Supporting Information

Highly Diastereoselective and Enantioselective Michael Addition of 5*H*-Oxazol-4-ones to α,β-Unsaturated Ketones Catalyzed by New Bifunctional Organocatalyst with Broad Substrate Scope and Applicability

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A: General Information and Starting Materials

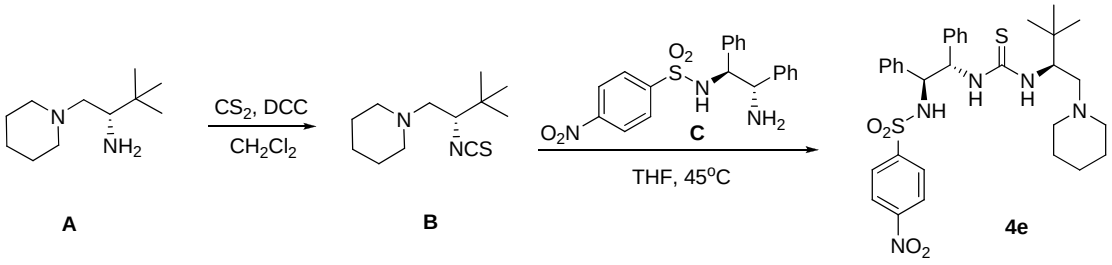
General Information. Proton nuclear magnetic resonance (^{1}H NMR) spectra and carbon nuclear magnetic resonance (^{13}C NMR) spectra were recorded on a Bruker AV-400 spectrometer (400 MHz and 100 MHz). Chemical shifts for protons are reported in parts per million downfield from tetramethylsilane and 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) and Low resolution mass spectrometry (ESI) were carried out using a Waters Quatro Macro triple quadrupole mass spectrometer. High resolution mass spectra (EI) were measured on a Waters Micromass GCT spectrometer. Optical rotations were measured on an Autopol III automatic polarimeter (Rudolph Research analytical). IR were measured on a Nicolet 6700. 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 IA, IC, AS-H, AD-H) as noted.

Starting Materials. All solvents and inorganic reagents were from commercial sources and used without purification unless otherwise noted. The pronucleophiles 5*H*-Oxazol-4-ones **5** were synthesized following the literature procedure.[1]

B: Experimental Procedure and Characterization of Catalysts

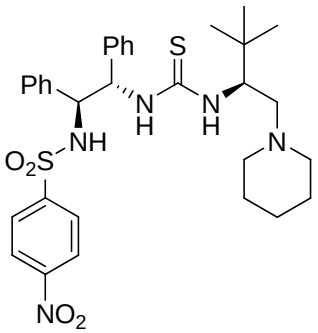
Synthetic route of new chiral Thiourea-Tertiary Amine catalyst 4e.

The primary amine **A** was synthesized following the literature procedure[2].



A **B** **4e**

***N*-((1*S*,2*S*)-2-(3-((*S*)-3,3-dimethyl-1-(piperidin-1-yl)butan-2-yl)thioureido)-1,2-diphenylethyl)-4-nitrobenzenesulfonamide (4e)**

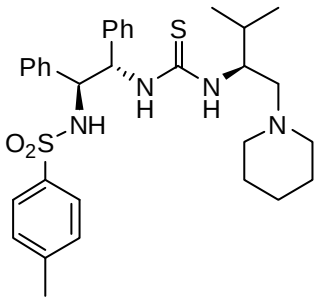


DCC (0.83 g, 4.0 mmol) and CS_2 (0.38 g, 5.0 mmol) were added into a solution of (*S*)-3,3-dimethyl-1-(piperidin-1-yl)butan-2-amine (0.74 g, 4.0 mmol) in CH_2Cl_2 at 0°C. The resulting mixture was stirred at room temperature for 12 h. After that the solvent was removed in vacuum and the residue was redissolved with ethyl ether. After filtration the filtrate was concentrated in vacuum to afford the crude product of isothiocyanate **B** as a light yellow oil, which was taken directly to the next step.

To a solution of the diamine **C** (1.19 g, 3.0 mmol) in THF (10 mL) was added isothiocyanate **B** (4.0 mmol). The resulting solution was stirred for 12h at 45°C. The reaction was concentrated in vacuum and the residue was purified by silica gel chromatography to afford catalysts 4e as a yellow solid (1.77 g) in 95% yield. Mp 100-101°C; $[\alpha]^{24}D$ - 53.3 (*c* 1.0, CH_2Cl_2); ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 10.46 (d, *J* = 9.2 Hz, 1H), 7.94-7.92 (m, 2H), 7.52-7.50 (m, 2H), 7.22-7.18 (m, 5H), 6.99-6.90 (m, 5H), 6.28 (d, *J* = 5.6 Hz, 1H), 6.14 (t, *J* = 20.4 Hz, 1H), 5.00 (d, *J* = 11.2 Hz, 1H), 3.10 (t, *J* = 11.6 Hz, 1H), 2.72-2.60 (m, 6H), 1.84-1.63 (m, 6H), 1.01 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 183.2, 149.0, 147.7, 137.7, 137.4, 128.4, 128.2, 128.1, 128.1, 128.0, 127.7, 123.4, 64.9, 63.7, 63.4, 63.0, 55.2, 33.7, 26.5, 25.2, 23.9; IR (KBr): 3020-3320(NH) cm^{-1}, 1520, 1345 (NO_2) cm^{-1}, 1166 (SO_2) cm^{-1}; HRMS (ESI): exact mass calculated for $[(M+H)^+]$ ($C_{32}H_{42}N_5O_4S_2$) requires m/z 624.2678, found m/z 624.2674.

Other new chiral Thiourea-Tertiary Amine catalysts **4a, 4b, 4c, 4d, 4f, 4g** were synthesized following the procedure of **4e.**

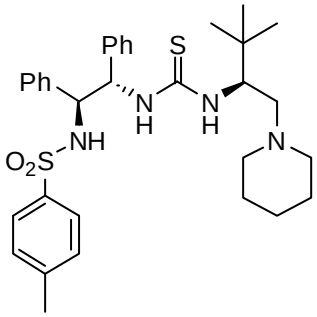
4-methyl-N-((1*S*,2*S*)-2-(3-((*S*)-3-methyl-1-(piperidin-1-yl)butan-2-yl)thioureido)-1,2-diphenylethyl)benzenesulfonamide (4a)



White solid. Mp 91-92°C; $[\alpha]^{24}_D$ – 2.5 (*c* 1.0, CH_2Cl_2); ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 10.27 (d, *J* = 9.2 Hz, 1H ）, 7.38（br, 1H）, 7.31-7.28 (m, 2H), 7.20-7.15 (m, 5H), 7.00-6.92 (m, 7H), 6.24-6.13 (m, 2H), 4.95 (d, *J* = 10.0 Hz, 1H), 3.29-3.27 (m, 1H), 2.70-2.60 (m, 5H), 2.45 (d, *J* = 14.0 Hz, 1H), 2.27 (s, 3H), 1.88-1.58 (m, 7H), 0.97 (d, *J* = 6.4 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 182.9,

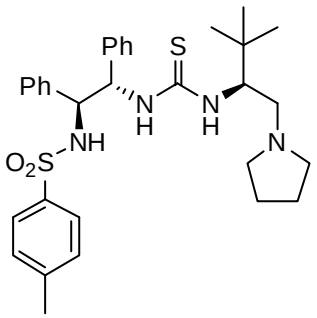
142.0, 137.8, 128.8, 128.3, 128.2, 127.9, 127.8, 127.2, 126.5, 55.0, 25.1, 24.0, 21.3, 18.2, 18.1; HRMS (ESI): exact mass calculated for $[(M+H)^+]$ ($C_{32}H_{43}N_4O_2S_2$) requires m/z 579.2827, found m/z 579.2832.

_N_-((1_S_,2_S_)-2-(3-((_S_)-3,3-dimethyl-1-(piperidin-1-yl)butan-2-yl)thioureido)-1,2-diphenylethyl)-4-methylbenzenesulfonamide (4b)



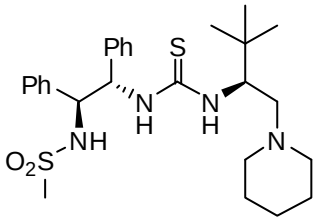
White solid. Mp 92-93°C; $[\alpha]^{24}_D$ – 13.2 (_c_ 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 10.36 (d, _J_ = 9.2 Hz, 1H), 7.54 (br, 1H), 7.28-7.25 (m, 2H), 7.20-7.16 (m, 5H), 7.00-6.91 (m, 7H), 6.25 (d, _J_ = 5.2 Hz, 1H), 6.13 (t, _J_ = 20.4 Hz, 1H), 4.97 (d, _J_ = 10.0 Hz, 1H), 3.09-3.07 (m, 1H), 2.69-2.63 (m, 6H), 2.27 (s, 3H), 1.80-1.61 (m, 6H), 1.01 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 183.1, 141.9, 139.0, 138.3, 137.9, 128.8, 128.3, 128.2, 128.0, 127.9, 127.8, 127.1, 126.5, 64.5, 63.9, 63.1, 62.9, 55.1, 33.7, 26.5, 25.1, 23.9, 21.3; HRMS (ESI): exact mass calculated for $[(M+H)^+]$ ($C_{33}H_{45}N_4O_2S_2$) requires m/z 593.2984, found m/z 593.2988.

_N_-((1_S_,2_S_)-2-(3-((_S_)-3,3-dimethyl-1-(pyrrolidin-1-yl)butan-2-yl)thioureido)-1,2-diphenylethyl)-4-methylbenzenesulfonamide (4c)



White solid. Mp 90-91°C; $[\alpha]^{24}_D$ - 11.3 (_c_ 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 10.91 (d, _J_ = 8.8 Hz, 1H), 7.59 (br, 1H), 7.32-7.30 (m, 2H), 7.18-7.16 (m, 3H), 7.04-7.02 (m, 2H), 6.98-6.92 (m, 7H), 6.29 (d, _J_ = 4.4 Hz, 1H), 5.98 (t, _J_ = 19.6 Hz, 1H), 4.83 (d, _J_ = 10.8 Hz, 1H), 3.12-3.10 (m, 1H), 2.97-2.92 (m, 2H), 2.83-2.68 (m, 5H), 2.27 (s, 3H), 2.11-2.02 (m, 4H), 1.00 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 183.4, 142.0, 138.9, 138.4, 138.3, 128.8, 128.3, 127.9, 127.8, 127.7, 127.1, 126.5, 65.1, 64.2, 64.0, 60.7, 54.7, 33.6, 26.5, 23.9, 21.3; HRMS (ESI): exact mass calculated for $[(M+H)^+]$ ($C_{32}H_{43}N_4O_2S_2$) requires m/z 579.2827, found m/z 579.2828.

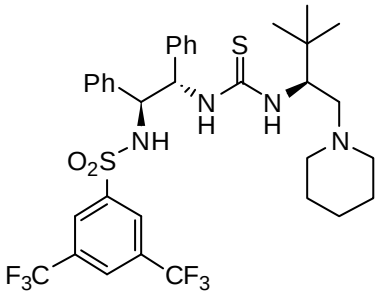
_N_-((1_S_,2_S_)-2-(3-((_S_)-3,3-dimethyl-1-(pyrrolidin-1-yl)butan-2-yl)thioureido)-1,2-diphenylethyl)methanesulfonamide (4d)



White solid. Mp 190-191°C; $[\alpha]^{24}_D$ - 0.7 (_c_ 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 10.37 (d, _J_ = 8.8 Hz, 1H), 7.46 (br, 1H), 7.36-7.34 (m, 2H), 7.27-7.20 (m, 8H), 6.26-6.21 (m, 2H), 4.94 (d, _J_ = 10.8 Hz, 1H), 3.08-3.05 (m,

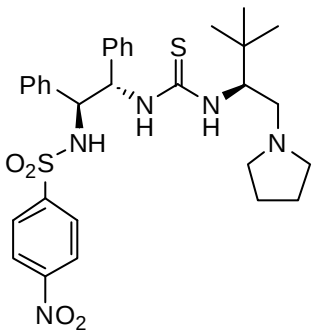
1H), 2.66 -2.57 (m, 5H), 2.37 (s, 3H), 1.78-1.58 (m, 6H), 0.99 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 183.1, 139.4, 137.9, 128.7, 128.4, 128.3, 128.0, 127.9, 64.1, 63.6, 63.1, 63.0, 55.1, 42.2, 33.7, 26.5, 25.2, 23.9; HRMS (ESI): exact mass calculated for $[(M+H)^+]$ ($C_{27}H_{41}N_4O_2S_2$) requires m/z 517.2617, found m/z 517.2625.

_N_-((1_S_,2_S_)-2-(3-((_S_)-3,3-dimethyl-1-(piperidin-1-yl)butan-2-yl)thioureido)-1,2-diphenylethyl)-3,5-bis(trifluoromethyl)benzenesulfonamide (4f)



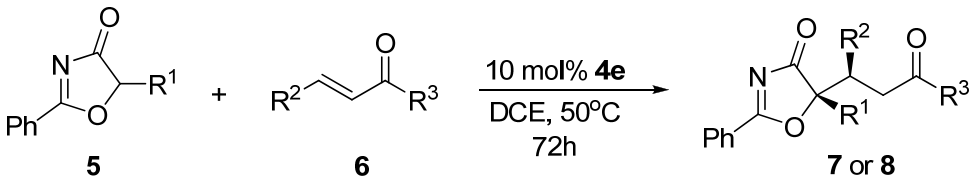
White solid. Mp 89-90°C; $[\alpha]^{24}_D$ – 37.9 (_c_ 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 10.37 (d, _J_ = 9.2 Hz, 1H), 8.45 (br, 1H), 7.81-7.73 (m, 2H), 7.21-7.19 (m, 5H), 6.99-6.91 (m, 5H), 6.30 (d, _J_ = 5.6 Hz, 1H), 6.16 (t, _J_ = 20.4 Hz, 1H), 4.98 (d, _J_ = 11.2 Hz, 1H), 3.10 (t, _J_ = 12.0 Hz, 1H), 2.73-2.60 (m, 6H), 1.81-1.63 (m, 6H), 1.02 (s, 9H)^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 183.3, 144.3, 137.3, 137.1, 132.0, 131.7, 128.4, 128.3, 128.2, 128.1, 127.9, 127.8, 126.9, 125.0, 123.7, 121.0, 64.9, 63.6, 63.4, 63.1, 55.2, 33.6, 26.5, 25.1, 23.9; HRMS (ESI): exact mass calculated for $[(M+H)^+]$ ($C_{34}H_{41}F_6N_4O_2S_2$) requires m/z 715.2575, found m/z 715.2578.

_N_-((1_S_,2_S_)-2-(3-((_S_)-3,3-dimethyl-1-(pyrrolidin-1-yl)butan-2-yl)thioureido)-1,2-diphenylethyl)-4-nitrobenzenesulfonamide (4g)



Yellow solid. Mp 99-100°C; $[\alpha]^{24}_D$ – 50.2 (_c_ 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 11.00 (d, _J_ = 8.4 Hz, 1H), 7.95-7.93 (m, 2H), 7.55-7.53 (m, 2H), 7.19-7.18 (m, 3H), 7.04-6.90 (m, 7H), 6.23 (d, _J_ = 5.2 Hz, 1H), 6.00 (t, _J_ = 19.6 Hz, 1H), 4.85 (d, _J_ = 10.8 Hz, 1H), 3.15 (t, _J_ = 12.4 Hz, 1H), 2.98-2.93 (m, 1H), 2.85-2.74 (m, 5H), 2.10-2.06 (m, 4H), 1.01 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 183.5, 149.0, 147.4, 137.8, 137.7, 128.5, 128.1, 127.9, 127.7, 127.6, 123.4, 65.5, 64.2, 64.0, 54.8, 33.6, 26.5, 24.0; HRMS (ESI): exact mass calculated for $[(M+H)^+]$ ($C_{31}H_{40}N_5O_4S_2$) requires m/z 610.2522, found m/z 610.2518.

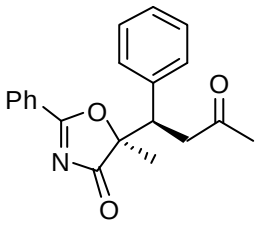
C: General Procedure for Asymmetric Michael Addition



5*H*-Oxazol-4-ones **5** (0.30 mmol, 1.0 equiv.) was added to a mixture of catalyst **4e** (0.03 mmol, 0.10 equiv.) and α,β-unsaturated ketones **6** (0.45 mmol, 1.5 equiv.) in CH_2ClCH_2Cl (0.6 mL) at 50°C. The reaction mixture was maintained at this temperature for 3 days and then the solvent was removed under vacuum. The residue was purified by silica gel chromatography to yield the desired addition product. The enantiomeric ratio was determined by HPLC analysis on chiral column.

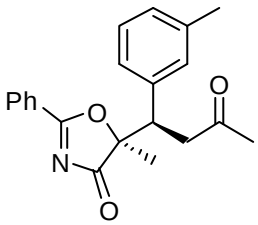
D: Characterization of Michael Addition Products

7a:(*S*)-5-methyl-5-((*R*)-3-oxo-1-phenylbutyl)-2-phenyloxazol-4(5*H*)-one



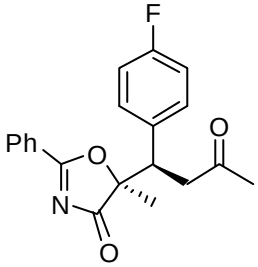
The product was obtained as a white solid(80.9 mg, 84% yield). Mp 118-119°C; $[\alpha]^{24}_{D}$ – 113.4 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.20-8.18 (m, 2H), 7.72-7.69 (m, 1H), 7.56-7.52 (m, 2H), 7.33-7.26 (m, 4H), 7.23-7.19 (m, 1H), 3.79 (dd, *J* = 3.6, 10.4 Hz, 1H), 3.03 (dd, *J* = 10.4, 16.8 Hz, 1H), 2.70 (dd, *J* = 3.6, 16.8 Hz, 1H), 1.96 (s, 3H), 1.42 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 204.8, 193.5, 185.5, 137.5, 135.4, 130.1, 129.1, 128.5, 127.8, 125.5, 89.8, 46.6, 43.4, 30.4, 21.6; IR (KBr): 1540 (NC=O)cm^{-1}, 1745 (C=O) cm^{-1}; HRMS (EI): exact mass calculated for M^+ ($C_{19}H_{19}NO_3$) requires m/z 321.1365, found m/z 321.1367; The enantiomeric excess was determined by HPLC. [IA column, 254 nm, *n*-Hexane: EtOH = 7:3, 0.8 mL/min]: 7.9 min (minor), 11.2 min (major), ee 96%.

7b:(*S*)-5-methyl-5-((*R*)-3-oxo-1-m-tolylbutyl)-2-phenyloxazol-4(5*H*)-one



The product was obtained as a white solid(97.5 mg, 97% yield). Mp 140-141°C; $[\alpha]^{24}_{D}$ – 100.5 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.20-8.17 (m, 2H), 7.72-7.68 (m, 1H), 7.56-7.52 (m, 2H), 7.17-7.10 (m, 3H), 7.02-7.00 (m, 1H), 3.74 (dd, *J* = 3.6, 10.4 Hz, 1H), 3.02 (dd, *J* = 10.4, 16.8 Hz, 1H), 2.68 (dd, *J* = 2.8, 16.8 Hz, 1H), 2.28 (s, 3H), 1.96 (s, 3H), 1.41 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 204.9, 193.6, 185.4, 138.0, 137.3, 135.4, 130.2, 130.0, 129.0, 128.5, 128.4, 125.7,125.6, 89.8, 46.6, 43.3, 30.4, 21.6, 21.4; IR (KBr): 1540 (NC=O) cm^{-1}, 1745 (C=O)cm^{-1}; HRMS (EI): exact mass calculated for M^+ ($C_{21}H_{21}NO_3$) requires m/z 335.1521, found m/z 335.1523; The enantiomeric excess was determined by HPLC. [IA column, 254 nm, *n*-Hexane: EtOH = 7:3, 1.0 mL/min]: 5.4 min (minor), 7.2 min (major), ee 99%.

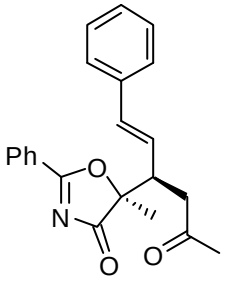
7c:(*S*)-5-((*R*)-1-(4-fluorophenyl)-3-oxobutyl)-5-methyl-2-phenyloxazol-4(5*H*)-one



The product was obtained as a white solid(95.6 mg, 94% yield). Mp 110-111°C; $[\alpha]^{24}_{D}$ – 77.4 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.18-8.16 (m, 2H), 7.71-7.69 (m, 1H), 7.57-7.53 (m, 2H), 7.31-7.28 (m, 2H), 6.99-6.94 (m, 2H), 3.79 (dd, *J* = 3.6, 10.4 Hz, 1H), 3.01 (dd, *J* = 10.8, 17.2 Hz, 1H), 2.73 (dd, *J* = 3.6, 17.2 Hz, 1H), 1.99 (s, 3H), 1.43 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 204.6, 193.4, 185.4, 163.4, 160.9, 135.5, 133.4, 133.3, 130.6, 130.5, 130.0, 129.1, 125.4, 115.6, 115.4, 89.6, 45.8, 43.4, 30.4, 21.6; IR

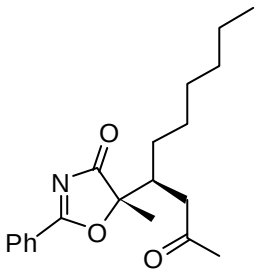
(KBr): 1540 (NC=O)cm^{-1}, 1740 (C=O)cm^{-1}; HRMS (EI): exact mass calculated for M^+ ($C_{20}H_{183}FNO_3$) requires m/z 339.1271, found m/z 335.1275; The enantiomeric excess was determined by HPLC. [IA column, 254 nm, *n*-Hexane: EtOH = 7:3, 0.8 mL/min]: 8.3 min (minor), 16.2 min (major), ee 96%.

7d:(*S*)-5-methyl-5-((*R*,*E*)-5-oxo-1-phenylhex-1-en-3-yl)-2-phenyloxazol-4(5*H*)-one



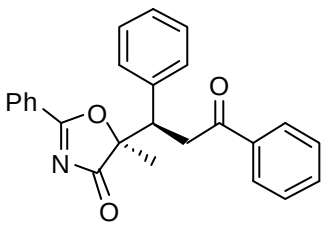
The product was obtained as a white solid(97.8 mg, 94% yield). Mp 113-114°C; $[\alpha]^{24}_D$ – 124.3 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.25-8.23 (m, 2H), 7.73-7.69 (m, 1H), 7.57-7.53 (m, 2H), 7.33-7.26 (m, 4H), 7.24-7.22 (m, 1H), 6.62 (d, *J* = 15.6 Hz, 1H), 5.96 (dd, *J* = 5.6, 15.6 Hz, 1H), 3.40 (ddd, *J* = 3.6, 9.6, 19.2 Hz, 1H), 2.67 (dd, *J* = 9.6, 16.8 Hz, 1H), 2.57 (dd, *J* = 3.6, 16.4 Hz, 1H), 2.10 (s, 3H), 1.60 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 205.0, 193.3, 185.6, 136.3, 135.7, 135.4, 130.1, 129.1, 128.5, 127.9, 126.5, 125.6, 124.8, 89.2, 44.5, 42.8, 30.5, 21.2; IR (KBr): 1545 (NC=O) cm^{-1}, 1745 (C=O)cm^{-1};HRMS (EI): exact mass calculated for M^+ ($C_{22}H_{21}NO_3$) requires m/z 347.1521, found m/z 347.1523; The enantiomeric excess was determined by HPLC. [IA column, 254 nm, *n*-Hexane: EtOH = 7:3, 0.8 mL/min]: 8.2 min (minor), 12.3 min (major), ee 97%.

7e:(*S*)-5-methyl-5-((*S*)-2-oxodecan-4-yl)-2-phenyloxazol-4(5*H*)-one



The product was obtained as a colorless oil(83.9 mg, 85% yield). $[\alpha]^{24}_D$ – 8.1 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.20-8.18 (m, 2H), 7.72-7.68 (m, 1H), 7.56-7.52 (m, 2H), 2.79 (dd, *J* = 5.2, 18.0 Hz, 1H), 2.72-2.66 (m, 1H), 2.67 (dd, *J* = 6.0, 17.6 Hz, 1H), 2.16 (s, 3H), 1.56-1.52 (m, 1H), 1.52 (s, 3H), 1.26-1.14 (m, 10H), 0.83-0.80(t, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 206.4, 193.7, 185.2, 135.3, 130.1, 129.0, 125.7, 89.8, 42.9, 38.8, 31.6, 30.2, 29.2, 29.1, 27.1, 22.5, 20.6, 14.0; HRMS (EI): exact mass calculated for M^+ ($C_{20}H_{27}NO_3$) requires m/z 329.1991, found m/z 329.1989; The enantiomeric excess was determined by HPLC. [IC column, 254 nm, *n*-Hexane: EtOH = 7:3, 0.8 mL/min]: 8.9 min (minor), 11.9 min (major), ee 93%.

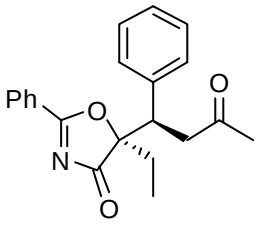
7f: (*S*)-5-methyl-5-((*R*)-3-oxo-1,3-diphenylpropyl)-2-phenyloxazol-4(5*H*)-one



The product was obtained as a white solid(100.0 mg, 87% yield). Mp 175-176°C; $[\alpha]^{24}_D$ + 7.0 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.23-8.21 (m, 2H), 7.84-7.83 (m, 2H), 7.74-7.70 (m, 1H), 7.58-7.49 (m, 3H), 7.41-7.35 (m, 4H), 7.28-7.24 (m, 2H), 7.20-7.17 (m, 1H),

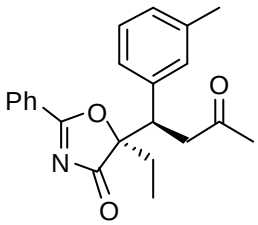
4.06 (dd, *J* = 3.6, 10.0 Hz, 1H), 3.61 (dd, *J* = 10.4, 16.8 Hz, 1H), 3.35 (dd, *J* = 3.6, 16.4 Hz, 1H), 1.51 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm), 196.6, 193.7, 185.5, 137.6, 136.5, 135.4, 133.3, 130.1, 129.1, 129.0, 128.6, 128.5, 128.1, 127.7, 125.6, 90.0, 47.0, 38.6, 21.8; HRMS (EI): exact mass calculated for M^+ ($C_{25}H_{21}NO_3$) requires m/z 383.1521, found m/z 383.1523; The enantiomeric excess was determined by HPLC. [IA column, 254 nm, *n*-Hexane: *i*-PrOH = 4:1, 1.0 mL/min]: 12.2 min (minor), 13.1 min (major), ee 99%.

7g: (*S*)-5-ethyl-5-((*R*)-3-oxo-1-phenylbutyl)-2-phenyloxazol-4(5*H*)-one



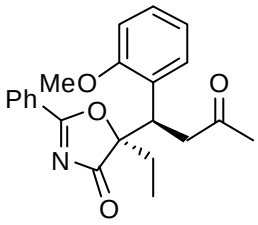
The product was obtained as a white solid(95.5 mg, 95% yield). Mp 104-105°C; $[\alpha]^{24}_D$ – 76.3 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.20-8.19 (m, 2H), 7.72-7.68 (m, 1H), 7.56-7.52 (m, 2H), 7.32-7.24 (m, 4H), 7.21-7.17 (m, 1H), 3.80 (dd, *J* = 3.6, 10.4 Hz, 1H), 3.03 (dd, *J* = 10.4, 16.8 Hz, 1H), 2.69 (dd, *J* = 3.6, 16.8 Hz, 1H), 1.94 (s, 3H), 1.92-1.84 (m, 1H), 1.77-1.67 (m, 1H), 0.75-0.72 (t, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 204.8, 193.1, 186.0, 137.7, 135.4, 130.0, 129.1, 128.5, 127.7, 125.4, 93.5, 46.1, 43.5, 30.4, 28.3, 7.2; HRMS (EI): exact mass calculated for M^+ ($C_{21}H_{21}NO_3$) requires m/z 335.1521, found m/z 335.1518; The enantiomeric excess was determined by HPLC. [IA column, 254 nm, *n*-Hexane: EtOH = 7:3, 0.80 mL/min]: 7.4 min (minor), 9.0 min (major), ee 97%.

7h: (*S*)-5-ethyl-5-((*R*)-3-oxo-1-m-tolylbutyl)-2-phenyloxazol-4(5*H*)-one



The product was obtained as a colorless oil(94.3 mg, 90% yield). $[\alpha]^{24}_D$ – 72.6 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.21-8.19 (m, 2H), 7.72-7.69 (m, 1H), 7.57-7.53 (m, 2H), 7.18-7.10 (m, 3H), 7.01-7.00 (m, 1H), 3.70 (dd, *J* = 3.2, 10.4 Hz, 1H), 3.02 (dd, *J* = 10.8, 16.8 Hz, 1H), 2.67 (dd, *J* = 3.2, 16.8 Hz, 1H), 2.3 (s, 3H), 1.96 (s, 3H), 1.92-1.85 (m, 1H), 1.78-1.69 (m, 1H), 0.76-0.72 (t, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 204.9, 193.2, 186.0, 137.9, 137.5, 135.4, 130.2, 130.0, 129.1, 128.4, 128.3, 125.7, 125.4, 93.6, 46.1, 43.4, 30.4, 28.2, 21.4, 7.2; HRMS (EI): exact mass calculated for M^+ ($C_{22}H_{23}NO_3$) requires m/z 349.1678, found m/z 349.1675; The enantiomeric excess was determined by HPLC. [IA column, 254 nm, *n*-Hexane: EtOH = 7:3, 0.80 mL/min]: 6.6 min (minor), 8.0 min (major), ee 97%.

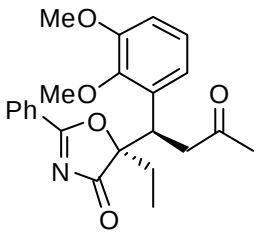
7i: (*S*)-5-ethyl-5-((*R*)-1-(2-methoxyphenyl)-3-oxobutyl)-2-phenyloxazol-4(5*H*)-one



The product was obtained as a colorless oil(90.9 mg, 83% yield). $[\alpha]^{24}_D$ – 70.1 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz,

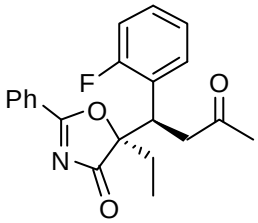
$CDCl_3$): δ (ppm) 8.20-8.19 (m, 2H), 7.71-7.68 (m, 1H), 7.55-7.52 (m, 2H), 7.28-7.17 (m, 2H), 6.95-6.83 (m, 2H), 4.54-4.50 (m, 1H), 3.86 (s, 3H), 2.95-2.85 (m, 1H), 2.66-2.62 (m, 1H), 2.04-1.97 (m, 1H), 1.94 (s, 3H), 1.78-1.67 (m, 1H), 0.72-0.68 (t, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 205.4, 193.3, 186.0, 157.7, 135.3, 130.0, 129.0, 128.7, 126.0, 125.4, 120.8, 111.0, 94.1, 55.8, 43.6, 37.1, 29.7, 27.4, 7.1; HRMS (EI): exact mass calculated for M^+ ($C_{22}H_{23}NO_4$) requires m/z 365.1627, found m/z 365.1628; The enantiomeric excess was determined by HPLC. [IA column, 254 nm, *n*-Hexane: EtOH = 7:3, 0.80 mL/min]: 6.9 min (minor), 7.9 min (major), ee 94%.

7j:(*S*)-5-((*R*)-1-(2,3-dimethoxyphenyl)-3-oxobutyl)-5-ethyl-2-phenyloxazol-4(5*H*)-one



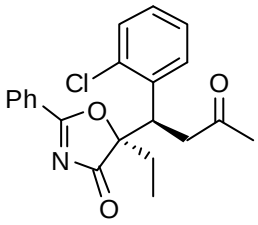
The product was obtained as a colorless oil(102.0 mg, 86% yield). $[\alpha]^{24}_D$ – 55.3 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.22-8.20 (m, 2H), 7.72-7.68 (m, 1H), 7.56-7.52 (m, 2H), 7.04-7.00 (m, 1H), 6.83-6.78 (m, 2H), 4.44-4.41 (m, 1H), 4.00 (s, 1H), 3.81 (s, 1H), 2.98 (dd, *J* = 12.0, 16.2 Hz, 1H), 2.61 (dd, *J* = 3.2, 16.8 Hz, 1H), 2.09-2.01 (m, 1H), 1.95 (s, 3H),1.71-1.62 (m, 1H), 0.68-0.65 (t, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 204.9, 193.4, 186.1, 152.7, 147.9, 135.4, 131.5, 130.1, 129.1, 125.4, 124.0, 118.9, 111.5, 94.1, 60.6, 55.6, 53.5, 43.0, 37.8, 30.4, 27.7, 7.1; HRMS (EI): exact mass calculated for M^+ ($C_{23}H_{25}NO_5$) requires m/z 395.1733, found m/z 395.1730; The enantiomeric excess was determined by HPLC. [IA column, 254 nm, *n*-Hexane: EtOH = 7:3, 0.80 mL/min]: 6.7 min (minor), 7.3 min (major), ee 92%.

7k: (*S*)-5-ethyl-5-((*R*)-1-(2-fluorophenyl)-3-oxobutyl)-2-phenyloxazol-4(5*H*)-one



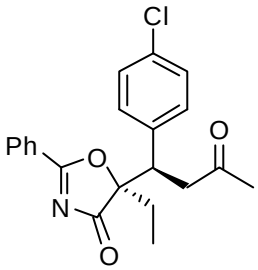
The product was obtained as a white solid(101.7 mg, 96% yield). Mp 81-82°C; $[\alpha]^{24}_D$ – 41.4 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.19-8.17 (m, 2H), 7.72-7.68 (m, 1H), 7.55-7.51 (m, 2H), 7.29-7.25 (m, 1H), 7.19-7.14 (m, 1H), 7.09-7.06 (m, 1H), 7.00-6.95 (m, 1H), 4.25 (d, *J* = 9.2 Hz, 1H), 3.08 (dd, *J* = 10.8, 17.2 Hz, 1H), 2.75 (dd, *J* = 2.8, 17.2 Hz, 1H), 2.03-1.94 (m, 1H), 1.98 (s, 3H), 1.82-1.73 (m, 1H), 0.77-0.73 (t, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 204.5, 192.8, 186.1, 162.4, 159.9, 135.5, 130.0, 129.3, 129.2, 129.1, 125.2, 124.8, 124.7, 124.4, 124.3, 115.7, 115.5, 93.1, 42.4, 30.0, 27.9, 7.1; HRMS (EI): exact mass calculated for M^+ ($C_{21}H_{20}FNO_3$) requires m/z 353.1427, found m/z 353.1428; The enantiomeric excess was determined by HPLC. [IA column, 254 nm, *n*-Hexane: EtOH = 7:3, 0.80 mL/min]: 7.7 min (minor), 11.2 min (major), ee 94%.

7l: (*S*)-5-((*R*)-1-(2-chlorophenyl)-3-oxobutyl)-5-ethyl-2-phenyloxazol-4(5*H*)-one



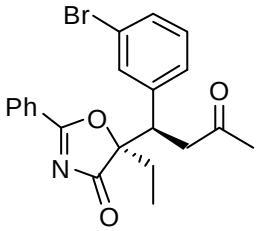
The product was obtained as a colorless oil(94.1 mg, 85% yield). $[\alpha]^{24}_{D}$ – 46.9 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.16-8.14 (m, 2H), 7.68-7.65 (m, 1H), 7.52-7.48 (m, 2H), 7.30-7.27 (m, 2H), 7.20-7.16 (m, 1H), 7.09-7.05 (m, 1H), 4.57 (dd, *J* = 3.6, 10.4 Hz, 1H), 3.04 (dd, *J* = 10.4, 16.8 Hz, 1H), 2.80 (dd, *J* = 3.6, 16.8 Hz, 1H), 2.09-2.00 (m, 1H), 1.96 (s, 3H),1.81-1.72 (m, 1H), 0.75-0.71 (t, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 204.5, 192.9, 186.0, 135.7, 135.6, 135.5, 130.0, 129.7, 129.1, 128.7, 128.2, 127.2, 125.1, 93.4, 43.2, 41.0, 30.0, 27.6, 7.2; HRMS (EI): exact mass calculated for M^+ ($C_{21}H_{20}ClNO_3$) requires m/z 369.1132, found m/z 369.1135; The enantiomeric excess was determined by HPLC. [IA column, 254 nm, *n*-Hexane: EtOH = 7:3, 0.80 mL/min]: 7.2 min (minor), 9.8 min (major), ee 90%.

7m: (*S*)-5-((*R*)-1-(4-chlorophenyl)-3-oxobutyl)-5-ethyl-2-phenyloxazol-4(5*H*)-one



The product was obtained as a colorless oil(105.2 mg, 95% yield). $[\alpha]^{24}_{D}$ – 85.4 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.19-8.17 (m, 2H), 7.73-7.69 (m, 1H), 7.57-7.53 (m, 2H), 7.26-7.22 (m, 4H), 3.80-3.77 (m, 1H), 3.00 (dd, *J* = 10.4, 17.2 Hz, 1H), 2.71-2.67 (m, 1H), 1.95 (s, 3H), 1.92-1.83 (m, 1H), 1.76-1.69 (m, 1H), 0.76-0.72 (t, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 204.5, 192.8, 186.0, 136.4, 135.6, 133.5, 130.4, 130.0, 129.1, 128.7, 125.2, 93.2, 45.4, 43.3, 30.4, 28.3, 7.1; HRMS (EI): exact mass calculated for M^+ ($C_{21}H_{20}ClNO_3$) requires m/z 369.1132, found m/z 369.1129; The enantiomeric excess was determined by HPLC. [IA column, 254 nm, *n*-Hexane: EtOH = 7:3, 0.80 mL/min]: 7.7 min (minor), 16.1 min (major), ee 97%.

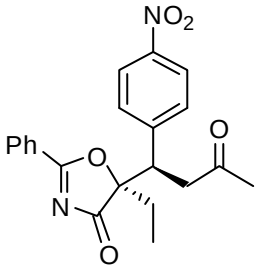
7n: (*S*)-5-((*R*)-1-(3-bromophenyl)-3-oxobutyl)-5-ethyl-2-phenyloxazol-4(5*H*)-one



The product was obtained as a white solid (122.0 mg, 98% yield). Mp 50-51°C; $[\alpha]^{24}_{D}$ - 86.9 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.20-8.18 (m, 2H), 7.72-7.70 (m, 1H), 7.58-7.54 (m, 2H), 7.47-7.46 (m, 1H), 7.33-7.31 (m, 1H), 7.26-7.24 (m, 1H), 7.16-7.12 (m, 1H), 3.78 (dd, *J* = 3.2, 10.4 Hz, 1H), 3.00 (dd, *J* = 10.4, 17.2 Hz, 1H), 2.69 (dd, *J* = 2.8, 17.6 Hz, 1H), 1.97 (s, 3H), 1.93-1.83 (m, 1H), 1.76-1.67 (m, 1H), 0.76-0.72 (t, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 204.3, 192.7, 186.0, 140.2, 135.6, 132.2, 130.8, 130.1, 129.2, 127.6, 125.2, 122.5, 93.1, 45.6, 43.2, 30.4, 28.2, 7.2; HRMS (EI): exact mass calculated for M^+ ($C_{21}H_{20}BrNO_3$) requires m/z 415.0606, found m/z 415.0615; The enantiomeric excess was determined by HPLC. [IA column, 254 nm,

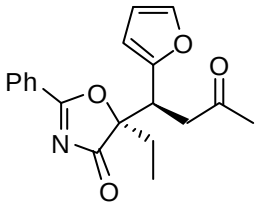
n-Hexane: EtOH = 7:3, 0.80 mL/min]: 7.7 min (minor), 11.9 min (major), ee 97%.

7o: (*S*)-5-ethyl-5-((*R*)-1-(4-nitrophenyl)-3-oxobutyl)-2-phenyloxazol-4(5*H*)-one



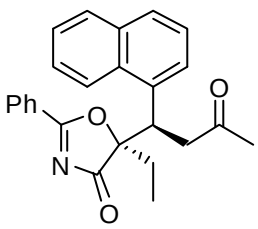
The product was obtained as a white solid (100.4 mg, 88% yield). Mp 146-147°C; $[\alpha]^{24}_{D}$ – 75.4 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.19-8.17 (m, 2H), 8.12-8.10 (m, 2H), 7.74-7.70 (m, 1H), 7.57-7.51 (m, 4H), 3.94 (dd, *J* = 2.8, 10.4 Hz, 1H), 3.10 (dd, *J* = 10.8, 18.0 Hz, 1H), 2.83-2.78 (m, 1H), 2.00 (s, 3H), 1.96-1.87 (m, 1H), 1.75-1.66 (m, 1H), 0.77-0.74 (t, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 204.1, 192.4, 186.1, 147.3, 145.7, 135.8, 130.1, 129.2, 124.9, 123.6, 92.6, 45.6, 43.1, 30.3, 28.3, 7.1; HRMS (EI):exact mass calculated for M^+ ($C_{21}H_{20}N_2O_5$) requires m/z 380.1372, found m/z 380.1374; The enantiomeric excess was determined by HPLC. [IA column, 254 nm, EtOH, 0.50 mL/min]: 10.0 min (minor), 19.2 min (major), ee 97%.

7p: (*S*)-5-ethyl-5-((*R*)-1-(furan-2-yl)-3-oxobutyl)-2-phenyloxazol-4(5*H*)-one



The product was obtained as a colorless oil(81.9 mg, 84% yield). $[\alpha]^{24}_{D}$ – 48.9 (c 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.20-8.18 (m, 2H), 7.72-7.68 (m, 1H), 7.55-7.52 (m, 2H), 7.28-7.27 (m, 1H), 6.22-6.17 (m, 2H), 3.95 (dd, *J* = 2.4, 10.8 Hz, 1H), 3.08 (dd, *J* = 10.8, 17.2 Hz, 1H), 2.64 (dd, *J* = 2.0, 17.2 Hz, 1H), 2.02 (s, 3H), 1.98-1.91 (m, 1H), 1.88-1.79 (m, 1H), 0.81-0.77 (t, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 204.6, 192.4, 186.1, 151.1，142.1，135.4, 130.1, 129.0, 125.4, 110.4, 108.6, 92.0, 41.2, 39.6, 30.2, 27.7, 7.2; HRMS (EI): exact mass calculated for M^+ ($C_{19}H_{19}NO_4$) requires m/z 325.1314, found m/z 325.1317; The enantiomeric excess was determined by HPLC. [IA column, 254 nm, *n*-Hexane: EtOH = 7:3, 0.80 mL/min]: 8.1 min (minor), 10.4 min (maior), ee 97%.

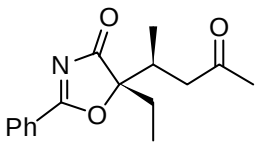
7q: (*S*)-5-ethyl-5-((*R*)-1-(naphthalen-1-yl)-3-oxobutyl)-2-phenyloxazol-4(5*H*)-one



The product was obtained as a colorless oil(112.1 mg, 97% yield). $[\alpha]^{24}_{D}$ – 106.9 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.27-8.25 (m, 2H), 7.84-7.81 (m, 4H), 7.73-7.69 (m, 1H), 7.58-7.50 (m, 3H), 7.49-7.42 (m, 2H), 4.02 (dd, *J* = 3.2, 17.2 Hz, 1H), 3.16 (dd, *J* = 10.8, 17.2 Hz, 1H), 2.75 (dd, *J* = 3.2, 16.8 Hz, 1H), 2.00-1.91 (m, 1H), 1.94 (s, 3H), 1.79-1.70 (m, 1H), 0.77-0.73 (t, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 204.7, 193.2, 186.2, 135.5, 135.3, 133.2, 132.8, 130.1, 129.2, 128.5, 128.4, 127.9, 127.6, 126.3, 126.1, 125.4, 93.7, 46.3, 43.7, 30.4, 28.5, 7.2; HRMS (EI): exact mass calculated for M^+

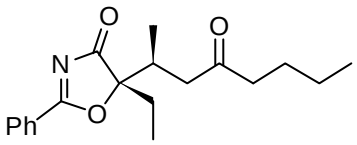
($C_{25}H_{23}NO_3$) requires m/z 385.1678, found m/z 385.1679; The enantiomeric excess was determined by HPLC. [IA column, 254 nm, *n*-Hexane: EtOH = 7:3, 0.80 mL/min]: 8.6 min (minor), 11.1 min (major), ee 98%.

7r: (*S*)-5-ethyl-5-((*S*)-4-oxopentan-2-yl)-2-phenyloxazol-4(5*H*)-one



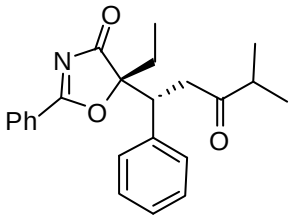
The product was obtained as a colorless oil(73.7 mg, 90% yield). $[\alpha]^{24}_D$ – 8.2 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.13-8.11 (m, 2H), 7.60-7.58 (m, 1H), 7.46-7.42 (m, 2H), 2.61-2.46 (m, 2H), 2.37-2.31 (m, 1H), 2.00-1.99 (m, 3H), 1.93-1.80 (m, 2H), 0.89-0.87 (m, 3H), 0.72-0.69 (t, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 206.0, 193.1, 185.8, 135.3, 129.9, 129.0, 125.4, 93.5, 44.3, 33.7, 30.4, 26.6, 14.0, 7.1; HRMS (EI): exact mass calculated for M^+ ($C_{16}H_{19}NO_3$) requires m/z 273.1365, found m/z 273.1366; The enantiomeric excess was determined by HPLC. [IC column, 254 nm, *n*-Hexane: EtOH = 7:3, 0.80 mL/min]: 10.5 min (minor), 12.6 min (major), ee 96%.

7s: (*S*)-5-ethyl-5-((*S*)-4-oxooctan-2-yl)-2-phenyloxazol-4(5*H*)-one



The product was obtained as a colorless oil(76.6 mg, 81% yield). $[\alpha]^{24}_D$ – 2.7 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.22-8.20 (m, 2H), 7.70-7.67 (m, 1H), 7.55-7.51 (m, 2H), 2.73-2.68 (m, 1H), 2.56-2.55 (m, 1H), 2.44-2.26 (m, 3H), 2.05-1.88 (m, 2H), 1.52-1.45 (m, 2H), 1.29-1.19 (m, 2H), 0.96-0.94 (m, 3H), 0.86-0.83 (t, 3H), 0.82-0.79 (t, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 208.6, 193.2, 185.9, 135.3, 130.0, 129.0, 125.5, 93.7, 43.4, 43.1, 33.8, 26.8, 25.8, 22.2, 14.1, 13.8, 7.2; HRMS (EI): exact mass calculated for M^+ ($C_{19}H_{25}NO_3$) requires m/z 315.1834, found m/z 315.1832; The enantiomeric excess was determined by HPLC. [IA column, 254 nm, *n*-Hexane: EtOH = 7:3, 0.60 mL/min]: 8.8 min (minor), 10.4 min (major), ee 98%.

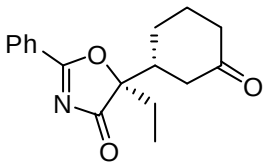
7t: (*S*)-5-ethyl-5-((*R*)-4-methyl-3-oxo-1-phenylpentyl)-2-phenyloxazol-4(5*H*)-one



The product was obtained as a colorless oil(93.7 mg, 86% yield). $[\alpha]^{24}_D$ – 73.0 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.20-8.18 (m, 2H), 7.72-7.68 (m, 1H), 7.56-7.52 (m, 2H), 7.31-7.29 (m, 2H), 7.26-7.22 (m, 2H), 7.19-7.15 (m, 1H), 3.85 (dd, *J* = 3.6, 17.2 Hz, 1H), 3.09 (dd, *J* = 10.4, 17.2 Hz, 1H), 2.68 (dd, *J* = 3.2, 16.8 Hz, 1H), 2.43-2.36 (m, 1H), 1.95-1.86 (m, 1H), 1.73-1.1.71 (m, 1H), 0.92-0.91 (m, 3H), 0.81-0.79 (m, 3H), 0.77-0.73 (t, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 210.7, 193.2, 186.0, 137.9, 135.3, 130.0, 129.1, 128.4, 127.5, 125.4, 93.7, 46.1, 41.0, 40.5,

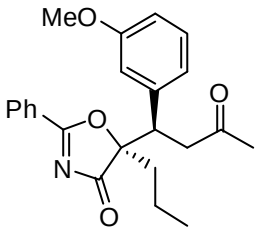
28.4, 17.8, 17.7, 7.2; HRMS (EI): exact mass calculated for M^+ ($C_{23}H_{25}NO_3$) requires m/z 363.1834, found m/z 363.1836; The enantiomeric excess was determined by HPLC. [AS-H column, 254 nm, *n*-Hexane: EtOH = 7:3, 0.60 mL/min]: 8.2 min (minor), 11.0 min (major), ee 99%.

7u: (*S*)-5-ethyl-5-((*R*)-3-oxocyclohexyl)-2-phenyloxazol-4(5*H*)-one



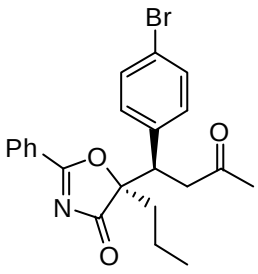
The product was obtained as a colorless oil(69.3 mg, 81% yield). $[\alpha]^{24}_D$ – 4.8 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.21-8.19 (m, 2H), 7.70-7.67 (m, 1H), 7.54-7.51 (m, 2H), 2.48-2.32 (m, 4H), 2.25-2.17 (m, 1H), 2.08-1.92 (m, 4H), 1.63-1.41 (m, 2H), 0.84-0.81 (t, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 209.0, 192.6, 186.0, 135.4, 130.1, 129.1, 125.3, 92.4, 43.0, 41.1, 40.9, 26.6, 24.8, 24.3, 7.2; HRMS (EI): exact mass calculated for M^+ ($C_{17}H_{19}NO_3$) requires m/z 285.1365, found m/z 285.1366; The enantiomeric excess was determined by HPLC. [IA column, 254 nm, *n*-Hexane: EtOH = 7:3, 0.60 mL/min]: 15.0min (minor), 16.3 min (major), ee 90%.

8a:(*S*)-5-((*R*)-1-(3-methoxyphenyl)-3-oxobutyl)-2-phenyl-5-propyloxazol-4(5*H*)-one



The product was obtained as a colorless oil(99.0 mg, 87% yield). $[\alpha]^{24}_D$ – 50.4 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.21-8.19 (m, 2H), 7.72-7.68 (m, 1H), 7.56-7.52 (m, 2H), 7.21-7.17 (m, 1H), 6.91-6.89 (m, 1H), 6.86-6.85 (m, 1H), 6.76-6.74 (m, 1H), 3.78-3.75 (m, 1H), 3.75 (s, 3H), 3.00 (dd, *J* = 2.8, 16.8 Hz, 1H), 2.63 (dd, *J* = 2.8, 16.8 Hz, 1H), 1.95 (s, 3H), 1.86-1.78 (m, 1H), 1.70-1.62 (m, 1H), 1.19-1.09 (m, 2H), 0.78-0.75 (t, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 204.7, 193.2, 186.0, 159.4, 139.2, 135.4, 130.0, 129.5, 129.1, 125.4, 121.4, 115.3, 112.7, 93.1, 55.1, 46.4, 43.4, 37.0, 30.4, 16.3, 13.7; HRMS (EI): exact mass calculated for M^+ ($C_{23}H_{25}NO_4$) requires m/z 379.1784, found m/z 379.1782; The enantiomeric excess was determined by HPLC. [AD-H column, 254 nm, *n*-Hexane: EtOH = 7:3, 0.60 mL/min]: 11.9min (minor), 15.1 min (major), ee 97%.

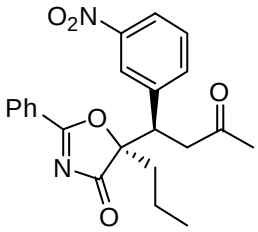
8b:(*S*)-5-((*R*)-1-(4-bromophenyl)-3-oxobutyl)-2-phenyl-5-propyloxazol-4(5*H*)-one



The product was obtained as a white solid (125.6 mg, 98% yield). Mp 113-114°C; $[\alpha]^{24}_D$ – 71.3 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.18-8.16 (m, 2H), 7.73-7.69 (m, 1H), 7.56-7.52 (m, 2H), 7.40-7.38 (m, 2H), 7.20-7.18 (m, 2H), 3.76 (dd, *J* = 2.8, 10.8 Hz, 1H), 2.99 (dd, *J* = 10.8, 17.2 Hz,

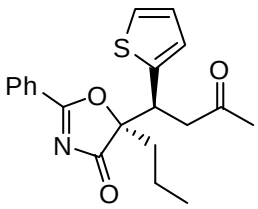
1H), 2.63 (dd, *J* = 2.4, 17.2 Hz, 1H), 1.95 (s, 3H), 1.84-1.76 (m, 1H), 1.78-1.76 (m, 1H), 1.67-1.59 (m, 1H), 1.18-1.09 (m, 1H), 0.78-0.75 (t, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 204.4, 192.9, 185.9, 136.9, 135.6, 131.6, 130.8, 130.0, 129.1, 125.2, 121.7, 92.7, 45.7, 43.2, 37.0, 30.4, 16.2, 13.7; HRMS (EI): exact mass calculated for M^+ ($C_{22}H_{22}BrNO_3$) requires m/z 427.0783, found m/z 427.0785; The enantiomeric excess was determined by HPLC. [IA column, 254 nm, *n*-Hexane: EtOH = 7:3, 1.0 mL/min]: 5.7min (minor), 9.4 min (major), ee 96%.

8c: (*S*)-5-((*R*)-1-(3-nitrophenyl)-3-oxobutyl)-2-phenyl-5-propyloxazol-4(5*H*)-one



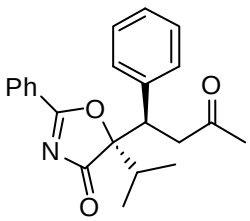
The product was obtained obtained as a white solid (110.0 mg, 93% yield). Mp 150-151°C; $[\alpha]^{24}_D$ – 41.5 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.23-8.18 (m, 3H), 8.07-8.05 (m, 1H), 7.74-7.67 (m, 2H), 7.58-7.54 (m, 2H), 7.49-7.45 (m, 1H), 3.93 (dd, *J* = 3.2, 10.8 Hz, 1H), 3.13 (dd, *J* = 10.8, 17.6 Hz, 1H), 2.80 (dd, *J* = 3.2, 17.2 Hz, 1H), 2.00 (s, 3H), 1.88-1.80 (m, 1H), 1.65-1.58 (m, 1H), 1.23-1.11 (m, 2H), 0.80-0.76 (t, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 204.1, 192.4, 185.9, 148.2, 140.2, 135.8, 135.6, 130.1, 1129.5, 129.2, 125.0, 123.7, 122.7, 92.3, 45.6, 43.0, 37.0, 30.3, 16.2, 13.7; HRMS(EI): exact mass calculated for M^+ ($C_{22}H_{21}N_2O_5$) requires m/z 394.1529, found m/z 394.1533; The enantiomeric excess was determined by HPLC. [IA column, 254 nm, *n*-Hexane: EtOH = 7:3, 1.0 mL/min]: 7.3 min (minor), 11.3 min (major), ee 95%.

8d: (*S*)-5-((*S*)-3-oxo-1-(thiophen-2-yl)butyl)-2-phenyl-5-propyloxazol-4(5*H*)-one



The product was obtained as a colorless oil(100.1 mg, 94% yield). $[\alpha]^{24}_D$ – 56.5 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.25-8.23 (m, 2H), 7.74-7.70 (m, 1H), 7.58-7.54 (m, 2H), 7.17-7.16 (m, 1H), 6.98-6.97 (m, 1H), 6.90-6.88 (m, 1H),4.13 (dd, *J* = 3.2, 10.8 Hz, 1H), 2.96 (dd, *J* = 2.8, 16.8 Hz, 1H), 2.63 (dd, *J* = 2.8, 16.8 Hz, 1H), 1.98 (s, 3H), 1.90-1.82 (m, 1H), 1.80-1.72 (m, 1H), 1.23-1.14 (m, 2H), 0.81-0.80 (t, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 204.3, 192.7, 186.0, 140.0, 135.5, 130.2,129.1, 127.5, 126.7, 125.3, 125.0, 92.5, 44.6, 41.6, 36.8, 30.5, 16.2, 13.8; HRMS (EI): exact mass calculated for M^+ ($C_{20}H_{21}NO_3S$) requires m/z 355.1242, found m/z 355.1239; The enantiomeric excess was determined by HPLC. [IA column, 254 nm, *n*-Hexane: EtOH = 7:3, 0.8 mL/min]: 7.6min (minor), 8.0 min (major), ee 97%.

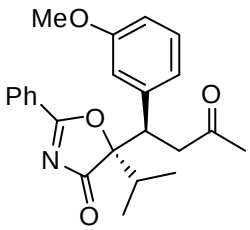
8e: (*S*)-5-isopropyl-5-((*R*)-3-oxo-1-phenylbutyl)-2-phenyloxazol-4(5*H*)-one



The product was obtained as a colorless oil(89.0 mg, 85% yield). $[\alpha]^{24}_D$ – 21.8 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ

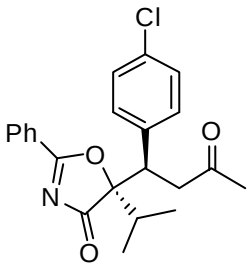
(ppm) 8.15-8.13 (m, 2H), 7.70-7.66 (m, 1H), 7.54-7.50 (m, 2H), 7.34-7.32 (m, 2H), 7.23-7.19 (m, 2H), 7.16-7.12 (m, 1H), 4.01 (dd, *J* = 2.8, 11.2 Hz, 1H), 3.19 (dd, *J* = 11.2, 17.2 Hz, 1H), 2.68 (dd, *J* = 2.8, 17.2 Hz, 1H), 2.18-2.15 (m, 1H), 1.96 (s, 3H), 1.00-0.97 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 205.1, 192.8, 185.8, 137.5, 135.2, 129.9, 129.1, 129.0, 128.4, 127.6, 125.3, 95.2, 43.8, 43.1, 31.9, 30.7, 16.3, 15.7; HRMS (EI): exact mass calculated for M^+ ($C_{22}H_{23}NO_3$) requires m/z 349.1678, found m/z 349.1677; The enantiomeric excess was determined by HPLC. [IC column, 254 nm, *n*-Hexane: *i*-PrOH = 7:3, 0.8 mL/min]: 17.9min (minor), 40.1 min (major), ee 98%.

8f:(*S*)-5-isopropyl-5-((*R*)-1-(3-methoxyphenyl)-3-oxobutyl)-2-phenyloxazol-4(5*H*)-one



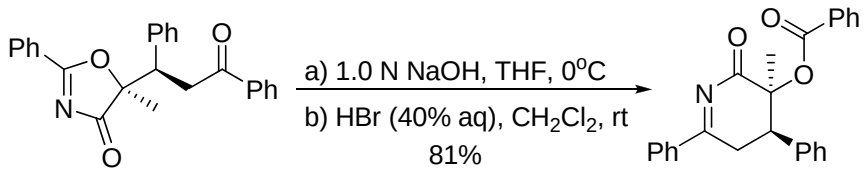
The product was obtained as a colorless oil(99.0 mg, 87% yield). $[\alpha]^{24}_D$ – 25.9 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.16-8.14 (m, 2H), 7.69-7.66 (m, 1H), 7.53-7.50 (m, 2H), 7.15-7.11 (m, 1H), 6.93-6.87 (m, 2H), 6.70-6.68 (m, 1H), 3.97 (dd, *J* = 3.2, 11.2 Hz, 1H), 3.71 (s, 3H), 3.14 (dd, *J* = 3.2, 16.8 Hz, 1H), 2.62 (dd, *J* = 3.2, 16.8 Hz, 1H), 2.20-2.11 (m, 1H), 1.96 (s, 3H), 1.00-0.94 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 205.0, 192.7, 185.8, 159.3, 139.0, 135.2, 129.9, 129.4, 129.0, 125.4, 121.4, 115.4, 112.7, 95.1, 55.1, 43.8, 43.1, 31.9, 30.7, 16.3, 15.7; HRMS (EI): exact mass calculated for M^+ ($C_{23}H_{25}NO_4$) requires m/z 379.1784, found m/z 379.1786; The enantiomeric excess was determined by HPLC. [IA column, 254 nm, *n*-Hexane: EtOH = 7:3, 1.0 mL/min]: 6.6min (minor), 9.2 min (major), ee 98%.

8g: (*S*)-5-((*R*)-1-(4-chlorophenyl)-3-oxobutyl)-5-isopropyl-2-phenyloxazol-4(5*H*)-one



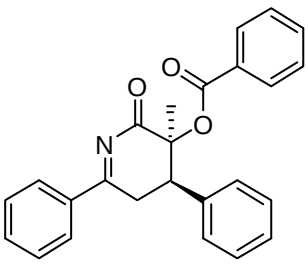
The product was obtained obtained as a white solid (104.6 mg, 91% yield). Mp 58-59°C; $[\alpha]^{24}_D$ – 20.2 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.14-8.12 (m, 2H), 7.69-7.67 (m, 1H), 7.54-7.50 (m, 2H), 7.28-7.26 (m, 2H), 7.19-7.17 (m, 2H), 7.16-7.12 (m, 1H), 3.98 (dd, *J* = 2.4, 11.2 Hz, 1H), 3.16 (dd, *J* = 11.2, 17.2 Hz, 1H), 2.67 (dd, *J* = 2.8, 17.2 Hz, 1H), 2.17-2.13 (m, 1H), 1.97 (s, 3H), 0.980-0.96 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 204.7, 192.5, 185.8, 136.2, 135.4, 133.4, 130.5, 129.9, 129.1, 128.6, 125.2, 94.9, 43.0, 42.9, 31.9, 30.7, 16.3, 15.7; HRMS (EI): exact mass calculated for M^+ ($C_{23}H_{22}ClNO_3$) requires m/z 383.1288, found m/z 383.1287; The enantiomeric excess was determined by HPLC. [IC column, 254 nm, *n*-Hexane: EtOH = 7:3, 0.8 mL/min]: 8.1min (minor), 11.6 min (major), ee 98%.

E: Derivatization of Addition Products

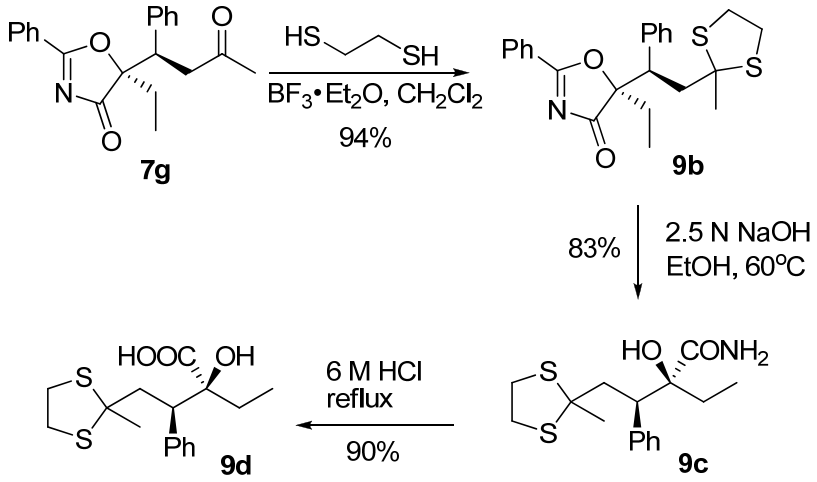


7f **9a**

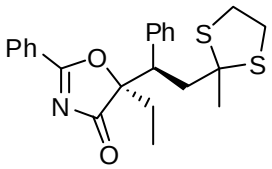
9a: (3*S*,4*R*)-3-methyl-2-oxo-4,6-diphenyl-2,3,4,5-tetrahydropyridin-3-yl benzoate



A 1.0 N NaOH aqueous solution (0.6 mL) was added dropwise to a stirred solution of (*S*)-5-methyl-5-((*R*)-3-oxo-1,3-diphenylpropyl)-2-phenylox azol-4(5*H*)-one **7f** (184 mg, 0.50 mmol) in THF (3.0 mL) at 0-5°C. After stirring at same temperature for 1 h, Et_2O (10 ml) and sat. NaCl aqueous solution (10 mL) were added to the reaction mixture. Then the mixture was transferred to a separatory funnel, and the organic phase was dried (Na_2SO_4) and concentrated. The obtained crude product was redissolved with CH_2Cl_2 (2 mL), then conc. HBr (40% aqueous solution, 1 mL) was added, the resulting solution was stirred for 2 hrs at room temperature. Then the mixture was diluted with CH_2Cl_2 (10 mL), washed with water (2x10 mL), and the organic phase was dried (Na_2SO_4) and concentrated. The crude product was purified by silica gel chromatography to afford **9a** (149 mg, 81%) as a white solid. Mp 162-163°C; $[\alpha]^{24}_D$ + 8.6 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.23-8.21 (m, 2H), 7.85-7.83 (m, 2H), 7.75-7.71 (m, 1H), 7.59-7.51 (m, 3H), 7.43-7.35 (m, 4H), 7.28-7.24 (m, 2H), 7.21-7.17 (m, 1H), 4.06 (dd, *J* = 3.6, 10.4 Hz, 1H), 3.61 (dd, *J* = 10.0, 16.8 Hz, 1H), 3.37 (dd, *J* = 3.6, 16.8 Hz, 1H), 1.52 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 196.5, 193.6, 185.4, 137.5, 136.5, 135.3, 133.2, 130.0, 129.0, 128.9, 128.5, 128.4, 128.0, 127.6, 125.6, 89.9, 47.0, 38.6, 21.8; IR (KBr): 1550 (NC=O) cm^{-1}, 1735 (O-C=O) cm^{-1};HRMS (EI): exact mass calculated for M^+ ($C_{25}H_{21}NO_3$) requires m/z 383.1521, found m/z 383.1523.

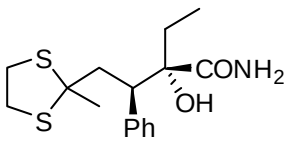


9b:(*S*)-5-ethyl-5-((*R*)-2-(2-methyl-1,3-dithiolan-2-yl)-1-phenylethyl)-2-phenyloxazol-4(5*H*)-one



To a stirred solution of addition product **7g** (167.2 mg, 0.5 mmol) and 1,2-ethanedithiol (0.07 mL, 0.8 mmol) in anhydrous dichloromethane (2 mL) at 0°C, was added a catalytic amount of BF_3•Et_2O, and the resultant was warmed up to room temperature and stirred overnight. Aqueous NaOH (5%) (1.0 mL) was then added, and the resulting mixture was extracted with dichloromethane. The combined organic layers were washed with brine, dried (Na_2SO_4) and concentrated. The residue was purified by flash chromatography to furnish **9b** (193.5 mg, 94%) as a white solid. Mp 47-48°C; $[\alpha]^{25}_D$ – 90.9 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.26-8.24 (m, 2H), 7.75-7.71 (m, 1H), 7.60-7.56 (m, 2H), 7.34-7.29 (m, 5H), 3.57 (d, *J* = 10.4 Hz, 1H), 3.28-3.17 (m, 4H), 2.55 (dd, *J* = 11.2, 14.0 Hz, 1H), 2.22 (d, *J* = 14.4 Hz, 1H), 1.91-1.80 (m, 1H), 1.65-1.56 (m, 1H), 1.41 (s, 3H), 0.74-0.71 (t, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 193.4, 186.2, 138.6, 135.3, 129.0, 128.5, 127.7, 125.5, 94.7, 66.0, 50.4, 44.8, 39.7, 38.8, 31.6, 28.6, 7.2; HRMS (ESI): exact mass calculated for $[M+Na]^+$ ($C_{23}H_{25}NNaO_2S_2$) requires m/z 434.1224, found m/z 434.1219.

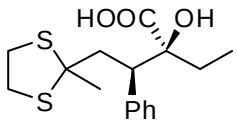
9c:(2*S*,3*R*)-2-ethyl-2-hydroxy-4-(2-methyl-1,3-dithiolan-2-yl)-3-phenylbutanamide



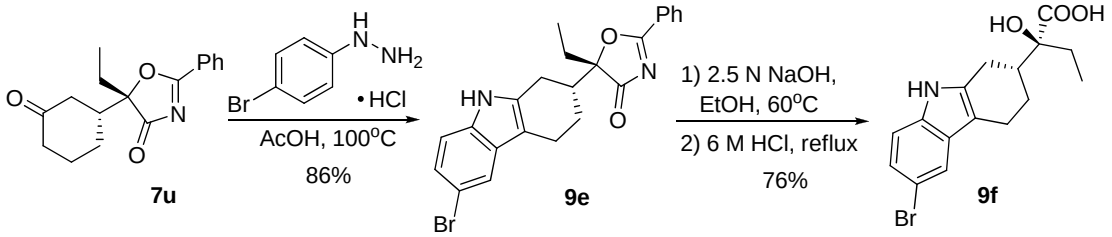
A 2.5 N NaOH aqueous solution (0.1 mL) was added to a stirred solution of **9b** (82.3 mg, 0.20 mmol) in ethanol (0.5 mL) . After stirring at 60°C for 1 h, the reaction mixture was diluted with water. The mixture was extracted three times with EtOAc, and the combined organic phase was washed with brine, dried ($MgSO_4$) and concentrated. The obtained crude product was chromatographed on silica (pet. ether /ethyl acetate = 1/1) to give **9c** (54.0 mg, 83%) as a white solid. Mp 125-126°C; $[\alpha]^{25}_D$ – 20.2 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.35-7.29 (m, 5H), 6.69 (br, 1H), 6.14 (br, 1H), 3.34 (d, *J* = 10.8 Hz, 1H), 3.28-3.20 (m, 4H), 2.72 (dd,

J = 10.8, 14.8 Hz, 1H), 2.65 (br, 1H), 2.38 (d, *J* = 14.4 Hz, 1H), 1.76-1.67 (m, 1H), 1.45 (s, 3H), 1.08-0.99 (m, 1H), 0.83-0.79 (t, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 177.2, 140.0, 128.4, 127.3, 81.8, 66.8, 51.8, 45.7, 39.6, 38.8, 32.0, 31.7, 7.7; IR (KBr): 3405 (OH) cm^{-1}, 3350, 1660 (C=ONH$_2$) cm^{-1}; HRMS (ESI): exact mass calculated for $[M+Na]^+$ ($C_{16}H_{23}NNaO_2S_2$) requires m/z 348.1068, found m/z 348.1062.

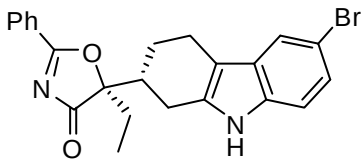
9d:(2*S*,3*R*)-2-ethyl-2-hydroxy-4-(2-methyl-1,3-dithiolan-2-yl)-3-phenylbutanoic acid



α-hydroxy amide **9c** (0.1 mmol, 32.5 mg) was refluxed in hydrochloric acid (6 N, 4 ml) for 8 h, after extraction with ethyl acetate and column chromatography using a silica gel column with a mixture of petroleum ether and ethyl acetate (1:1) as an eluent, give α-hydroxy acid **9d** (29.4 mg, 90%) as white solid. Mp 141-142°C; $[\alpha]^{25}_D$ – 0.19 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.39-7.36(m, 2H), 7.34-7.26 (m, 3H), 3.34-3.22 (m, 5H), 2.75 (dd, *J* = 10.4, 14.4 Hz, 1H), 2.38 (dd, *J* = 1.2, 14.4 Hz, 1H), 1.71-1.64(m, 1H), 1.45 (s, 3H), 1.19-1.14 (m, 1H), 0.81-0.78 (t, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 180.8, 139.7, 128.2, 127.3, 81.6, 77.4, 77.0, 76.7, 66.5, 51.7, 46.5, 32.2, 30.8, 7.8; IR (KBr): 3415 (OH) cm^{-1}, 3150, 1712 (COOH) cm^{-1}; HRMS (ESI): exact mass calculated for $[M+Na]^+$ ($C_{16}H_{22}NaO_3S_2$) requires m/z 349.0908, found m/z 349.0905.



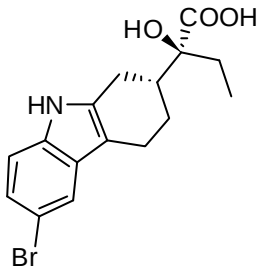
9e:(*S*)-5-ethyl-5-((7*R*)-5,6,7,8,9,9a-hexahydro-4a*H*-carbazol-7-yl)-2-phenyloxazol-4(5*H*)-one



4-Bromophenylhydrazine hydrochloride (55.9 mg, 0.25 mmol) was added to a solution of **7u** (57.1 mg, 0.20 mmol) in 0.5 mL of acetic acid, and the reaction mixture was heated for 1.5 h at 100 °C. After this time, TLC analysis indicates complete conversion of **7u**. The reaction mixture was cooled to room temperature and then poured into 2 mL of water and extracted three times with AcOEt. The organic layers were combined, washed with 10% Na_2CO_3, and dried ($MgSO_4$) and concentrated. The crude reaction mixture was purified by column chromatography using (pet. ether /ethyl acetate = 5/1) to give **9d** (75.2 mg, 86%) as a white solid. Mp >180°C; $[\alpha]^{25}_D$ – 39.4 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.27-8.22 (m, 3H), 7.74-7.70 (m, 1H), 7.57-7.53 (m, 3H), 7.20-7.14 (m, 2H), 2.88-2.72 (m, 3H), 2.66-2.59 (m, 1H), 2.55-2.48 (m, 1H), 2.27-2.17 (m, 2H), 2.14-2.07 (m, 1H), 1.69-1.59 (m, 1H),

0.96-0.93 (t, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 193.5,. 186.3, 135.4, 134.8, 133.8, 130.1, 129.1, 129.0, 125.4, 123.9, 120.4, 112.4, 112.1, 109.2, 93.3, 40.1, 27.1, 23.4, 23.3, 20.4, 7.3; HRMS (ESI): exact mass calculated for $[M+H]^+$ ($C_{23}H_{22}BrN_2O_2$) requires m/z 437.0865, found m/z 437.0859.

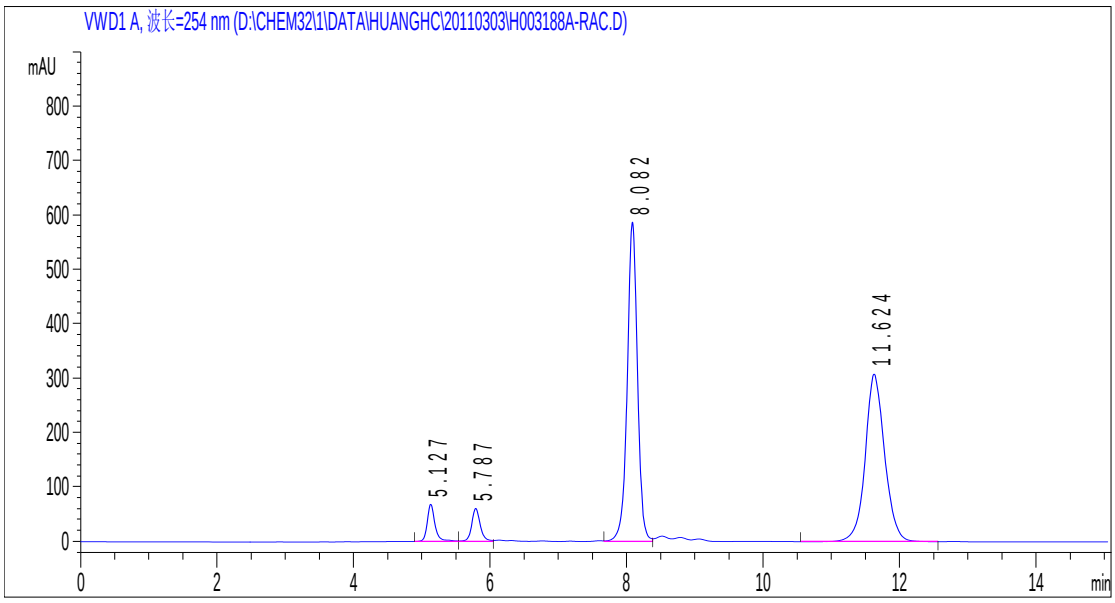
9f:(*S*)-2-((*R*)-6-bromo-2,3,4,9-tetrahydro-1*H*-carbazol-2-yl)-2-hydroxybutanoic acid



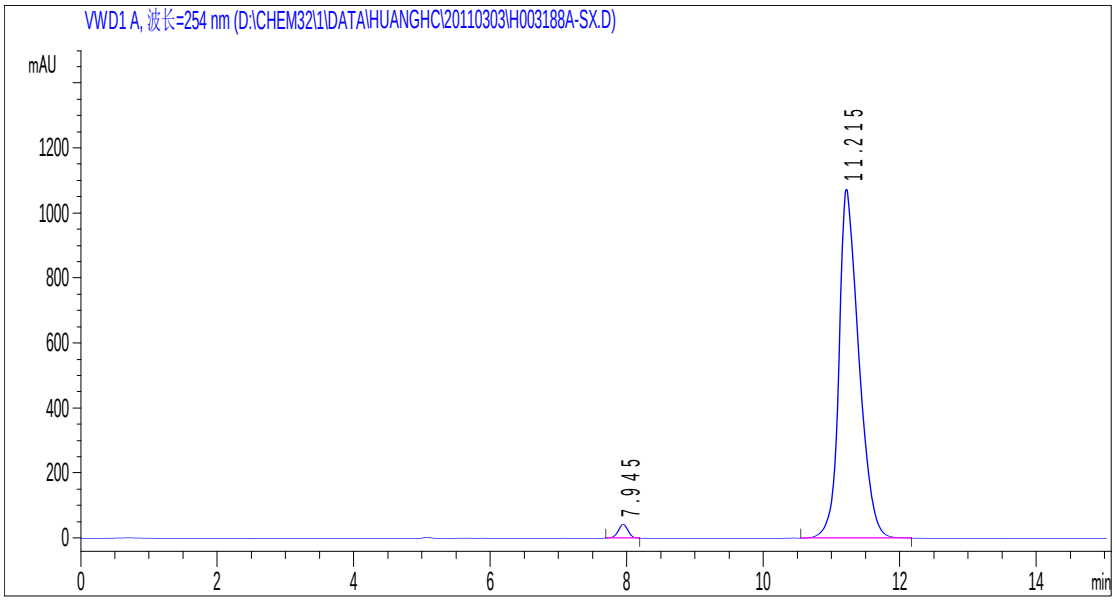
white solid. Mp 154-156°C; $[\alpha]^{25}_D$ – 0.25 (*c* 0.6, CH_2Cl_2); ^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) 10.79 (br, 1H),7.44-7.43 (m, 1H), 7.26-7.23 (m, 2H), 7.16-7.14 (m, 1H), 7.05-7.02 (m, 1H), 4.78 (br, 1H), 2.76-2.70 (m, 2H), 2.46-2.42 (m, 1H), 2.13-1.99 (m, 2H), 1.74-1.70 (m, 2H), 1.39-1.33 (m, 1H), 0.82-0.79 (t, 3H). ^{13}C NMR (100 MHz, DMSO-d_6): δ (ppm) 176.7, 136.6, 134.5, 128.7, 122.1, 119.4, 112.3, 110.5, 107.7, 78.4, 42.1, 29.0, 23.9, 22.9, 20.4, 8.0; HRMS (ESI): exact mass calculated for $[M+Na]^+$ ($C_{16}H_{18}BrNNaO_3$) requires m/z 374.0368, found m/z 374.0373.

F: HPLC Charts of Michael Addition Products

7a:(*S*)-5-methyl-5-((*R*)-3-oxo-1-phenylbutyl)-2-phenyloxazol-4(5*H*)-one

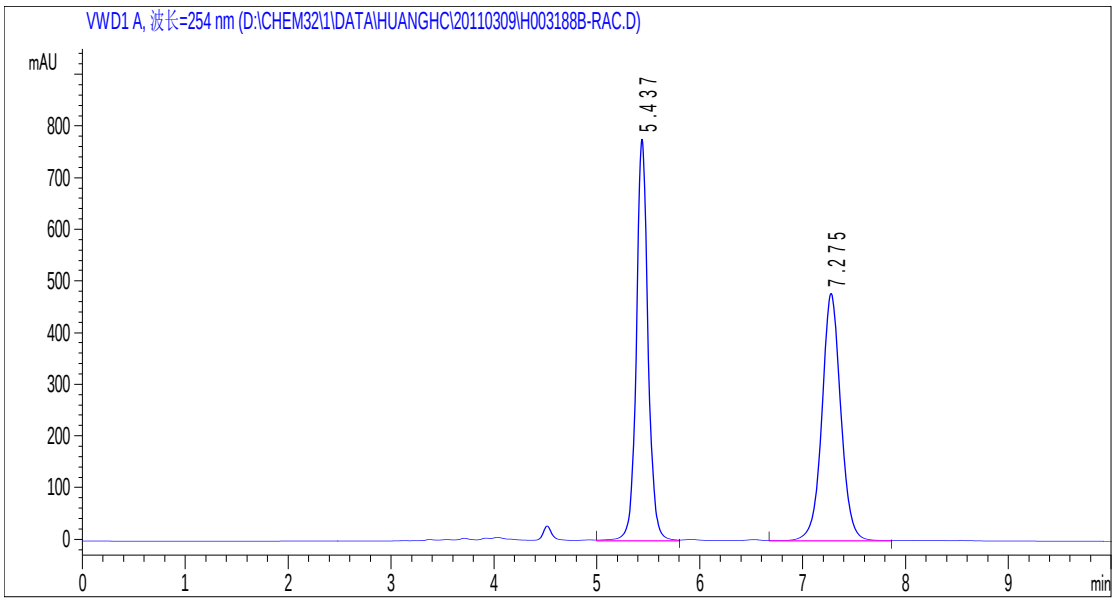


#	Time	Area	Height	Width	Symmetry	Area %
1	5.127	578	69.1	0.1238	0.722	4.313
2	5.787	559.5	61.5	0.1382	0.85	4.175
3	8.082	6146.3	587.3	0.1629	1.006	45.860
4	11.624	6118.4	308.1	0.2987	0.841	45.653

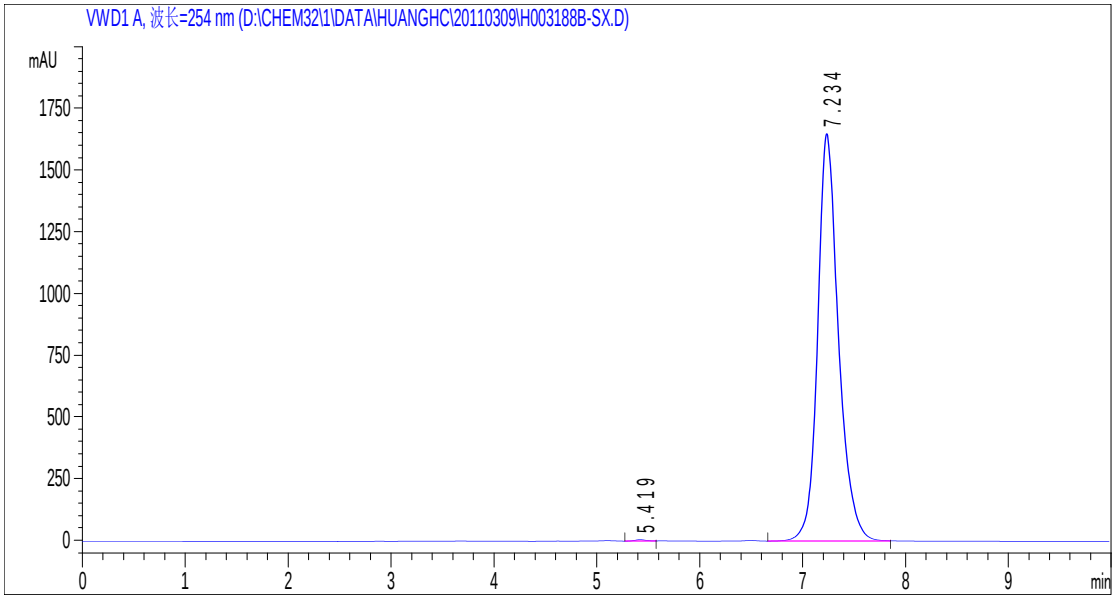


#	Time	Area	Height	Width	Symmetry	Area %
1	7.945	449.4	43.3	0.1731	0.978	2.020
2	11.215	21801	1074.8	0.3381	0.588	97.980

7b:(*S*)-5-methyl-5-((*R*)-3-oxo-1-m-tolylbutyl)-2-phenyloxazol-4(5*H*)-one

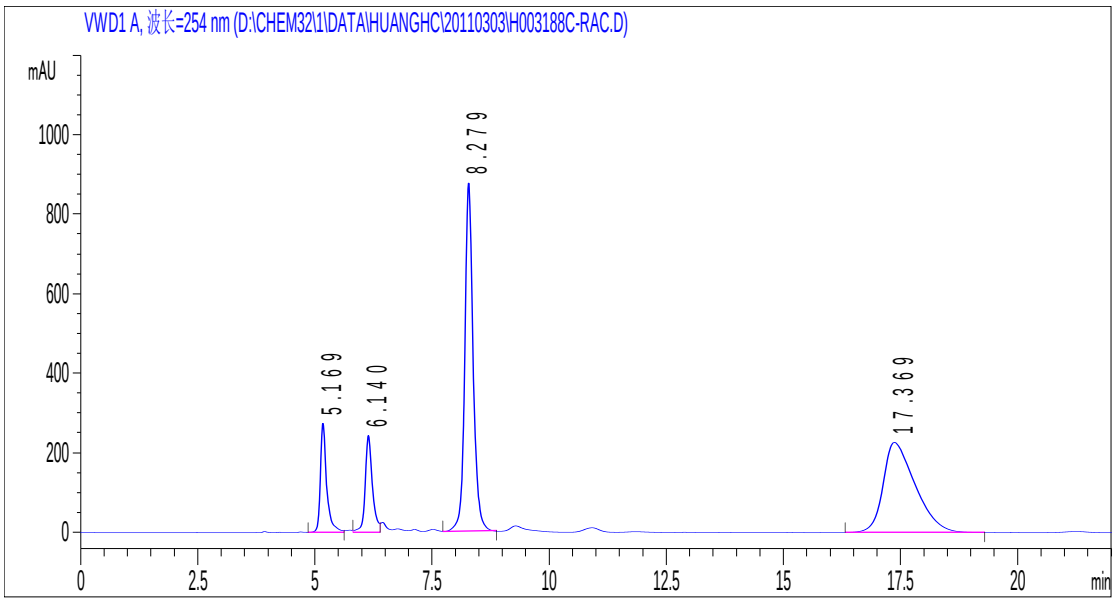


#	Time	Area	Height	Width	Symmetry	Area %
1	5.437	6153.2	778.6	0.1199	0.911	49.977
2	7.275	6158.9	479.4	0.195	0.926	50.023

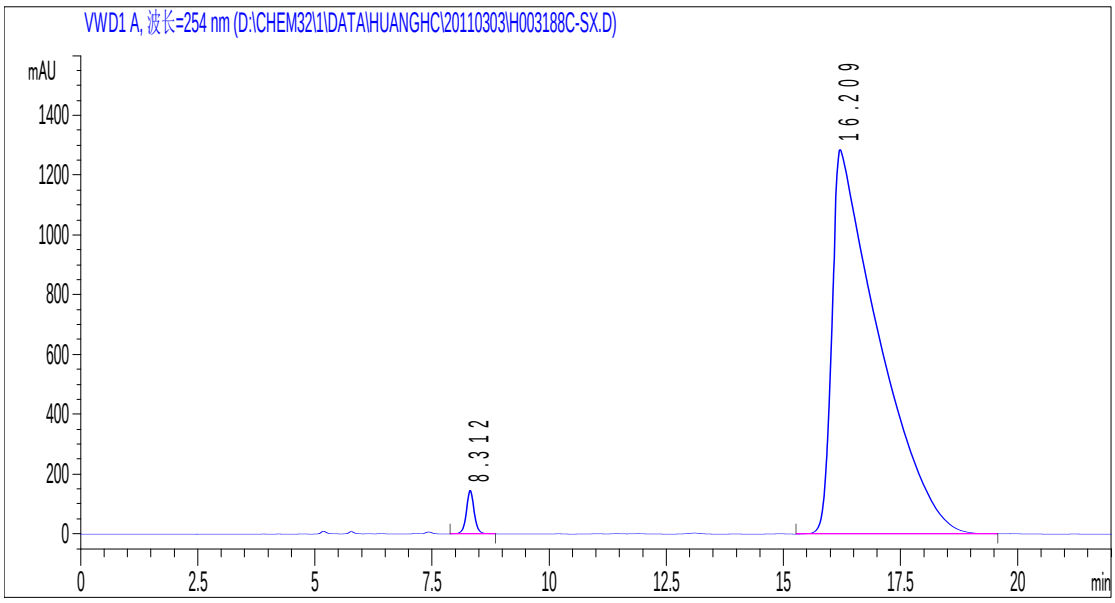


#	Time	Area	Height	Width	Symmetry	Area %
1	5.419	54.2	6.3	0.1278	0.78	0.232
2	7.234	23279.4	1651.1	0.235	0.767	99.768

7c:(*S*)-5-((*R*)-1-(4-fluorophenyl)-3-oxobutyl)-5-methyl-2-phenyloxazol-4(5*H*)-one

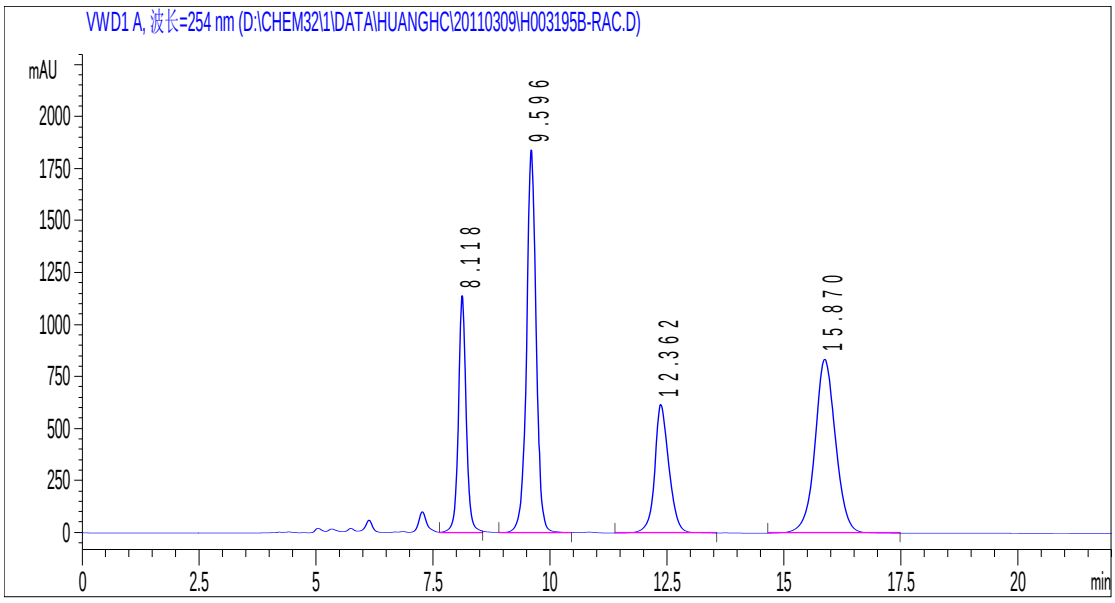


#	Time	Area	Height	Width	Symmetry	Area %
1	5.169	2611	275	0.1399	0.619	9.669
2	6.14	2655.2	244.1	0.1618	0.78	9.833
3	8.279	10923.5	877	0.2076	0.856	40.453
4	17.369	10813.1	226.9	0.7191	0.533	40.044

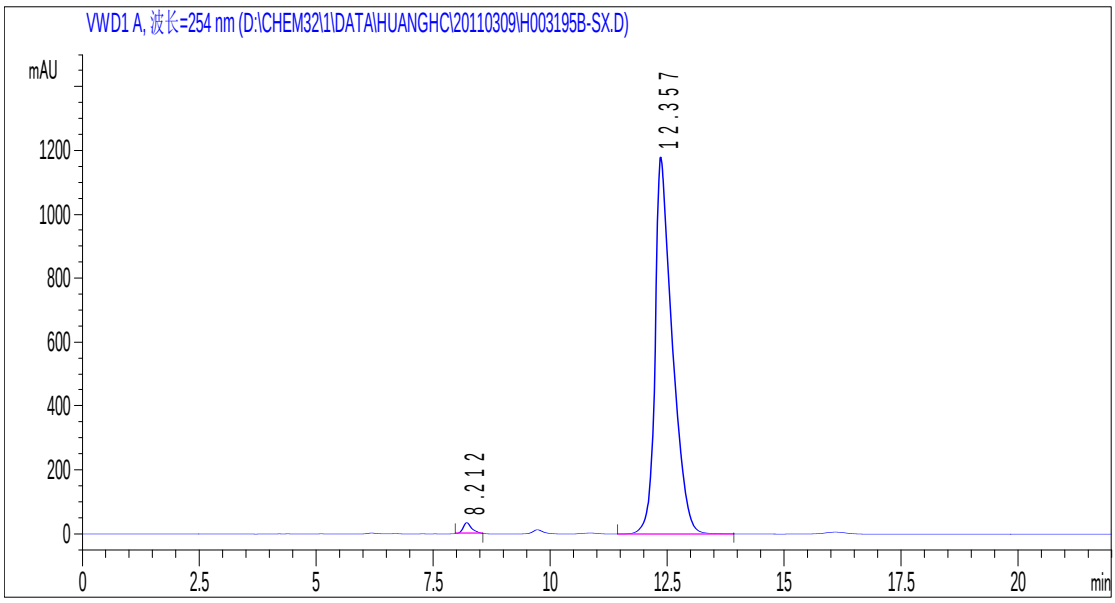


#	Time	Area	Height	Width	Symmetry	Area %
1	8.312	1720.4	146	0.1811	0.922	1.885
2	16.209	89560.1	1286	0.9231	0.201	98.115

7d:(*S*)-5-methyl-5-((*R*,*E*)-5-oxo-1-phenylhex-1-en-3-yl)-2-phenyloxazol-4(5*H*)-one

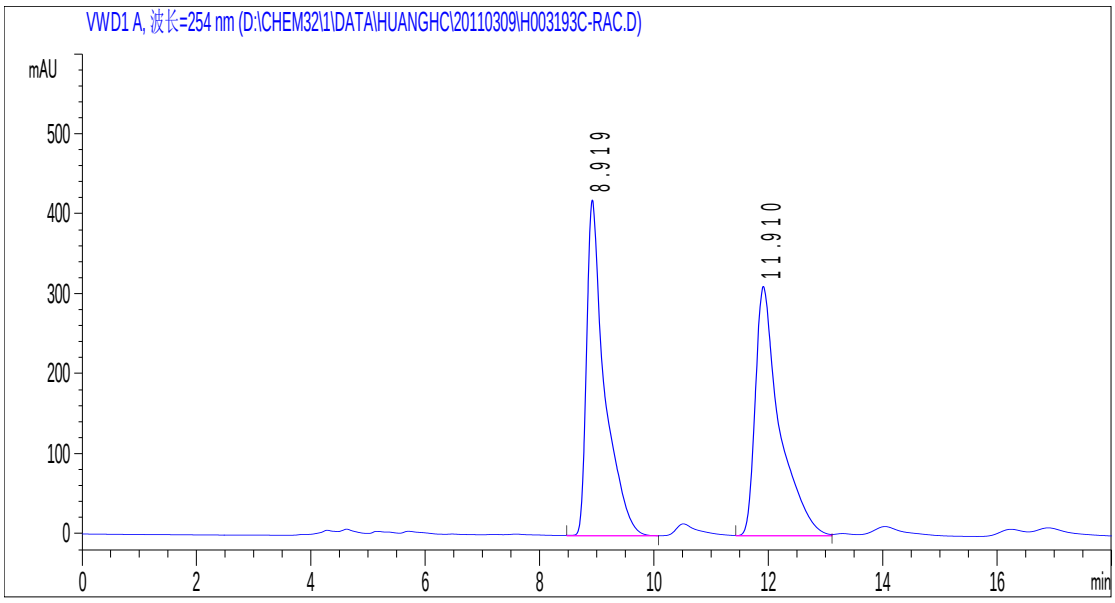


#	Time	Area	Height	Width	Symmetry	Area %
1	8.118	13319.1	1141.9	0.1944	0.917	16.962
2	9.596	26495.7	1842.3	0.2173	0.956	33.742
3	12.362	13017.1	618.3	0.314	0.724	16.577
4	15.87	25692.8	836.8	0.466	0.894	32.719

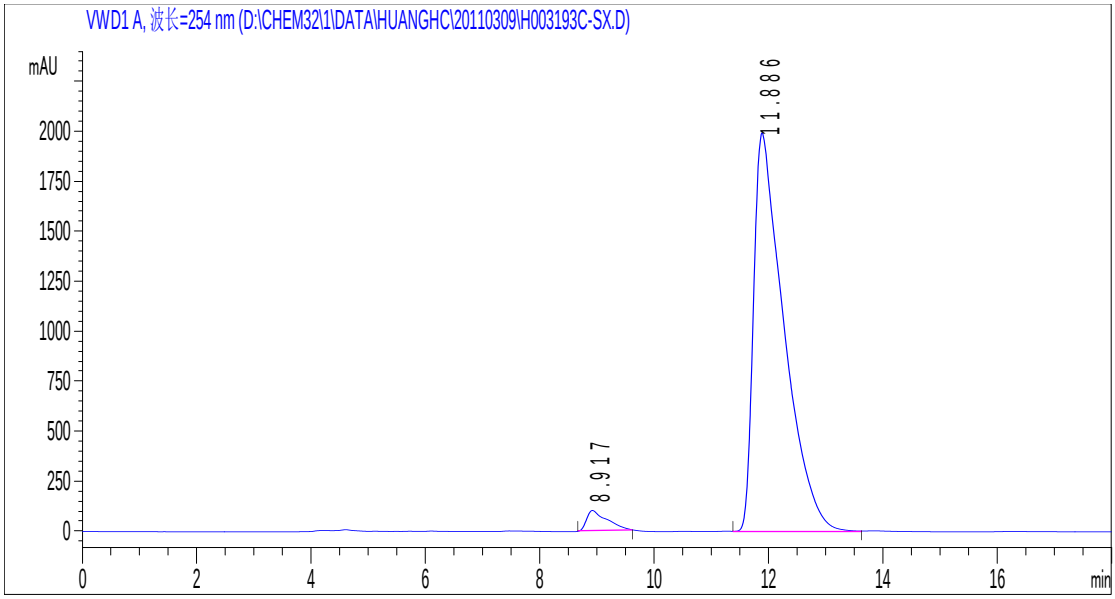


#	Time	Area	Height	Width	Symmetry	Area %
1	8.212	462.2	35	0.2203	0.703	1.513
2	12.357	30090.2	1181.5	0.4245	0.482	98.487

7e:(*S*)-5-methyl-5-((*S*)-2-oxodecan-4-yl)-2-phenyloxazol-4(5*H*)-one

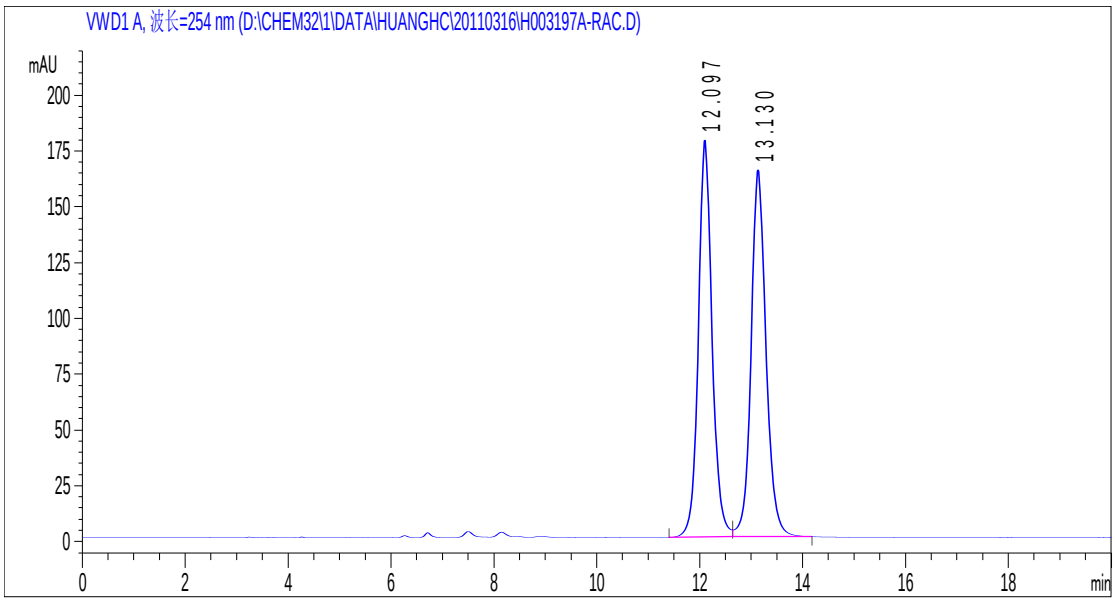


#	Time	Area	Height	Width	Symmetry	Area %
1	8.919	9190.1	419.9	0.3106	0.427	50.026
2	11.91	9180.4	312.2	0.4187	0.453	49.974

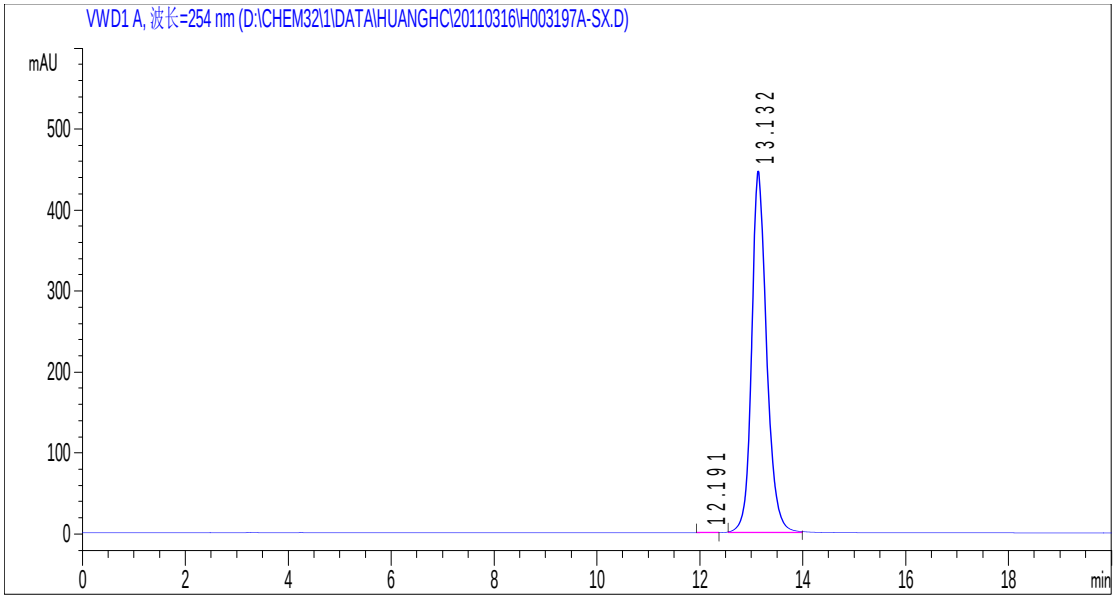


#	Time	Area	Height	Width	Symmetry	Area %
1	8.917	2604.6	103.3	0.4204	0.38	3.413
2	11.886	73711.8	1995.2	0.5126	0.365	96.587

7f: (*S*)-5-methyl-5-((*R*)-3-oxo-1,3-diphenylpropyl)-2-phenyloxazol-4(5*H*)-one

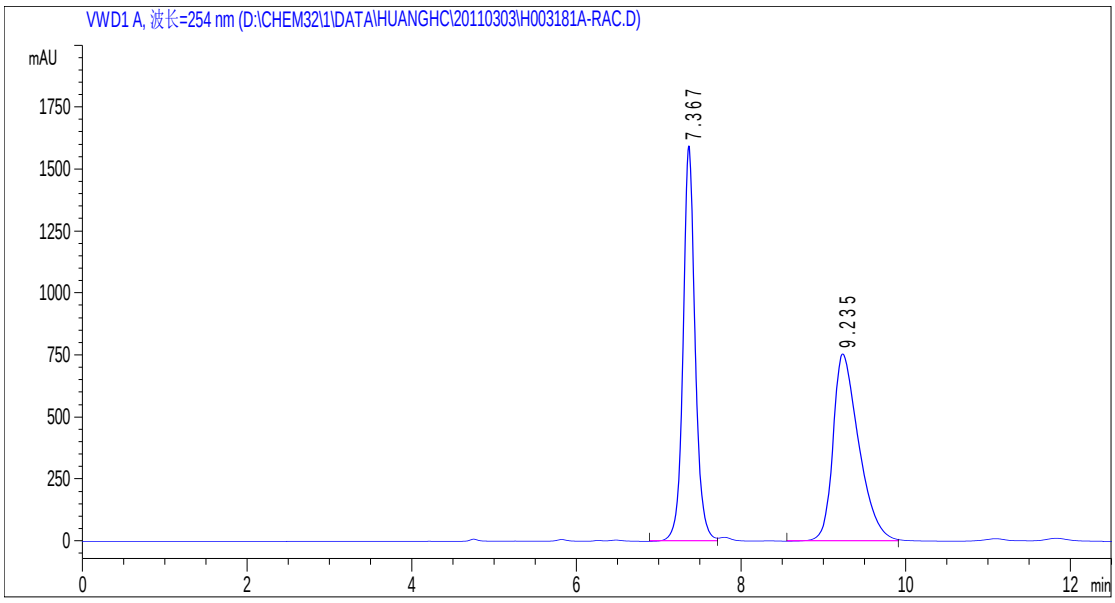


#	Time	Area	Height	Width	Symmetry	Area %
1	12.097	3302.4	178.1	0.2804	0.864	49.753
2	13.13	3335.2	164.6	0.3048	0.823	50.247

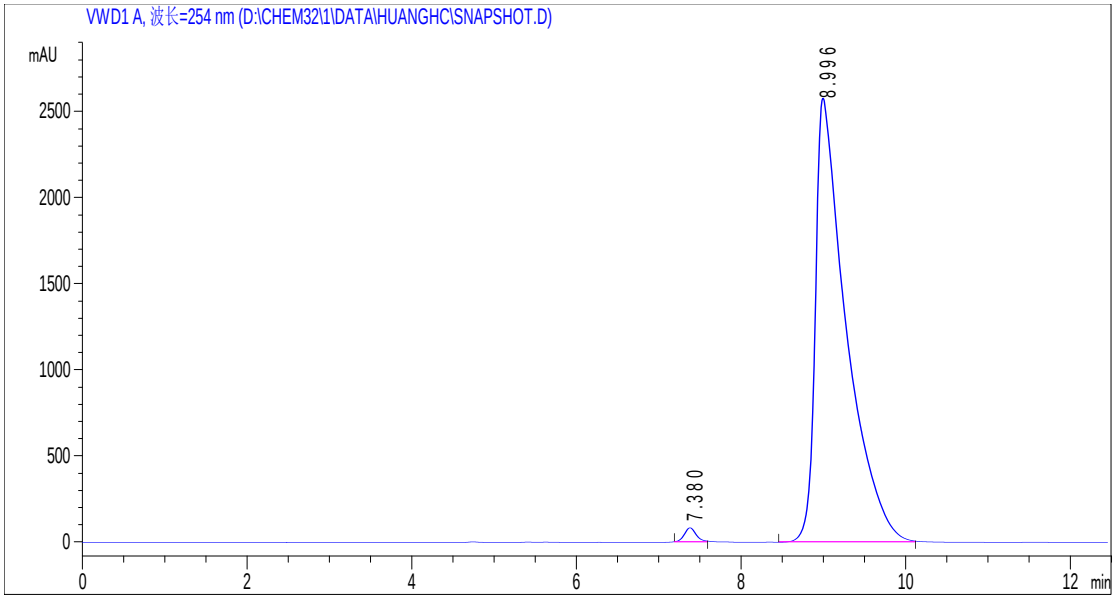


#	Time	Area	Height	Width	Symmetry	Area %
1	12.191	12.7	7.5E-1	0.2826	1.026	0.140
2	13.132	9066.1	446.8	0.3382	0.768	99.860

7g: (*S*)-5-ethyl-5-((*R*)-3-oxo-1-phenylbutyl)-2-phenyloxazol-4(5*H*)-one

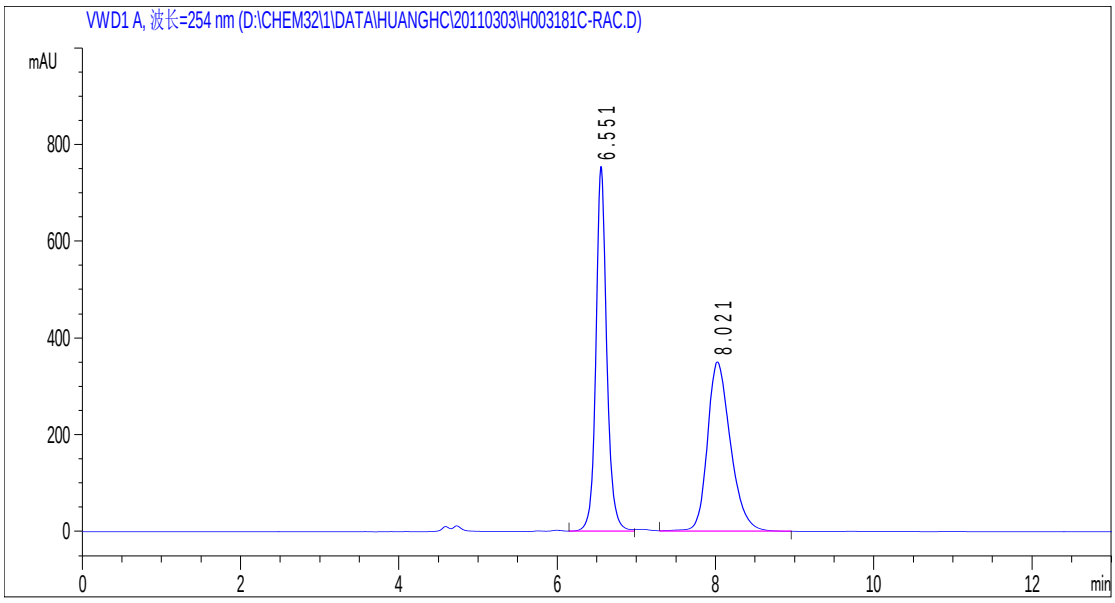


#	Time	Area	Height	Width	Symmetry	Area %
1	7.367	16215.4	1595.1	0.1521	0.884	49.579
2	9.235	16490.7	756.2	0.3635	0.586	50.421

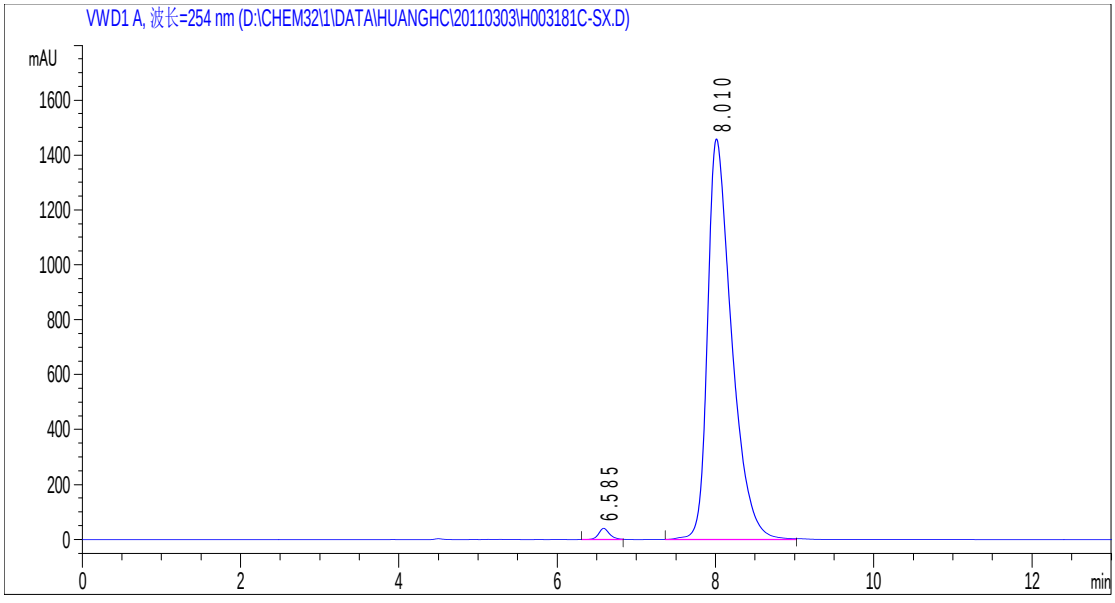


#	Time	Area	Height	Width	Symmetry	Area %
1	7.38	883.8	84.7	0.174	0.872	1.299
2	8.996	67176.5	2579.7	0.434	0.328	98.701

7h: (*S*)-5-ethyl-5-((*R*)-3-oxo-1-m-tolylbutyl)-2-phenyloxazol-4(5*H*)-one

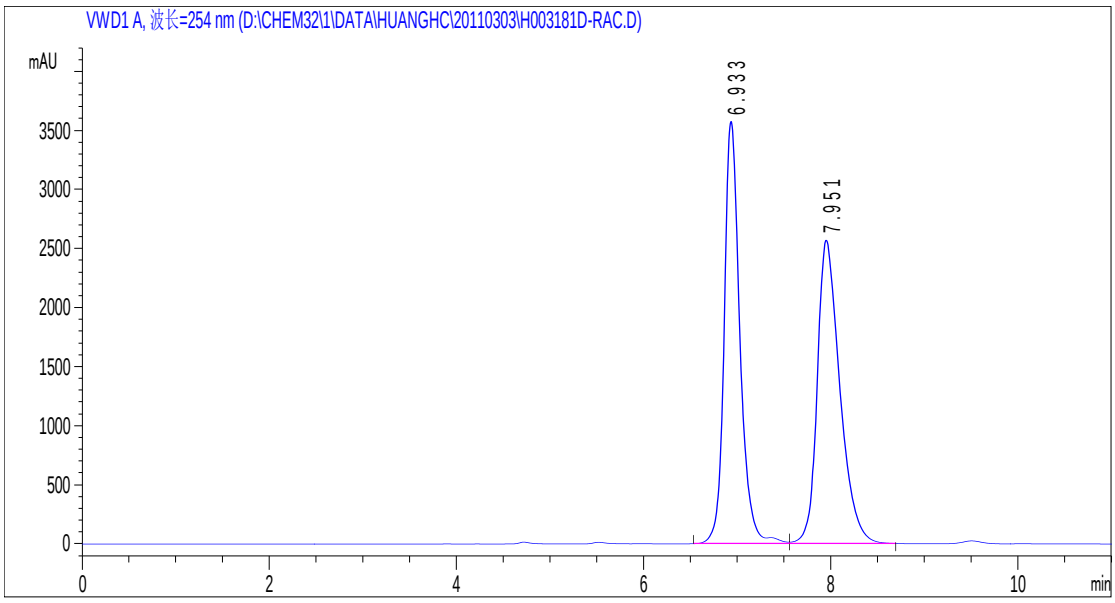


#	Time	Area	Height	Width	Symmetry	Area %
1	6.551	7194.5	754.8	0.1432	0.847	50.147
2	8.021	7152.2	350.8	0.3092	0.73	49.853

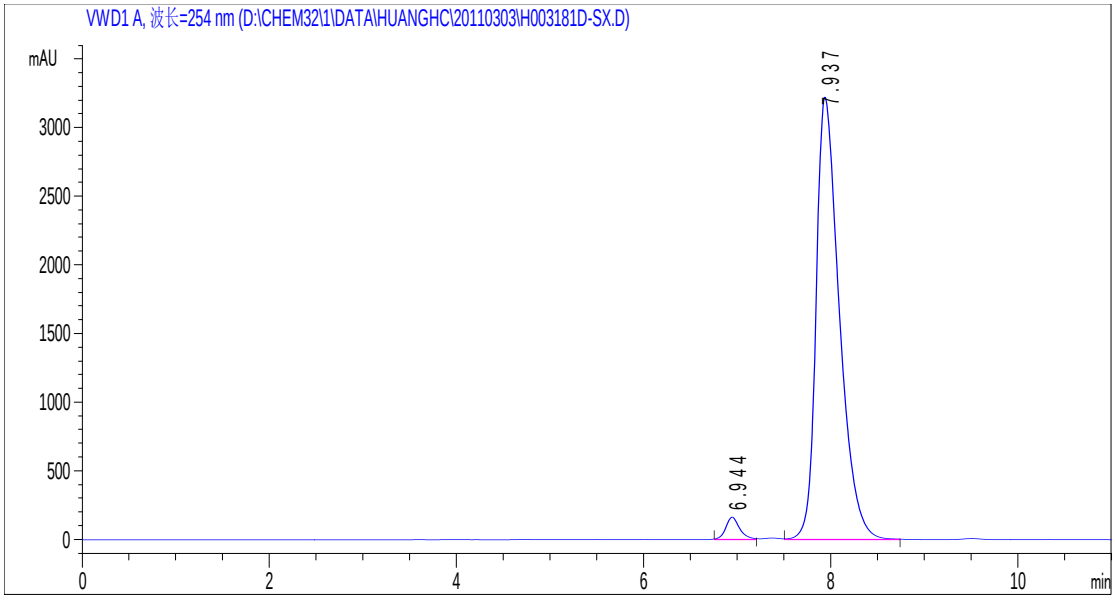


#	Time	Area	Height	Width	Symmetry	Area %
1	6.585	408.6	41.4	0.1646	0.834	1.305
2	8.01	30902.6	1460.3	0.3527	0.571	98.695

7i: (*S*)-5-ethyl-5-((*R*)-1-(2-methoxyphenyl)-3-oxobutyl)-2-phenyloxazol-4(5*H*)-one

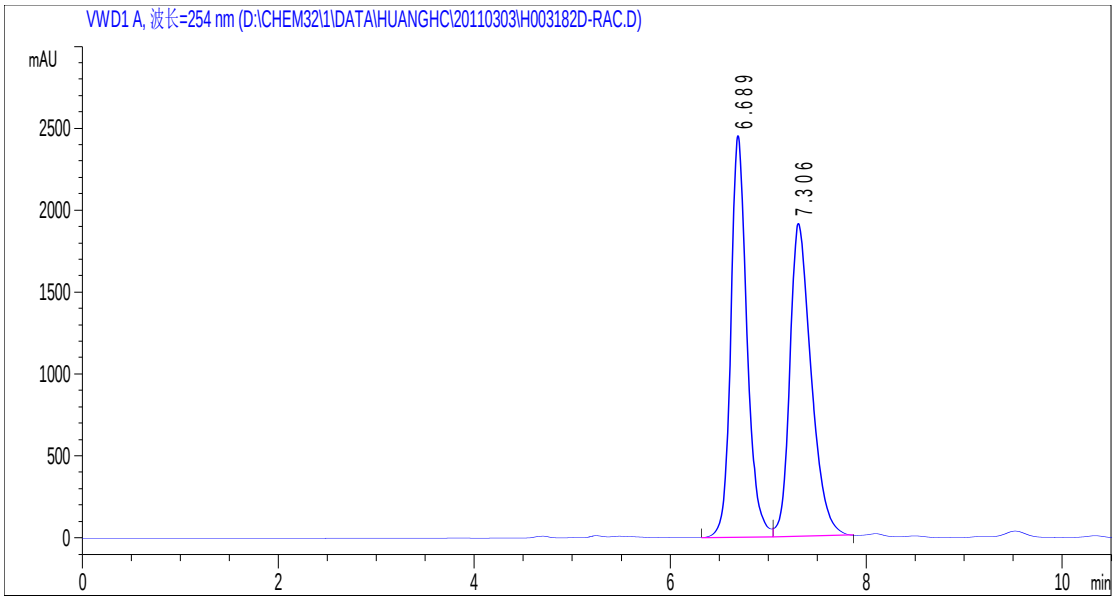


#	Time	Area	Height	Width	Symmetry	Area %
1	6.933	41841.3	3575.4	0.195	0.751	49.369
2	7.951	42911.5	2566.1	0.2787	0.646	50.631

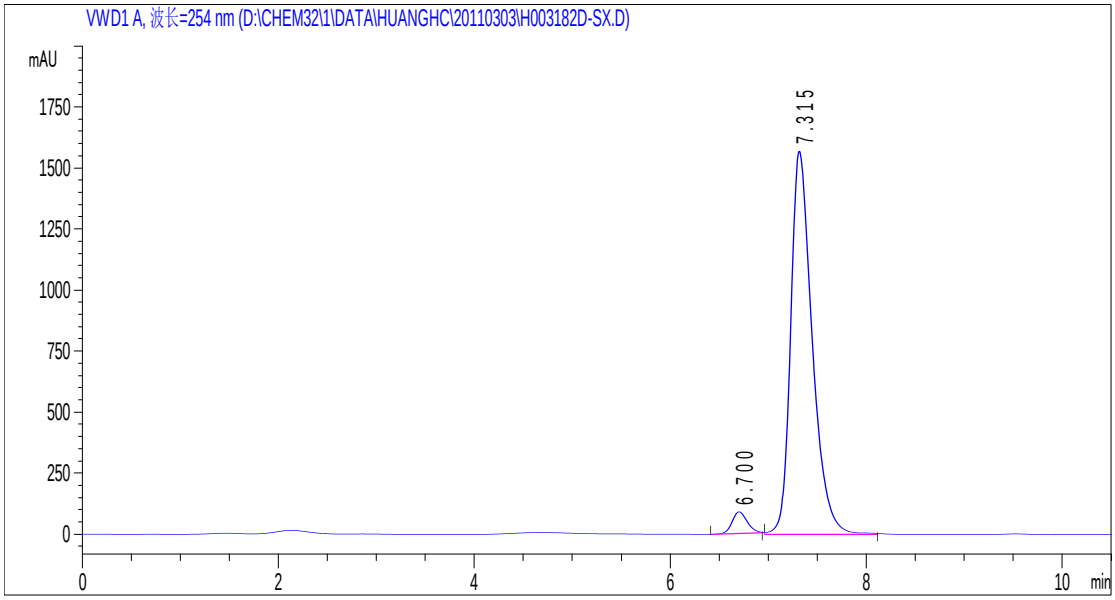


#	Time	Area	Height	Width	Symmetry	Area %
1	6.944	1730.5	165	0.1748	0.799	3.007
2	7.937	55815.8	3224.9	0.2885	0.593	96.993

7j:(*S*)-5-((*R*)-1-(2,3-dimethoxyphenyl)-3-oxobutyl)-5-ethyl-2-phenyloxazol-4(5*H*)-one

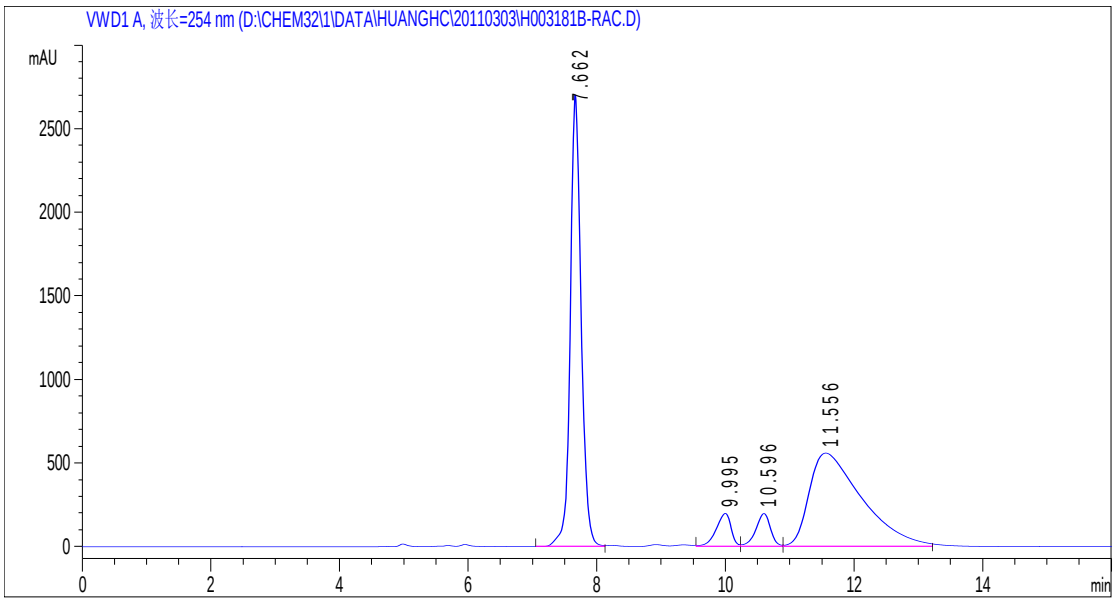


#	Time	Area	Height	Width	Symmetry	Area %
1	6.689	28270.3	2455.7	0.1919	0	49.363
2	7.306	28999.8	1911.7	0.2528	0	50.637

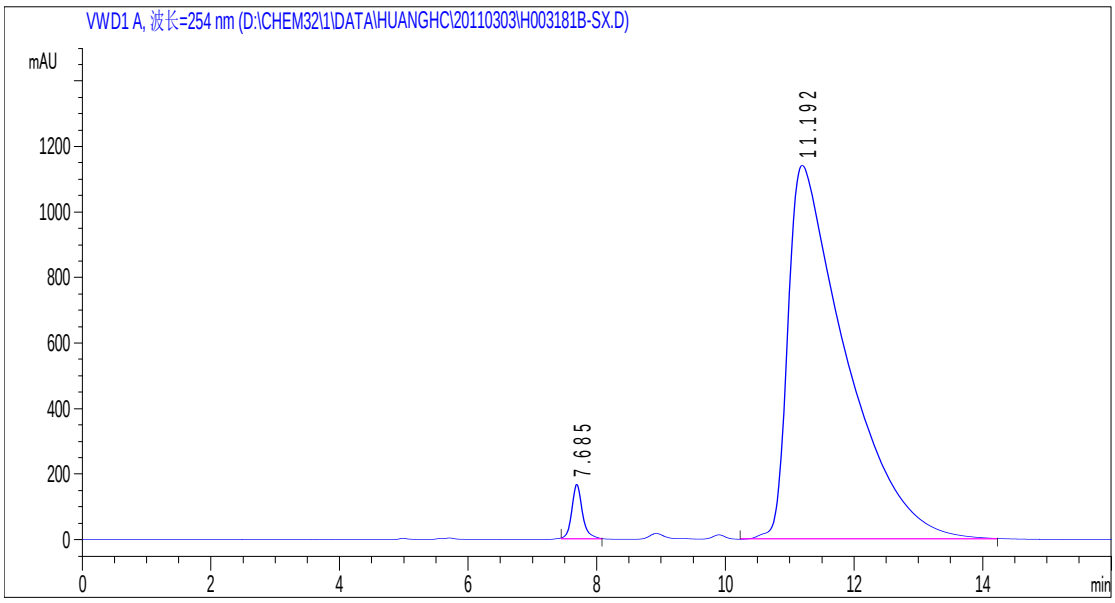


#	Time	Area	Height	Width	Symmetry	Area %
1	6.7	1004.5	90.8	0.1844	0.854	4.017
2	7.315	24002.9	1570.4	0.2547	0.657	95.983

7k: (*S*)-5-ethyl-5-((*R*)-1-(2-fluorophenyl)-3-oxobutyl)-2-phenyloxazol-4(5*H*)-one

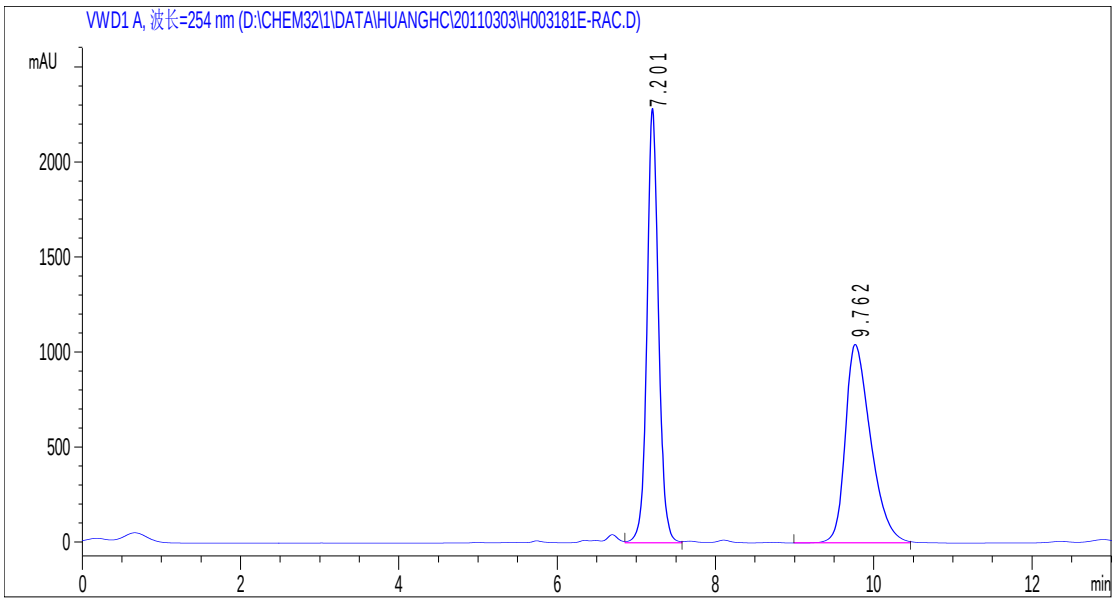


#	Time	Area	Height	Width	Symmetry	Area %
1	7.662	31776.9	2703.1	0.1779	0.822	45.299
2	9.995	3250.4	199.4	0.2499	1.556	4.634
3	10.596	3179.3	198.2	0.2425	1.213	4.532
4	11.556	31942.7	559.8	0.951	0.445	45.535

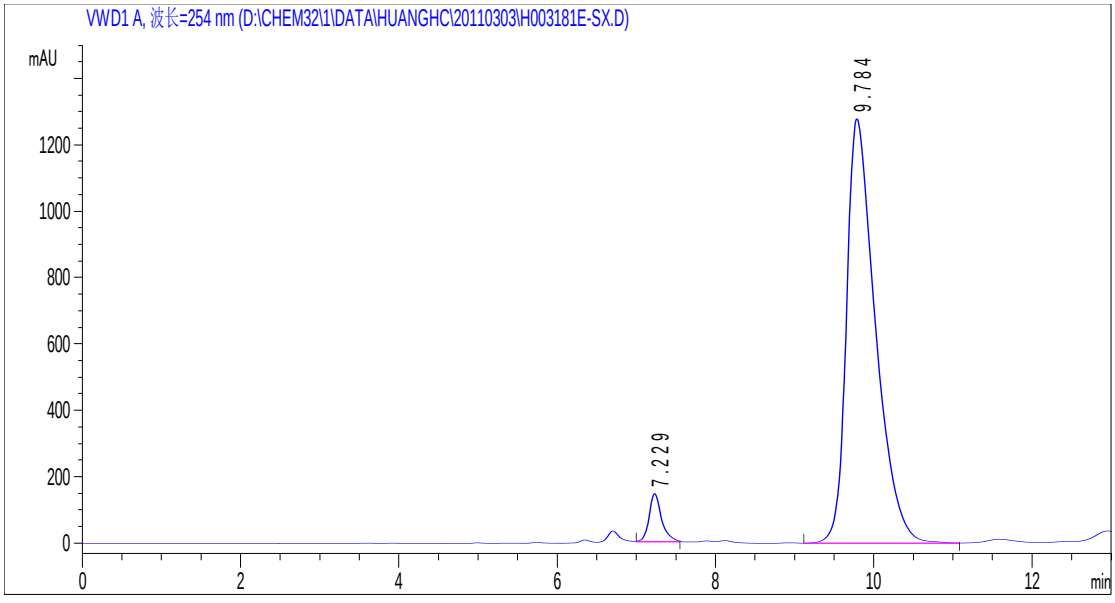


#	Time	Area	Height	Width	Symmetry	Area %
1	7.685	1993.6	168.4	0.1973	0.83	2.709
2	11.192	71588.7	1141.9	1.0449	0.318	97.291

7l: (*S*)-5-((*R*)-1-(2-chlorophenyl)-3-oxobutyl)-5-ethyl-2-phenyloxazol-4(5*H*)-one

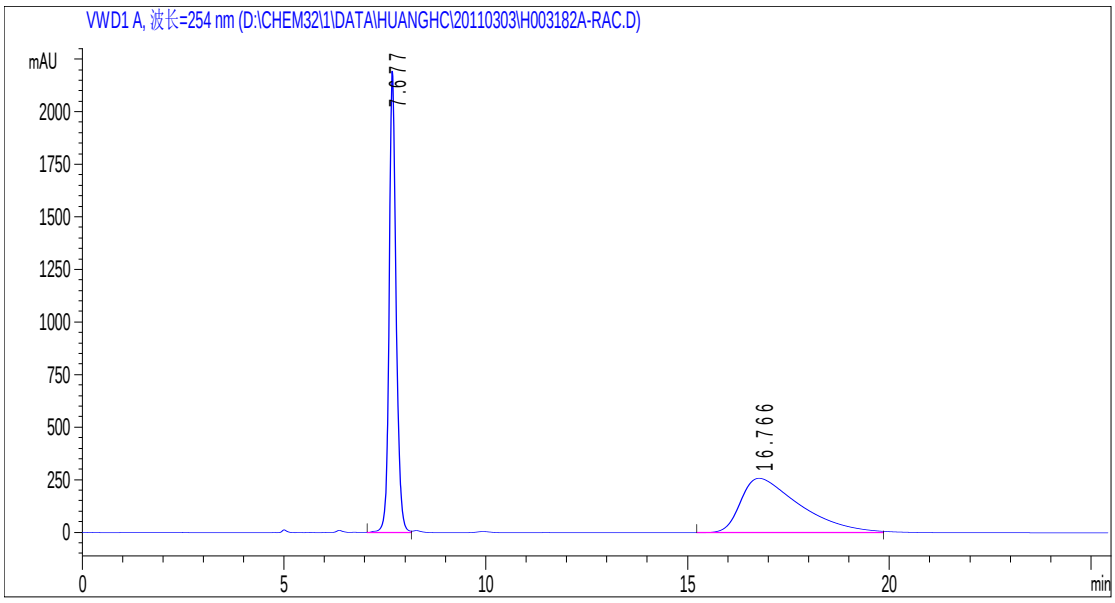


#	Time	Area	Height	Width	Symmetry	Area %
1	7.201	23235.7	2286.3	0.155	0.874	49.848
2	9.762	23376.9	1044.9	0.3729	0.622	50.152

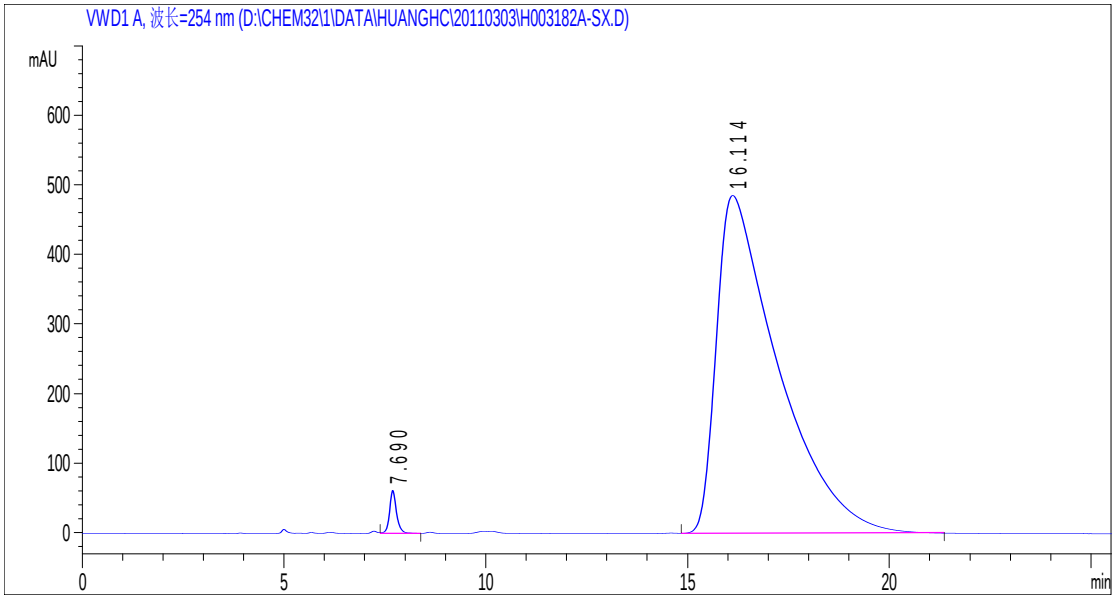


#	Time	Area	Height	Width	Symmetry	Area %
1	7.229	1605.4	145.7	0.1836	0.777	4.702
2	9.784	32537.3	1279.4	0.3782	0.535	95.298

7m: (*S*)-5-((*R*)-1-(4-chlorophenyl)-3-oxobutyl)-5-ethyl-2-phenyloxazol-4(5*H*)-one

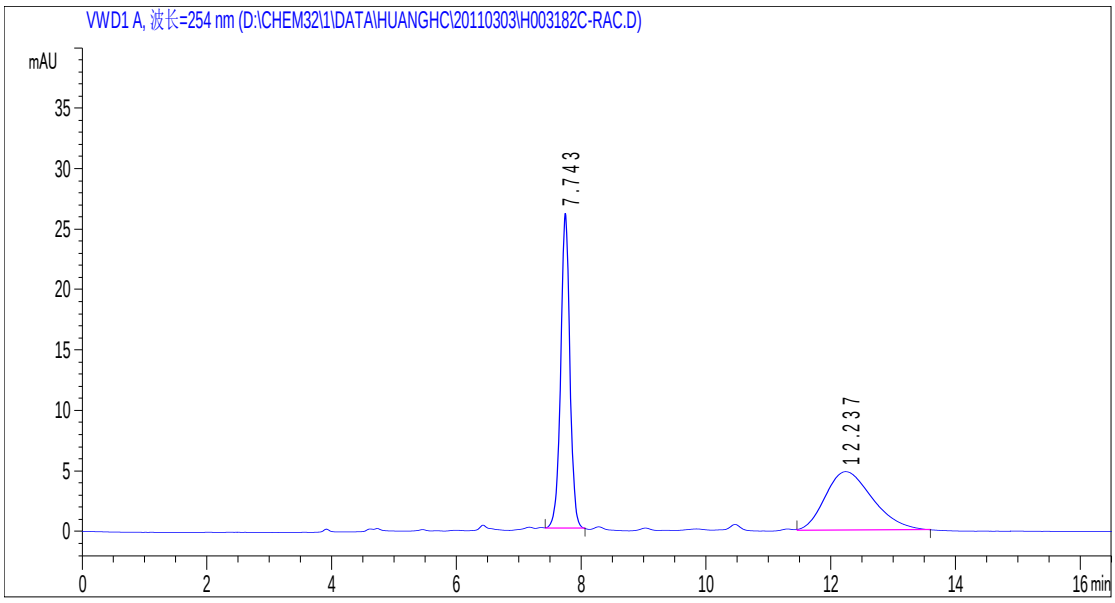


#	Time	Area	Height	Width	Symmetry	Area %
1	7.677	26407.4	2195.2	0.1797	0.787	50.011
2	16.766	26396.3	258.9	1.6992	0.44	49.989

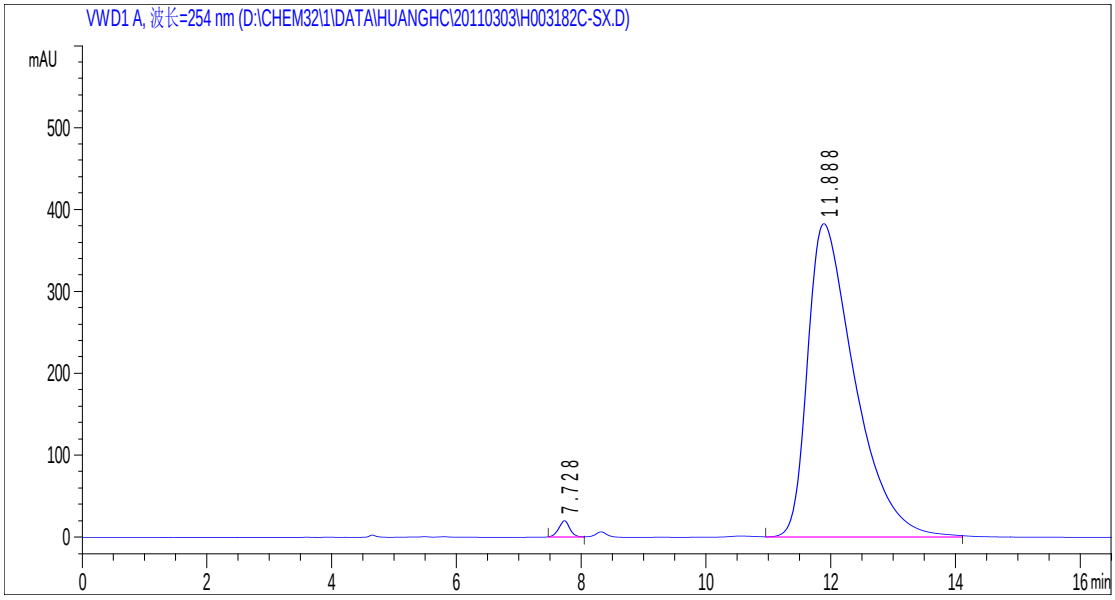


#	Time	Area	Height	Width	Symmetry	Area %
1	7.69	758.3	62	0.1821	0.787	1.449
2	16.114	51580.3	485.9	1.5019	0.333	98.551

7n: (*S*)-5-((*R*)-1-(3-bromophenyl)-3-oxobutyl)-5-ethyl-2-phenyloxazol-4(5*H*)-one

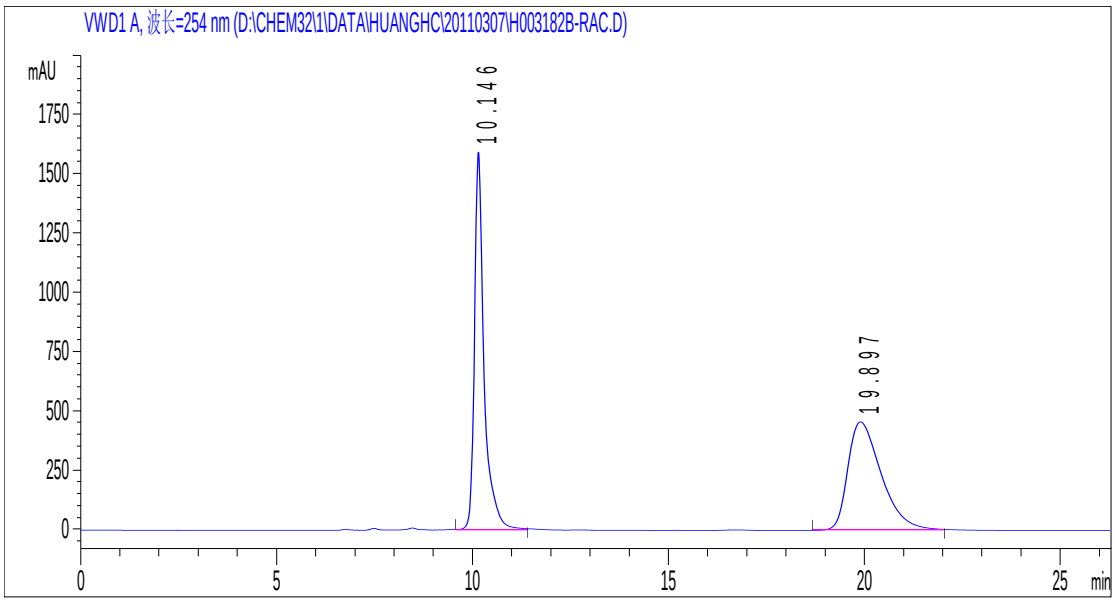


#	Time	Area	Height	Width	Symmetry	Area %
1	7.743	267.3	26.1	0.1708	1.002	50.666
2	12.237	260.3	4.9	0.7841	0.72	49.334

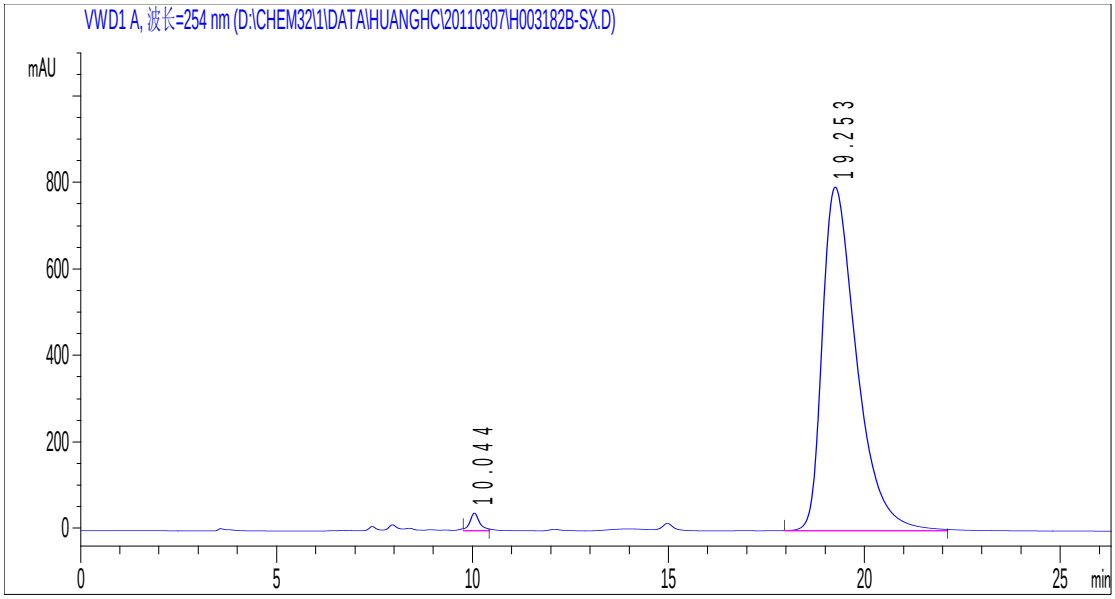


#	Time	Area	Height	Width	Symmetry	Area %
1	7.728	259	20.3	0.2126	1.019	1.272
2	11.888	20107	382.7	0.8756	0.512	98.728

7o: (*S*)-5-ethyl-5-((*R*)-1-(4-nitrophenyl)-3-oxobutyl)-2-phenyloxazol-4(5*H*)-one

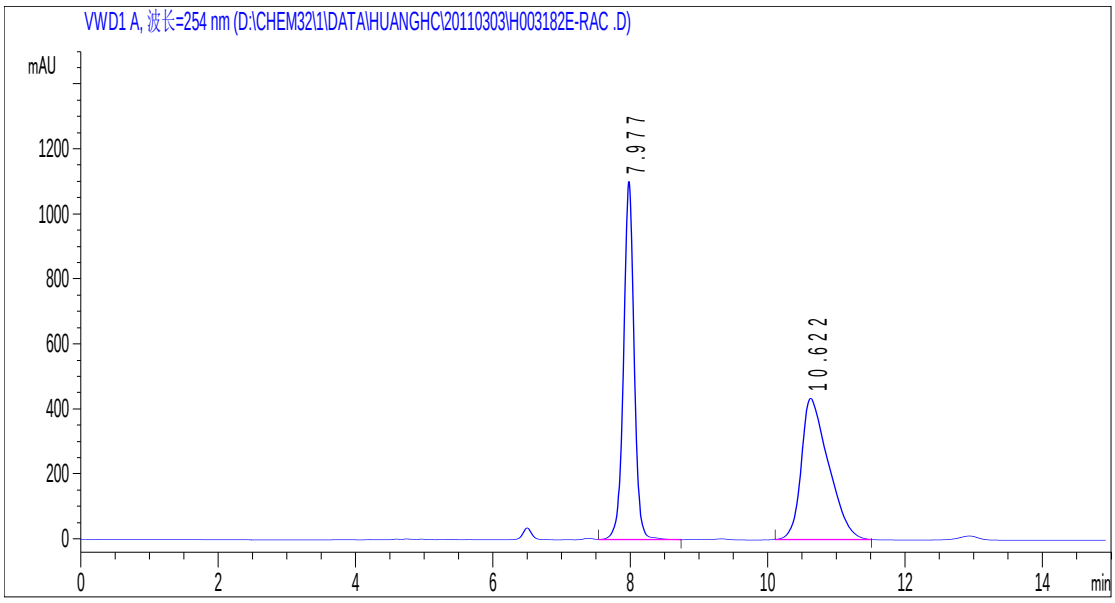


#	Time	Area	Height	Width	Symmetry	Area %
1	10.146	27422.4	1595.9	0.2864	0.663	50.062
2	19.897	27355.1	458.1	0.9952	0.585	49.938

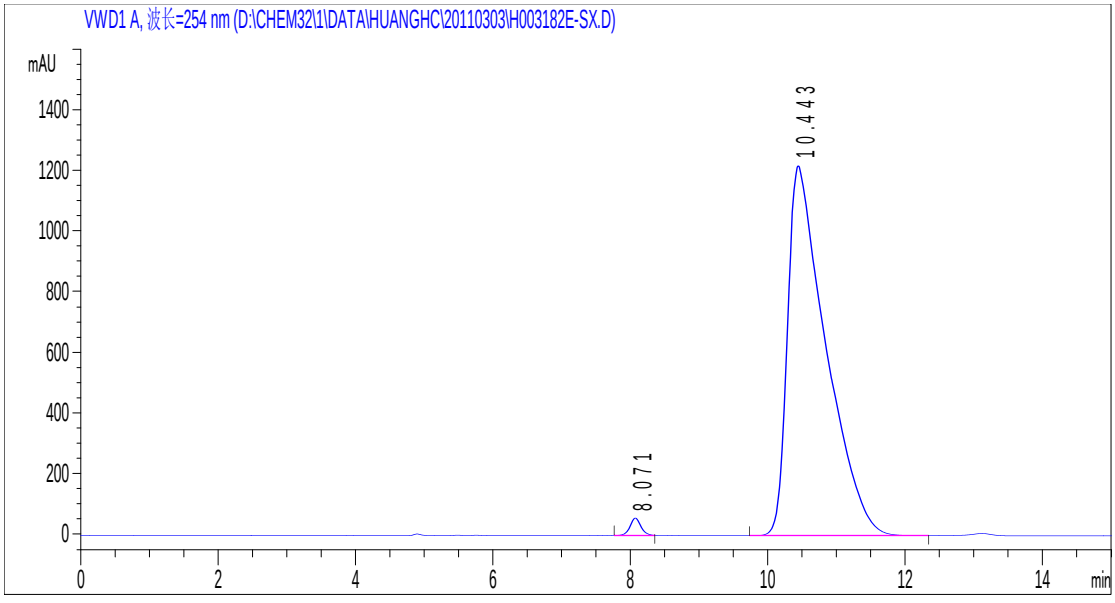


#	Time	Area	Height	Width	Symmetry	Area %
1	10.044	732	41.5	0.2938	0.818	1.494
2	19.253	48252.1	794.5	1.0121	0.586	98.506

7p: (*S*)-5-ethyl-5-((*R*)-1-(furan-2-yl)-3-oxobutyl)-2-phenyloxazol-4(5*H*)-one

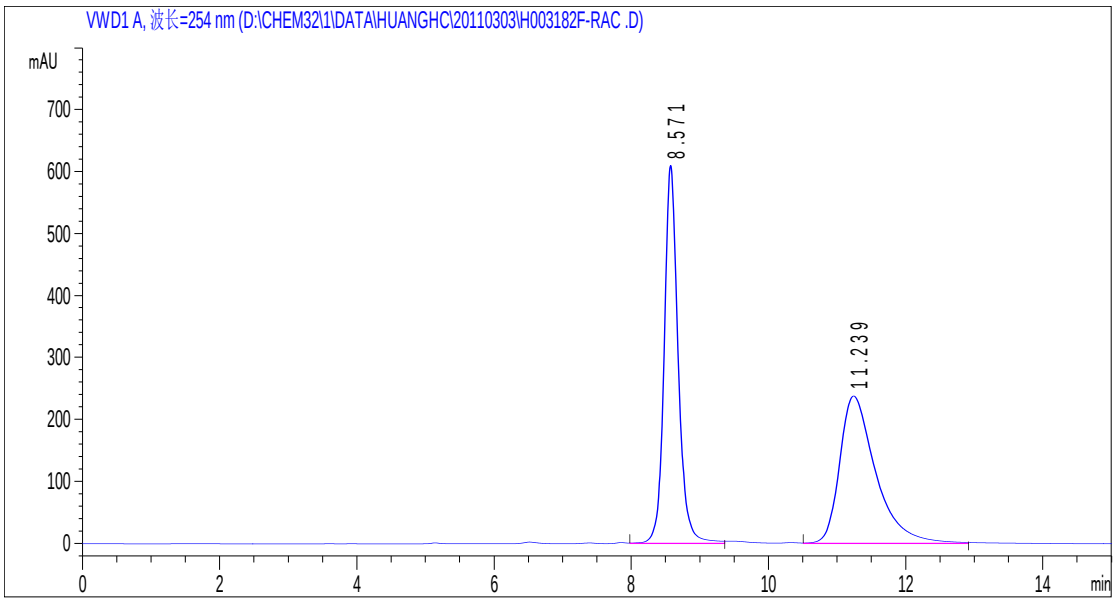


#	Time	Area	Height	Width	Symmetry	Area %
1	7.977	11853.5	1103.2	0.1632	0.997	49.567
2	10.622	12060.5	436.1	0.461	0.521	50.433

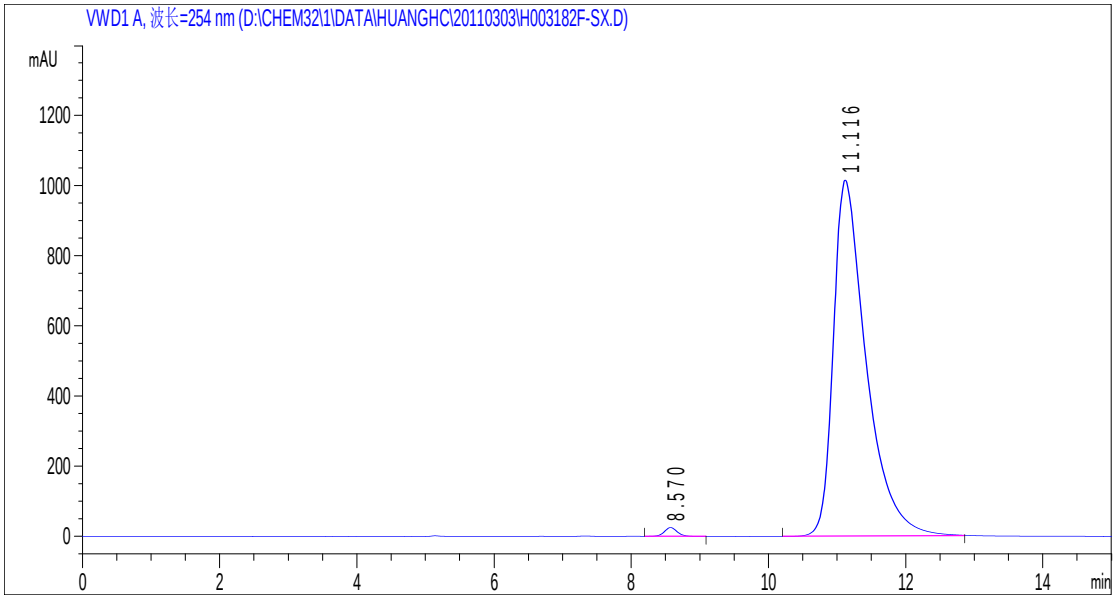


#	Time	Area	Height	Width	Symmetry	Area %
1	8.071	666.9	58.3	0.1906	0.93	1.393
2	10.443	47206.8	1219.8	0.5403	0.37	98.607

7q: (*S*)-5-ethyl-5-((*R*)-1-(naphthalen-1-yl)-3-oxobutyl)-2-phenyloxazol-4(5*H*)-one

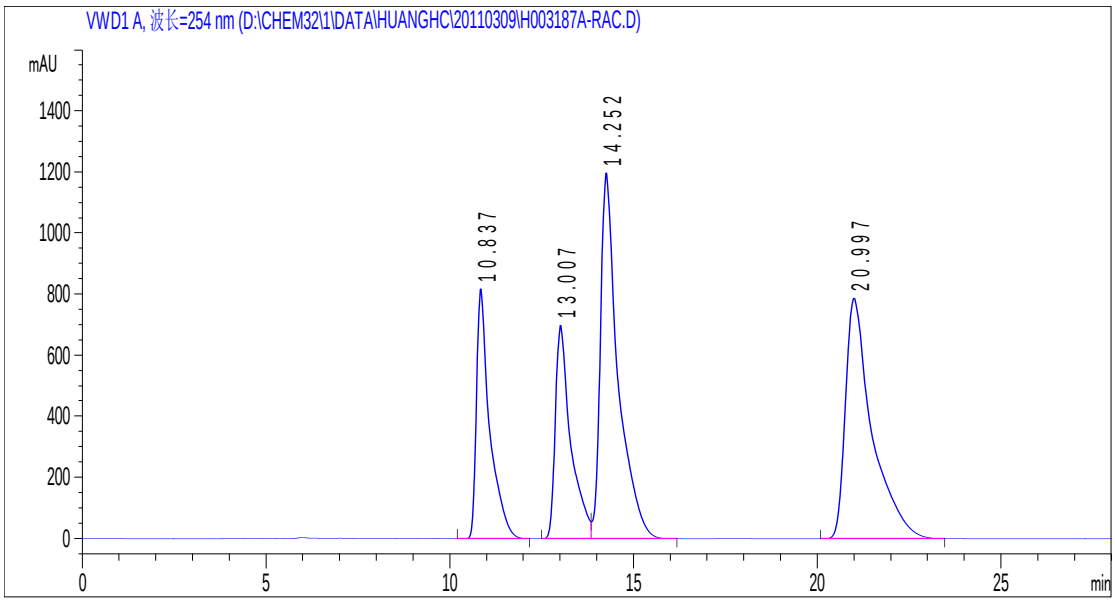


#	Time	Area	Height	Width	Symmetry	Area %
1	8.571	8687.8	610.6	0.2141	0.811	49.846
2	11.239	8741.7	238.4	0.6111	0.609	50.154

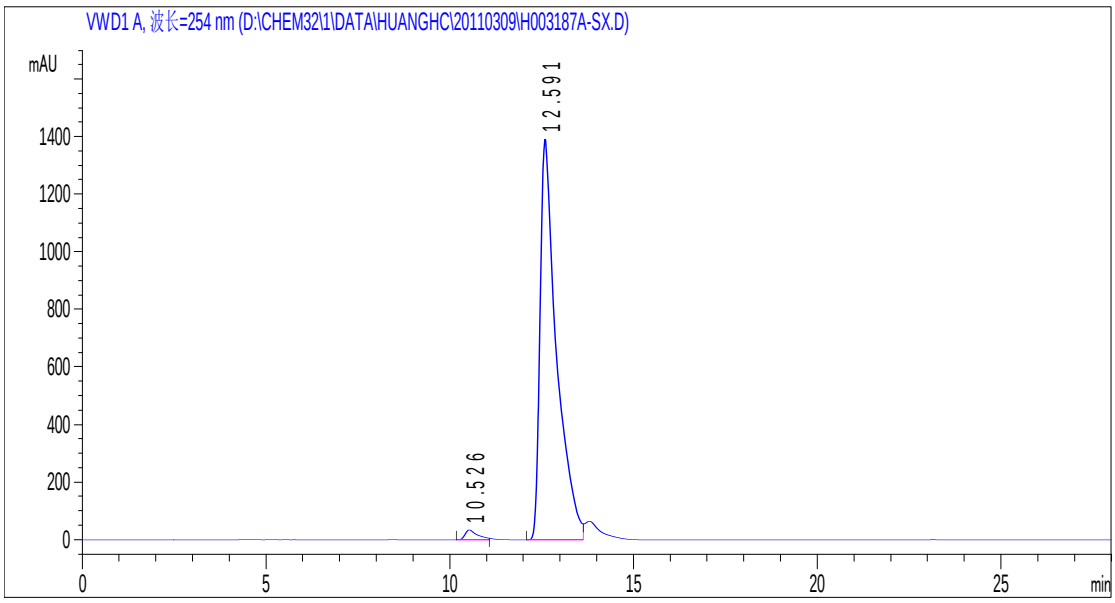


#	Time	Area	Height	Width	Symmetry	Area %
1	8.57	338.7	25.4	0.2019	0.915	0.987
2	11.116	33968.7	1017.3	0.5565	0.544	99.013

7r: (*S*)-5-ethyl-5-((*S*)-4-oxopentan-2-yl)-2-phenyloxazol-4(5*H*)-one

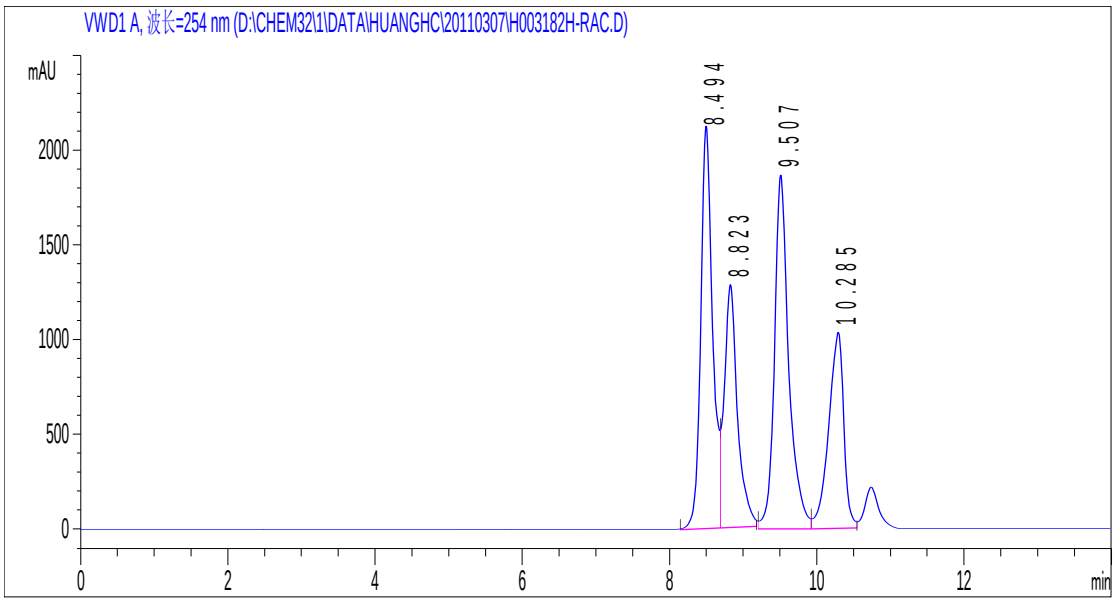


#	Time	Area	Height	Width	Symmetry	Area %
1	10.837	20450.4	818.1	0.3571	0.437	17.014
2	13.007	20330.5	699.1	0.4164	0.465	16.914
3	14.252	40021.7	1198.2	0.4785	0.456	33.296
4	20.997	39395.9	788.3	0.7199	0.448	32.776

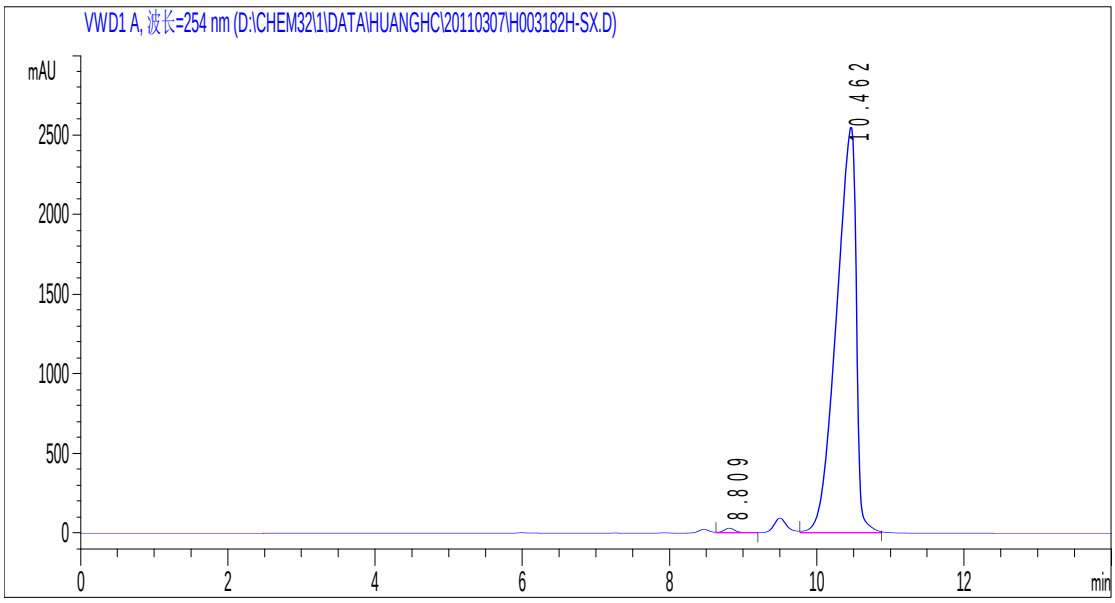


#	Time	Area	Height	Width	Symmetry	Area %
1	10.526	813.6	34.5	0.3931	0.483	1.841
2	12.591	43372.5	1392.3	0.4435	0.409	98.159

7s: (*S*)-5-ethyl-5-((*S*)-4-oxooctan-2-yl)-2-phenyloxazol-4(5*H*)-one

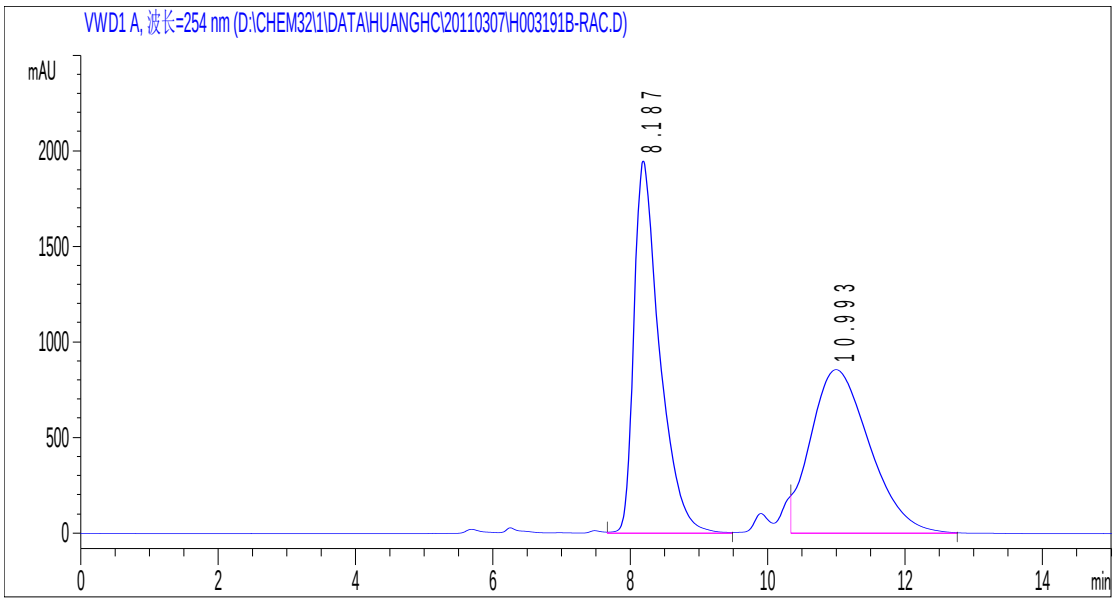


#	Time	Area	Height	Width	Symmetry	Area %
1	8.494	24081.7	2127.4	0.1887	0	30.144
2	8.823	15693.3	1284.5	0.2036	0.74	19.644
3	9.507	25239.1	1865.8	0.2015	0.73	31.593
4	10.285	14874.5	1034.5	0.2172	1.559	18.619

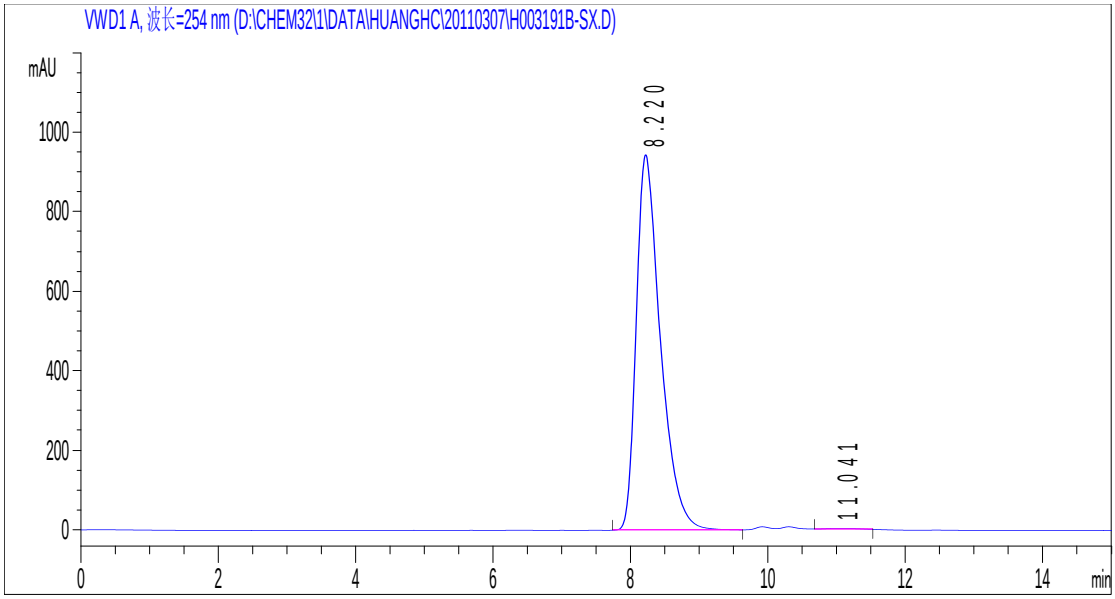


#	Time	Area	Height	Width	Symmetry	Area %
1	8.809	410.9	31.8	0.1887	0.718	0.855
2	10.462	47673.9	2553.8	0.3111	2.631	99.145

7t: (*S*)-5-ethyl-5-((*R*)-4-methyl-3-oxo-1-phenylpentyl)-2-phenyloxazol-4(5*H*)-one

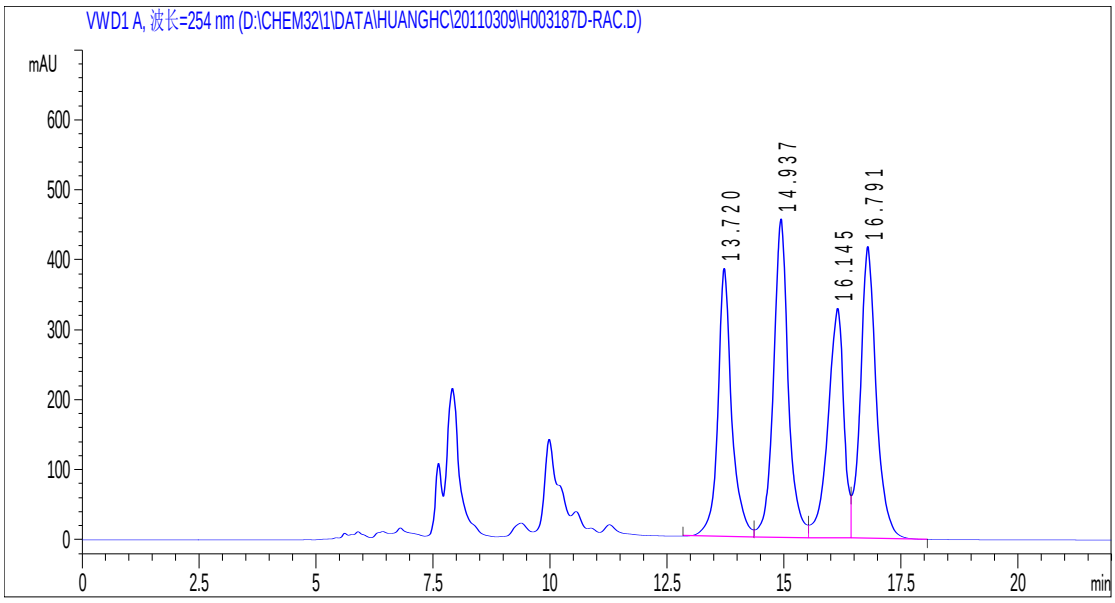


#	Time	Area	Height	Width	Symmetry	Area %
1	8.187	50904.2	1949	0.3862	0.532	49.843
2	10.993	51225	857.6	0.9955	0.731	50.157

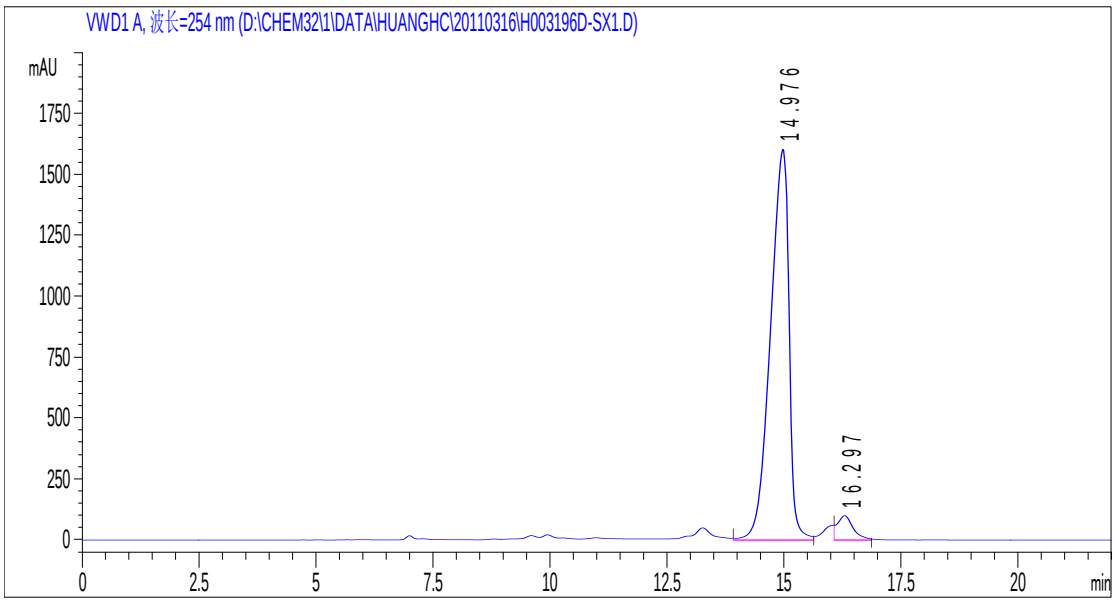


#	Time	Area	Height	Width	Symmetry	Area %
1	8.22	23150.8	944.2	0.3676	0.594	99.517
2	11.041	112.3	3.1	0.6002	0	0.483

7u: (*S*)-5-ethyl-5-((*R*)-3-oxocyclohexyl)-2-phenyloxazol-4(5*H*)-one

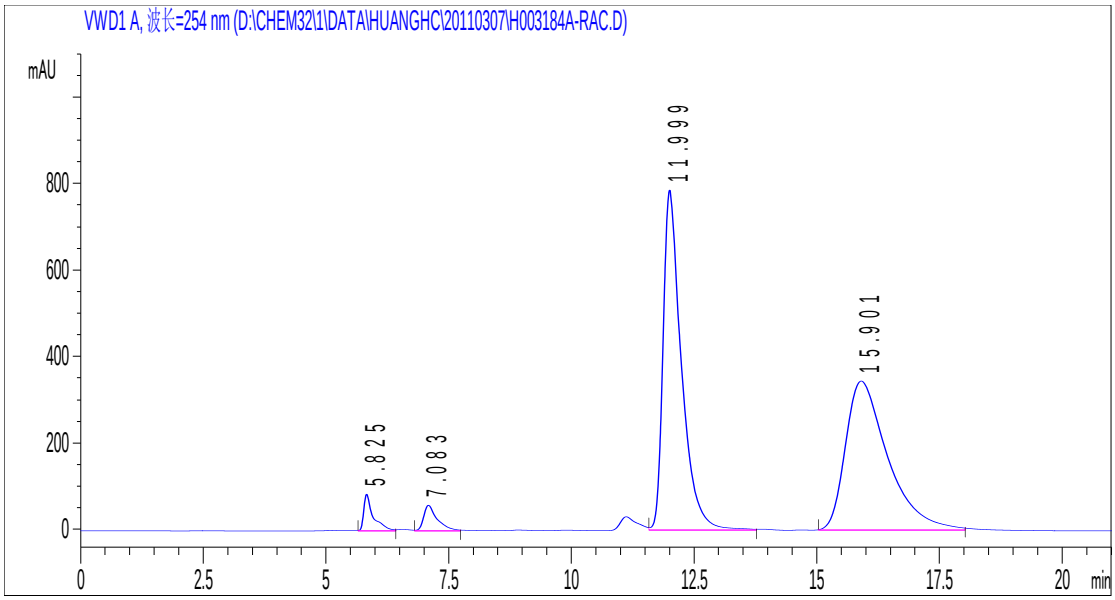


#	Time	Area	Height	Width	Symmetry	Area %
1	13.72	7926.6	383.5	0.3023	0.809	22.237
2	14.937	10070.6	455.4	0.3279	0.994	28.252
3	16.145	7800.4	328.7	0.3598	1.516	21.883
4	16.791	9847.8	417.5	0.3494	0.816	27.627

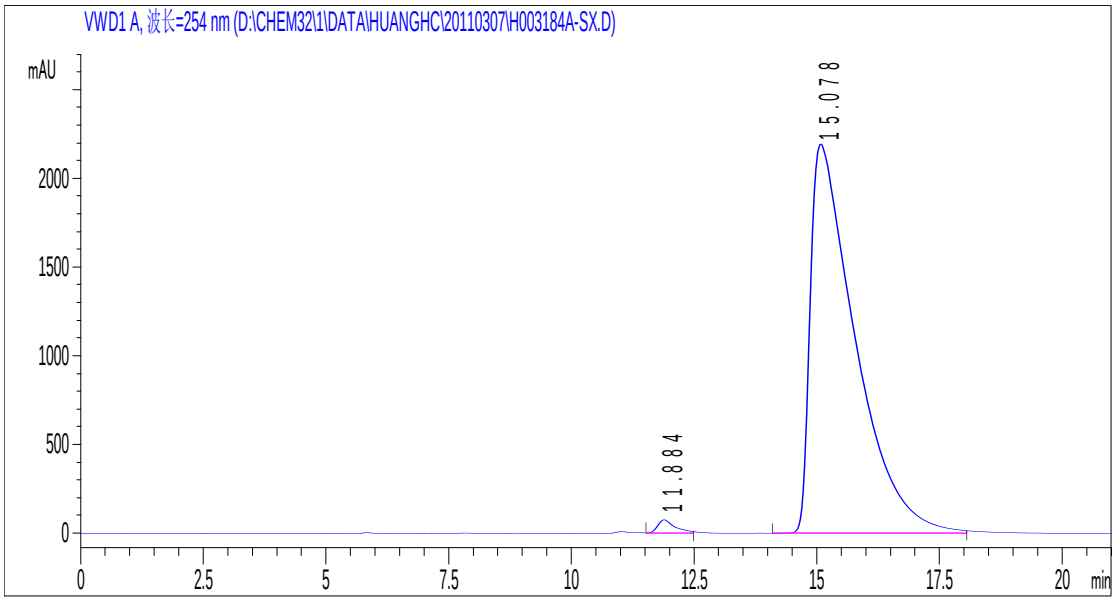


#	Time	Area	Height	Width	Symmetry	Area %
1	14.976	44226.4	1604	0.4353	1.942	94.979
2	16.297	2338	100.4	0.3882	0.787	5.021

8a:(*S*)-5-((*R*)-1-(3-methoxyphenyl)-3-oxobutyl)-2-phenyl-5-propyloxazol-4(5*H*)-one

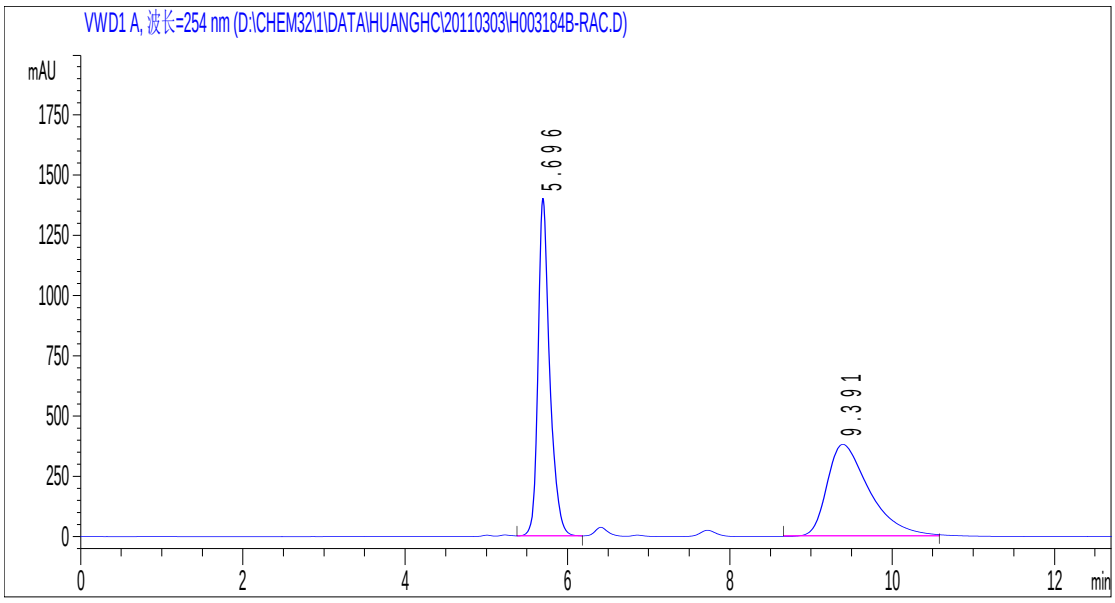


#	Time	Area	Height	Width	Symmetry	Area %
1	5.825	1149.1	84.7	0.1933	0.389	2.620
2	7.083	1146.4	59.3	0.3222	0.534	2.613
3	11.999	20662.3	787.5	0.3789	0.519	47.102
4	15.901	20909.6	346	1.0071	0.576	47.665

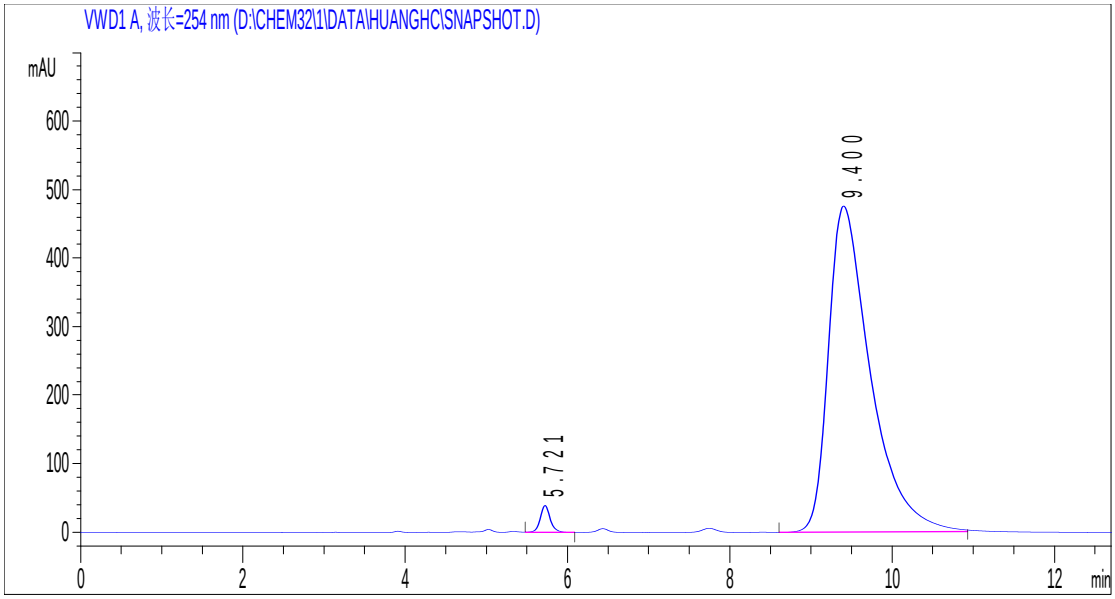


#	Time	Area	Height	Width	Symmetry	Area %
1	11.884	1956.2	76.9	0.4241	0.555	1.381
2	15.078	139693.8	2195.3	1.0605	0.299	98.619

8b:(*S*)-5-((*R*)-1-(4-bromophenyl)-3-oxobutyl)-2-phenyl-5-propyloxazol-4(5*H*)-one

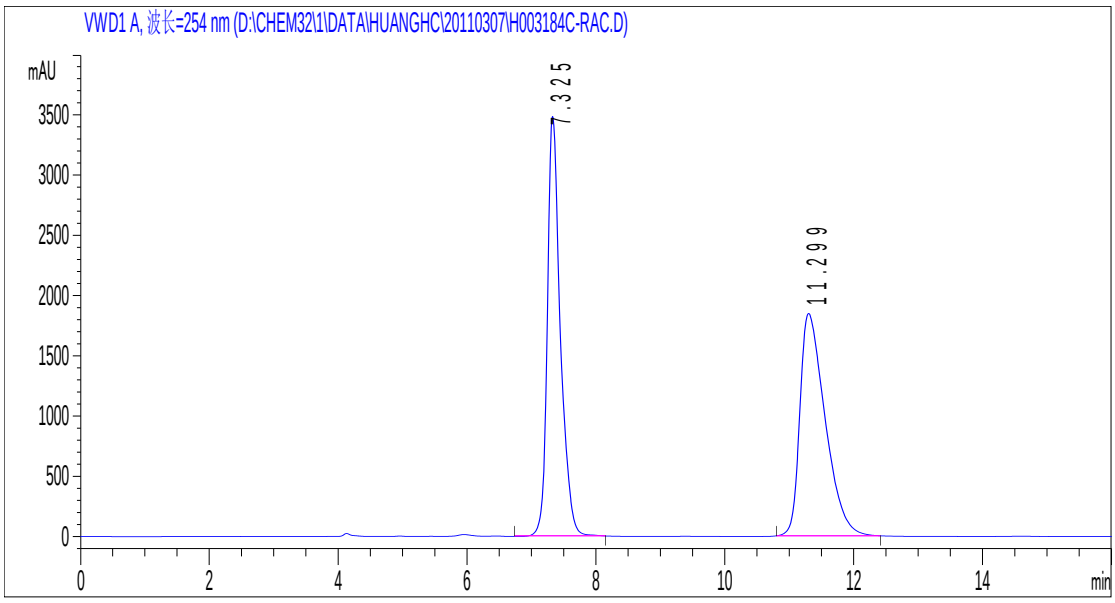


#	Time	Area	Height	Width	Symmetry	Area %
1	5.696	14103.8	1402.2	0.1494	0.697	50.160
2	9.391	14013.7	383.4	0.6091	0.574	49.840

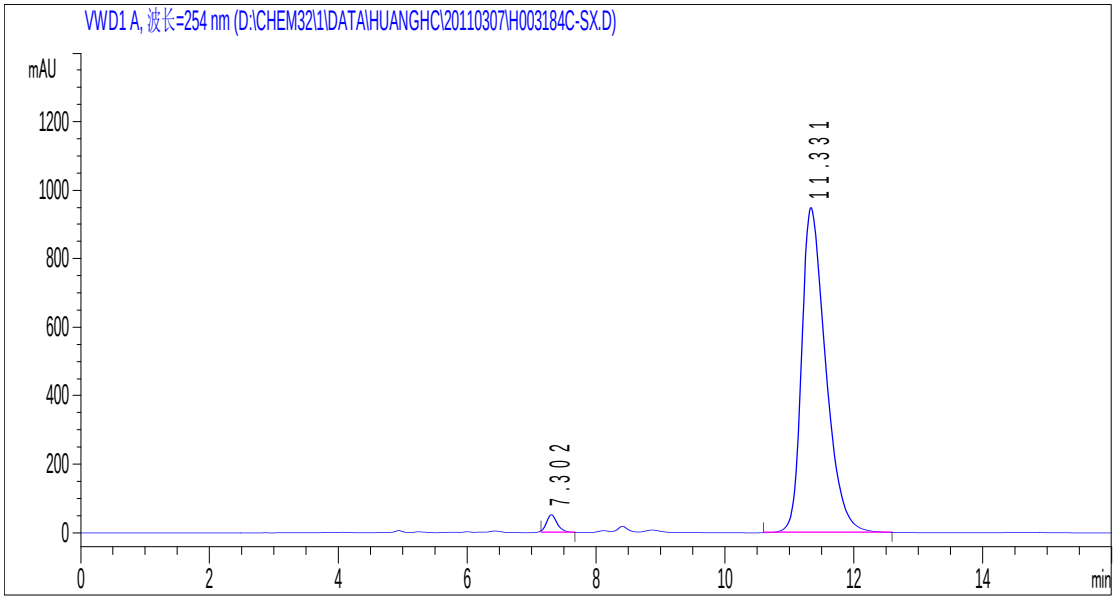


#	Time	Area	Height	Width	Symmetry	Area %
1	5.721	340.7	39.4	0.1329	0.892	1.944
2	9.4	17185.2	476.5	0.6011	0.539	98.056

8c: (*S*)-5-((*R*)-1-(3-nitrophenyl)-3-oxobutyl)-2-phenyl-5-propyloxazol-4(5*H*)-one

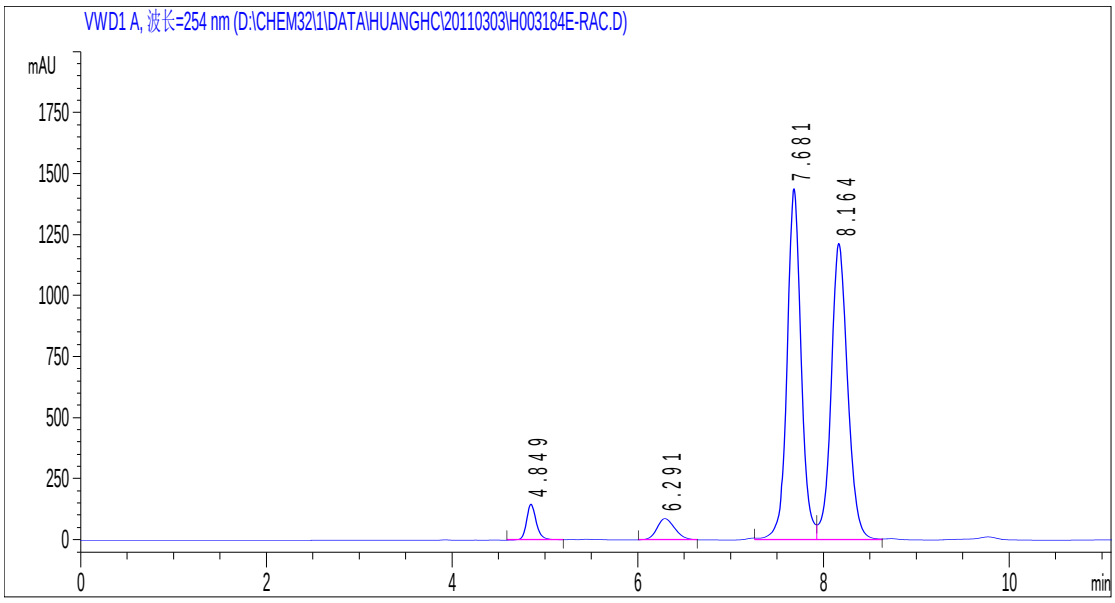


#	Time	Area	Height	Width	Symmetry	Area %
1	7.325	49064.7	3493	0.2341	0.659	49.118
2	11.299	50827.6	1854.1	0.4569	0.53	50.882

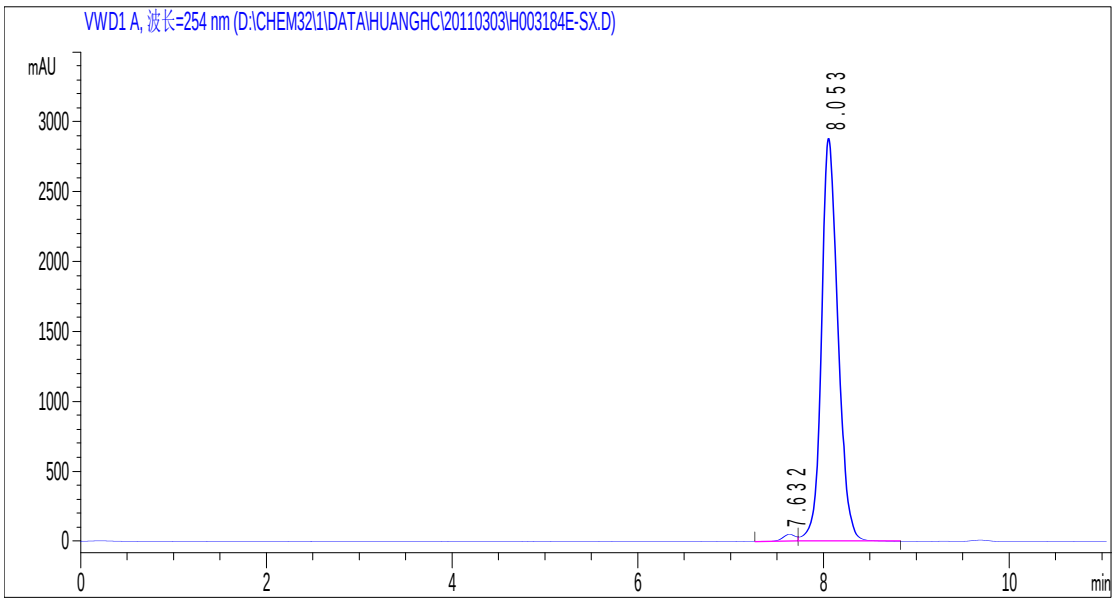


#	Time	Area	Height	Width	Symmetry	Area %
1	7.302	631.6	52.9	0.1989	0.789	2.496
2	11.331	24676.8	950	0.4329	0.616	97.504

8d: (*S*)-5-((*S*)-3-oxo-1-(thiophen-2-yl)butyl)-2-phenyl-5-propyloxazol-4(5*H*)-one

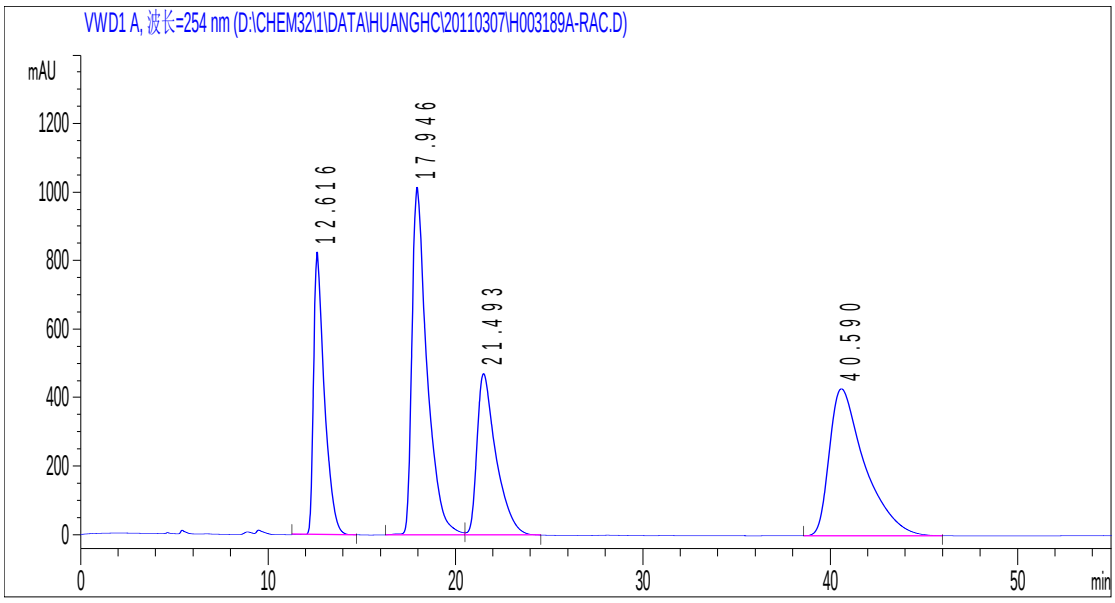


#	Time	Area	Height	Width	Symmetry	Area %
1	4.849	1121.4	148.6	0.1258	0.785	3.431
2	6.291	1227.3	88.9	0.2301	0.782	3.755
3	7.681	15258.9	1441.6	0.1764	0.967	46.681
4	8.164	15079.9	1214.3	0.1886	0.835	46.133

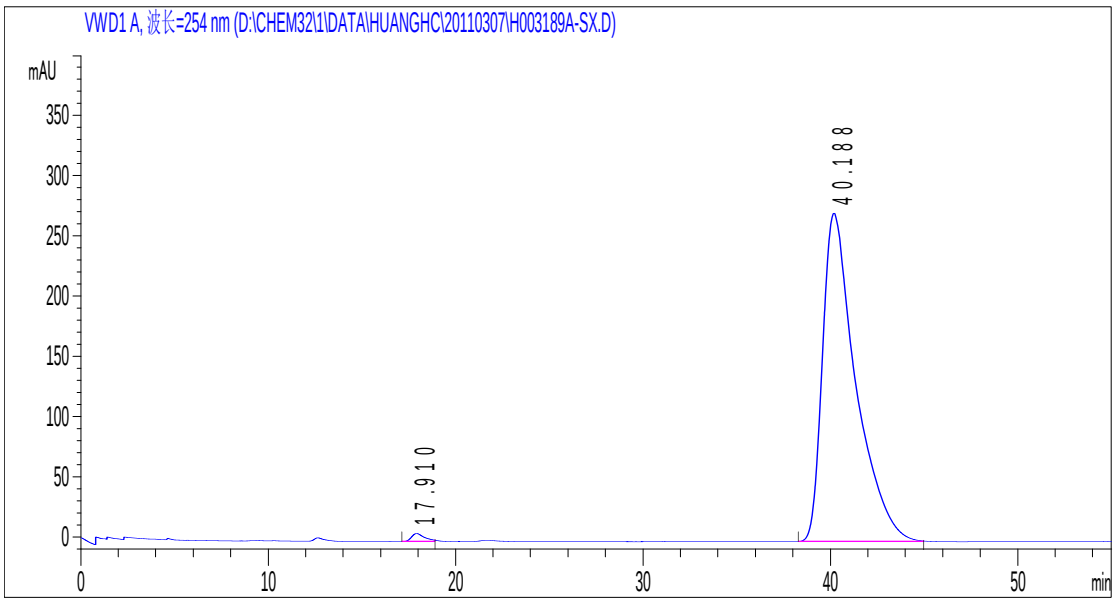


#	Time	Area	Height	Width	Symmetry	Area %
1	7.632	542.7	52.3	0.1731	1.204	1.495
2	8.053	35762.8	2887.4	0.2064	0.737	98.505

8e: (*S*)-5-isopropyl-5-((*R*)-3-oxo-1-phenylbutyl)-2-phenyloxazol-4(5*H*)-one

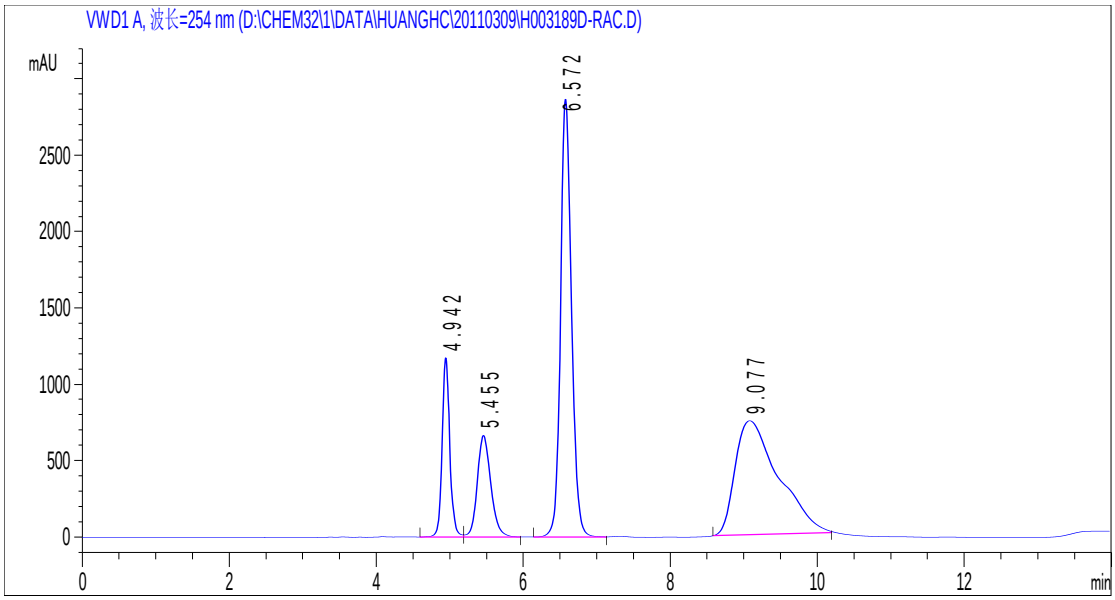


#	Time	Area	Height	Width	Symmetry	Area %
1	12.616	33204.7	825.7	0.5798	0.467	18.476
2	17.946	57018.4	1015.5	0.8181	0.472	31.726
3	21.493	33298.8	471.8	1.0272	0.488	18.528
4	40.59	56199.1	429.4	1.923	0.48	31.270

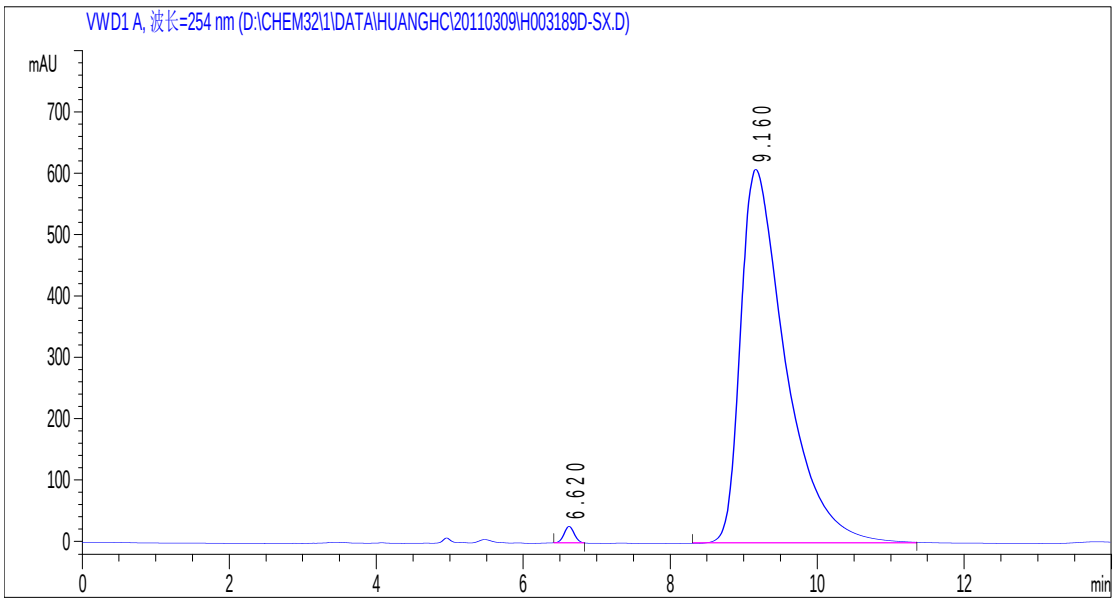


#	Time	Area	Height	Width	Symmetry	Area %
1	17.91	328.3	6.7	0.8167	0.591	0.967
2	40.188	33624.7	273.1	1.8036	0.49	99.033

8f:(*S*)-5-isopropyl-5-((*R*)-1-(3-methoxyphenyl)-3-oxobutyl)-2-phenyloxazol-4(5*H*)-one

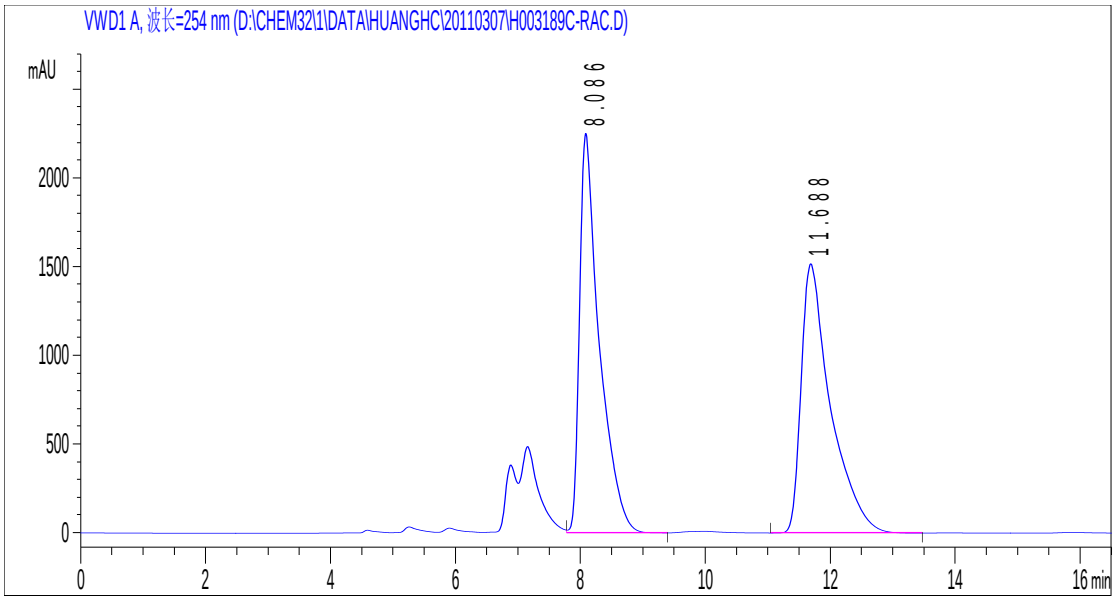


#	Time	Area	Height	Width	Symmetry	Area %
1	4.942	8606.4	1178.1	0.11	0.87	11.075
2	5.455	8715	669.7	0.1999	0.792	11.215
3	6.572	29844.4	2871.6	0.1591	0.799	38.406
4	9.077	30541.9	747.3	0.6812	0.495	39.304

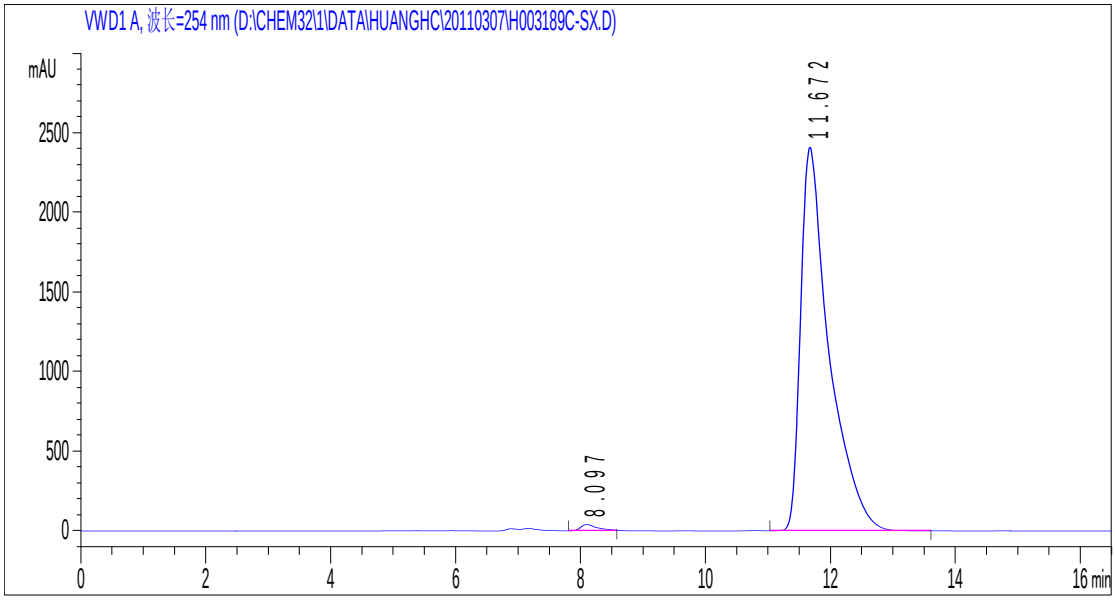


#	Time	Area	Height	Width	Symmetry	Area %
1	6.62	285.7	27.9	0.1705	0.951	1.088
2	9.16	25983.1	608.7	0.7114	0.492	98.912

8g:(*S*)-5-((*R*)-1-(4-chlorophenyl)-3-oxobutyl)-5-isopropyl-2-phenyloxazol-4(5*H*)-one



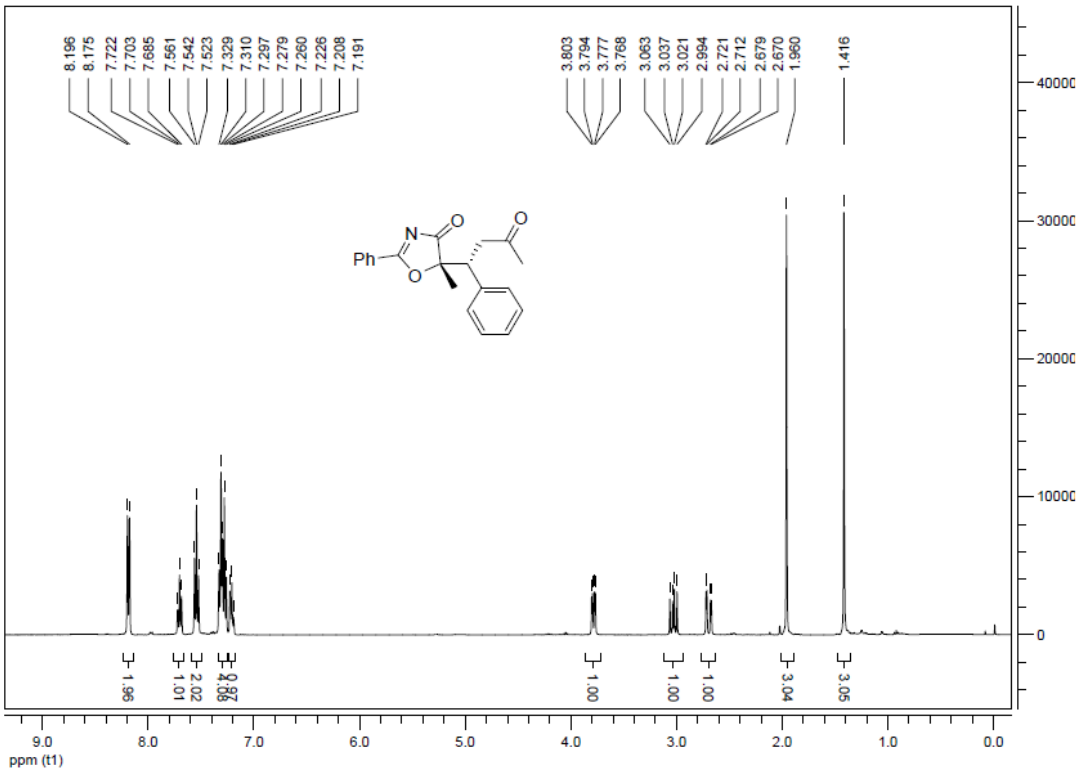
#	Time	Area	Height	Width	Symmetry	Area %
1	8.086	49696.3	2252	0.3128	0.427	50.043
2	11.688	49611.2	1518.4	0.4714	0.448	49.957

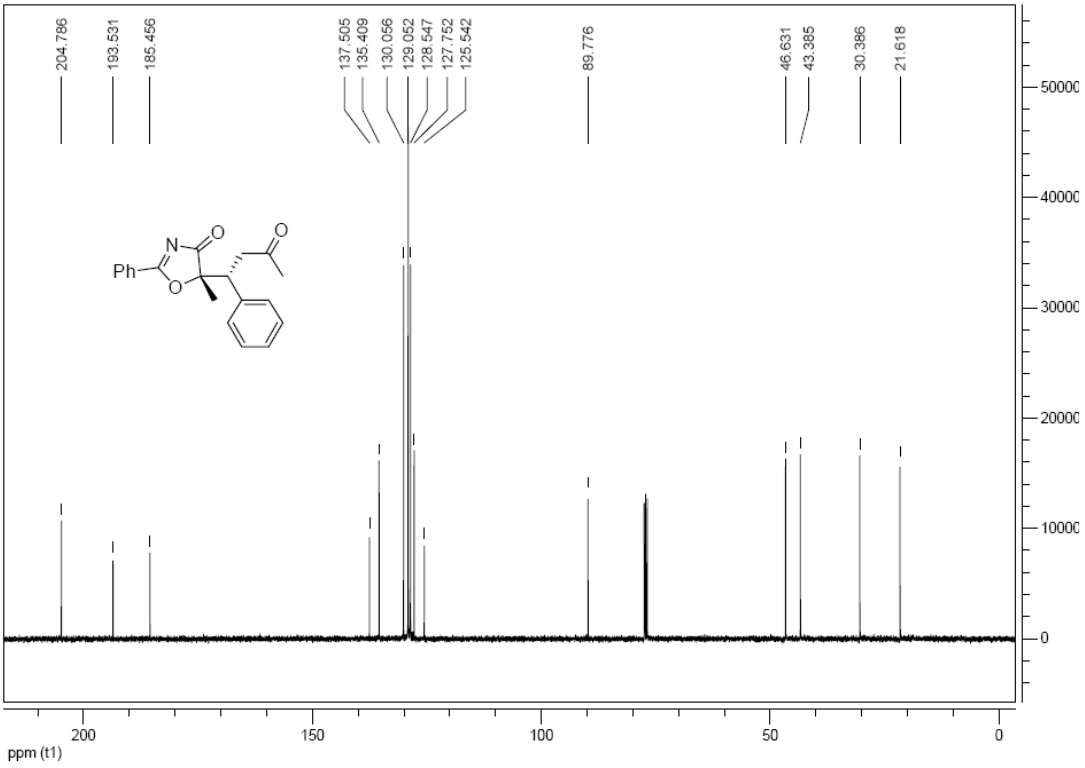


#	Time	Area	Height	Width	Symmetry	Area %
1	8.097	804.4	40.6	0.3301	0.53	1.039
2	11.672	76587.6	2411.7	0.4579	0.446	98.961

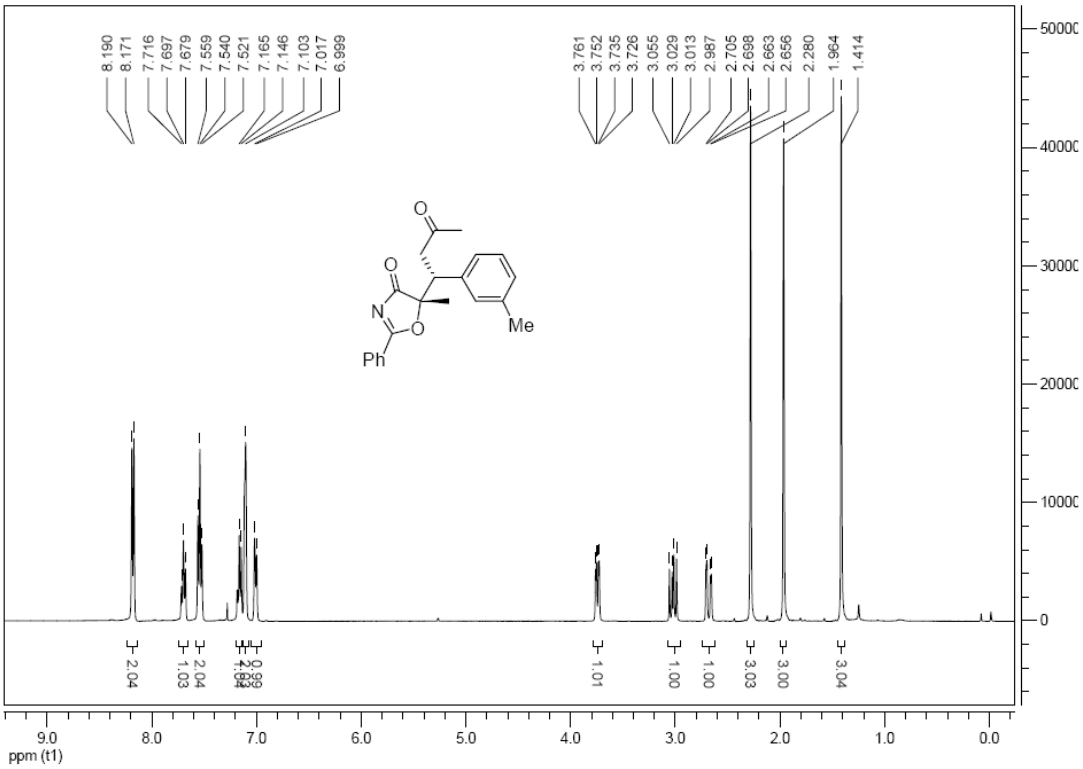
G: NMR Spectra of Michael Addition Products

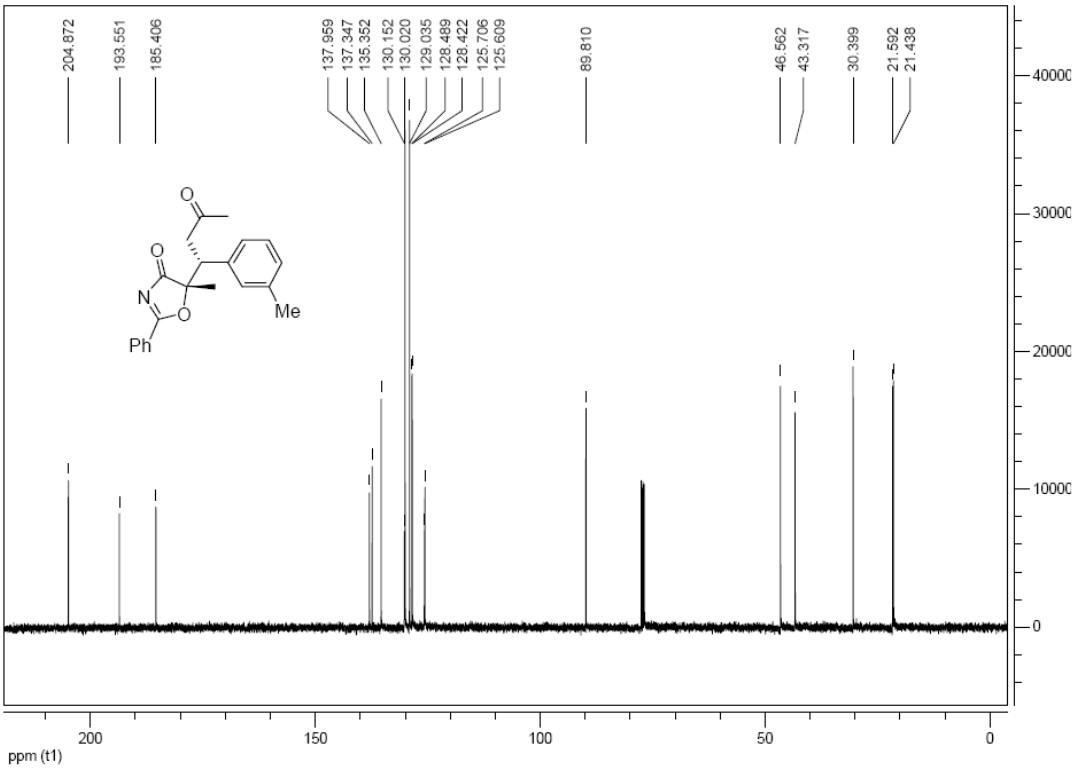
7a:(*S*)-5-methyl-5-((*R*)-3-oxo-1-phenylbutyl)-2-phenyloxazol-4(5*H*)-one



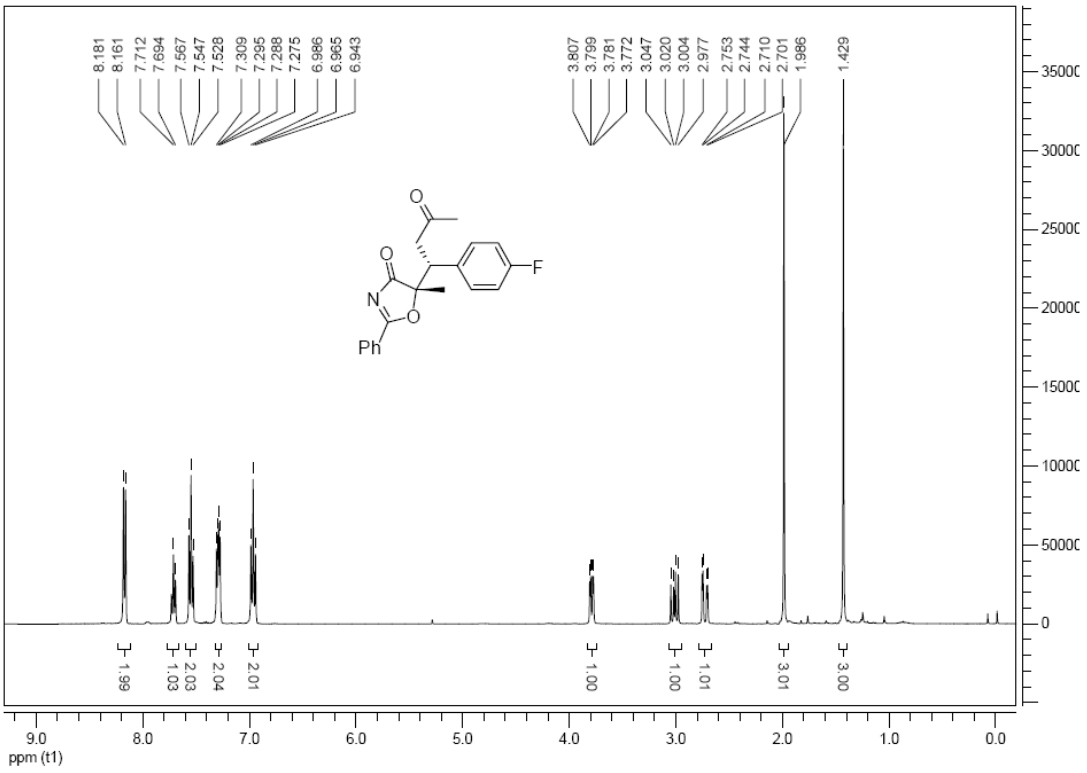


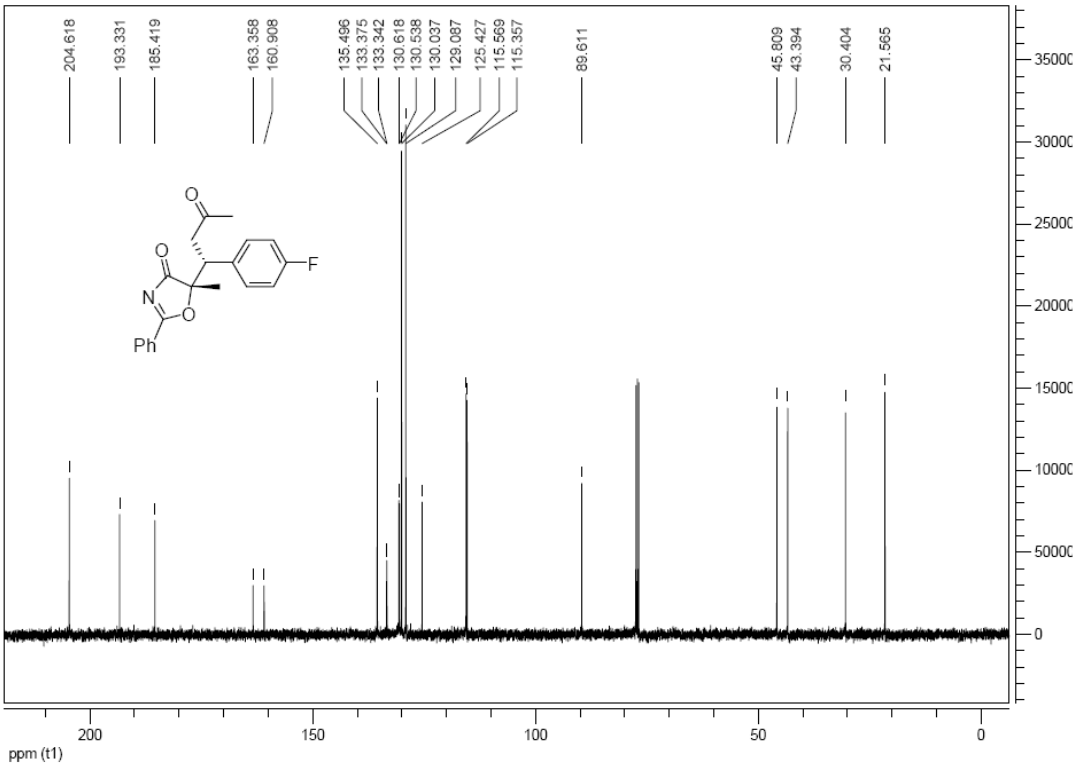
7b:(*S*)-5-methyl-5-((*R*)-3-oxo-1-m-tolylbutyl)-2-phenyloxazol-4(5*H*)-one



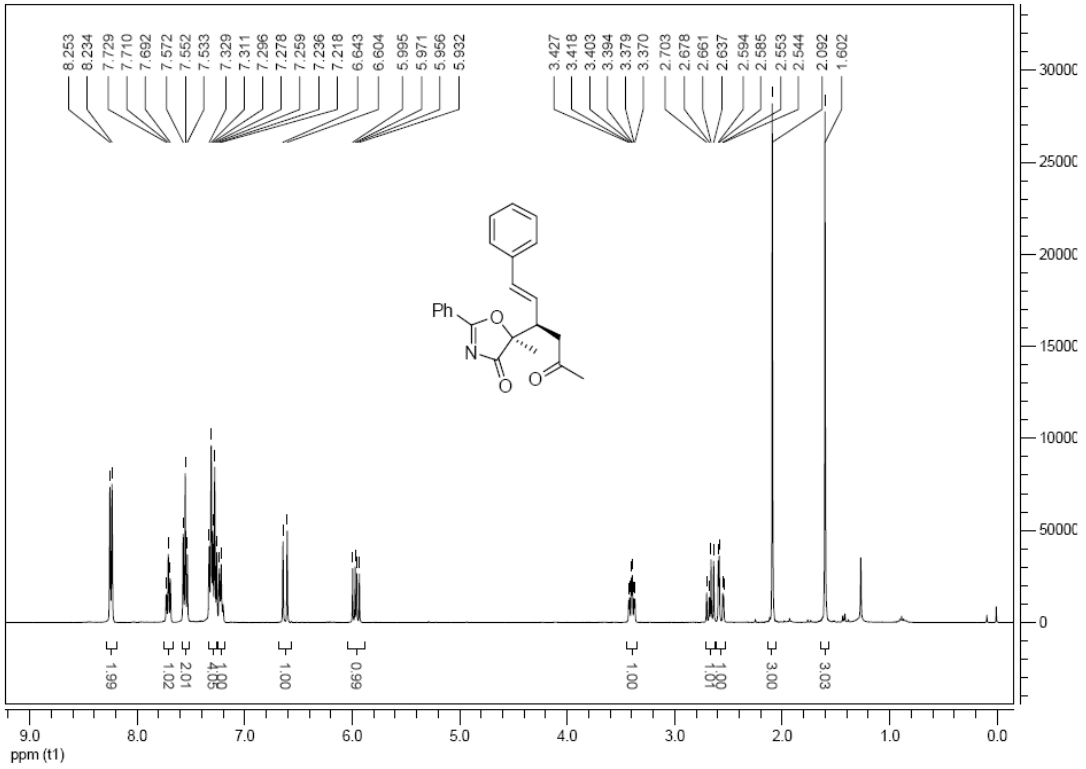


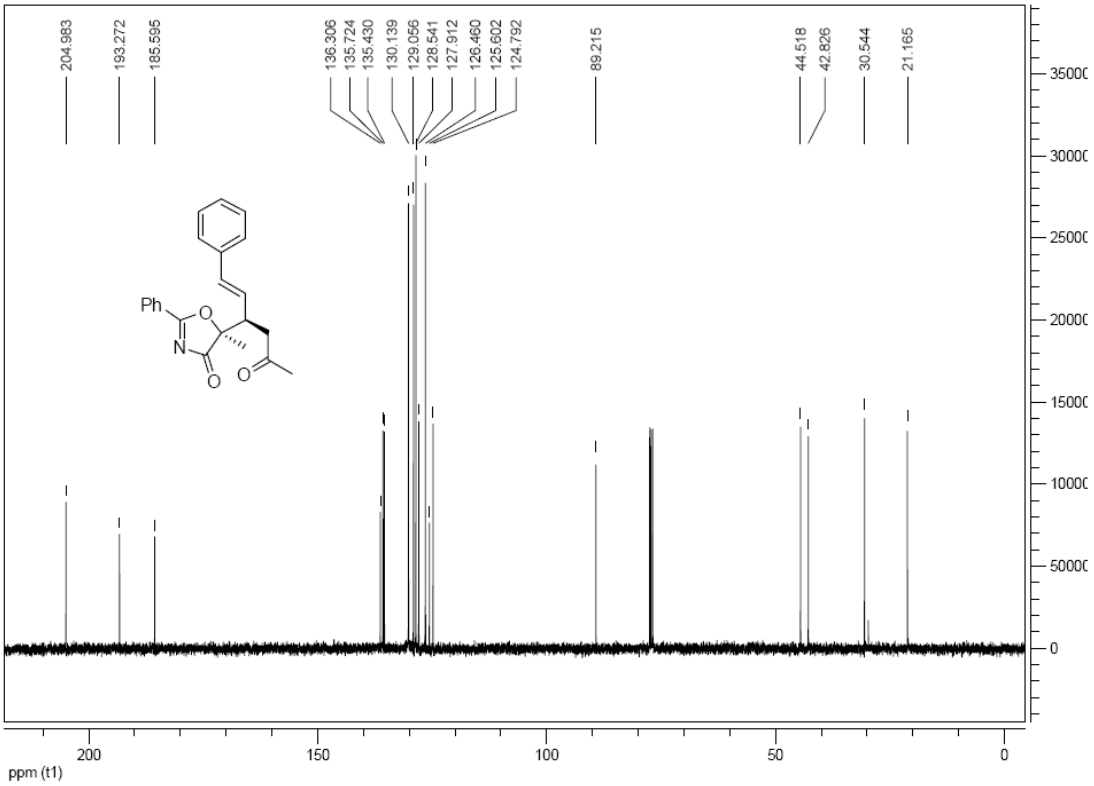
7c:(*S*)-5-((*R*)-1-(4-fluorophenyl)-3-oxobutyl)-5-methyl-2-phenyloxazol-4(5*H*)-one



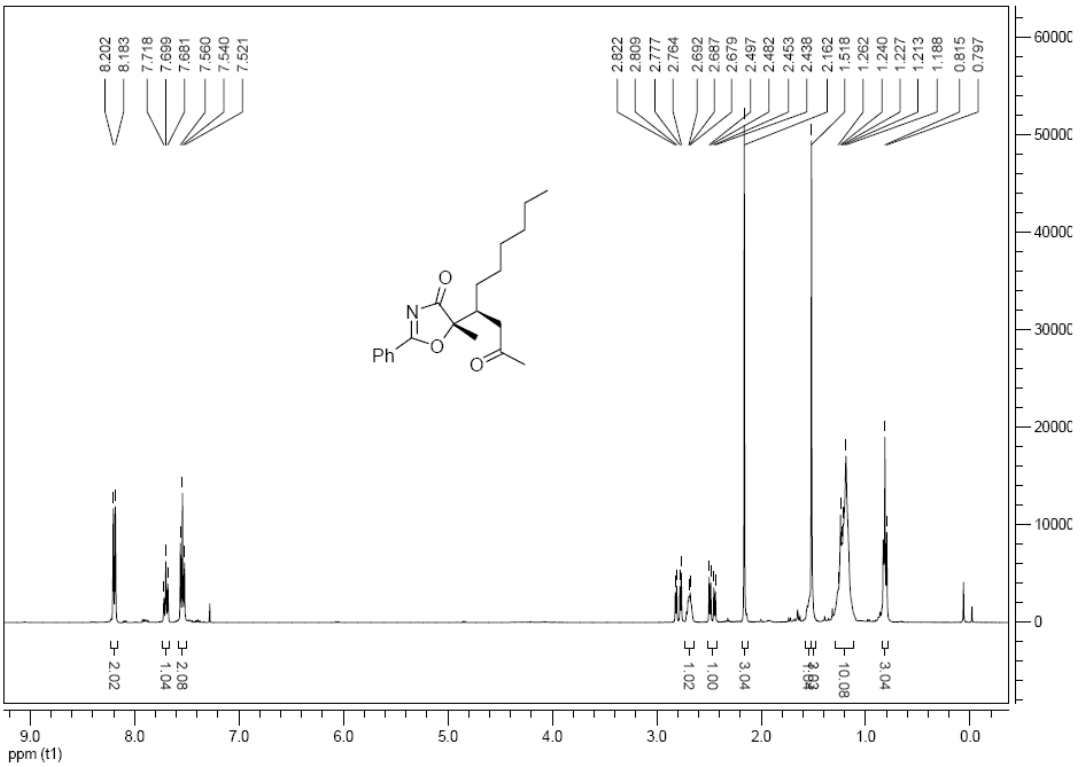


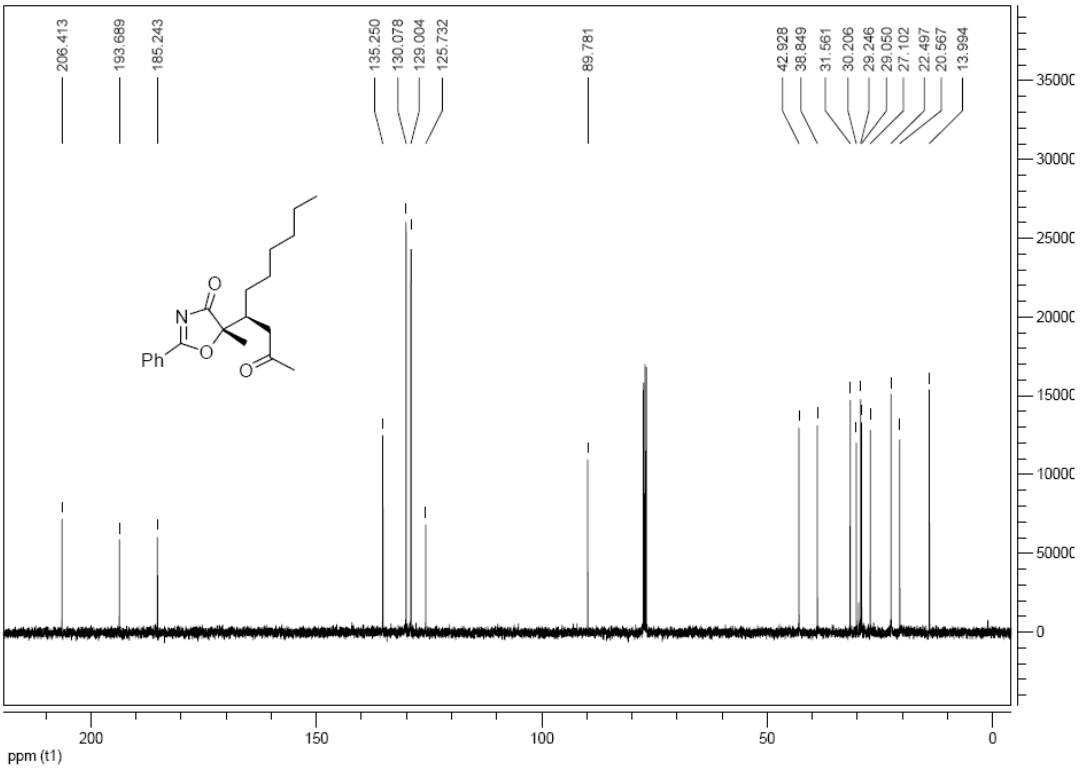
7d:(*S*)-5-methyl-5-((*R*,*E*)-5-oxo-1-phenylhex-1-en-3-yl)-2-phenyloxazol-4(5*H*)-one



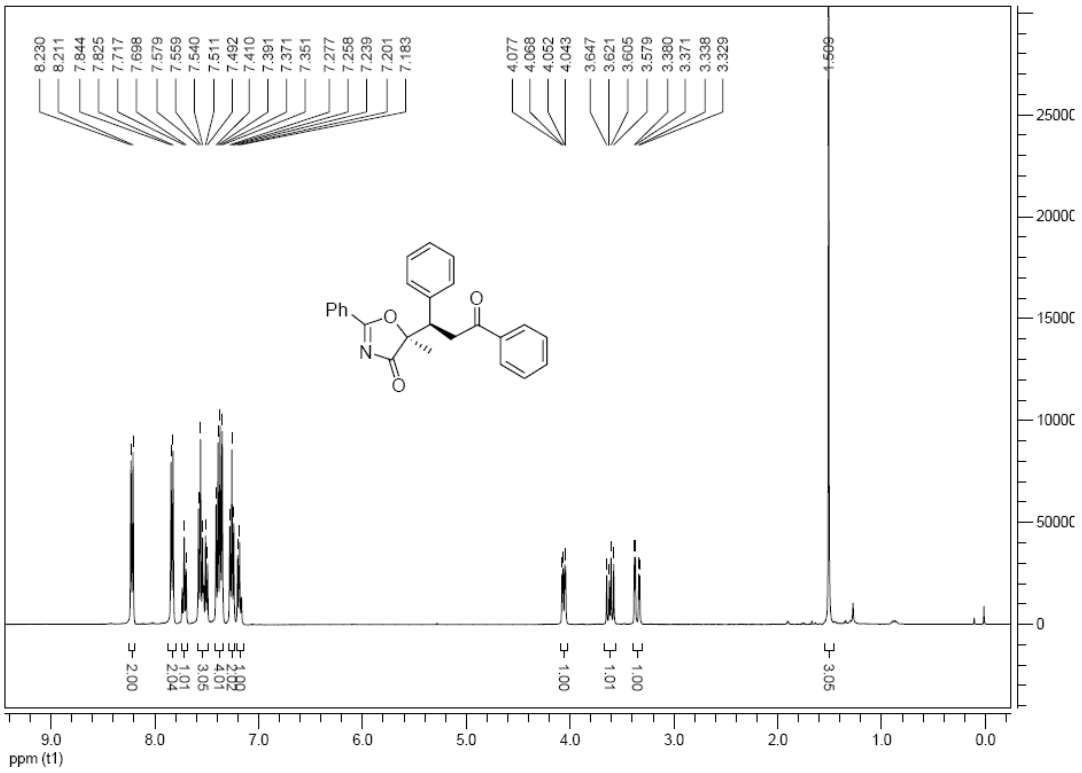


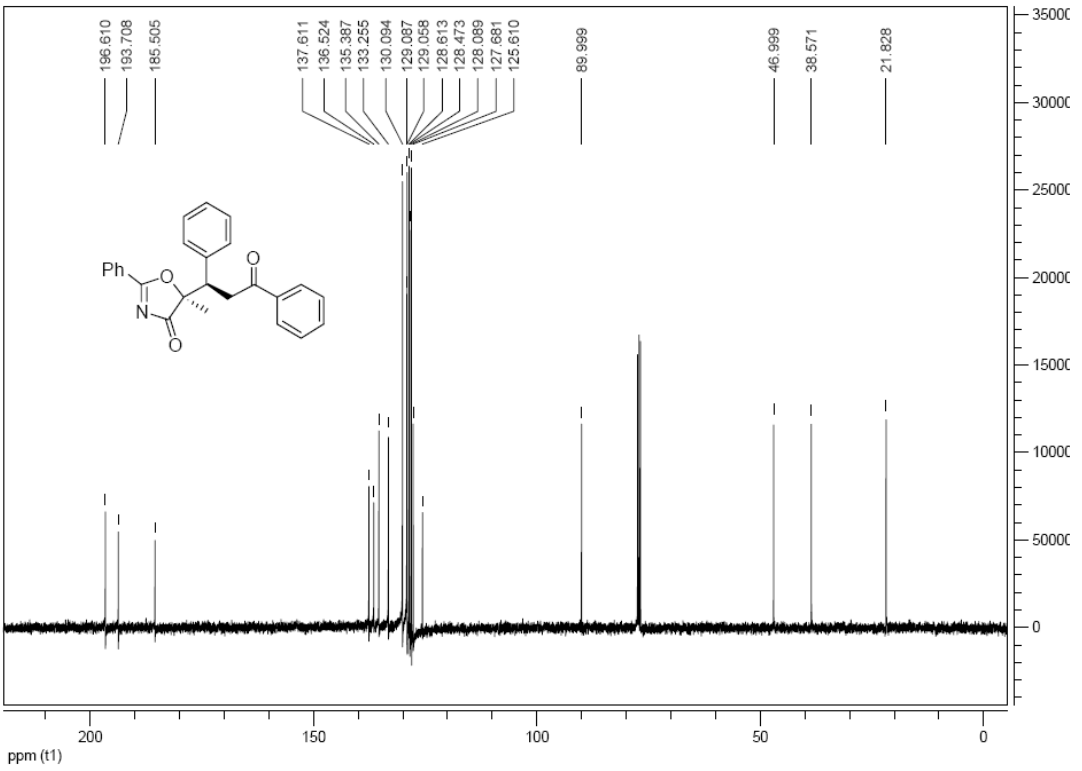
7e:(*S*)-5-methyl-5-((*S*)-2-oxodecan-4-yl)-2-phenyloxazol-4(5*H*)-one



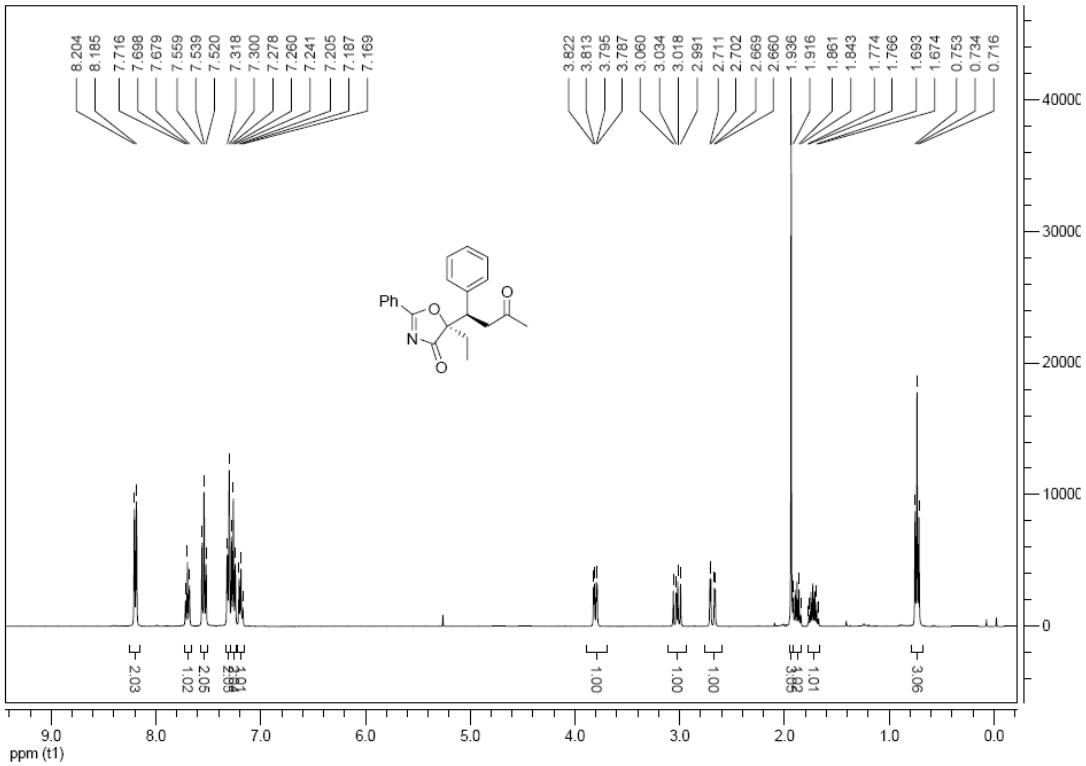


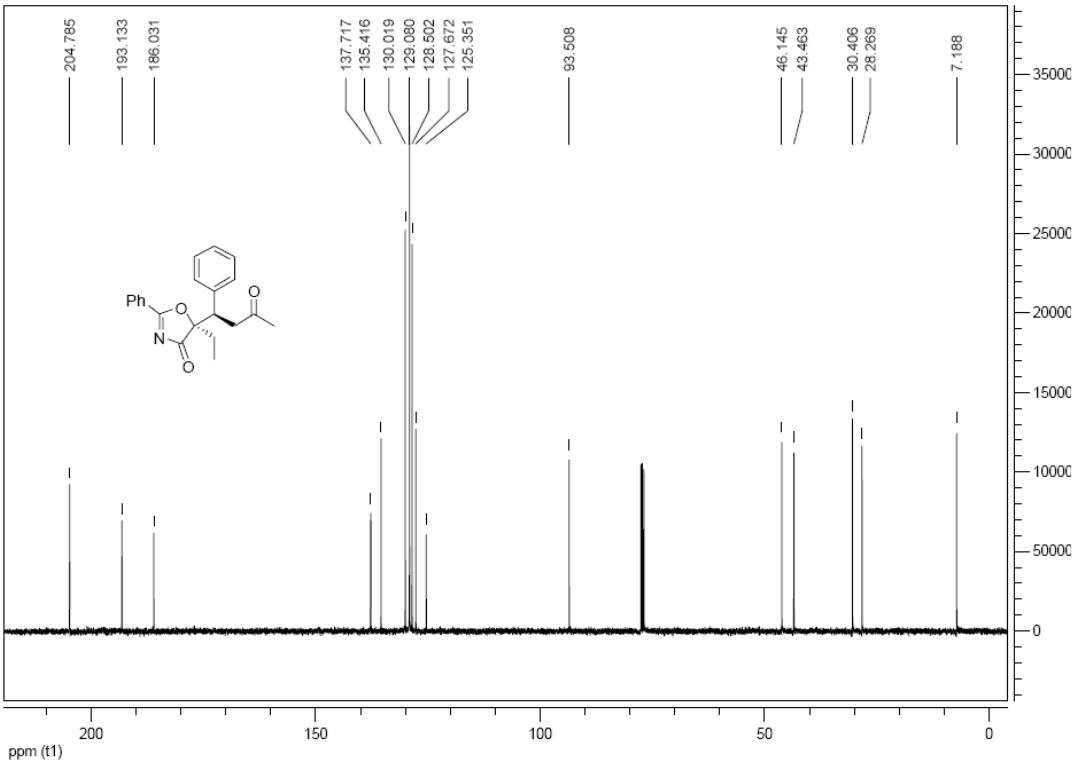
7f: (*S*)-5-methyl-5-((*R*)-3-oxo-1,3-diphenylpropyl)-2-phenyloxazol-4(5*H*)-one



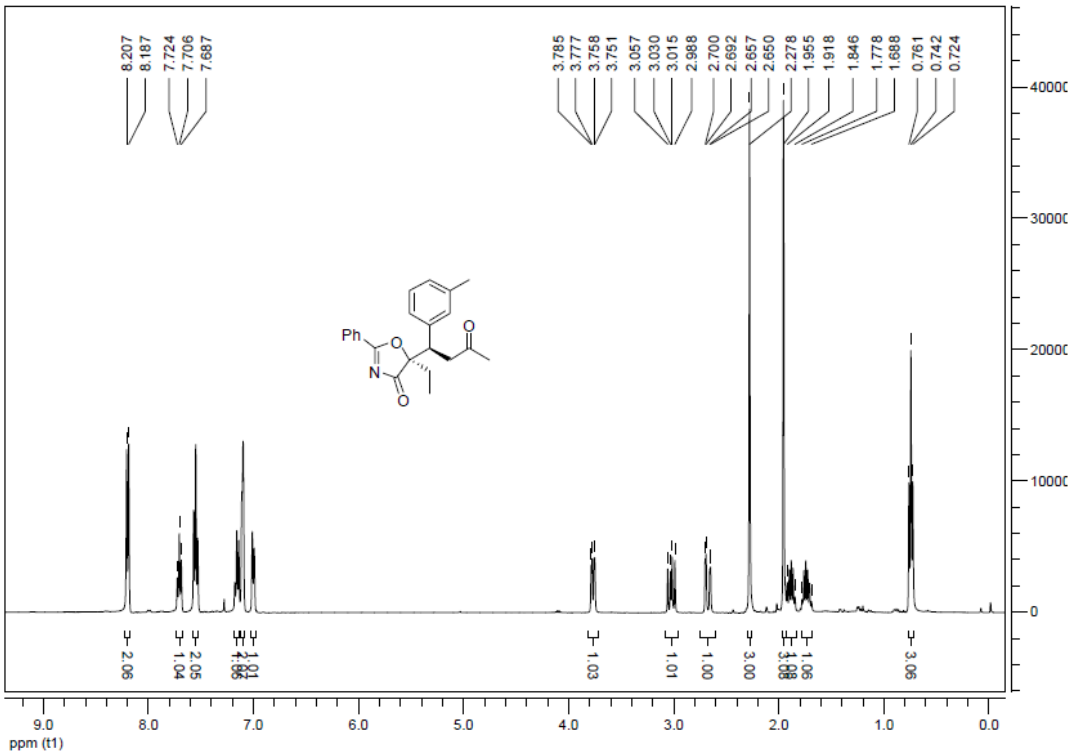


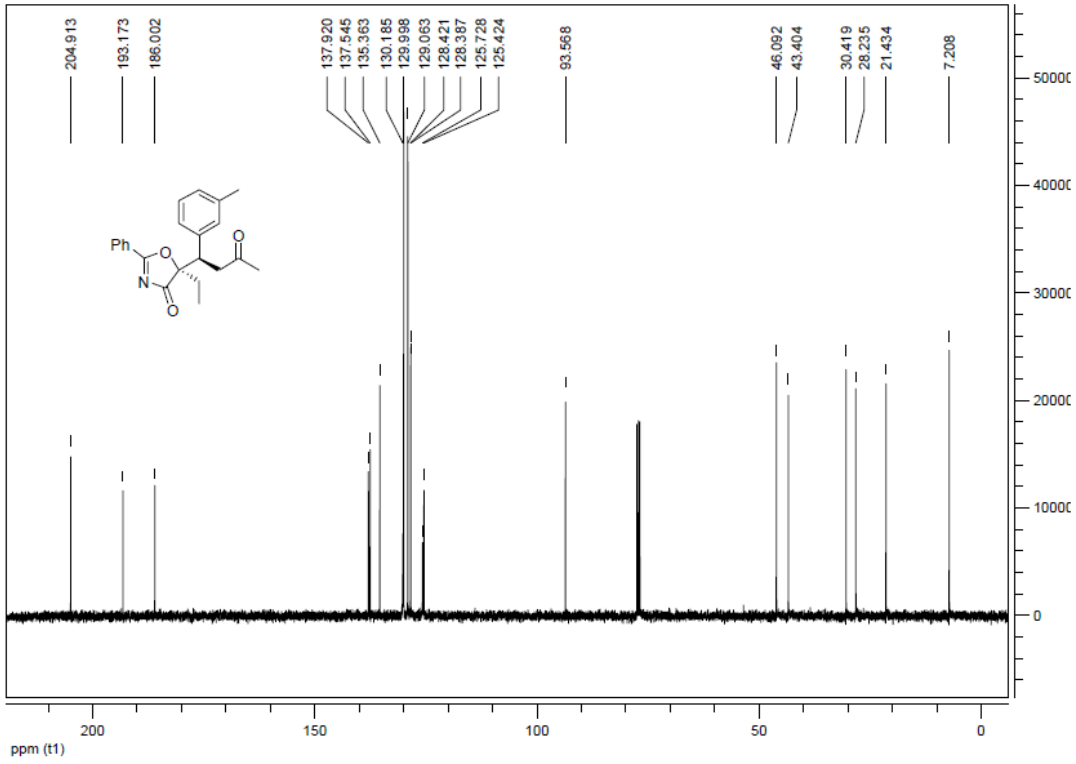
7g: (*S*)-5-ethyl-5-((*R*)-3-oxo-1-phenylbutyl)-2-phenyloxazol-4(5*H*)-one



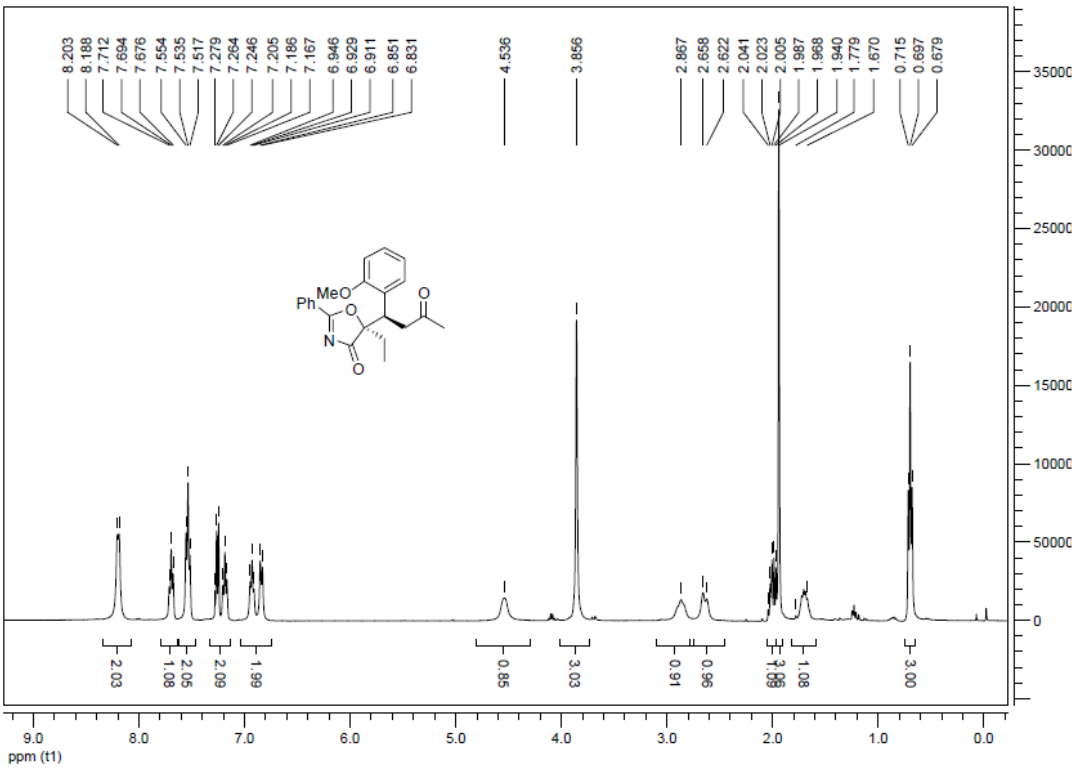


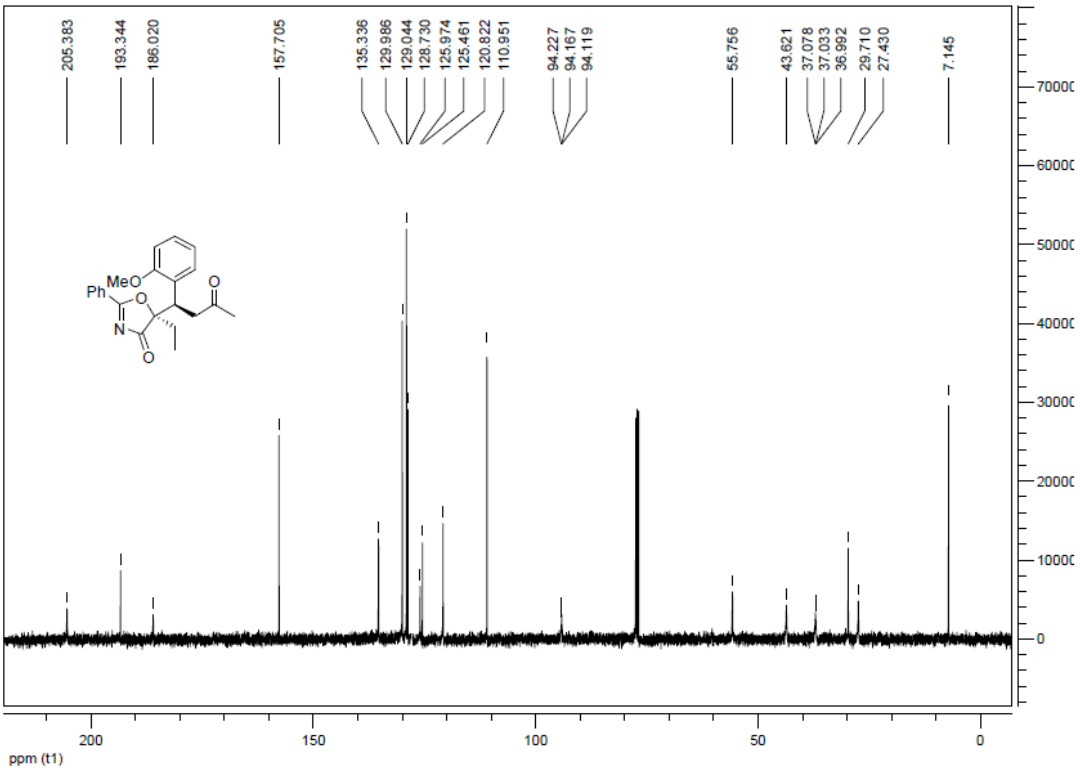
7h: (*S*)-5-ethyl-5-((*R*)-3-oxo-1-m-tolylbutyl)-2-phenyloxazol-4(5*H*)-one



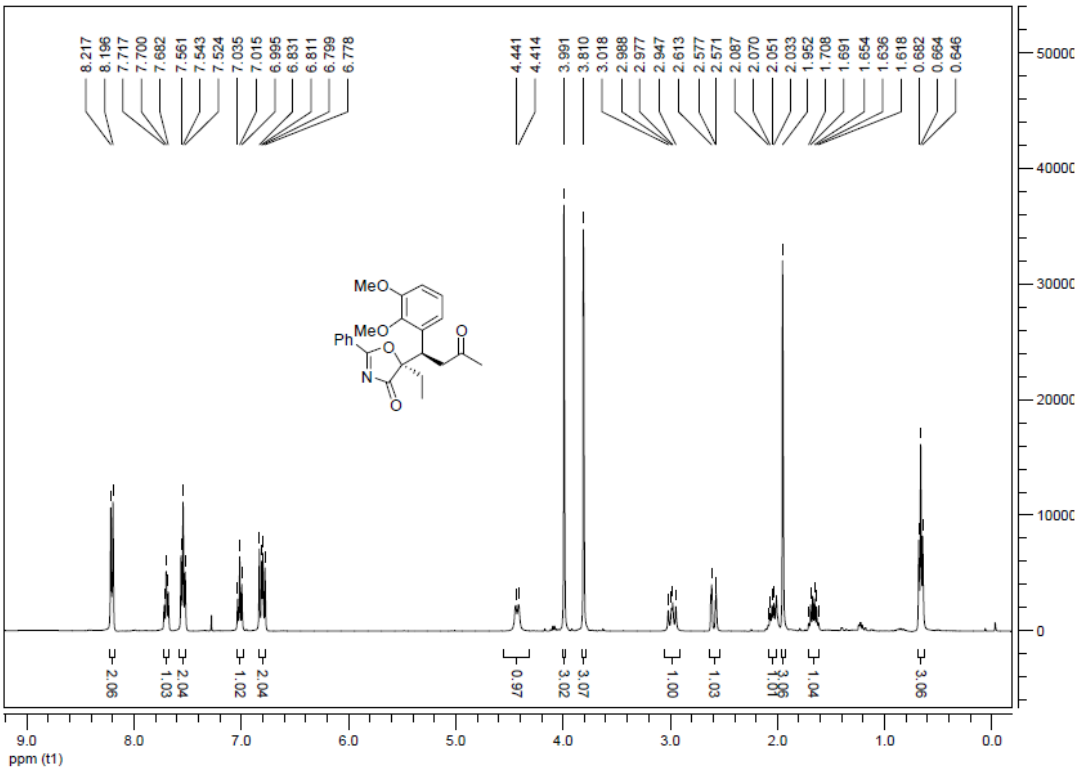


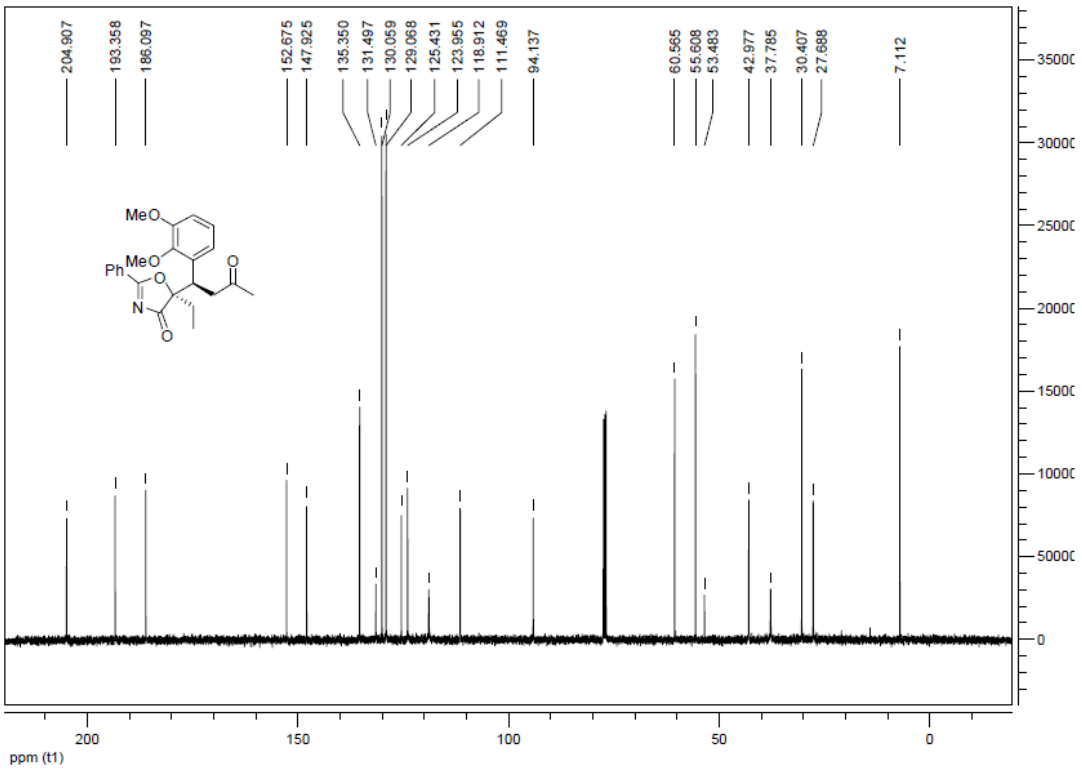
7i: (*S*)-5-ethyl-5-((*R*)-1-(2-methoxyphenyl)-3-oxobutyl)-2-phenyloxazol-4(5*H*)-one



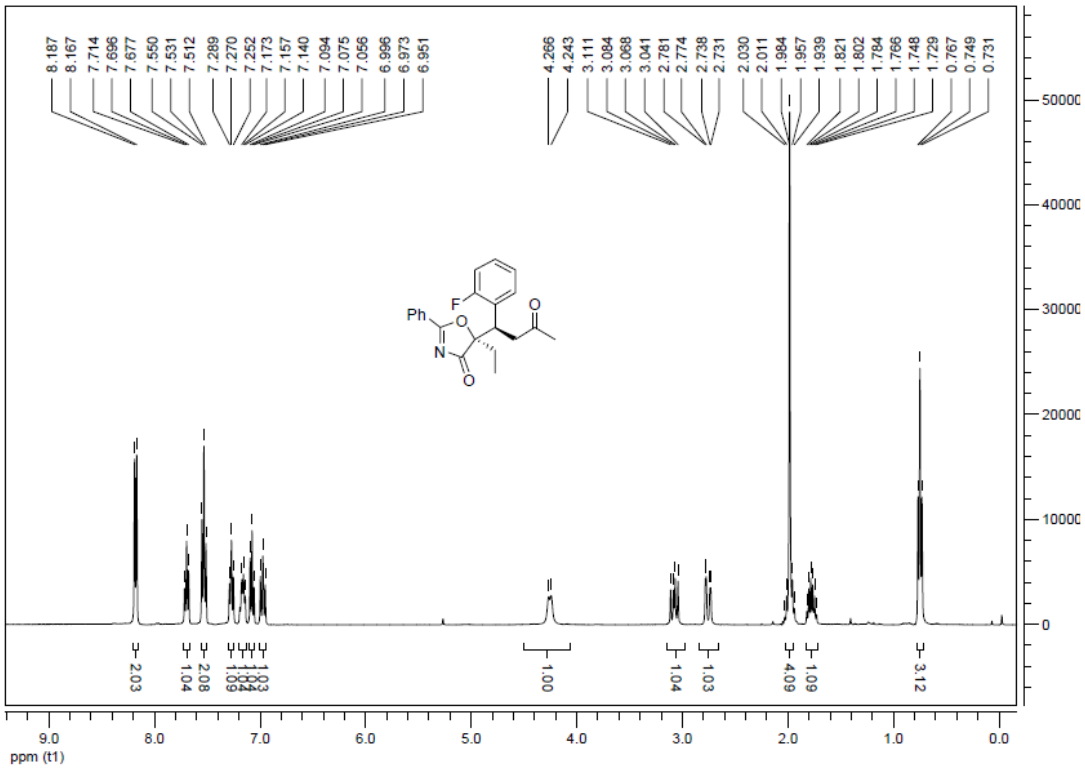


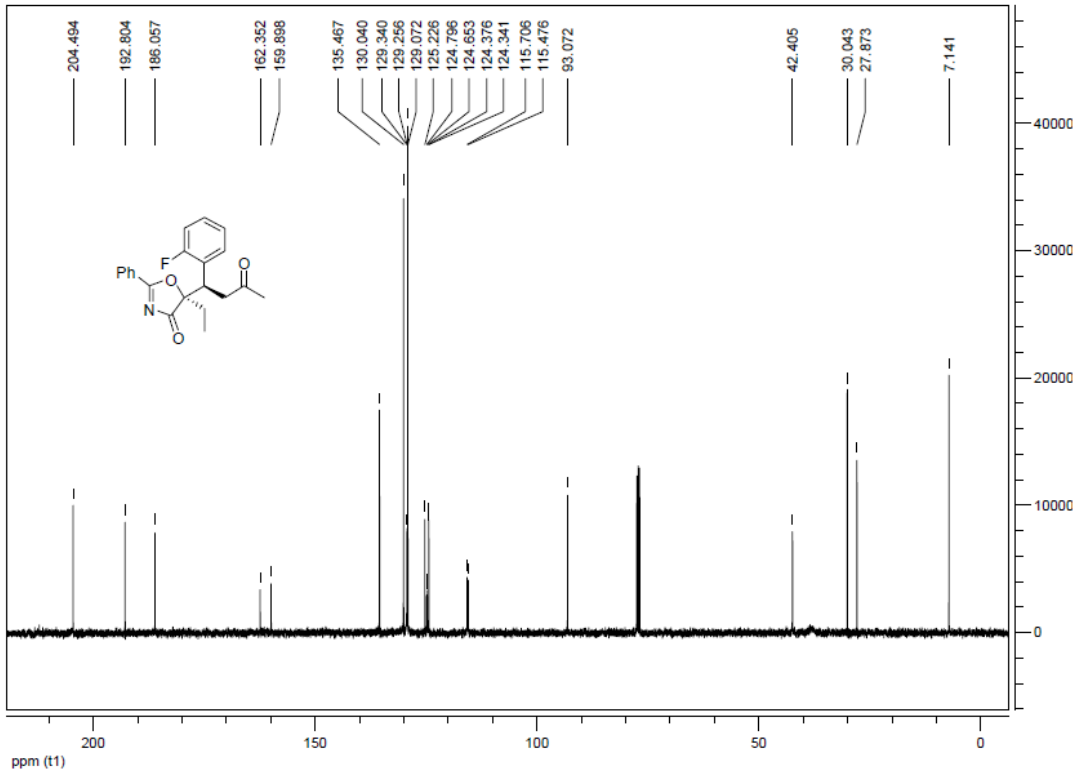
7j:(*S*)-5-((*R*)-1-(2,3-dimethoxyphenyl)-3-oxobutyl)-5-ethyl-2-phenyloxazol-4(5*H*)-one



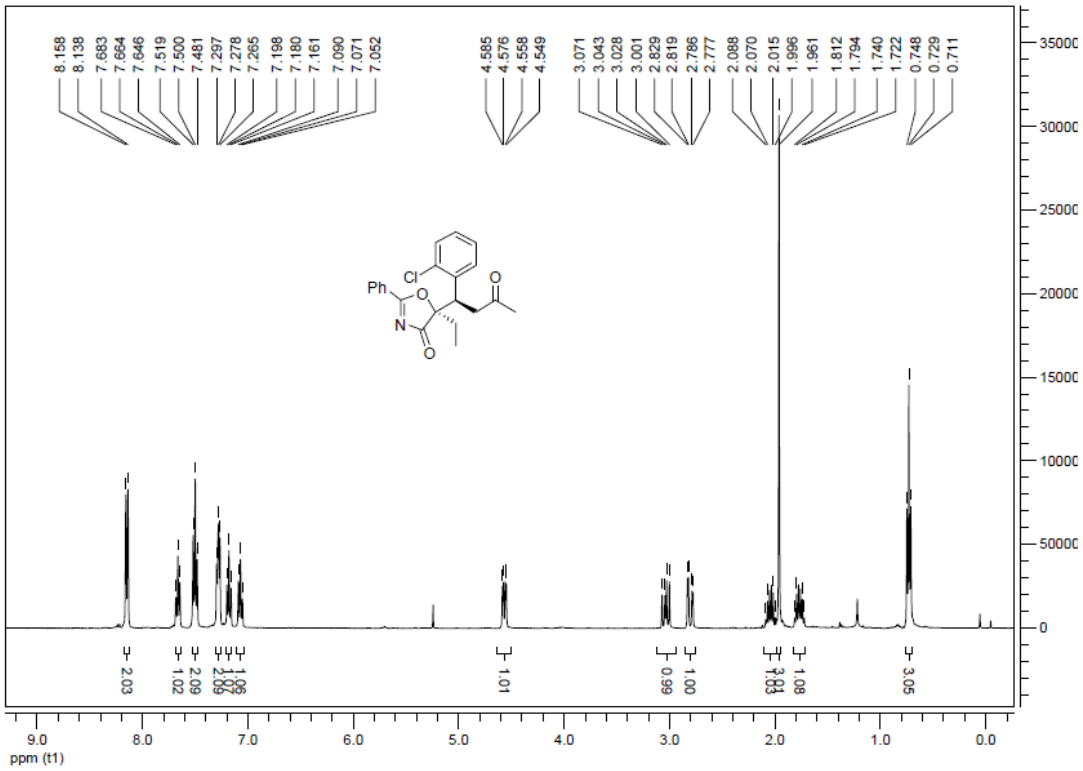


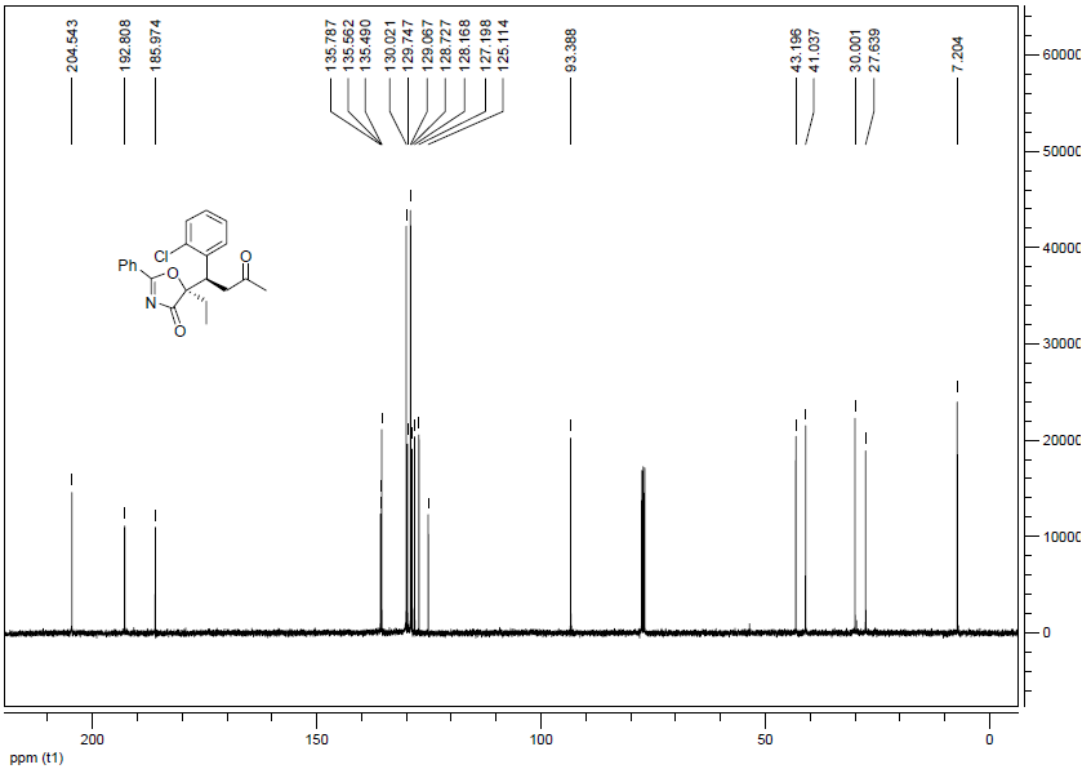
7k: (*S*)-5-ethyl-5-((*R*)-1-(2-fluorophenyl)-3-oxobutyl)-2-phenyloxazol-4(5*H*)-one



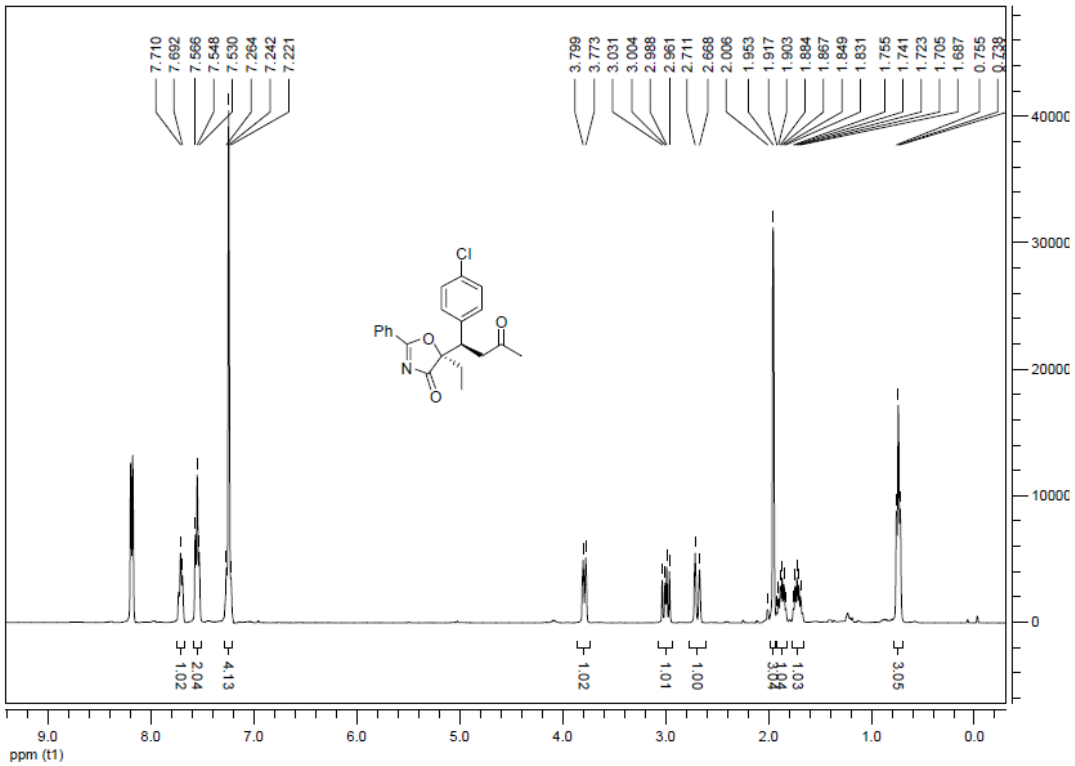


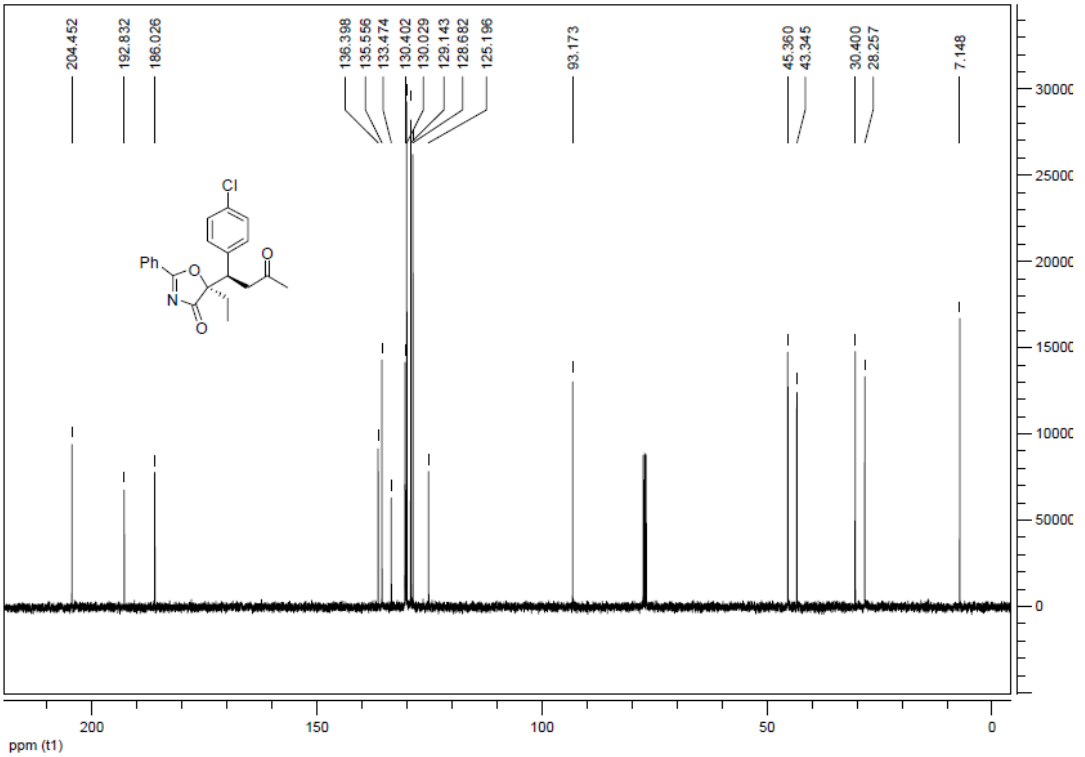
7l: (*S*)-5-((*R*)-1-(2-chlorophenyl)-3-oxobutyl)-5-ethyl-2-phenyloxazol-4(5*H*)-one



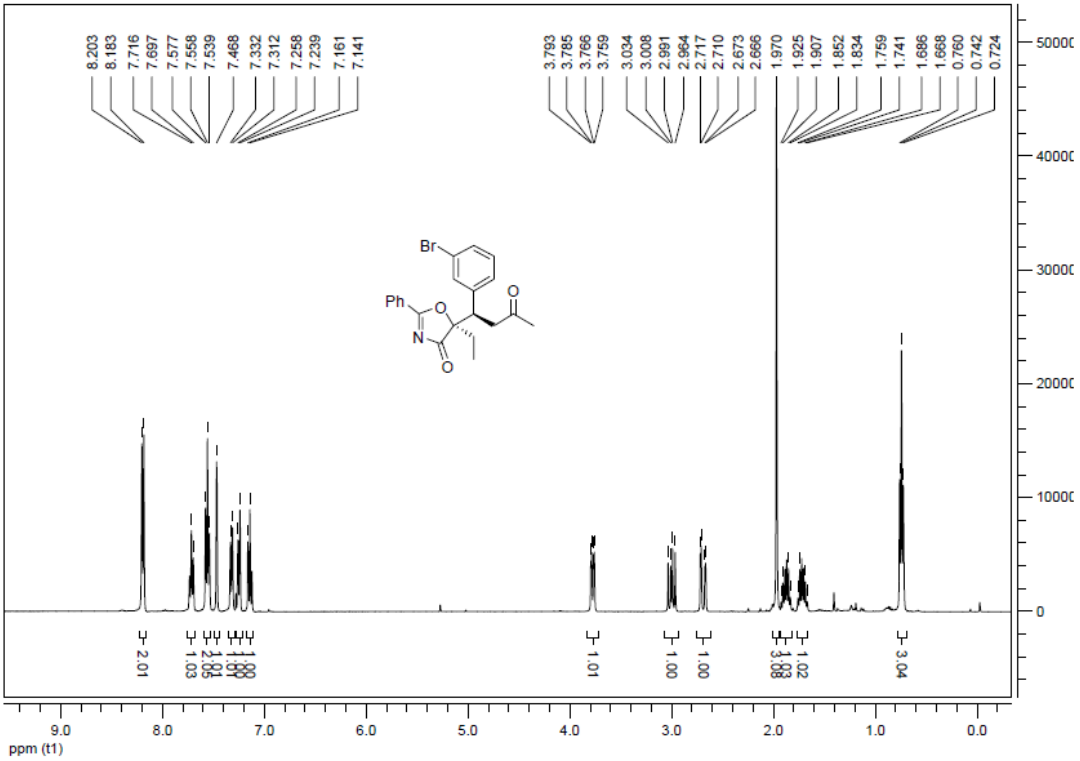


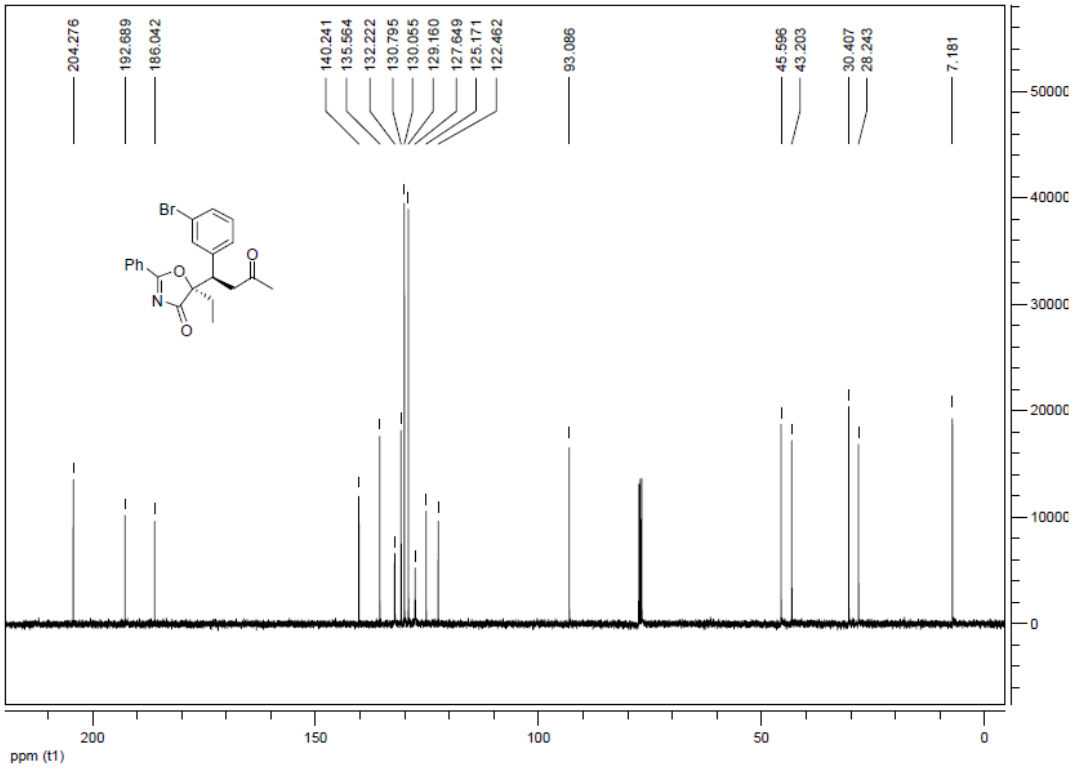
7m: (*S*)-5-((*R*)-1-(4-chlorophenyl)-3-oxobutyl)-5-ethyl-2-phenyloxazol-4(5*H*)-one



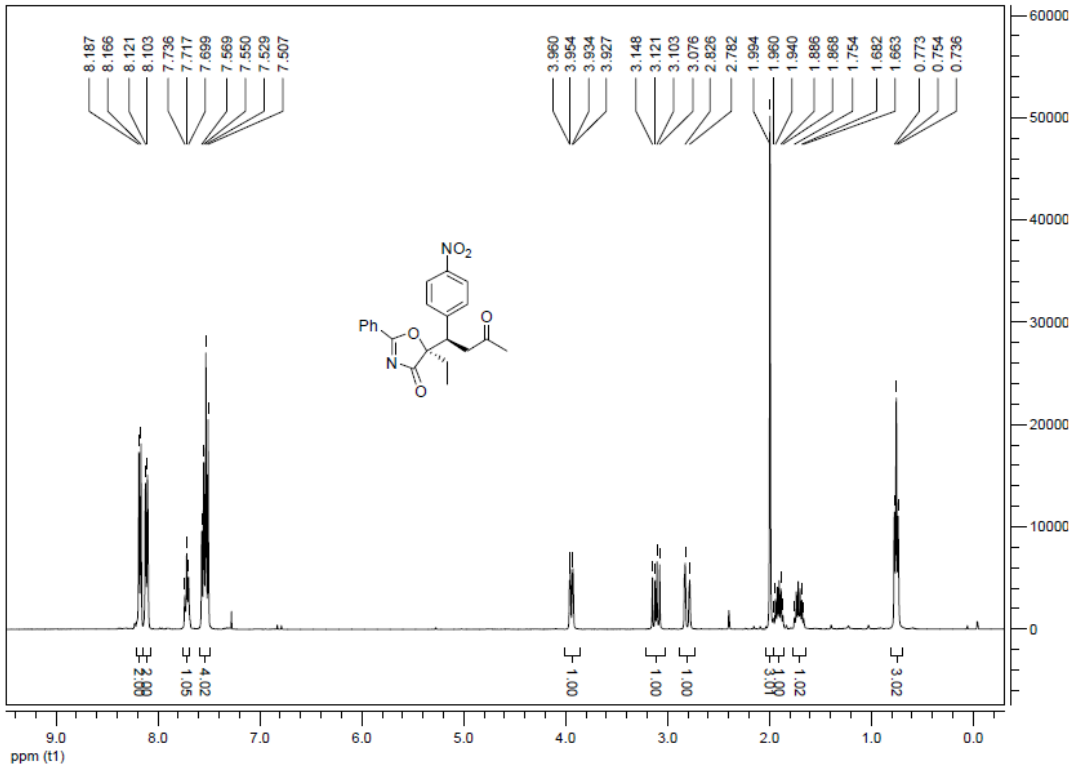


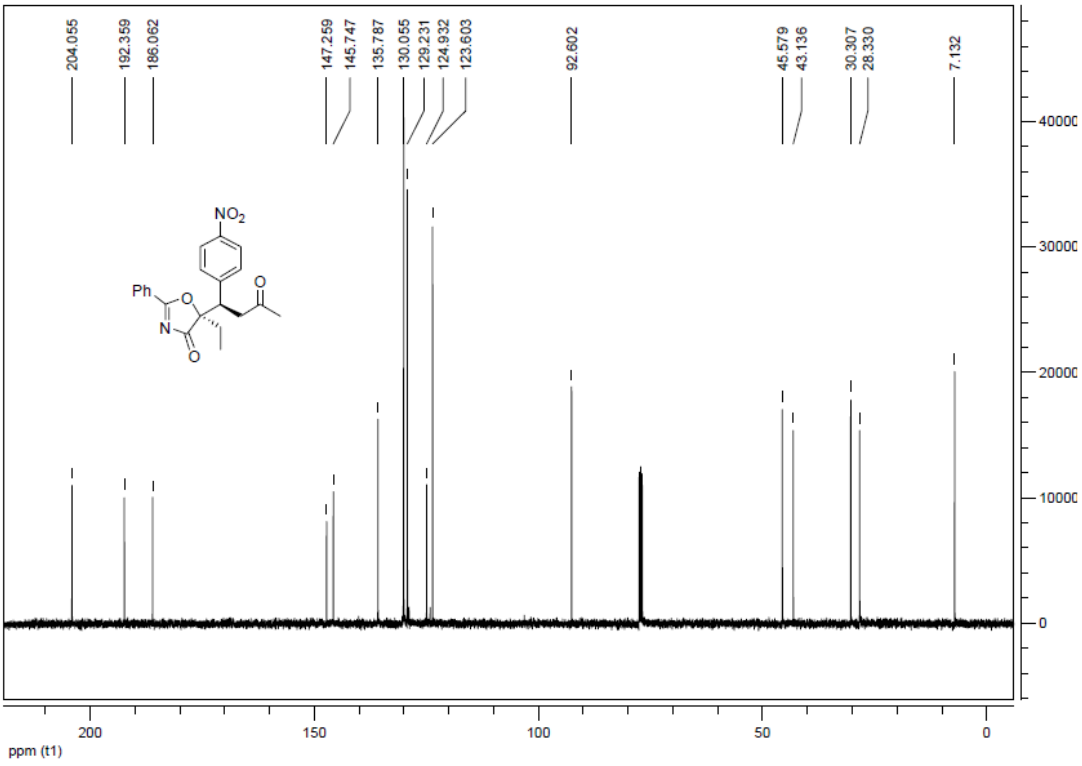
7n: (*S*)-5-((*R*)-1-(3-bromophenyl)-3-oxobutyl)-5-ethyl-2-phenyloxazol-4(5*H*)-one



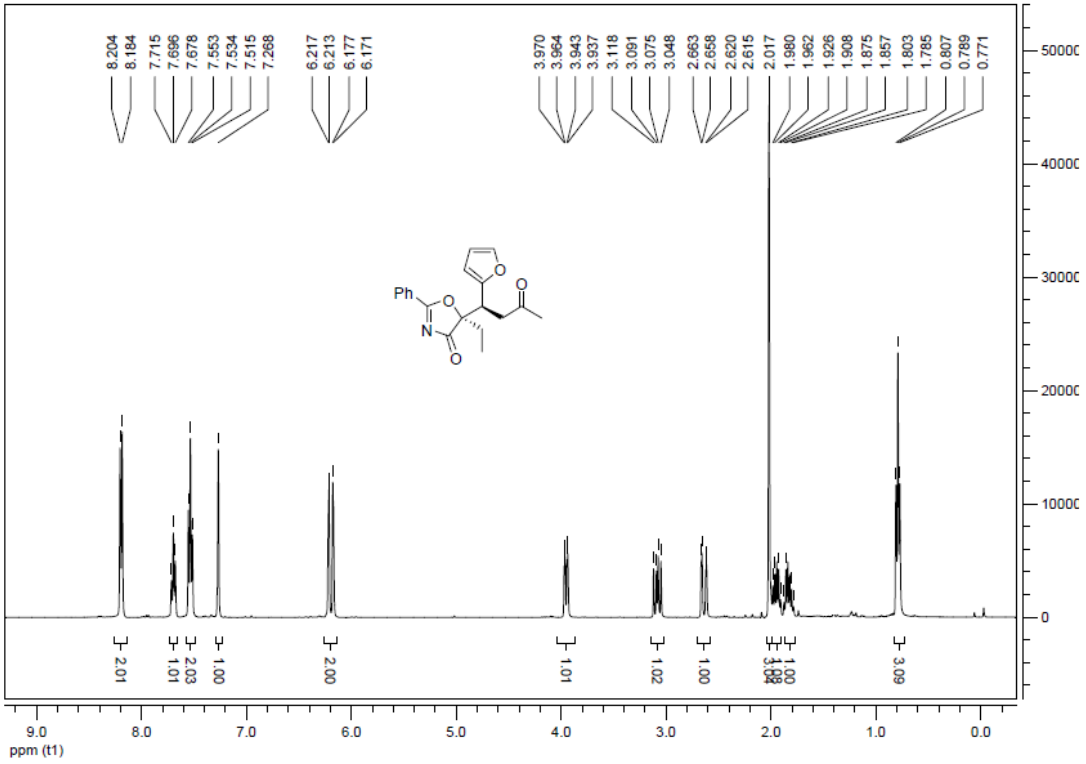


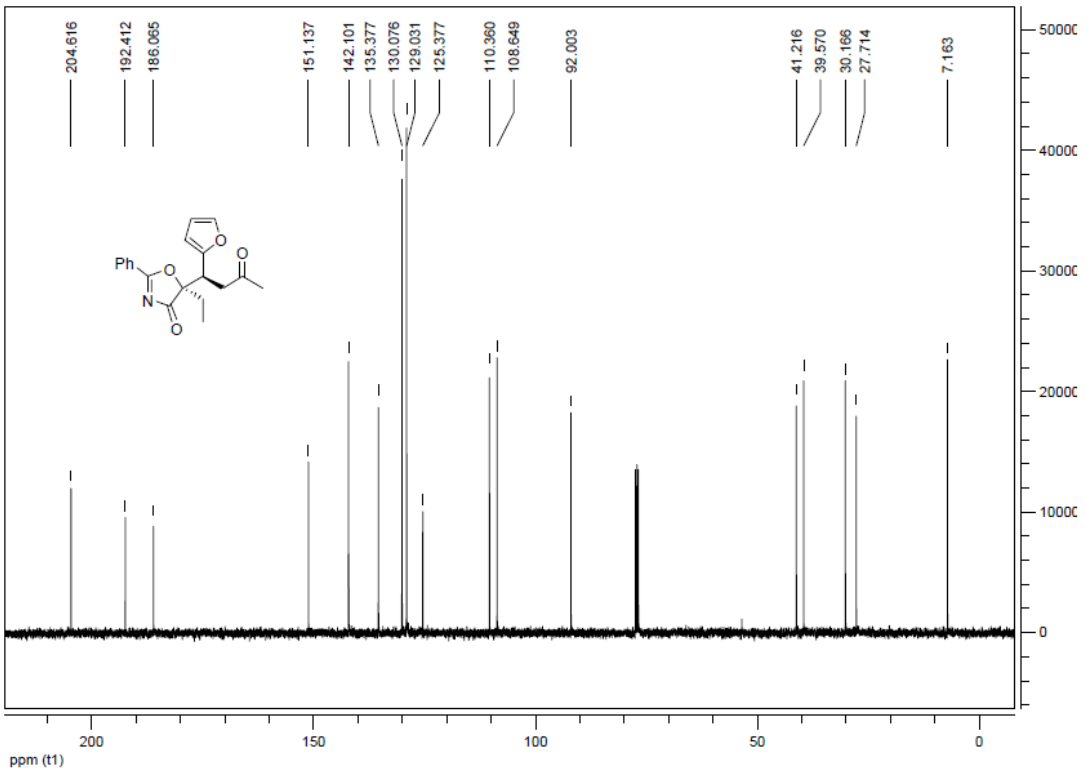
7o: (*S*)-5-ethyl-5-((*R*)-1-(4-nitrophenyl)-3-oxobutyl)-2-phenyloxazol-4(5*H*)-one



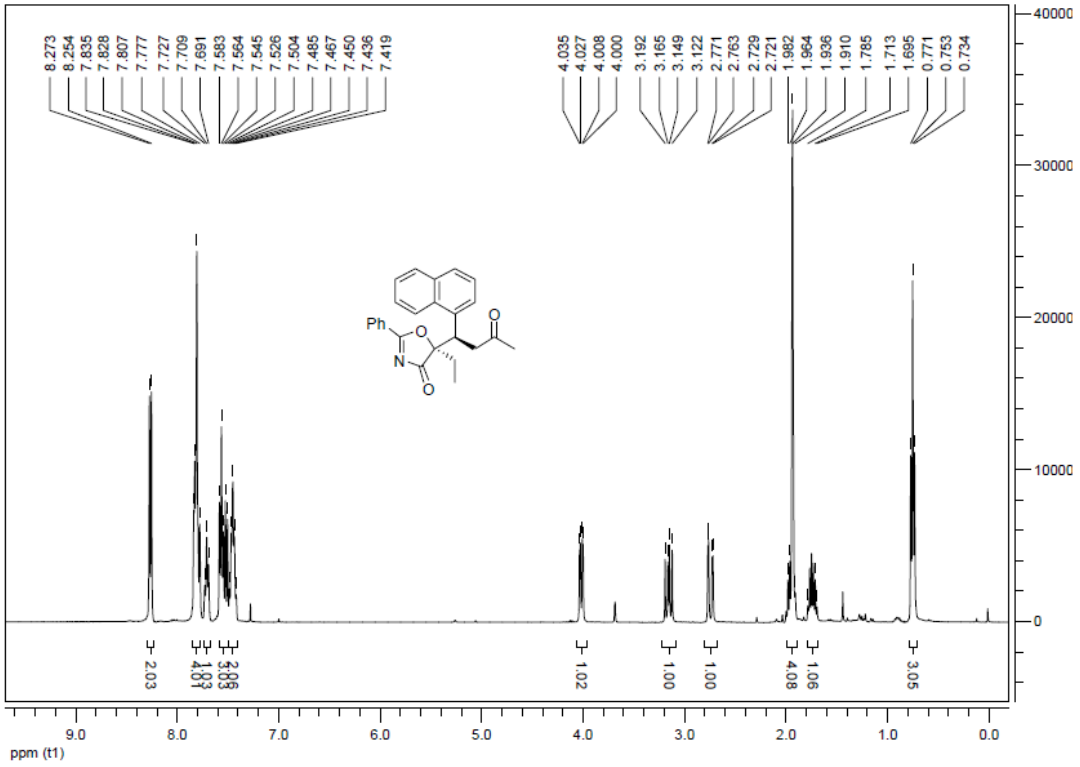


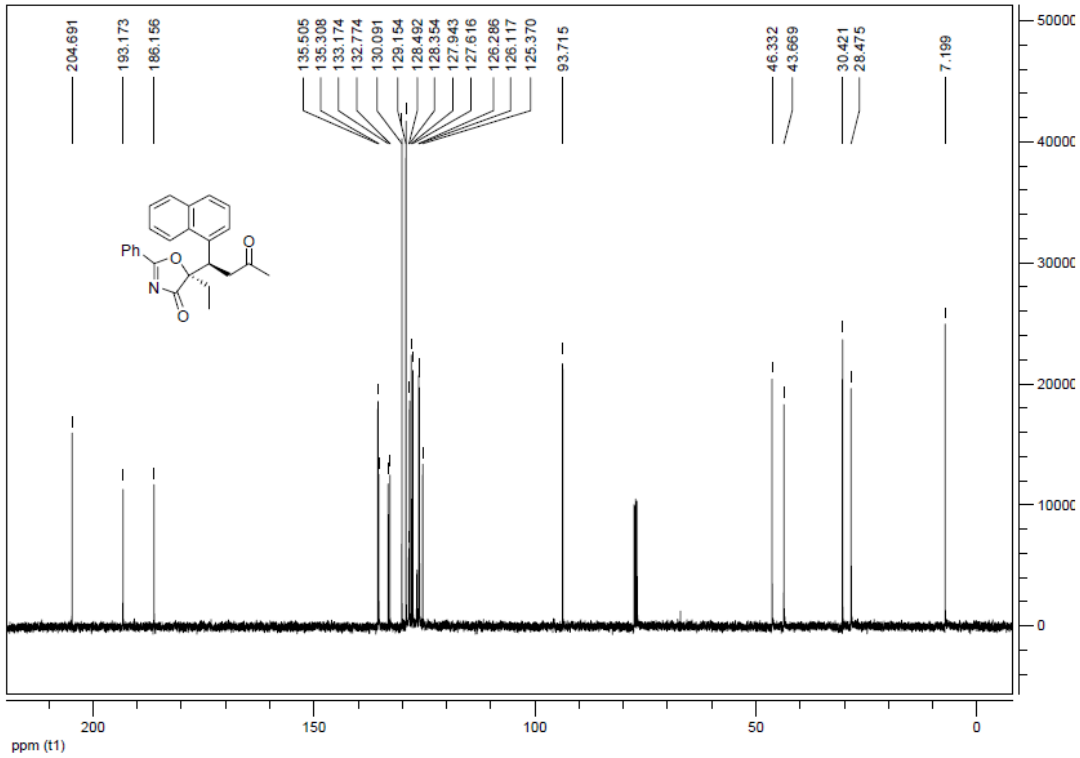
7p: (*S*)-5-ethyl-5-((*R*)-1-(furan-2-yl)-3-oxobutyl)-2-phenyloxazol-4(5*H*)-one



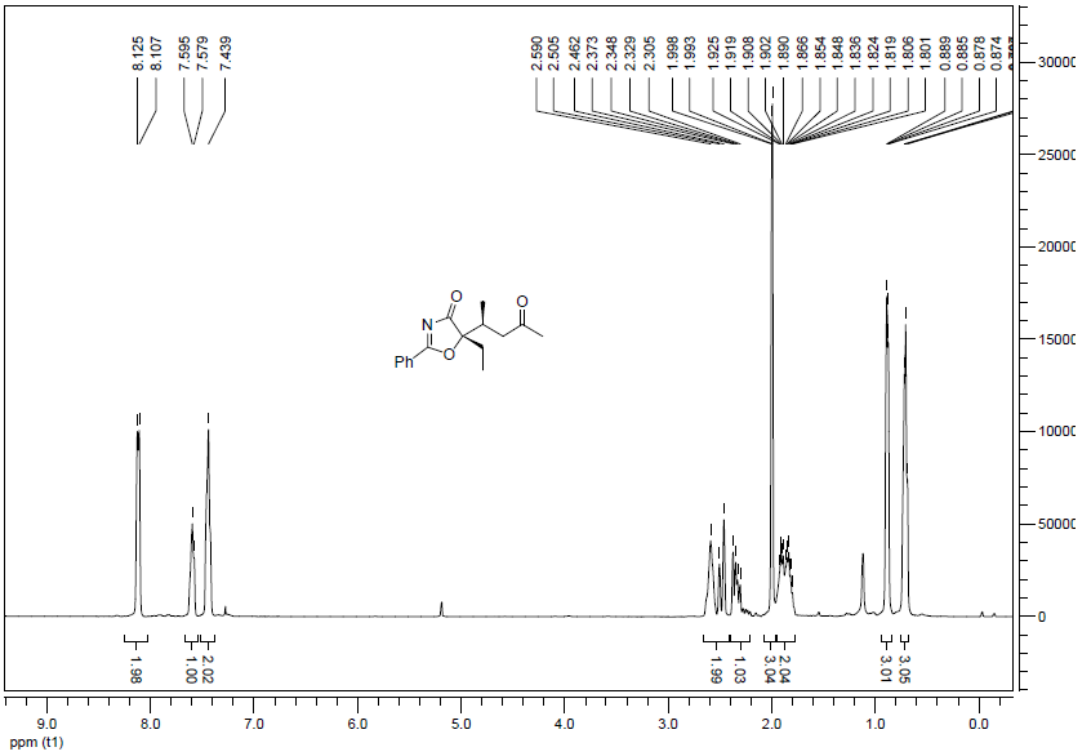


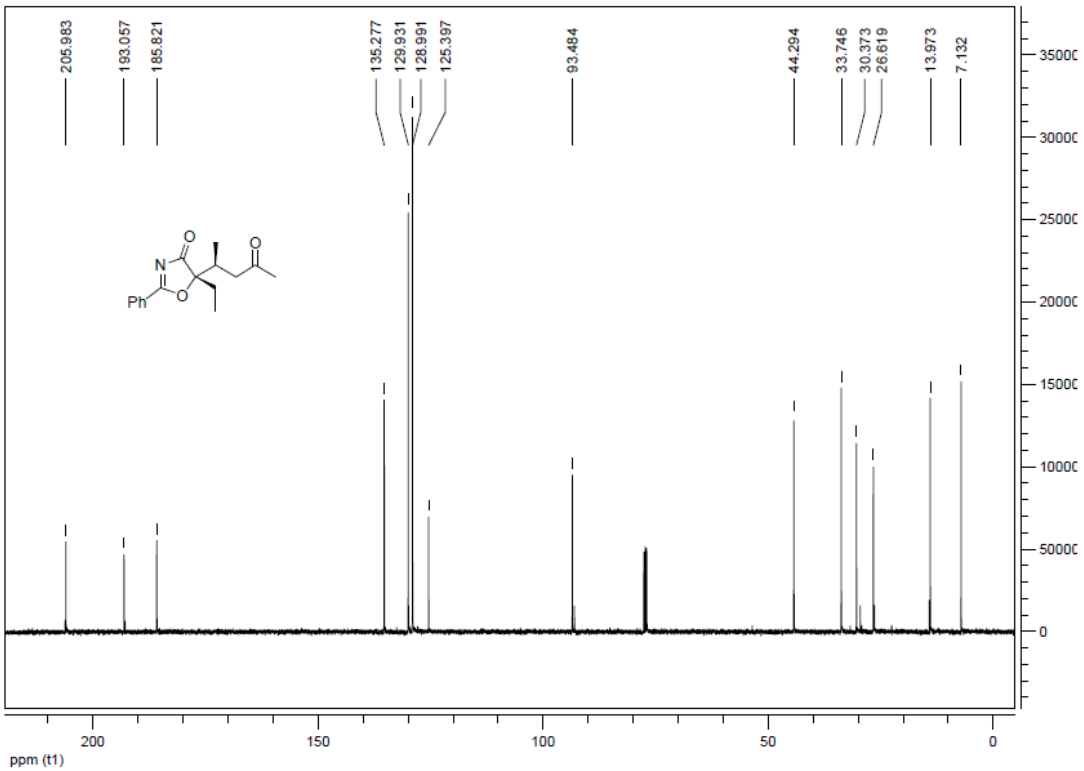
7q: (*S*)-5-ethyl-5-((*R*)-1-(naphthalen-1-yl)-3-oxobutyl)-2-phenyloxazol-4(5*H*)-one



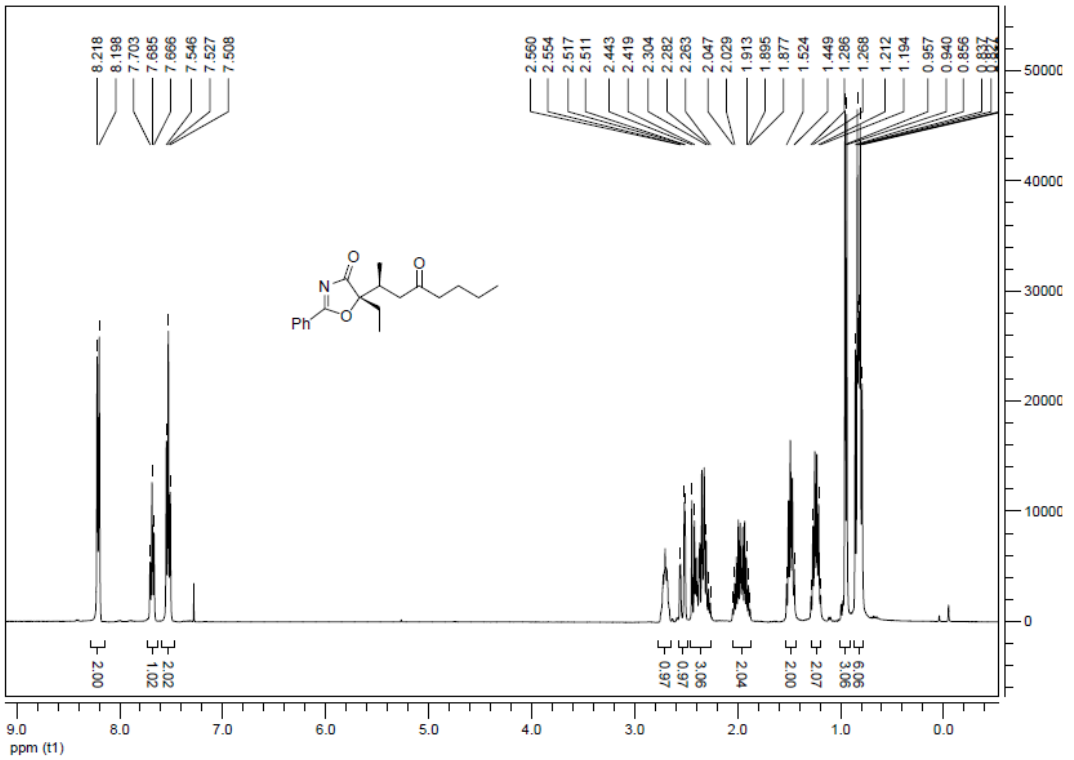


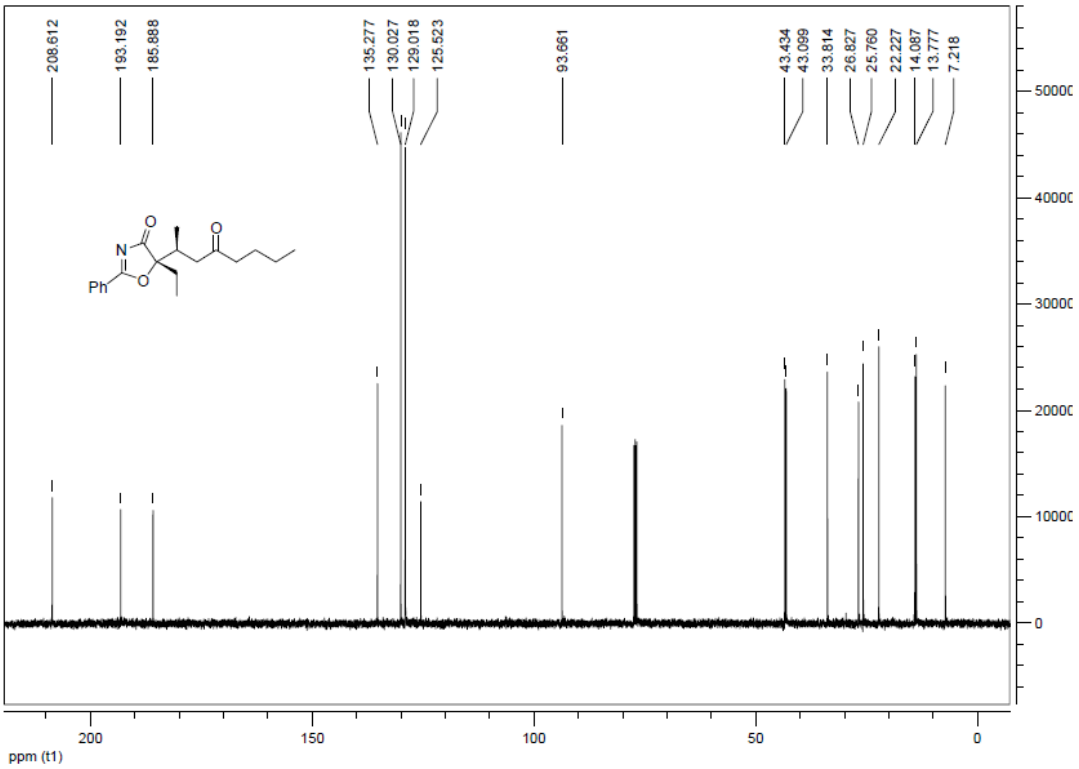
7r: (*S*)-5-ethyl-5-((*S*)-4-oxopentan-2-yl)-2-phenyloxazol-4(5*H*)-one



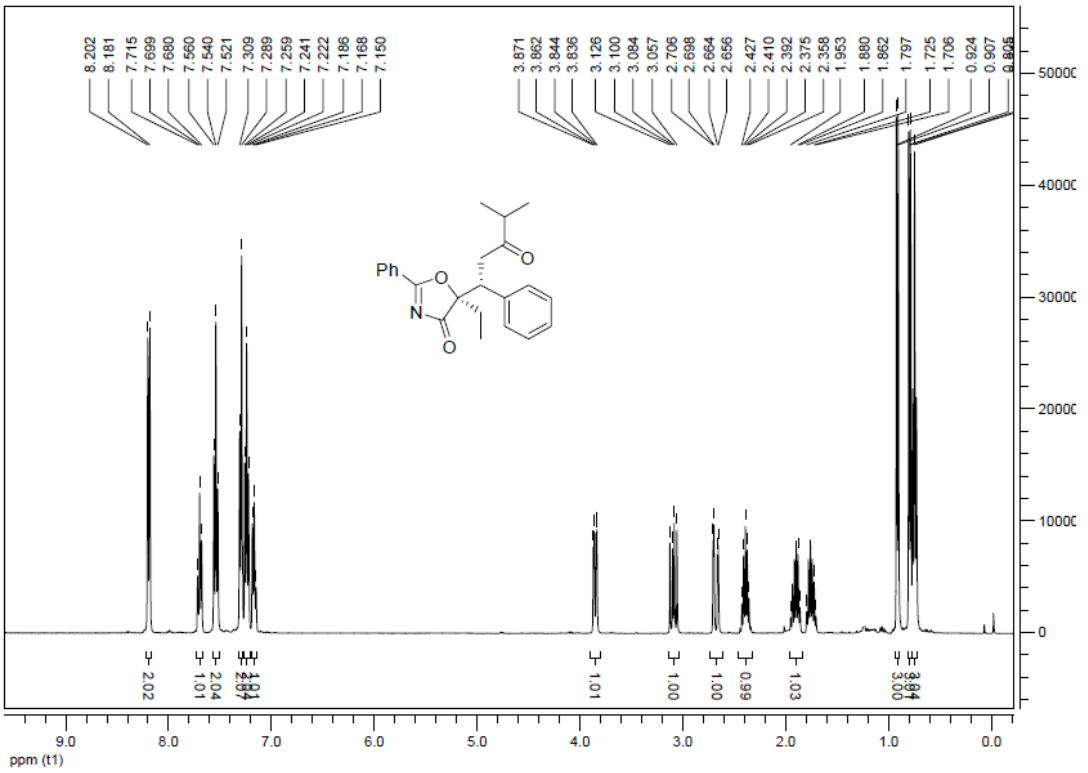


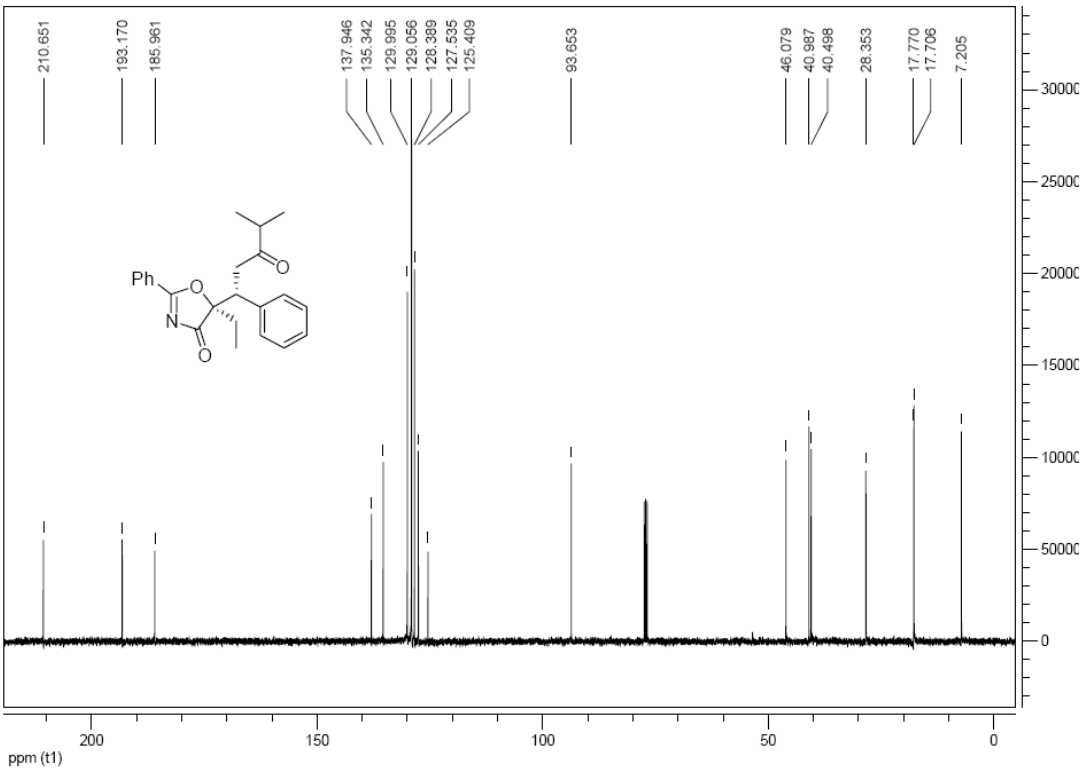
7s: (*S*)-5-ethyl-5-((*S*)-4-oxooctan-2-yl)-2-phenyloxazol-4(5*H*)-one



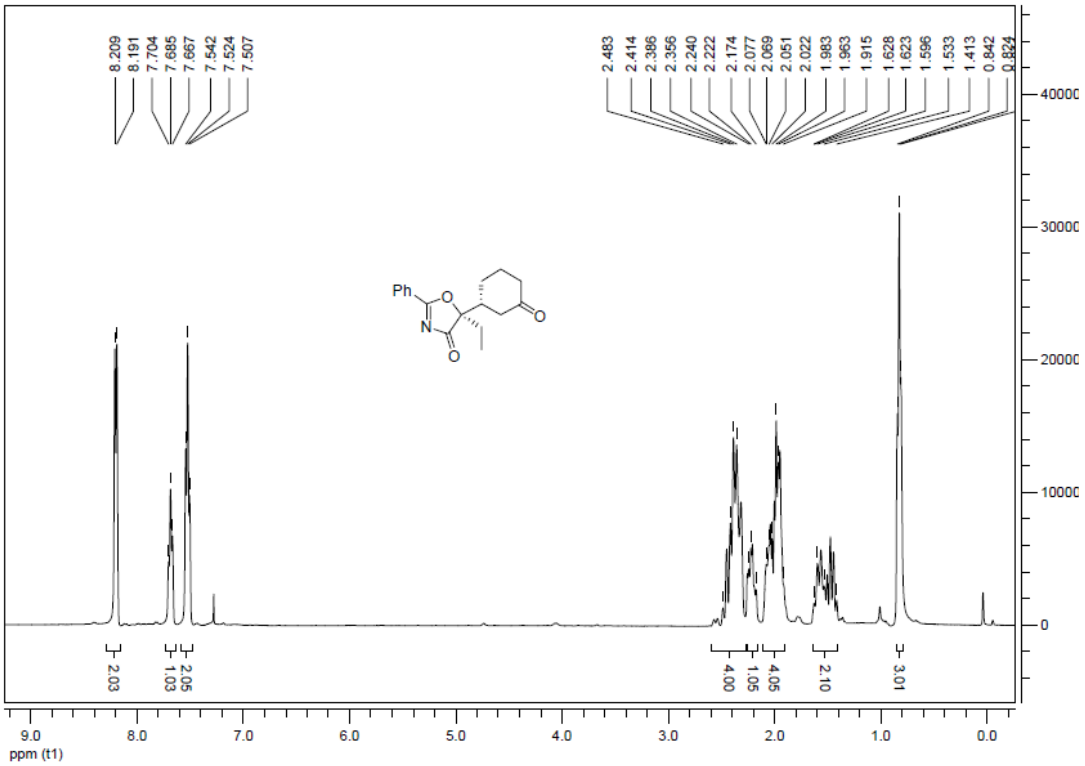


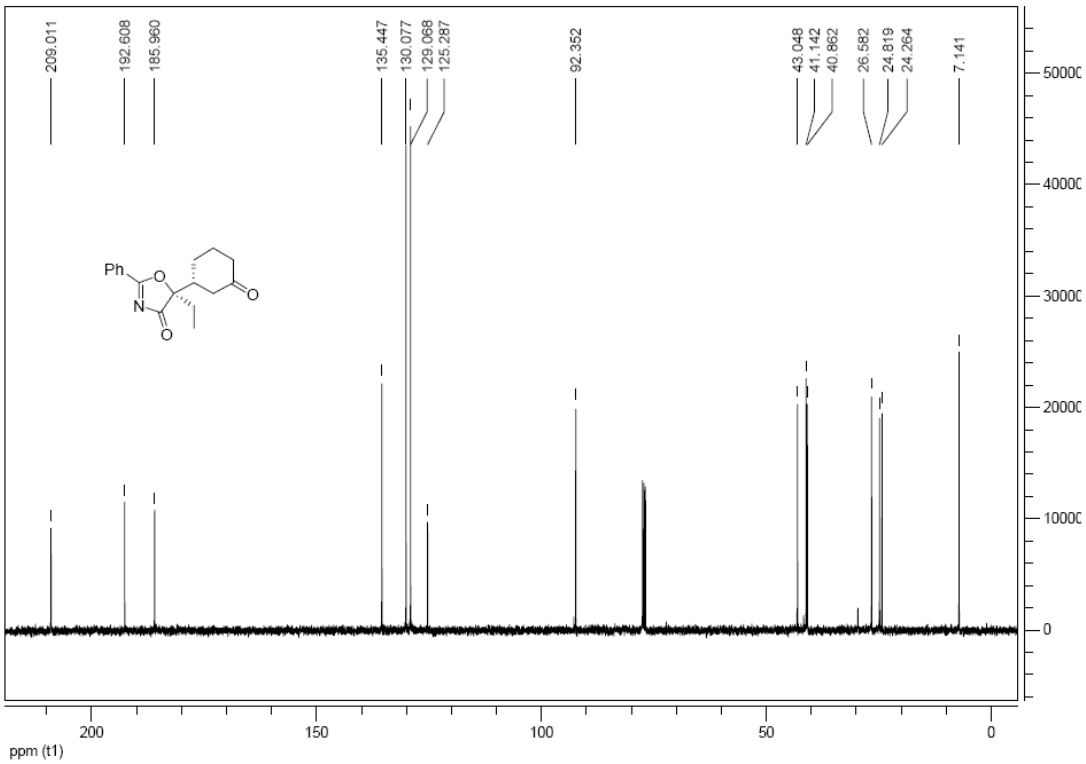
7t: (*S*)-5-ethyl-5-((*R*)-4-methyl-3-oxo-1-phenylpentyl)-2-phenyloxazol-4(5*H*)-one



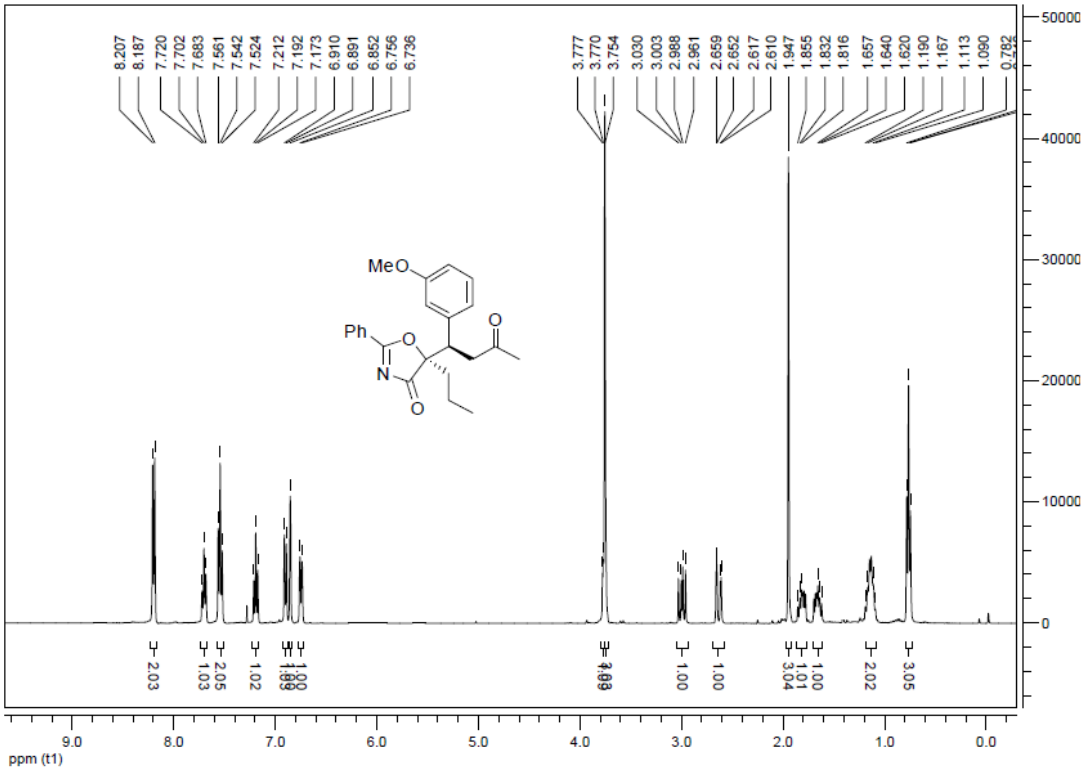


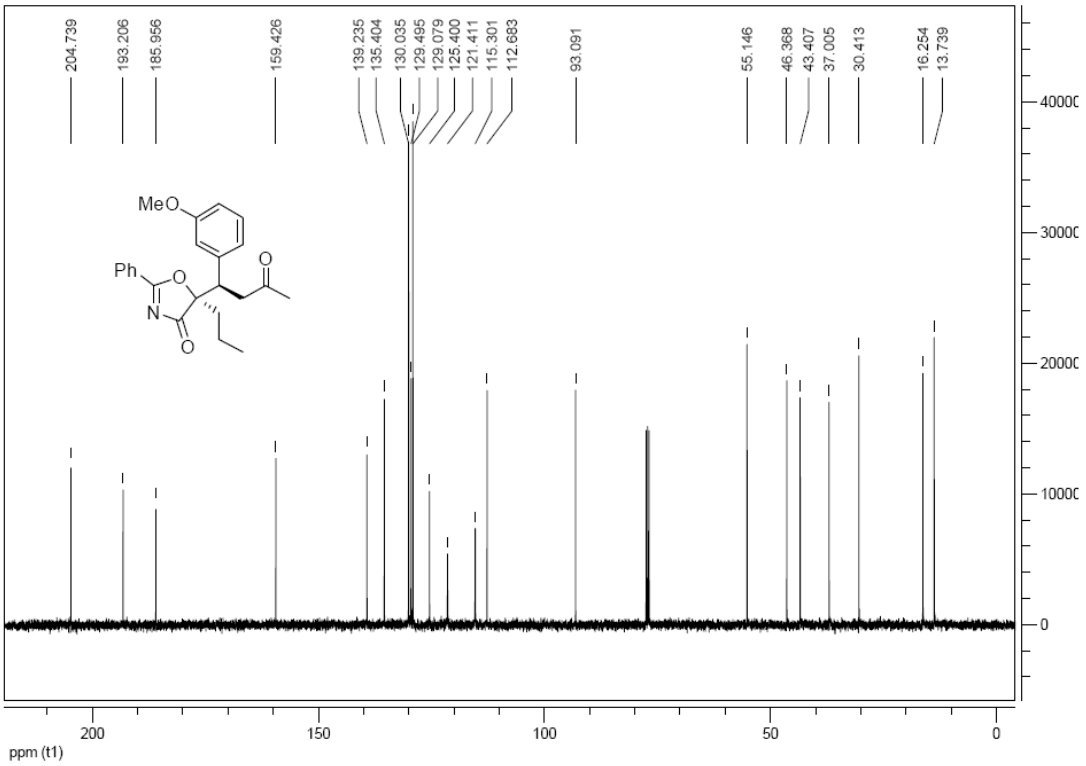
7u: (*S*)-5-ethyl-5-((*R*)-3-oxocyclohexyl)-2-phenyloxazol-4(5*H*)-one



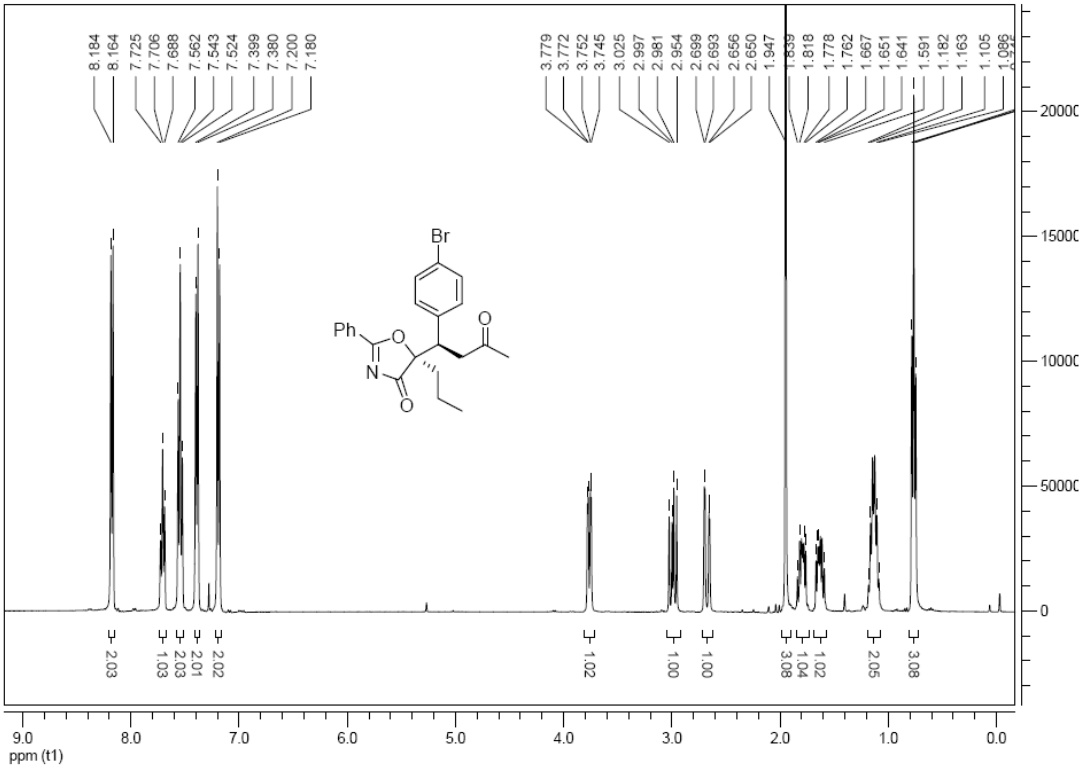


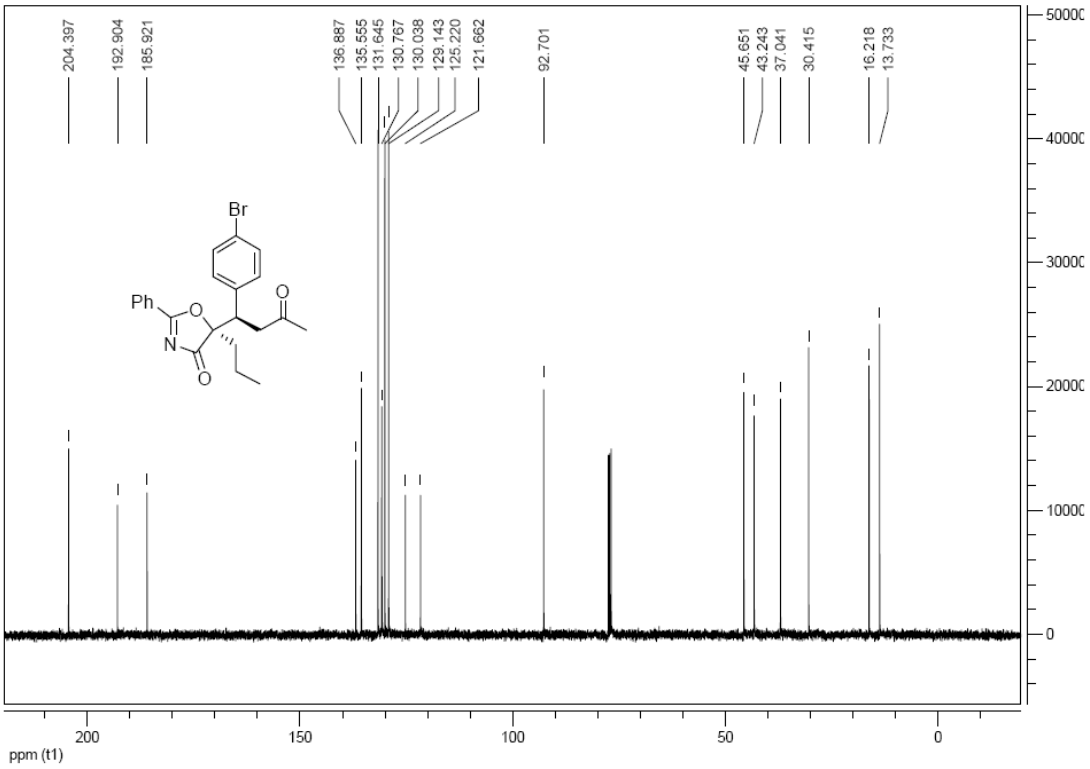
8a:(*S*)-5-((*R*)-1-(3-methoxyphenyl)-3-oxobutyl)-2-phenyl-5-propyloxazol-4(5*H*)-one



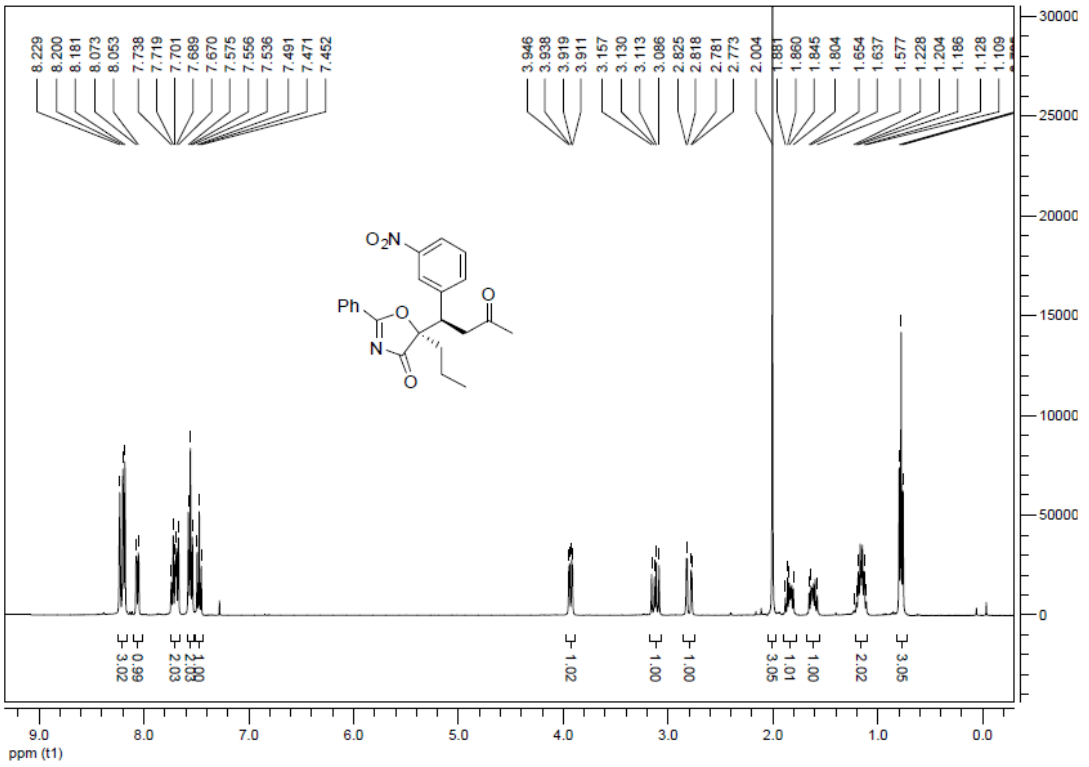


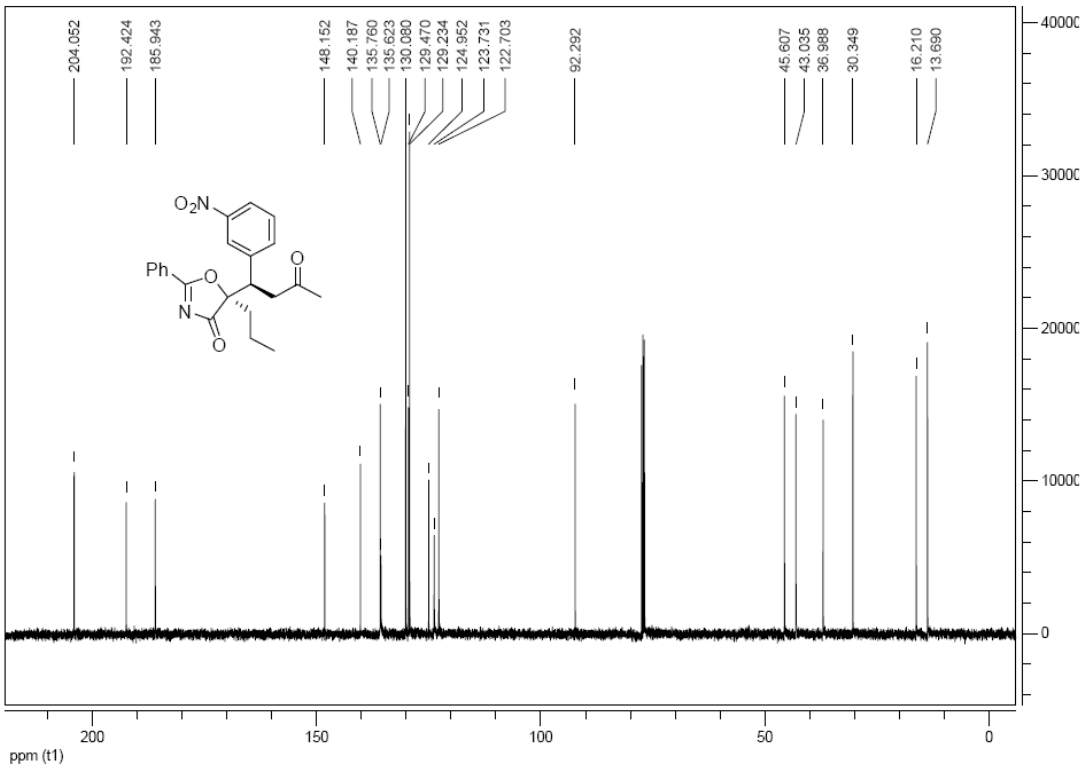
8b:(*S*)-5-((*R*)-1-(4-bromophenyl)-3-oxobutyl)-2-phenyl-5-propyloxazol-4(5*H*)-one



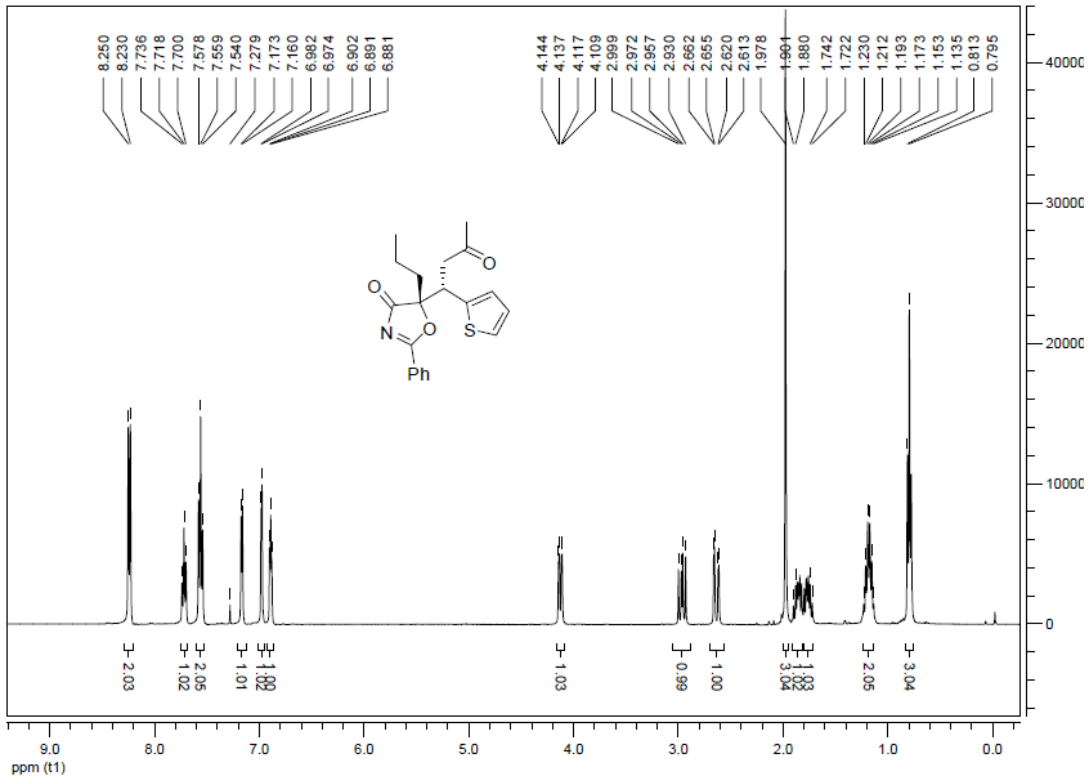


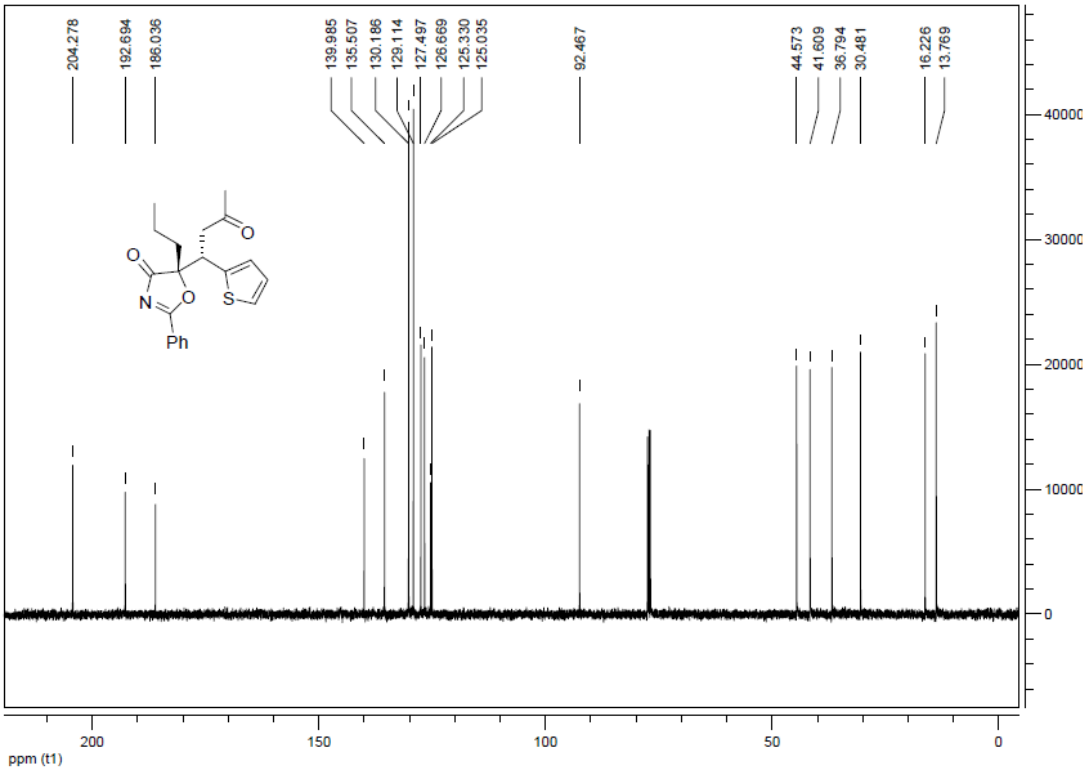
8c: (*S*)-5-((*R*)-1-(3-nitrophenyl)-3-oxobutyl)-2-phenyl-5-propyloxazol-4(5*H*)-one



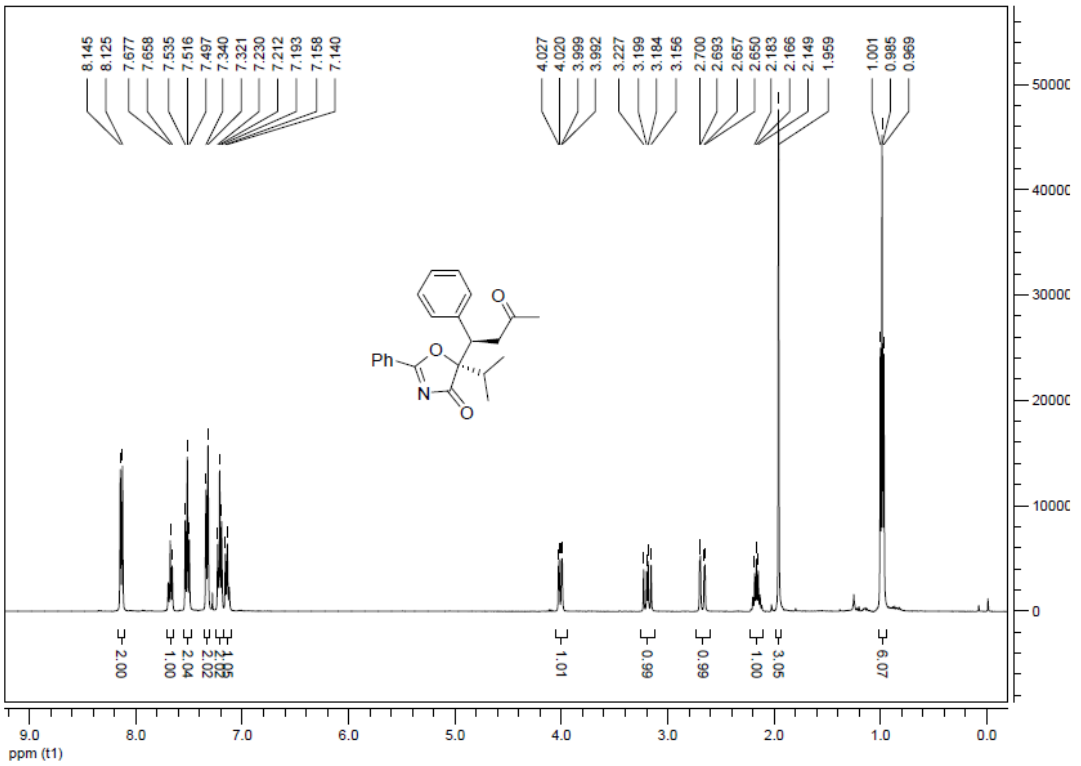


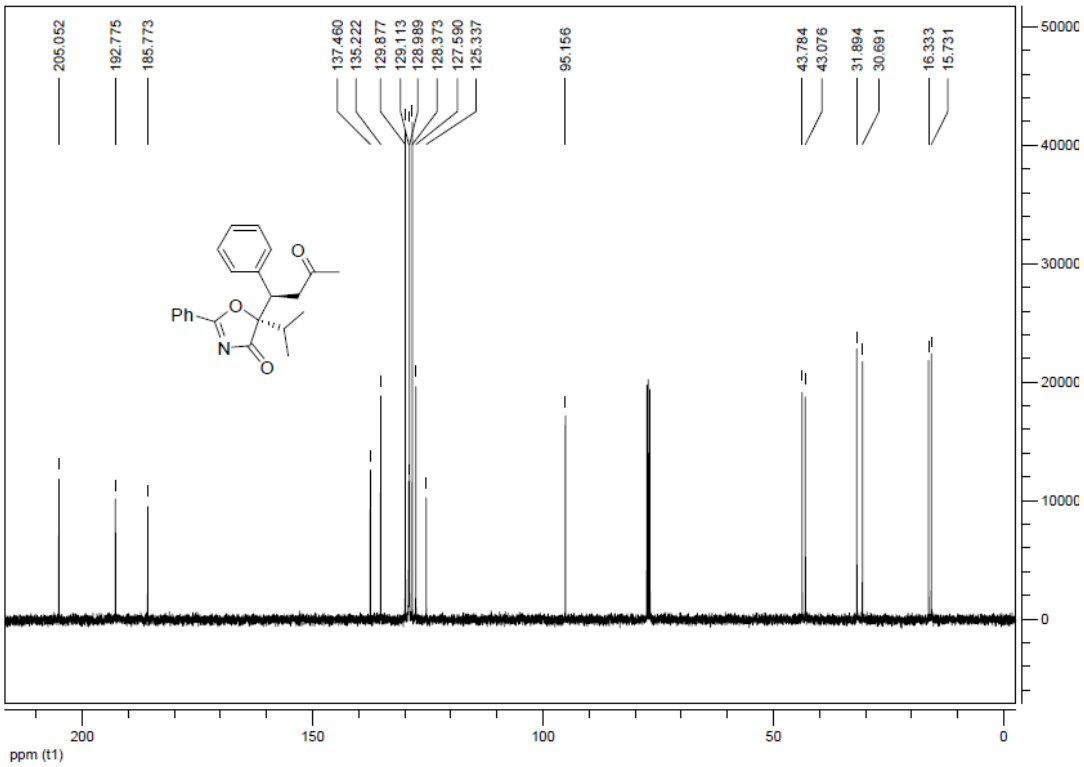
8d: (*S*)-5-((*S*)-3-oxo-1-(thiophen-2-yl)butyl)-2-phenyl-5-propyloxazol-4(5*H*)-one



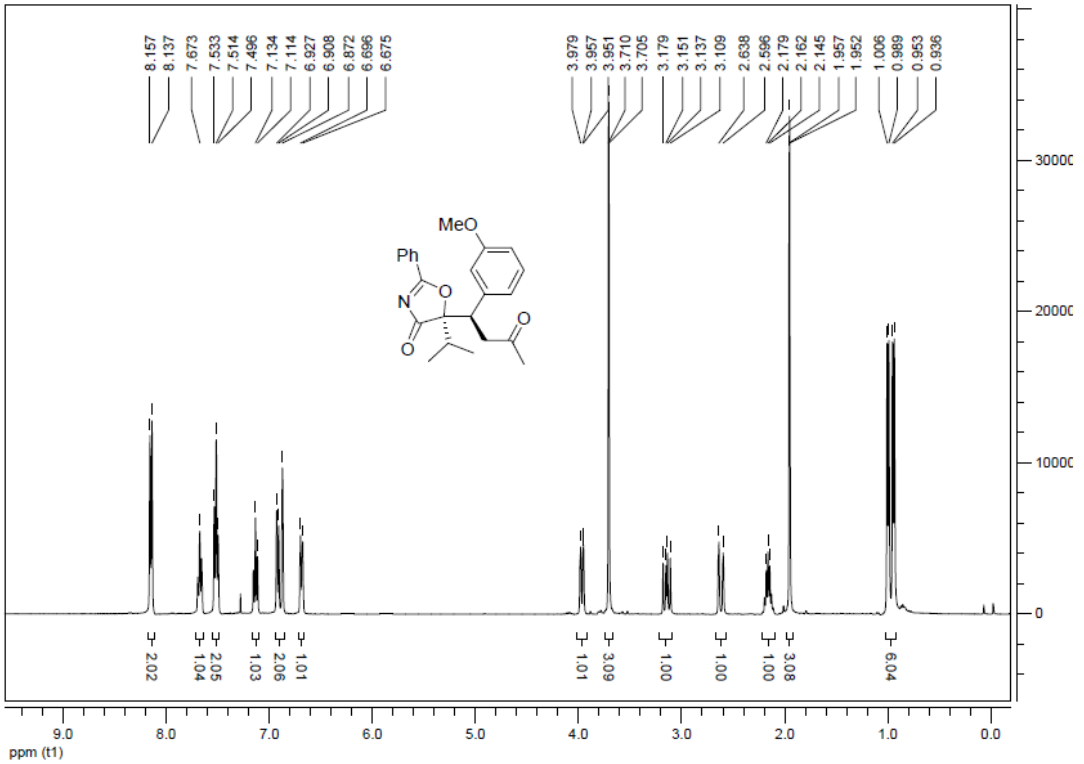


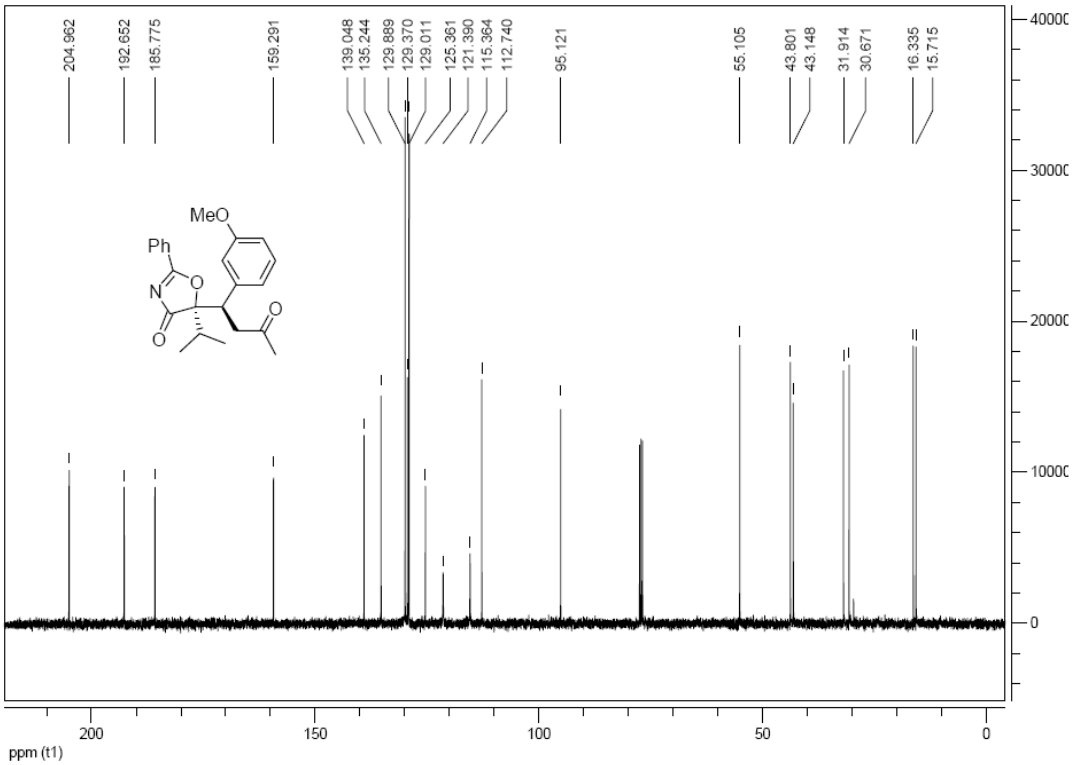
8e: (*S*)-5-isopropyl-5-((*R*)-3-oxo-1-phenylbutyl)-2-phenyloxazol-4(5*H*)-one



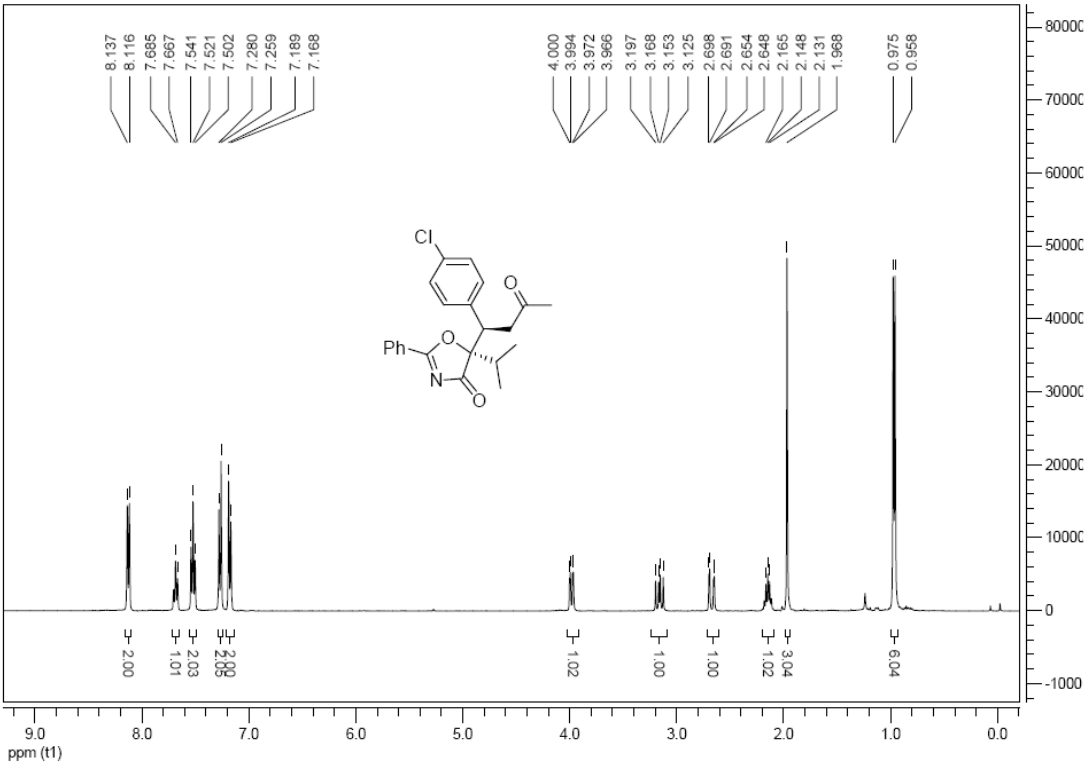


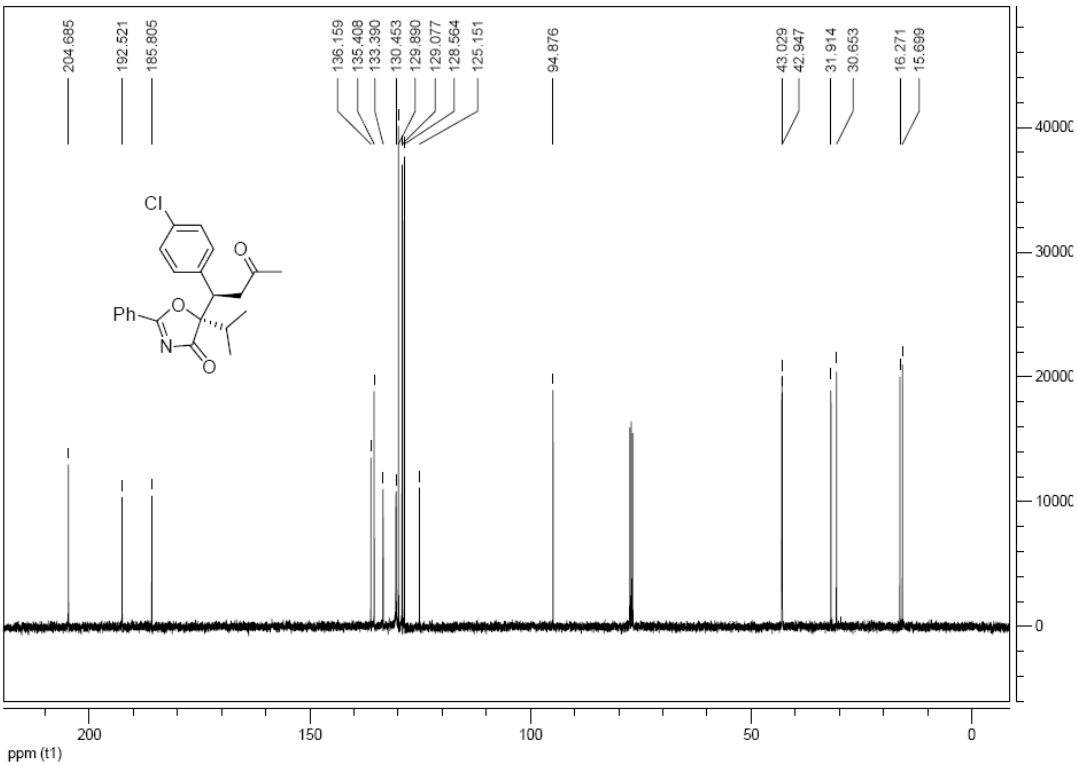
8f:(*S*)-5-isopropyl-5-((*R*)-1-(3-methoxyphenyl)-3-oxobutyl)-2-phenyloxazol-4(5*H*)-one



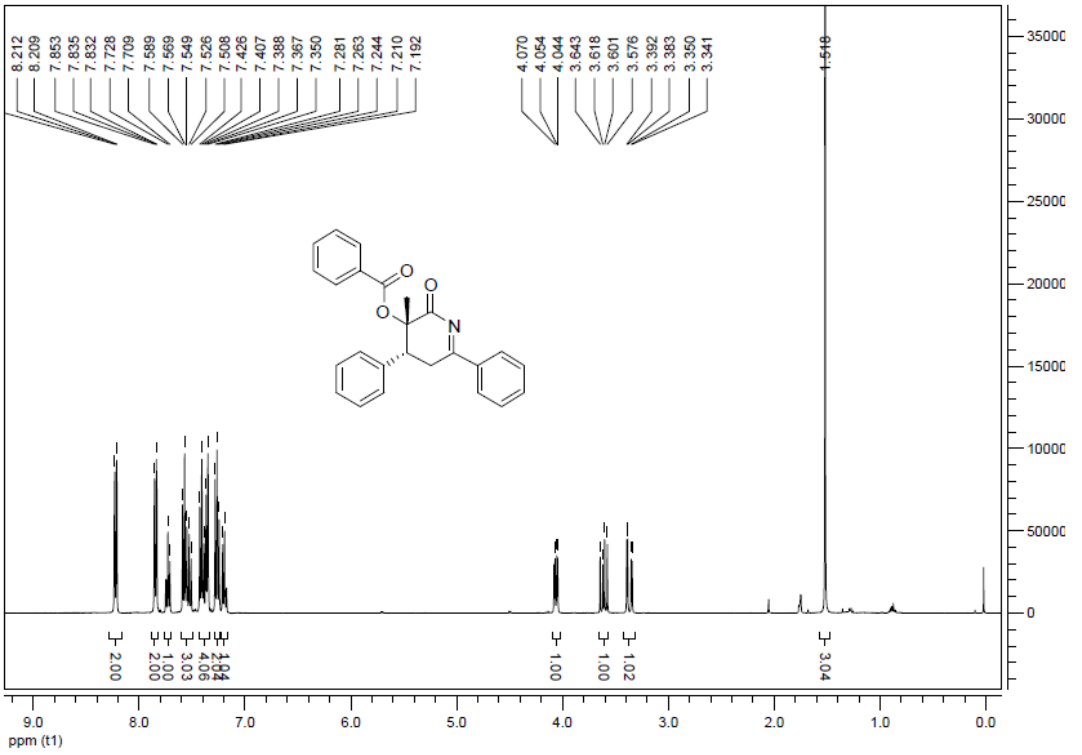


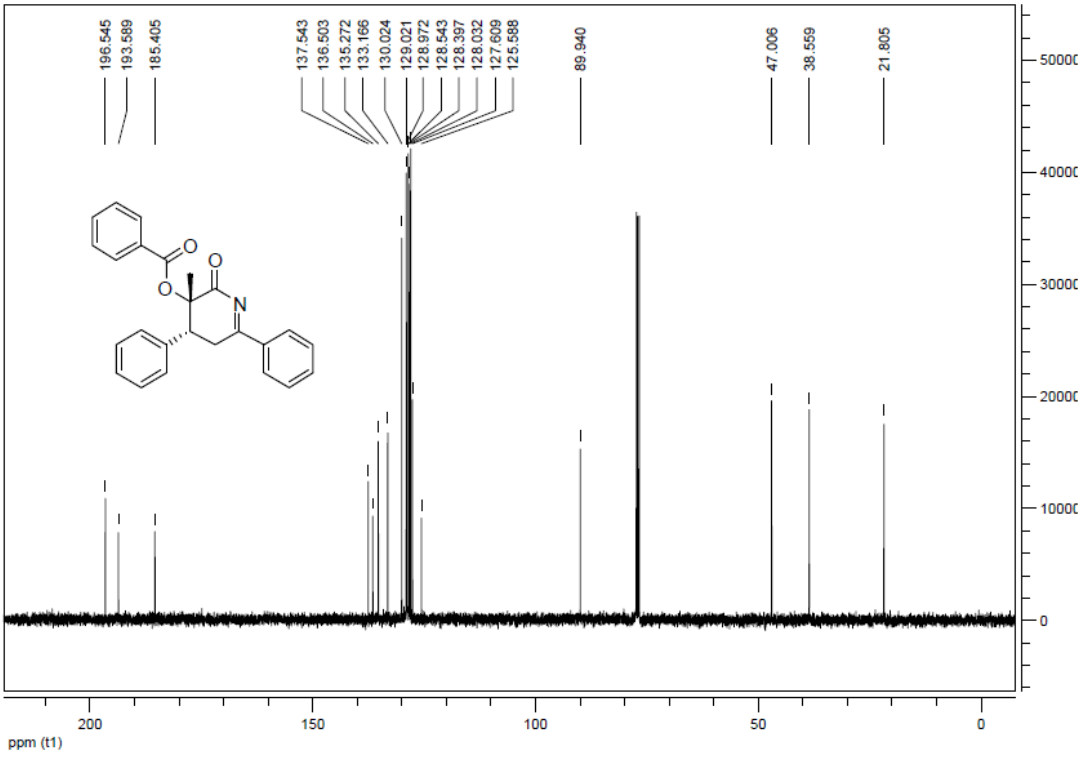
8g:(*S*)-5-((*R*)-1-(4-chlorophenyl)-3-oxobutyl)-5-isopropyl-2-phenyloxazol-4(5*H*)-one



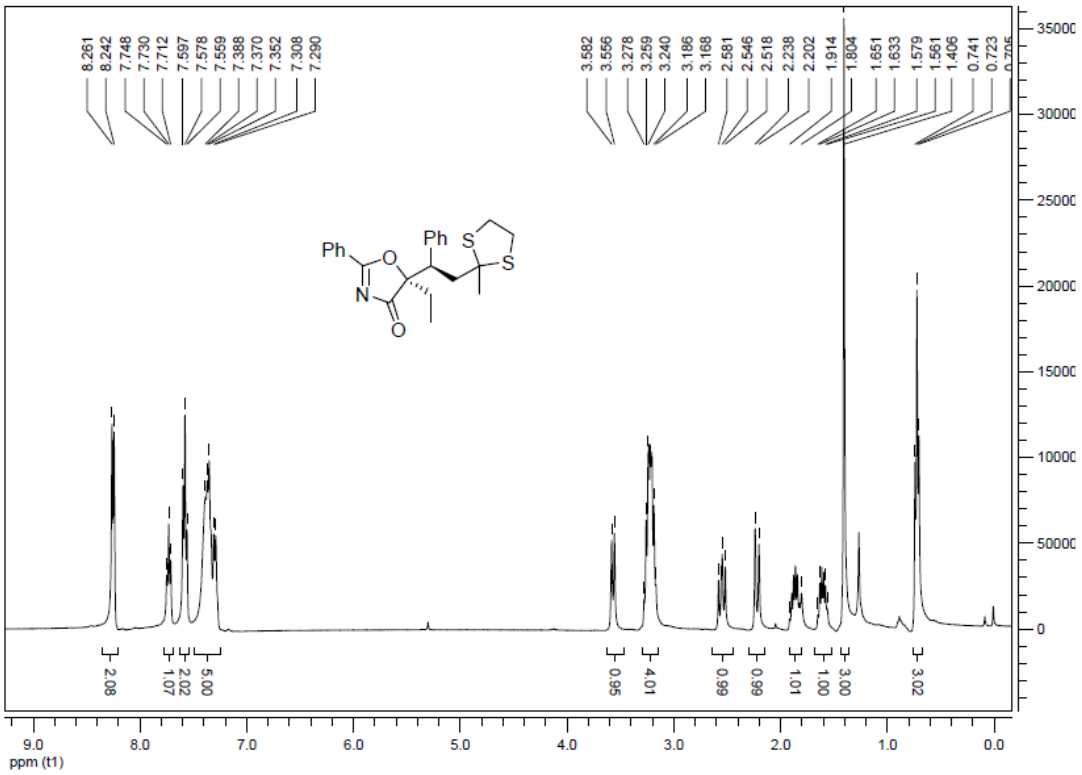


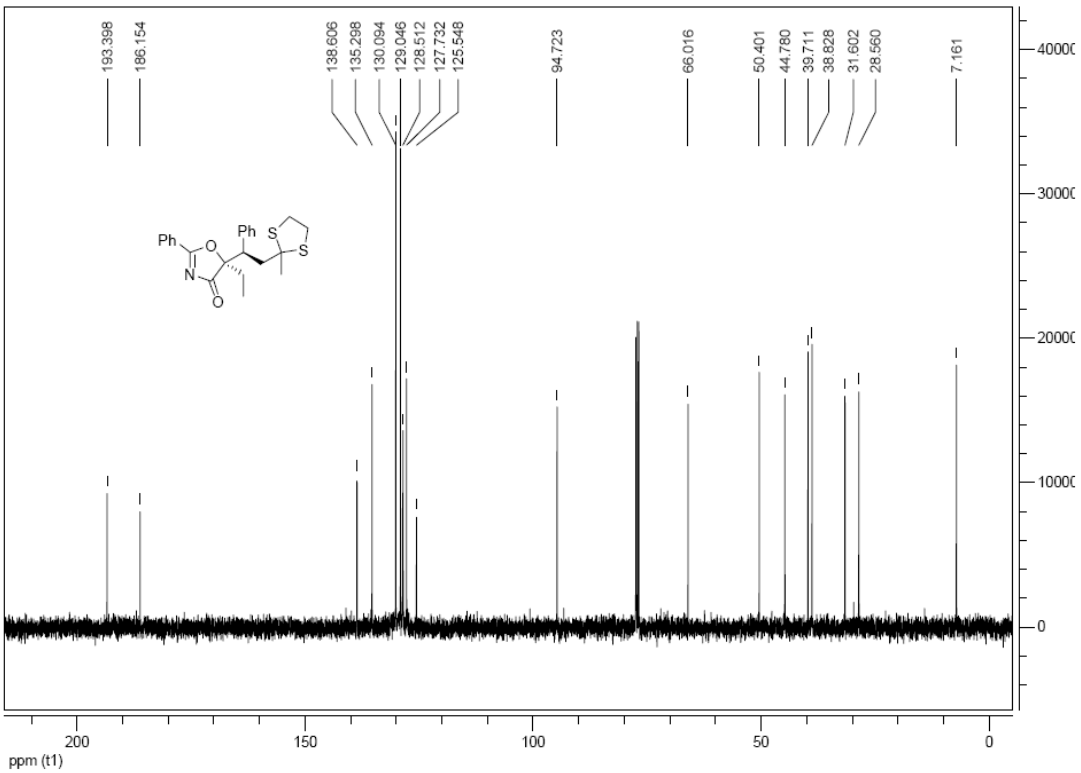
9a: (3*S*,4*R*)-3-methyl-2-oxo-4,6-diphenyl-2,3,4,5-tetrahydropyridin-3-yl benzoate



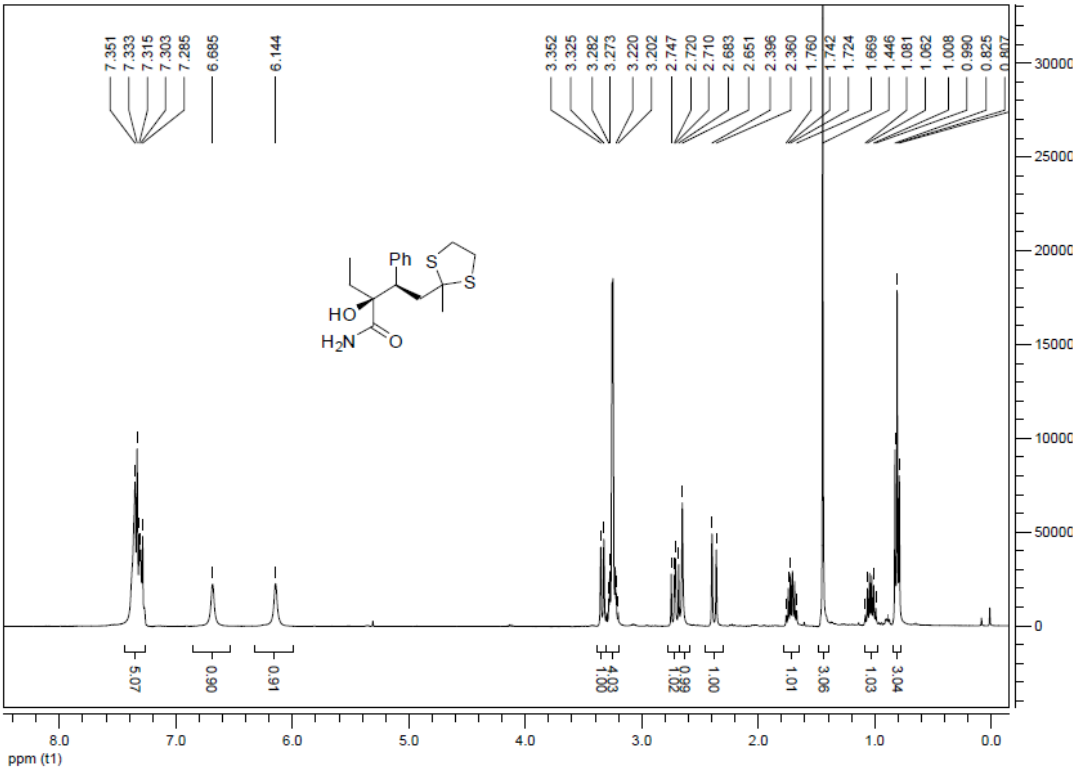


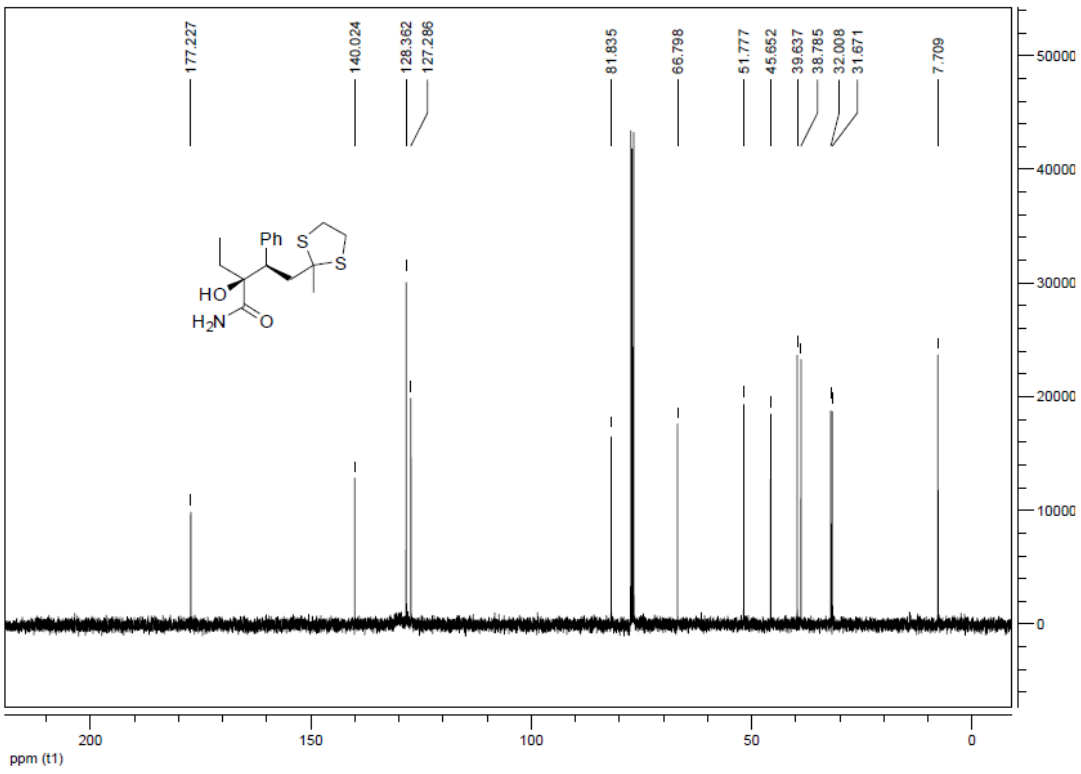
9b:(*S*)-5-ethyl-5-((*R*)-2-(2-methyl-1,3-dithiolan-2-yl)-1-phenylethyl)-2-phenyloxazol-4(5*H*)-one



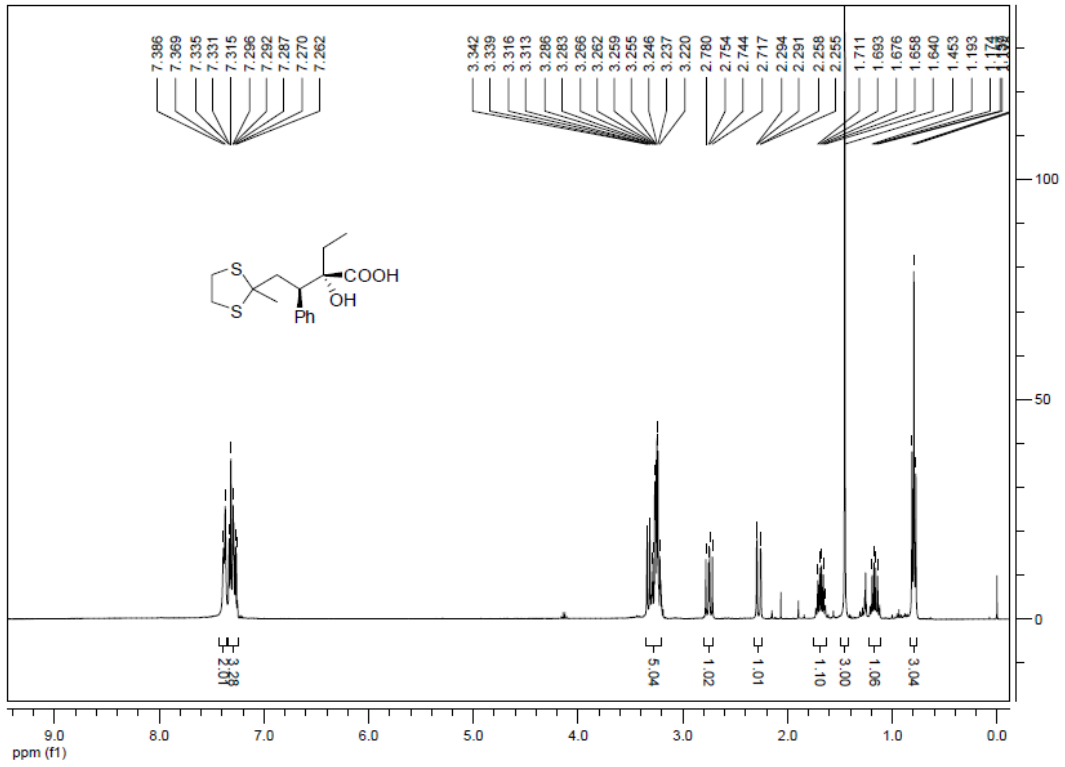


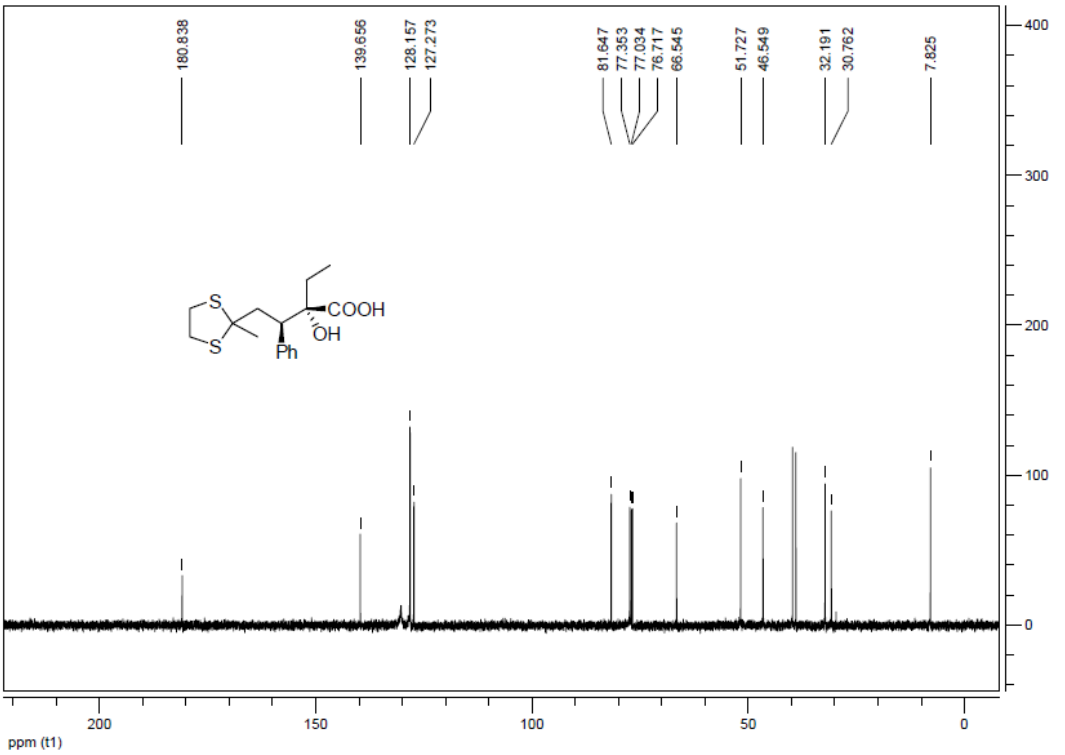
9c:(2*S*,3*R*)-2-ethyl-2-hydroxy-4-(2-methyl-1,3-dithiolan-2-yl)-3-phenylbutanamide



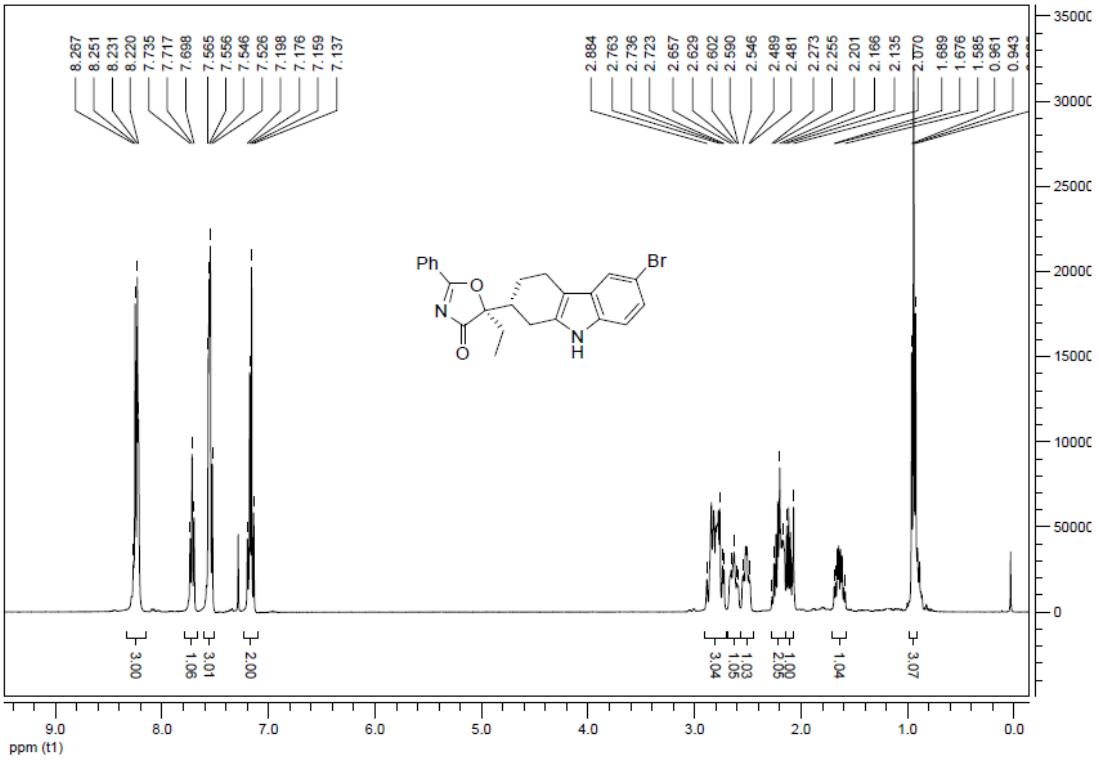


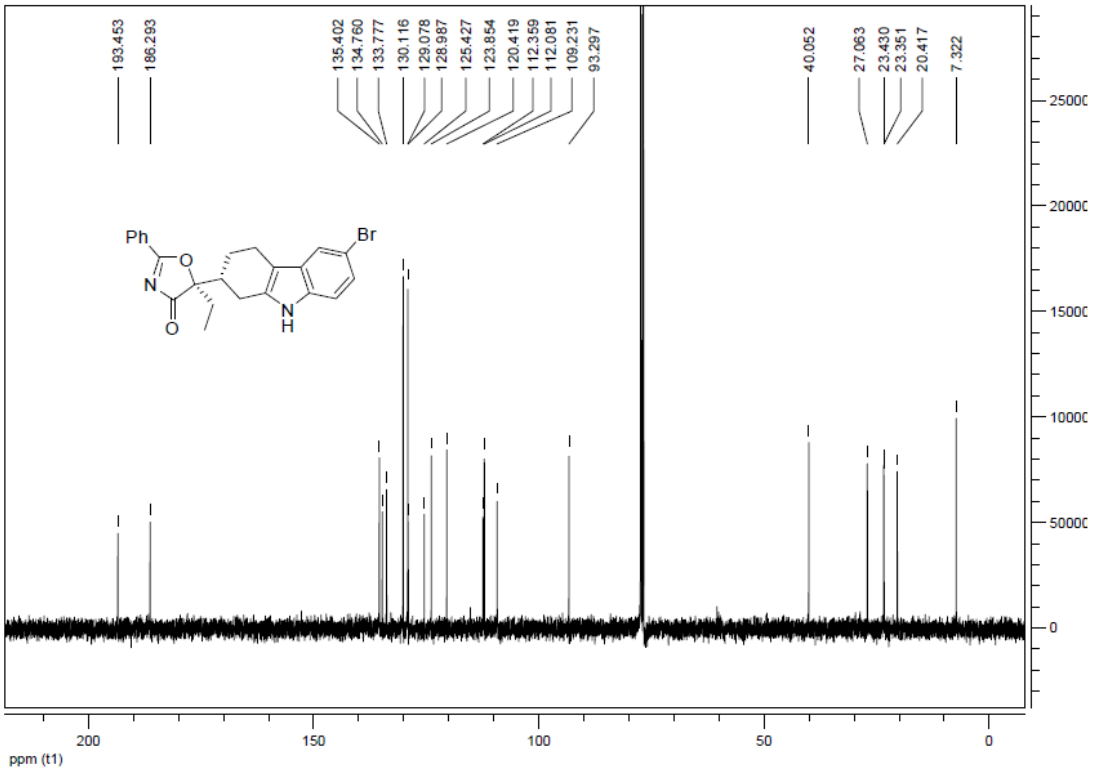
9d: (2*S*,3*R*)-2-ethyl-2-hydroxy-4-(2-methyl-1,3-dithiolan-2-yl)-3-phenylbutanoic acid



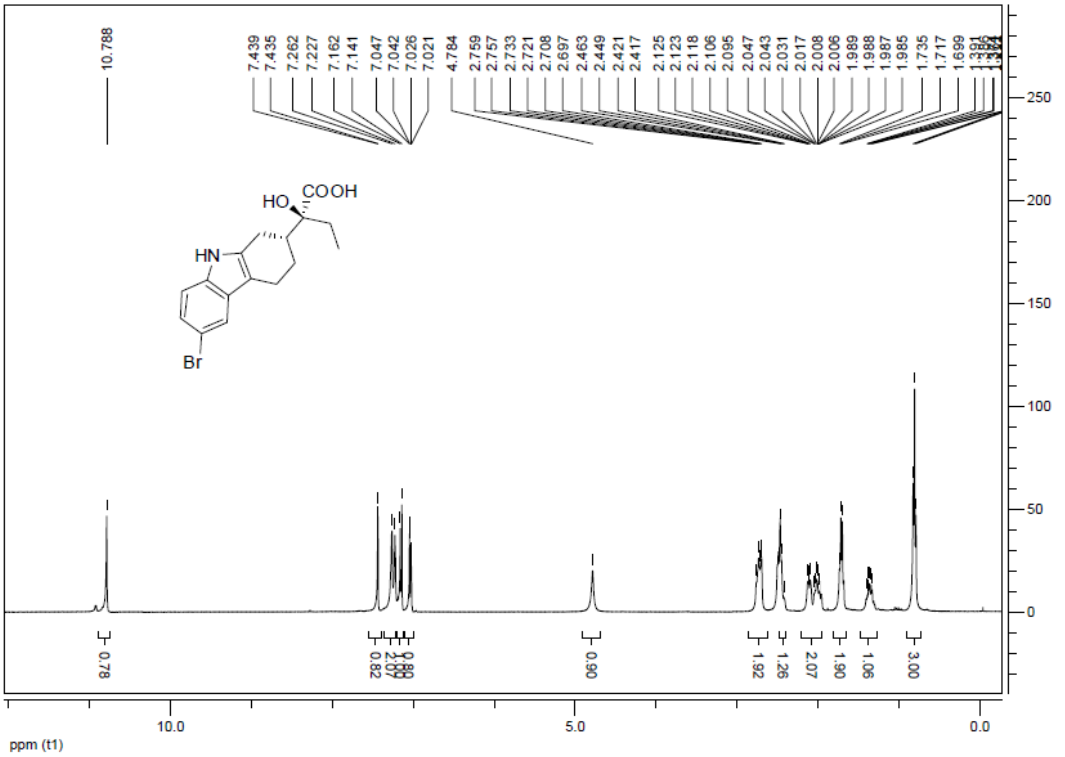


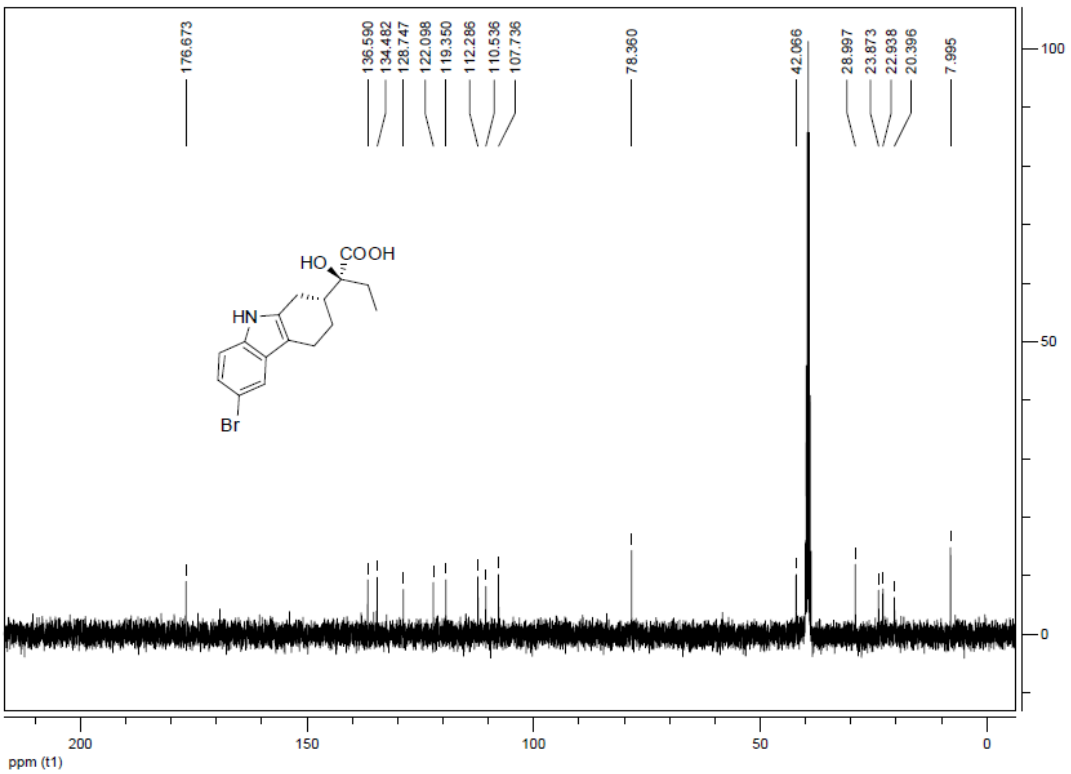
9e:(*S*)-5-ethyl-5-((7*R*)-5,6,7,8,9,9a-hexahydro-4a*H*-carbazol-7-yl)-2-phenyloxazol-4(5*H*)-one



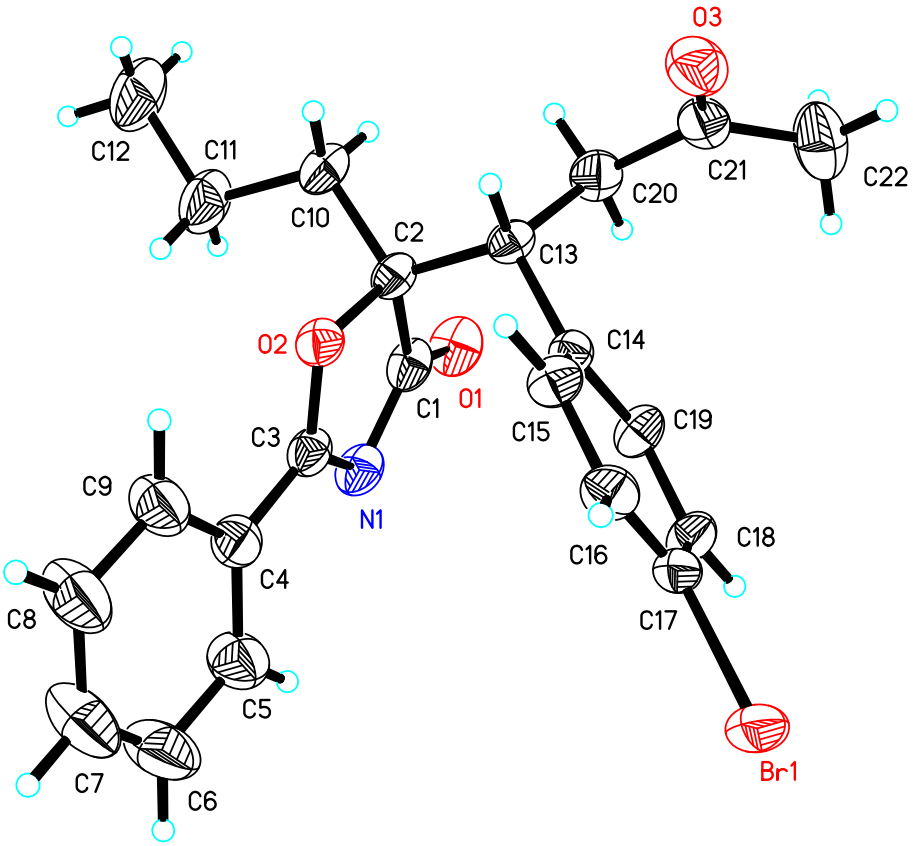


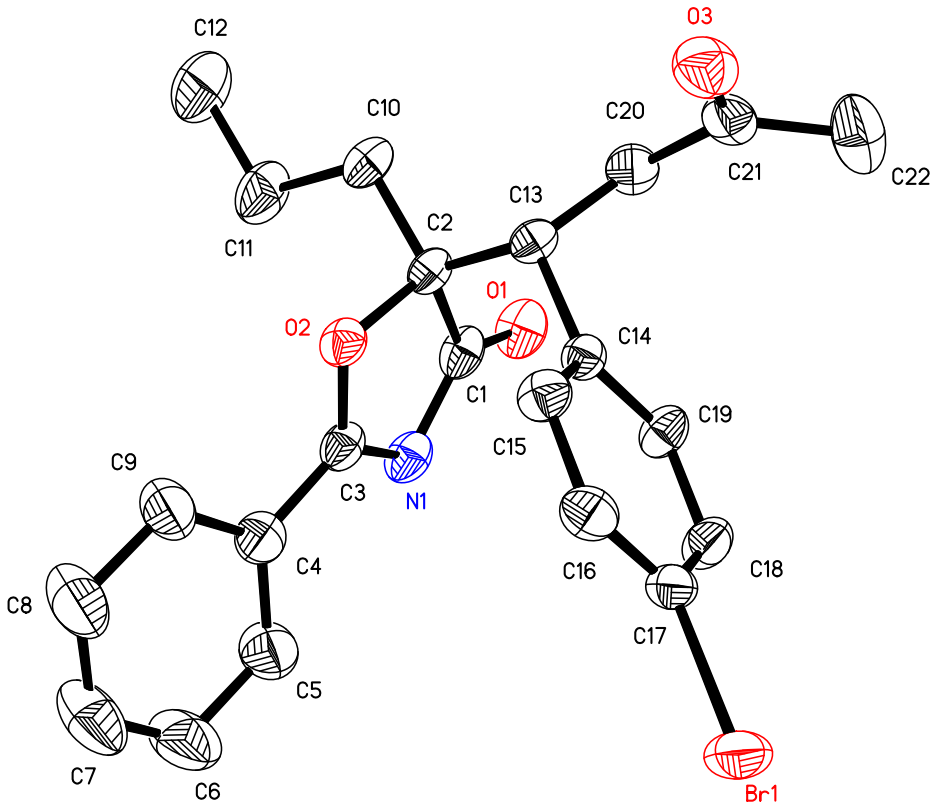
9f:(*S*)-2-((*R*)-6-bromo-2,3,4,9-tetrahydro-1H-carbazol-2-yl)-2-hydroxybutanoic acid





H: Absolute Configuration and X-Ray Analysis Data of 8b




C12
O3
C10
C20
C21
C22
C13
C11
C2
O1
O2
C14
C1
C19
C15
C9
C3
N1
C4
C16
C18
C8
C17
C5
C7
C6
Br1

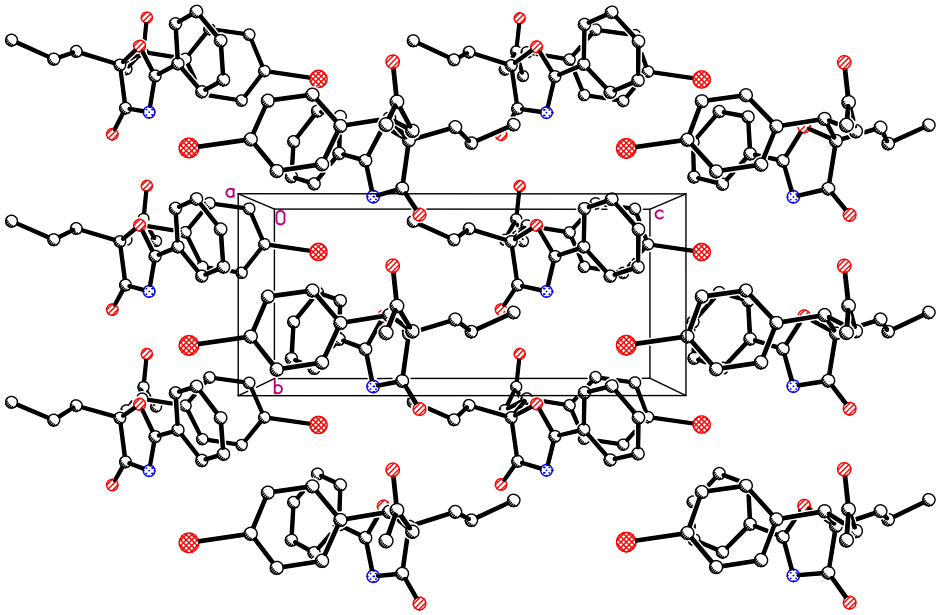

a
0
c
b

Table 1. Crystal data and structure refinement for 8b.

Identification code	mo_dm1197_0m
Empirical formula	C22 H22 Br N O3
Formula weight	428.32
Temperature	296(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)
Unit cell dimensions	a = 12.773(3) A alpha = 90 deg. b = 6.0463(13) A beta = 90.851(3) deg. c = 13.400(3) A gamma = 90 deg.
Volume	1034.8(4) A^3
Z, Calculated density	2, 1.375 Mg/m^3
Absorption coefficient	2.007 mm^-1
F(000)	440
Crystal size	0.58 x 0.25 x 0.08 mm
Theta range for data collection	1.52 to 27.00 deg.
Limiting indices	-16<=h<=16, -7<=k<=7, -17<=l<=16
Reflections collected / unique	7395 / 4172 [R(int) = 0.0220]
Completeness to theta = 27.00	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8559 and 0.3890
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4172 / 1 / 246

Goodness-of-fit on F^2	0.960
Final R indices [I>2sigma(I)]	R1 = 0.0374, wR2 = 0.1150
R indices (all data)	R1 = 0.0468, wR2 = 0.1319
Absolute structure parameter	0.009(12)
Largest diff. peak and hole	0.473 and -0.617 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for mo_dm1197_0m.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Br(1)	1277(1)	2574(1)	11247(1)	77(1)
N(1)	3323(2)	4851(5)	7119(3)	57(1)
O(1)	2001(2)	5892(4)	5995(2)	70(1)
O(2)	3253(2)	1151(3)	6871(2)	49(1)
O(3)	-532(2)	-1421(6)	6540(3)	78(1)
C(1)	2520(3)	4491(5)	6410(3)	54(1)
C(2)	2397(2)	2020(5)	6251(2)	46(1)
C(3)	3692(2)	2903(5)	7317(2)	50(1)
C(4)	4570(2)	2415(7)	7995(3)	58(1)
C(5)	4959(4)	4018(8)	8625(4)	80(1)
C(6)	5819(5)	3538(12)	9242(6)	104(2)
C(7)	6259(4)	1547(10)	9220(6)	103(2)
C(8)	5893(4)	-89(10)	8601(6)	102(2)
C(9)	5023(3)	346(8)	7990(5)	80(1)
C(10)	2584(3)	1302(6)	5169(3)	57(1)
C(11)	3673(4)	1981(9)	4787(4)	84(1)
C(12)	3859(5)	970(18)	3772(4)	115(3)
C(13)	1384(2)	1044(5)	6677(2)	44(1)
C(14)	1327(2)	1442(5)	7793(2)	41(1)
C(15)	1656(3)	-208(6)	8454(3)	50(1)
C(16)	1639(3)	106(6)	9477(3)	57(1)
C(17)	1308(2)	2126(6)	9842(2)	52(1)
C(18)	968(3)	3772(7)	9218(3)	60(1)
C(19)	977(3)	3425(5)	8192(3)	51(1)
C(20)	384(3)	1826(7)	6124(3)	59(1)
C(21)	-562(3)	545(8)	6446(3)	61(1)
C(22)	-1533(3)	1819(12)	6655(5)	100(2)

Table 3. Bond lengths [A] and angles [deg] for mo_dm1197_0m.

Br(1)-C(17)	1.904(3)
N(1)-C(3)	1.294(5)
N(1)-C(1)	1.405(5)
O(1)-C(1)	1.206(5)
O(2)-C(3)	1.335(4)
O(2)-C(2)	1.461(4)
O(3)-C(21)	1.196(6)
C(1)-C(2)	1.517(5)
C(2)-C(10)	1.535(5)
C(2)-C(13)	1.540(4)
C(3)-C(4)	1.464(5)
C(4)-C(5)	1.373(6)
C(4)-C(9)	1.378(6)
C(5)-C(6)	1.396(8)
C(5)-H(5)	0.9300
C(6)-C(7)	1.329(9)
C(6)-H(6)	0.9300
C(7)-C(8)	1.368(9)
C(7)-H(7)	0.9300
C(8)-C(9)	1.396(7)
C(8)-H(8)	0.9300
C(9)-H(9)	0.9300
C(10)-C(11)	1.545(5)
C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700
C(11)-C(12)	1.513(8)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-H(12A)	0.9600
C(12)-H(12B)	0.9600
C(12)-H(12C)	0.9600
C(13)-C(14)	1.517(4)
C(13)-C(20)	1.541(4)
C(13)-H(13)	0.9800
C(14)-C(19)	1.390(4)
C(14)-C(15)	1.395(4)
C(15)-C(16)	1.384(5)
C(15)-H(15)	0.9300
C(16)-C(17)	1.384(5)
C(16)-H(16)	0.9300

C(17)-C(18)	1.366(5)
C(18)-C(19)	1.391(5)
C(18)-H(18)	0.9300
C(19)-H(19)	0.9300
C(20)-C(21)	1.504(6)
C(20)-H(20A)	0.9700
C(20)-H(20B)	0.9700
C(21)-C(22)	1.490(7)
C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600

C(3)-N(1)-C(1)	104.9(3)
C(3)-O(2)-C(2)	106.0(2)
O(1)-C(1)-N(1)	126.4(3)
O(1)-C(1)-C(2)	124.9(4)
N(1)-C(1)-C(2)	108.7(3)
O(2)-C(2)-C(1)	101.5(3)
O(2)-C(2)-C(10)	108.1(3)
C(1)-C(2)-C(10)	113.2(3)
O(2)-C(2)-C(13)	106.1(2)
C(1)-C(2)-C(13)	114.2(3)
C(10)-C(2)-C(13)	112.6(3)
N(1)-C(3)-O(2)	118.8(3)
N(1)-C(3)-C(4)	125.7(3)
O(2)-C(3)-C(4)	115.5(3)
C(5)-C(4)-C(9)	119.8(4)
C(5)-C(4)-C(3)	120.4(4)
C(9)-C(4)-C(3)	119.8(4)
C(4)-C(5)-C(6)	119.4(5)
C(4)-C(5)-H(5)	120.3
C(6)-C(5)-H(5)	120.3
C(7)-C(6)-C(5)	120.3(5)
C(7)-C(6)-H(6)	119.9
C(5)-C(6)-H(6)	119.9
C(6)-C(7)-C(8)	121.9(5)
C(6)-C(7)-H(7)	119.1
C(8)-C(7)-H(7)	119.1
C(7)-C(8)-C(9)	118.7(5)
C(7)-C(8)-H(8)	120.6
C(9)-C(8)-H(8)	120.6
C(4)-C(9)-C(8)	119.9(5)
C(4)-C(9)-H(9)	120.1
C(8)-C(9)-H(9)	120.1

C(2)-C(10)-C(11)	113.0(3)
C(2)-C(10)-H(10A)	109.0
C(11)-C(10)-H(10A)	109.0
C(2)-C(10)-H(10B)	109.0
C(11)-C(10)-H(10B)	109.0
H(10A)-C(10)-H(10B)	107.8
C(12)-C(11)-C(10)	110.1(4)
C(12)-C(11)-H(11A)	109.6
C(10)-C(11)-H(11A)	109.6
C(12)-C(11)-H(11B)	109.6
C(10)-C(11)-H(11B)	109.6
H(11A)-C(11)-H(11B)	108.1
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-C(2)	111.0(2)
C(14)-C(13)-C(20)	111.9(2)
C(2)-C(13)-C(20)	113.6(3)
C(14)-C(13)-H(13)	106.6
C(2)-C(13)-H(13)	106.6
C(20)-C(13)-H(13)	106.6
C(19)-C(14)-C(15)	117.9(3)
C(19)-C(14)-C(13)	122.5(3)
C(15)-C(14)-C(13)	119.6(3)
C(16)-C(15)-C(14)	121.5(3)
C(16)-C(15)-H(15)	119.3
C(14)-C(15)-H(15)	119.3
C(17)-C(16)-C(15)	118.7(3)
C(17)-C(16)-H(16)	120.7
C(15)-C(16)-H(16)	120.7
C(18)-C(17)-C(16)	121.5(3)
C(18)-C(17)-Br(1)	119.3(3)
C(16)-C(17)-Br(1)	119.1(3)
C(17)-C(18)-C(19)	119.2(3)
C(17)-C(18)-H(18)	120.4
C(19)-C(18)-H(18)	120.4
C(14)-C(19)-C(18)	121.2(3)
C(14)-C(19)-H(19)	119.4
C(18)-C(19)-H(19)	119.4
C(21)-C(20)-C(13)	111.6(3)
C(21)-C(20)-H(20A)	109.3

C(13)-C(20)-H(20A)	109.3
C(21)-C(20)-H(20B)	109.3
C(13)-C(20)-H(20B)	109.3
H(20A)-C(20)-H(20B)	108.0
O(3)-C(21)-C(22)	121.3(4)
O(3)-C(21)-C(20)	121.1(4)
C(22)-C(21)-C(20)	117.5(4)
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (Å^2 x 10^3) for mo_dm1197_0m.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Br(1)	76(1)	112(1)	44(1)	-14(1)	-2(1)	-23(1)
N(1)	66(2)	39(1)	66(2)	-6(1)	15(1)	-1(1)
O(1)	84(2)	41(1)	85(2)	10(1)	11(2)	12(1)
O(2)	53(1)	34(1)	60(1)	-5(1)	5(1)	1(1)
O(3)	76(2)	79(2)	78(2)	0(2)	4(1)	-18(2)
C(1)	62(2)	36(2)	62(2)	2(1)	19(2)	3(1)
C(2)	55(1)	38(2)	47(2)	-4(1)	8(1)	6(1)
C(3)	51(1)	40(2)	58(2)	-8(1)	14(1)	-4(1)
C(4)	54(1)	54(2)	66(2)	-6(2)	8(1)	-9(2)
C(5)	74(3)	62(2)	102(4)	-16(2)	-11(2)	-4(2)
C(6)	92(4)	97(4)	123(5)	-19(3)	-35(3)	-18(3)
C(7)	70(3)	84(4)	152(6)	9(3)	-38(3)	-14(3)
C(8)	68(3)	78(3)	158(6)	-10(4)	-33(3)	7(2)
C(9)	61(2)	65(2)	112(4)	-14(2)	-19(2)	6(2)
C(10)	72(2)	51(2)	49(2)	-4(1)	17(2)	3(2)
C(11)	85(3)	89(3)	79(3)	-5(2)	39(2)	-6(2)
C(12)	106(4)	157(7)	82(4)	-12(4)	46(4)	6(4)
C(13)	54(2)	37(1)	40(2)	-2(1)	4(1)	0(1)
C(14)	43(1)	38(1)	43(2)	-1(1)	2(1)	1(1)
C(15)	60(2)	42(2)	50(2)	0(1)	-1(1)	6(1)
C(16)	58(2)	61(2)	50(2)	8(2)	-9(1)	4(2)
C(17)	46(1)	70(2)	40(1)	-7(1)	0(1)	-10(1)
C(18)	63(2)	60(2)	56(2)	-14(2)	11(2)	5(2)
C(19)	64(2)	43(2)	47(2)	3(1)	7(1)	14(1)
C(20)	62(2)	69(2)	44(2)	6(1)	-3(1)	3(2)
C(21)	56(2)	89(3)	37(2)	7(2)	-6(1)	-7(2)
C(22)	60(2)	128(5)	110(4)	24(3)	4(2)	13(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for mo_dm1197_0m.

	x	y	z	U(eq)
H(5)	4651	5411	8641	95
H(6)	6086	4617	9670	125
H(7)	6831	1257	9636	123
H(8)	6218	-1465	8588	122
H(9)	4748	-759	7580	95
H(10A)	2049	1957	4740	69
H(10B)	2514	-292	5123	69
H(11A)	3714	3580	4741	101
H(11B)	4210	1483	5254	101
H(12A)	3839	-613	3824	172
H(12B)	4531	1424	3536	172
H(12C)	3323	1457	3312	172
H(13)	1424	-561	6583	52
H(15)	1891	-1549	8202	60
H(16)	1846	-1019	9911	68
H(18)	733	5108	9477	72
H(19)	744	4541	7766	62
H(20A)	275	3386	6257	70
H(20B)	473	1646	5411	70
H(22A)	-2053	843	6919	149
H(22B)	-1794	2474	6048	149
H(22C)	-1378	2962	7132	149

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