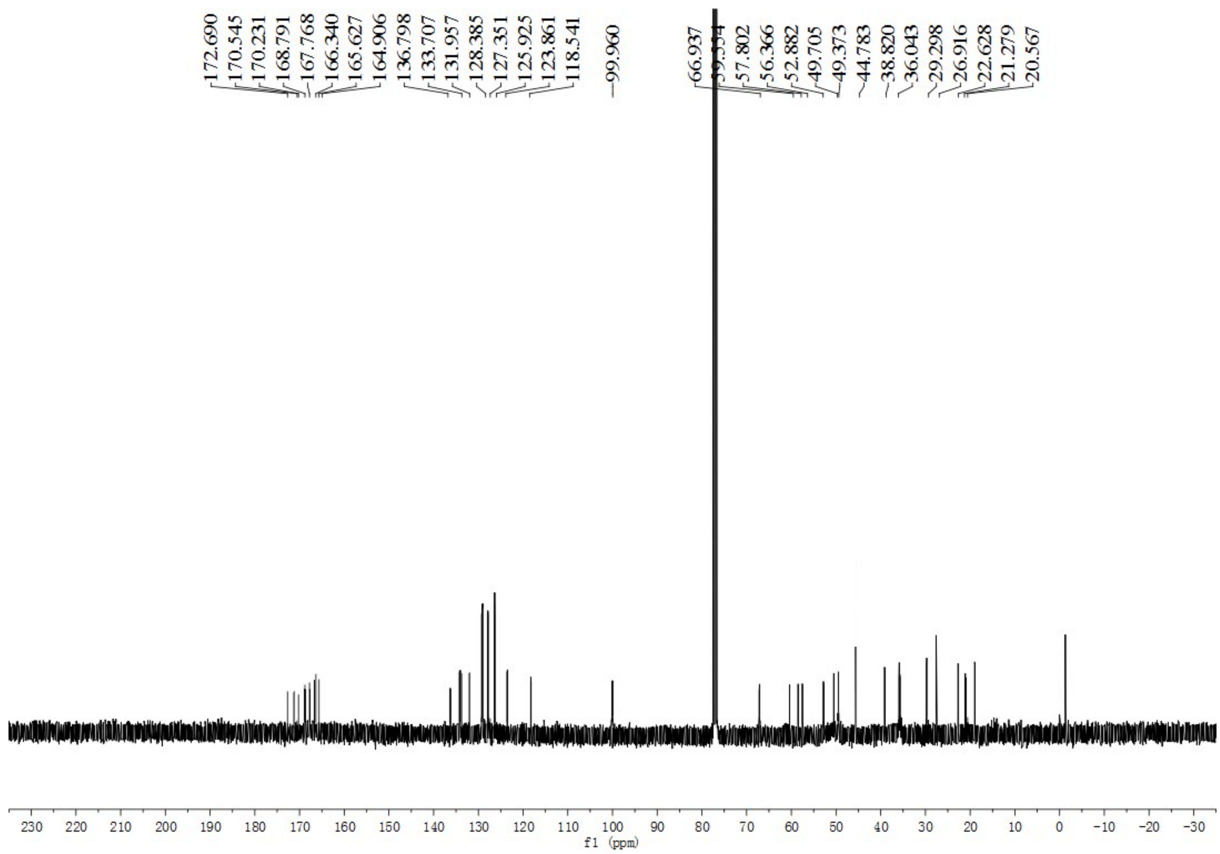


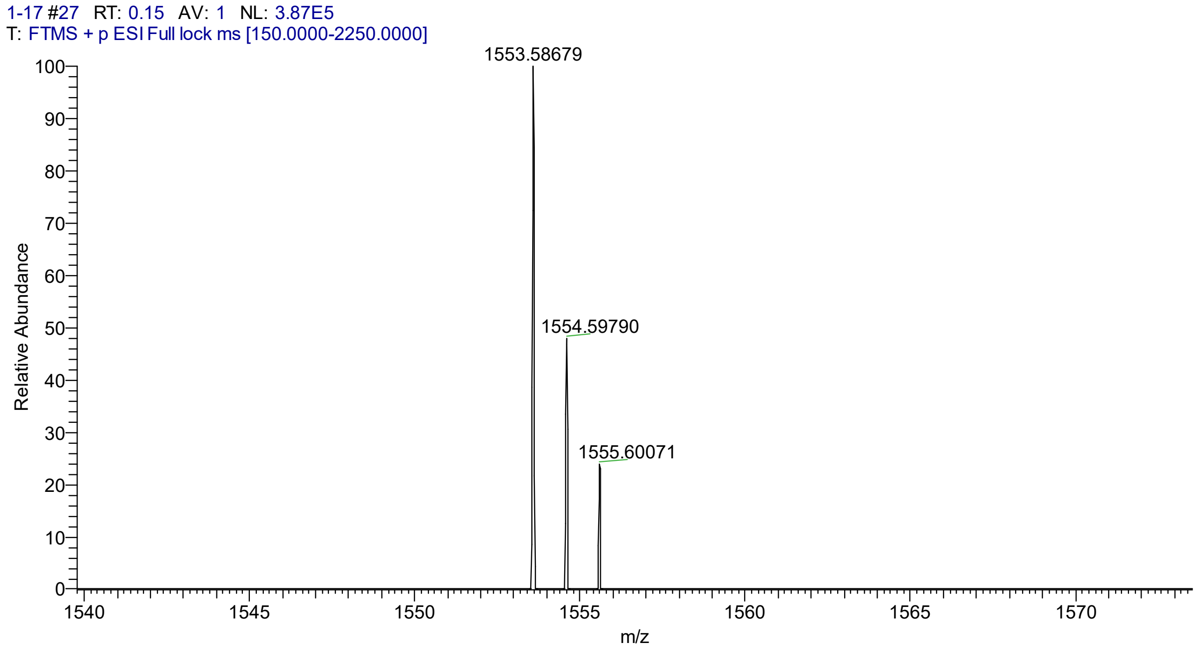




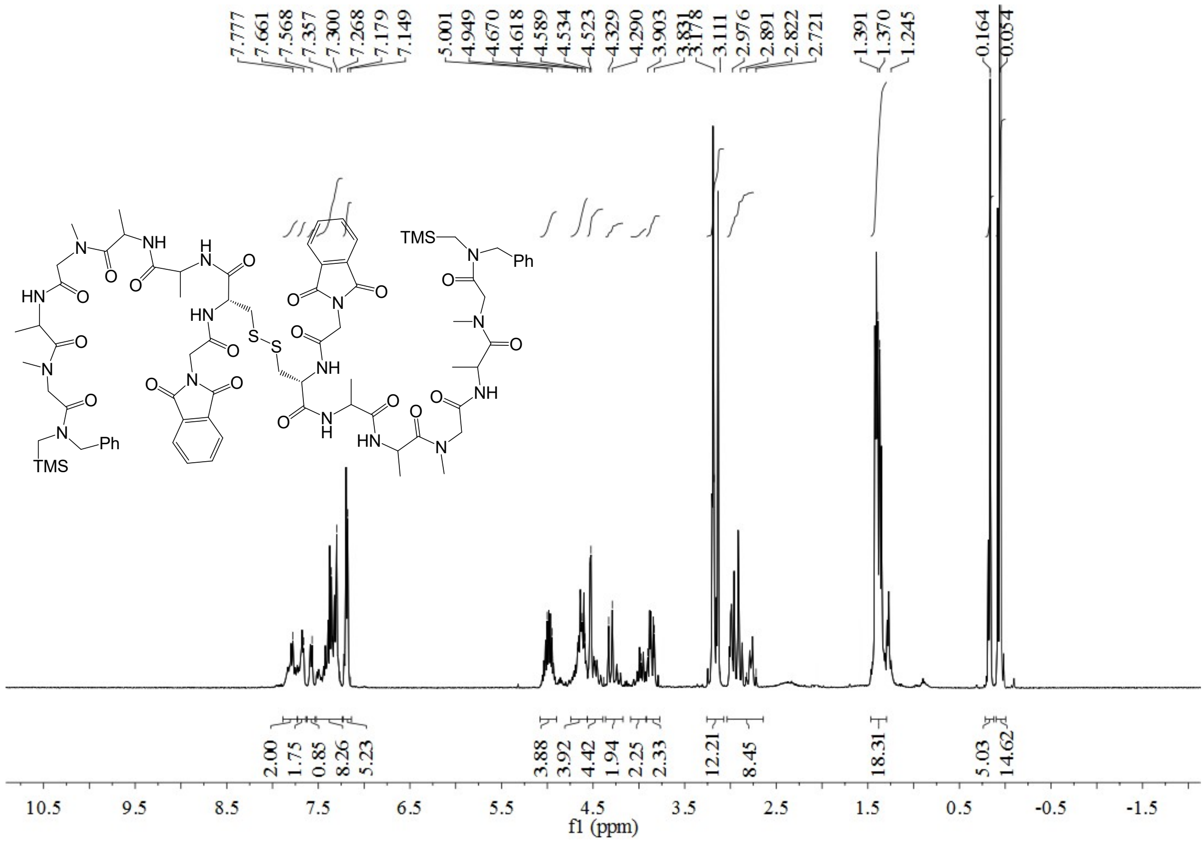
(16) ^{1}H, ^{13}C-NMR and HRMS of **4h.**

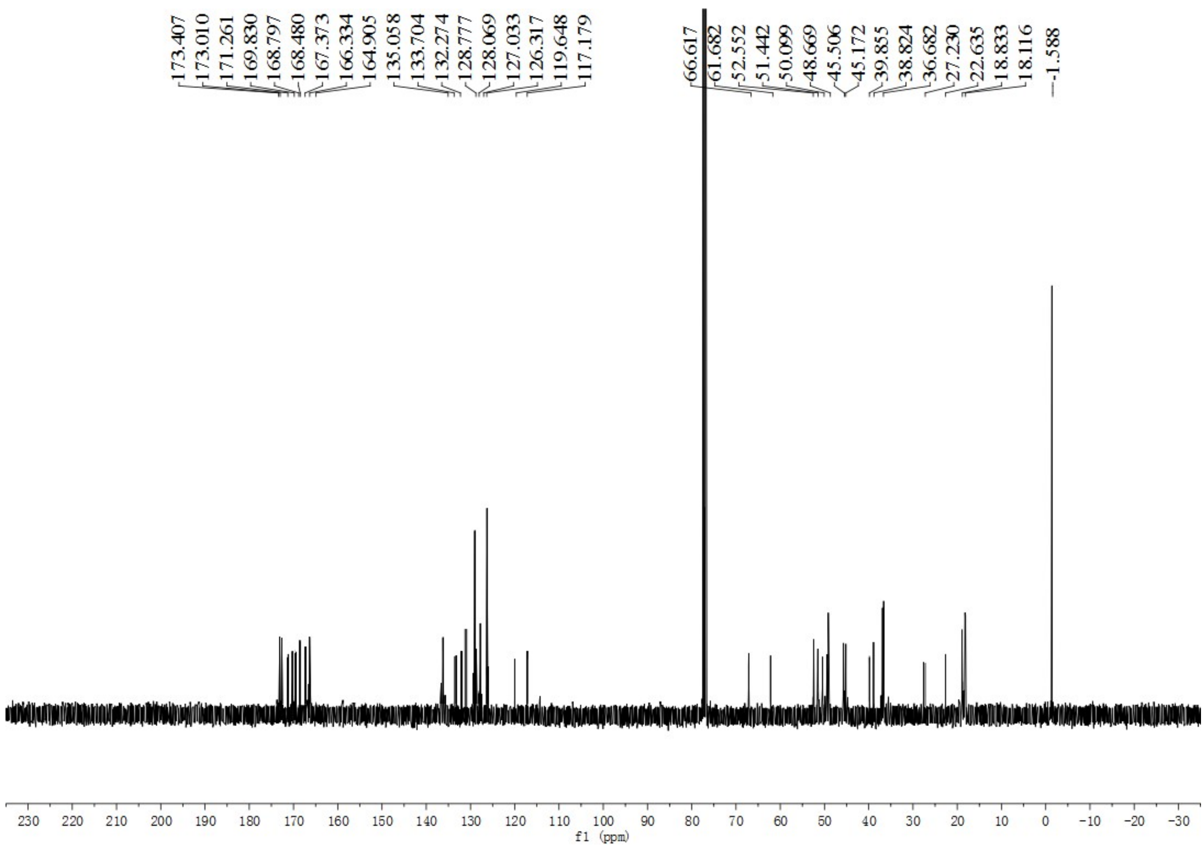


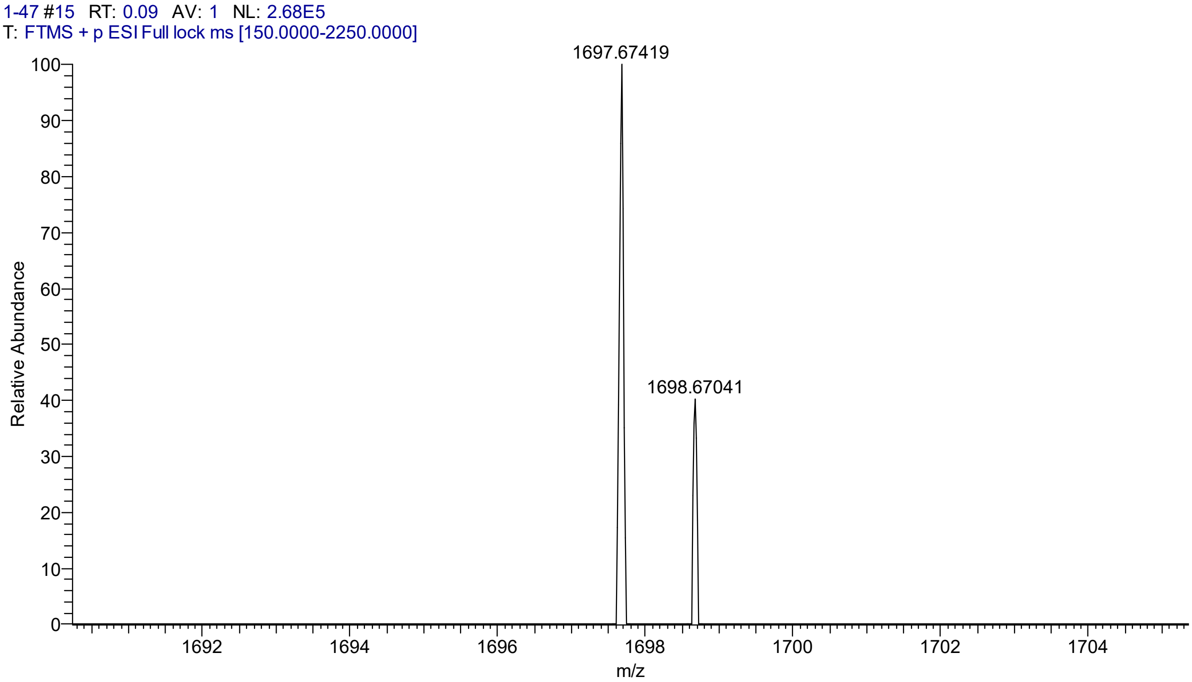

172.690
170.545
170.231
168.791
167.768
166.340
165.627
164.906
136.798
133.707
131.957
128.385
127.351
125.925
123.861
118.541
99.960
66.937
57.802
56.366
52.882
49.705
49.373
44.783
38.820
36.043
29.298
26.916
22.628
21.279
20.567
f1 (ppm)


1-17 #27 RT: 0.15 AV: 1 NL: 3.87E5
T: FTMS + p ESI Full lock ms [150.0000-2250.0000]
1553.58679
1554.59790
1555.60071
Relative Abundance
m/z

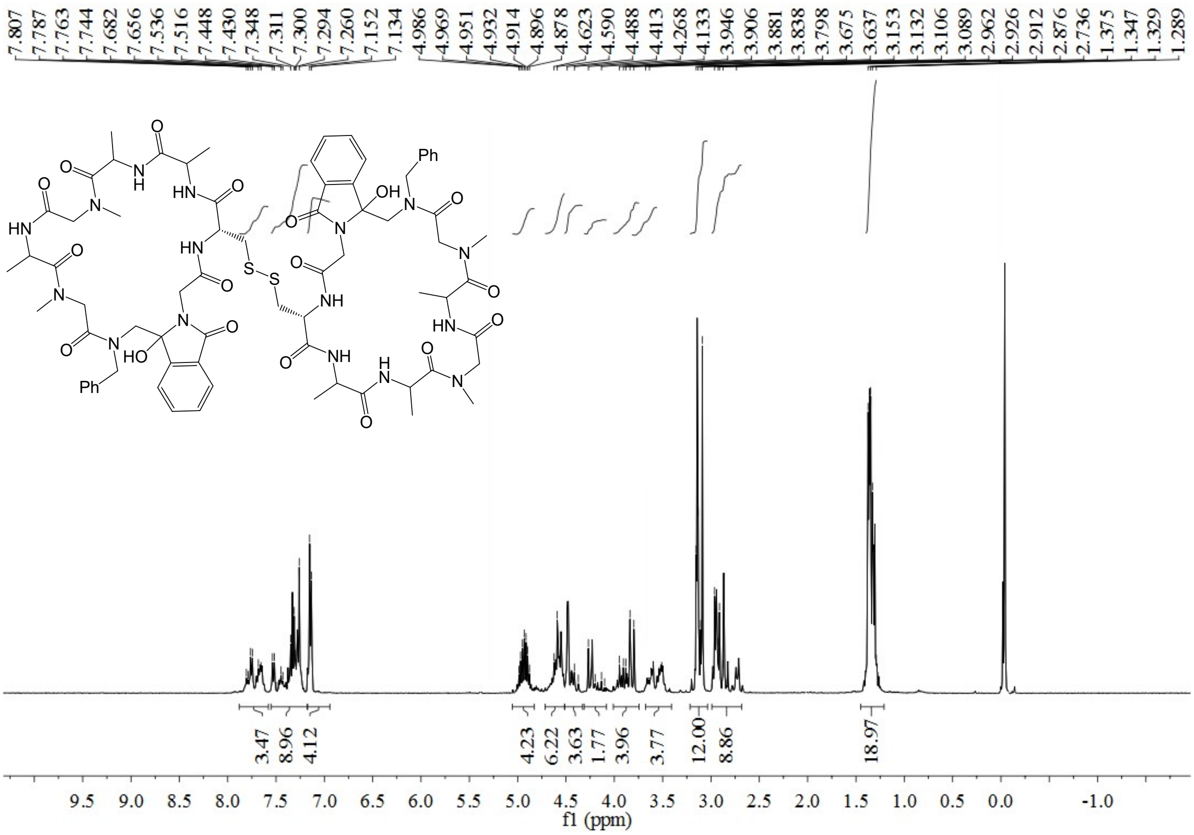
(17) ^{1}H, ^{13}C-NMR and HRMS of **3i.**

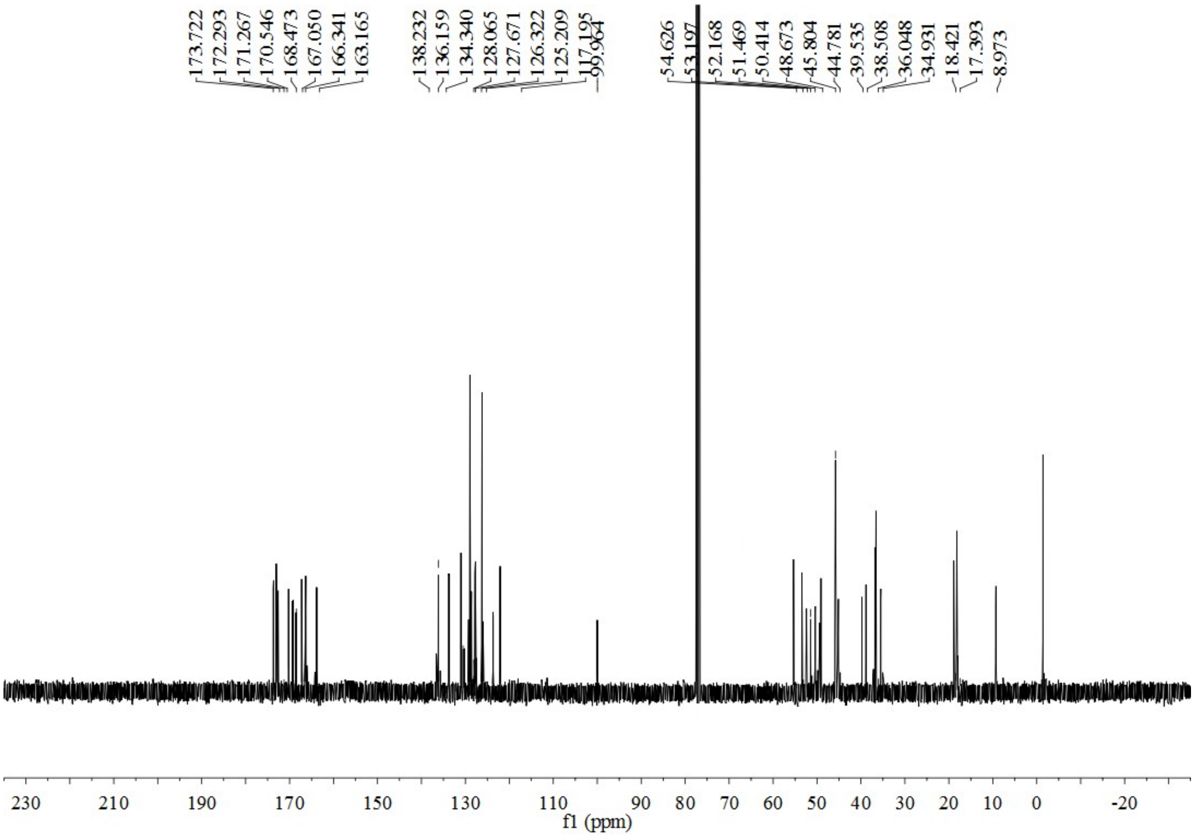


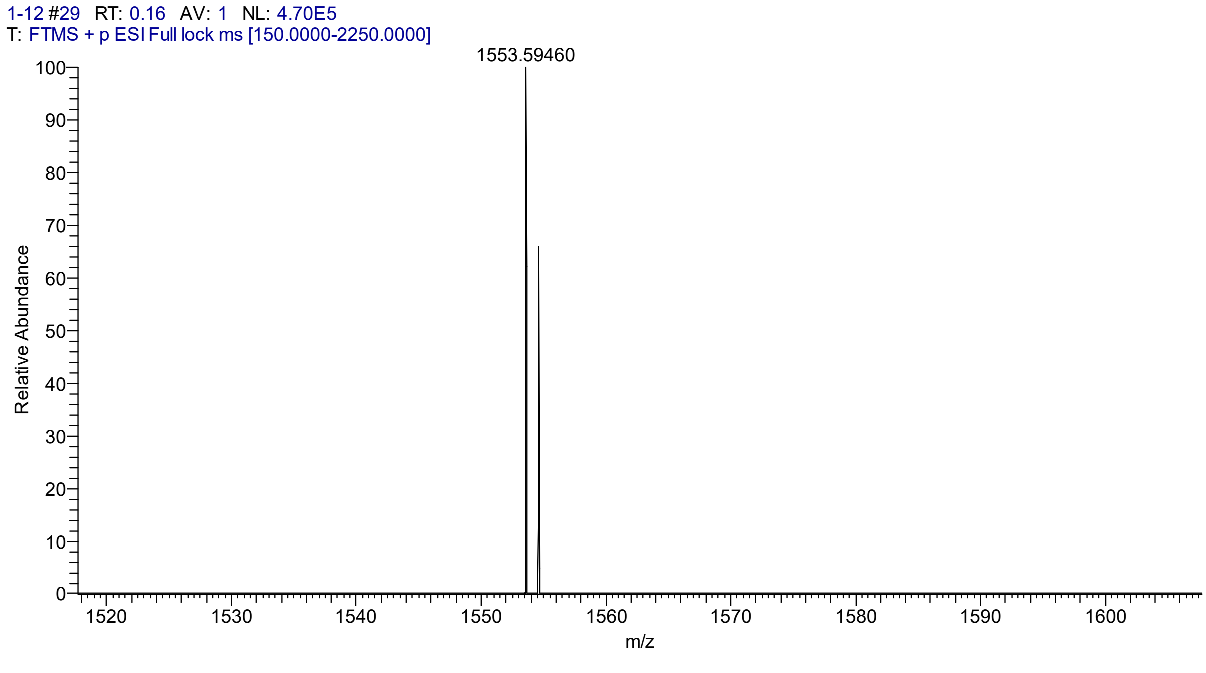




(18) ^{1}H, ^{13}C-NMR and HRMS of **4i.**




173.722
172.293
171.267
170.546
168.473
167.050
166.341
163.165
138.232
136.159
134.340
128.065
127.671
126.322
125.209
117.195
99.964
54.626
53.197
52.168
51.469
50.414
48.673
45.804
44.781
39.535
38.508
36.048
34.931
18.421
17.393
8.973
230 210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20
f1 (ppm)


1-12 #29 RT: 0.16 AV: 1 NL: 4.70E5
T: FTMS + p ESI Full lock ms [150.0000-2250.0000]
1553.59460
Relative Abundance
100 90 80 70 60 50 40 30 20 10 0
1520 1530 1540 1550 1560 1570 1580 1590 1600
m/z