Supporting Information

Aminocatalyzed Asymmetric Diels-Alder Reaction of 2,4-Dienals and Rhodanine/Hydantoin Derivatives †

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A: General Information and Starting Materials

General Information. Proton nuclear magnetic resonance (^{1}H NMR) spectra and carbon nuclear magnetic resonance (^{13}C NMR) spectra were recorded on a Bruker AV-400 spectrometer (400 MHz and 100 MHz). Chemical shifts for protons are reported in parts per million downfield from tetramethylsilane and are referenced to residual protium in the NMR solvent ($CDCl_3$: δ 7.26) Chemical shifts for carbon are reported in parts per million downfield from tetramethylsilane and are referenced to the carbon resonances of the solvent ($CDCl_3$: δ 77.16). Data are represented as follows: chemical shift, integration, multiplicity (br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants in Hertz (Hz). High resolution mass spectrometry (ESI) were carried out using a Waters Quatro Macro triple quadrupole mass spectrometer Mass spectra (EI) were measured on a Waters Micromass GCT spectrometer. Optical rotations were measured on an Autopol III automatic polarimeter (Rudolph Research analytical). Melting points were measured on a XT3A apparatus. High Performance Liquid Chromatography (HPLC) was performed on an Agilent 1200 Series chromatographs using chiral columns (DAICEL CHIRALPAK AD-H, IA, IC) as noted.

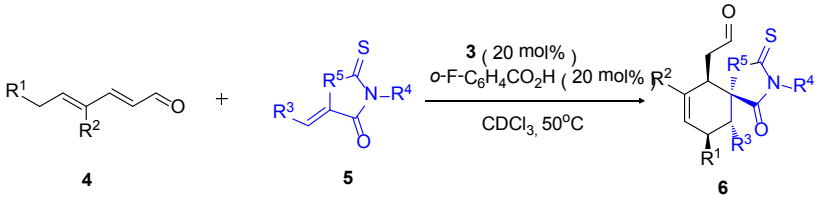
Starting Materials. All solvents and inorganic reagents were from commercial sources and used without purification unless otherwise noted. 2,4-dienals **4** were synthesized following the literature procedure[1]. Substrates **5** were synthesized following the literature procedure[2-4].

Reference.

1 Z.-J. Jia, Q, Zhou, Q.-Q. Zhou, P.-Q, Chen, Y.-C. Cheng, *Angew. Chem. Int. Ed.*, **2011**, *50*, 8638.
2 N. K. El-Aasar, K. F. Saied. *J. Heterocylic. Chem.,* **2008**, *45*, 645.
3 Y. Dürüst, F. Nohout. *Synth. Commun*., **1999**, *29*, 1997.
4 N. Faucher, P. Martres, A. Laroze, O. Pineau, F. Potvain, D. Grillot. *Bioorg. Med. Chem. Lett.* **2008**, *18*, 710.

B: Experimental Details

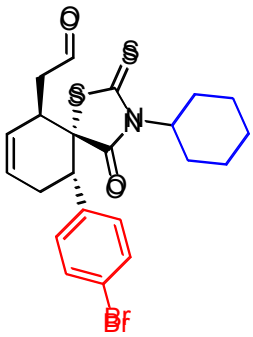
General procedure for the asymmetric Diels-Alder reaction



To a solution of catalyst **3** (0.02 mmol, 0.20 equiv.) and *o*-F-$C_6H_4CO_2H$ (0.02 mmol, 0.20 equiv.) in $CDCl_3$ (1.0 mL), was added **4** (0.20 mmol, 2.0 equiv), then substrate **5** (0.10 mmol, 1.0 equiv.) was added. The reaction mixture was stirred at 50°C for a specified time and then the solvent was removed under vacuum. The residue was purified by silica gel chromatography (petroleum ether/ethyl acetate) to afford the desired product.

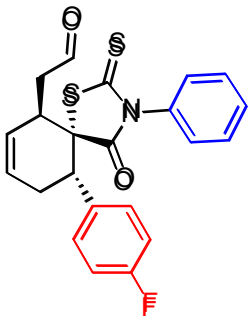
C: Characterization of Diels-Alder Raction Products

6a:2-((5S,6R,10S)-10-(4-bromophenyl)-3-cyclohexyl-4-oxo-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



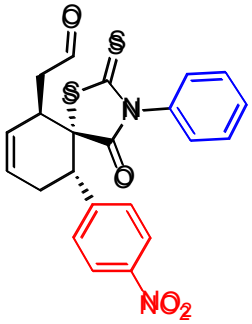
The product was obtained in 90% yield, yellow oil. $[\alpha]^{25}_{D}$ – -18.9 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.74 (s, 1H), 7.39-7.37 (m, 2H), 7.24-7.21 (m, 2H), 5.91-5.87 (m, 1H), 5.76-5.72 (m, 1H), 4.49 (brs, 1H), 3.59-3.49 (m, 2H), 3.37 (q, *J* = 5.6 Hz, 1H), 2.60-2.59 (m, 2H), 2.45-2.37 (m, 1H), 2.02-1.93 (m, 1H), 1.76-1.73 (m, 1H), 1.63-1.38 (m, 4H), 1.21-0.96 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 200.3, 198.8, 177.0, 136.4, 131.3, 131.1, 128.4, 127.4, 122.1, 58.0, 45.2, 42.1, 40.1, 30.3, 27.3, 26.6, 25.9, 25.8, 25.0; HRMS (EI): exact mass calculated for M^+ ($C_{22}H_{24}BrNO_2S_2$) requires m/z 477.0432, found m/z 477.0435; The enantiomeric excess was determined by HPLC after **6a** was converted to the corresponding α,β-unsaturated ester (Ph_3P=$CHCO_2Me$ in THF, r.t). [IA column, 254nm, *n*-Hexane: EtOH = 7:3, 0.80 mL/min]: 6.2 min (minor), 7.1 min (major), ee 94%.

6b:2-((5S,6R,10S)-10-(4-fluorophenyl)-4-oxo-3-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



The product was obtained in 82% yield, yellow solid. Mp 87-89 °C. $[\alpha]^{25}_{D}$ -16.4 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.71 (s, 1H), 7.41-7.35 (m, 5H), 7.04-7.00 (m, 2H), 5.96-5.93 (m, 1H), 5.82-5.78 (m, 1H), 3.80 (brs, 1H), 3.61 (dd, *J* = 19.2, 8.8 Hz, 1H), 3.52 (dd, *J* = 11.2, 5.6 Hz, 1H), 2.72-2.58 (m, 2H), 2.46 (m, 1H). ^{13}C NMR(100 MHz, $CDCl_3$): δ 199.3, 199.1, 176.4, 163.8, 161.4, 134.7, 133.1, 133.0, 131.3, 131.2, 129.6, 129.4, 128.2, 128.0, 127.5, 115.4, 115.2, 67.3, 45.6, 42.0, 40.1, 30.2; HRMS (EI): exact mass calculated for M^+ ($C_{22}H_{18}FNO_2S_2$) requires m/z 411.0763, found m/z 411.0762; The enantiomeric excess was determined by HPLC after **6b** was converted to the corresponding α,β-unsaturated ester (Ph_3P=$CHCO_2Me$ in THF, r.t). [IA column, 254nm, *n*-Hexane: EtOH = 7:3, 0.80 mL/min]: 8.6 min (minor), 9.4 min (major), ee 93%.

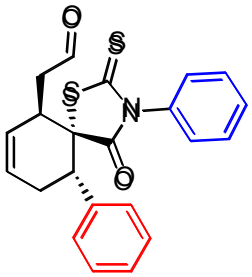
6c:2-((5S,6R,10S)-10-(4-nitrophenyl)-4-oxo-3-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



The product was obtained in 91% yield, yellow solid. Mp 105-107°C. $[\alpha]^{25}_{D}$ – 45.7 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.71 (s, 1H), 8.19-8.17 (m, 2H), 7.64-7.61 (m, 2H), 7.46-7.35 (m, 3H), 6.00-5.97 (m, 1H), 5.85-5.81 (m, 1H), 3.84 (brs, 1H), 3.67-3.55 (m, 2H), 2.76-2.62 (m, 2H), 2.52 (m, 1H). ^{13}C NMR(100 MHz, $CDCl_3$): δ 198.9, 198.4, 176.1, 147.7,

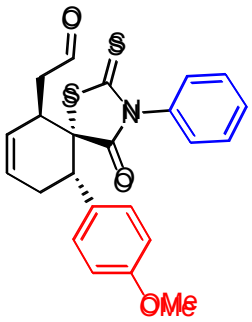
145.0, 134.5, 130.7, 129.7, 129.5, 128.4, 127.8, 127.0, 123.4, 66.7, 45.4, 42.4, 40.5, 29.8; HRMS (EI): exact mass calculated for M^+ ($C_{22}H_{18}N_2O_4S_2$) requires m/z 438.0708, found m/z 438.0710; The enantiomeric excess was determined by HPLC after **6c** was converted to the corresponding α,β-unsaturated ester ($Ph_3P{=}CHCO_2Me$ in THF, r.t). [IC column, 254nm, *n*-Hexane: EtOH = 7:3, 1.0 mL/min]: 10.4 min (major), 12.0 min (minor), ee 90%.

6d:2-((5S,6R,10S)-4-oxo-3,10-diphenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



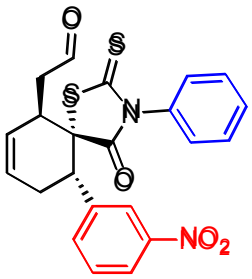
The product was obtained in 84% yield, brown oil. $[\alpha]^{25}_D$ –14.8 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.72 (s, 1H), 7.43-7.41 (m, 2H), 7.36-7.32 (m, 6H), 5.98-5.94 (m, 1H), 5.83-5.79 (m, 1H), 3.80 (brs, 1H), 3.65 (dd, *J* = 18.8, 8.4 Hz, 1H), 3.52 (dd, *J* = 11.6, 5.6 Hz, 1H), 2.79-2.71 (m, 1H), 2.61 (dd, *J* = 18.8, 4.0 Hz, 1H), 2.49 (m, 1H). ^{13}C NMR(100 MHz, $CDCl_3$): δ 199.7, 199.2, 176.4, 137.3, 134.8, 129.6, 129.5, 129.3, 128.5, 128.3, 128.2, 128.1, 127.7, 67.4, 45.6, 42.9, 40.0, 30.0; HRMS (EI): exact mass calculated for M^+ ($C_{22}H_{19}NO_2S_2$) requires m/z 393.0857, found m/z 393.0852; The enantiomeric excess was determined by HPLC after **6d** was converted to the corresponding α,β-unsaturated ester ($Ph_3P{=}CHCO_2Me$ in THF, r.t). [IA column, 254nm, *n*-Hexane: EtOH = 7:3, 0.80 mL/min]: 7.4 min (MINOR), 8.4 min (mAJOR), ee 91%.

6e:2-((5S,6R,10S)-10-(4-methoxyphenyl)-4-oxo-3-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



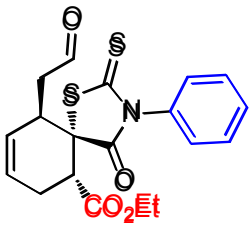
The product was obtained in 64% yield. yellow solid. Mp 71-73°C; $[\alpha]^{25}_D$ – 13.9 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.72 (s, 1H), 7.34-7.32 (m, 5H), 6.86-6.84 (m, 4H), 5.96-5.94 (m, 1H), 5.82-5.78 (m, 1H), 3.81 (s, 4H), 3.64 (dd, *J* = 18.8, 8.4 Hz, 1H), 3.49 (dd, *J* = 11.6, 5.2 Hz, 1H), 2.73-2.58 (m, 2H), 2.46 (m, 1H). ^{13}C NMR(100 MHz, $CDCl_3$): δ 199.8, 199.2, 176.5, 159.6, 134.9, 130.6, 129.4, 129.3, 129.2, 128.2, 128.1, 127.8, 113.8, 67.7, 55.4, 45.6, 42.0, 40.0, 30.2; HRMS (EI): exact mass calculated for M^+ ($C_{23}H_{21}NO_3S_2$) requires m/z 423.0963, found m/z 423.0960; The enantiomeric excess was determined by HPLC after **6e** was converted to the corresponding α,β-unsaturated ester ($Ph_3P{=}CHCO_2Me$ in THF, r.t). [IA column, 254nm, *n*-Hexane: EtOH = 7:3, 0.80 mL/min]: 8.8 min (minor), 10.2 min (major), ee 91%.

6f:2-((5S,6R,10S)-10-(3-nitrophenyl)-4-oxo-3-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



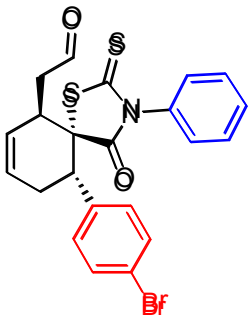
The product was obtained in 95% yield, brown solid. Mp 60-62 °C. $[\alpha]^{25}_{D}$ – 12.7 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.72 (s, 1H), 8.30-8.22 (m, 2H), 7.83-7.81 (m, 1H), 7.56-7.52 (m, 1H), 7.35-7.33 (m, 3H), 6.01-5.98 (m, 1H), 5.86-5.82 (m, 1H), 3.85 (brs, 1H), 3.69-3.57 (m, 2H), 2.30-2.72 (m, 1H), 2.66 (dd, *J* = 19.2, 3.2 Hz, 1H), 2.55 (m, 1H). ^{13}C NMR(100 MHz, $CDCl_3$): δ 199.0, 198.3, 176.2, 148.1, 139.8, 135.6, 134.5, 129.7, 129.5, 129.4, 128.4, 127.9, 127.0, 124.8, 123.2, 66.7, 45.4, 42.2, 40.4, 29.9; HRMS (EI): exact mass calculated for M^+ ($C_{22}H_{18}N_2O_4S_2$) requires m/z 438.0708, found m/z 438.0712; The enantiomeric excess was determined by HPLC after **6f** was converted to the corresponding α,β-unsaturated ester (Ph_3P=$CHCO_2Me$ in THF, r.t). [IA column, 254nm, *n*-Hexane: EtOH = 4:1, 1.0 mL/min]: 10.8 min (minor), 11.8 min (major), ee 92%.

6g:(5S,6S,10R)-ethyl-4-oxo-10-(2-oxoethyl)-3-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-8-ene-6-carboxylate



The product was obtained in 93% yield, yellow oil. $[\alpha]^{25}_{D}$ –111.4 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.64 (s, 1H), 7.54-7.44 (m, 3H), 7.34-7.32 (m, 2H), 5.87-5.85 (m, 1H), 5.76-5.72 (m, 1H), 4.19 (q, *J* = 7.2 Hz, 2H), 3.72 (brs, 1H), 3.39 (dd, *J* = 11.6, 6.4 Hz, 1H), 3.26 (dd. *J* = 18.8, 8.4 Hz, 1H), 2.79 (m, 1H), 2.48 (dd, *J* = 19.2, 4.0 Hz, 1H), 2.42-2.34 (m, 1H), 1.26 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR(100 MHz, $CDCl_3$): δ 200.4, 198.7, 177.9, 171.0, 135.6, 129.5, 129.4, 128.6, 128.5, 126.1, 61.8, 61.7, 45.4, 41.9, 40.0, 26.6; HRMS (EI): exact mass calculated for M^+ ($C_{19}H_{19}NO_4S_2$) requires m/z 389.0755, found m/z 389.0760; The enantiomeric excess was determined by HPLC after **6g** was converted to the corresponding α,β-unsaturated ester (Ph_3P=$CHCO_2Me$ in THF, r.t). [AD-H column, 254nm, *n*-Hexane: EtOH = 7:3, 0.60 mL/min]: 14.2 min (major), 18.2 min (minor), ee 94%.

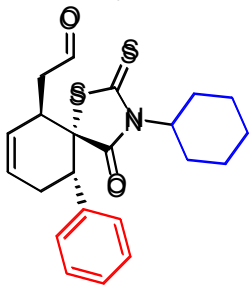
6h:2-((5S,6R,10S)-10-(4-bromophenyl)-4-oxo-3-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



The product was obtained in 76% yield, brown solid. Mp 146-148 °C; $[\alpha]^{25}_{D}$ – 30.5 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.72 (s, 1H), 7.46-7.44 (m, 2H), 7.36-7.28 (m, 5H), 5.96-5.93 (m, 1H), 5.82-5.78 (m, 1H), 3.80 (brs, 1H), 3.60 (dd, *J* = 18.8, 8.4 Hz, 1H), 3.48 (dd, *J* = 11.6, 5.6 Hz, 1H), 2.72-2.58 (m, 2H), 2.47 (m, 1H). ^{13}C NMR(100 MHz, $CDCl_3$): δ 199.2, 199.0, 176.3, 136.3, 134.7, 131.5, 131.2, 129.6, 129.4, 128.3, 128.0, 127.4, 122.4, 67.0, 45.5, 42.3, 40.0, 29.9; HRMS (EI): exact mass calculated for M^+ ($C_{22}H_{18}BrNO_2S_2$) requires m/z 470.9962, found m/z 470.9960; The enantiomeric excess was determined by HPLC after **6h** was converted

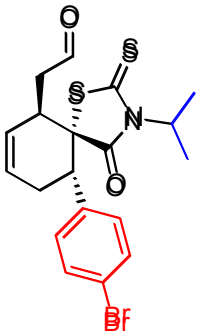
to the corresponding α,β-unsaturated ester ($Ph_3P=CHCO_2Me$ in THF, r.t). [IA column, 254nm, *n*-Hexane: EtOH = 9:1, 1.0 mL/min]: 11.8 min (minor), 13.3 min (major), ee 93%.

6i:2-((5S,6R,10S)-3-cyclohexyl-4-oxo-10-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl) acetaldehyde



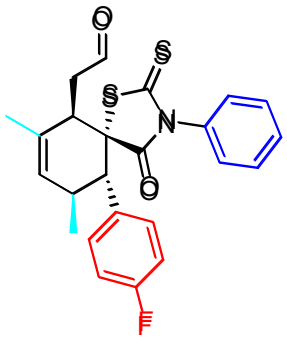
The product was obtained in 88% yield, yellow oil. $[\alpha]^{25}_D$ +19.7 (*c* 1.0, CH_2Cl_2); ^1H NMR (400 MHz, $CDCl_3$): δ 9.75 (s, 1H), 7.35-7.33 (m, 2H), 7.24-7.23 (m, 3H), 5.91-5.89 (m, 1H), 5.76-5.72 (m, 1H), 4.46 (brs, 1H), 3.61-3.53 (m, 2H), 3.40 (dd, *J* = 11.6, 5.6 Hz, 1H), 2.66-2.50 (m, 2H), 2.43 (m, 1H), 2.01-1.92 (m, 1H), 1.74-1.71 (m, 1H), 1.53-1.42 (m, 4H), 1.25-1.00 (m, 4H). ^{13}C NMR(100 MHz, $CDCl_3$): δ 200.8, 198.9, 177.1, 137.3, 129.4, 128.4, 128.3, 128.2, 128.0, 127.7, 57.9, 45.3, 42.6, 40.2, 30.4, 27.3, 26.5, 25.9, 25.8, 25.0; HRMS (EI): exact mass calculated for M^+ ($C_{22}H_{25}NO_2S_2$) requires m/z 399.1327, found m/z 399.1320; The enantiomeric excess was determined by HPLC after **6i** was converted to the corresponding α,β-unsaturated ester ($Ph_3P=CHCO_2Me$ in THF, r.t). [IA column, 254nm, *n*-Hexane: EtOH = 9:1, 1.0 mL/min]: 4.6 min (minor), 5.0 min (major), ee 94%.

6j:2-((5S,6R,10S)-10-(4-bromophenyl)-3-isopropyl-4-oxo-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



The product was obtained in 89% yield, yellow solid. Mp 168-169 °C; $[\alpha]^{25}_D$ +77.0 (*c* 1.0, CH_2Cl_2); ^1H NMR (400 MHz, $CDCl_3$): δ 9.74 (s, 1H), 7.39-7.37 (m, 2H), 7.24-7.22 (m 2H), 5.91-5.88 (m, 1H), 5.76-7-5.73 (m, 1H), 4.89-4.82 (m, 1H), 3.60-3.51 (m, 2H), 3.38 (dd, *J* = 11.6, 5.6 Hz, 1H), 2.60-2.52 (m, 2H), 2.41 (m, 1H), 1.21 (d, *J* = 6.8 Hz, 3H), 0.66 (d, *J* = 5.6 Hz, 3H). ^{13}C NMR(100 MHz, $CDCl_3$): δ 200.1, 198.8, 176.9, 136.3, 131.3, 131.1, 128.4, 127.4, 122.1, 50.0, 45.2, 42.0, 40.1, 30.3, 18.0, 17.3; HRMS (EI): exact mass calculated for M^+ ($C_{19}H_{20}BrNO_2S_2$) requires m/z 437.0119, found m/z 437.0120; The enantiomeric excess was determined by HPLC after **6j** was converted to the corresponding α,β-unsaturated ester ($Ph_3P=CHCO_2Me$ in THF, r.t). [IA column, 254nm, *n*-Hexane: *i*-PrOH = 7:3, 0.70 mL/min]: 5.5 min (minor), 6.0 min (major) ee 93%.

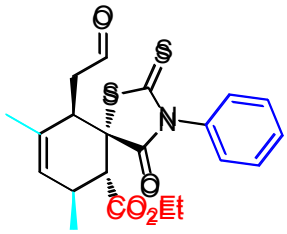
6k:2-((5S,6R,9S,10S)-10-(4-fluorophenyl)-7,9-dimethyl-4-oxo-3-phenyl-2-thioxo-1-thia-3-aza spiro[4.5]dec-7-en-6-yl)acetaldehyde



The product was obtained in 98% yield, yellow solid. Mp 51-53°C; $[\alpha]^{25}_D$ +82.8 (*c* 1.0, CH_2Cl_2); ^1H NMR (400 MHz, $CDCl_3$): δ 9.74 (s, 1H), 7.40-7.35 (m, 5H), 7.07-7.00 (m, 2H), 5.55 (s, 1H), 3.65-3.52 (m, 2H), 3.04 (d, *J* = 10.8 Hz, 1H), 2.75 (brs, 1H), 2.62 (dd, *J* = 18.8, 1.2 Hz, 1H), 1.79 (s, 3H), 0.90 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR(100 MHz, $CDCl_3$): δ

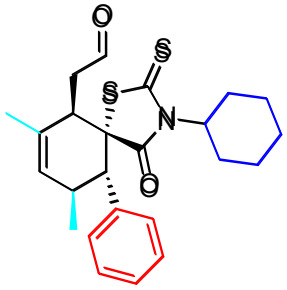
199.9, 199.3, 176.4, 163.8, 161.3, 134.7, 133.4, 132.2, 132.1, 131.4, 129.6, 129.5, 129.4, 128.0, 115.4, 115.2, 68.2, 49.3, 44.2, 43.7, 35.0, 29.7, 22.0, 19.4; HRMS (EI): exact mass calculated for M^+ ($C_{24}H_{22}FNO_2S_2$) requires m/z 439.1076, found m/z 439.1072; The enantiomeric excess was determined by HPLC after **6k** was converted to the corresponding α,β-unsaturated ester ($Ph_3P{=}CHCO_2Me$ in THF, r.t). [IA column, 254nm, *n*-Hexane: EtOH = 15:1, 0.8 mL/min]: 9.7 min (minor), 11.0 min (major), ee 96%.

6l:(5S,6S,7S,10R)-ethyl-7,9-dimethyl-4-oxo-10-(2-oxoethyl)-3-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-8-ene-6-carboxylate



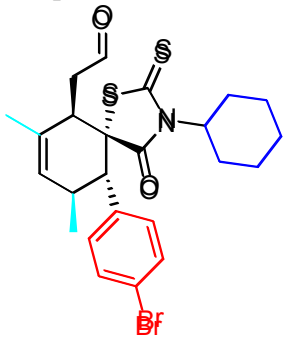
The product was obtained in 91% yield, pale yellow solid. Mp 120-121°C; $[\alpha]^{25}_D$ – 18.5 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.67 (s, 1H), 7.53-7.43 (m, 3H), 7.28-7.26 (m, 2H), 5.42 (s, 1H), 4.20 (q, *J* = 7.2 Hz, 2H), 3.50 (d, *J* = 8.8 Hz, 1H), 3.24 (dd, *J* = 19.2, 8.8 Hz, 1H), 2.99 (d, *J* = 10.4 Hz, 1H), 2.64 (brs, 1H), 2.49 (dd, *J* = 19.2, 2.0 Hz, 1H), 1.73 (s, 3H), 1.28-1.24 (m, 6H). ^{13}C NMR(100 MHz, $CDCl_3$): δ 201.0, 198.9, 177.5, 171.4, 135.5, 133.9, 129.6, 129.4, 128.9, 128.5, 63.9, 61.7, 48.6, 43.9, 43.7, 32.4, 22.0, 21.4, 14.2; HRMS (EI): exact mass calculated for M^+ ($C_{21}H_{23}NO_4S_2$) requires m/z 417.1068, found m/z 417.1071; The enantiomeric excess was determined by HPLC after **6l** was converted to the corresponding α,β-unsaturated ester ($Ph_3P{=}CHCO_2Me$ in THF, r.t). [IA column, 254nm, *n*-Hexane: EtOH = 7:3, 0.8 mL/min]: 5.7 min (minor), 6.5 min (major), ee 96%.

6m:2-((5S,6R,9S,10S)-3-cyclohexyl-7,9-dimethyl-4-oxo-10-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



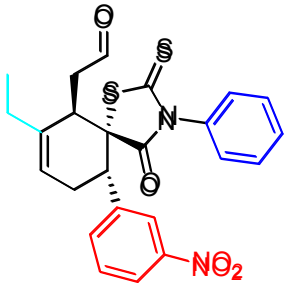
The product was obtained in 94% yield, yellow solid. Mp 146-148°C; $[\alpha]^{25}_D$ +109.3 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.80 (s, 1H), 7.33-7.31 (m, 2H), 7.25-7.22 (m, 3H), 5.50 (s, 1H), 4.44 (brs, 1H), 3.54 (dd, *J* = 18.8, 9.2 Hz, 1H), 3.39 (d, *J* = 8.8 Hz, 1H), 2.92 (d, *J* = 10.8 Hz, 1H), 2.69 (brs, 1H), 2.54 (dd, *J* = 18.8, 1.6 Hz, 1H), 1.97-1.89 (m, 1H), 1.74-1.69 (m, 4H), 1.52-1.40 (m, 4H), 1.17-0.97 (m, 4H), 0.86 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR(100 MHz, $CDCl_3$): δ 201.4, 199.2, 177.0, 136.3, 133.5, 129.7, 128.2, 127.9, 55.8, 49.9, 44.0, 43.8, 35.1, 27.2, 26.4, 25.9, 25.8, 25.0, 21.9, 19.4; HRMS (EI): exact mass calculated for M^+ ($C_{24}H_{29}NO_2S_2$) requires m/z 427.1640, found m/z 427.1636; The enantiomeric excess was determined by HPLC after **6m** was converted to the corresponding α,β-unsaturated ester ($Ph_3P{=}CHCO_2Me$ in THF, r.t). [IC column, 254nm, *n*-Hexane:EtOH = 49:1, 1.0 mL/min]: 5.2 min (minor), 5.6 min (major), ee 97%.

6n:2-((5S,6R,9S,10S)-10-(4-bromophenyl)-3-cyclohexyl-7,9-dimethyl-4-oxo-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



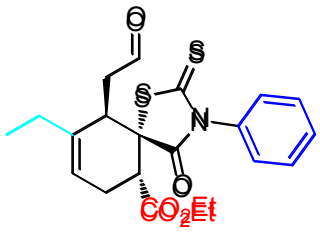
The product was obtained in 95% yield, yellow solid. Mp 102-104°C; $[\alpha]^{25}_{D}$ +63.4 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.77 (s, 1H), 7.39-7.36 (m, 2H), 7.22-7.20 (m, 2H), 5.48 (s, 1H), 4.47 (brs, 1H), 3.50 (dd, J = 18.8, 9.2 Hz, 1H), 3.39 (d, *J* = 9.2 Hz, 1H), 2.89 (d, *J* = 10.4 Hz, 1H), 2.63 (brs, 1H), 2.54 (dd, *J* = 18.8, 1.6 Hz, 1H), 1.99-1.89 (m, 1H), 1.73 (s, 4H), 1.69-1.52 (m, 4H), 1.19-0.98 (m, 4H), 0.85 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): (ppm) 200.9, 199.0, 176.9, 135.5, 133.6, 131.3, 129.4, 122.0, 57.9, 49.4, 43.9, 43.7, 35.0, 27.2, 26.6, 25.9, 25.8, 24.9, 21.9, 19.4; HRMS (EI): exact mass calculated for M^+ ($C_{24}H_{28}BrNO_2S_2$) requires m/z 505.0745, found m/z 505.0750; The enantiomeric excess was determined by HPLC after **6n** was converted to the corresponding α,β-unsaturated ester (Ph_3P=$CHCO_2Me$ in THF, r.t). [IA column, 254nm, *n*-Hexane: EtOH = 49:1, 1.0 mL/min]: 3.8 min (minor), 4.1 min (major), ee 97%.

6o:2-((5S,6R,10S)-7-ethyl-10-(3-nitrophenyl)-4-oxo-3-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



The product was obtained in 98% yield, yellow solid. Mp 168-170°C; $[\alpha]^{25}_{D}$ – 33.6 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.74 (s, 1H) 8.29-8.28 (m, 1H), 8.22-8.20 (m, 2H), 7.82-7.81 (m, 1H), 7.54-7.50 (m, 1H), 7.34 (brs, 3H), 5.69 (s, 1H), 3.77 (d, *J* = 8.8 Hz, 1H), 3.70 (dd, *J* = 11.2, 6.0 Hz, 1H), 3.59 (dd, *J* = 19.2, 9.2 Hz, 1H), 2.74-2.53 (m, 3H), 2.18-2.09 (m, 1H), 2.01-1.94 (m, 1H), 1.11 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR(100 MHz, $CDCl_3$): δ 199.2, 198.7, 176.2, 148.0, 140.3, 139.9, 135.6, 134.5, 129.6, 129.5, 129.4, 127.9, 124.8, 123.1, 120.7, 67.2, 44.3, 42.1, 41.9, 30.0, 27.8, 12.6; HRMS (EI): exact mass calculated for M^+ ($C_{24}H_{22}N_2O_4S_2$) requires m/z 466.1021, found m/z 466.1019; The enantiomeric excess was determined by HPLC after **6o** was converted to the corresponding α,β-unsaturated ester (Ph_3P=$CHCO_2Me$ in THF, r.t). [IA column, 254nm, *n*-Hexane: EtOH = 9:1, 1.0 mL/min]: 11.1 min (minor), 12.7 min (major), ee 97%.

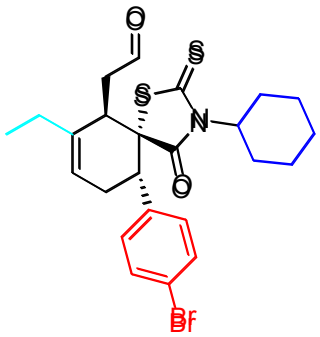
6p:(5S,6S,10R)-ethyl-9-ethyl-4-oxo-10-(2-oxoethyl)-3-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-8-ene-6-carboxylate



The product was obtained in 95% yield. pale yellow solid. Mp 106-107°C; $[\alpha]^{25}_{D}$ – 87.9 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.66 (s, 1H), 7.54-7.41 (m, 3H), 7.34-7.32 (m, 2H), 5.56 (s, 1H), 4.19 (q, *J* = 7.2 Hz, 2H), 3.62 (d, *J* = 8.8 Hz, 1H), 3.41 (dd, *J* = 11.6, 6.8 Hz, 1H), 3.26 (dd, *J* = 19.6, 9.2 Hz, 1H), 2.81-2.73 (m, 1H), 2.48 (dd, *J* = 19.6, 2.0 Hz, 1H), 2.38-2.30 (m, 1H), 2.11-2.02 (m, 1H), 1.94-1.89 (m, 1H),

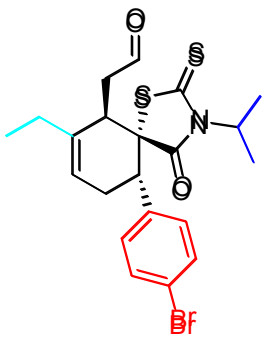
1.26 (t, J = 7.2 Hz, 3H), 1.06 (t, J = 7.2 Hz, 3H). ^{13}C NMR(100 MHz, $CDCl_3$): δ 200.8, 198.9, 178.0, 171.2, 140.6, 135.6, 129.5, 129.4, 128.6, 119.7, 62.3, 61.6, 44.4, 42.1, 41.6, 27.8, 26.4, 14.2, 12.3; HRMS (EI): exact mass calculated for M^+ ($C_{21}H_{23}NO_4S_2$) requires m/z 417.1068, found m/z 417.1070; The enantiomeric excess was determined by HPLC after **6p** was converted to the corresponding α,β-unsaturated ester (Ph_3P=$CHCO_2Me$ in THF, r.t). [IA column, 254nm, *n*-Hexane: EtOH = 49:1, 1.0 mL/min]: 15.3 min (minor), 17.2 min (major), ee 97%.

6q:2-((5S,6R,10S)-10-(4-bromophenyl)-3-cyclohexyl-7-ethyl-4-oxo-2-thioxo-1-thia-3-azaspiro [4.5]dec-7-en-6-yl)acetaldehyde



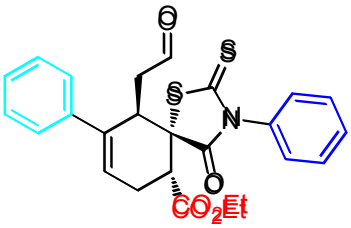
The product was obtained in 93% yield, off-white solid. Mp 170-171°C; $[\alpha]^{25}_D$ – 77.5 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.78 (s, 1H), 7.39-7.36 (m, 2H), 7.24-7.22 (m, 2H), 5.59 (s, 1H), 4.48 (brs, 1H), 3.58-3.48 (m, 2H), 3.41 (dd, J = 11.6, 6.0 Hz, 1H), 2.53-2.38 (m, 3H), 2.11-2.02 (m, 1H), 1.97-1.89 (m, 2H), 1.74 (d, J = 12.8 Hz, 1H), 1.62-1.40 (m, 4H), 1.25-1.03 (m, 7H). ^{13}C NMR(100 MHz, $CDCl_3$): δ 200.8, 199.0, 177.1, 140.4, 136.4, 131.3, 131.1, 122.0, 121.0, 57.9, 44.2, 41.8, 41.7, 30.3, 27.8, 27.2, 26.6, 25.9, 25.8, 25.0, 12.5; HRMS (EI): exact mass calculated for M^+ ($C_{24}H_{28}BrNO_2S_2$) requires m/z 505.0745, found m/z 505.0740; The enantiomeric excess was determined by HPLC after **6q** was converted to the corresponding α,β-unsaturated ester (Ph_3P=$CHCO_2Me$ in THF, r.t). [IA column, 254nm, *n*-Hexane: EtOH = 49:1, 1.0 mL/min]: 7.0 min (minor),7.8 min (major), ee 97%.

6r:2-((5S,6R,10S)-10-(4-bromophenyl)-7-ethyl-3-isopropyl-4-oxo-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



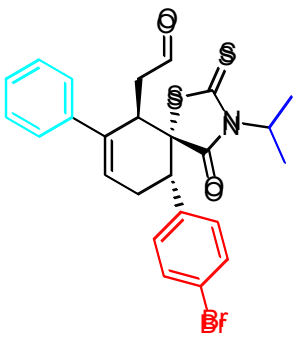
The product was obtained in 98% yield, off-white solid. Mp 125-126°C; $[\alpha]^{25}_D$ +99.5 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.78 (s, 1H), 7.39-7.37 (m, 2H), 7.27-7.23 (m, 2H), 5.59 (s, 1H), 4.89-4.82 (m, 1H), 3.60-3.49 (m, 2H), 3.42 (dd, J = 11.2, 6.0 Hz, 1H), 2.54-2.40 (m, 3H), 2.11-2.02 (m, 1H), 1.94-1.84 (m, 1H), 1.21 (d, J = 6.8 Hz, 3H), 1.05 (t, J = 7.2 Hz, 3H), 0.66 (d, J = 5.6 Hz, 3H). ^{13}C NMR(100 MHz, $CDCl_3$): δ 200.5, 199.0, 177.0, 140.4, 136.4, 131.3, 131.1, 122.0, 121.1, 63.6, 49.9, 44.2, 41.7, 30.3, 27.7, 18.0, 17.3, 12.5; HRMS (EI): exact mass calculated for M^+ ($C_{21}H_{24}BrNS_2O_2$) requires m/z 465.0432, found m/z 465.0430; The enantiomeric excess was determined by HPLC after **6r** was converted to the corresponding α,β-unsaturated ester (Ph_3P=$CHCO_2Me$ in THF, r.t). [IA column, 254nm, *n*-Hexane: i-PrOH = 19:1, 1.0 mL/min]: 6.5 min (minor), 7.8 min (major), ee 97%.

6s:(5S,6S,10R)-ethyl-4-oxo-10-(2-oxoethyl)-3,9-diphenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-8-ene-6-carboxylate



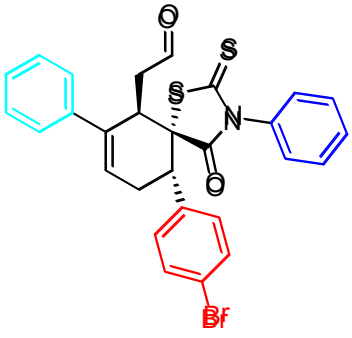
The product was obtained in 95% yield, pale yellow oil. $[\alpha]^{25}_{D}$ – 92.2 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.50 (s, 1H), 7.55-7.45 (m, 3H), 7.38-7.29 (m, 7H), 6.06-6.05 (m, 1H), 4.36 (d, *J* = 9.2 Hz, 1H), 4.22 (q, *J* = 7.2 Hz, 2H), 3.50 (dd, *J* = 12.0, 6.8 Hz, 1H), 3.24 (dd, *J* = 19.6, 9.6 Hz, 1H), 2.96 (m, 1H), 2.60-2.52 (m, 1H), 2.37 (dd, *J* = 19.2, 1.2 Hz, 1H), 1.28 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): (ppm) 200.4, 198.7, 177.8, 171.0, 139.6, 138.8, 135.7, 129.6, 129.5, 128.9, 128.6, 128.3, 126.4, 123.8, 62.3, 61.7, 44.4, 42.1, 41.5, 29.7, 27.2, 14.2; HRMS (EI): exact mass calculated for M^+ ($C_{25}H_{23}NO_4S_2$) requires m/z 465.1086, found m/z 465.1087; The enantiomeric excess was determined by HPLC after **6s** was converted to the corresponding α,β-unsaturated ester (Ph_3P=$CHCO_2Me$ in THF, r.t). [IA column, 254nm, *n*-Hexane: EtOH = 4:1, 1.0 mL/min]: 6.5 min (minor), 7.3 min (major), ee 99%.

6t:2-((5R,6R,10S)-10-(4-bromophenyl)-3-isopropyl-4-oxo-7-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



The product was obtained in 91% yield, pale yellow solid. Mp 206-207°C; $[\alpha]^{25}_{D}$ – 86.4 (c 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.63 (s, 1H), 7.42-7.40 (m, 2H), 7.33-7.26 (m, 7H), 6.10-6.08 (m, 1H), 4.93-4.86 (m, 1H), 4.26 (d, *J* = 9.2 Hz, 1H), 3.57-3.48 (m, 2H), 2.79-2.71 (m, 1H), 2.60 (m, 1H), 2.40 (dd, *J* = 19.2, 1.2 Hz, 1H), 1.24 (d, *J* = 6.8 Hz, 3H), 0.69 (d, *J* = 5.6 Hz, 3H). ^{13}C NMR(100 MHz, $CDCl_3$): δ 200.1, 198.7, 176.9, 139.5, 139.0, 136.1, 131.4, 131.2, 128.8, 128.2, 126.5, 125.1, 122.2, 50.0, 44.3, 41.7, 41.5, 30.9, 18.0, 17.4; HRMS (EI): exact mass calculated for M^+ ($C_{25}H_{24}BrNO_2S_2$) requires m/z 513.0432, found m/z 513.0429; The enantiomeric excess was determined by HPLC after **6t** was converted to the corresponding α,β-unsaturated ester (Ph_3P=$CHCO_2Me$ in THF, r.t). [IA column, 254nm, *n*-Hexane: *i*-PrOH = 7:3, 0.70 mL/min]: 7.5 min (minor), 9.0 min (major), ee 99%.

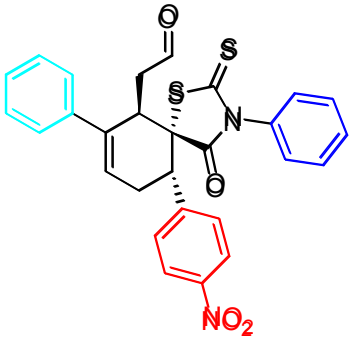
6u:2-((5R,6R,10S)-10-(4-bromophenyl)-4-oxo-3,7-diphenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



The product was obtained in 87% yield, yellow solid. Mp 223-225°C; $[\alpha]^{25}_{D}$ – 74.6 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.59 (s, 1H), 7.48-7.46 (m, 2H), 7.38-7.30 (m, 11H), 6.17-6.15 (m, 1H), 4.62 (d, *J* = 9.2 Hz, 1H), 3.62-3.53 (m, 2H), 2.90-2.83 (m, 1H), 2.67 (m, 1H), 2.47 (dd, *J* = 19.2, 1.6 Hz, 1H), . ^{13}C NMR(100 MHz, $CDCl_3$): δ 199.2, 199.0, 176.3, 139.3, 139.0, 136.1, 134.7, 131.5, 131.3, 129.6, 129.5, 128.9, 128.3,

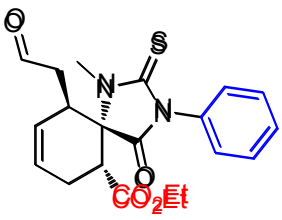
128.0, 126.5, 125.1, 122.4, 67.6, 44.5, 41.7, 30.5, 29.7; HRMS (EI): exact mass calculated for M^+ ($C_{28}H_{22}BrNO_2S_2$) requires m/z 547.0275, found m/z 547.0280; The enantiomeric excess was determined by HPLC after **6u** was converted to the corresponding α,β-unsaturated ester ($Ph_3P{=}CHCO_2Me$ in THF, r.t). [IA column, 254nm, *n*-Hexane: EtOH = 4:1, 1.0 mL/min]: 6.7 min (major), 7.6 min (minor), ee 99%.

6v:2-((5R,6R,10S)-10-(4-nitrophenyl)-4-oxo-3,7-diphenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



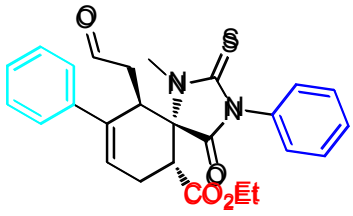
The product was obtained in 98% yield, pale yellow solid. Mp 203-205°C; $[\alpha]^{25}_D$ – 86.0 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.59 (s, 1H), 8.21-8.19 (m, 2H), 7.68-7.66 (m, 2H), 7.39-7.32 (m, 9H), 6.19-6.17 (m, 1H), 4.51 (d, *J* = 9.2 Hz, 1H), 3.76 (dd, *J* = 12.0, 6.0 Hz, 1H), 3.59 (dd, *J* = 19.2, 9.6 Hz, 1H), 2.94-2.87 (m, 1H), 2.71 (m, 1H), 2.51 (dd, *J* = 19.2, 1.6 Hz, 1H). ^{13}C NMR(100 MHz, $CDCl_3$): δ 199.0, 198.4, 176.0, 147.7, 144.8, 139.4, 138.8, 134.5, 130.7, 129.8, 129.6, 129.0, 128.4, 127.9, 126.5, 124.6, 123.4, 67.3, 44.4, 42.2, 41.8, 30.6; HRMS (EI): exact mass calculated for M^+ ($C_{28}H_{22}N_2O_4S_2$) requires m/z 514.1021, found m/z 514.1023; The enantiomeric excess was determined by HPLC after **6v** was converted to the corresponding α,β-unsaturated ester ($Ph_3P{=}CHCO_2Me$ in THF, r.t). [IA column, 254nm, *n*-Hexane: EtOH = 4:1, 1.0 mL/min]: 9.0 min (major), 12.3 min (minor), ee 99%.

6w:(5S,6R,10R)-ethyl-1-methyl-4-oxo-10-(2-oxoethyl)-3-phenyl-2-thioxo-1,3-diazaspiro[4.5]dec-8-ene-6-carboxylate



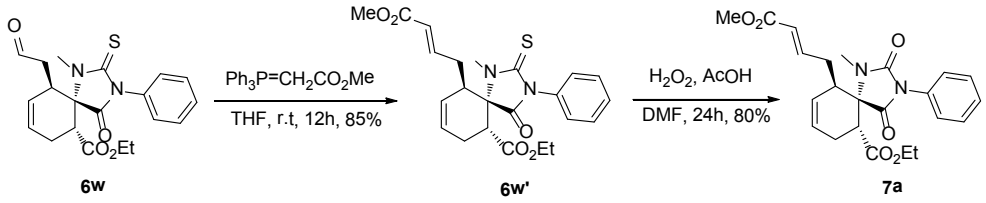
The product was obtained in 82% yield, pale yellow oil. $[\alpha]^{25}_D$ – 118.0 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.61 (s, 1H), 7.50-7.42 (m, 3H), 7.36-7.26 (m, 2H), 5.98-5.95 (m, 1H), 5.79-5.76 (m, 1H), 4.18 (q, *J* = 7.2 Hz), 3.47 (s, 3H), 3.28-3.22 (m, 3H), 2.83-2.75 (m, 1H), 2.59-2.51 (m, 1H), 2.45-2.37 (m, 1H), 1.24 (t, *J* = 7.2 Hz, 3H) ^{13}C NMR(100 MHz, $CDCl_3$): δ 198.6, 182.9, 174.8, 170.3, 133.9, 129.1, 129.0, 128.5, 128.2, 125.4, 65.8, 61.7, 45.5, 41.9, 35.9, 32.2, 25.2, 14.2; HRMS (EI): exact mass calculated for M^+ ($C_{20}H_{22}N_2O_4S$) requires m/z 386.1300, found m/z 386.1299; The enantiomeric excess was determined by HPLC after **6w** was converted to the corresponding α,β-unsaturated ester ($Ph_3P{=}CHCO_2Me$ in THF, r.t). [IA column, 254nm, *n*-Hexane: EtOH = 7:3, 0.8 mL/min]: 11.5 min (minor), 12.0 min (major), ee 92%.

6x:(5S,6R,10R)-ethyl-1-methyl-4-oxo-10-(2-oxoethyl)-3,9-diphenyl-2-thioxo-1,3-diazaspiro[4.5]dec-8-ene-6-carboxylate



The product was obtained in 86% yield, pale yellow solid. $[\alpha]^{25}_{D}$ – 90.6 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.48 (s, 1H), 7.51-7.32 (m, 10H), 6.20 (s, 1H), 4.21 (q, *J* = 7.2 Hz, 2H), 3.89 (d, *J* = 10.0 Hz, 1H), 3.52 (s, 3H), 3.44 (dd, *J* = 11.6, 8.4 Hz, 1H), 3.31 (dd, *J* = 19.2, 10.0 Hz, 1H), 3.03-2.95 (m, 1H), 2.84-2.76 (m, 1H), 2.28 (d, *J* = 19.2 Hz, 1H), 1.26 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR(100 MHz, $CDCl_3$): δ 198.5, 183.2, 174.9, 170.3, 138.8, 138.6, 134.0, 129.1, 129.0, 128.6, 128.4, 126.0, 123.5, 66.1, 61.8, 44.7, 40.9, 37.8, 32.4, 26.0, 14.2; HRMS (EI): exact mass calculated for M^+ ($C_{26}H_{26}N_2O_4S$) requires m/z 462.1613, found m/z 462.1618; The enantiomeric excess was determined by HPLC after **6x** was converted to the corresponding α,β-unsaturated ester (Ph_3P=$CHCO_2Me$ in THF, r.t). [IA column, 254nm, *n*-Hexane: EtOH = 7:3, 0.8 mL/min]: 9.2 min (minor), 12.4 min (major), ee 97%.

D: Elaboration of Diels-Alder Cycloaddition Adduct



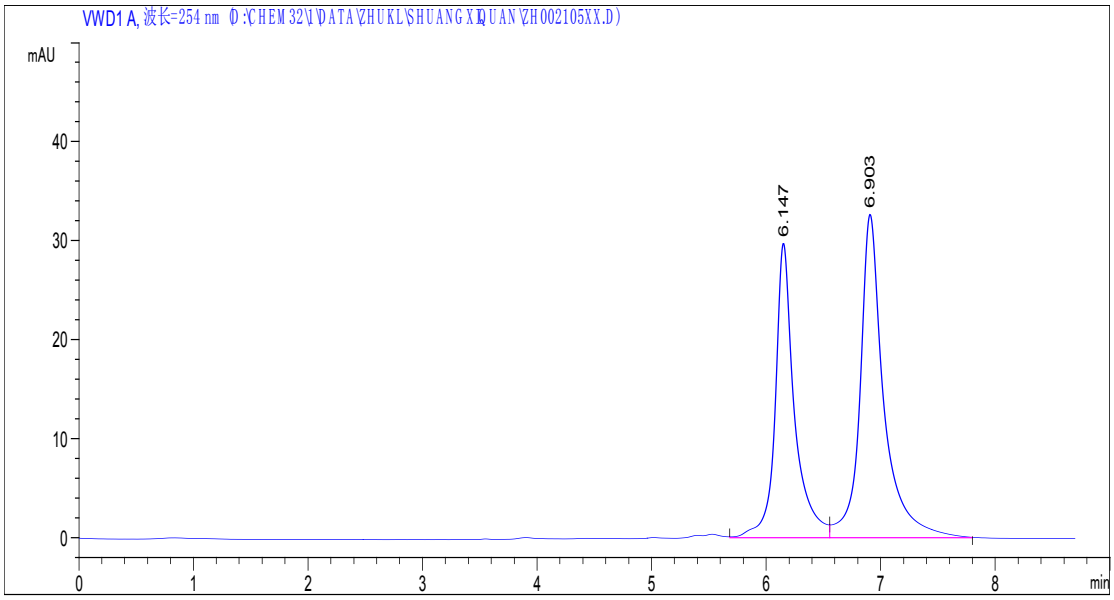
6w **6w'** **7a**

7a:(5S,6R,10R)-ethyl-10-(4-methoxy-4-oxobut-2-enyl)-1-methyl-2,4-dioxo-3-phenyl-1,3-diaza spiro[4.5]dec-8-ene-6-carboxylate

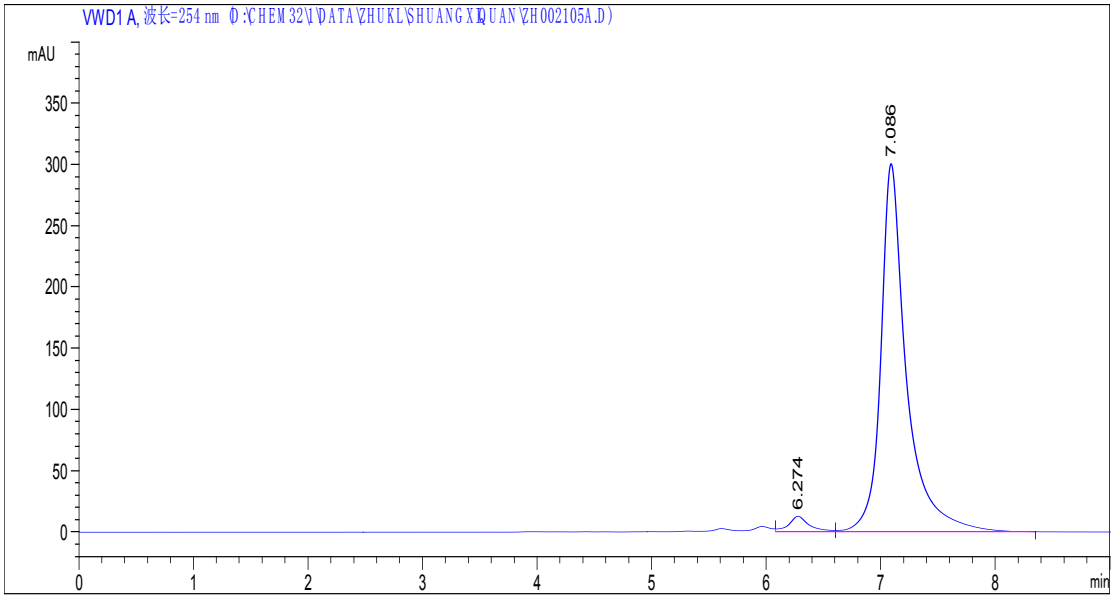
To a solution of **6w** (58.0 mg, 0.15 mmol) in THF (0.3 ml) was added $Ph_3P{=}CH_2CO_2Me$ (77.0 mg, 0.23 mmol), the reaction mixture was tirred at room temperature. After 2h, solvent was removed in vacuum. The residue was purified by silica gel chromatography to afford **6w'** (56.2 mg, 85%). To a solution of **6w'** (44.2 mg, 0.1 mmol) in DMF (0.5 ml) was added AcOH (50 µl) , the mixture was stirred for 20min at room temperature. Hydrogen peroxide (30%, 0.25 ml) was added, the mixture was heated to 50^{o}C and TLC monitored. After 24h, the mixture was cooled, diluted with H_2O (2 ml) and extracted with EtOAc (2 ml×2). The organic phase was washed with brine, dried with Na_2SO_4, and concentrated in vacuum. The residue was purified by silica gel chromatography to give the product **7a** as colorless oil (34 mg, 80% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.51-7.42 (m, 3H), 7.33-7.32 (m, 2H), 6.93-6.86 (m, 1H), 5.96-5.87 (m, 2H), 5.80-5.78 (m, 1H), 4.19 (q, *J* = 7.2 Hz, 2H), 3.73 (m, 3H), 3.37 (s, 3H), 3.25-3.21 (m, 1H), 2.94-2.84 (m, 2H), 2.52-2.37 (m, 2H), 2.37-2.29 (m, 1H), 1.27 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 182.6, 173.0, 170.9, 166.4, 144.8, 133.6, 129.2, 129.1, 128.3, 126.7, 125.8, 123.8, 67.8, 61.8, 51.6, 43.0, 39.1, 33.5, 32.0, 25.9, 14.2; HRMS (EI): exact mass calculated for M^+ ($C_{233}H_{26}N_2O_6$) requires m/z 426.1791, found m/z 426.1795. [IA column, 254nm, *n*-Hexane: *i*-PrOH = 7:3, 0.8 mL/min]: 11.01 min (minor), 11.94 min (major), ee 91%.

E: HPLC Charts of Diels-Alder Raction Products

6a:2-((5S,6R,10S)-10-(4-bromophenyl)-3-cyclohexyl-4-oxo-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde

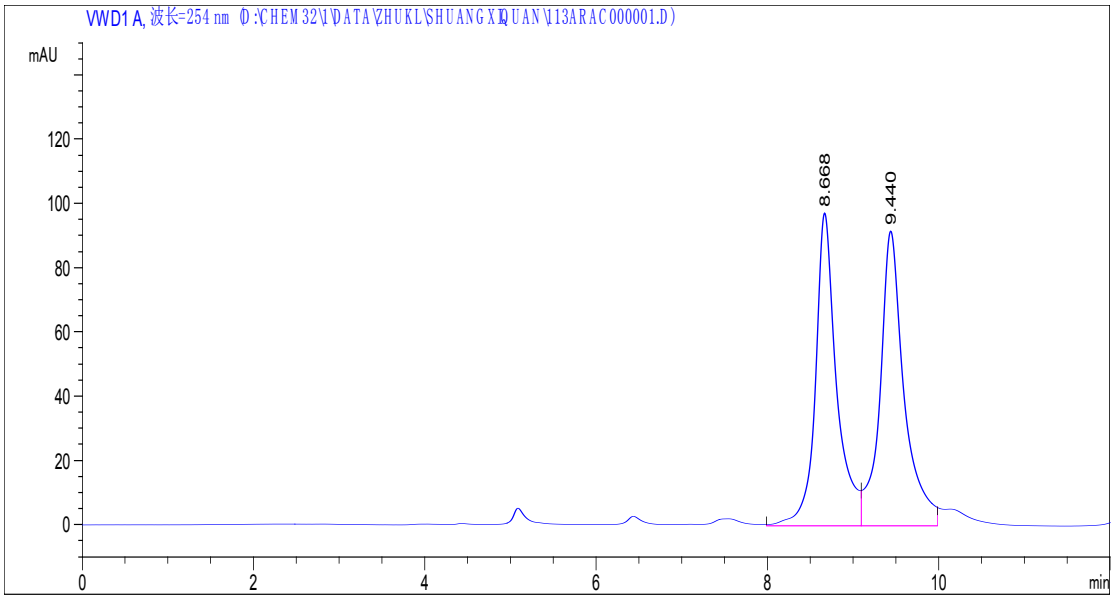


#	Time	Area	Height	Width	Symmetry	Area %
1	6.147	349.5	29.8	0.166	0.714	47.465
2	6.903	473.6	32.7	0.2055	0.686	52.535

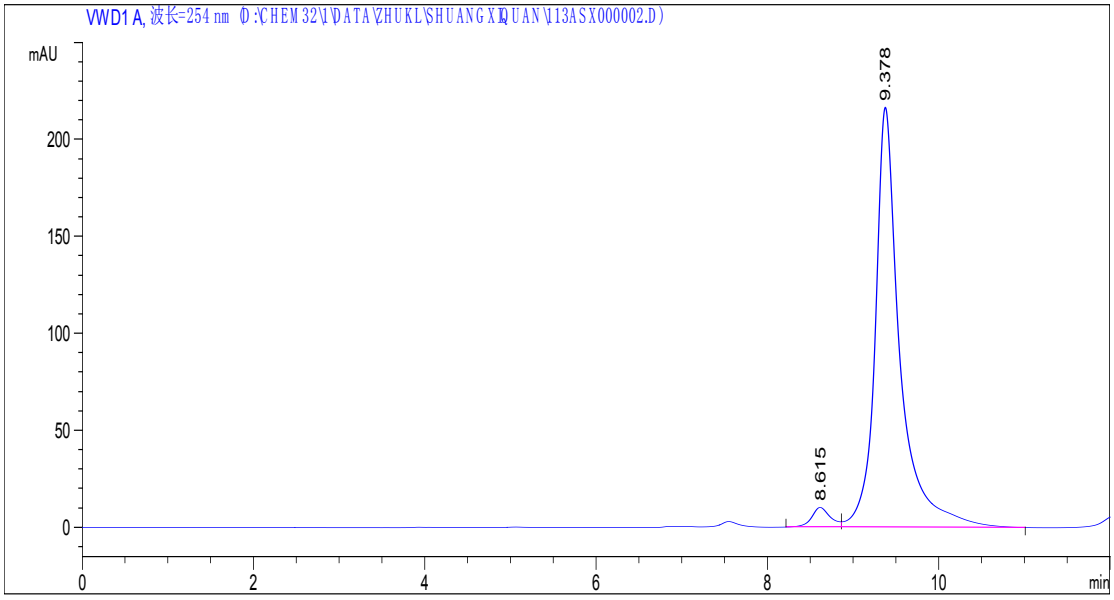


#	Time	Area	Height	Width	Symmetry	Area %
1	6.274	163.9	12.8	0.181	0.761	3.273
2	7.086	4694.1	300.7	0.2229	0.631	96.827

6b:2-((5S,6R,10S)-10-(4-fluorophenyl)-4-oxo-3-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde

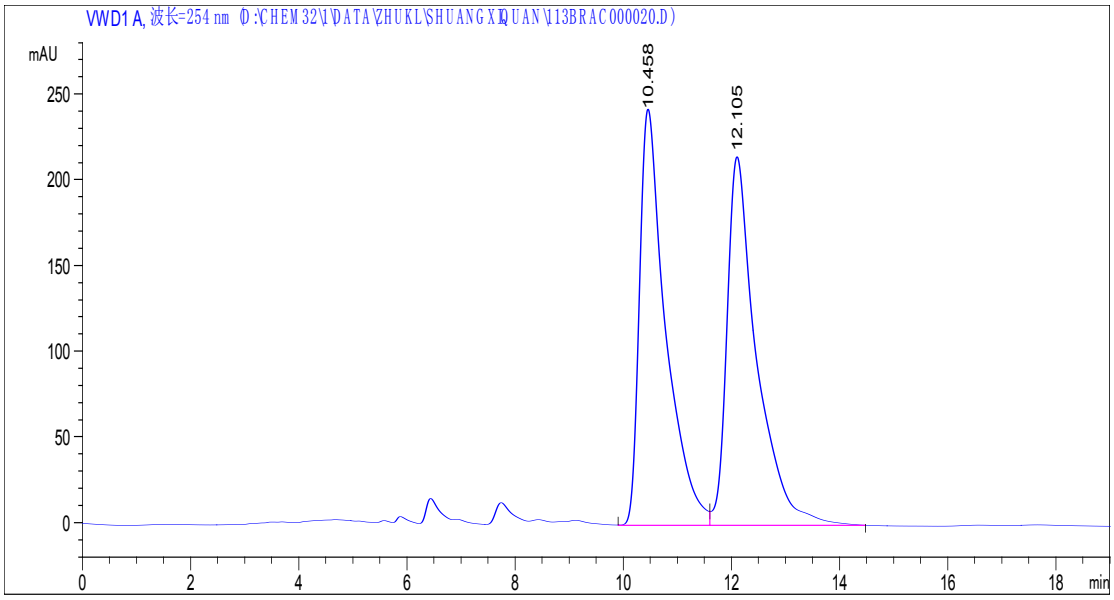


#	Time	Area	Height	Width	Symmetry	Area %
1	8.668	1680.1	97.4	0.2874	0.758	48.359
2	9.44	1794.1	91.8	0.3257	0.768	51.641

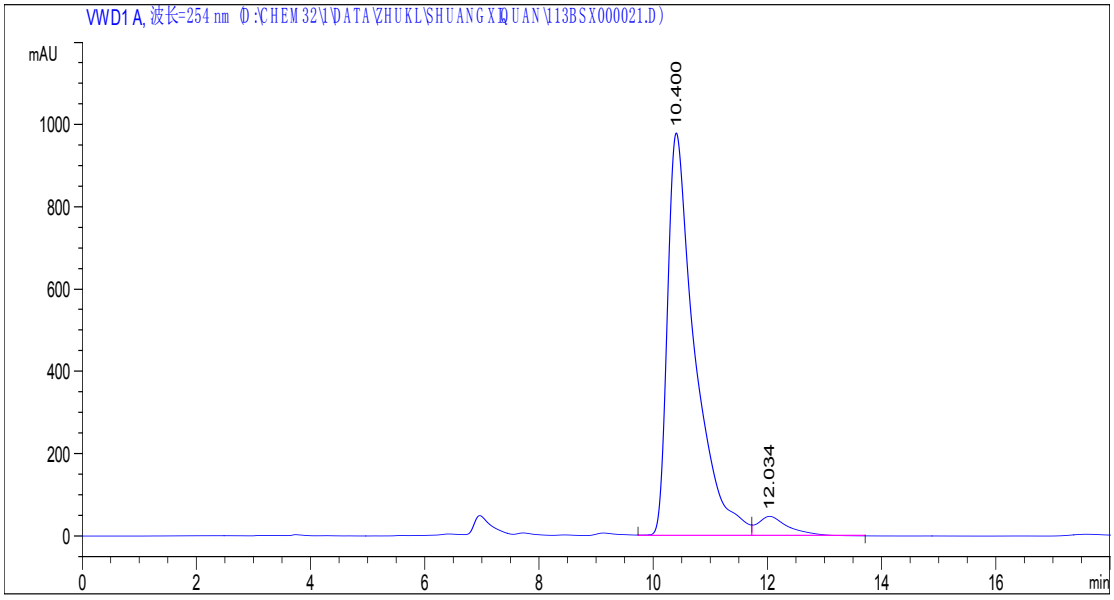


#	Time	Area	Height	Width	Symmetry	Area %
1	8.615	157	10.2	0.2241	0.816	3.483
2	9.378	4351.6	216.6	0.2868	0.642	96.517

6c:2-((5S,6R,10S)-10-(4-nitrophenyl)-4-oxo-3-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde

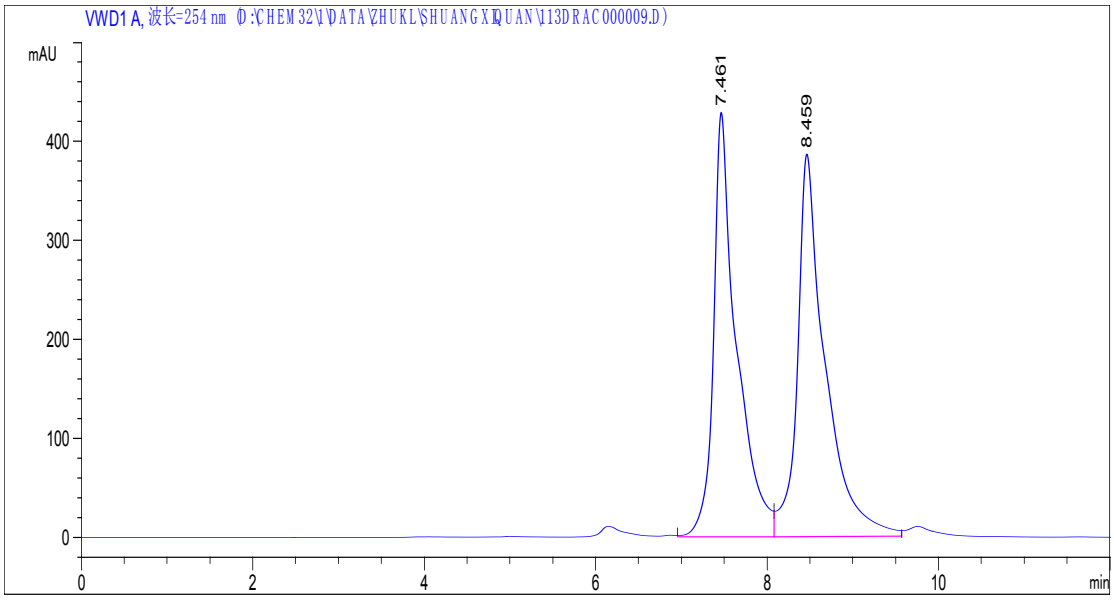


#	Time	Area	Height	Width	Symmetry	Area %
1	10.458	8179.2	242.7	0.4863	0.445	49.846
2	12.105	8229.9	215	0.5484	0.473	50.154

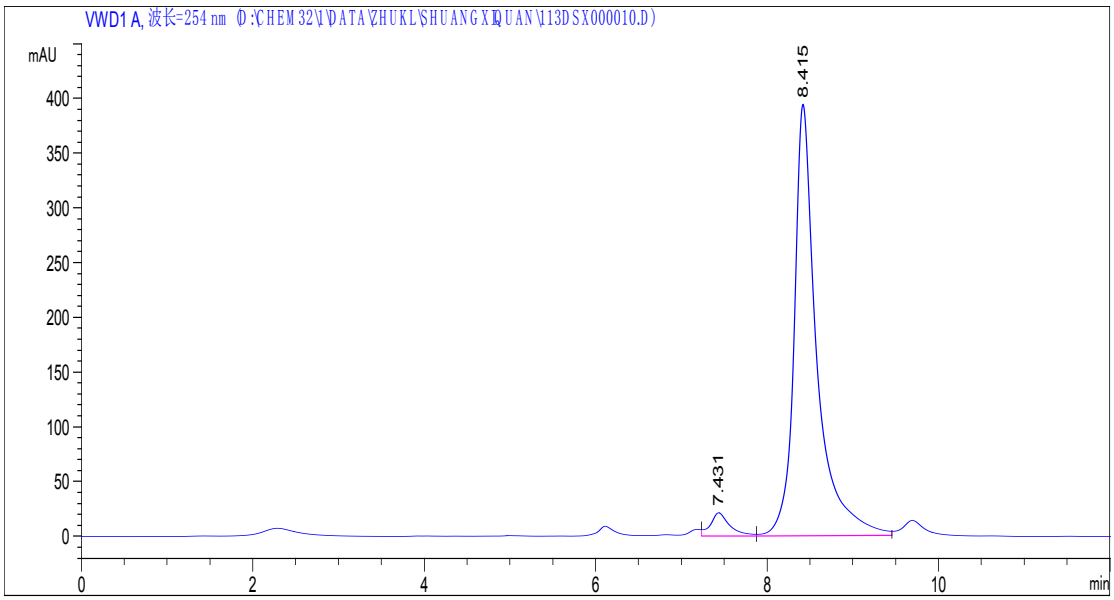


#	Time	Area	Height	Width	Symmetry	Area %
1	10.4	32542.7	979.3	0.478	0.44	94.745
2	12.034	1804.8	47.6	0.5385	0.549	5.255

6d:2-((5S,6R,10S)-4-oxo-3,10-diphenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde

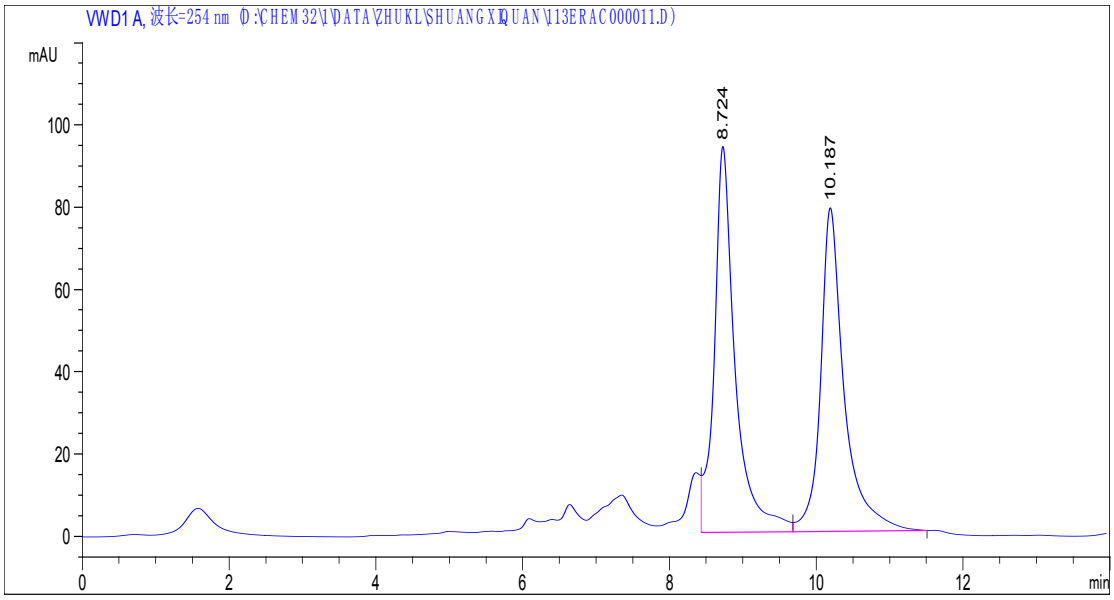


#	Time	Area	Height	Width	Symmetry	Area %
1	7.461	7975.6	428.8	0.2534	0.484	47.830
2	8.459	8699.5	386.6	0.3077	0.488	52.170

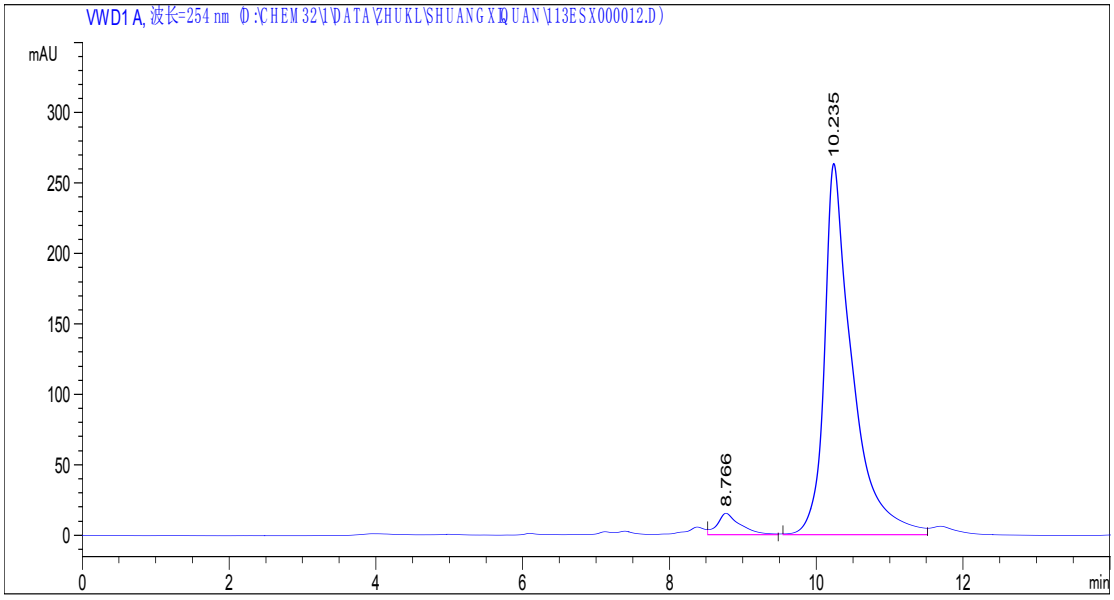


#	Time	Area	Height	Width	Symmetry	Area %
1	7.431	335.3	21.3	0.2233	0.689	4.417
2	8.415	7255.8	394.2	0.2614	0.597	95.583

6e:2-((5S,6R,10S)-10-(4-methoxyphenyl)-4-oxo-3-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde

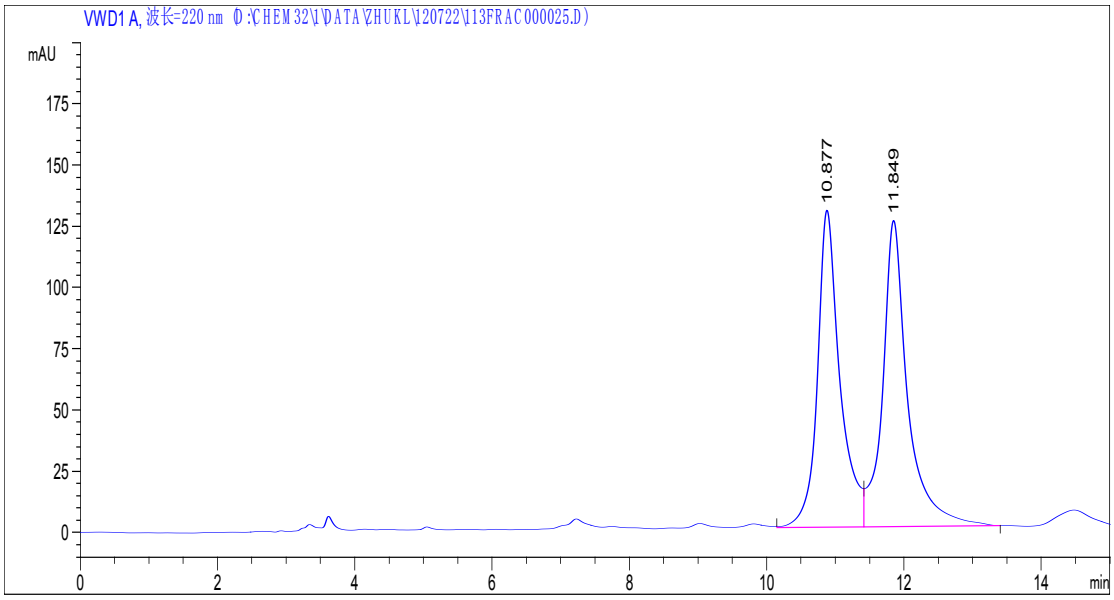


#	Time	Area	Height	Width	Symmetry	Area %
1	8.724	1863.1	93.9	0.281	0.643	51.419
2	10.187	1760.3	78.7	0.3192	0.661	48.581

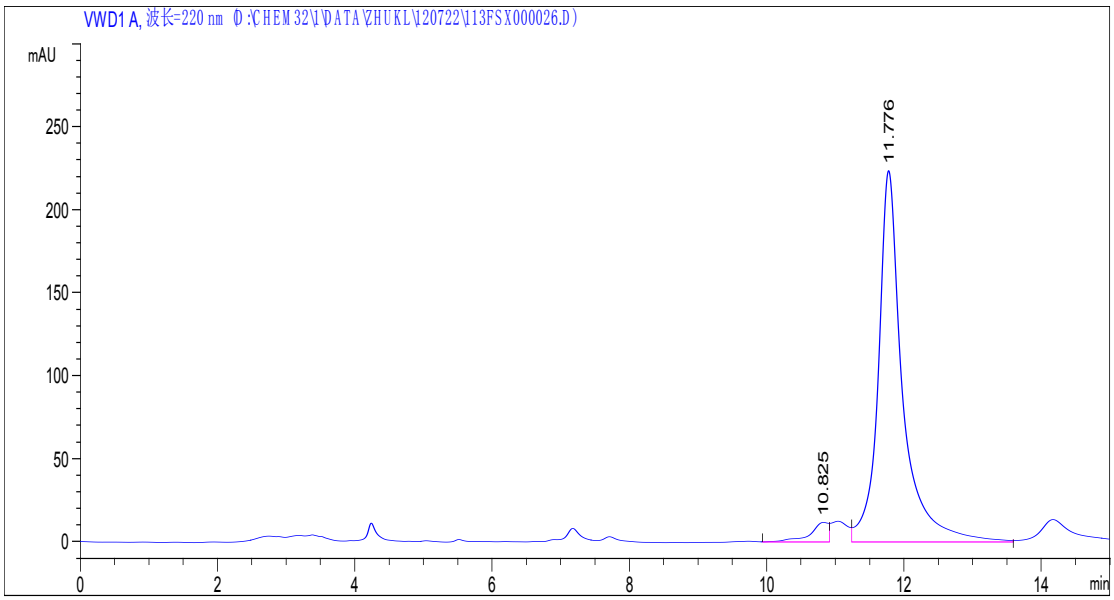


#	Time	Area	Height	Width	Symmetry	Area %
1	8.766	345.7	15.5	0.3047	0.552	4.726
2	10.235	6970.1	263.8	0.3621	0.493	95.274

6f:2-((5S,6R,10S)-10-(3-nitrophenyl)-4-oxo-3-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde

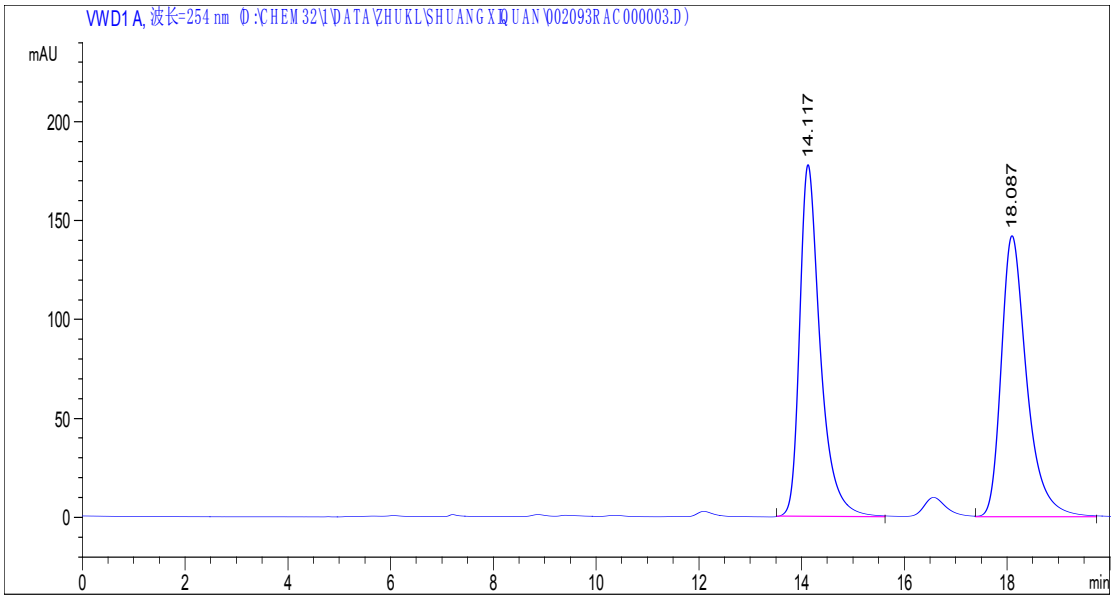


#	Time	Area	Height	Width	Symmetry	Area %
1	10.877	2954.5	129.5	0.3274	0.709	48.242
2	11.849	3169.9	125	0.3598	0.722	51.758

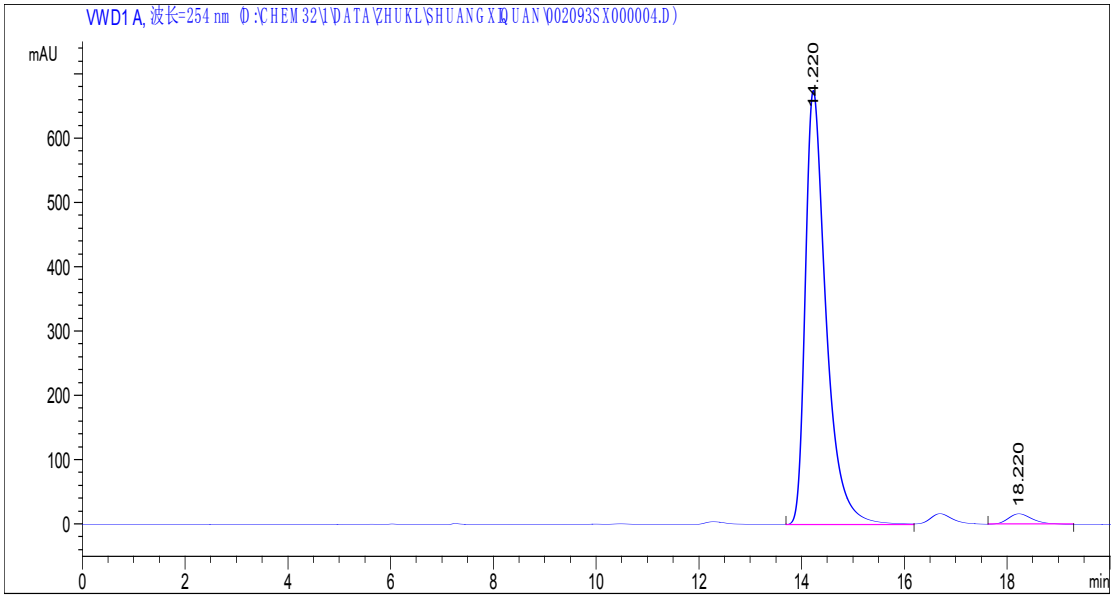


#	Time	Area	Height	Width	Symmetry	Area %
1	10.825	234.6	12	0.276	3.156	4.060
2	11.776	5543.5	224	0.3513	0.68	95.940

6g:(5S,6S,10R)-ethyl-4-oxo-10-(2-oxoethyl)-3-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-8-ene-6-carboxylate

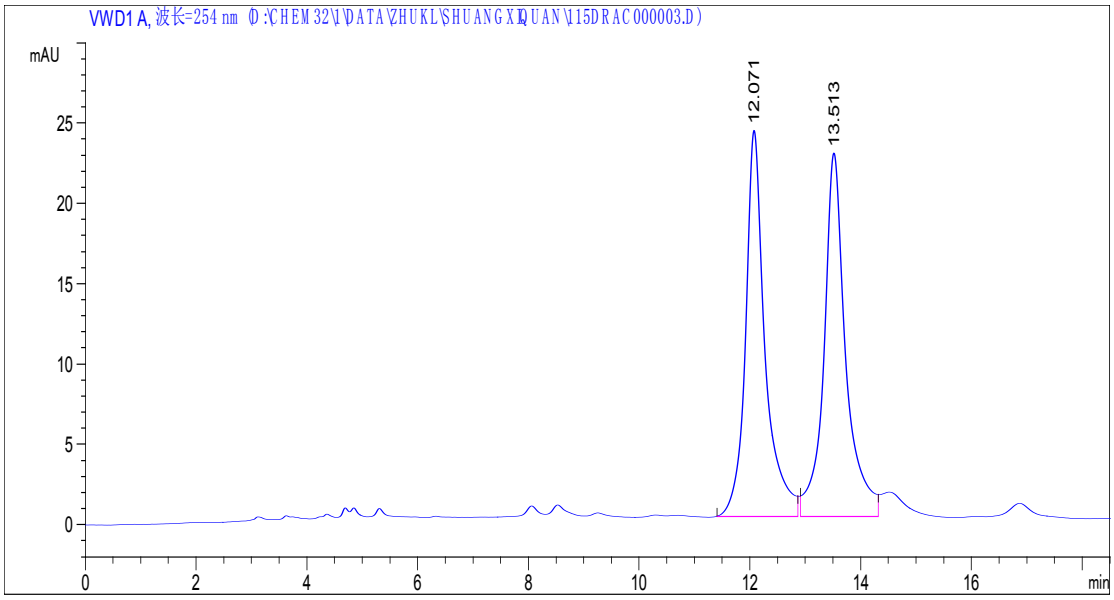


#	Time	Area	Height	Width	Symmetry	Area %
1	14.117	4961.4	178	0.4183	0.633	50.255
2	18.087	4911	142.2	0.5194	0.676	49.745

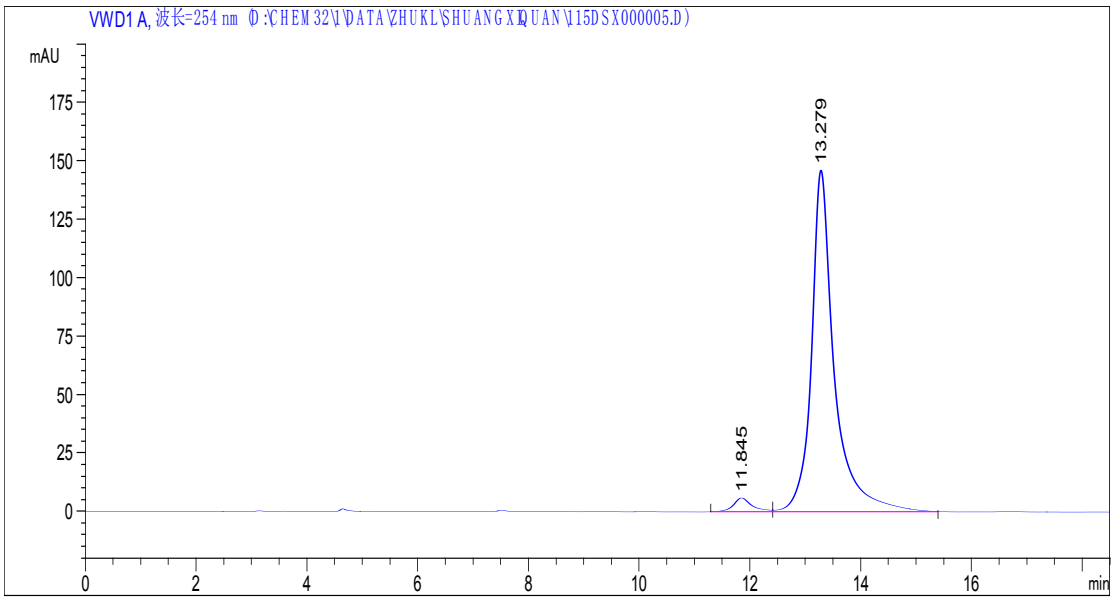


#	Time	Area	Height	Width	Symmetry	Area %
1	14.22	18954.7	675	0.4208	0.576	97.068
2	18.22	572.4	16.7	0.516	0.731	2.932

6h:2-((5S,6R,10S)-10-(4-bromophenyl)-4-oxo-3-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde

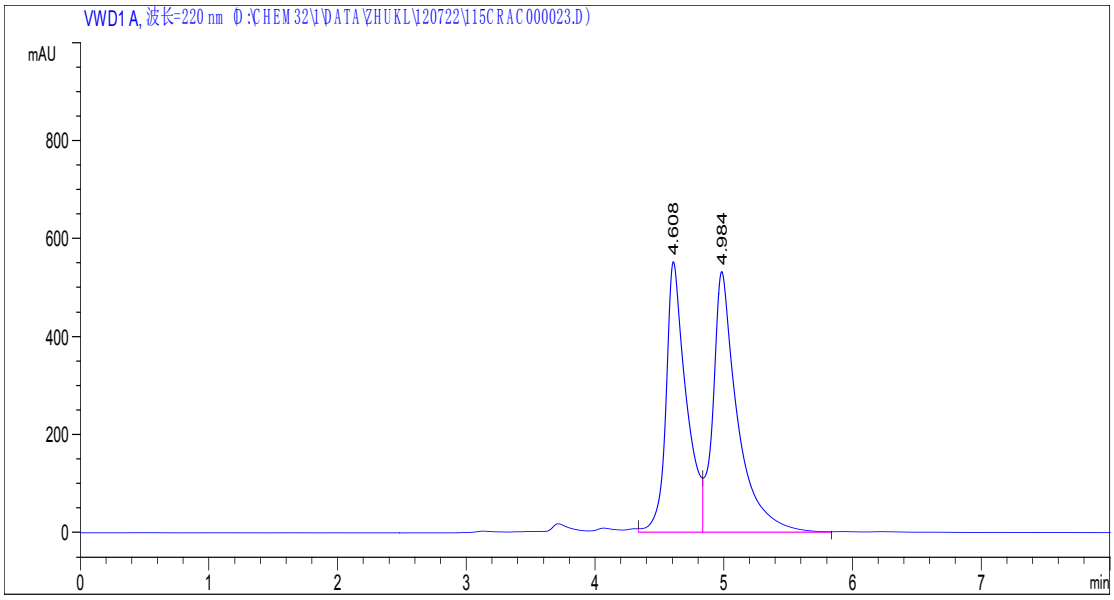


#	Time	Area	Height	Width	Symmetry	Area %
1	12.071	588.4	24	0.3525	0.73	48.775
2	13.513	618	22.6	0.39	0.8	51.225

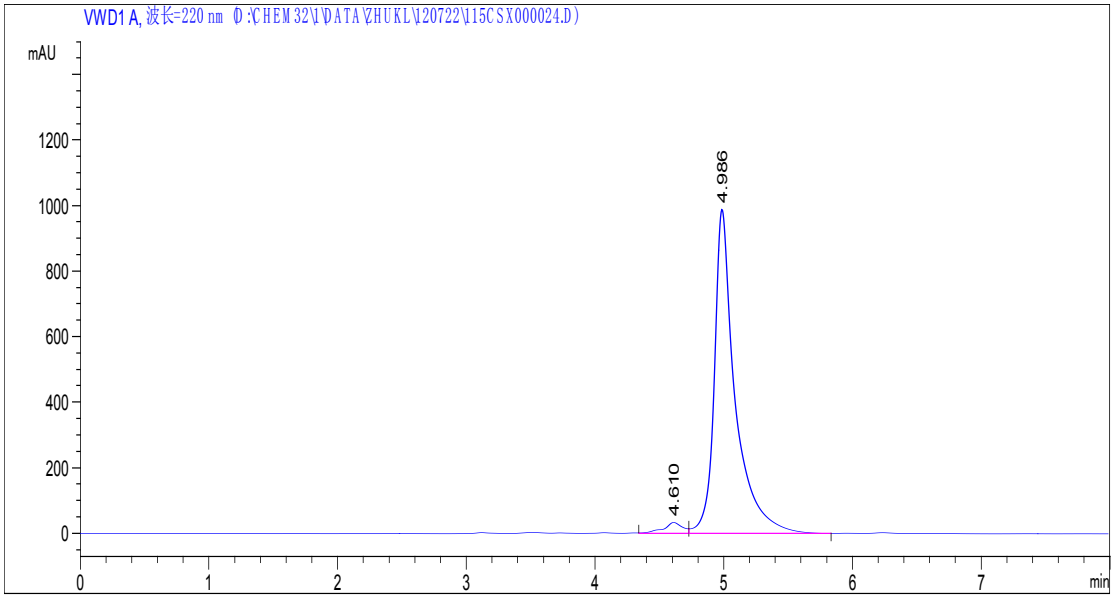


#	Time	Area	Height	Width	Symmetry	Area %
1	11.845	143.4	6	0.3475	0.746	3.309
2	13.279	4190	146.2	0.4058	0.667	96.691

6i:2-((5S,6R,10S)-3-cyclohexyl-4-oxo-10-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl) acetaldehyde

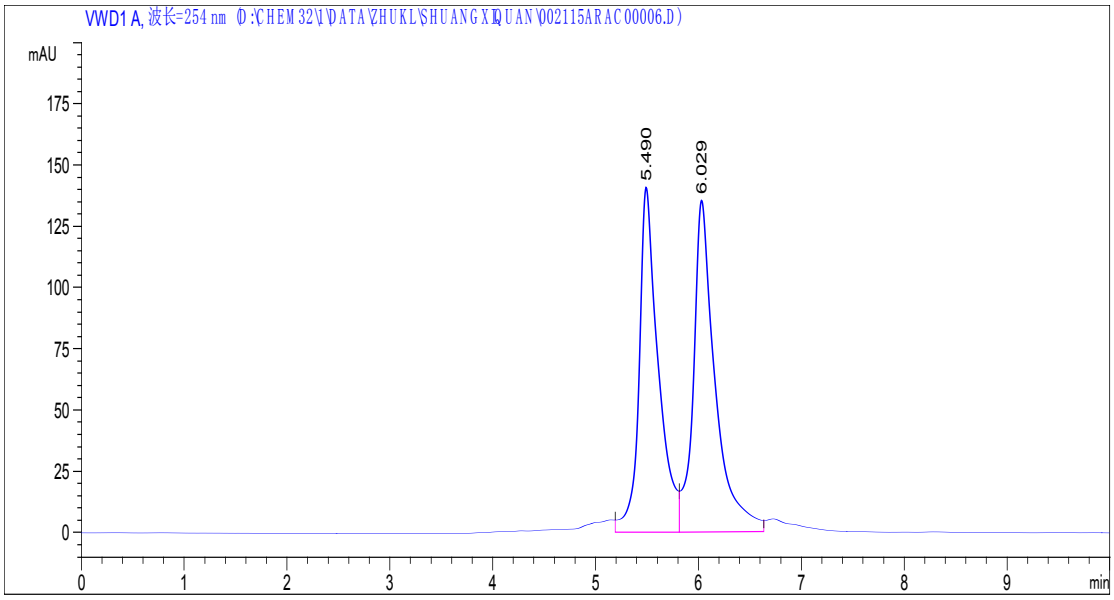


#	Time	Area	Height	Width	Symmetry	Area %
1	4.608	6051.2	553.5	0.1523	0.565	48.089
2	4.984	7078.1	533	0.184	0.509	51.911

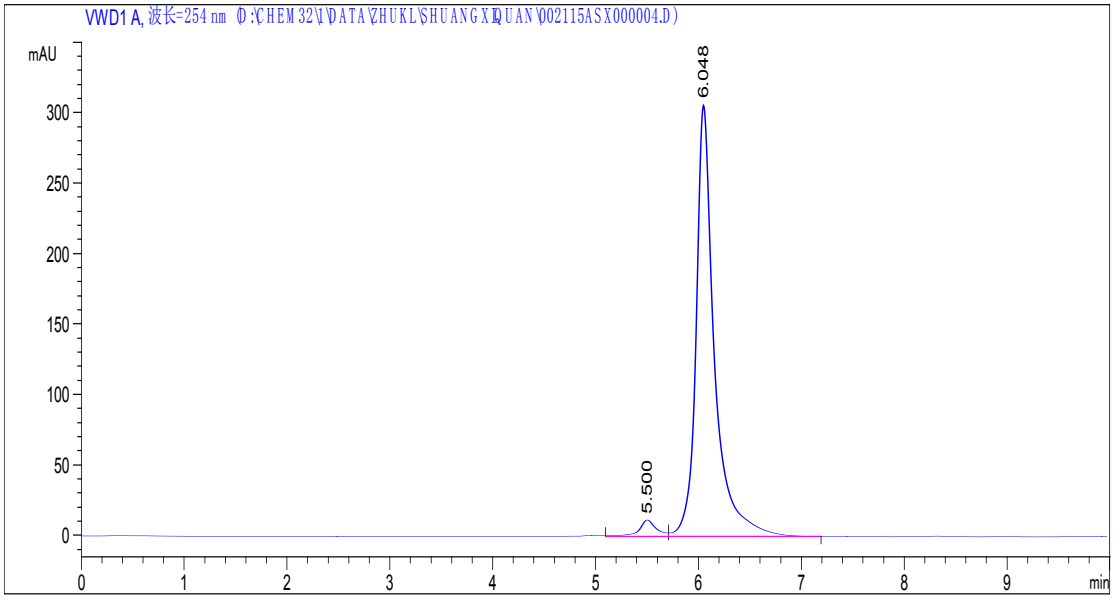


#	Time	Area	Height	Width	Symmetry	Area %
1	4.61	372.6	34.6	0.149	1.277	3.224
2	4.986	11185	990.7	0.1579	0.547	96.776

6j:2-((5S,6R,10S)-10-(4-bromophenyl)-3-isopropyl-4-oxo-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde

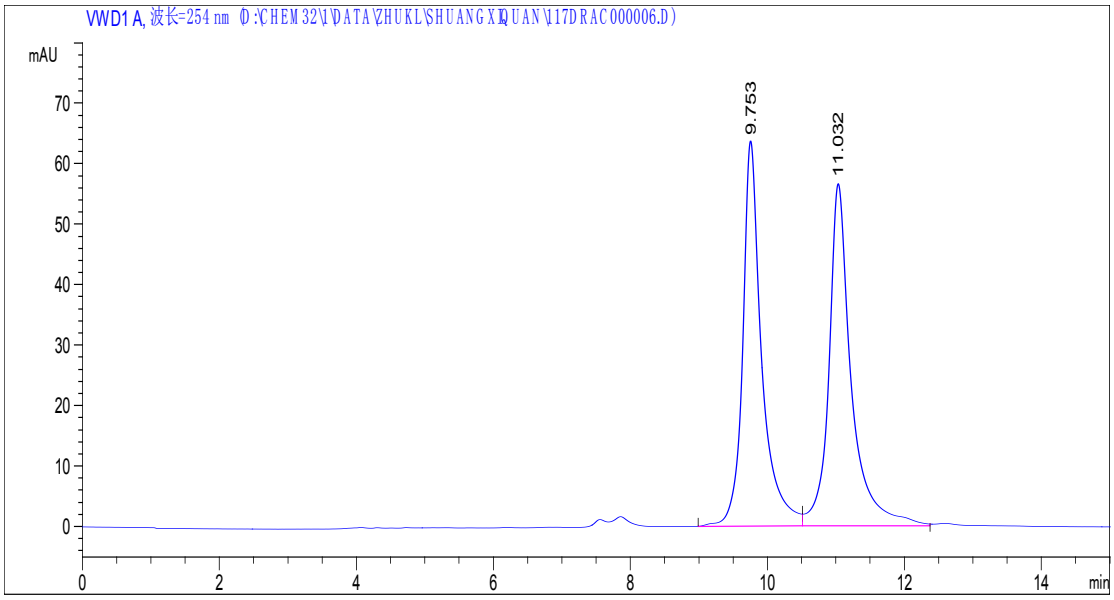


#	Time	Area	Height	Width	Symmetry	Area %
1	5.49	1831.6	140.9	0.1793	0.584	47.783
2	6.029	2001.5	135.6	0.2043	0.567	52.217

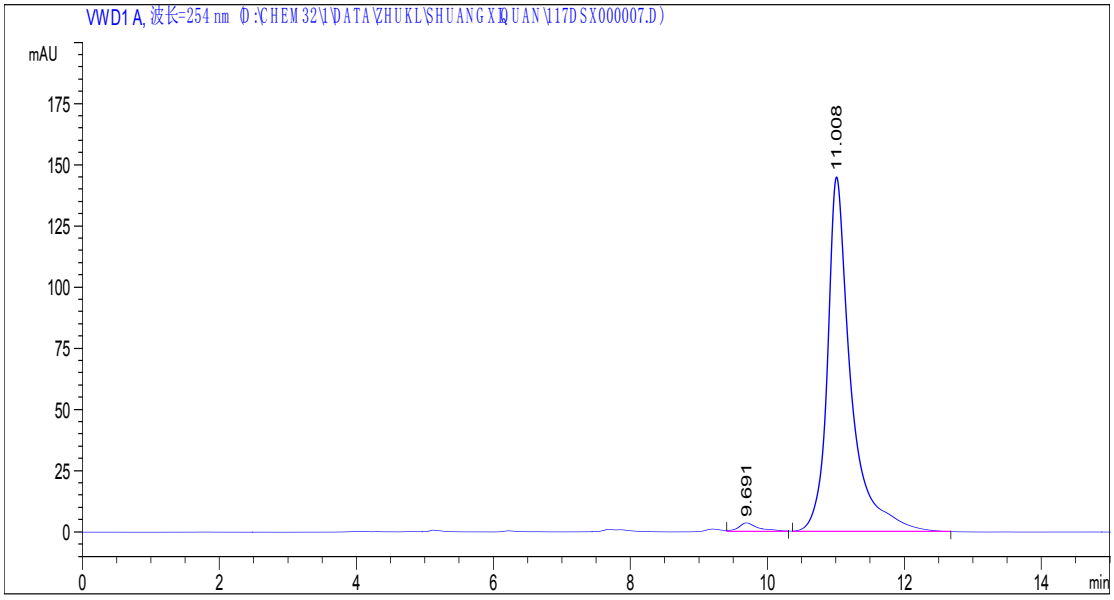


#	Time	Area	Height	Width	Symmetry	Area %
1	5.5	145.6	11.8	0.1726	0.966	3.684
2	6.048	3806.5	306.1	0.1785	0.631	96.316

6k:2-((5S,6R,9S,10S)-10-(4-fluorophenyl)-7,9-dimethyl-4-oxo-3-phenyl-2-thioxo-1-thia-3-aza spiro[4.5]dec-7-en-6-yl)acetaldehyde

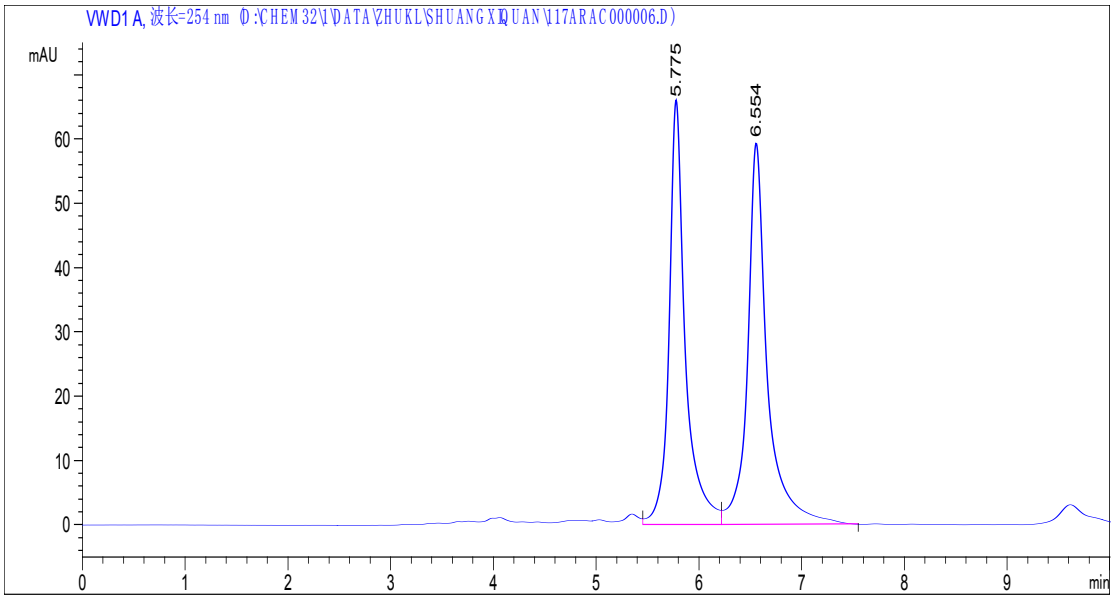


#	Time	Area	Height	Width	Symmetry	Area %
1	9.753	1231.3	63.7	0.275	0.673	48.882
2	11.032	1287.6	56.6	0.3237	0.675	51.118

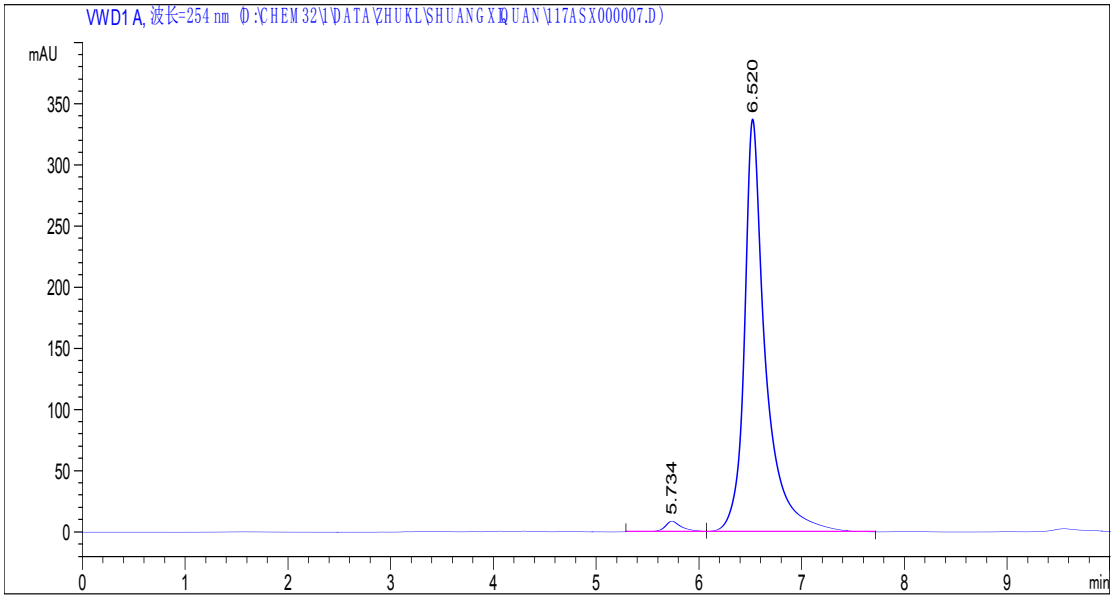


#	Time	Area	Height	Width	Symmetry	Area %
1	9.691	80.4	3.7	0.3059	0.573	2.282
2	11.008	3442.3	144.9	0.3354	0.602	97.718

6l:(5S,6S,7S,10R)-ethyl-7,9-dimethyl-4-oxo-10-(2-oxoethyl)-3-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-8-ene-6-carboxylate

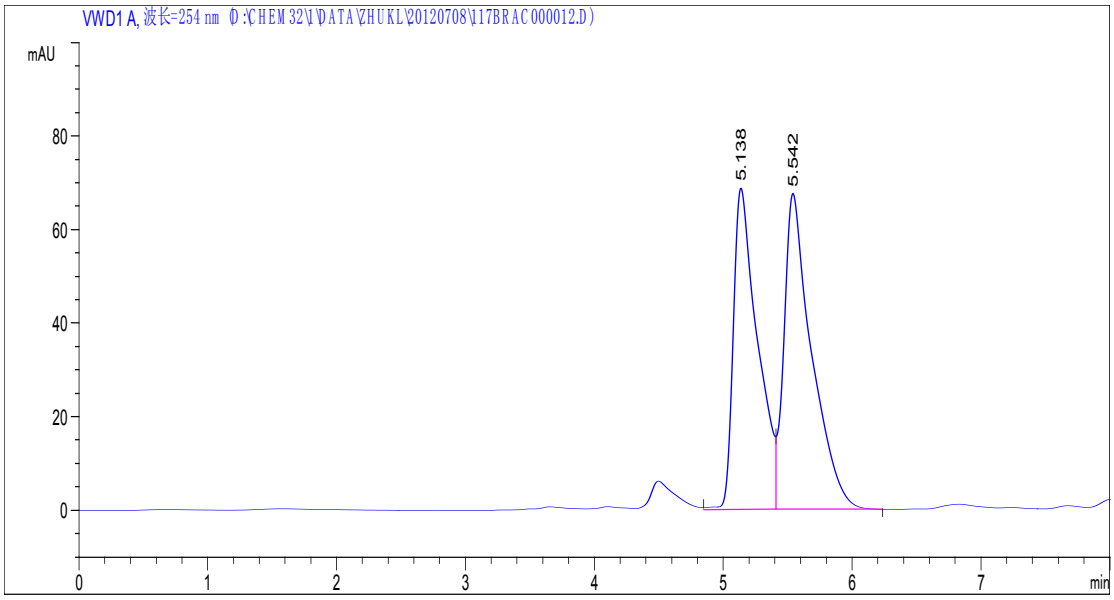


#	Time	Area	Height	Width	Symmetry	Area %
1	5.775	727.2	66.1	0.1575	0.716	48.843
2	6.554	792.7	59.4	0.1907	0.712	51.157

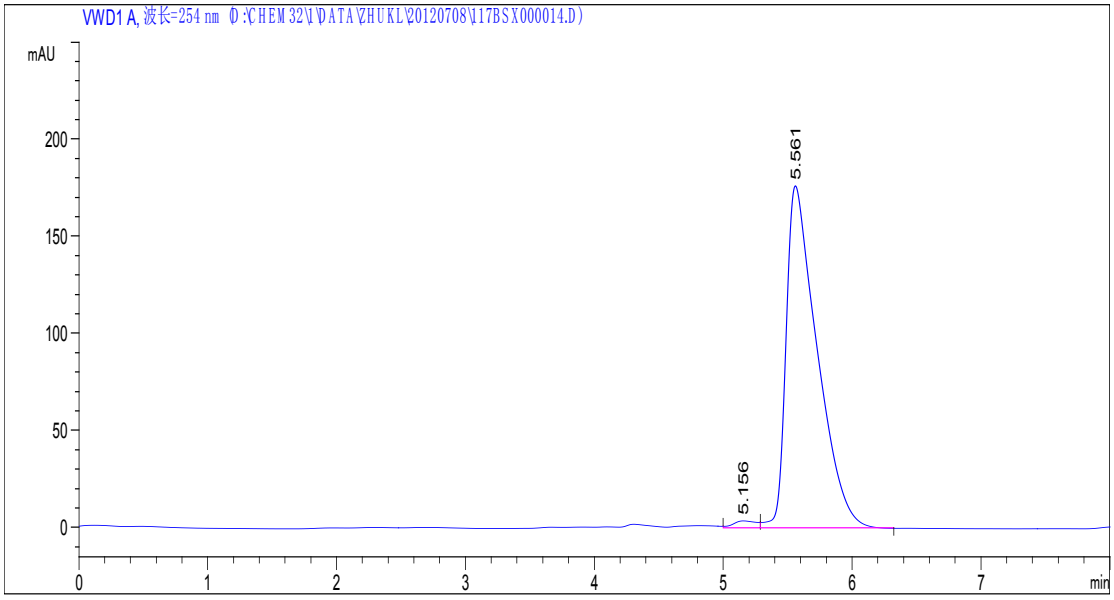


#	Time	Area	Height	Width	Symmetry	Area %
1	5.734	105.2	8.8	0.1705	0.696	2.136
2	6.52	4820	337.2	0.2032	0.605	97.864

6m:2-((5S,6R,9S,10S)-3-cyclohexyl-7,9-dimethyl-4-oxo-10-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde

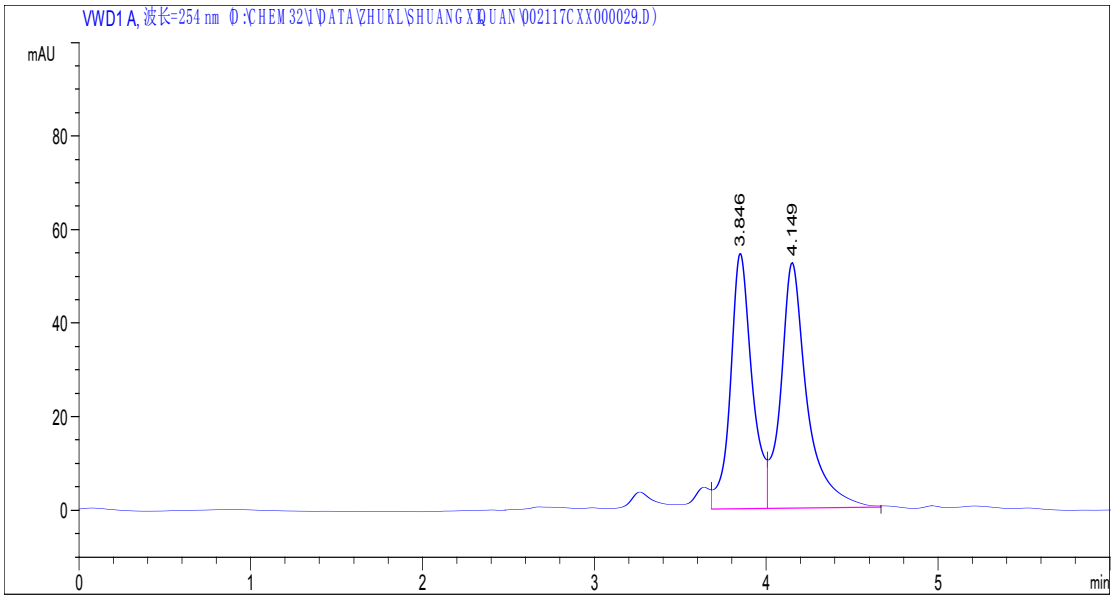


#	Time	Area	Height	Width	Symmetry	Area %
1	5.138	894.5	68.8	0.1837	0.439	46.902
2	5.542	1012.7	67.6	0.2082	0.445	53.098

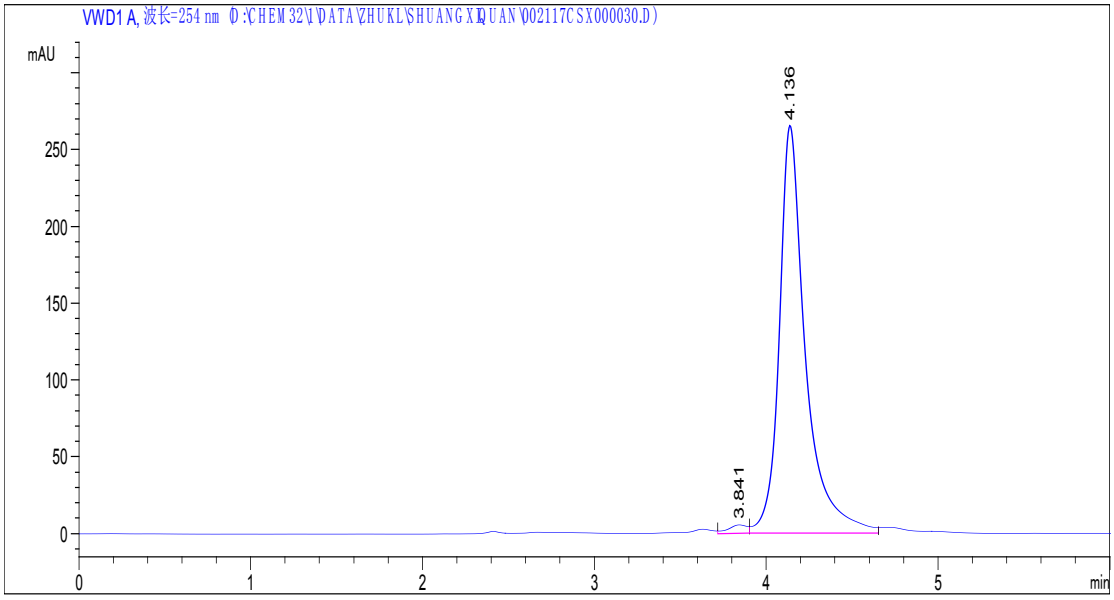


#	Time	Area	Height	Width	Symmetry	Area %
1	5.156	49.1	3.8	0.1872	0.824	1.632
2	5.561	2957.5	176.4	0.2393	0.408	98.368

6n:2-((5S,6R,9S,10S)-10-(4-bromophenyl)-3-cyclohexyl-7,9-dimethyl-4-oxo-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde

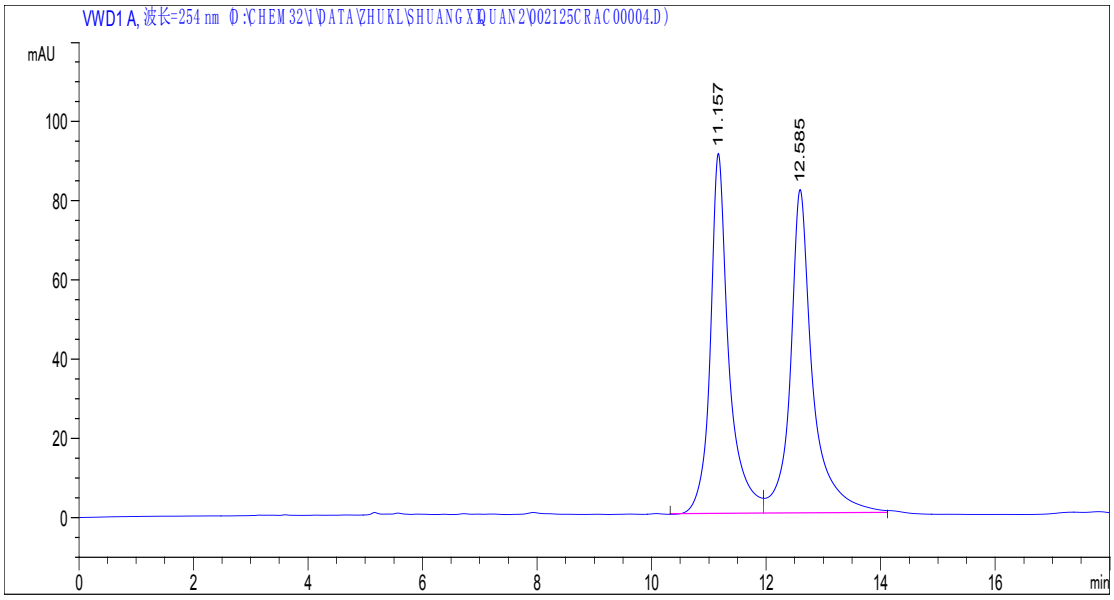


#	Time	Area	Height	Width	Symmetry	Area %
1	3.846	479.2	54.7	0.1284	0.797	47.101
2	4.149	560.2	52.6	0.1519	0.686	52.899

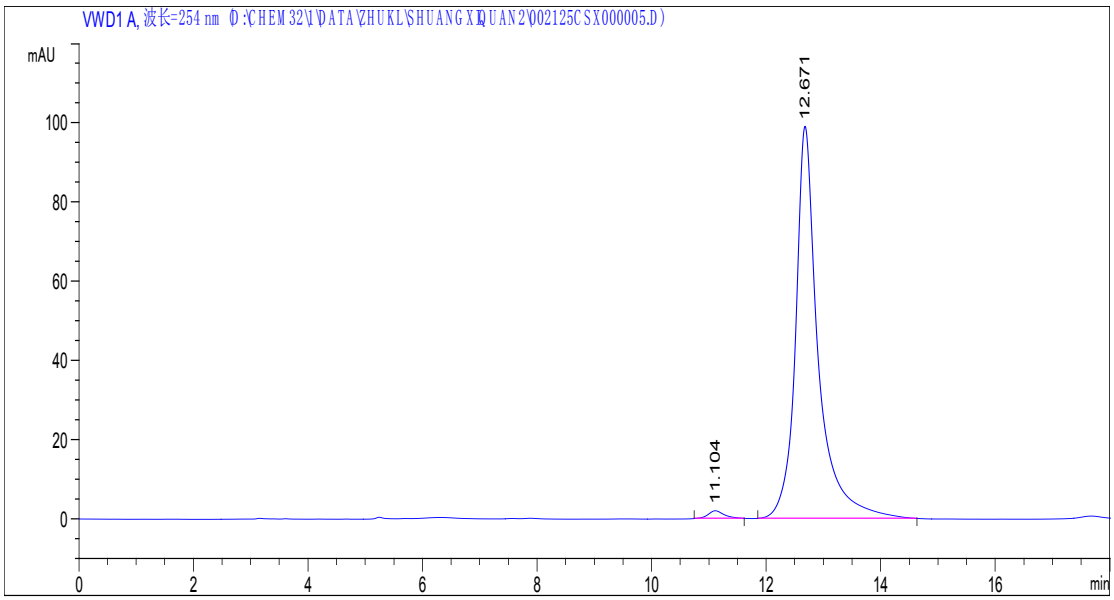


#	Time	Area	Height	Width	Symmetry	Area %
1	3.841	44.3	5.7	0.1132	1.411	1.546
2	4.136	2819.2	265.6	0.1544	0.642	98.454

6o:2-((5S,6R,10S)-7-ethyl-10-(3-nitrophenyl)-4-oxo-3-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde

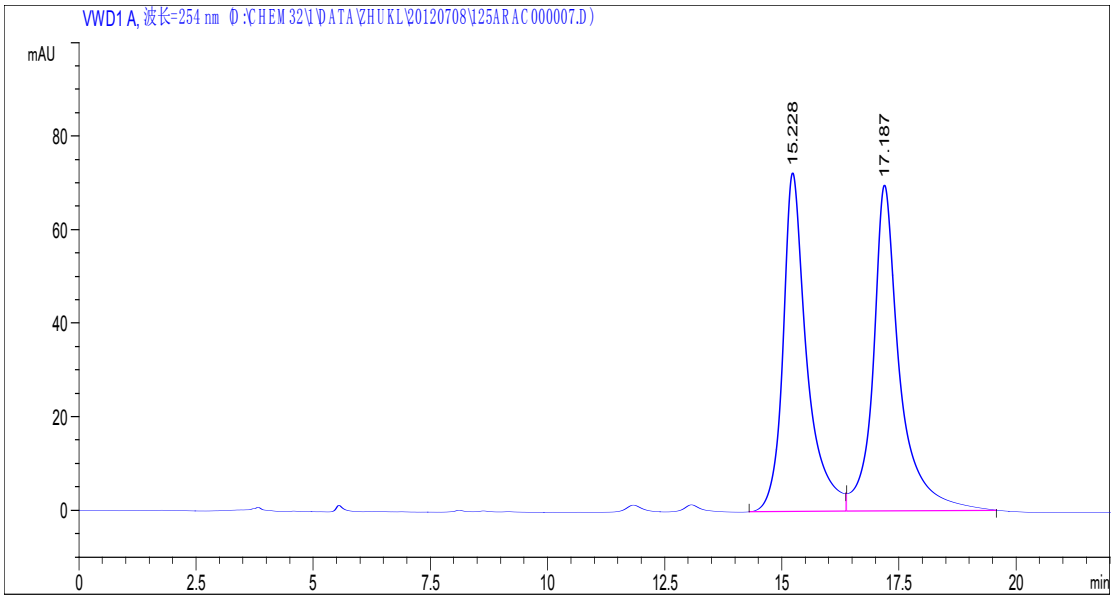


#	Time	Area	Height	Width	Symmetry	Area %
1	11.157	2060.8	91.1	0.3237	0.718	48.123
2	12.585	2221.6	81.8	0.3868	0.731	51.877

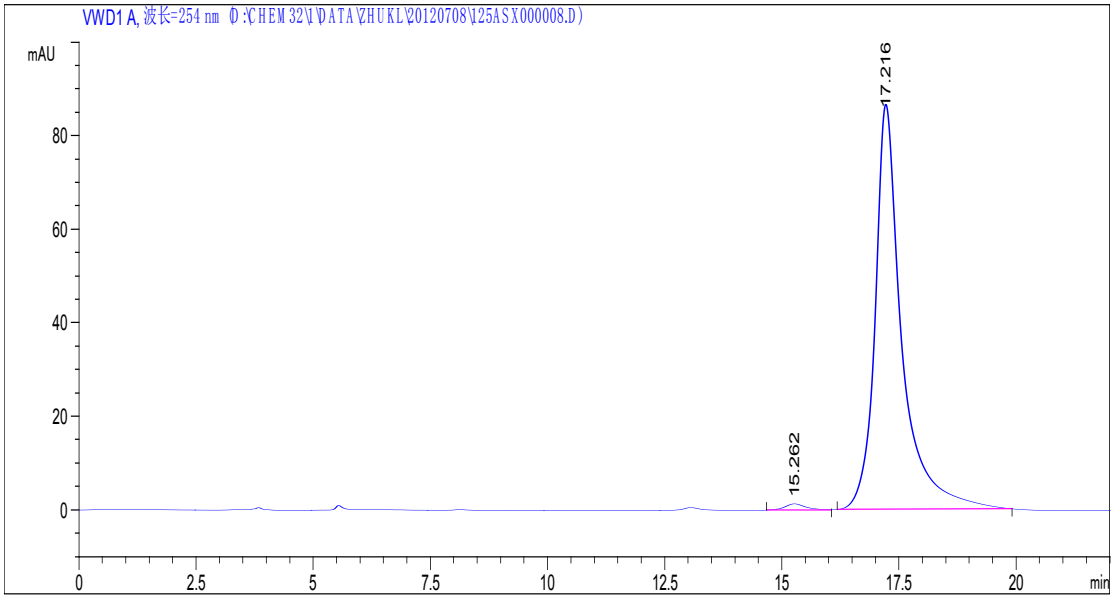


#	Time	Area	Height	Width	Symmetry	Area %
1	11.104	40.9	2	0.2994	0.767	1.476
2	12.671	2727	99.1	0.3938	0.667	98.524

6p:(5S,6S,10R)-ethyl-9-ethyl-4-oxo-10-(2-oxoethyl)-3-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-8-ene-6-carboxylate

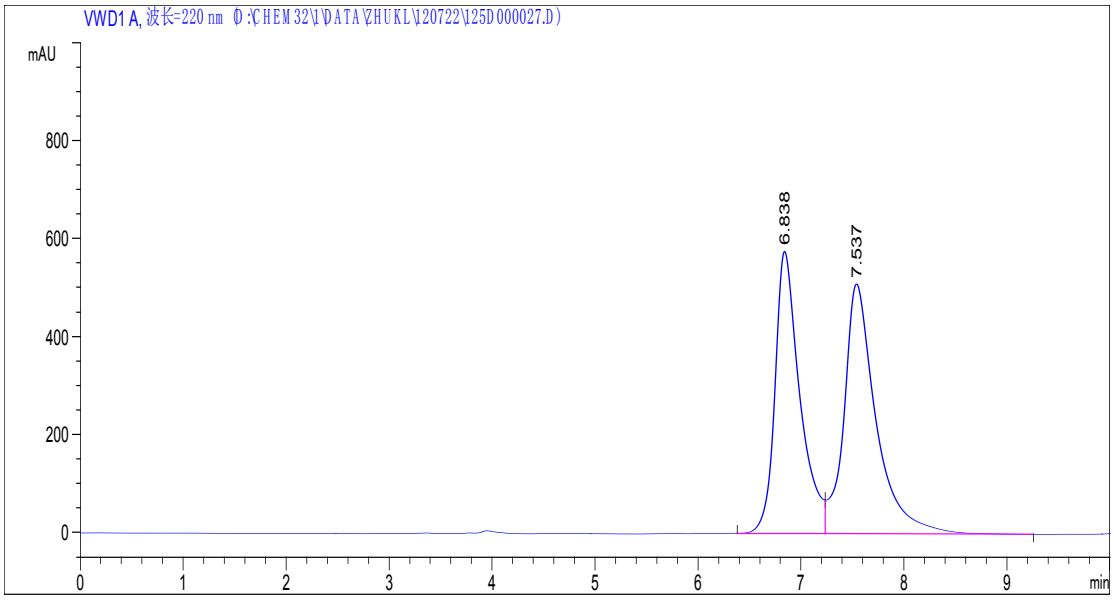


#	Time	Area	Height	Width	Symmetry	Area %
1	15.228	2570.1	72.5	0.5095	0.649	48.232
2	17.187	2758.4	69.8	0.5614	0.689	51.768

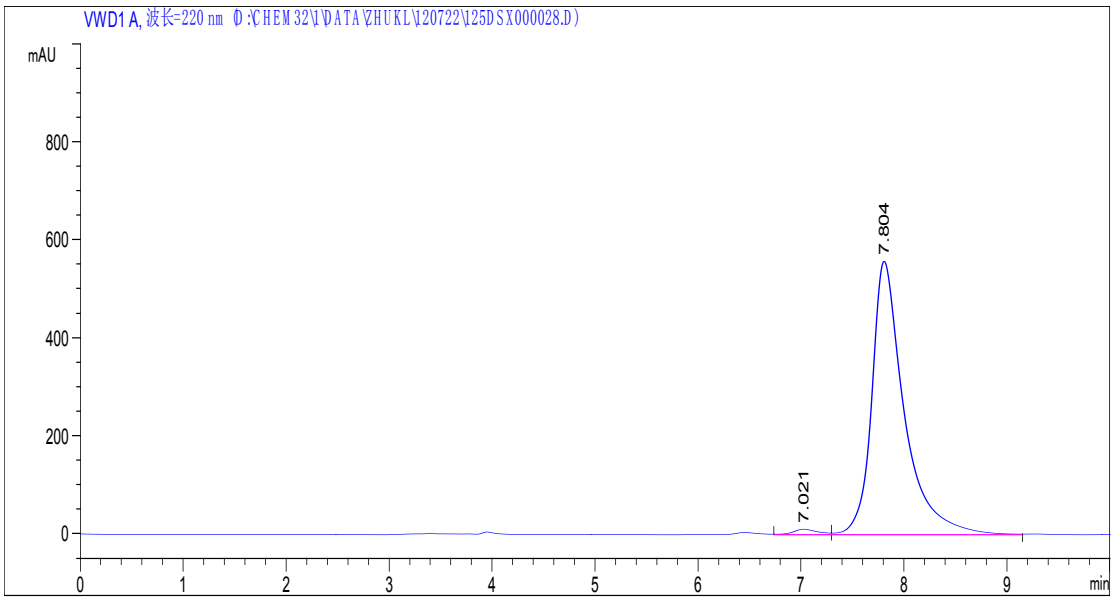


#	Time	Area	Height	Width	Symmetry	Area %
1	15.262	47	1.4	0.559	0.822	1.347
2	17.216	3444	86.7	0.574	0.616	98.653

6q:2-((5S,6R,10S)-10-(4-bromophenyl)-3-cyclohexyl-7-ethyl-4-oxo-2-thioxo-1-thia-3-azaspiro [4.5]dec-7-en-6-yl)acetaldehyde

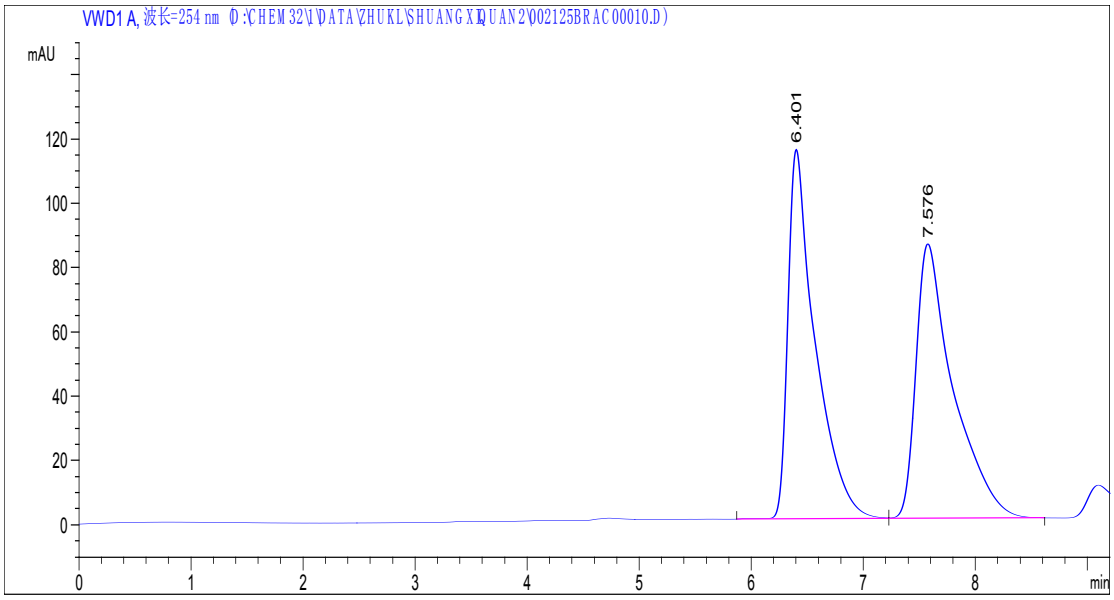


#	Time	Area	Height	Width	Symmetry	Area %
1	6.838	9721.5	576.9	0.2446	0.604	48.817
2	7.537	11043.6	510.6	0.3106	0.599	51.183

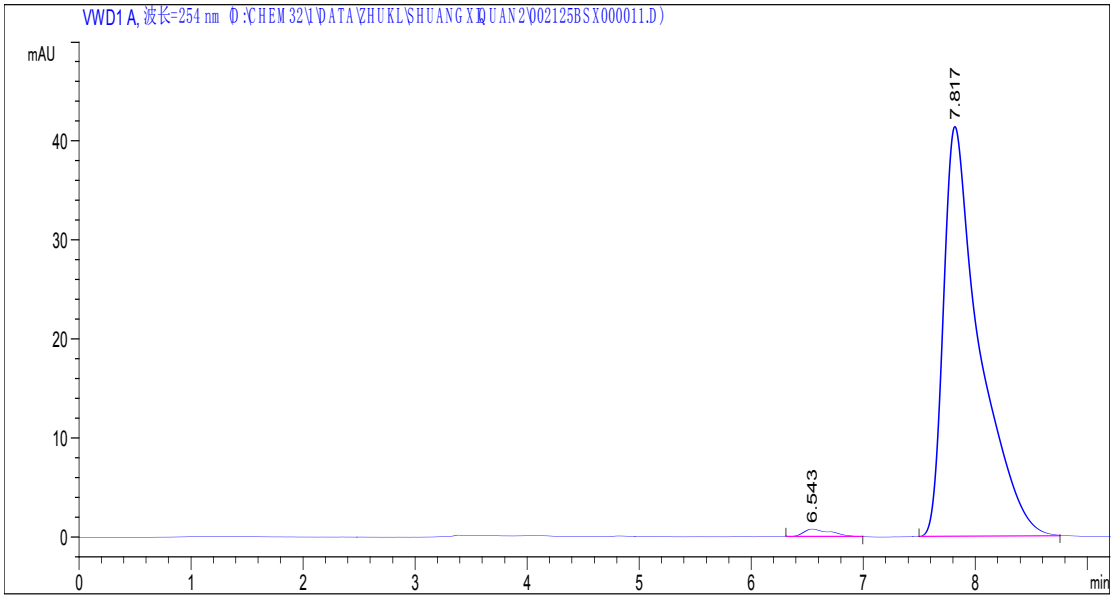


#	Time	Area	Height	Width	Symmetry	Area %
1	7.021	193.7	11.4	0.2456	0.733	1.561
2	7.804	12213.4	557.9	0.3165	0.578	98.439

6r:2-((5S,6R,10S)-10-(4-bromophenyl)-7-ethyl-3-isopropyl-4-oxo-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde

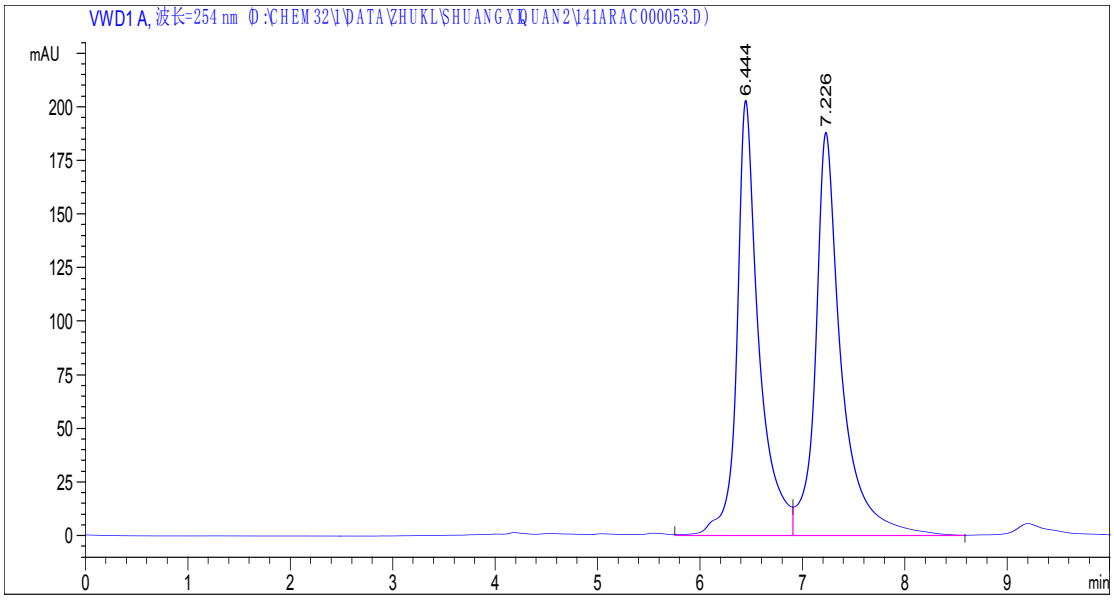


#	Time	Area	Height	Width	Symmetry	Area %
1	6.401	1942	114.8	0.2367	0.404	49.685
2	7.576	1966.6	85.4	0.327	0.428	50.315

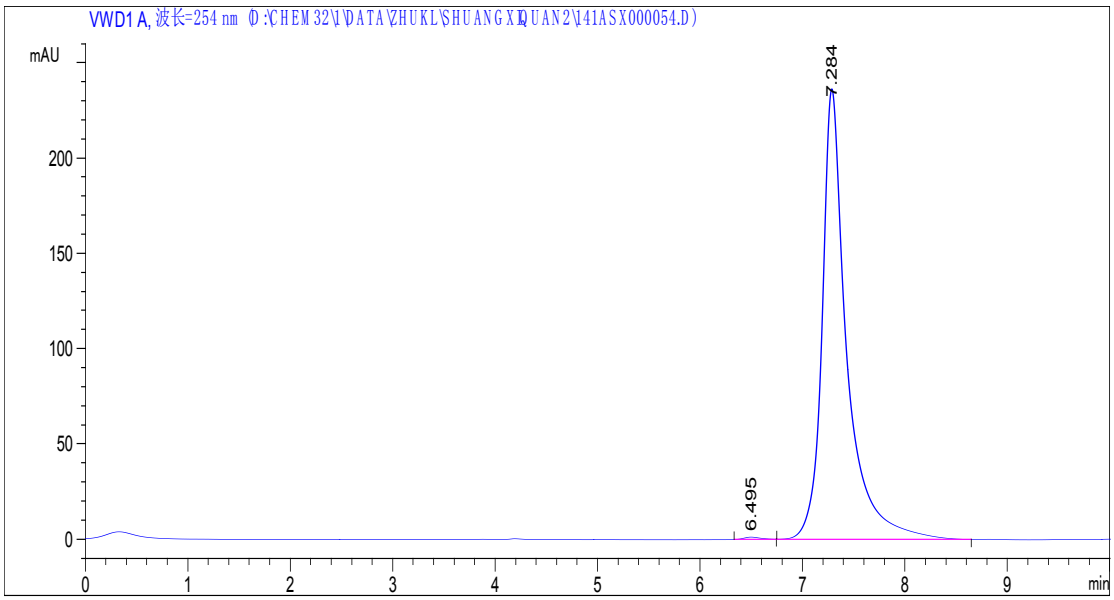


#	Time	Area	Height	Width	Symmetry	Area %
1	6.543	13.2	7.6E-1	0.29	0.429	1.411
2	7.817	924.7	41.4	0.3173	0.426	98.589

6s:(5S,6S,10R)-ethyl-4-oxo-10-(2-oxoethyl)-3,9-diphenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-8-ene-6-carboxylate

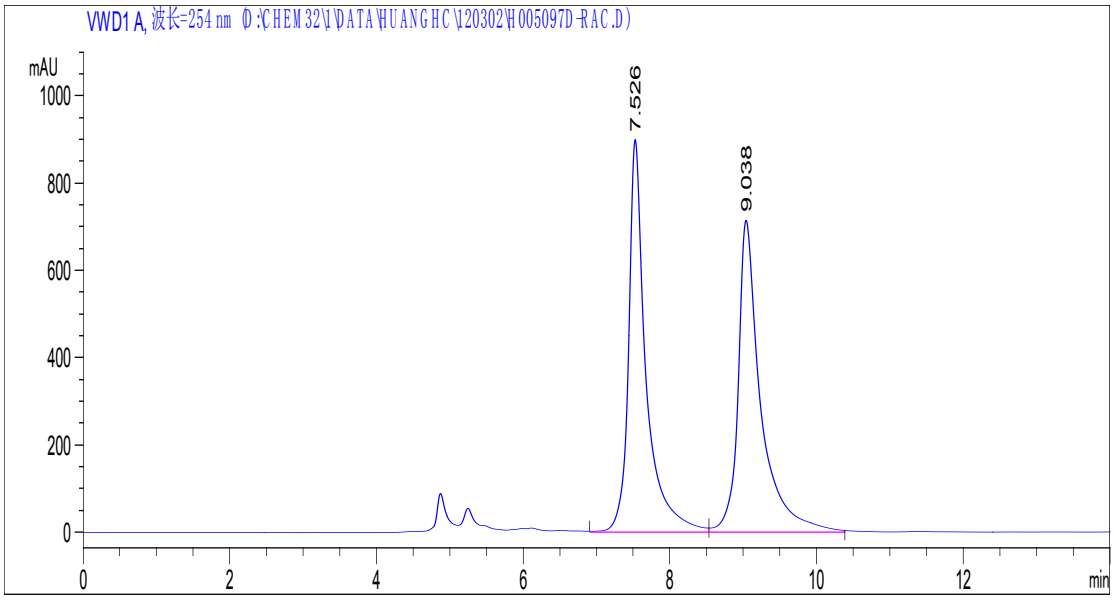


#	Time	Area	Height	Width	Symmetry	Area %
1	6.444	3050.8	203.2	0.2116	0.646	48.823
2	7.226	3328.5	188.2	0.2515	0.615	51.177

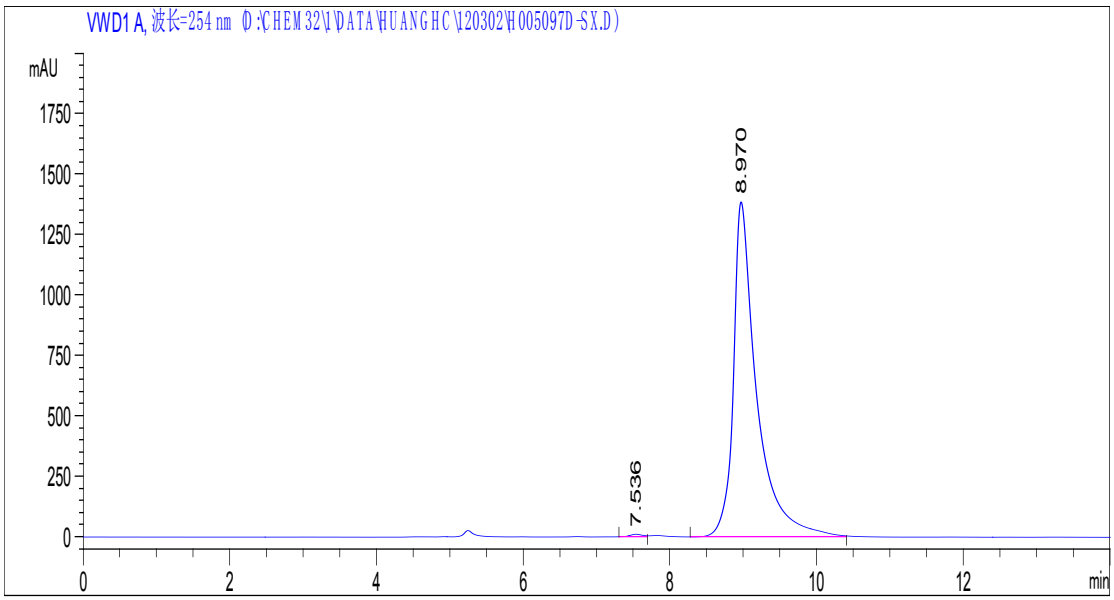


#	Time	Area	Height	Width	Symmetry	Area %
1	6.495	18.3	1.4	0.2154	0.685	0.459
2	7.284	3973.7	236.6	0.2381	0.596	99.541

6t:2-((5R,6R,10S)-10-(4-bromophenyl)-3-isopropyl-4-oxo-7-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde

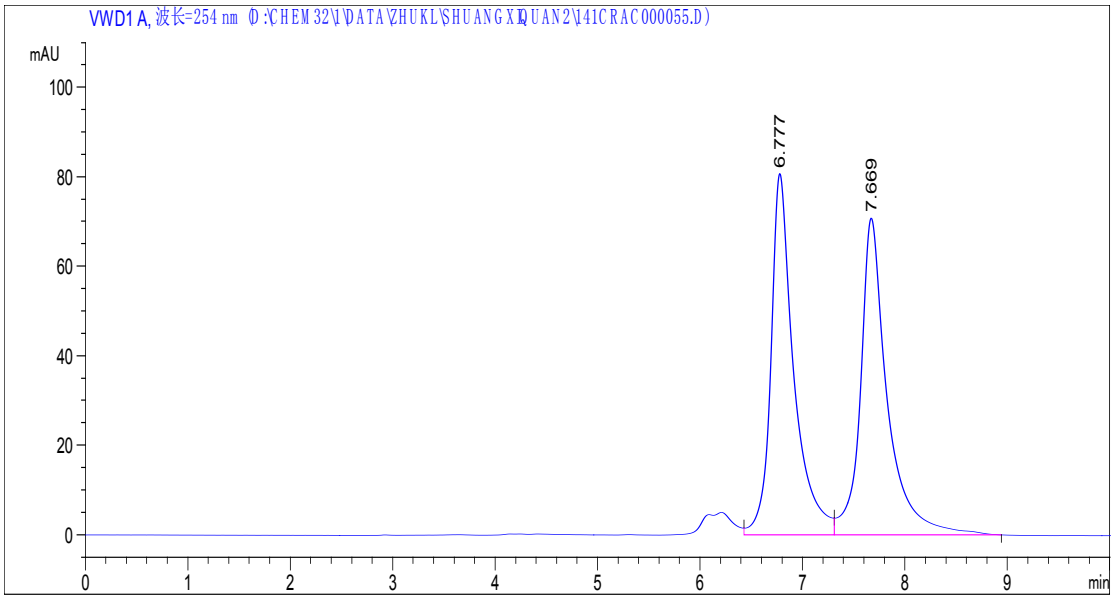


#	Time	Area	Height	Width	Symmetry	Area %
1	7.526	14907.7	899.2	0.2342	0.572	49.391
2	9.038	15275.4	714.4	0.3564	0.53	50.609

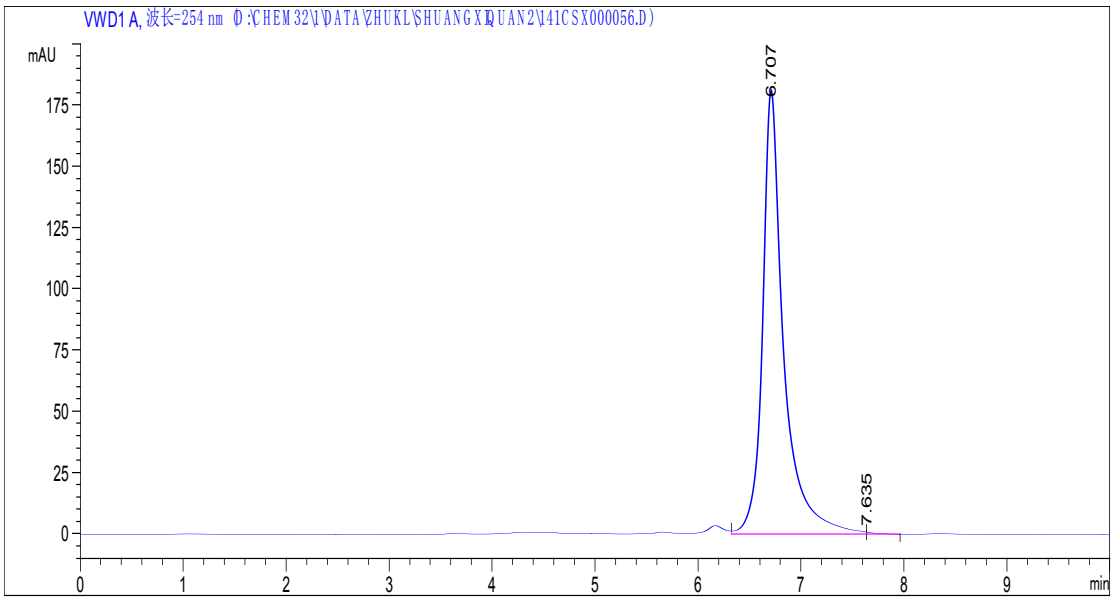


#	Time	Area	Height	Width	Symmetry	Area %
1	7.536	131.7	10.8	0.2041	0.849	0.428
2	8.97	30663.1	1386.5	0.3686	0.486	99.572

6u:2-((5R,6R,10S)-10-(4-bromophenyl)-4-oxo-3,7-diphenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde

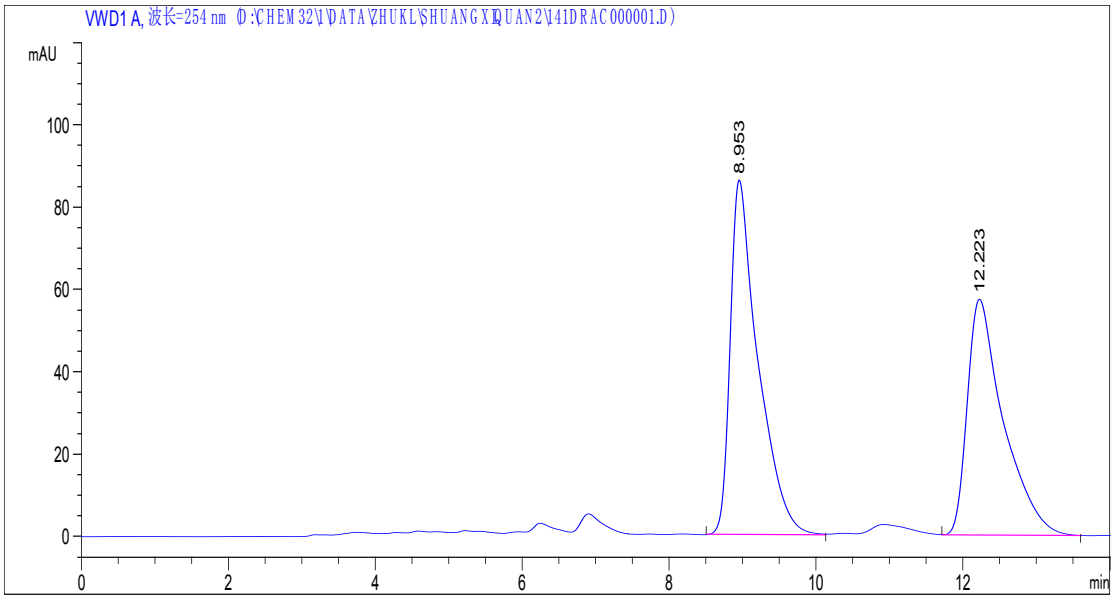


#	Time	Area	Height	Width	Symmetry	Area %
1	6.777	1258.2	80.8	0.2211	0.606	49.309
2	7.669	1293.5	70.8	0.2582	0.626	50.691

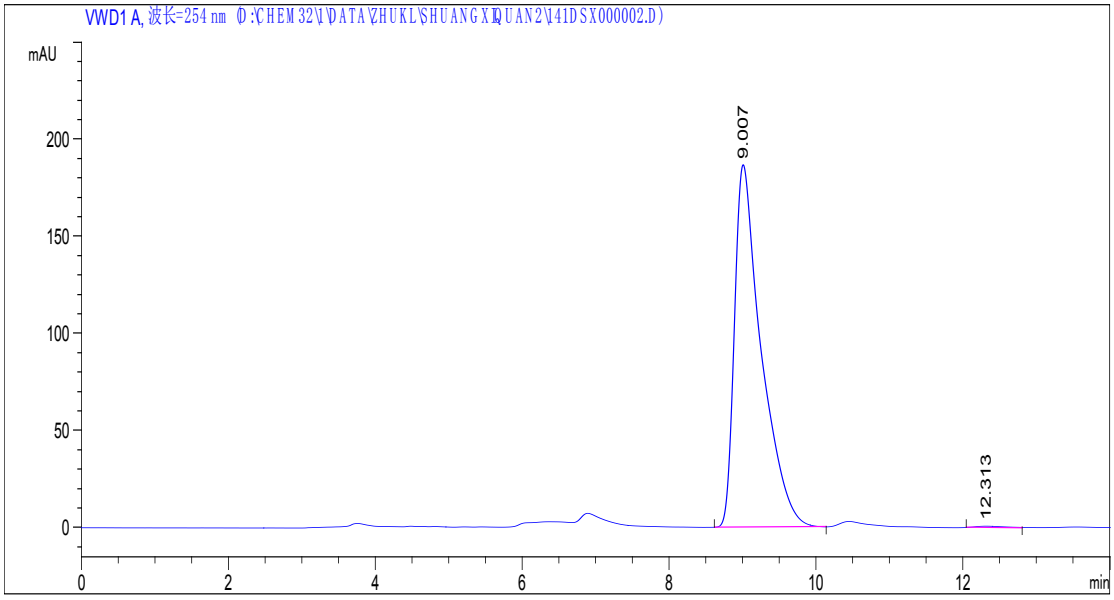


#	Time	Area	Height	Width	Symmetry	Area %
1	6.707	2588.2	181.5	0.2328	0	99.778
2	7.635	5.8	9.1E-1	0.1055	0	0.222

6v:2-((5R,6R,10S)-10-(4-nitrophenyl)-4-oxo-3,7-diphenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde

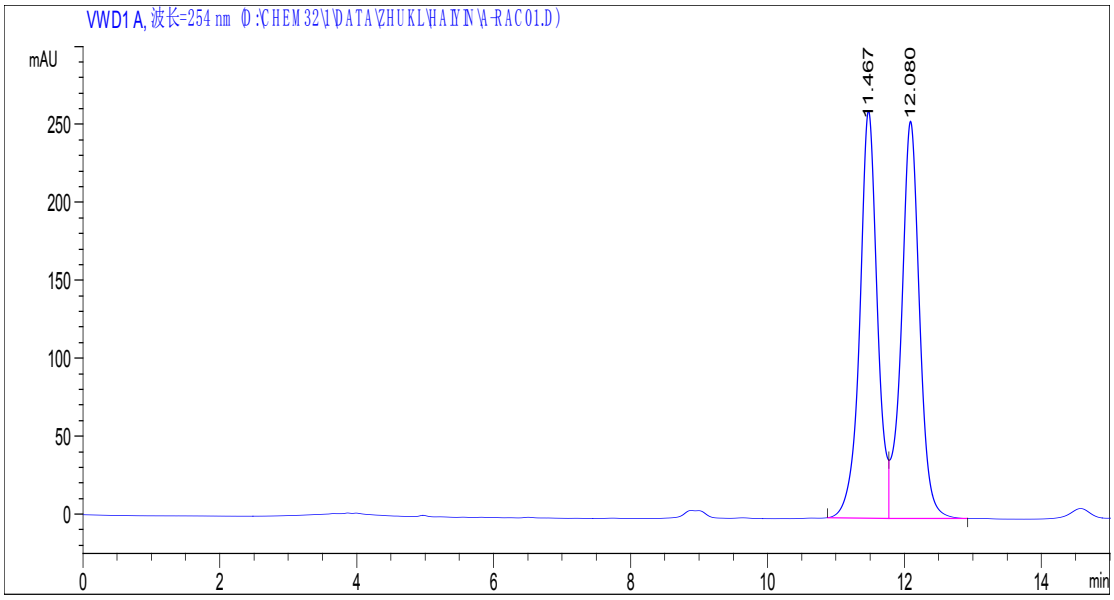


#	Time	Area	Height	Width	Symmetry	Area %
1	8.953	2271.8	86.3	0.3743	0.442	50.673
2	12.223	1960.9	57.4	0.4903	0.469	49.327

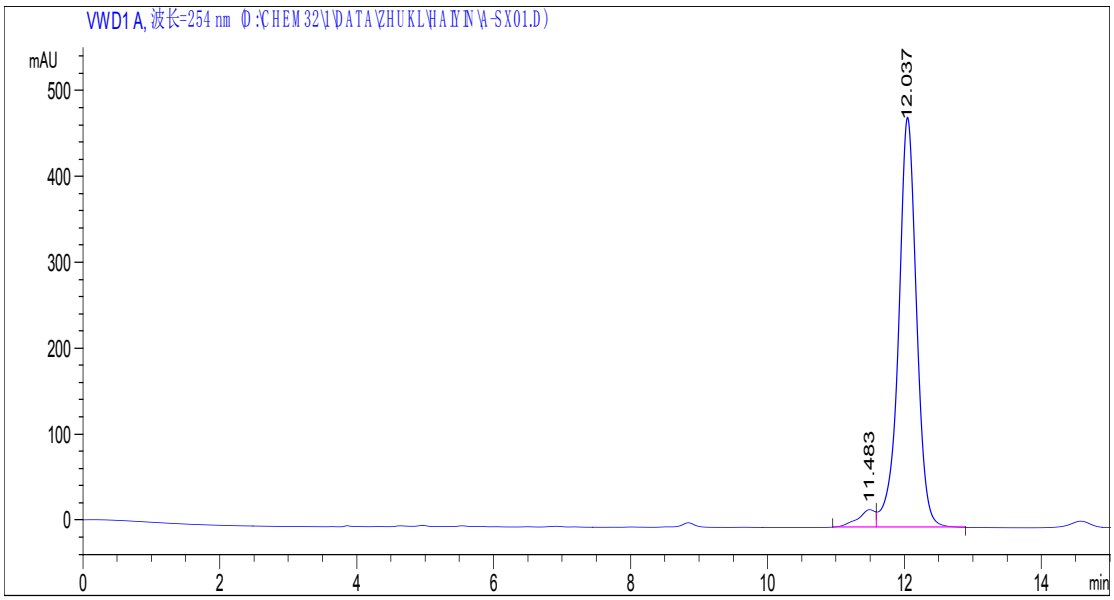


#	Time	Area	Height	Width	Symmetry	Area %
1	9.007	4713.7	186.7	0.3616	0.444	99.504
2	12.313	23.5	8.1E-1	0.4819	0.527	0.496

6w:(5S,6R,10R)-ethyl-1-methyl-4-oxo-10-(2-oxoethyl)-3-phenyl-2-thioxo-1,3-diazaspiro[4.5]dec-8-ene-6-carboxylate

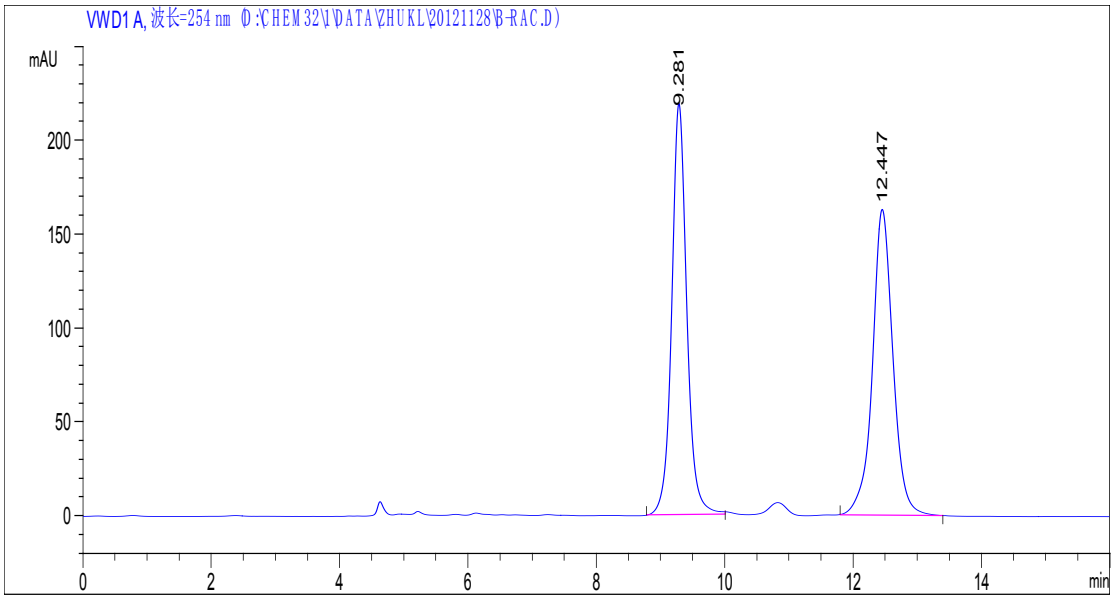


#	Time	Area	Height	Width	Symmetry	Area %
1	11.467	4655.3	261.3	0.2661	0.984	49.829
2	12.08	4687.2	254.5	0.276	0.966	50.171

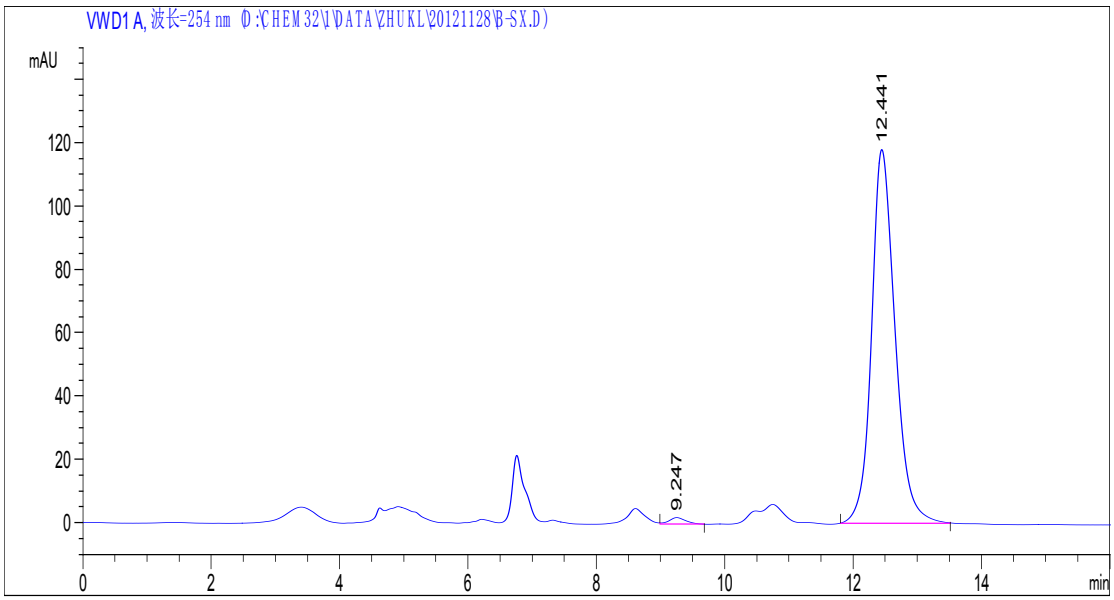


#	Time	Area	Height	Width	Symmetry	Area %
1	11.483	380.8	20.7	0.2608	2.294	4.180
2	12.037	8728.3	477.4	0.2744	0.985	95.820

6x:(5S,6R,10R)-ethyl-1-methyl-4-oxo-10-(2-oxoethyl)-3,9-diphenyl-2-thioxo-1,3-diazaspiro[4.5]dec-8-ene-6-carboxylate

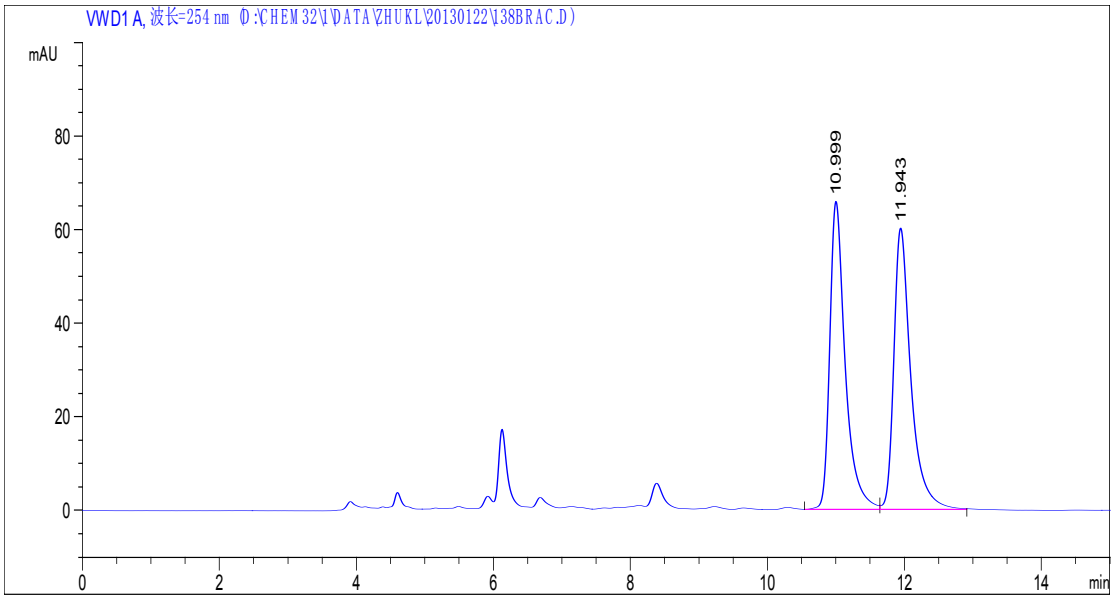


#	Time	Area	Height	Width	Symmetry	Area %
1	9.281	3587.9	219.2	0.2463	0.872	49.665
2	12.447	3636.4	163.1	0.3359	0.895	50.335

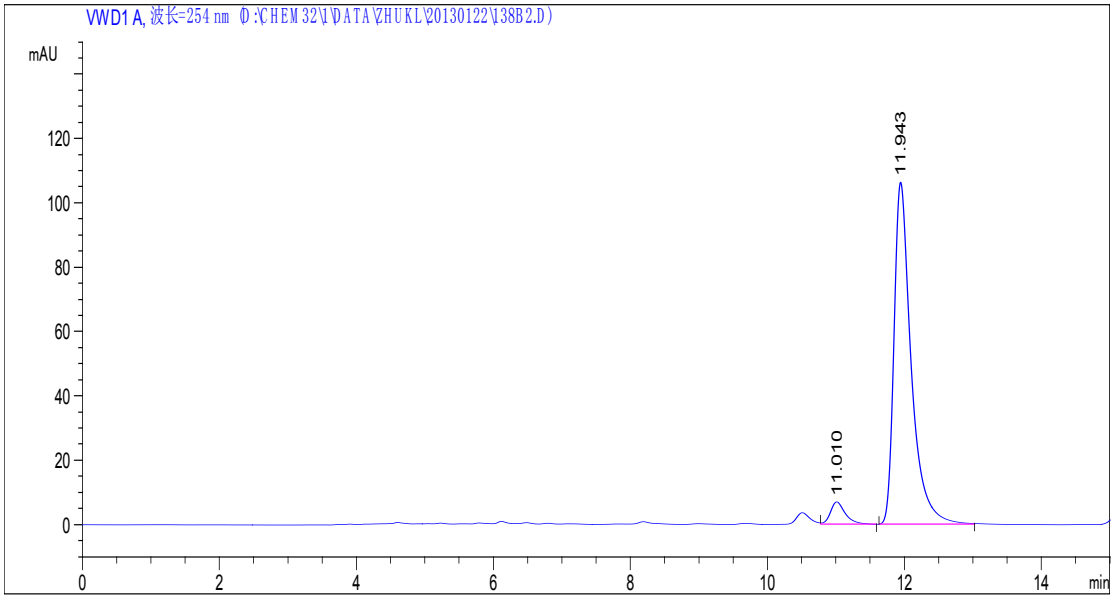


#	Time	Area	Height	Width	Symmetry	Area %
1	9.247	37.2	2.1	0.2659	0.813	1.218
2	12.441	3014.6	118.1	0.388	0.744	98.782

7a:(5S,6R,10R)-ethyl-10-(4-methoxy-4-oxobut-2-enyl)-1-methyl-2,4-dioxo-3-phenyl-1,3-diaza spiro[4.5]dec-8-ene-6-carboxylate



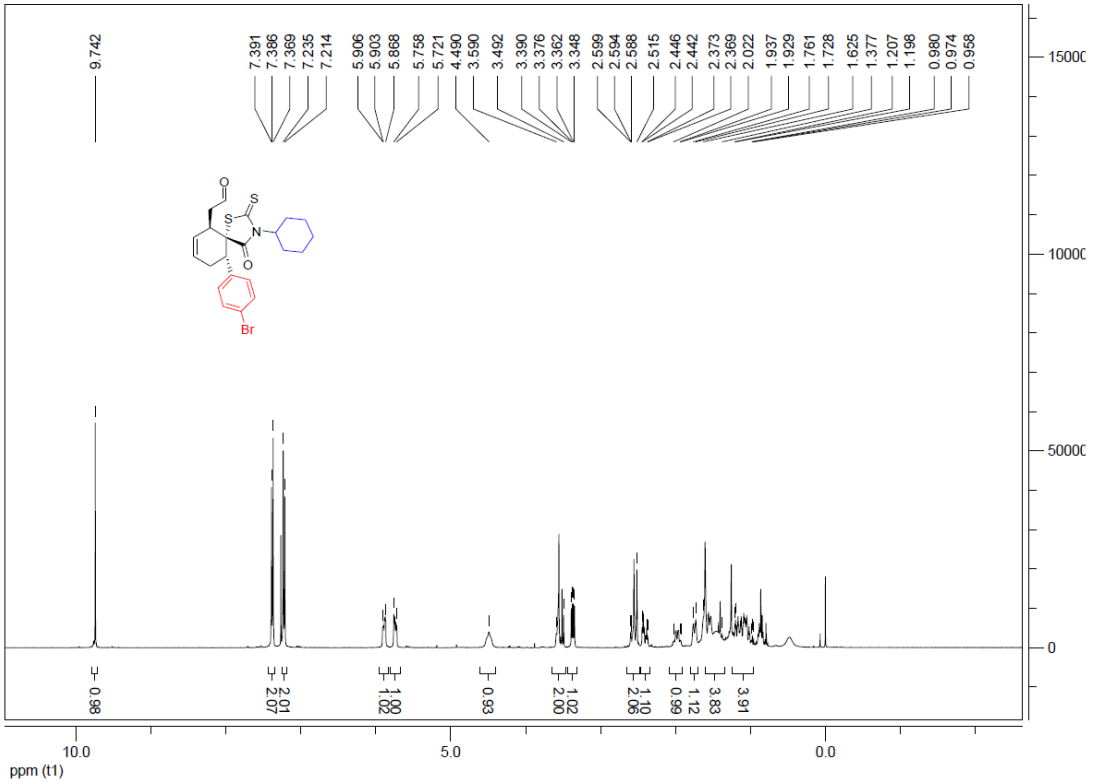
#	Time	Area	Height	Width	Symmetry	Area %
1	10.999	1032.3	65.8	0.2341	0.623	49.839
2	11.943	1039	60.1	0.2571	0.608	50.161

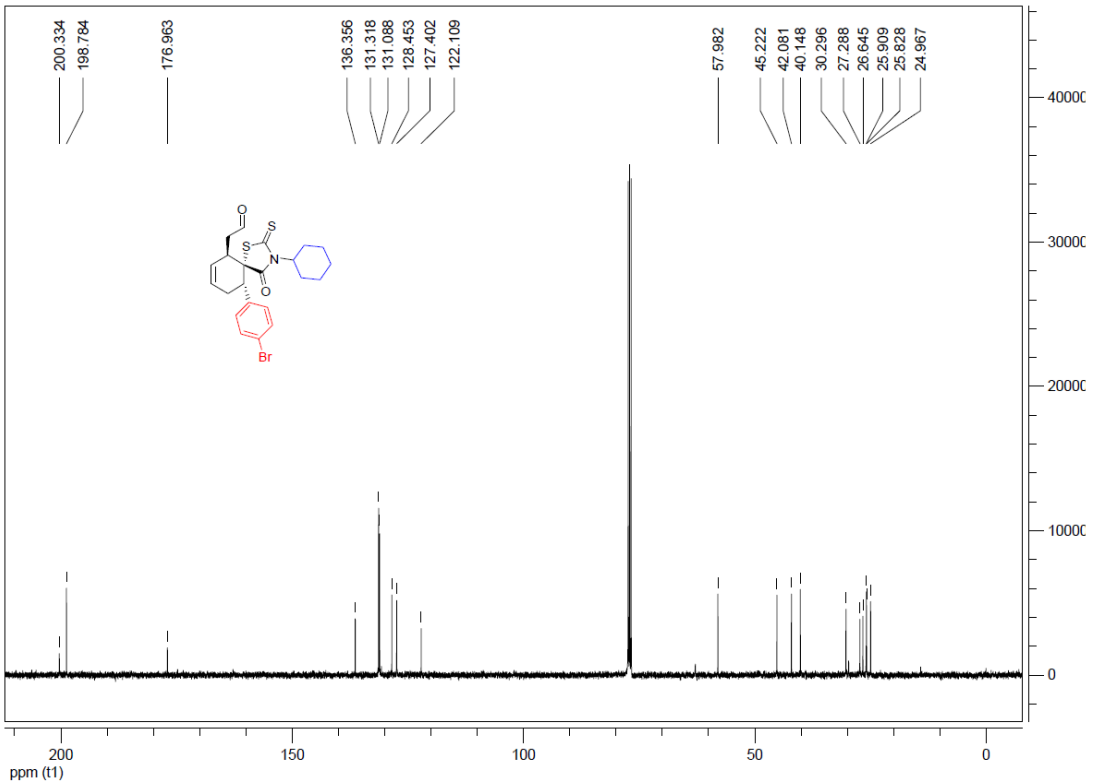


#	Time	Area	Height	Width	Symmetry	Area %
1	11.01	106.8	7	0.2276	0.688	4.466
2	11.943	1847.8	106.3	0.2566	0.577	95.534

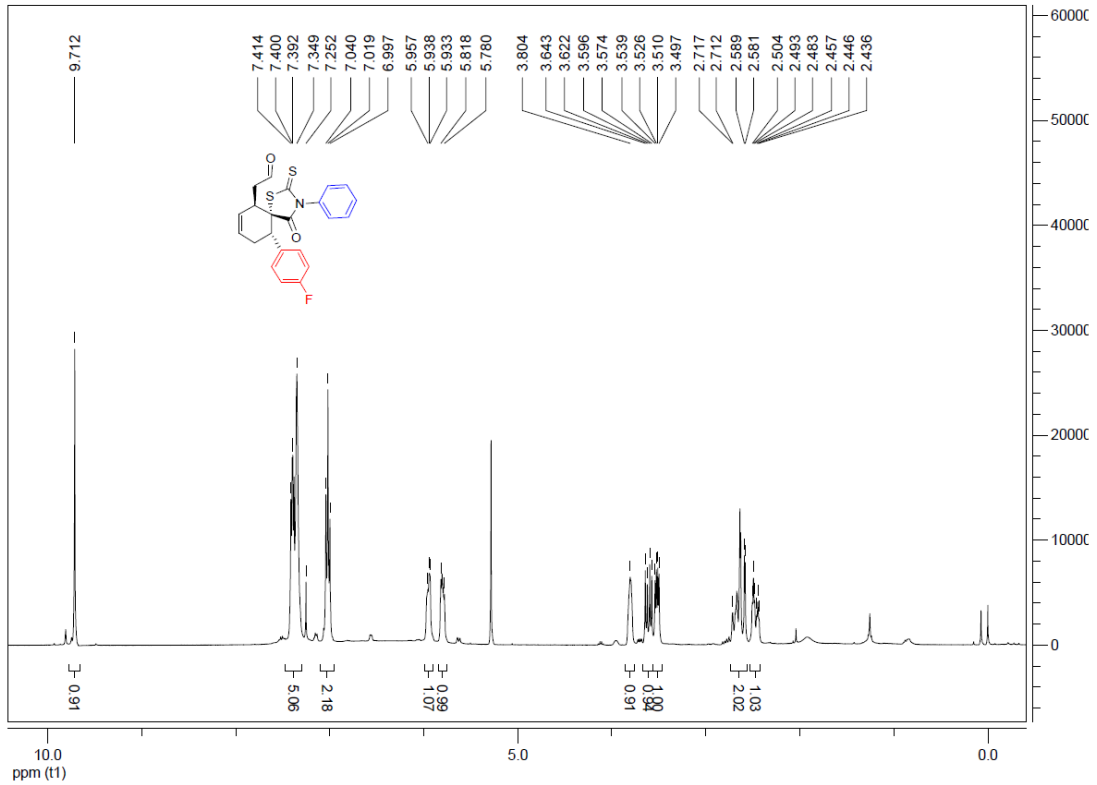
F: NMR Spectra of Diels-Alder Raction Products

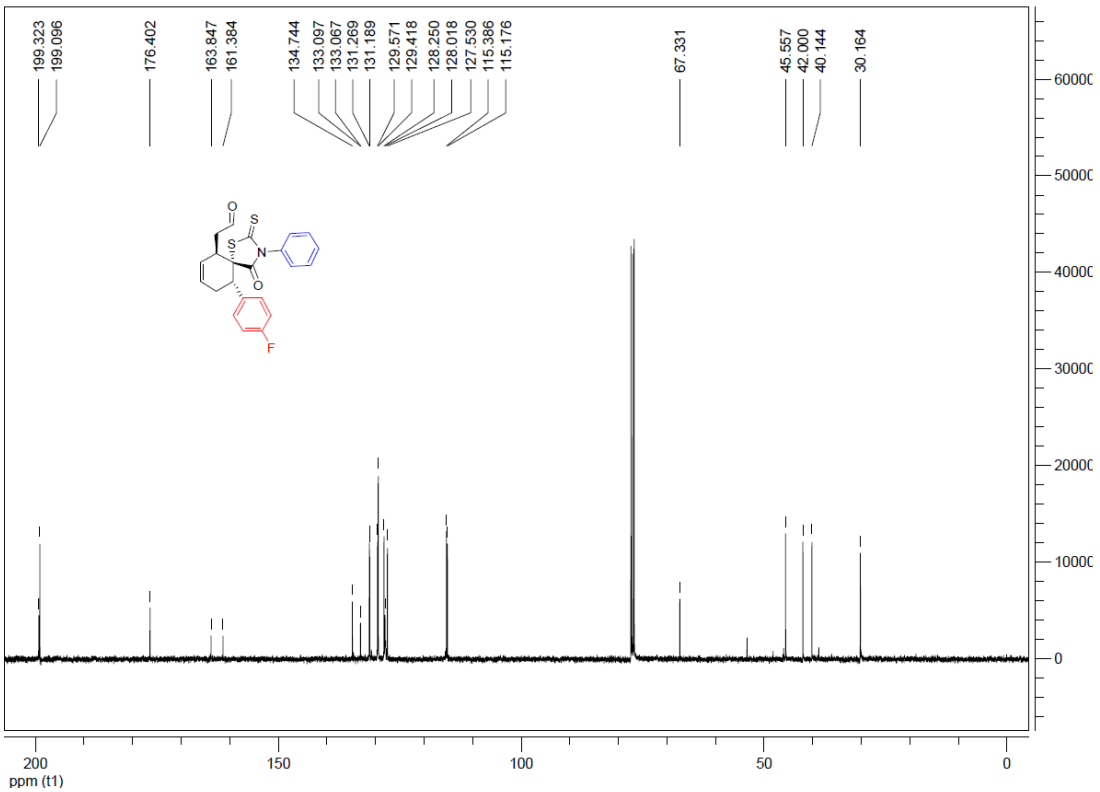
6a:2-((5S,6R,10S)-10-(4-bromophenyl)-3-cyclohexyl-4-oxo-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



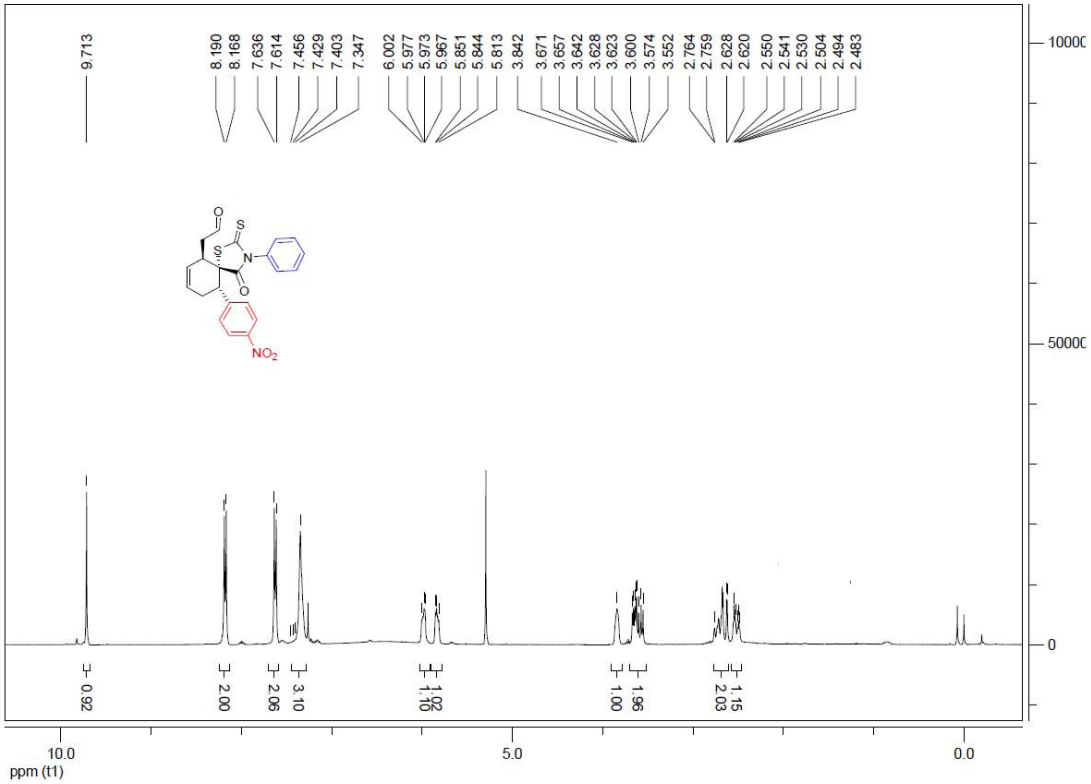


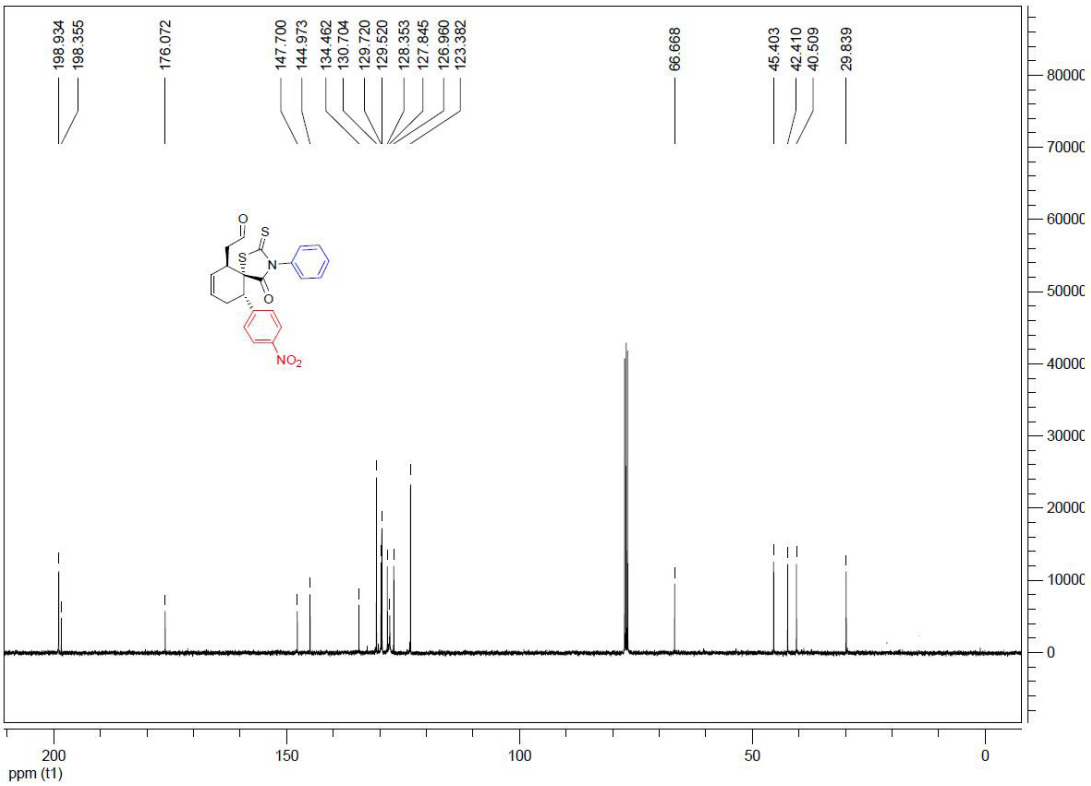
6b:2-((5S,6R,10S)-10-(4-fluorophenyl)-4-oxo-3-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



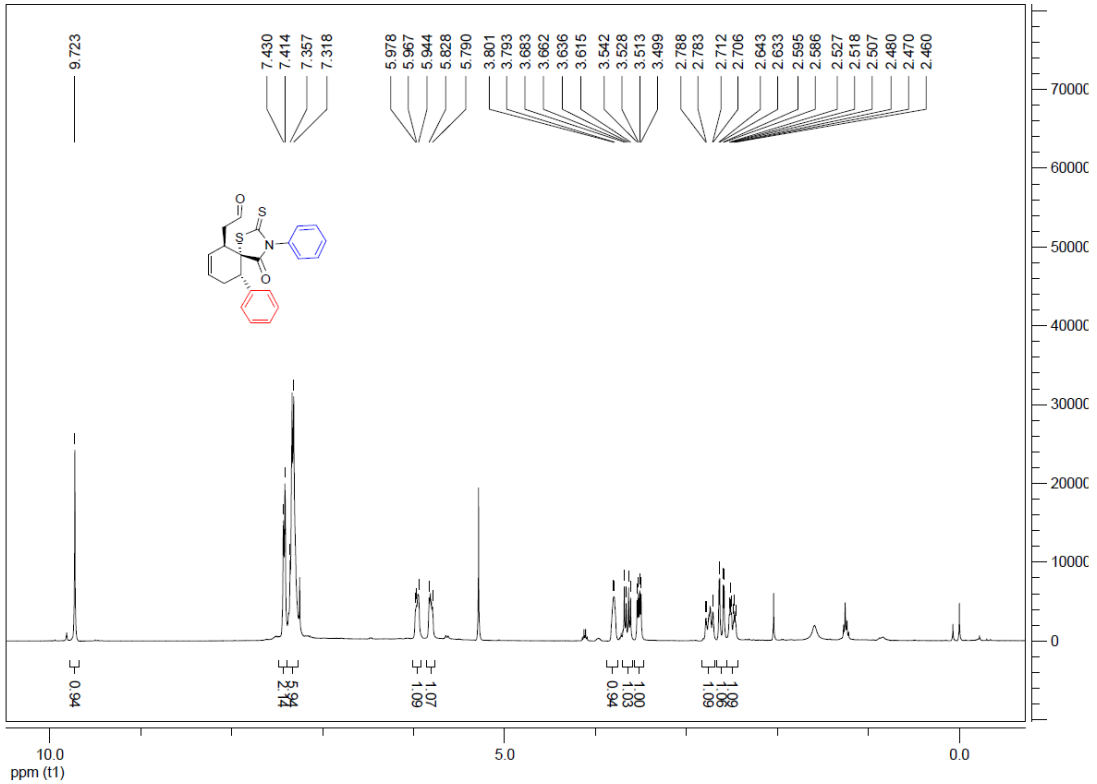


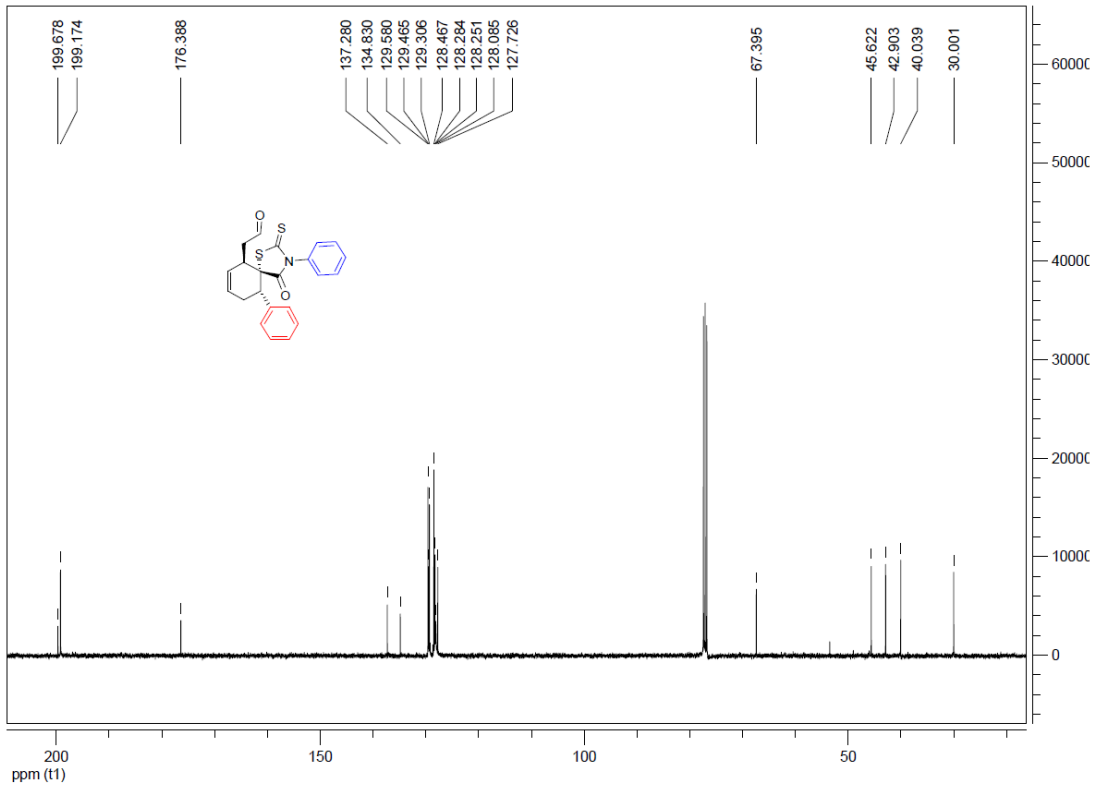
6c:2-((5S,6R,10S)-10-(4-nitrophenyl)-4-oxo-3-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



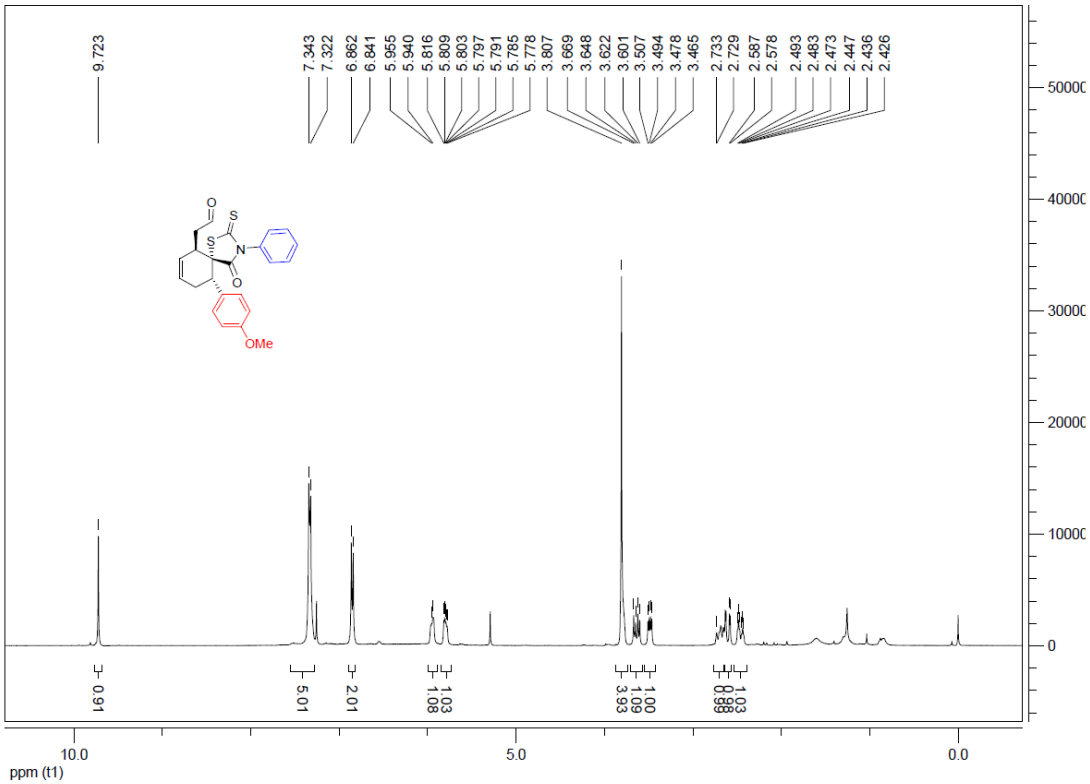


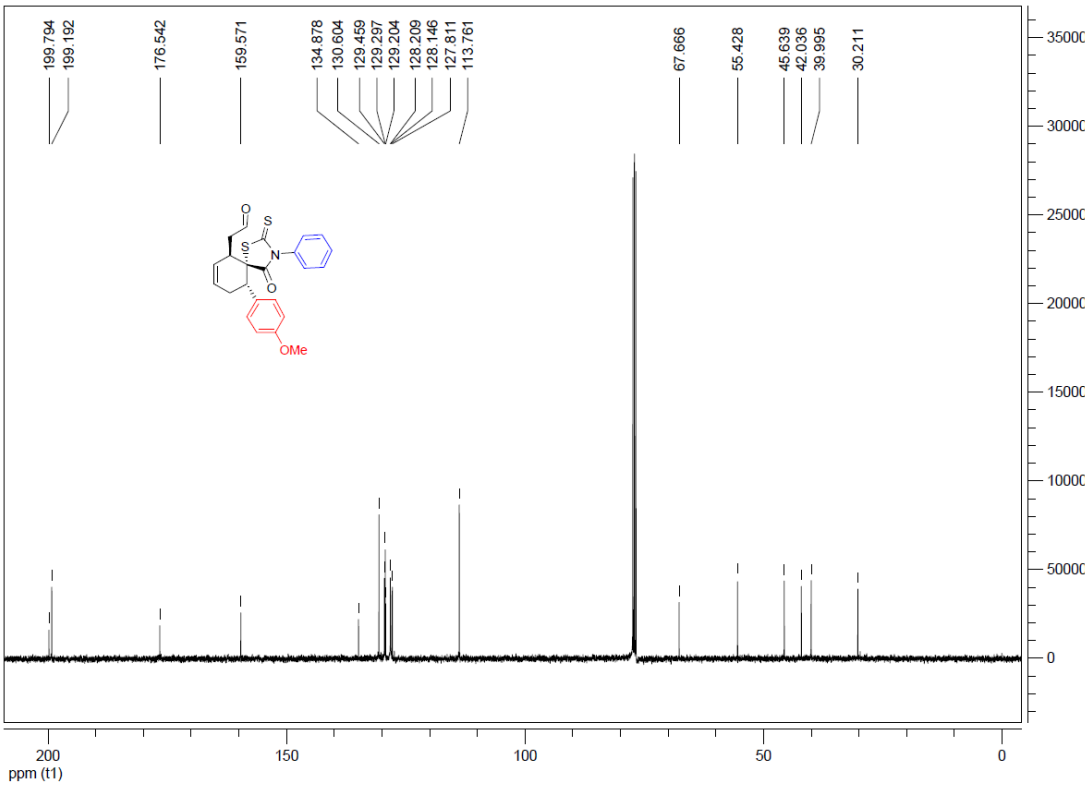
6d:2-((5S,6R,10S)-4-oxo-3,10-diphenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



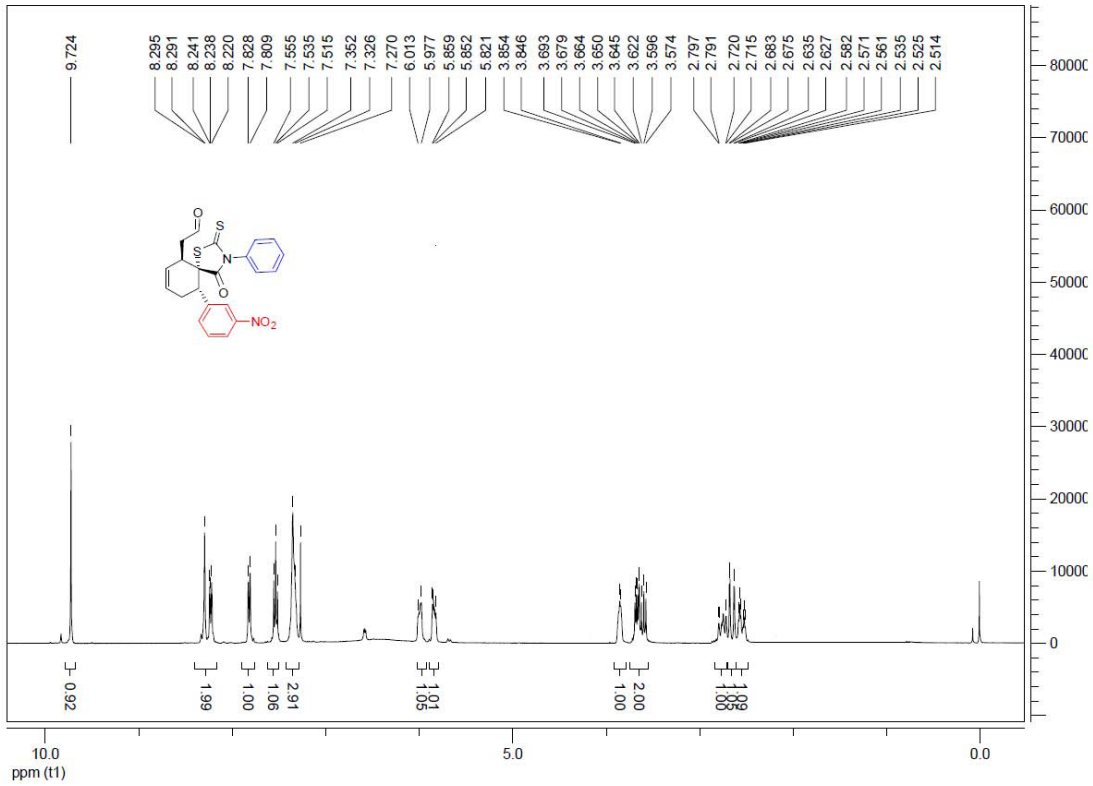


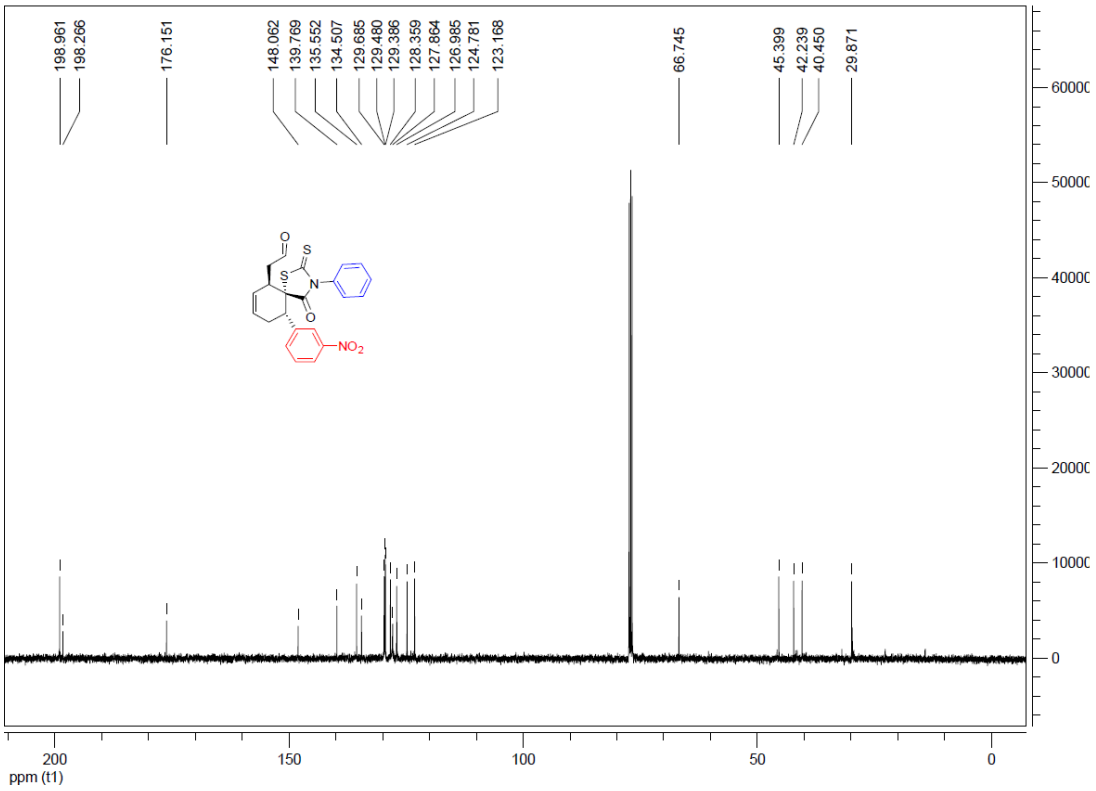
6e:2-((5S,6R,10S)-10-(4-methoxyphenyl)-4-oxo-3-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



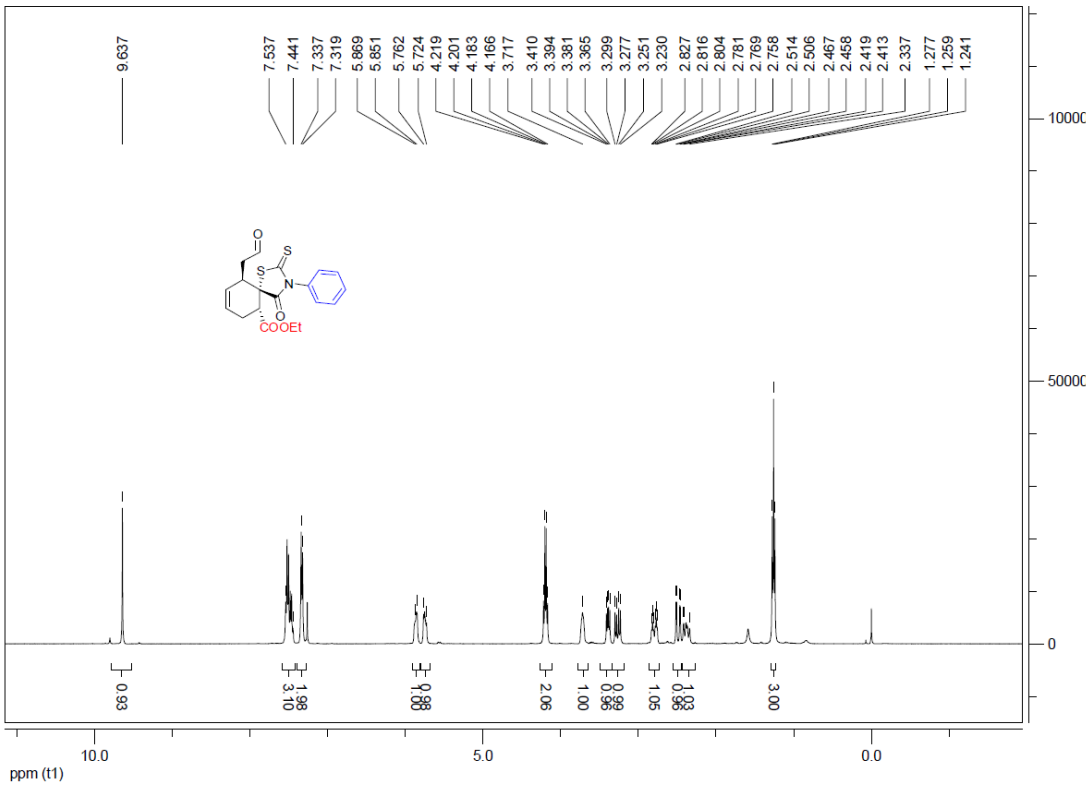


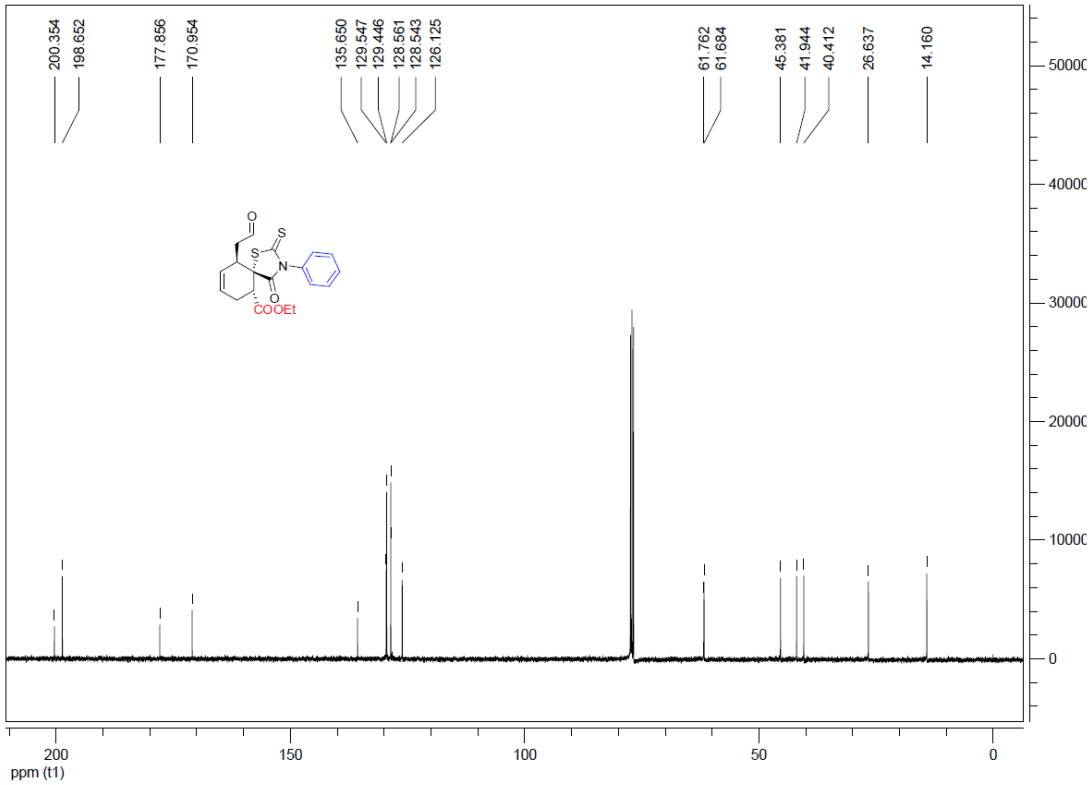
6f:2-((5S,6R,10S)-10-(3-nitrophenyl)-4-oxo-3-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



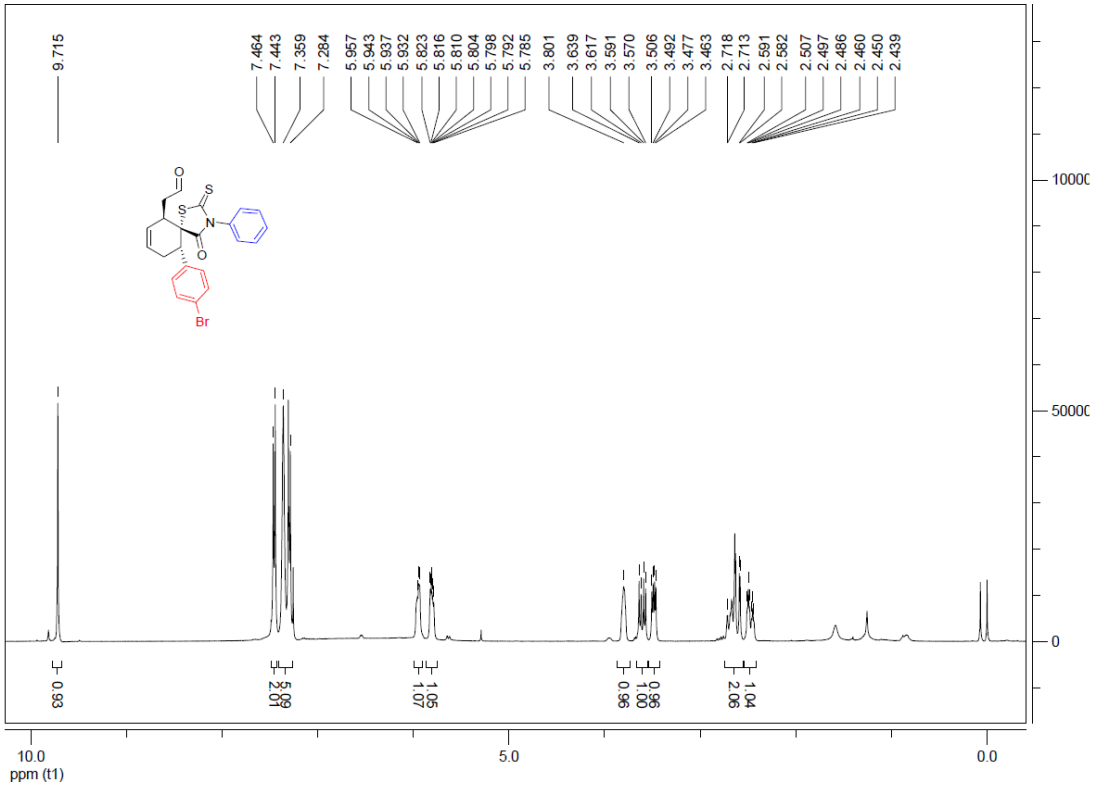


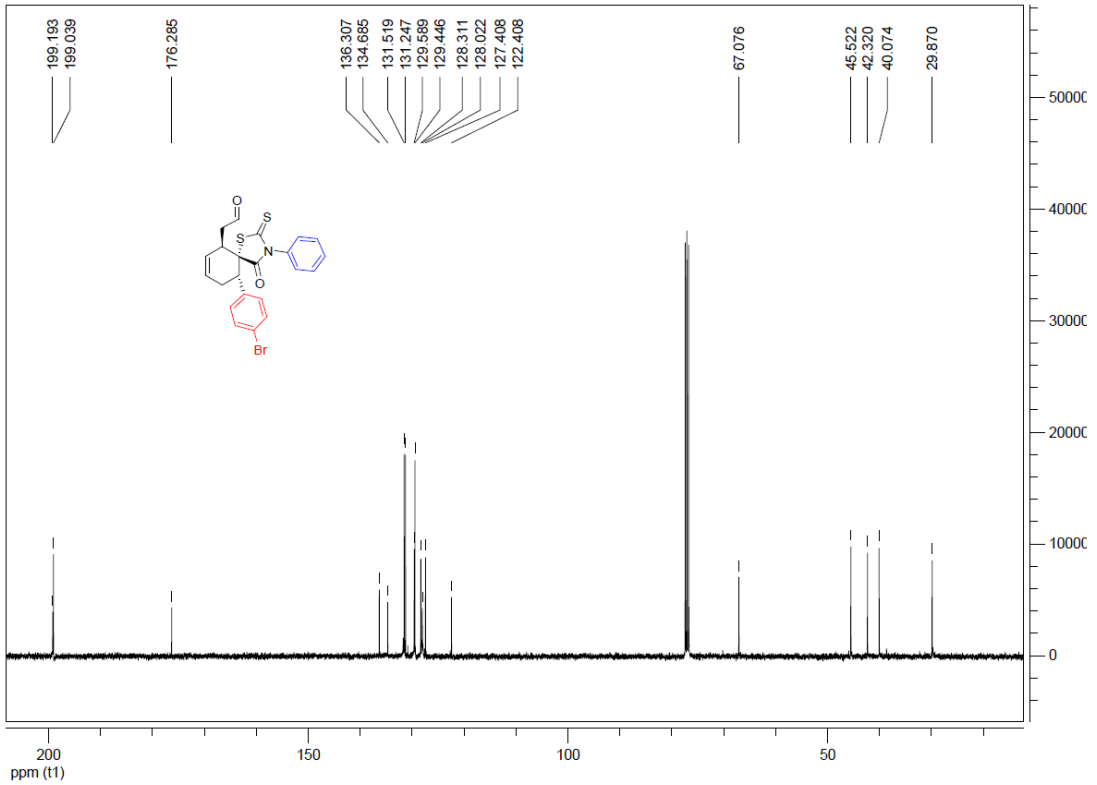
6g:(5S,6S,10R)-ethyl-4-oxo-10-(2-oxoethyl)-3-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-8-ene-6-carboxylate



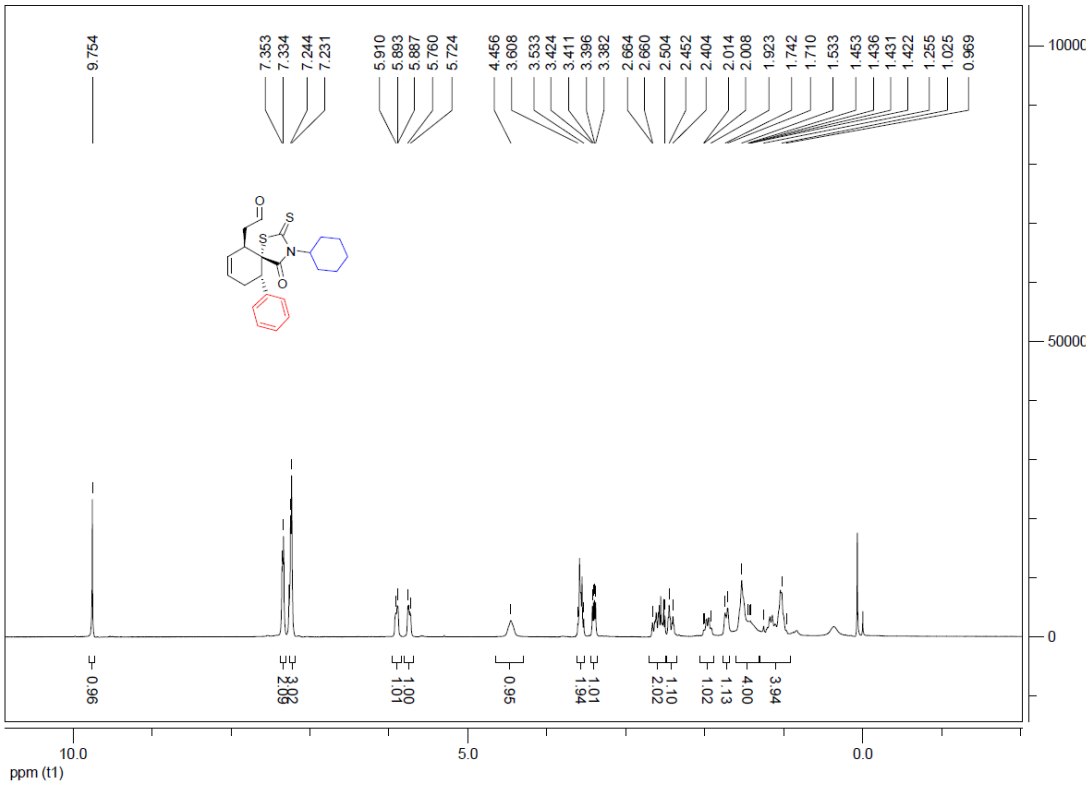


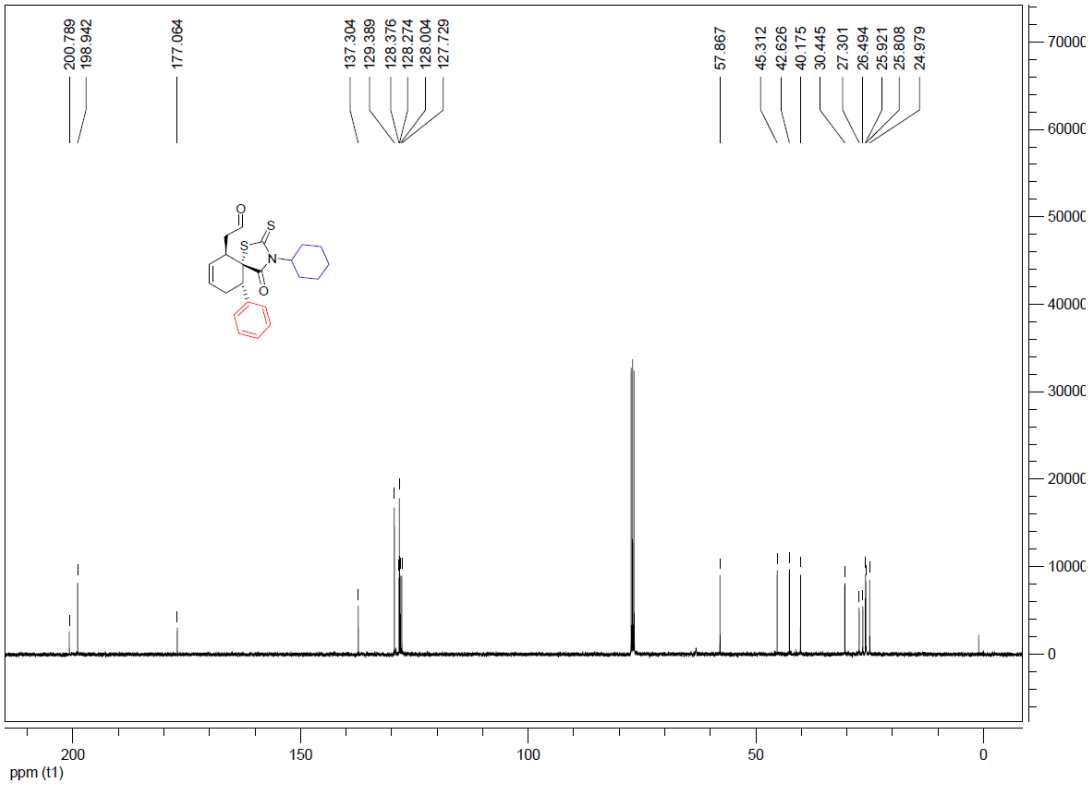
6h:2-((5S,6R,10S)-10-(4-bromophenyl)-4-oxo-3-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



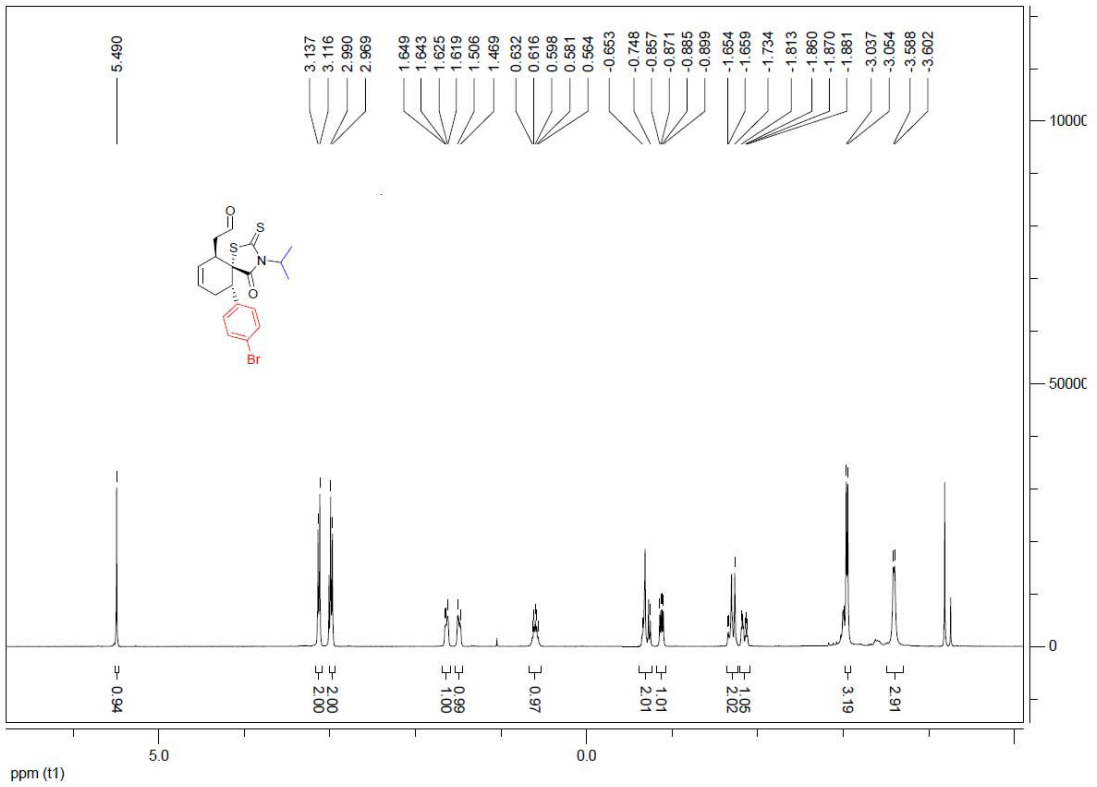


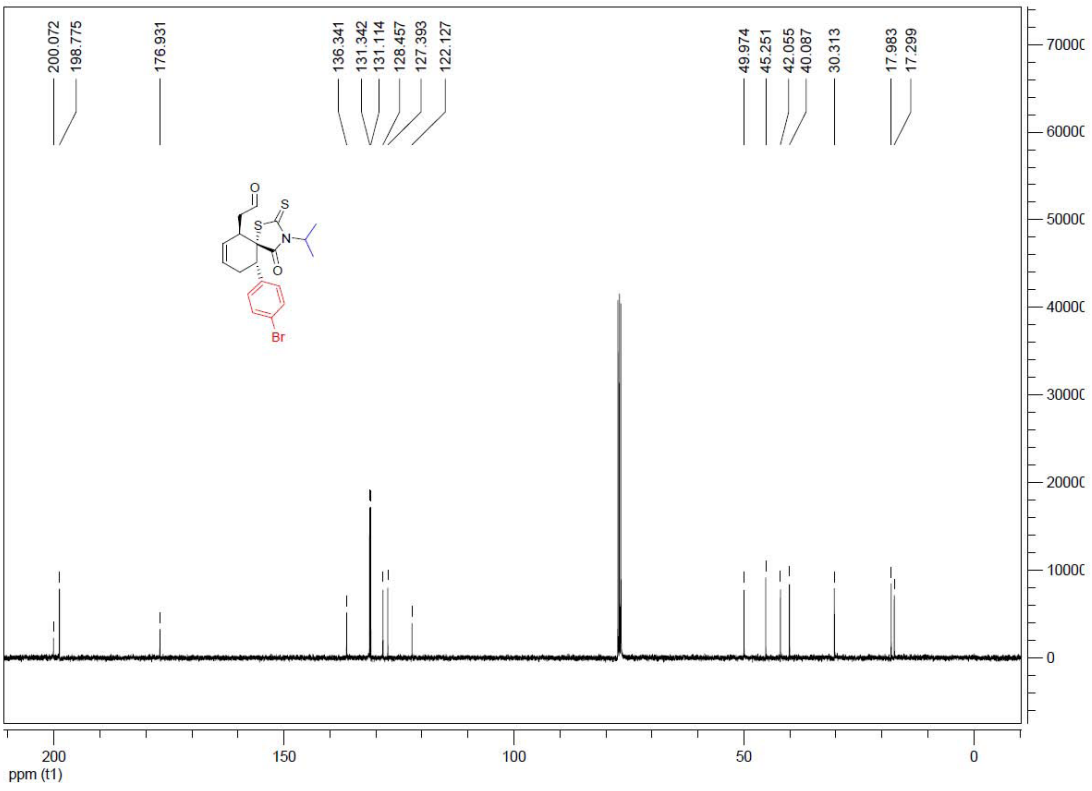
6i:2-((5S,6R,10S)-3-cyclohexyl-4-oxo-10-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl) acetaldehyde



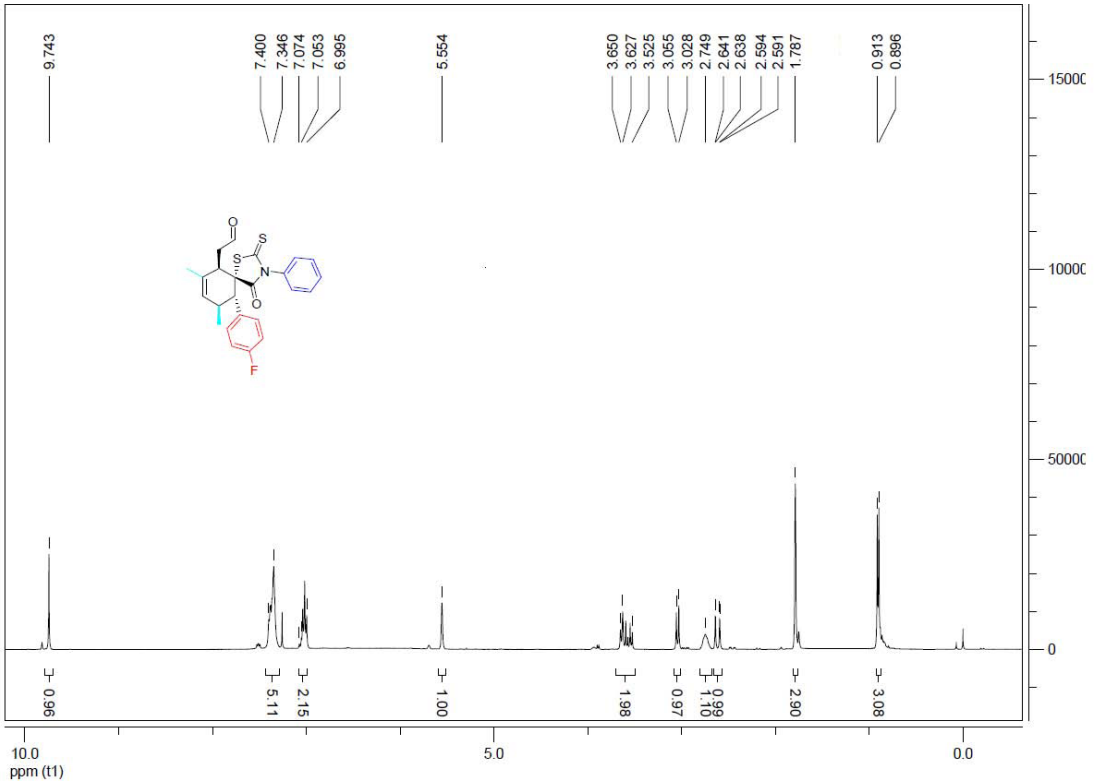


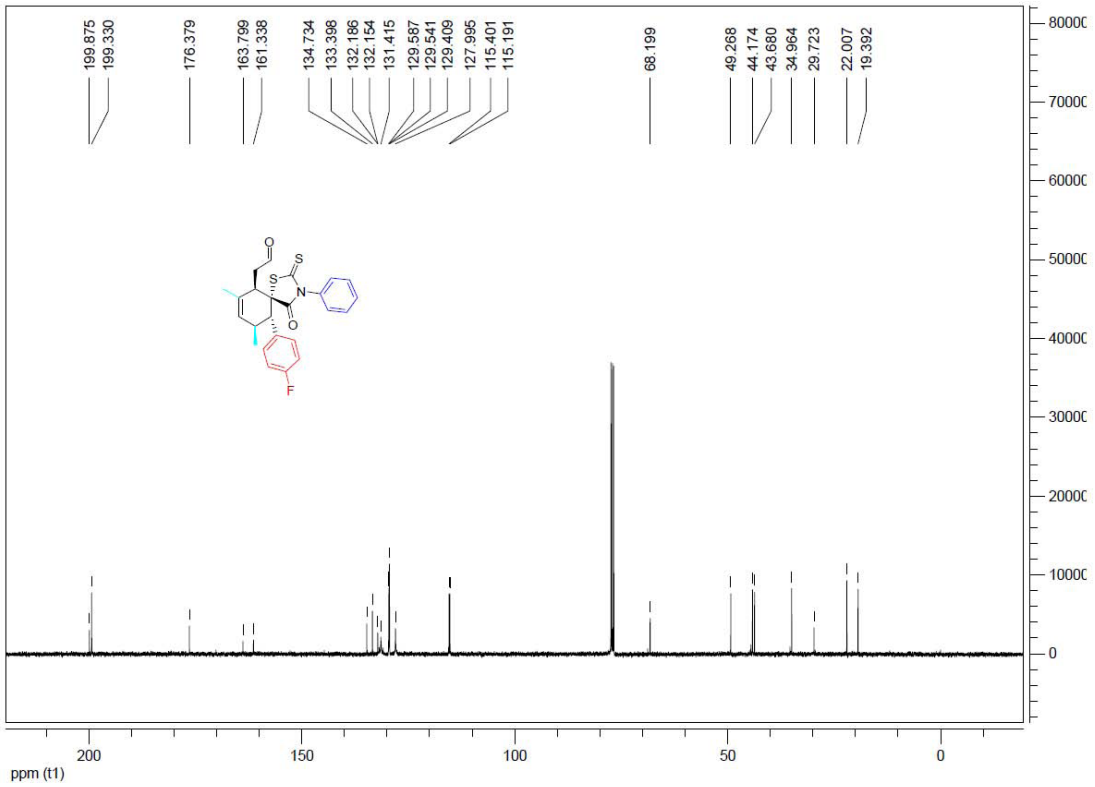
6j:2-((5S,6R,10S)-10-(4-bromophenyl)-3-isopropyl-4-oxo-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



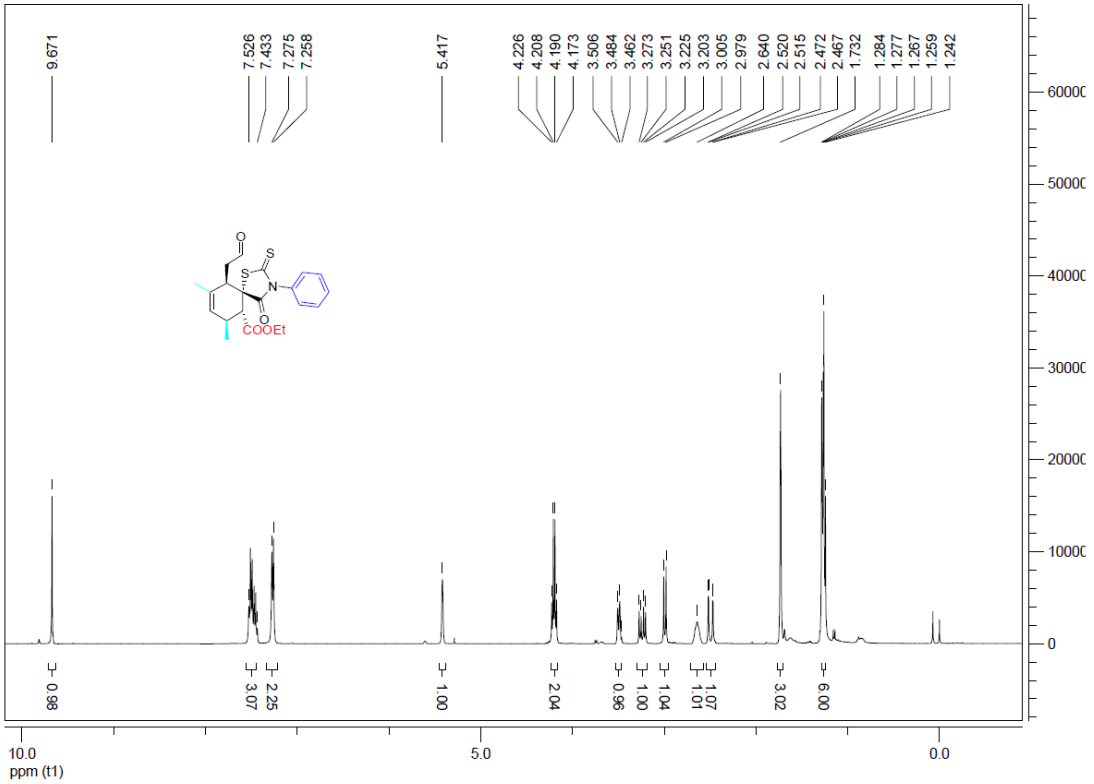


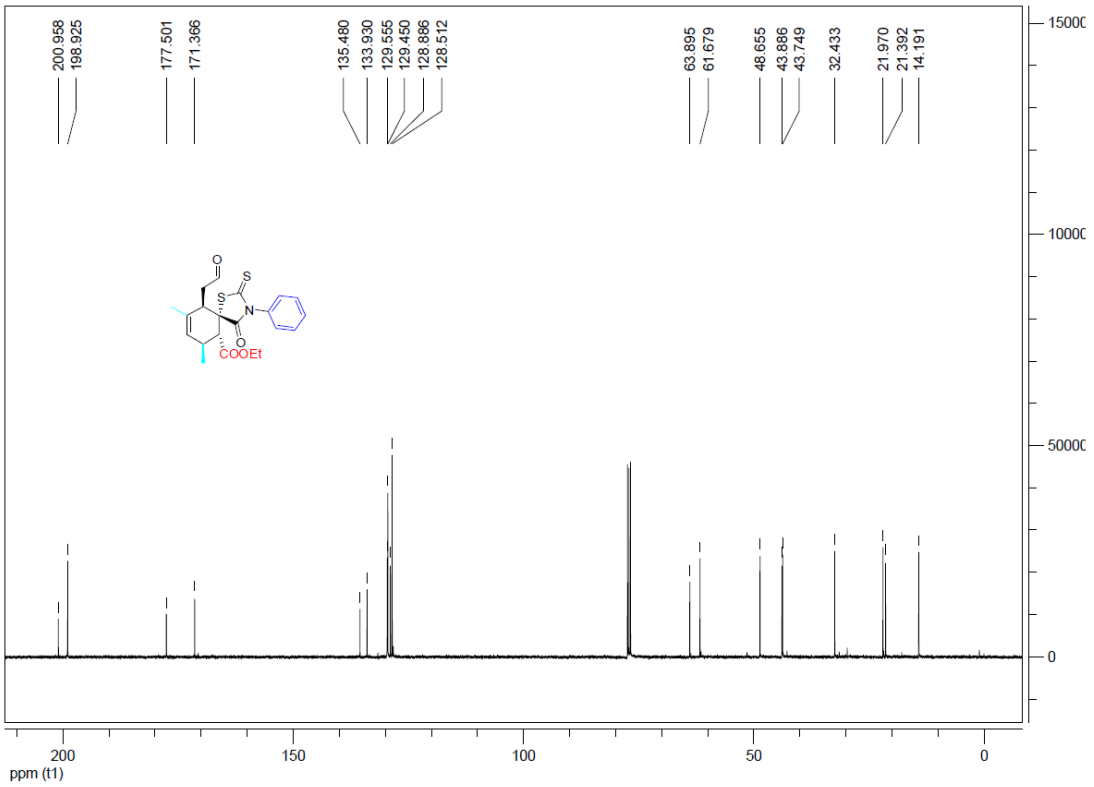
6k:2-((5S,6R,9S,10S)-10-(4-fluorophenyl)-7,9-dimethyl-4-oxo-3-phenyl-2-thioxo-1-thia-3-aza spiro[4.5]dec-7-en-6-yl)acetaldehyde



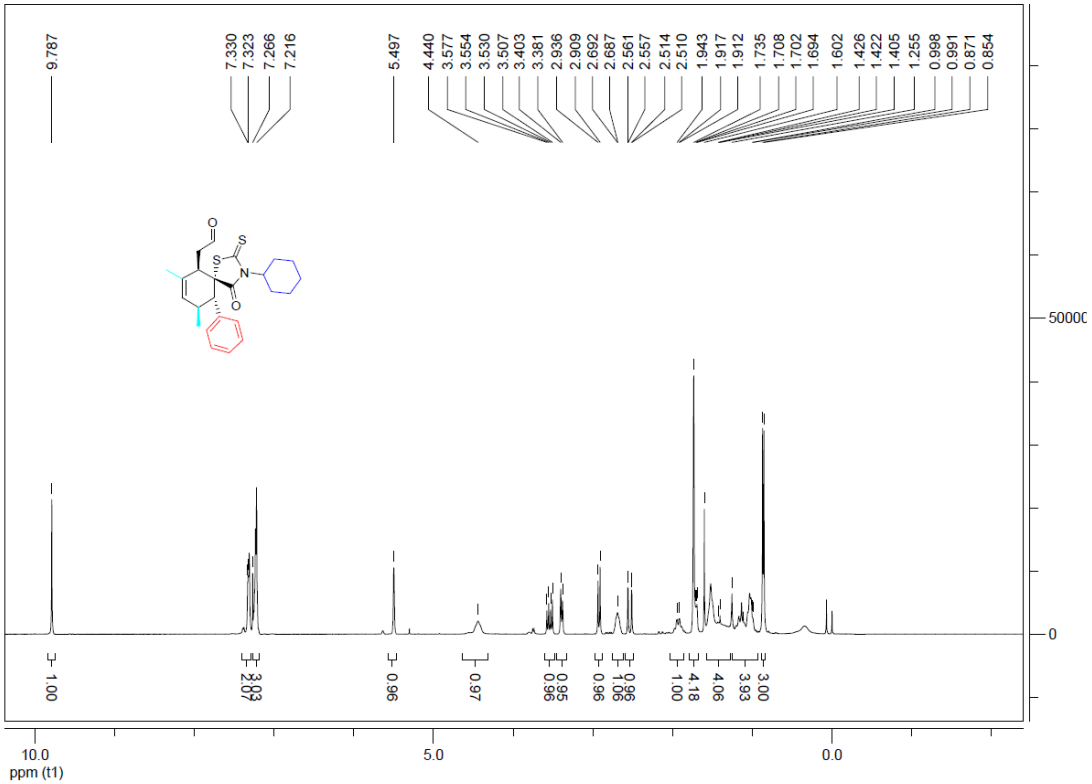


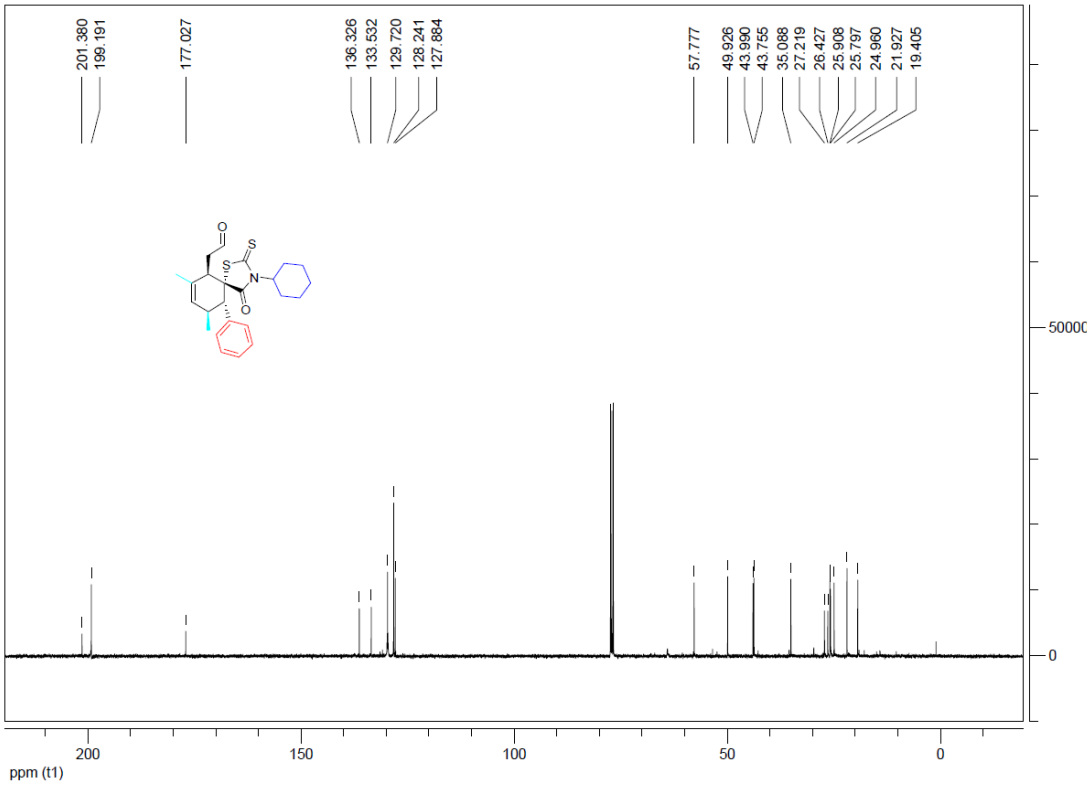
6l:(5S,6S,7S,10R)-ethyl-7,9-dimethyl-4-oxo-10-(2-oxoethyl)-3-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-8-ene-6-carboxylate



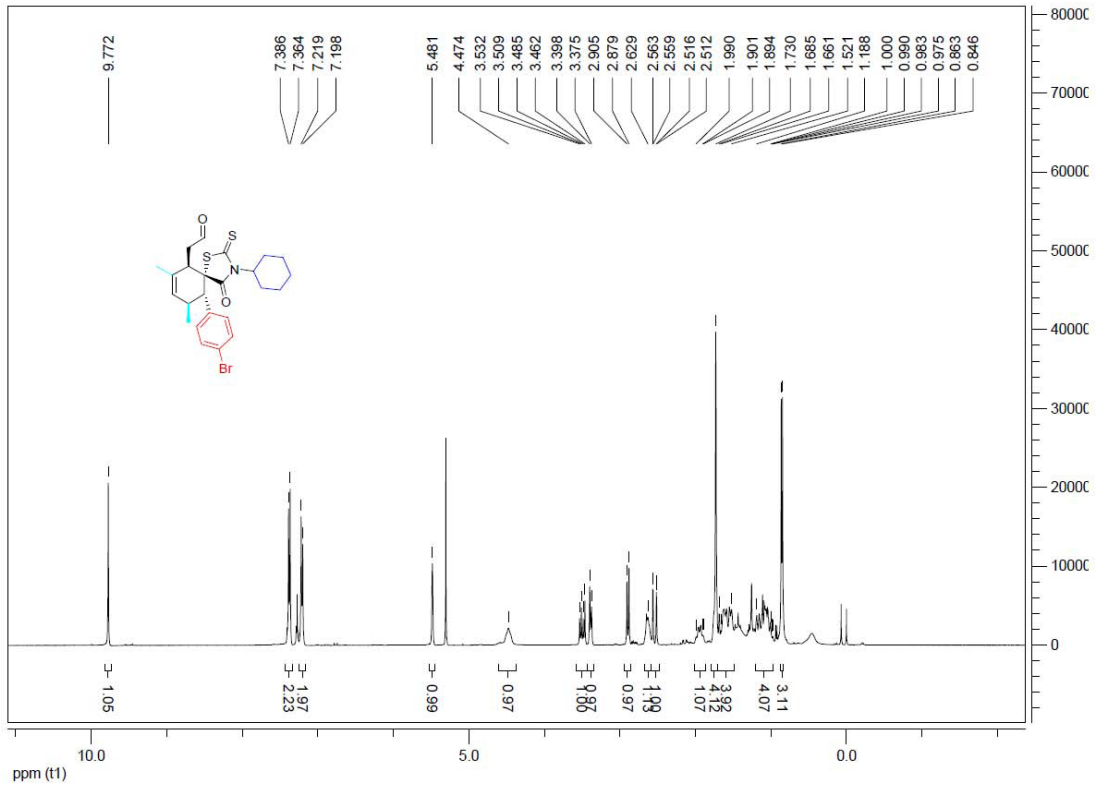


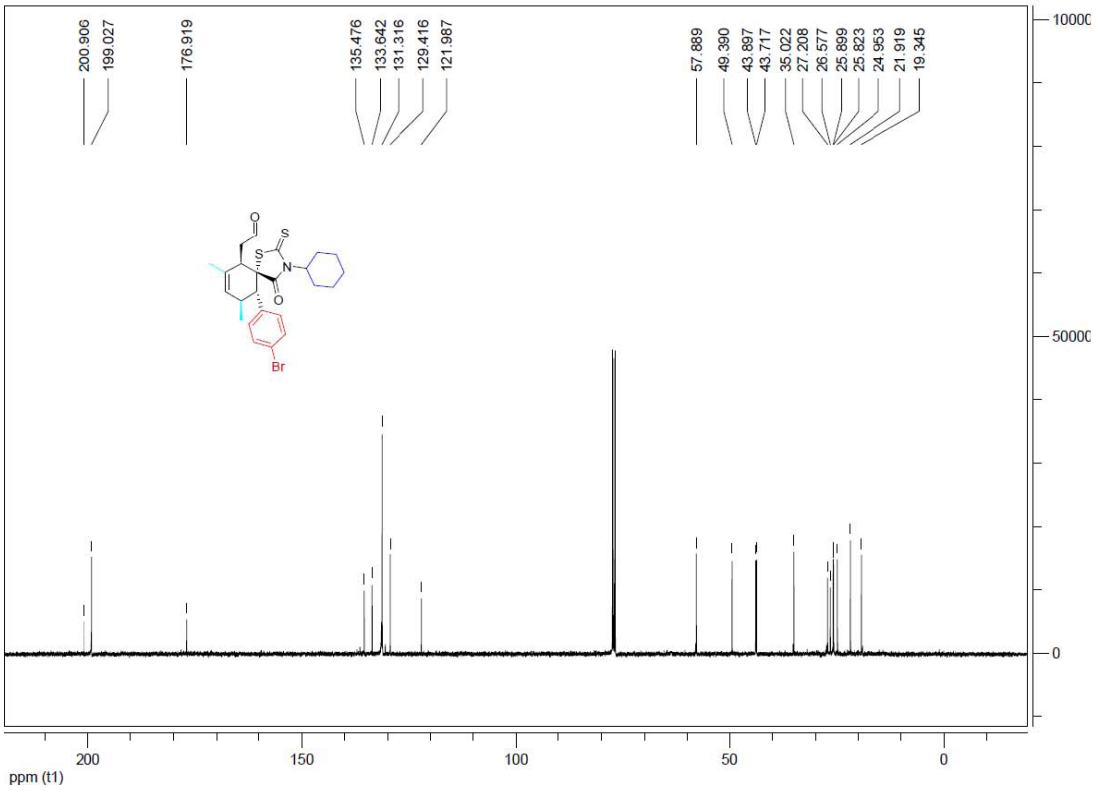
6m:2-((5S,6R,9S,10S)-3-cyclohexyl-7,9-dimethyl-4-oxo-10-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



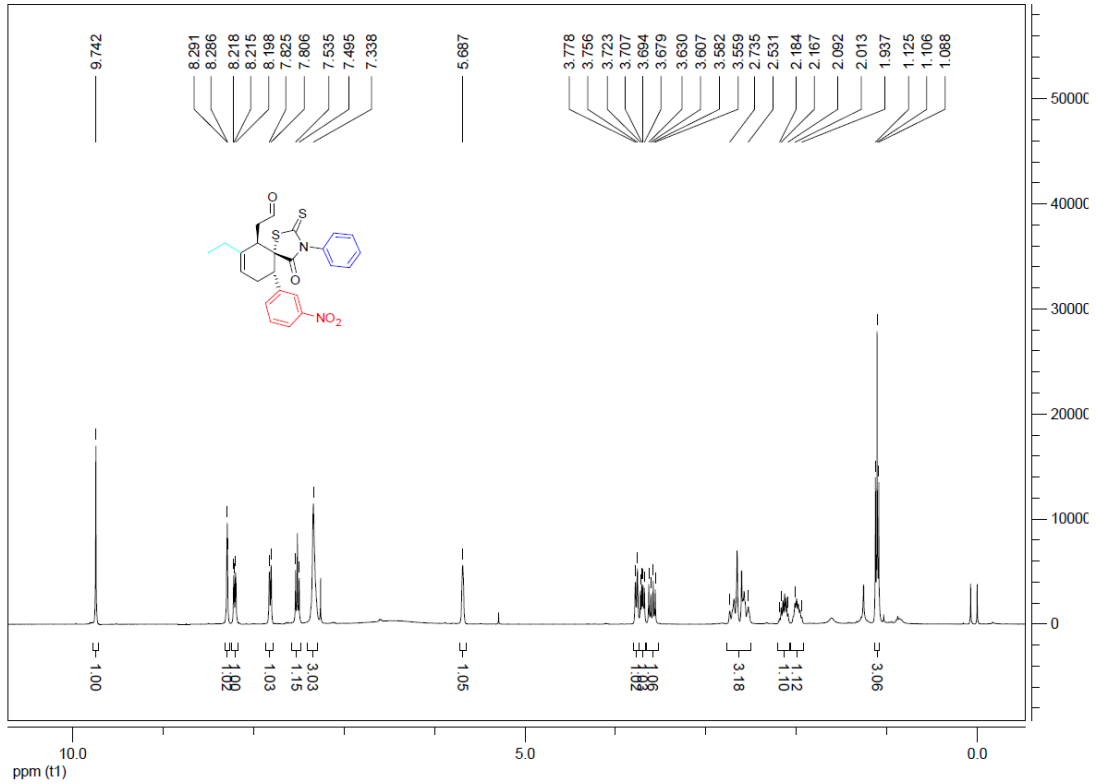


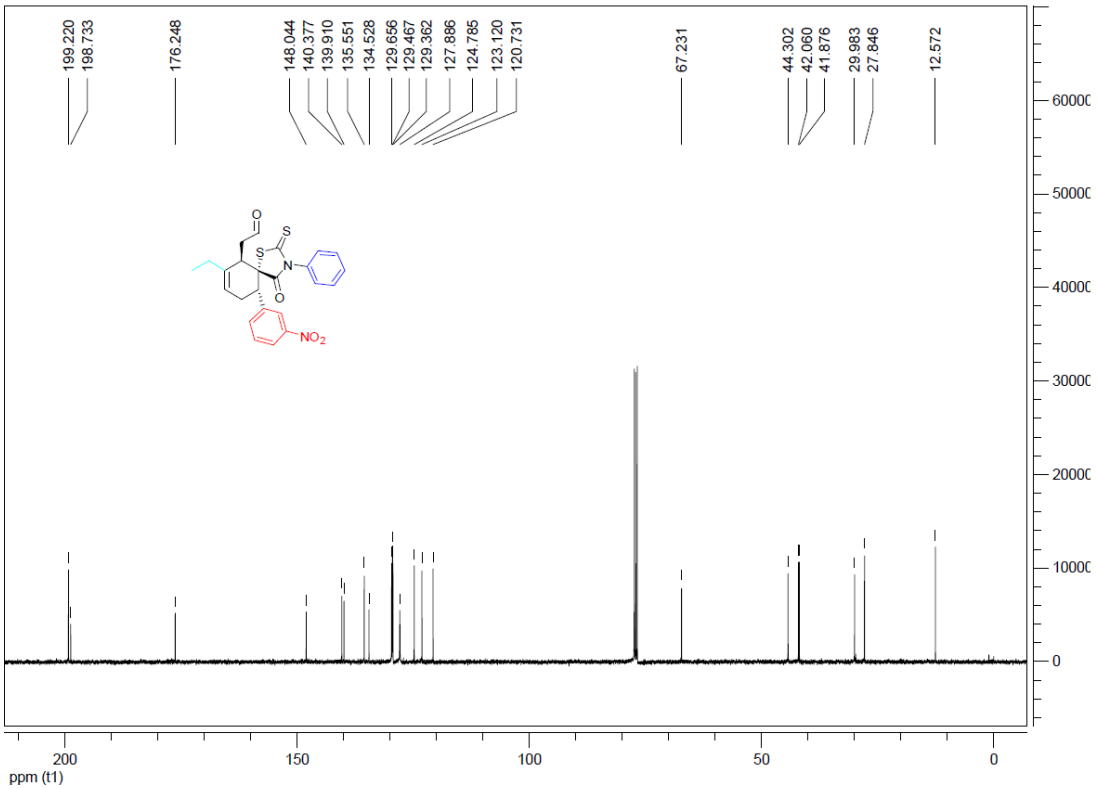
6n:2-((5S,6R,9S,10S)-10-(4-bromophenyl)-3-cyclohexyl-7,9-dimethyl-4-oxo-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



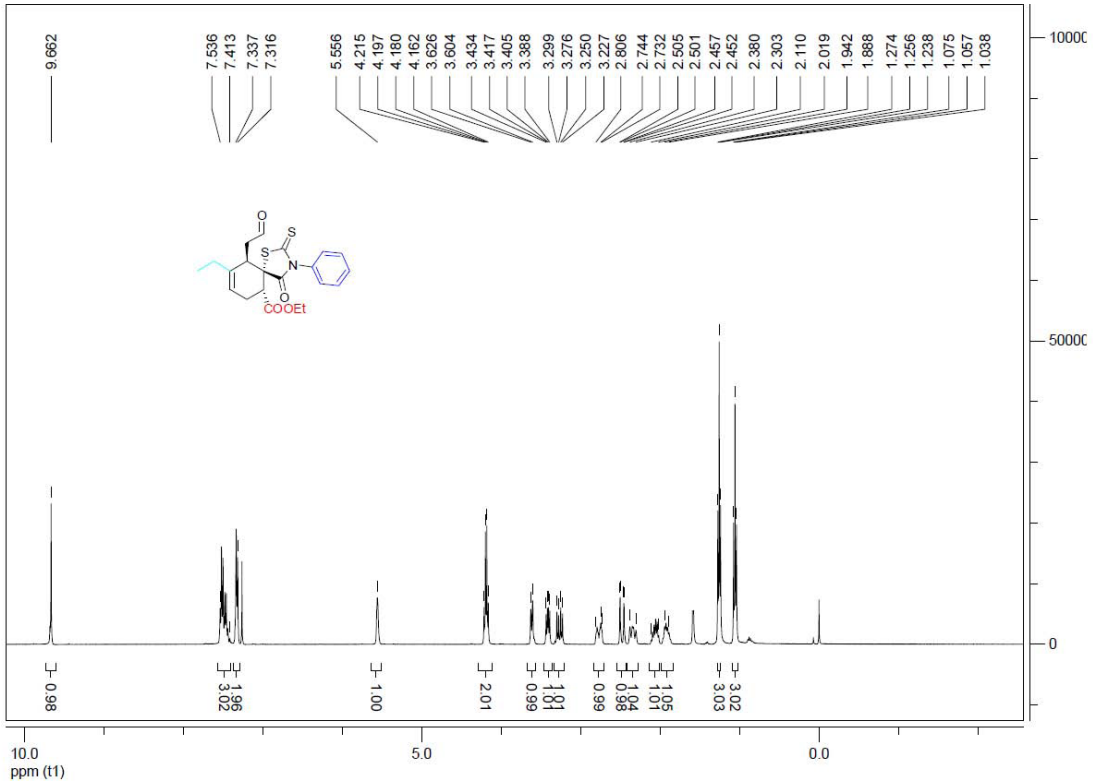


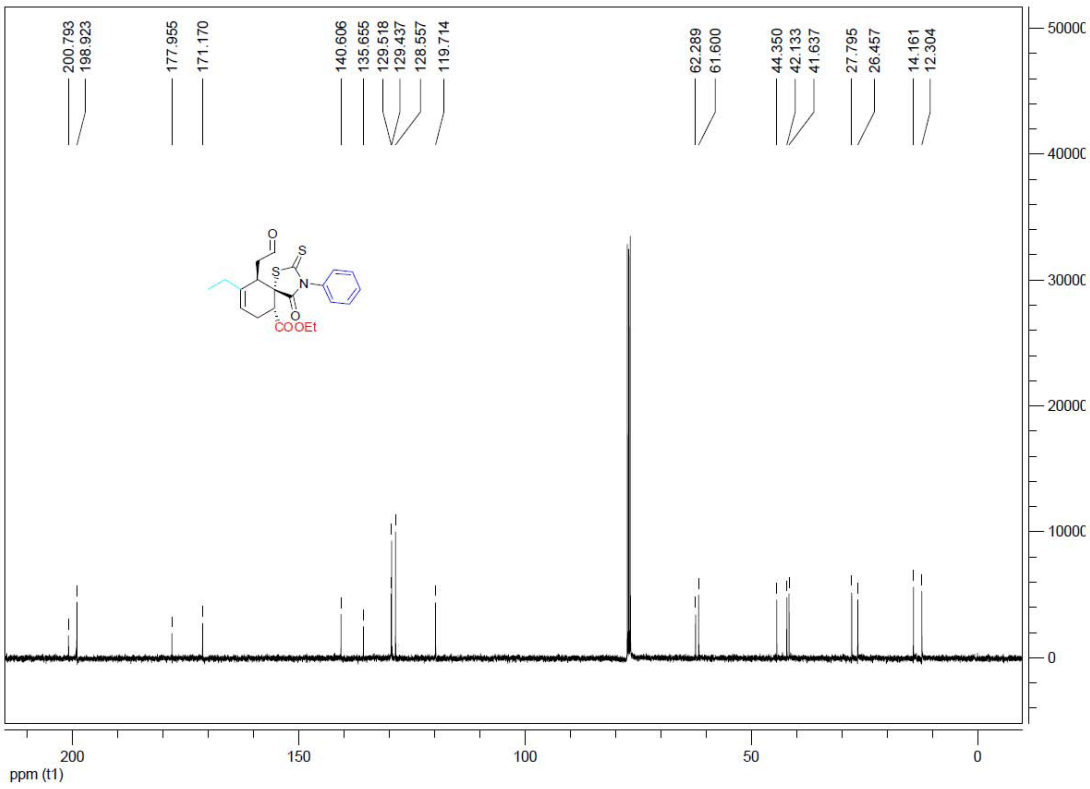
6o:2-((5S,6R,10S)-7-ethyl-10-(3-nitrophenyl)-4-oxo-3-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



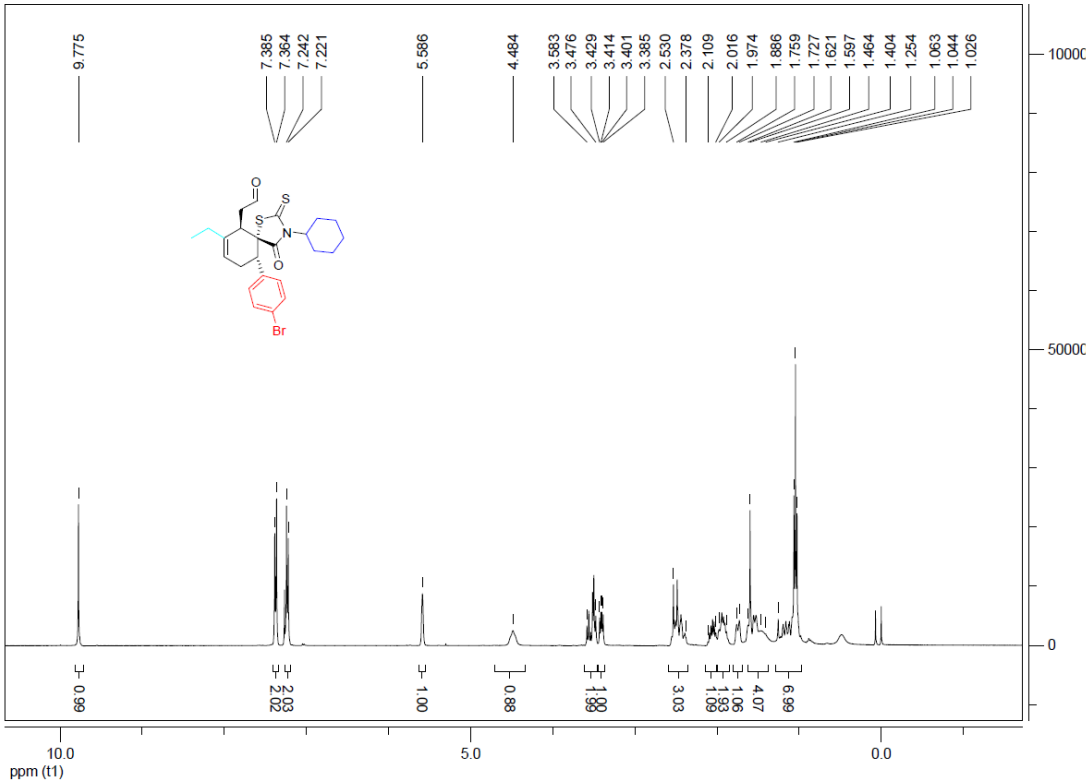


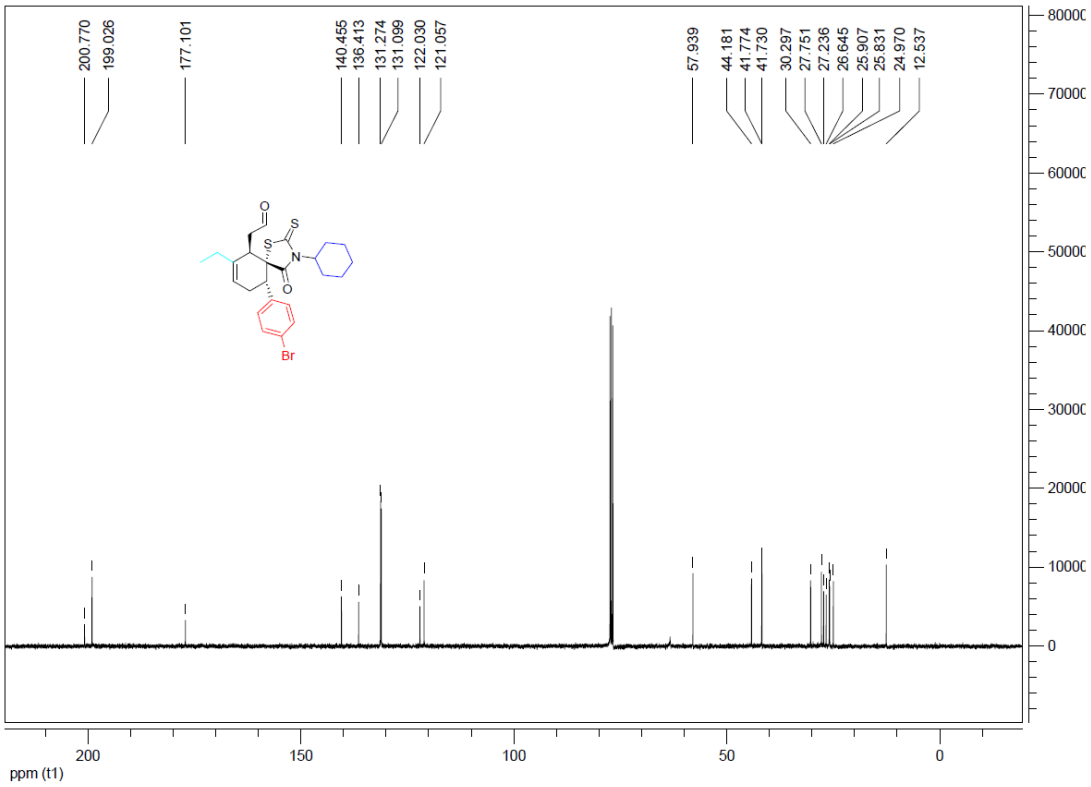
6p:(5S,6S,10R)-ethyl-9-ethyl-4-oxo-10-(2-oxoethyl)-3-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-8-ene-6-carboxylate



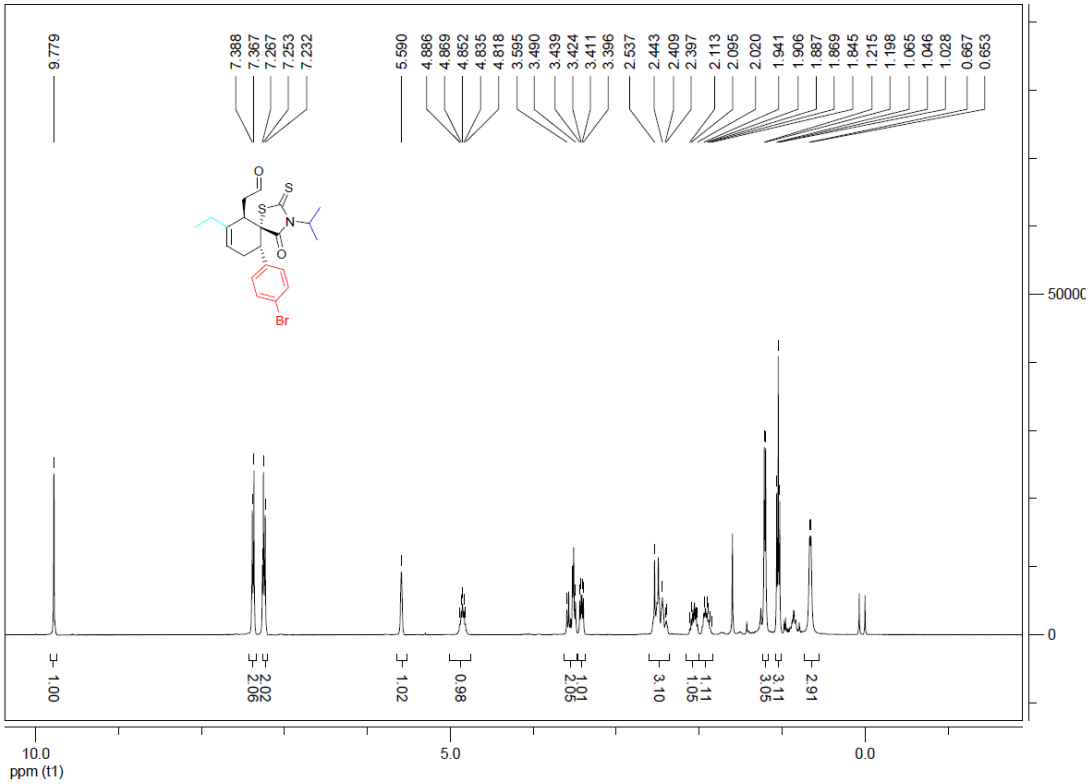


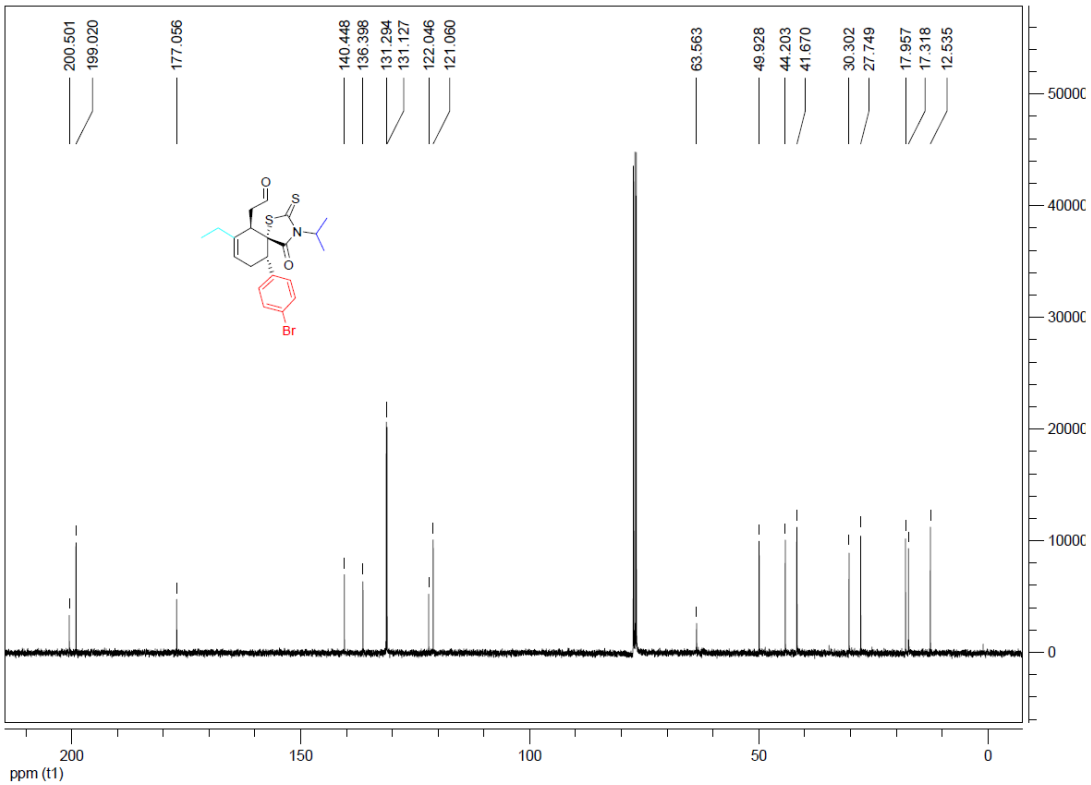
6q:2-((5S,6R,10S)-10-(4-bromophenyl)-3-cyclohexyl-7-ethyl-4-oxo-2-thioxo-1-thia-3-azaspiro [4.5]dec-7-en-6-yl)acetaldehyde



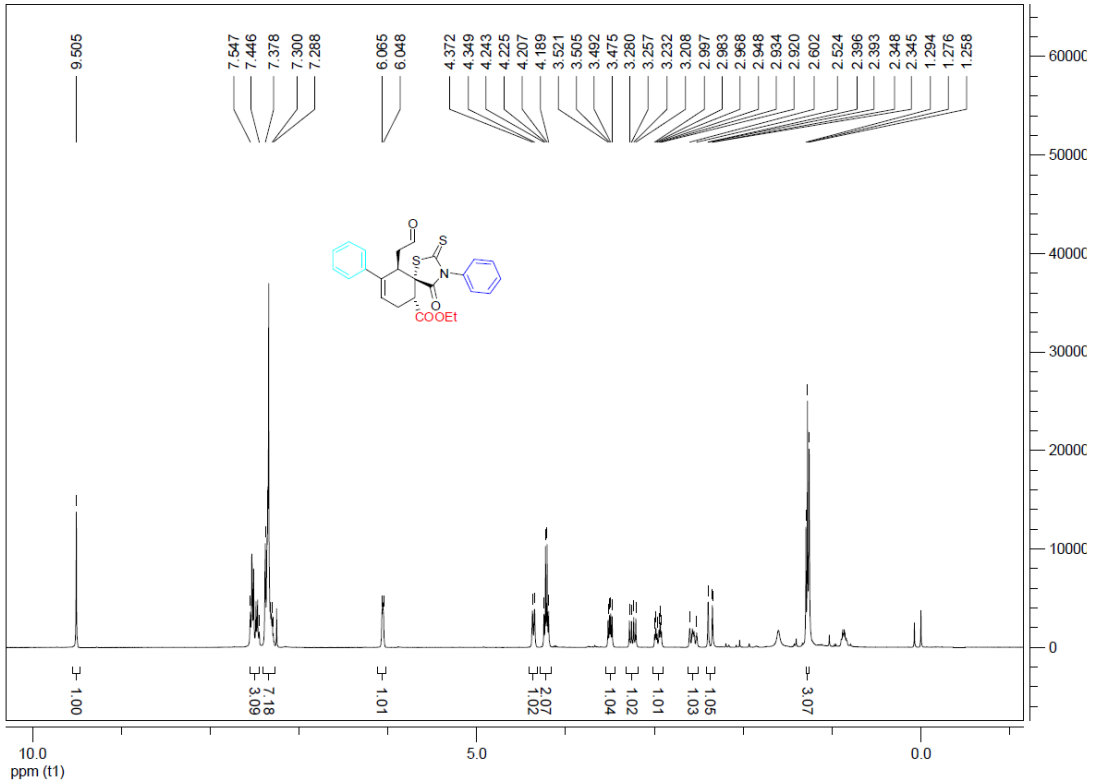


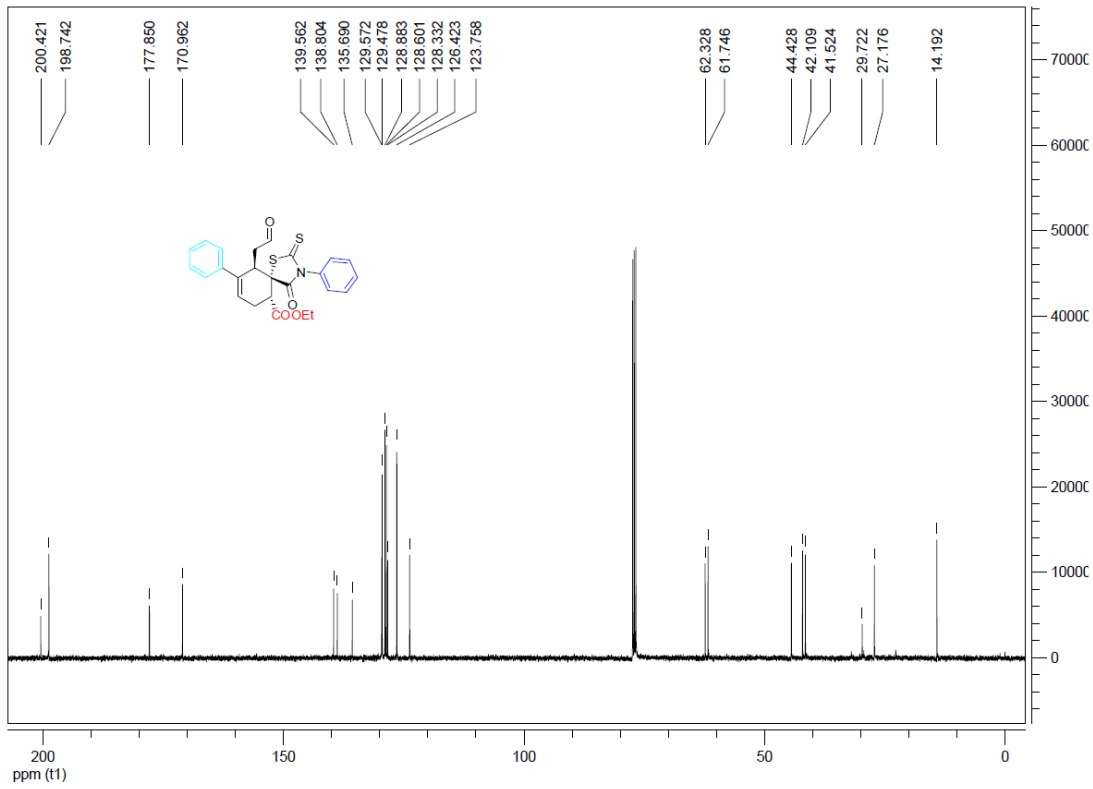
6r:2-((5S,6R,10S)-10-(4-bromophenyl)-7-ethyl-3-isopropyl-4-oxo-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



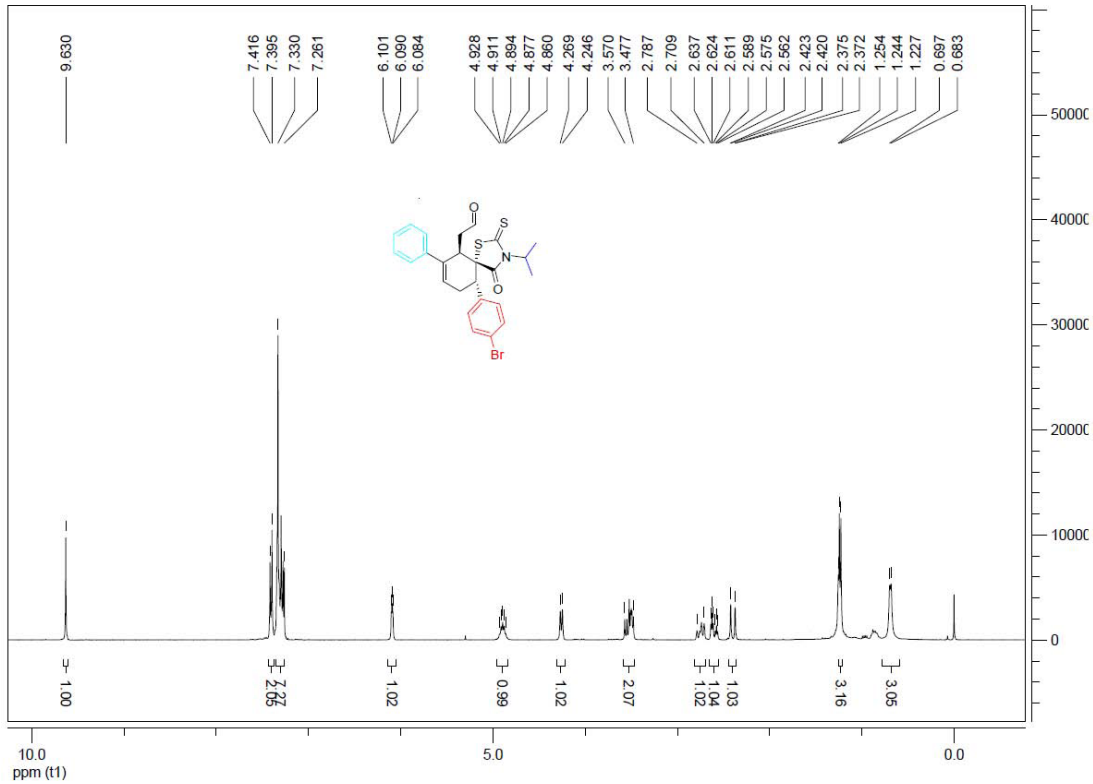


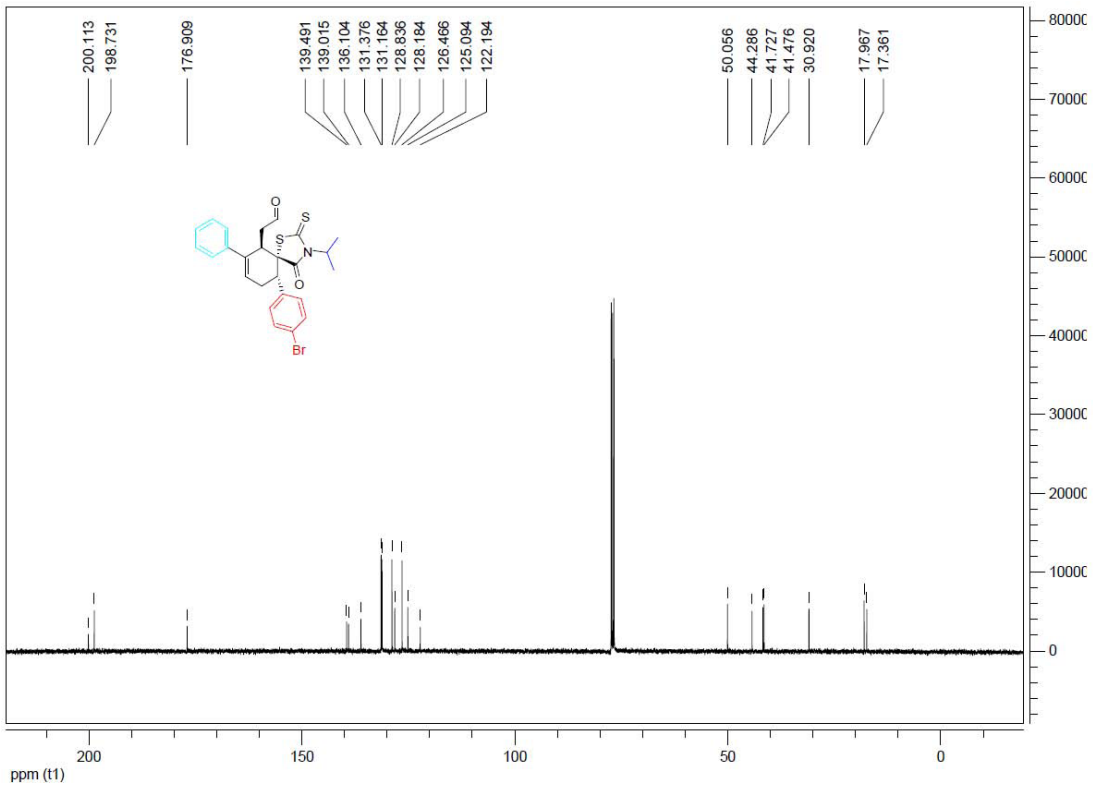
6s:(5S,6S,10R)-ethyl-4-oxo-10-(2-oxoethyl)-3,9-diphenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-8-ene-6-carboxylate



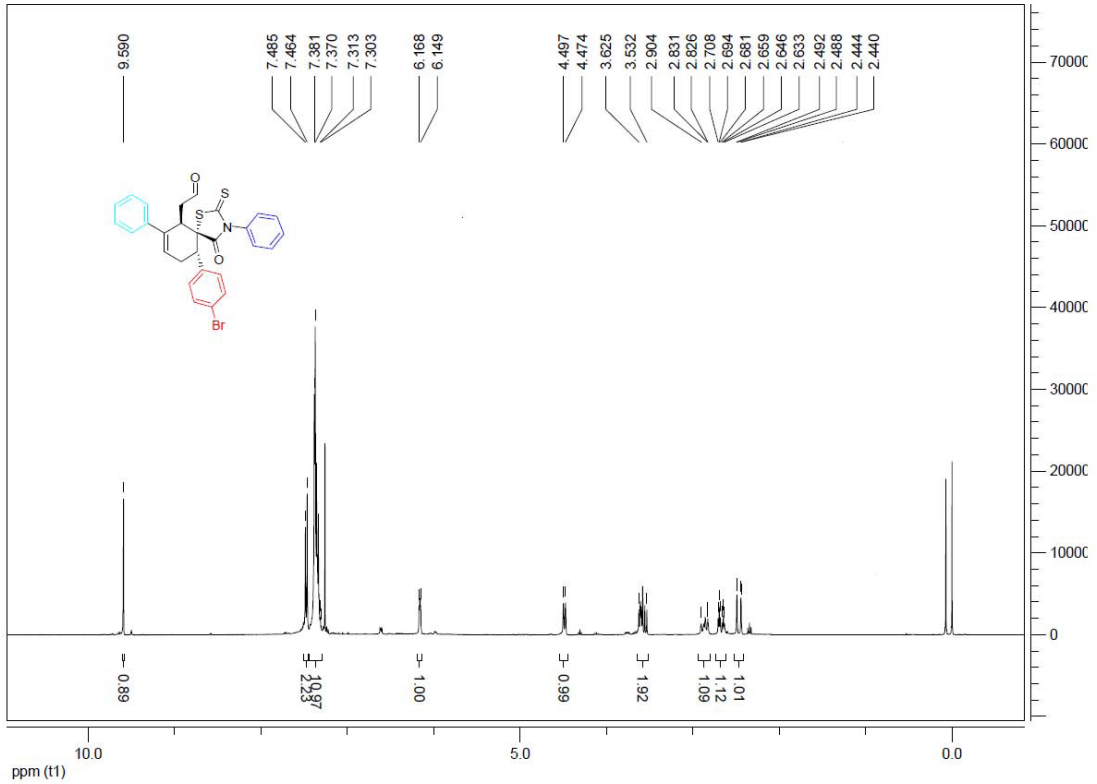


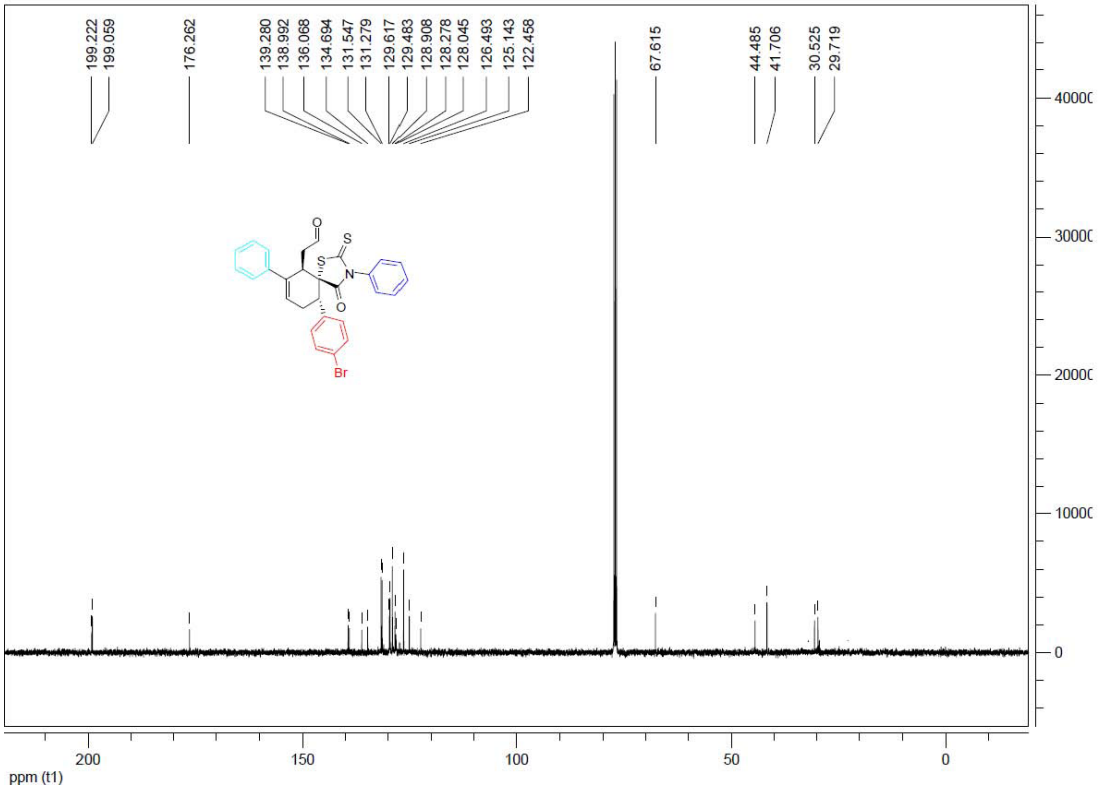
6t:2-((5R,6R,10S)-10-(4-bromophenyl)-3-isopropyl-4-oxo-7-phenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



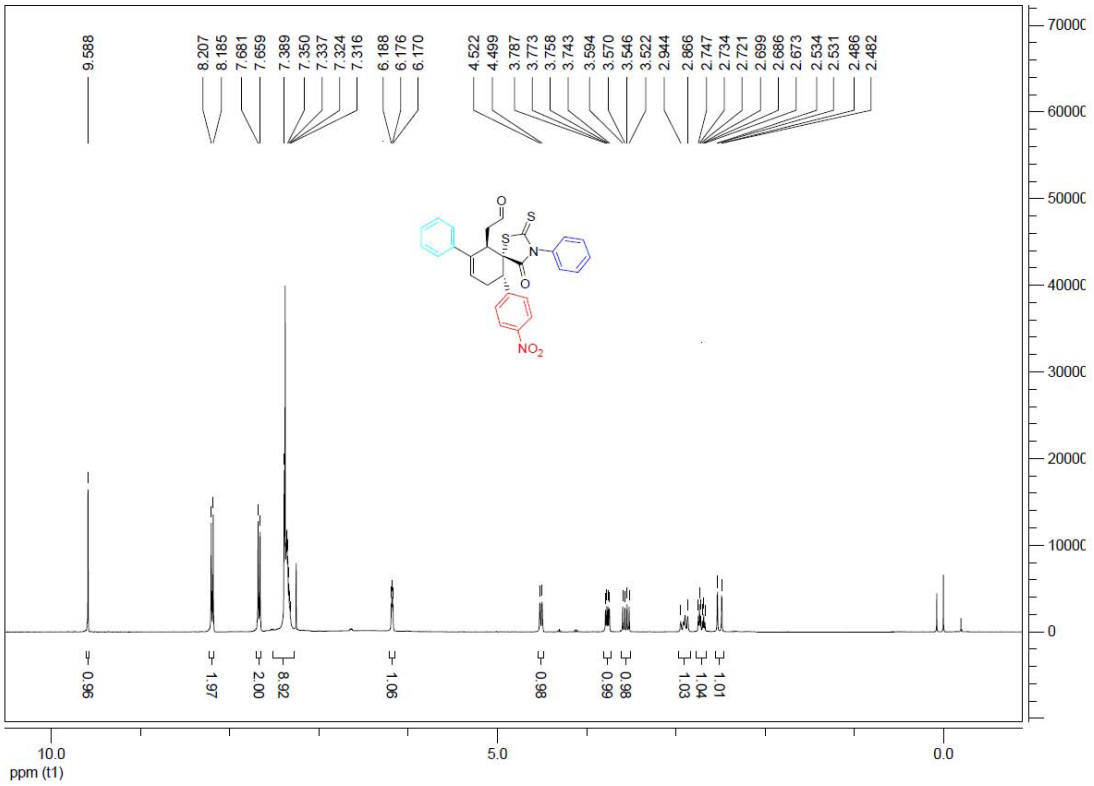


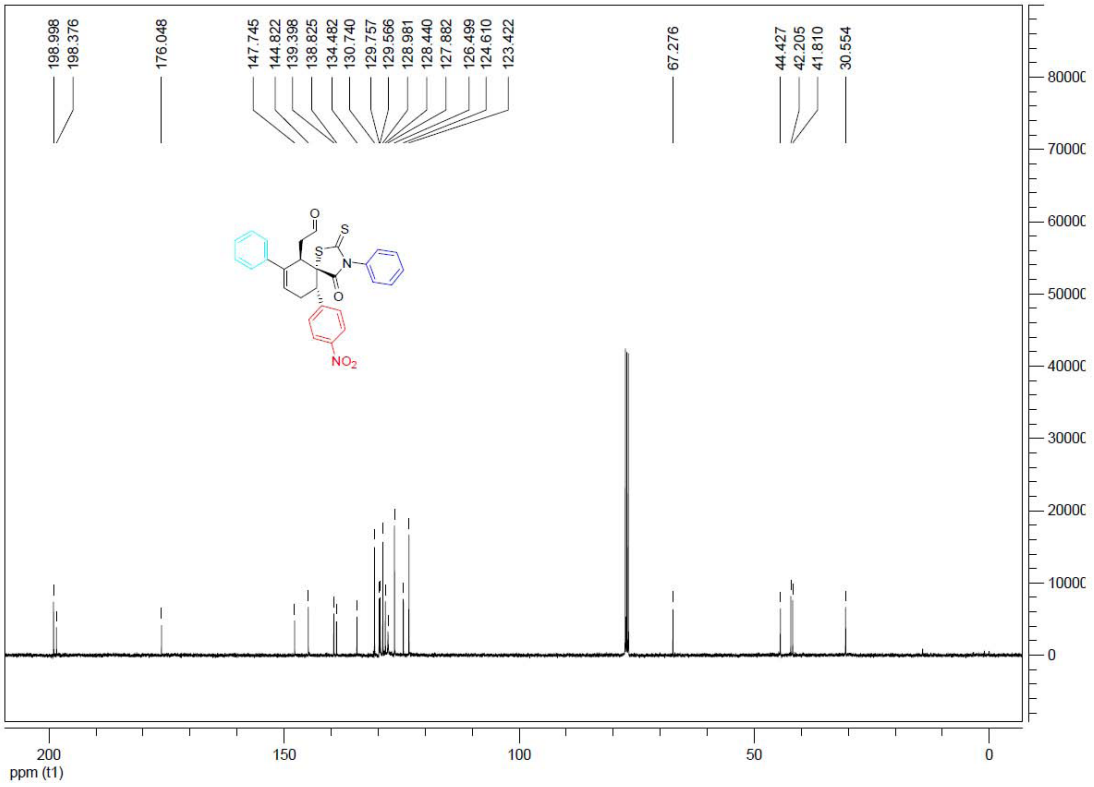
6u:2-((5R,6R,10S)-10-(4-bromophenyl)-4-oxo-3,7-diphenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



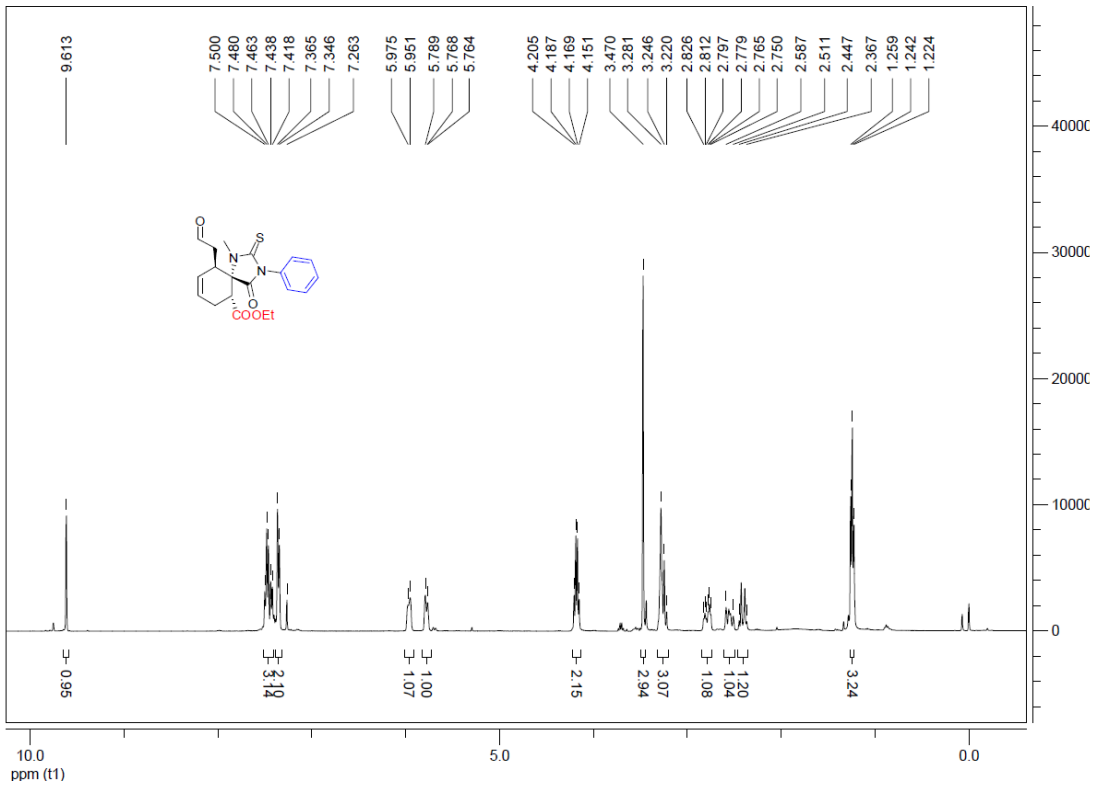


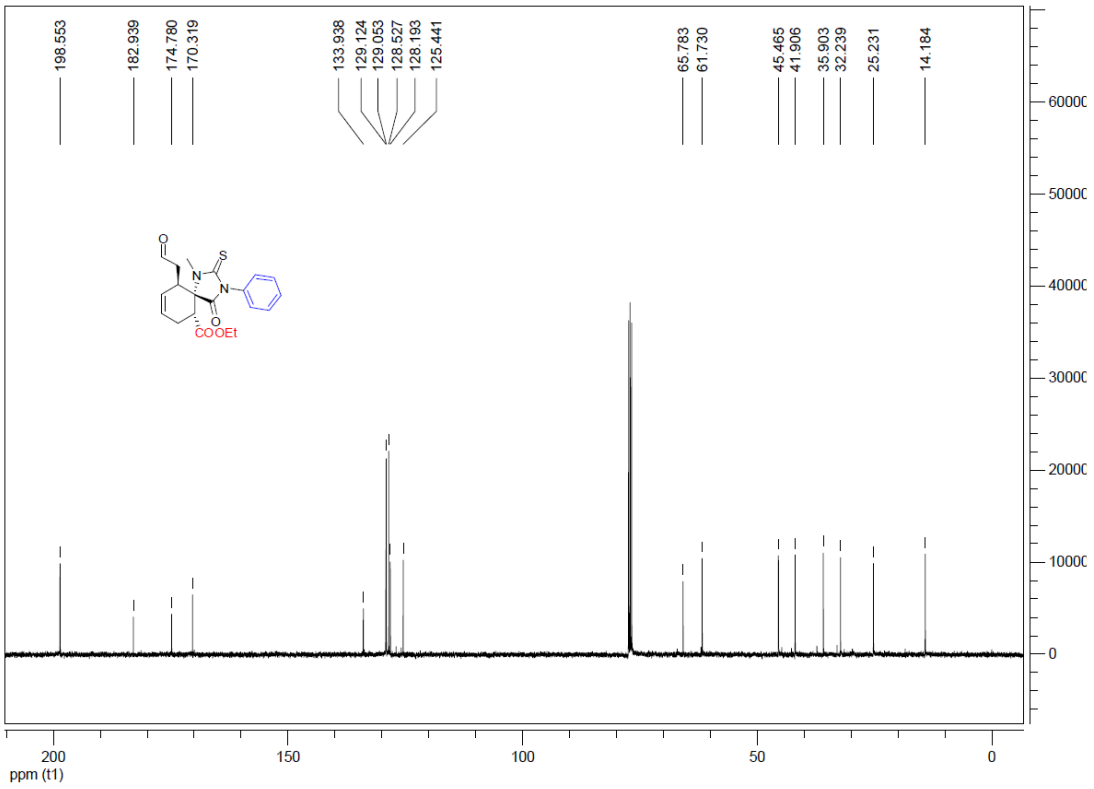
6v:2-((5R,6R,10S)-10-(4-nitrophenyl)-4-oxo-3,7-diphenyl-2-thioxo-1-thia-3-azaspiro[4.5]dec-7-en-6-yl)acetaldehyde



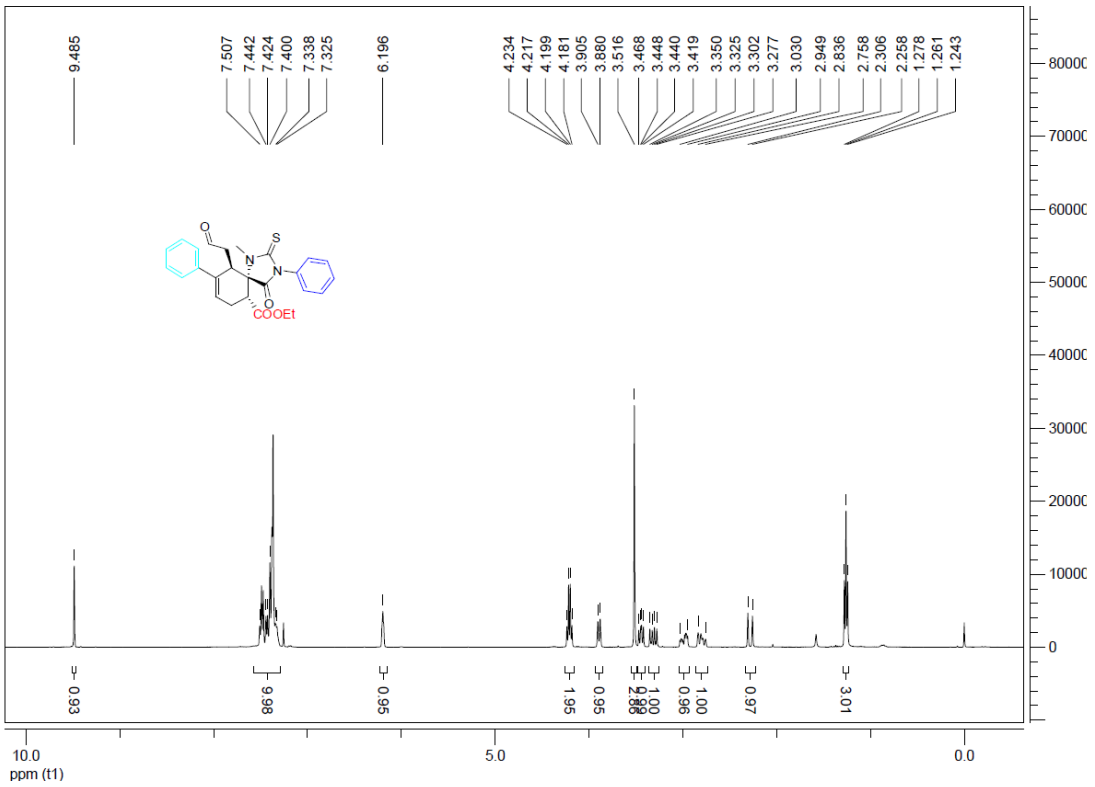


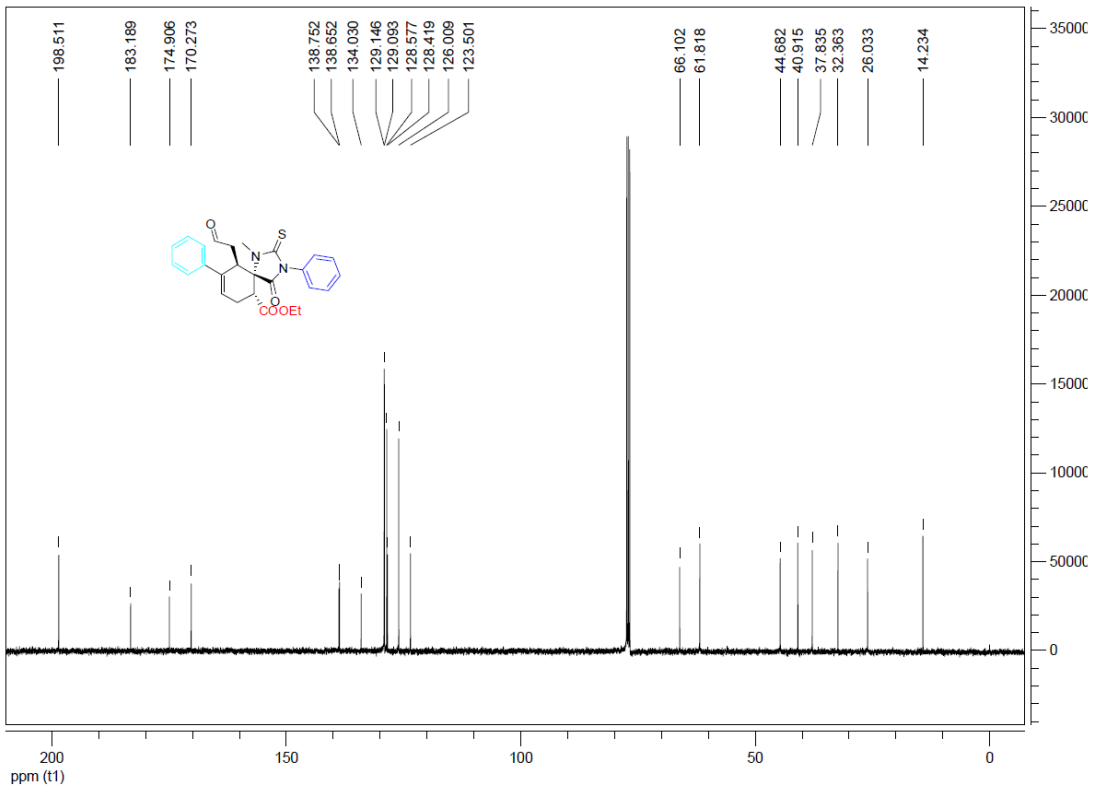
6w:(5S,6R,10R)-ethyl-1-methyl-4-oxo-10-(2-oxoethyl)-3-phenyl-2-thioxo-1,3-diazaspiro[4.5]dec-8-ene-6-carboxylate



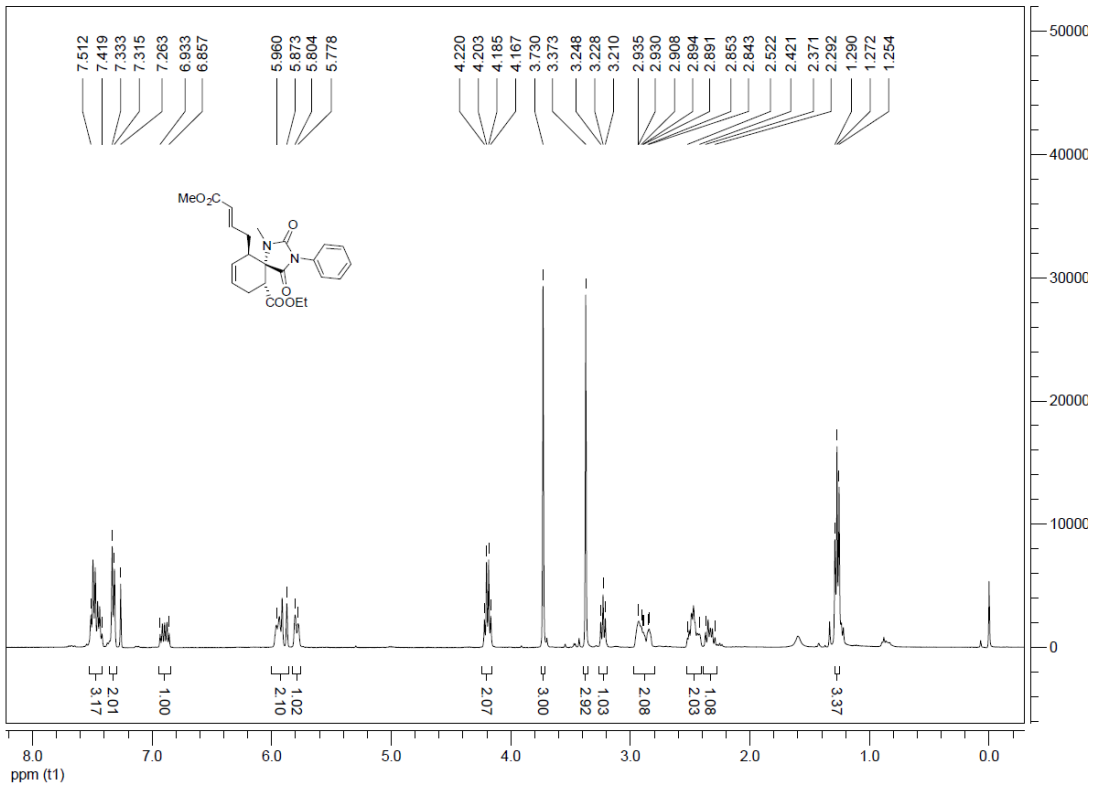


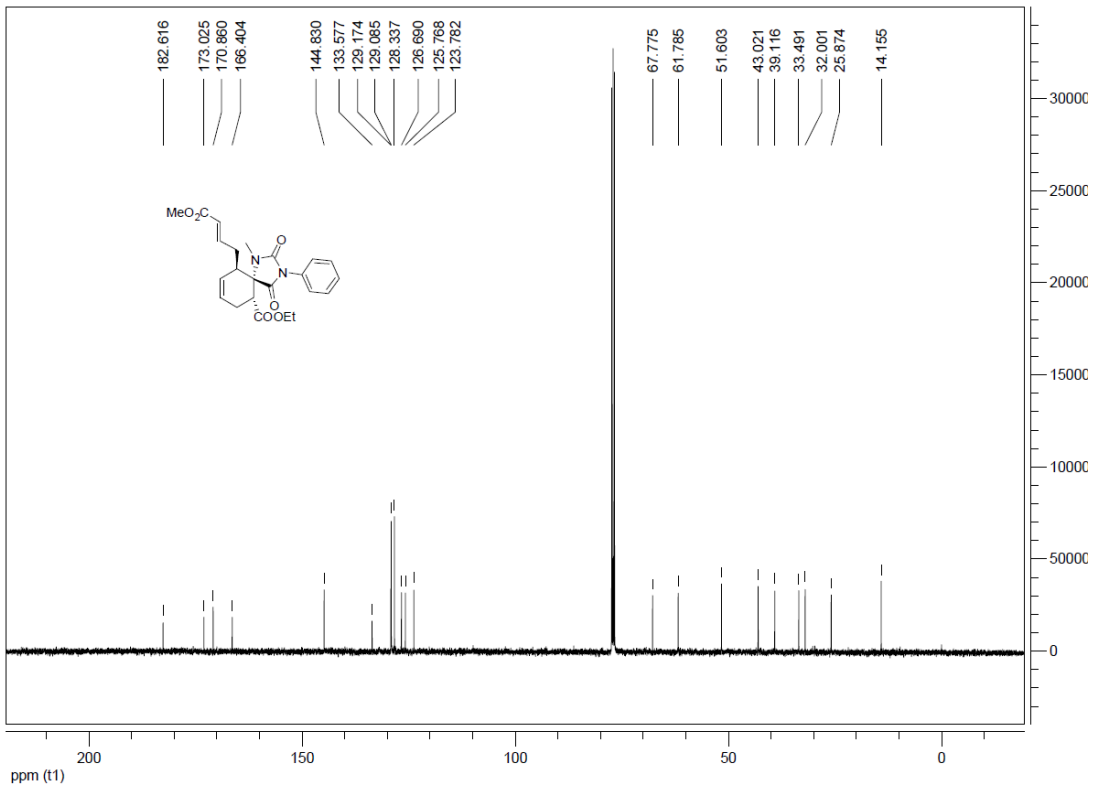
6x:(5S,6R,10R)-ethyl1-methyl-4-oxo-10-(2-oxoethyl)-3,9-diphenyl-2-thioxo-1,3-diazaspiro[4.5]dec-8-ene-6-carboxylate



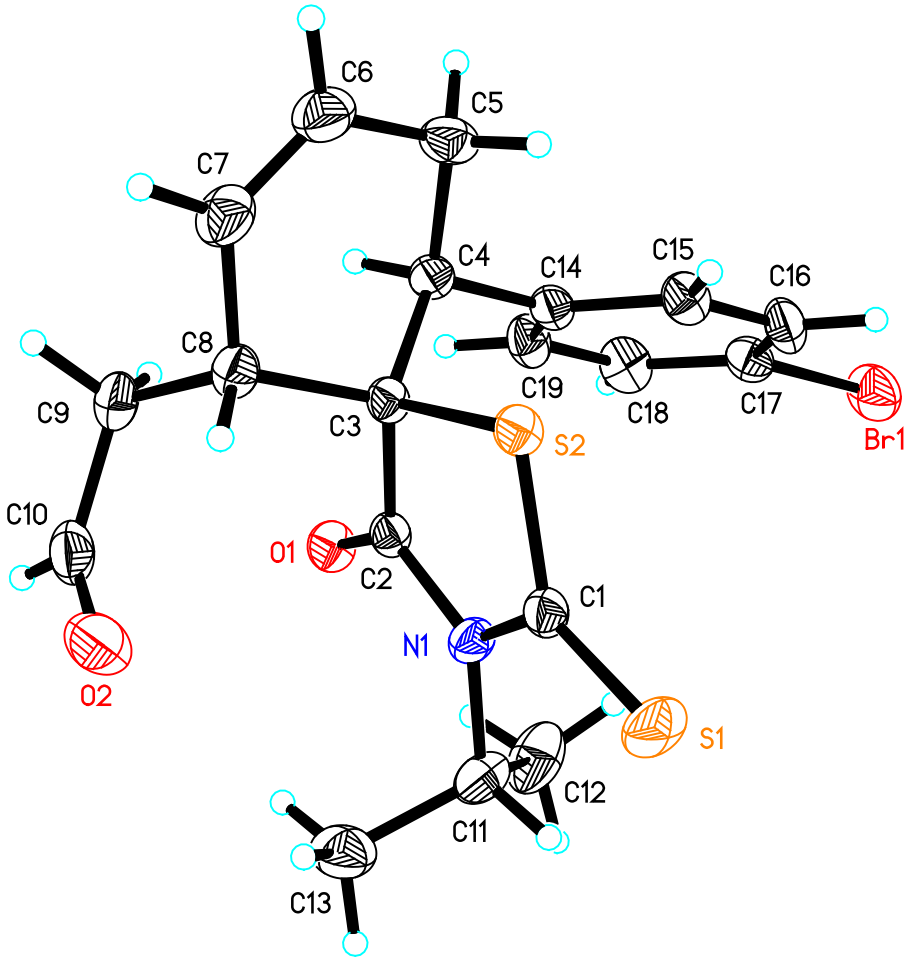


7a:(5S,6R,10R)-ethyl-10-(4-methoxy-4-oxobut-2-enyl)-1-methyl-2,4-dioxo-3-phenyl-1,3-diaza spiro[4.5]dec-8-ene-6-carboxylate





G: Absolute Configuration and X-Ray Analysis Data



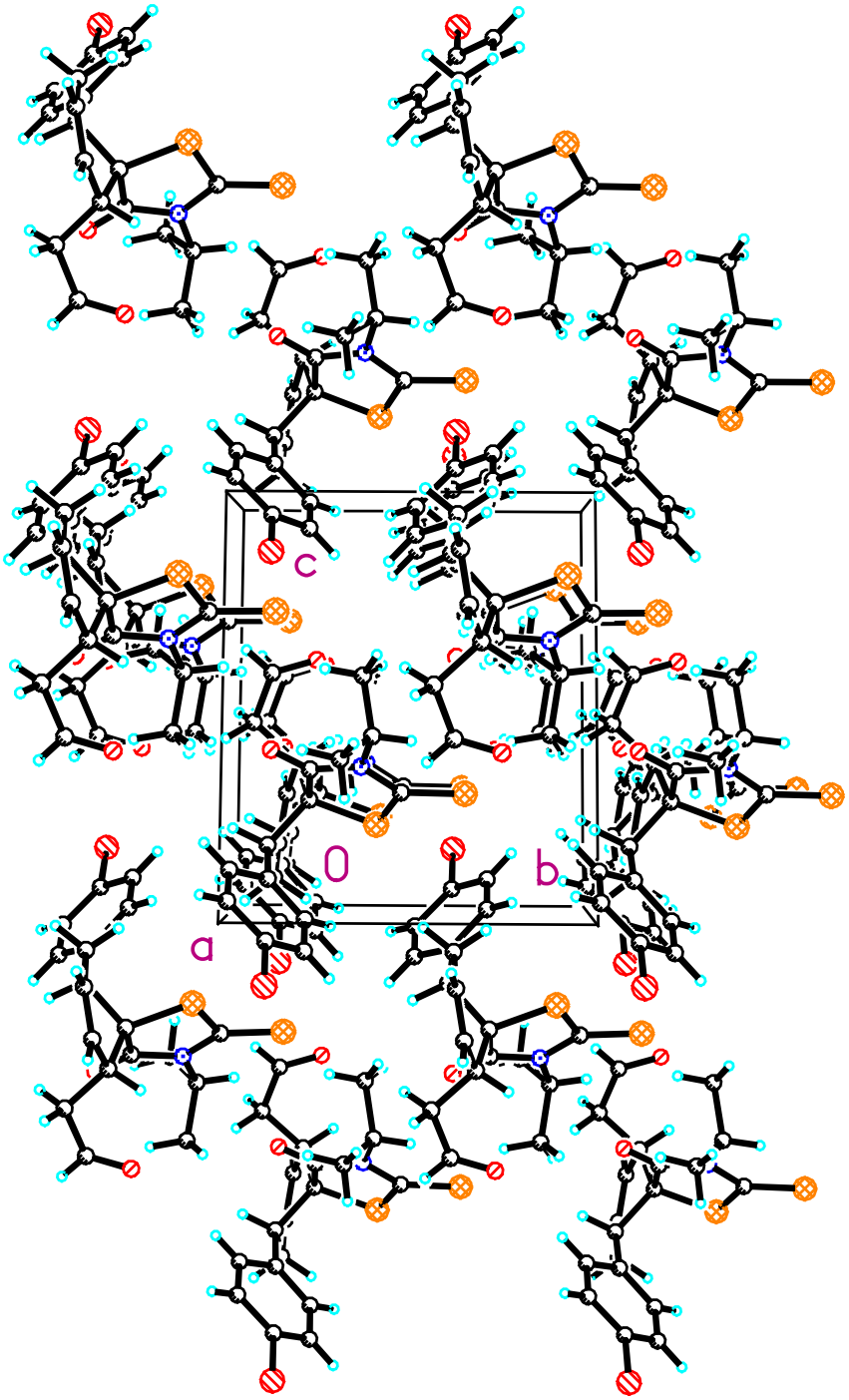


Table 1. Crystal data and structure refinement for **6j**.

Identification code	**6j**
Empirical formula	$C_{19}H_{20}BrNO_2S_2$
Formula weight	438.39
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2(1)
Unit cell dimensions	a = 9.9067 (13) Å α = 90 °. b = 9.1539 (13) Å β = 106 °. c = 10.9950 (15) Å γ = 90 °.
Volume	956.9 (2) $Å^3$
Z,	2
Calculated density	1.521 Mg/m^3
Absorption coefficient	2.378 mm^{-1}
F(000)	448
Crystal size	0.312 x 0.211 x 0.156 mm^3
θ range for data collection	1.93 to 25.99 °.
Limiting indices	$-12\le h\le 11$, $-11\le k\le 7$, $-13\le l\le 13$
Reflections collected / unique	5756 / 2911 [R_{int} = 0.0302]
Completeness to θ = 26.00º	100.0 %
Absorption correction(μ)	Empirical
Max. and min. transmission	1.00000 and 0.43771
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2911 / 1 / 229
Goodness-of-fit on F^2	1.065
Final R indices [I>2σ(I)]	R_1 = 0.0299, wR_2 = 0.0733
R indices (all data)	R_1 = 0.0329, wR_2 = 0.0745
Absolute structure parameter	0.005(8)
Largest diff. peak and hole	0.426 and -0.354 e^-. $Å^{-3}$