Catalytic Hetero-Ene Reactions of 5-Methyleneoxazoline: Highly Enantioselective Synthesis of 2,5-Disubstituted Oxazole Derivatives**

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Supporting Information

Contents:

1. General remarks

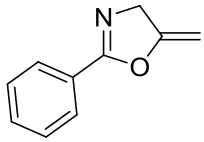
^{1}H NMR spectra were recorded on commercial instruments (400 MHz). Chemical shifts were reported in ppm from tetramethylsilane with the solvent resonance as the internal standard ($CDCl_3$, δ = 7.26). Spectra are reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz), integration, and assignment. ^{13}C NMR spectra were collected on commercial instruments (100 MHz) with complete proton decoupling. Chemical shifts are reported in ppm from the tetramethylsilane with the solvent resonance as internal standard ($CDCl_3$, δ = 77.0). The enantiomeric excess was determined by HPLC analysis on commercial chiral columns. Optical rotations were measured on a commercial polarimeter and reported as follows: $[\alpha]^{T}_{D}$ (c = g/100 mL, solvent). HR-ESIMS spectra were recorded using a commercial apparatus and methanol or acetonitrile was used to dissolve the sample. Unless otherwise indicated, reagents obtained from commercial sources were used without further purification. Solvents were dried and distilled prior to use according to the standard methods. Starting materials of alkylideneoxazolines were prepared according to the previous reports. [1] All α-ketoesters were prepared according to the literatures.[2] The synthesis method of glyoxal derivatives were according to the reported procedure.[3]

2. General procedure for chiral *N,N'*-dioxide preparation

The *N,N'*-dioxide ligands **L1**-**L6** were synthesized by the same procedure in the literature.[4]

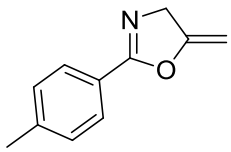
3. Characterization of alkylideneoxazolines 2

5-methylene-2-phenyl-4,5-dihydrooxazole 2a



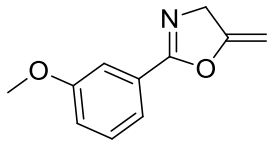
^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.09 – 7.78 (m, 2H), 7.51 – 7.22 (m, 3H), 4.73 (d, *J* = 2.8 Hz, 1H), 4.56 (s, 2H), 4.27 (d, *J* = 2.4 Hz, 1H). ^{13}C NMR (100MHz, $CDCl_3$) δ = 163.71, 158.87, 131.79, 128.48, 128.00, 126.79, 83.74, 57.76.

5-methylene-2-(p-tolyl)-4,5-dihydrooxazole 2b



^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.00 – 7.73 (m, 2H), 7.32 – 7.20 (m, 2H), 4.80 (dd, *J* = 5.6 Hz, 2.8 Hz, 1H), 4.64 (t, *J* = 2.8 Hz, 1H), 4.35 (dd, *J* = 5.2 Hz, 2.8 Hz, 1H), 2.41 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 163.82, 158.93, 142.31, 129.25, 127.97, 123.95, 83.57, 57.72, 21.65.

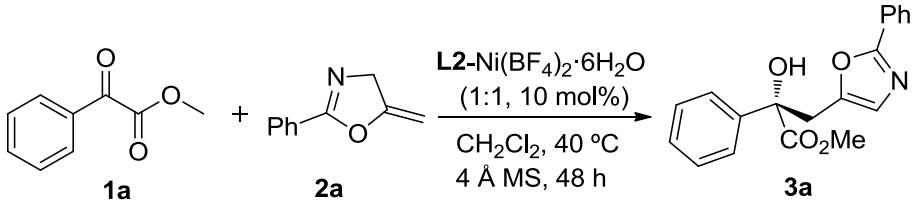
2-(3-methoxyphenyl)-5-methylene-4,5-dihydrooxazole 2c



^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.52 – 7.44 (m, 1H), 7.44 – 7.37 (m, 1H), 7.30 – 7.21 (m, 1H), 7.02 – 6.91 (m, 1H), 4.73 (dd, *J* = 6.0 Hz, 2.8 Hz, 1H), 4.56 (t, *J* = 2.4 Hz, 1H), 4.27 (dd, *J* = 5.2 Hz, 2.8 Hz, 1H), 3.76 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 162.61, 158.50, 157.74, 128.53, 126.87, 119.42, 117.55, 111.14, 82.80, 56.68, 54.35.

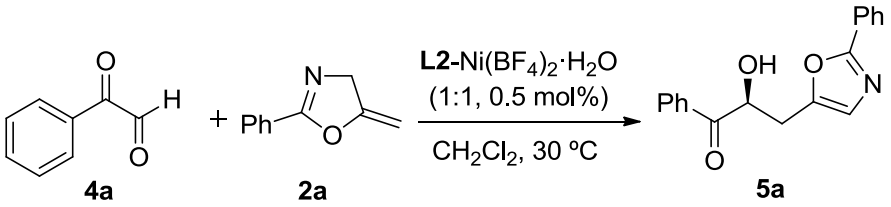
4. Typical procedure for the asymmetric hetero-ene reaction of dicarbonyl compounds

(a) Typical procedure for the asymmetric hetero-ene reaction of α-ketoesters



A dry reaction tube was charged with **L2**-Ni$(BF_4)_2$•$6H_2O$ (1:1, 10 mol%), 4 Å M.S. (20.0 mg), and α-ketoester **1a** (0.2 mmol). CH_2Cl_2 (1.0 mL) was added, and the mixture was stirred at 30 ^oC for 0.5 h. Then, the methyleneoxazoline **2a** (2.0 equiv) was added to the reaction mixture at 40 ^oC. The reaction mixture was stirred at 40 ^oC for 48 h. The crude reaction mixture was purified by flash chromatography on silica gel (petroleum ether/ethyl acetate = 4/1) to afford the corresponding product **3a** in 97% yield as a colourless liquid. The enantiomeric excess of **3a** was determined to be >99% ee by using chiral HPLC analysis.

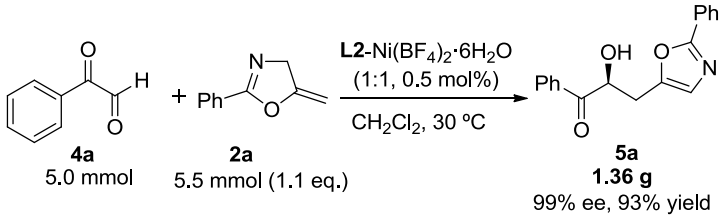
(b) Typical procedure for the asymmetric hetero-ene reaction of glyoxal derivatives



1) The preparation of the catalyst solution. In a 2.0 mL of volumetric flask, Ni$(BF_4)_2$ $6H_2O$ (3.4 mg, 0.01 mmol) and **L2** (6.5 mg, 0.01 mmol) were added, then 2.0 mL THF were added and stirred.

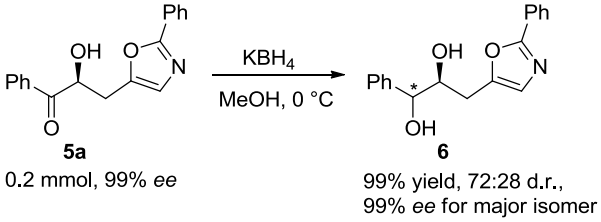
2) In a test tube, 100 μL (0.5 mol%) of the catalyst solution was added, and THF was removed under vacuum. Later, phenylglyoxal **4a** (0.1 mmol) and 1.0 mL of CH_2Cl_2 were added under air. The mixture was stirred at 30 ^oC for 0.5 h. and then the methyleneoxazoline **2a** (1.1 equiv) was added to the reaction mixture at 30 ^oC. After being stirred at 30 ^oC for 24 h, the crude reaction mixture was purified by flash chromatography on silica gel (petroleum ether/ethyl acetate = 3/1) to afford the corresponding product **5a** in 99% yield as a yellow amorphous solid. The enantiomeric excess of **5a** was determined to be >99% ee by using chiral HPLC analysis.

(c) Asymmetric hetero-ene reaction of phenylglyoxal on a gram scale.



A flask (100 mL) was charged with $Ni(BF_4)_2$ $6H_2O$ (8.5 mg, 0.025 mmol), **L2** (16.2 mg, 0.025 mmol) and phenylglyoxal **4a** (5 mmol). Then, CH_2Cl_2 (20 mL) was added and the mixture was stirred at 30 ℃ for 0.5 h. Finally, the methyleneoxazoline **2a** (0.88 g, 5.5 mmol, 1.1 equiv) and CH_2Cl_2 (10 mL) were added under stirring. The reaction mixture was stirred at 30 ℃ for 24 h. After evaporation of the solvents, the residue was purified by flash chromatography (petroleum ether/ethyl acetate = 2/1) on silica gel to afford the product **5a** as a yellow solid (1.362 g, 93% yield, 99% ee).

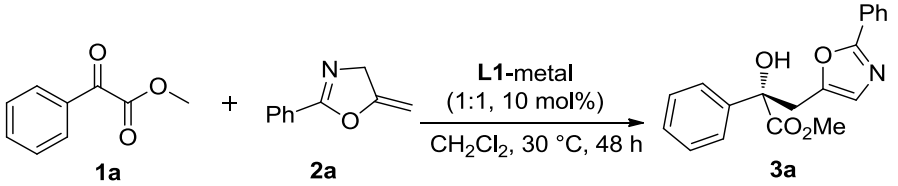
5. Experimental procedure for the transformations of the products 5a



To a solution of adducts **5a** (58.7 mg, 0.20 mmol) in CH_3OH (1.0 mL) was added KBH_4(16.2 mg, 1.5 equiv) at 0 ℃. The mixture was allowed to stir for 1 h. Excess of KBH_4 was quenched with cold water. Organic layer was extracted with CH_2Cl_2, dried over anhydrous Na_2SO_4 and the solvent was evaporated by rotary evaporator. The residue was then purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 2/1) to afford **6** (58.8 mg, 99% yield) as a white solid.

6. Optimization of the reaction conditions

6.1 Screening of metal.[a]

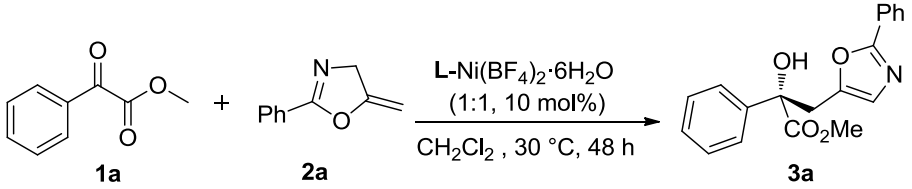


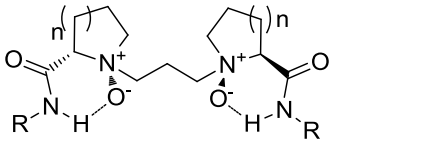
Entry	Ligand	Metal	Yield [%][b]	Ee [%][c]
1	**L1**	$Cu(OTf)_2$	0	–
2	**L1**	$Zn(OTf)_2$	0	–
3	**L1**	$Mg(OTf)_2$	7	98
4	**L1**	$Yb(OTf)_3$	29	83
5	**L1**	$Y(OTf)_3$	69	87
6	**L1**	$Sc(OTf)_3$	trace	–
7	**L1**	$Co(BF_4)_2$ $6H_2O$	8	98

8	**L1**	$Ni(BF_4)_2$ $6H_2O$	16	>99

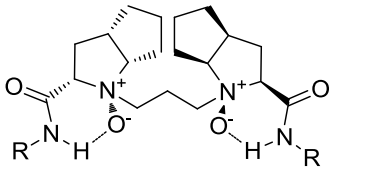
[a] Unless otherwise noted, all reactions were carried out with **1a** (0.1 mmol) and 1.1 equiv of **2a** in CH_2Cl_2(1.0 mL) at 30 ℃ for 48 h. [b] Yield of isolated product. [c] Determined by HPLC analysis using a Chiralcel IB column.

6.2 Screening of the ligands.[a]





L1: n = 1, R = 2,6-diisopropanylphenyl
L2: n = 2, R = 2,6-diisopropanylphenyl
L4: n = 2, R = phenyl
L5: n = 1, R = phenyl

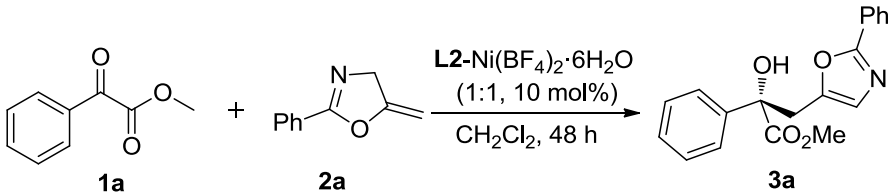


L3: R = 2,6-diisopropanylphenyl
L6: R = 2,4,6-triisopropanylphenyl

Entry	Ligand	Metal	Yield [%][b]	Ee [%][c]
1	**L1**	$Ni(BF_4)_2$ $6H_2O$	16	>99
2	**L2**	$Ni(BF_4)_2$ $6H_2O$	59	>99
3	**L3**	$Ni(BF_4)_2$ $6H_2O$	31	97
4	**L4**	$Ni(BF_4)_2$ $6H_2O$	7	92
5	**L5**	$Ni(BF_4)_2$ $6H_2O$	9	75
6	**L6**	$Ni(BF_4)_2$ $6H_2O$	41	>99

[a] Unless otherwise noted, all reactions were carried out with **1a** (0.1 mmol) and 1.1 equiv of **2a** in CH_2Cl_2(1.0 mL) at 30 ℃ for 48 h. [b] Yield of isolated product. [c] Determined by HPLC analysis using a Chiralcel IB column.

6.3 Optimization of other conditions.[a]



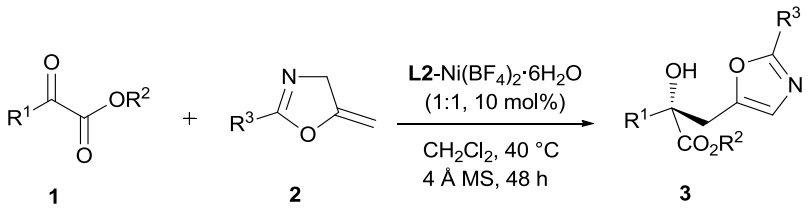
Entry	T[℃]	solvent	additive	Yield [%][b]	Ee [%][c]
1	30	CH_2Cl_2	–	59	>99
2	30	$CHCl_3$	–	39	>99
3	30	CH_2ClCH_2Cl	–	54	>99
4	30	CH_2Cl_2	3 Å MS(20 mg)	80	>99
5	30	CH_2Cl_2	4 Å MS(20 mg)	81	>99
6	30	CH_2Cl_2	5 Å MS(20 mg)	58	>99
7	40	CH_2Cl_2	–	64	>99
8	40	CH_2Cl_2	4 Å MS(20 mg)	86	>99

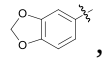
9	40	CH_2Cl_2	4 Å MS(10 mg)	75	>99
10	40	CH_2Cl_2	4 Å MS(50 mg)	71	>99
11[d]	40	CH_2Cl_2	4 Å MS(20 mg)	93	>99
12[e]	40	CH_2Cl_2	4 Å MS(20 mg)	95	>99
13[e,f]	40	CH_2Cl_2	4 Å MS(20 mg)	97	>99

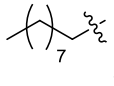
[a] Unless otherwise noted, all reactions were carried out with **1a** (0.1 mmol) and 1.1 equiv of **2a** in CH_2Cl_2 (1.0 mL) at 30 ℃ for 48 h. [b] Yield of isolated product. [c] Determined by HPLC analysis using a Chiralcel IB column. [d] 1.5 equiv of **2a** was used. [e] 2.0 equiv of **2a** was used. [f] The reaction was carried out with **1a** (0.2 mmol) in CH_2Cl_2 (1.0 mL).

7. Full list of substrates

Table 1. Substrate scope for the catalytic asymmetric hetero-ene reaction of α-ketoesters.

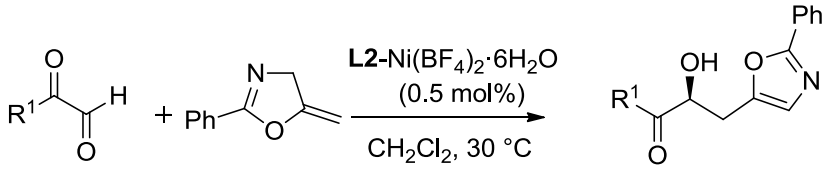


Entry[a]	**1**, R^1, R^2	**2**, R^3	Yield[b] (%)	*ee*[c] (%)
1	**1a**, C_6H_5, Me	**2a**, C_6H_5	97 **(3a)**	>99
2	**1a**[2], C_6H_5, Et	**2a**, C_6H_5	99 **(3a**[2]**)**	>99
3	**1a**[3], C_6H_5, iPr	**2a**, C_6H_5	98 **(3a**[3]**)**	>99
4	**1a**[4], C_6H_5, *t*Bu	**2a**, C_6H_5	98 **(3a**[4]**)**	>99
5	**1b**, 3-MeC_6H_4, Me	**2a**, C_6H_5	95 **(3b)**	>99
6	**1c**, 4-MeC_6H_4, Me	**2a**, C_6H_5	77 **(3c)**	>99
7[d]	**1d**, 2-MeOC_6H_4, Me	**2a**, C_6H_5	42 **(3d)**	99
8	**1e**, 3-MeOC_6H_4, Me	**2a**, C_6H_5	97 **(3e)**	>99 (*S*)[e]
9	**1f**, 4-MeOC_6H_4, Me	**2a**, C_6H_5	63 **(3f)**	>99
10	**1g**,  , Me	**2a**, C_6H_5	66 **(3g)**	>99
11	**1h**, 3-FC_6H_4, Me	**2a**, C_6H_5	99 **(3h)**	>99
12	**1i**, 4-FC_6H_4, Me	**2a**, C_6H_5	95 **(3i)**	>99
13	**1j**, 3-ClC_6H_4, Me	**2a**, C_6H_5	98 **(3j)**	>99
14	**1k**, 4-ClC_6H_4, Me	**2a**, C_6H_5	99 **(3k)**	>99
15	**1l**, 3-F_3CC_6H_4, Me	**2a**, C_6H_5	99 **(3l)**	>99
16	**1m**, 4-F_3CC_6H_4, Me	**2a**, C_6H_5	97 **(3m)**	99
17	**1n**, 3-CH_2=CHC_6H_4, Me	**2a**, C_6H_5	97 **(3n)**	>99
18	**1o**, 4-CH_2=CHC_6H_4, Me	**2a**, C_6H_5	95 **(3o)**	>99
19	**1p**, 3,5-$Me_2C_6H_3$, Me	**2a**, C_6H_5	93 **(3p)**	>99
20	**1q**, 3-iPrC_6H_4, Me	**2a**, C_6H_5	95 **(3q)**	>99
21	**1r**, 4-*t*BuC_6H_4, Me	**2a**, C_6H_5	96 **(3r)**	>99
22	**1s**, 4-PhC_6H_4, Me	**2a**, C_6H_5	95 **(3s)**	>99

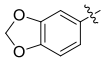
23	**1t**, 2-naphthyl, Me	**2a**, C_6H_5	98 **(3t)**	>99
24	**1u**, 2-thienyl, Et	**2a**, C_6H_5	98 **(3u)**	99
25	**1v**, 2-furyl, Me	**2a**, C_6H_5	96 **(3v)**	>99
26	**1w**, *c*-hexyl, Me	**2a**, C_6H_5	40 **(3w)**	>99
27	**1x**, Me, Me	**2a**, C_6H_5	84 **(3x)**	>99
28	**1y**,  , Et	**2a**, C_6H_5	75**(3y)**	>99
29	**1a**, C_6H_5, Me	**2b**, 3-$MeOC_6H_4$	91**(3ba)**	>99
30	**1a**, C_6H_5, Me	**2c**, 4-MeC_6H_4	98 **(3ca)**	>99

[a] Unless otherwise noted, all reactions were carried out with 10 mol% of **L2**-Ni$(BF_4)_2$•$6H_2O$, 0.2 mmol of α-ketoester **1**, 2.0 equiv of **2**, and 20 mg of 4 Å MS in CH_2Cl_2 (1.0 mL) at 40 °C for 48 h. [b] Isolated yield. [c] Determined by HPLC analysis. [d] The reaction was carried out for 96 h. [e] The absolute configuration was determined by X-ray analysis.

Table 2. Substrate scope for the catalytic asymmetric hetero-ene reaction of glyoxal derivatives.



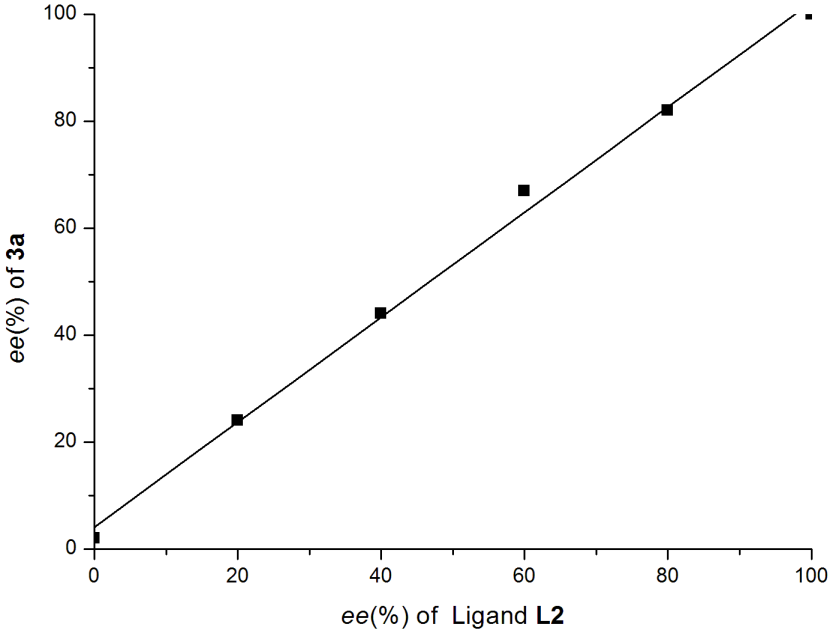
4 **2a** **5**

Entry	R^1	Product	Yield[%][b]	*ee*[%][c]
1	Ph	**5a**	99	>99
2	2-MeC_6H_4	**5b**	98	>99
3	3-MeC_6H_4	**5c**	96	>99
4	4-MeC_6H_4	**5d**	97	99
5	3-$MeOC_6H_4$	**5e**	86	>99
6	4-$MeOC_6H_4$	**5f**	92	>99
7	3,4-$(MeO)_2C_6H_3$	**5g**	99	>99
8		**5h**	83	>99
9	3-ClC_6H_4	**5i**	98	>99
10	4-ClC_6H_4	**5j**	90	99
11	3,4-$Cl_2C_6H_3$	**5k**	93	98
12	4-FC_6H_4	**5l**	84	99
13	4-BrC_6H_4	**5m**	93	>99(*S*)[d]
14[e]	3-$O_2NC_6H_4$	**5n**	70	95
15[e]	4-$O_2NC_6H_4$	**5o**	83	97
16	4-$F_3CC_6H_4$	**5p**	94	98
17	4-NCC_6H_4	**5q**	60	97
18	1-naphthyl	**5r**	99	>99
19	2-naphthyl	**5s**	99	>99
20	2-thienyl	**5t**	99	98
21	c-hexyl	**5u**	84	96
22[f]	Me	**5v**	97	96
23	OEt	**5w**	99	99

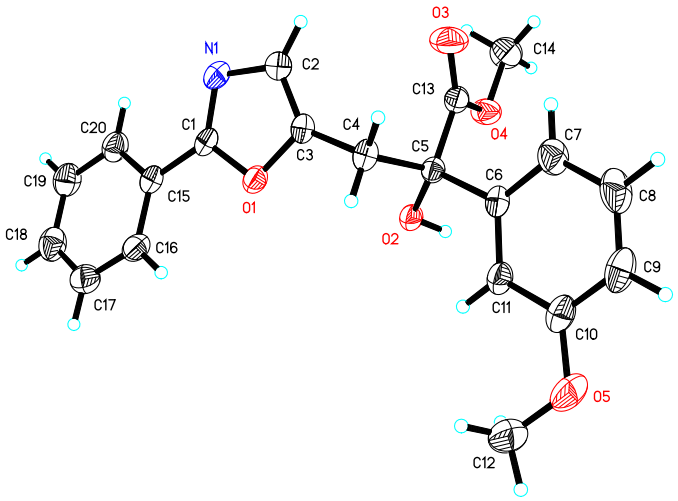
[a] Unless otherwise noted, all reactions were carried out with 0.5 mol% L2-Ni$(BF_4)_2$•$6H_2O$, 0.1 mmol of glyoxal derivative (glyoxylate), and 1.1 equiv of **2a** in CH_2Cl_2 (1.0 mL) at 30 °C for 24 h. [b] Isolated yield. [c] Determined by HPLC analysis. [d] The absolute configuration was determined by X-ray analysis. [e] The reaction was carried out for 48 h. [f] Using 2.5 mol% of the catalyst.

8. Proposed mechanism

8.1 Nonlinear effect

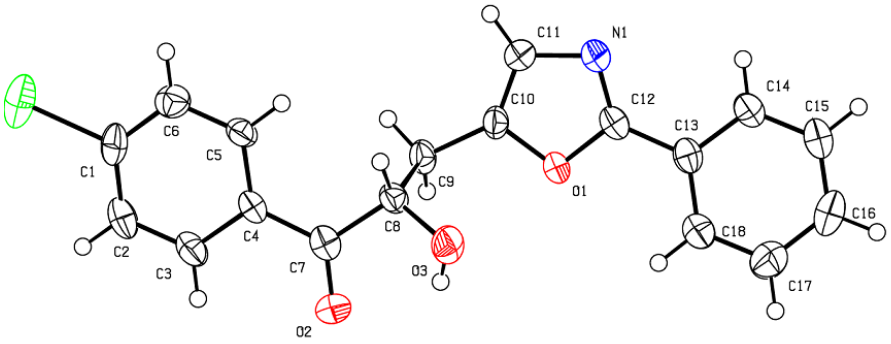


8.2 X-ray crystallographic structure of the product **3h**.



Single crystals of $C_{20}H_{19}NO_5$ **3h** were crystallized from mixed solvents of CH_2Cl_2 and petroleum ether. The absolute configuration of C5 is *S*. The thermal ellipsoids' level is 30 % for the above crystal structure.

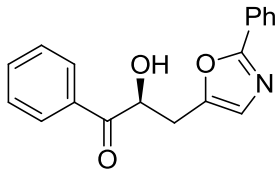
7.3 X-ray crystallographic structure of the product **5m**.



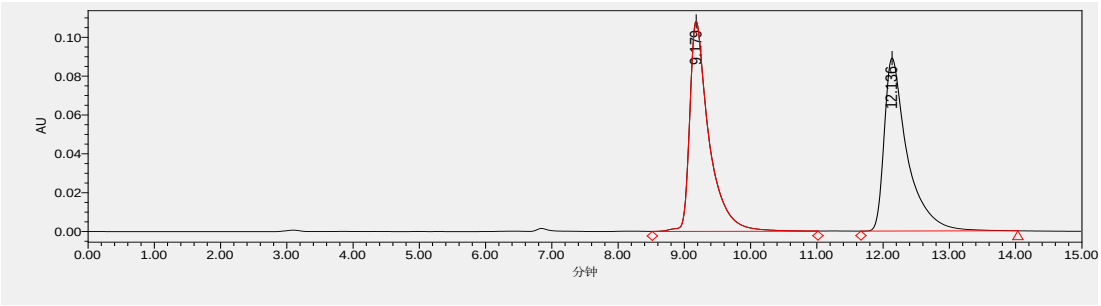
Single crystals of $C_{18}H_{14}BrNO_3$ **5m** were crystallized from mixed solvents of CH_2Cl_2 and petroleum ether. The absolute configuration of C8 is *S*. The thermal ellipsoids' level is 30 % for the above crystal structure.

9. Characterization of the hetero-ene reaction products

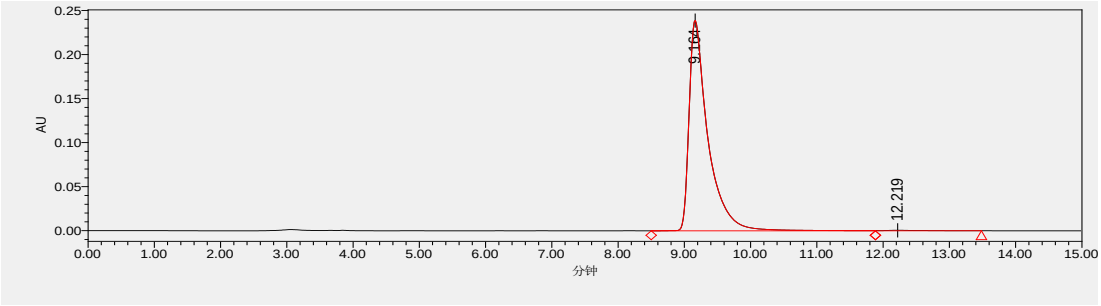
2-hydroxy-1-phenyl-3-(2-phenyloxazol-5-yl)propan-1-one 5a

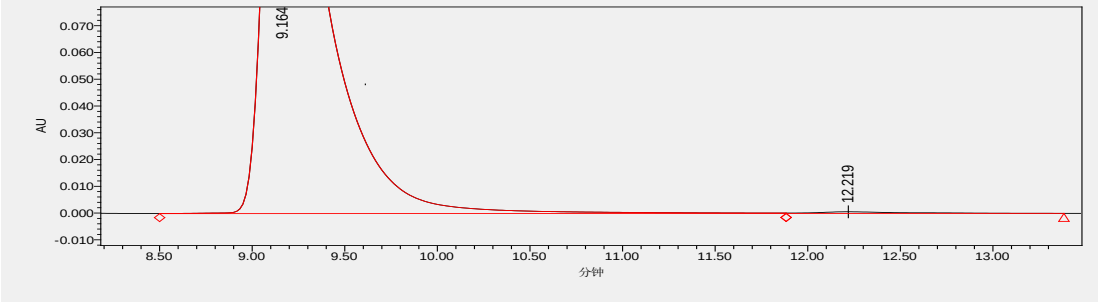


($C_{18}H_{15}NO_3$) a yellow amorphous solid; 99% yield, >99% ee. $[\alpha]_D^{20}$ = –15.8 (*c* 0.512 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 9.16 min (major), 12.22 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.90 – 7.74 (m, 4H), 7.58 – 7.48 (m, 1H), 7.45 – 7.36 (m, 2H), 7.34 – 7.24 (m, 3H), 6.82 (s, 1H), 5.40 – 5.15 (t, *J* = 5.6 Hz, 1H), 4.04 (s, 1H), 3.21 (dd, *J* = 15.6, 4.4 Hz, 1H), 3.01 (dd, *J* = 15.6, 6.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 200.27, 161.27, 147.53, 134.28, 133.59, 130.17, 129.06, 128.71, 128.57, 127.39, 126.31, 126.13, 71.33, 32.44. ESI-HRMS: calcd for $C_{18}H_{16}NO_3^+$ ([M+H$^+$]) 294.1125, found 294.1128.



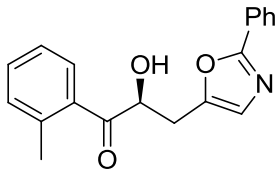
	Retention Time	Area	% Area	Height
1	9.179	2189876	50.40	108241
2	12.136	2154935	49.60	89118



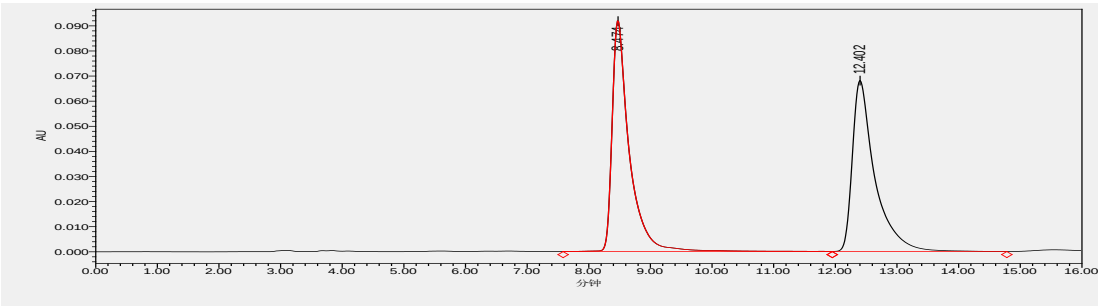


	Retention Time	Area	% Area	Height
1	9.164	4724319	99.57	238971
2	12.219	20308	0.43	614

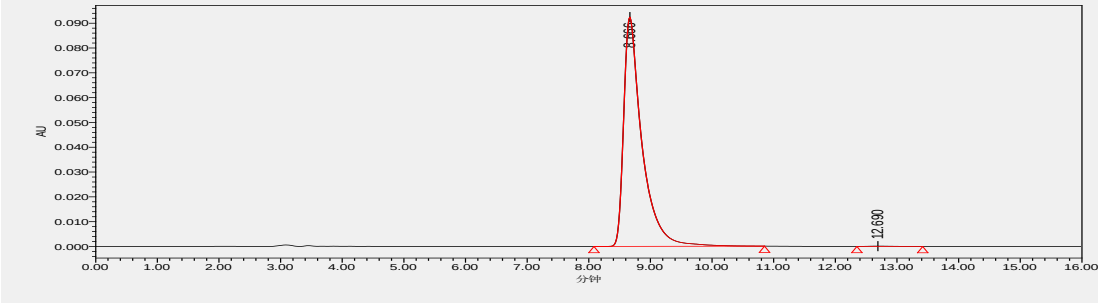
2-hydroxy-3-(2-phenyloxazol-5-yl)-1-(o-tolyl)propan-1-one 5b

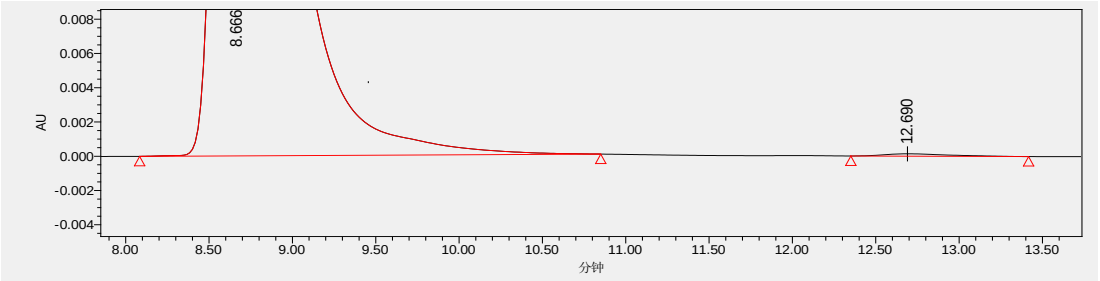


($C_{19}H_{17}NO_3$) a white amorphous solid; 98% yield, >99% ee. $[\alpha]_D^{20}$ = −13.7 (*c* 1.124 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB，n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 8.67 min (major), 12.69 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.90 – 7.76 (m, 2H), 7.72 – 7.57 (m, 2H), 7.47 – 7.24 (m, 5H), 6.83 (s, 1H), 5.38 – 5.22 (m, 1H), 3.91 (d, *J* = 6.4 Hz, 1H), 3.27 – 3.12 (m, 1H), 3.04 (m, 1H), 2.34 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 199.50, 160.22, 146.41, 138.02, 134.07, 132.59, 129.11, 128.00, 127.87, 127.66, 126.42, 125.33, 125.08, 124.67, 70.29, 31.58, 20.32. ESI-HRMS: calcd for $C_{19}H_{17}NNaO_3^+$ ([M+Na$^+$]) 330.1101, found 330.1102.



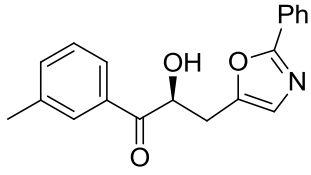
	Retention Time	Area	% Area	Height
1	8.474	1791378	50.99	92180
2	12.402	1721917	49.01	68165





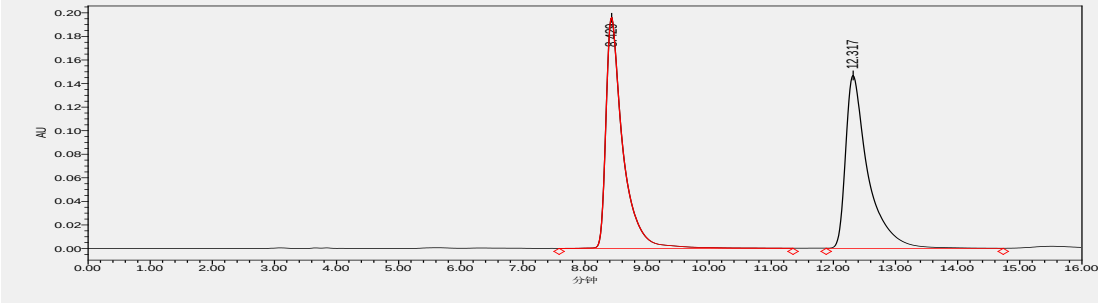
	Retention Time	Area	% Area	Height
1	8.666	1900867	99.80	92429
2	12.690	3749	0.20	138

2-hydroxy-3-(2-phenyloxazol-5-yl)-1-(m-tolyl)propan-1-one 5c

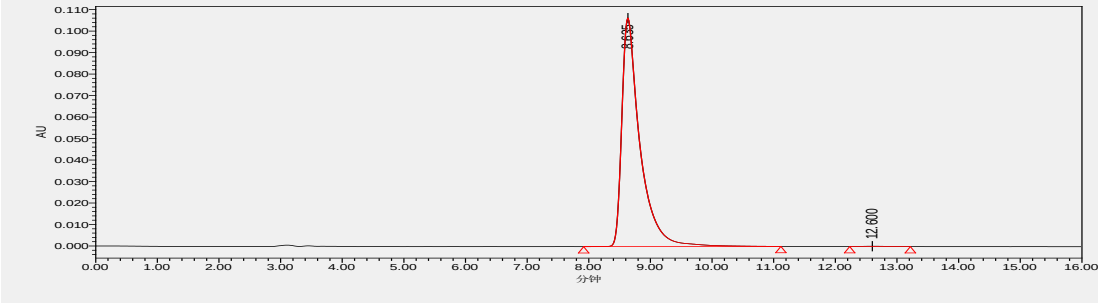


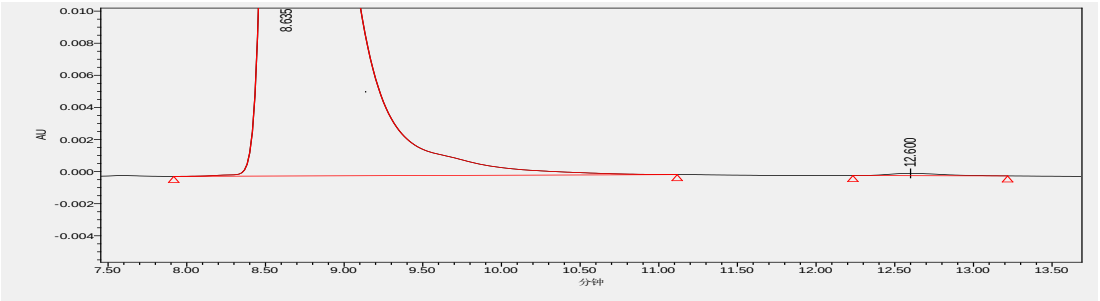
($C_{19}H_{17}NO_3$) a white amorphous solid; 96% yield, >99% ee.

$[\alpha]_D^{20}$ = −15.8 (*c* 1.154 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB，n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 8.64 min (major), 12.60 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.05 – 7.65 (m, 4H), 7.53 – 7.28 (m, 5H), 6.91 (s, 1H), 5.39 (dd, *J* = 11.2, 6.4 Hz, 1H), 4.12 (d, *J* = 6.8 Hz, 1H), 3.29 (dd, *J* = 15.6, 4.8 Hz, 1H), 3.11 (dd, *J* = 15.5, 6.4 Hz, 1H), 2.40 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 200.53, 161.22, 147.50, 139.02, 135.10, 133.63, 130.15, 129.05, 128.90, 128.70, 127.41, 126.35, 126.10, 125.72, 71.33, 32.54, 21.37. ESI-HRMS: calcd for $C_{19}H_{17}NNaO_3^+$ ([M+Na$^+$]) 330.1101, found 330.1101.



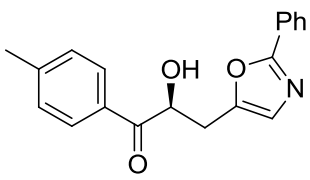
	Retention Time	Area	% Area	Height
1	8.429	3725571	50.42	196025
2	12.317	3664008	49.58	146823





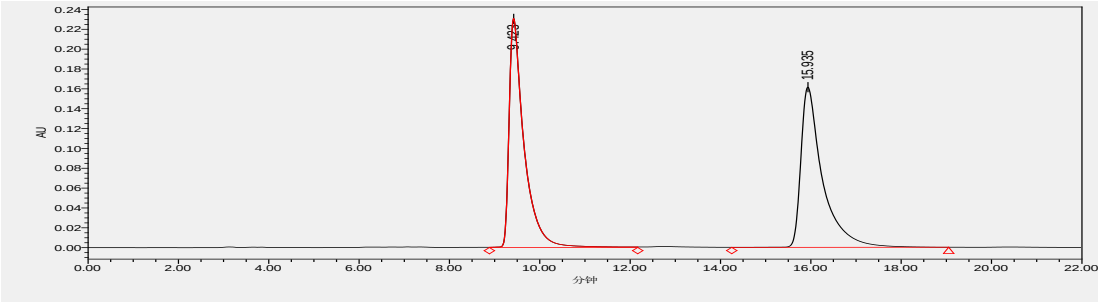
	Retention Time	Area	% Area	Height
1	8.635	2166982	99.84	106400
2	12.600	3368	0.16	145

2-hydroxy-3-(2-phenyloxazol-5-yl)-1-(p-tolyl)propan-1-one 5d

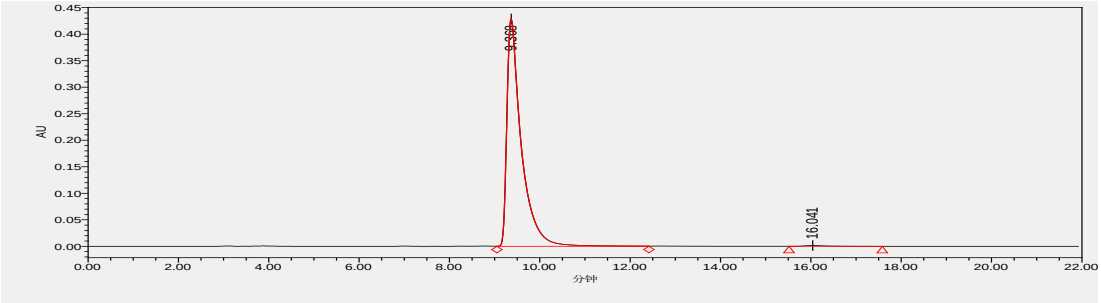


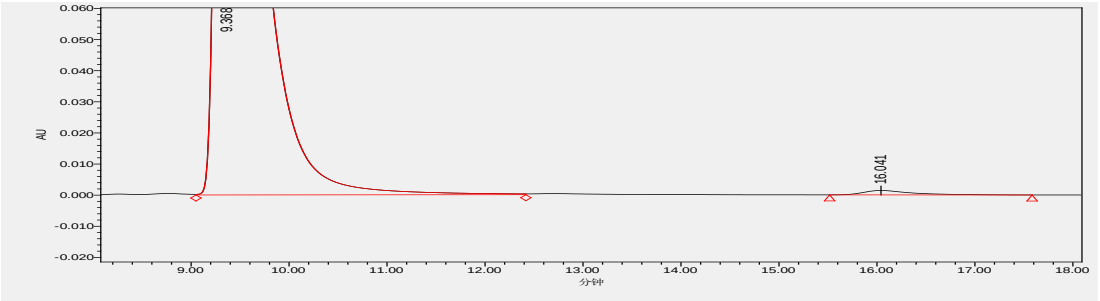
($C_{19}H_{17}NO_3$) a white amorphous solid; 97% yield, 99% ee. $[\alpha]_D^{20}$ = −37.3 (*c* 1.068 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB，n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254

nm, retention time: 9.37 min (major), 16.04 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.93 – 7.63 (m, 4H), 7.44 – 7.11 (m, 5H), 6.83 (s, 1H), 5.28 (dd, *J* = 11.2, 6.4 Hz, 1H), 4.04 (d, *J* = 6.8 Hz, 1H), 3.20 (dd, *J* = 15.6, 4.4 Hz, 1H), 3.00 (dd, *J* = 15.6, 6.4 Hz, 1H), 2.31 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 199.80, 161.22, 147.63, 145.46, 130.94, 130.13, 129.76, 128.69, 127.44, 126.29, 126.11, 71.20, 32.65, 21.81. ESI-HRMS: calcd for $C_{19}H_{17}NNaO_3^+$ ([M+Na^+]) 330.1101, found 330.1103.



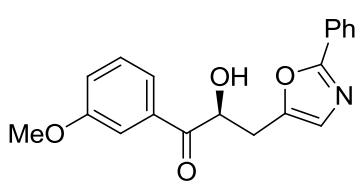
	Retention Time	Area	% Area	Height
1	9.423	5309888	49.79	231081
2	15.935	5353801	50.21	161486





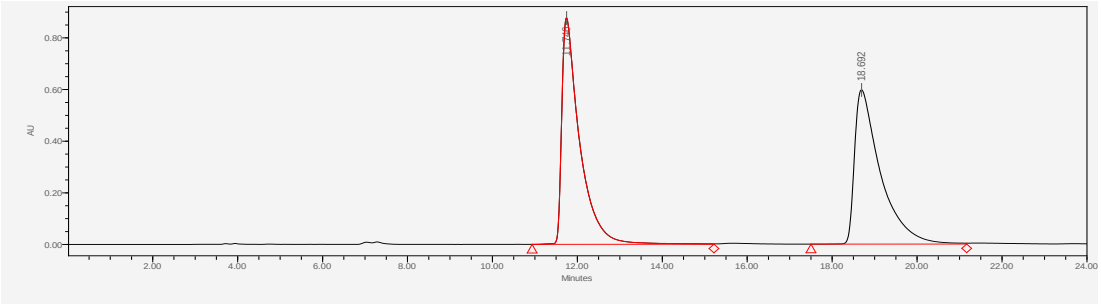
	Retention Time	Area	% Area	Height
1	9.368	9473719	99.48	428907
2	16.041	49699	0.52	1423

2-hydroxy-1-(3-methoxyphenyl)-3-(2-phenyloxazol-5-yl)propan-1-one 5e

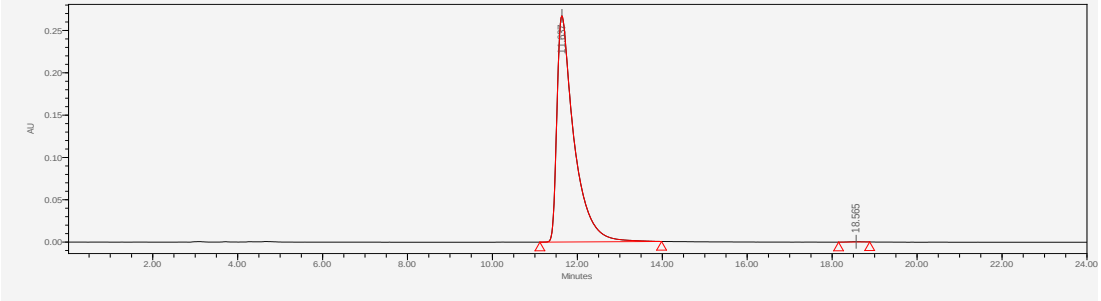


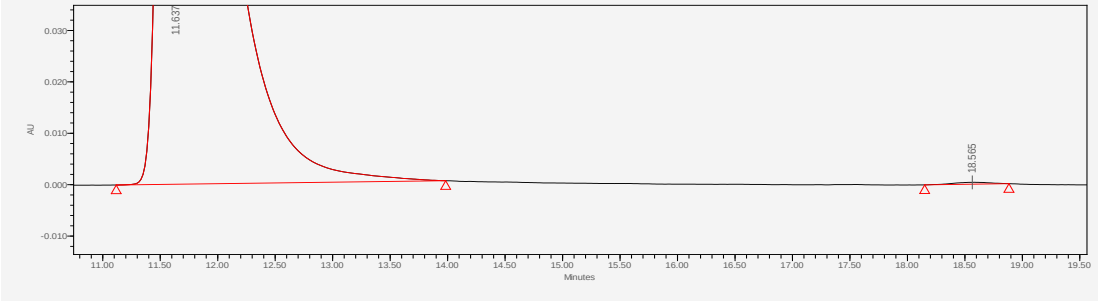
($C_{19}H_{17}NO_4$) a yellow viscous liquid; 86% yield, >99% ee. $[\alpha]_D^{20}$ = +4.0 (*c* 1.276 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB，n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 11.64 min (major), 18.57 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.95 – 7.66 (m, 2H), 7.48 – 7.22 (m, 6H), 7.15 – 6.98 (m, 1H), 6.82 (s, 1H), 5.28 (s, 1H), 4.00 (s,

1H), 3.74 (s, 3H), 3.21 (dd, *J* = 15.2, 4.4 Hz, 1H), 3.02 (dd, *J* = 15.6, 6.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 200.18, 161.25, 160.09, 147.48, 134.91, 130.14, 130.03, 128.68, 127.42, 126.35, 126.12, 120.92, 120.60, 112.98, 71.44, 55.48, 32.55. ESI-HRMS: calcd for $C_{19}H_{17}NNaO_4^+$ ([M+Na$^+$]) 346.1050, found 346.1057.



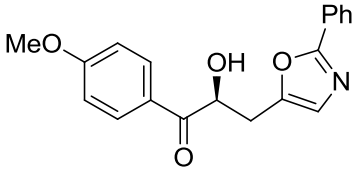
	Retention Time	Area	% Area	Height
1	11.746	25696832	50.39	877085
2	18.692	25304055	49.61	597721





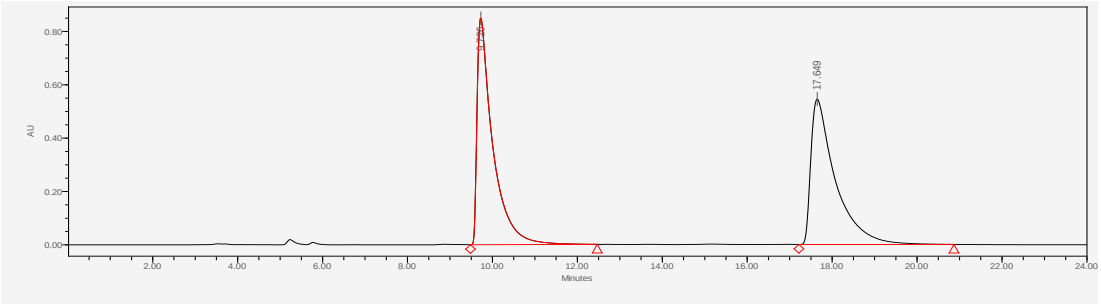
	Retention Time	Area	% Area	Height
1	11.637	7480915	99.89	267390
2	18.565	8006	0.11	359

2-hydroxy-1-(4-methoxyphenyl)-3-(2-phenyloxazol-5-yl)propan-1-one 5f

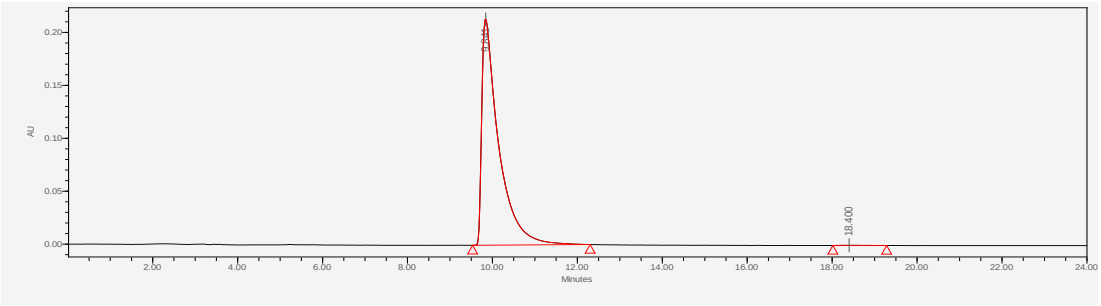


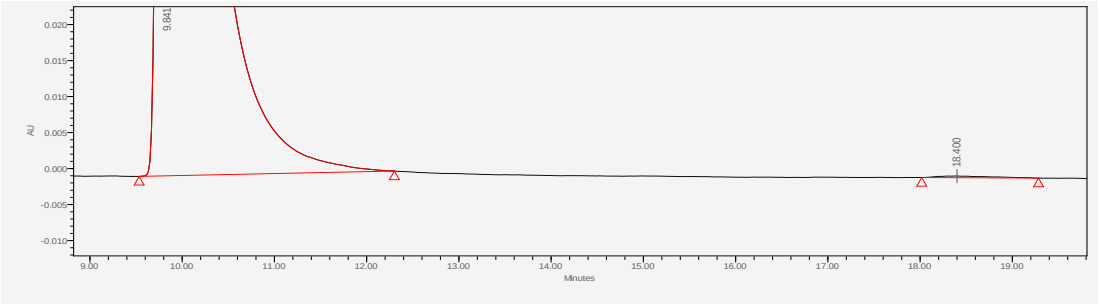
($C_{19}H_{17}NO_4$) a yellow viscous liquid; 92% yield, >99% ee. $[\alpha]_D^{20}$ = −32.3 (*c* 1.188 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB，n-hexane/2-propanol = 70/30, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 9.84 min (major), 18.40 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.00 – 7.81 (m, 4H), 7.52 – 7.36 (m, 3H), 7.03 – 6.89 (m, 3H), 5.34 (dd, *J* = 11.2, 6.8 Hz, 1H), 4.13 (d, *J* = 6.8 Hz, 1H), 3.85 (s, 3H), 3.28 (dd, *J* = 15.6, 4.4 Hz, 1H), 3.08 (dd, *J* = 15.6, 6.8 Hz,

1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 198.45, 164.42, 161.20, 147.75, 130.96, 130.12, 128.69, 127.46, 126.25, 126.21, 126.09, 114.30, 70.91, 55.61, 32.88. ESI-HRMS: calcd for $C_{19}H_{17}NNaO_4^+$ ([M+Na$^+$]) 346.1050, found 346.1055.



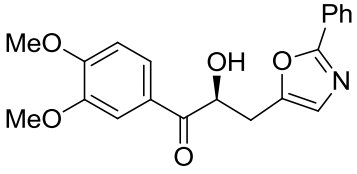
	Retention Time	Area	% Area	Height
1	9.726	21804311	50.05	851865
2	17.649	21760023	49.95	545560





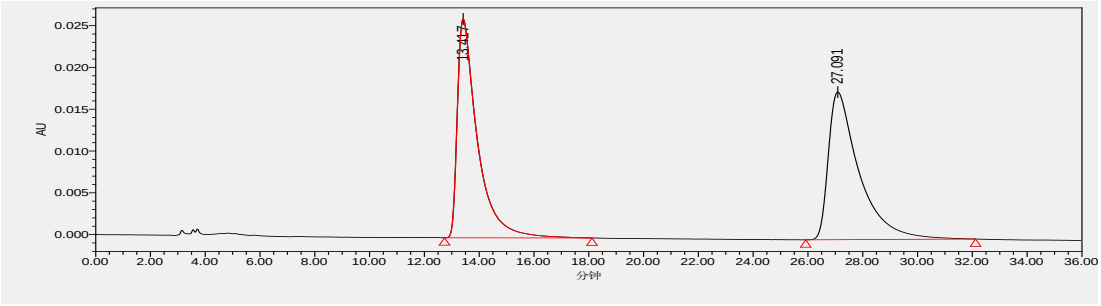
	Retention Time	Area	% Area	Height
1	9.841	5899475	99.84	214016
2	18.400	9696	0.16	226

1-(3,4-dimethoxyphenyl)-2-hydroxy-3-(2-phenyloxazol-5-yl)propan-1-one 5g

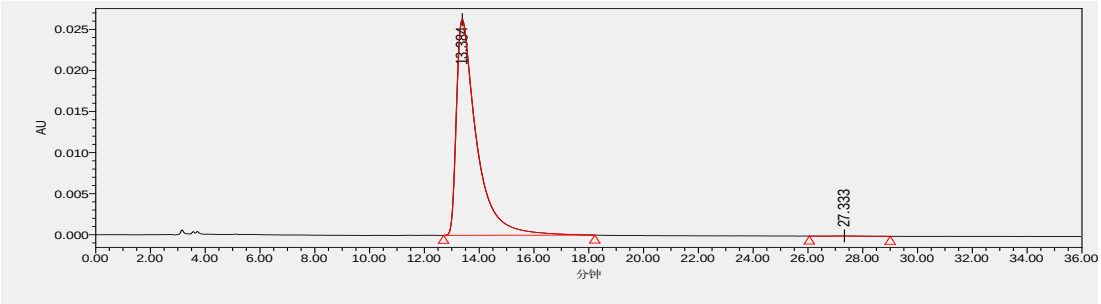


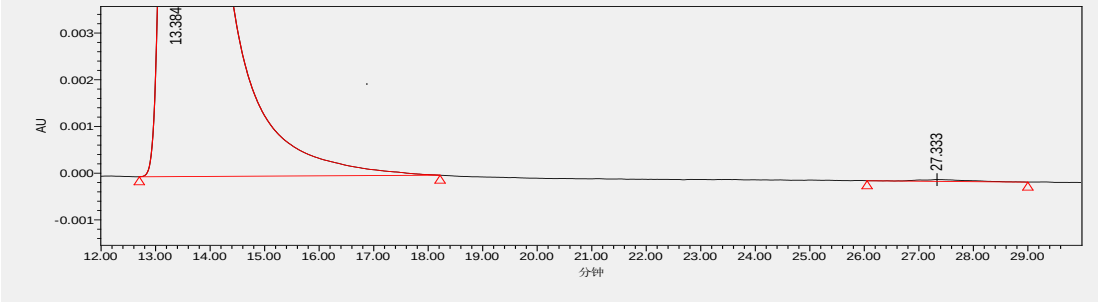
($C_{20}H_{19}NO_5$) a yellow amorphous solid; 99% yield, >99% ee. $[\alpha]_D^{20}$ = −15.6 (*c* 0.860 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB，n-hexane/2-propanol = 70/30, flow rate = 1.0 mL/min, λ = 254 nm, retention time:13.38 min (major), 27.33 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.96 – 7.81 (m, 2H), 7.61 – 7.49 (m, 2H), 7.48 – 7.34 (m, 3H), 7.00 – 6.81 (m, 2H), 5.36 (dd, *J* = 11.2, 6.4 Hz, 1H), 4.07 (d, *J* = 6.8 Hz, 1H), 3.93 (s, 6H), 3.30 (dd, *J* = 15.6, 4.8 Hz, 1H), 3.13 (dd, *J* = 15.6, 6.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 198.57, 161.20, 154.29, 149.52, 147.66, 130.15, 128.68, 127.43, 126.47, 126.29, 126.06, 123.23, 110.56, 110.28, 70.88, 56.16,

56.04, 33.13. ESI-HRMS: calcd for $C_{20}H_{19}NNaO_5^+$ ([M+Na^+]) 376.1155, found 376.1161.



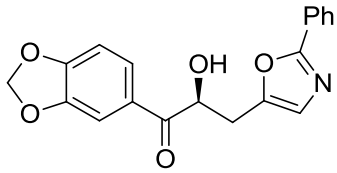
	Retention Time	Area	% Area	Height
1	13.417	1331908	49.13	26177
2	27.091	1379107	50.87	17671



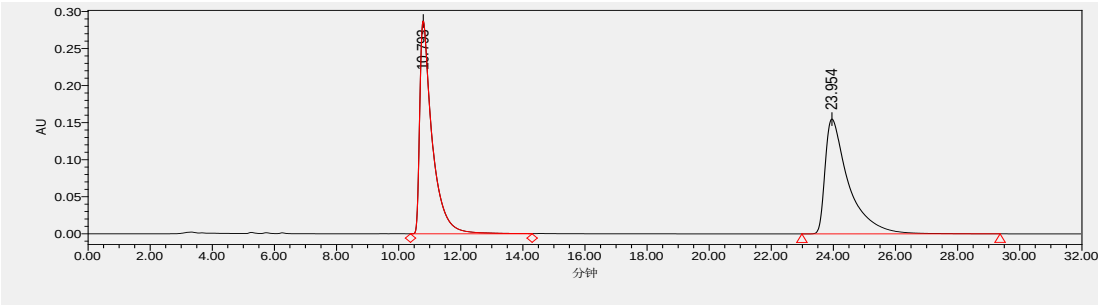


	Retention Time	Area	% Area	Height
1	13.384	1335030	99.82	26268
2	27.333	2461	0.18	38

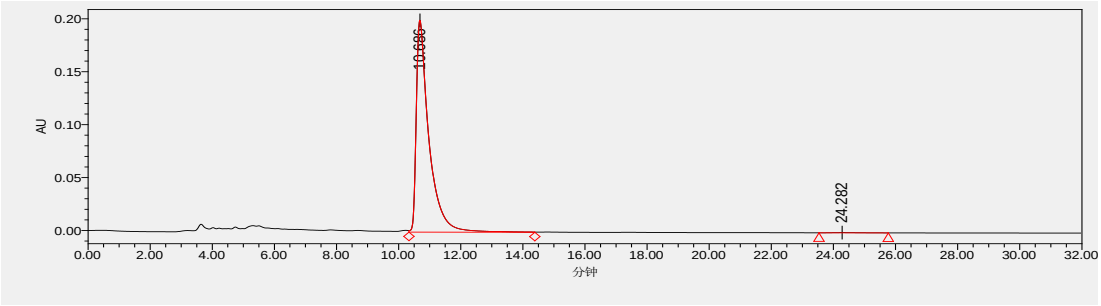
1-(benzo[d][1,3]dioxol-5-yl)-2-hydroxy-3-(2-phenyloxazol-5-yl)propan-1-one 5h

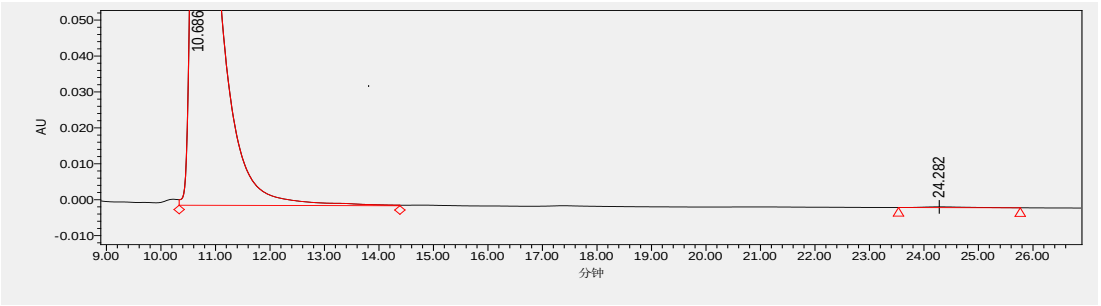


($C_{19}H_{15}NO_5$) a yellow amorphous solid; 83% yield, >99% ee. $[\alpha]_D^{20}$ = −16.5 (*c* 0.838 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB，n-hexane/2-propanol = 70/30, flow rate = 1.0 mL/min, λ = 254 nm, retention time:10.69 min (major), 24.28 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.92 – 7.71 (m, 2H), 7.51 – 7.39 (m, 1H), 7.38 – 7.22 (m, 4H), 6.92 – 6.70 (m, 2H), 5.95 (s, 2H), 5.21 (dd, *J* = 11.2, 6.4 Hz, 1H), 3.99 (d, *J* = 6.8 Hz, 1H), 3.18 (dd, *J* = 15.6, 4.8 Hz, 1H), 3.00 (dd, *J* = 15.2, 6.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 198.18, 161.24, 152.81, 148.58, 147.60, 130.14, 128.71, 128.05, 127.41, 126.30, 126.10, 125.04, 108.35, 108.20, 102.20, 71.02, 32.90. ESI-HRMS: calcd for $C_{19}H_{15}NNaO_5^+$ ([M+Na^+]) 360.0842, found 360.0847.



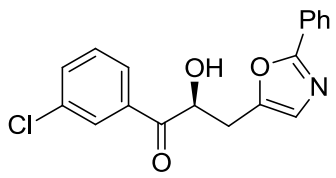
	Retention Time	Area	% Area	Height
1	10.793	8028907	49.73	287875
2	23.954	8115455	50.27	155033



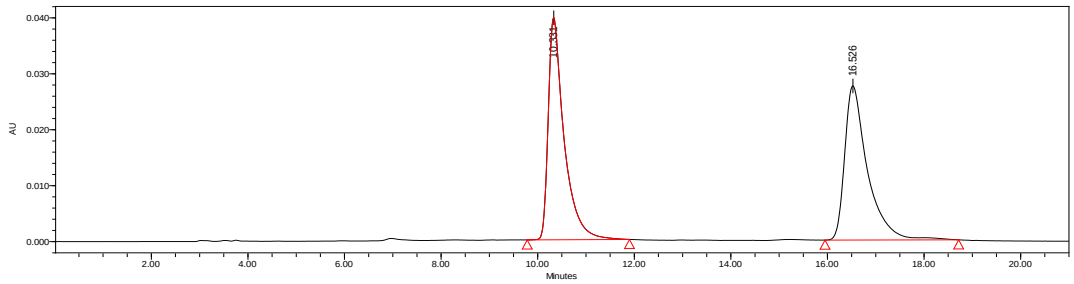


	Retention Time	Area	% Area	Height
1	10.686	5678798	99.78	200197
2	24.282	12393	0.22	215

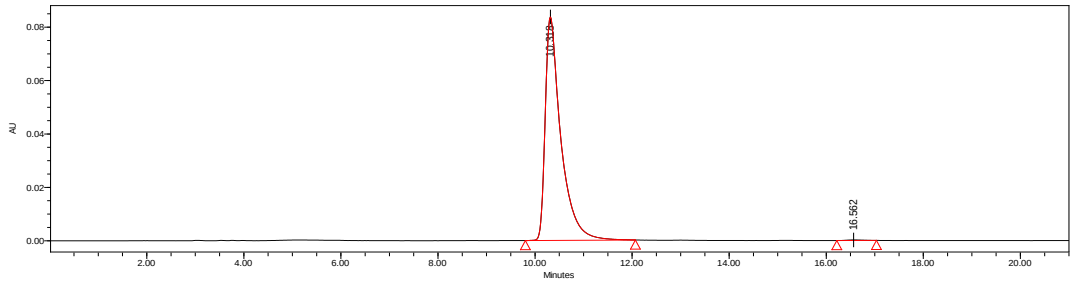
1-(3-chlorophenyl)-2-hydroxy-3-(2-phenyloxazol-5-yl)propan-1-one 5i

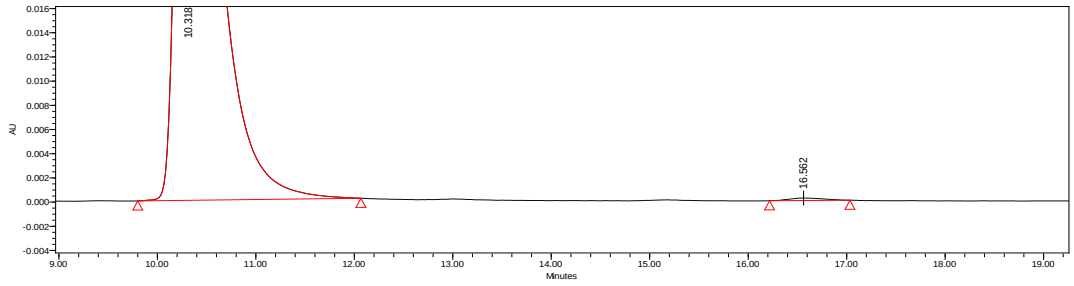


($C_{18}H_{14}ClNO_3$) a red viscous liquid; 98% yield, >99% ee. $[\alpha]_D^{20}$ = −13.7 (*c* 1.198 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB，n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 10.32 min (major), 16.56 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.97 – 7.62 (m, 4H), 7.56 – 7.43 (m, 1H), 7.42 – 7.21 (m, 4H), 6.83 (s, 1H), 5.25 (t, *J* = 5.6 Hz, 1H), 4.05 (s, 1H), 3.20 (dd, *J* = 15.6, 4.8 Hz, 1H), 3.03 (dd, *J* = 15.6, 6.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 198.21, 160.32, 146.07, 134.42, 134.29, 133.06, 129.30, 129.22, 127.71, 127.60, 126.18, 125.49, 125.44, 125.07, 70.52, 31.18. ESI-HRMS: calcd for $C_{18}H_{14}{}^{34.9689}ClNNaO_3^+$ ([M+Na^+]) 350.0554, found 350.0557.



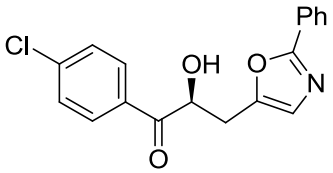
	Retention Time	Area	% Area	Height
1	10.331	904079	50.02	39716
2	16.526	903236	49.98	27585



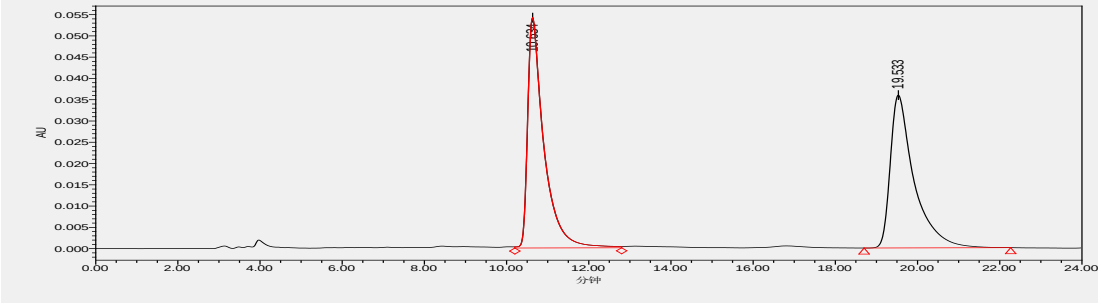


	Retention Time	Area	% Area	Height
1	10.318	1872753	99.74	83721
2	16.562	4951	0.26	207

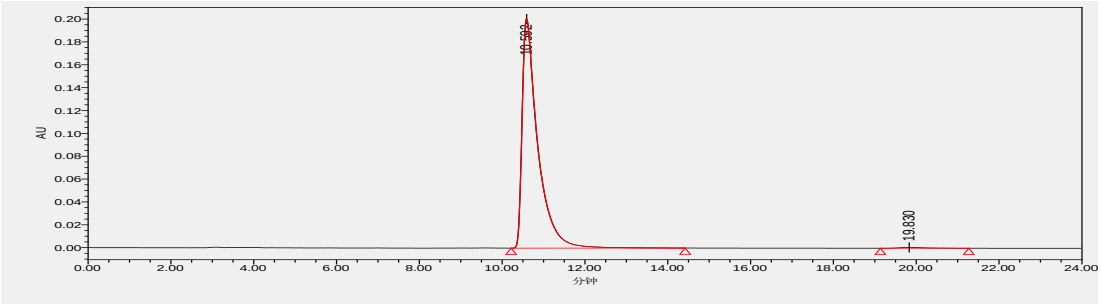
1-(4-chlorophenyl)-2-hydroxy-3-(2-phenyloxazol-5-yl)propan-1-one 5j

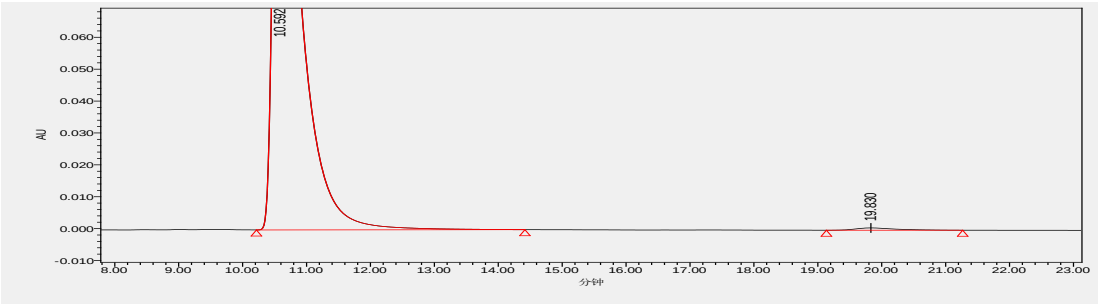


($C_{18}H_{14}ClNO_3$) a red amorphous solid; 90% yield, 99% ee. $[\alpha]_D^{20}$ = −51.5 (*c* 1.092 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB，n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 10.59 min (major), 19.83 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.01 – 7.78 (m, 4H), 7.58 – 7.32 (m, 5H), 6.91 (s, 1H), 5.34 (dd, *J* = 11.6, 6.4 Hz, 1H), 4.15 (d, *J* = 6.8 Hz, 1H), 3.28 (dd, *J* = 15.6, 4.4 Hz, 1H), 3.10 (dd, *J* = 15.6, 6.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 199.12, 161.32, 147.25, 140.83, 131.93, 130.26, 129.95, 129.44, 128.75, 127.27, 126.44, 126.08, 71.38, 32.34. ESI-HRMS: calcd for $C_{18}H_{14}{}^{34.9689}ClNNaO_3^+$ ([M+Na$^+$]) 350.0554, found 350.0560.



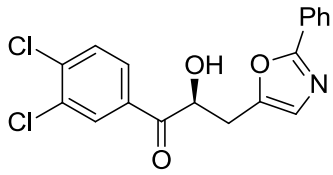
	Retention Time	Area	% Area	Height
1	10.634	1488597	50.86	54140
2	19.533	1438189	49.14	35925



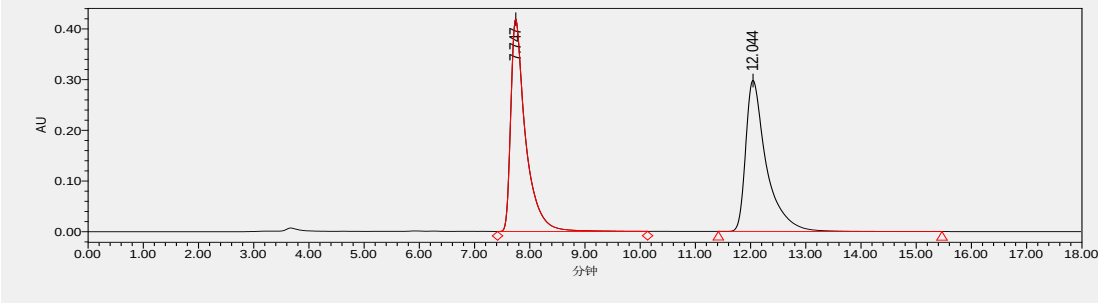


	Retention Time	Area	% Area	Height
1	10.592	5251664	99.41	200948
2	19.830	31250	0.59	719

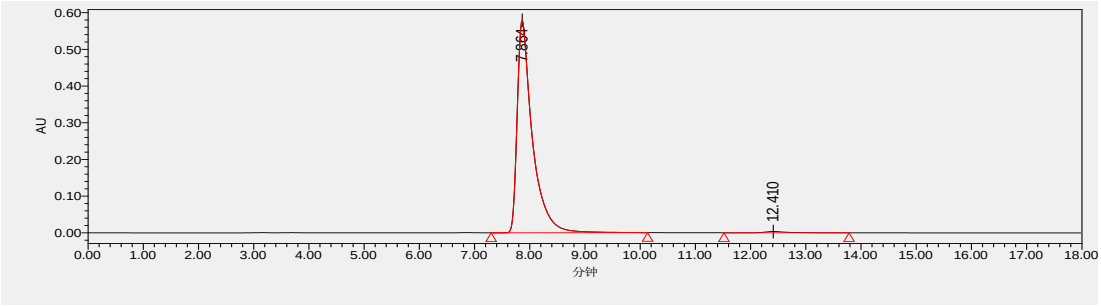
1-(3,4-dichlorophenyl)-2-hydroxy-3-(2-phenyloxazol-5-yl)propan-1-one 5k



($C_{18}H_{13}Cl_2NO_3$) a white amorphous solid; 93% yield, 98% ee. $[\alpha]_D^{20}$ = −49.7 (*c* 0.998 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB，n-hexane/2-propanol = 70/30, flow rate = 1.0 mL/min, λ = 254 nm, retention time:7.86 min (major), 12.41 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ =8.05 – 7.88 (m, 1H), 7.83 – 7.71 (m, 2H), 7.70 – 7.60 (m, 1H), 7.54-7.41 (m, 1H), 7.40 – 7.24 (m, 3H), 6.83 (s, 1H), 5.21 (dd, *J* = 11.6, 6.0 Hz, 1H), 4.11 (d, *J* = 6.8 Hz, 1H), 3.19 (dd, *J* = 15.2, 4.8 Hz, 1H), 3.04 (dd, *J* = 15.2, 6.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 198.33, 161.40, 146.97, 138.89, 133.91, 133.36, 131.13, 130.53, 130.34, 128.79, 127.43, 127.11, 126.56, 126.07, 71.61, 32.15. ESI-HRMS: calcd for $C_{18}H_{13}{}^{34.9689}Cl_2NNaO_3^+$ ([M+Na$^+$]) 384.0165, found 384.0163.

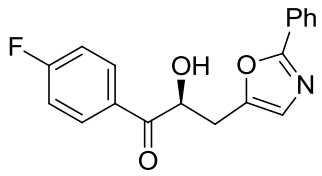


	Retention Time	Area	% Area	Height
1	7.747	7791227	50.20	419193
2	12.044	7728290	49.80	298167

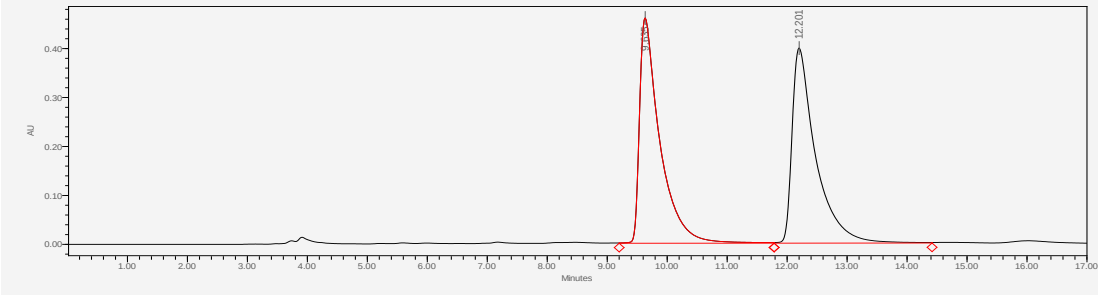


	Retention Time	Area	% Area	Height
1	7.864	11039609	99.13	579196
2	12.410	96645	0.87	3479

1-(4-fluorophenyl)-2-hydroxy-3-(2-phenyloxazol-5-yl)propan-1-one 5l

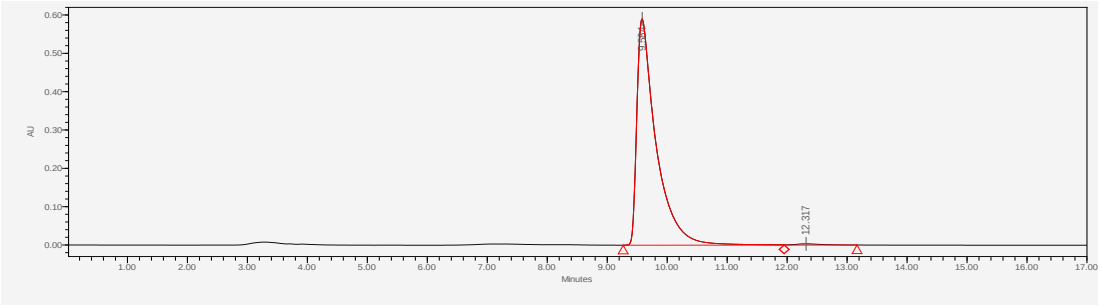


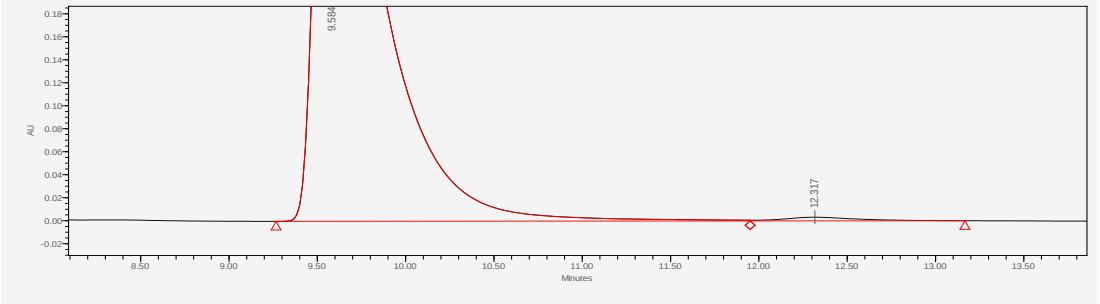
($C_{18}H_{14}FNO_3$) a yellow amorphous solid; 84% yield, 99% ee. $[\alpha]_D^{20}$ = −6.5 (*c* 0.978 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 9.58 min (major), 12.32 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.12 – 7.78 (m, 4H), 7.49 – 7.33 (m, 3H), 7.24 – 7.08 (m, 2H), 6.91 (s, 1H), 5.35 (dd, *J* = 11.2, 6.4 Hz, 1H), 4.18 (d, *J* = 6.8 Hz, 1H), 3.29 (dd, *J* = 15.6, 4.8 Hz, 1H), 3.10 (dd, *J* = 15.6, 6.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 198.65, 166.29 (d, *J* = 255.6 Hz), 161.29, 147.36, 131.34 (d, *J* = 9.5 Hz), 130.25, 130.01(d, *J* = 3.1 Hz), 128.74, 127.30, 126.39, 126.07, 116.35 (d, *J* =21.9 Hz), 71.26, 32.43. ESI-HRMS: calcd for $C_{18}H_{14}FNNaO_3^+$ ([M+Na$^+$]) 334.0850, found 334.0850.



	Retention Time	Area	% Area	Height

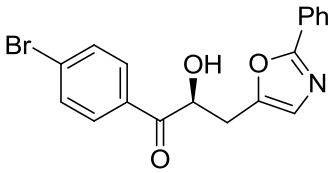
1	9.635	10841962	49.93	460394
2	12.201	10873911	50.07	398751



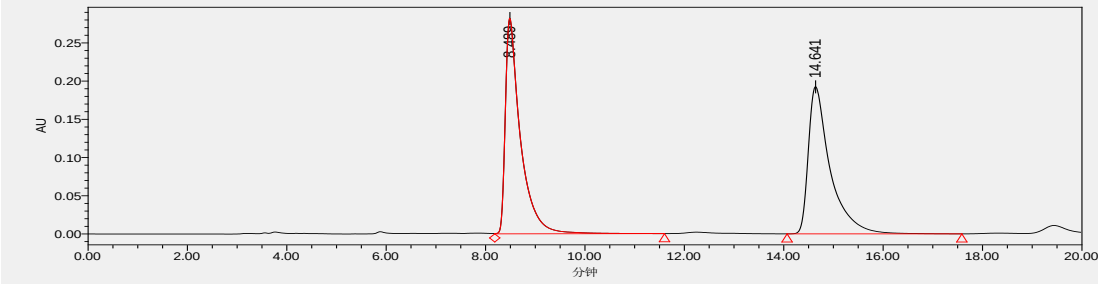


	Retention Time	Area	% Area	Height
1	9.584	13160696	99.30	590837
2	12.317	92707	0.70	3212

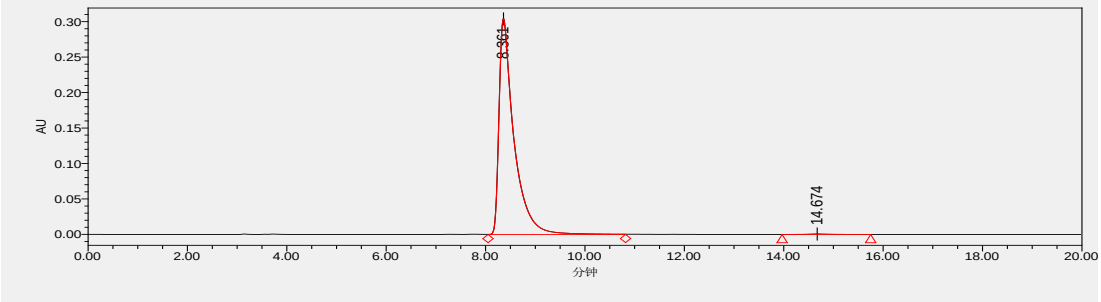
1-(4-bromophenyl)-2-hydroxy-3-(2-phenyloxazol-5-yl)propan-1-one 5m

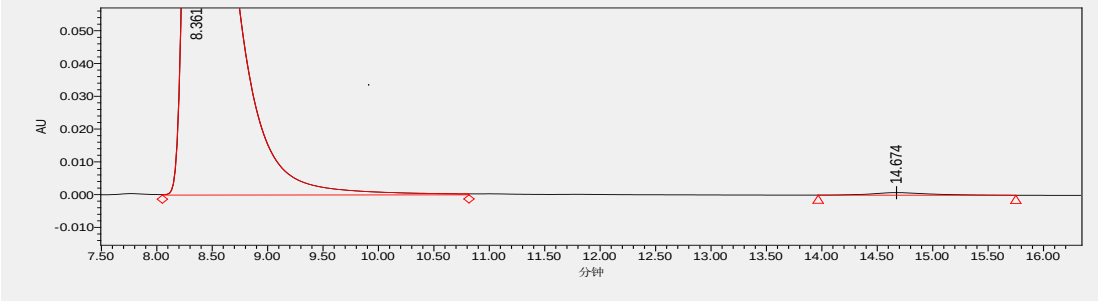


($C_{18}H_{14}BrNO_3$) a red amorphous solid; 93% yield, >99% ee. $[\alpha]_D^{20}$ = −59.7 (*c* 0.906 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB, n-hexane/2-propanol = 70/30, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 8.36 min (major), 14.67 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.95 – 7.72 (m, 4H), 7.71 – 7.59 (m, 2H), 7.52 – 7.34 (m, 3H), 6.91 (s, 1H), 5.33 (dd, *J* = 11.2, 6.4 Hz, 1H), 4.10 (d, *J* = 6.8 Hz, 1H), 3.28 (dd, *J* = 15.6, 4.8 Hz, 1H), 3.10 (dd, *J* = 15.6, 6.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 199.36, 161.33, 147.20, 132.44, 132.33, 130.27, 129.99, 129.63, 128.76, 127.27, 126.46, 126.09, 71.38, 32.35. ESI-HRMS: calcd for $C_{18}H_{14}{}^{78.9183}BrNNaO_3^+$ ([M+Na^+]) 394.0049, found 394.0055.



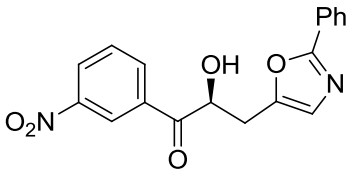
	Retention Time	Area	% Area	Height
1	8.489	5944144	50.29	282694
2	14.641	5874768	49.71	192740



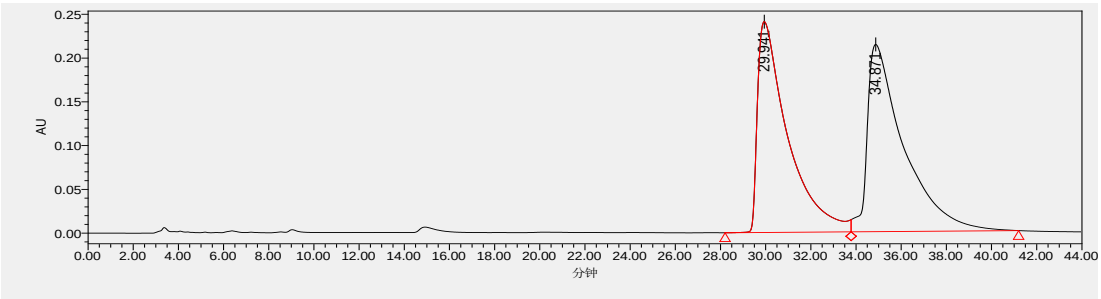


	Retention Time	Area	% Area	Height
1	8.361	6354525	99.56	304433
2	14.674	28214	0.44	780

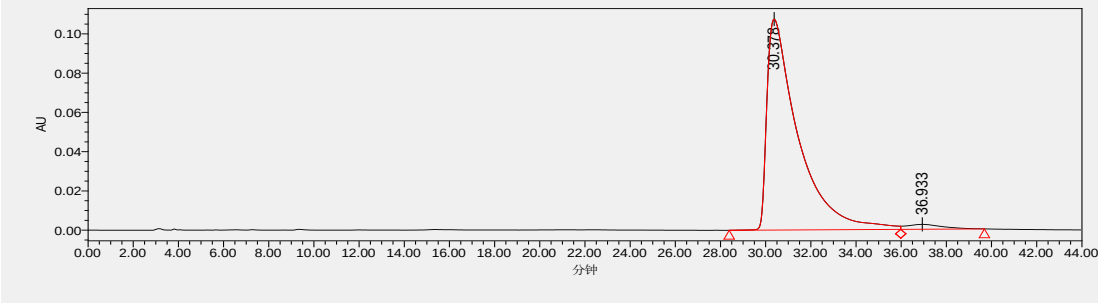
2-hydroxy-1-(3-nitrophenyl)-3-(2-phenyloxazol-5-yl)propan-1-one 5n



($C_{18}H_{14}N_2O_5$) a yellow amorphous solid; 70% yield, 95% ee. $[\alpha]_D^{20}$ = −16.5 (*c* 0.310 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB, n-hexane/2-propanol = 85/15, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 30.38 min (major), 36.93 min (minor). ^{1}H NMR (400 MHz, DMSO) δ = 8.86 – 8.65 (m, 1H), 8.54 – 8.37 (m, 2H), 7.98 – 7.74 (m, 3H), 7.61 – 7.40 (m, 3H), 7.09 (s, 1H), 6.21 (d, *J* = 7.6 Hz, 1H), 5.37 (dd, *J* = 12.8, 7.2 Hz, 1H), 3.28 (dd, *J* = 15.6, 5.2 Hz, 1H), 3.16 (dd, *J* = 15.6, 7.6 Hz, 1H). ^{13}C NMR (100 MHz, DMSO) δ = 198.27, 159.74, 149.26, 147.84, 136.25, 134.91, 130.41, 130.18, 128.98, 127.40, 127.05, 125.81, 125.50, 123.28, 71.22, 29.74. ESI-HRMS: calcd for $C_{18}H_{15}N_2O_5^+$ ([M+H$^+$]) 339.0975, found 339.0980.

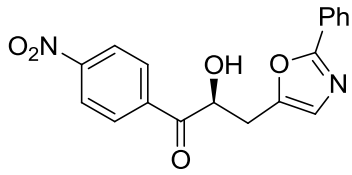


	Retention Time	Area	% Area	Height
1	29.941	22368875	48.33	240846
2	34.871	23913284	51.67	213885

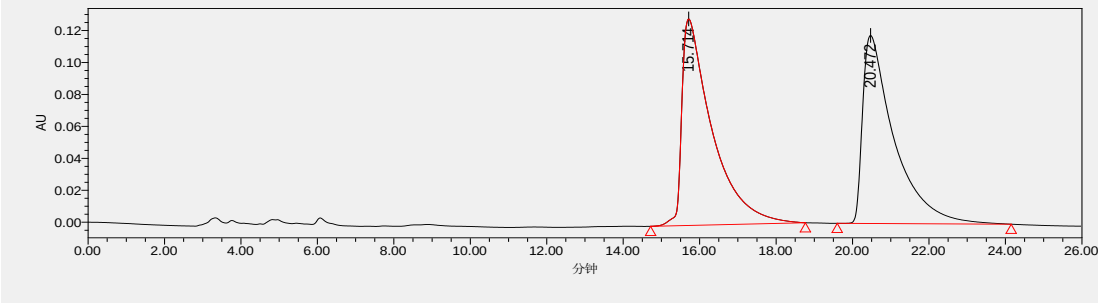


	Retention Time	Area	% Area	Height
1	30.378	10305287	97.41	107442
2	36.933	274401	2.59	2485

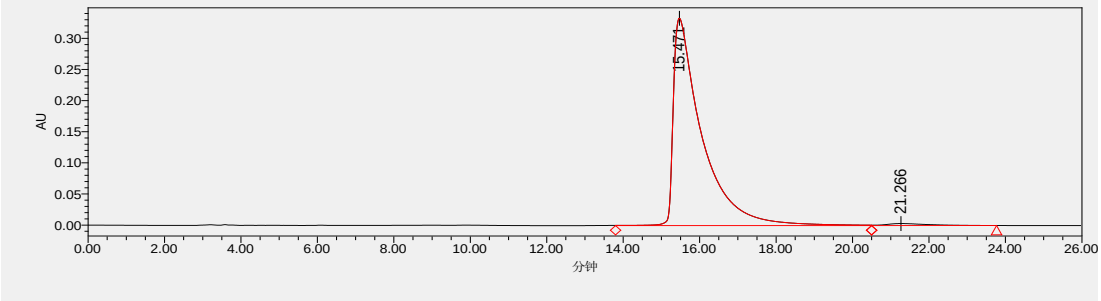
2-hydroxy-1-(4-nitrophenyl)-3-(2-phenyloxazol-5-yl)propan-1-one 5o



($C_{18}H_{14}N_2O_5$) a yellow amorphous solid; 83% yield, 97% ee. $[\alpha]_D^{20}$ = −29.9 (*c* 0.566 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB, n-hexane/2-propanol = 75/25, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 15.47 min (major), 21.27 min (minor). ^{1}H NMR (400 MHz, DMSO) δ = 8.49 – 8.12 (m, 4H), 7.98 – 7.83 (m, 2H), 7.63 – 7.38 (m, 3H), 7.08 (s, 1H), 6.13 (d, *J* = 7.2 Hz, 1H), 5.34 (dd, *J* = 12.8, 7.6 Hz, 1H), 3.25 (dd, *J* = 15.6, 4.8 Hz, 1H), 3.13 (dd, *J* = 15.6, 7.6 Hz, 1H). ^{13}C NMR (100 MHz, DMSO) δ = 199.09, 159.73, 149.75, 149.27, 139.95, 130.19, 130.14, 129.01, 127.05, 125.78, 125.51, 123.68, 71.20, 29.66. ESI-HRMS: calcd for $C_{18}H_{15}N_2O_5^+$ ([M+H$^+$]) 339.0975, found 339.0985.



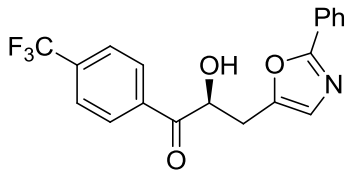
	Retention Time	Area	% Area	Height
1	15.714	7078253	51.26	129239
2	20.472	6731280	48.74	117774



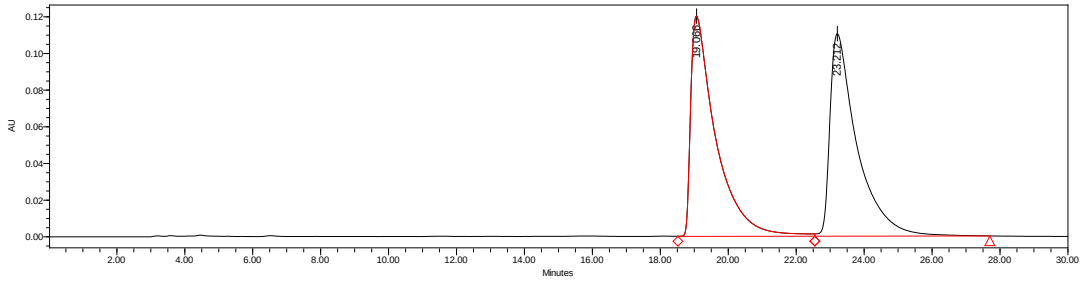
	Retention Time	Area	% Area	Height
1	15.471	17260399	98.61	333276

2	21.266	242889	1.39	3209

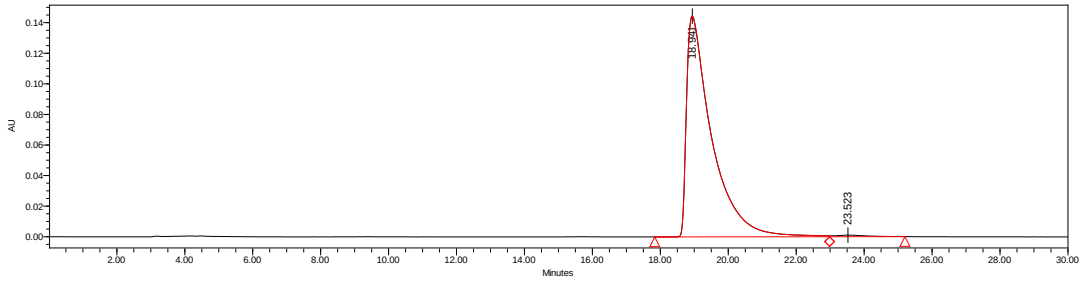
2-hydroxy-3-(2-phenyloxazol-5-yl)-1-(4-(trifluoromethyl)phenyl)propan-1-one 5p



($C_{19}H_{14}F_3NO_3$) a yellow amorphous solid; 94% yield, 98% ee. $[\alpha]_D^{20}$ = −27.0 (*c* 0.452 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB, n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 18.94 min (major), 23.52 min (minor). ^{1}H NMR (400 MHz, DMSO) δ = 8.45 – 8.10(m, 2H), 8.03 – 7.77 (m, 4H), 7.61 – 7.35 (m, 3H), 7.10 (s, 1H), 6.09 (d, *J* = 7.2 Hz, 1H), 5.37 (d, *J* = 6.4 Hz, 1H) , 3.27 (dd, *J* = 15.6, 4.8 Hz, 1H), 3.15 (dd, *J* = 15.2, 7.2 Hz, 1H). ^{13}C NMR (100 MHz, DMSO) δ = 199.31, 159.73, 149.29, 138.35, 132.50 (q, *J* =37.2 Hz), 130.13, 129.51 , 128.96, 127.09, 125.75, 125.53 (d, *J* = 6.1 Hz), 125.05, 122.34 , 71.08 , 29.83. ESI-HRMS: calcd for $C_{19}H_{15}F_3NO_3^+$ ([M+H$^+$]) 362.0999, found 362.1006.

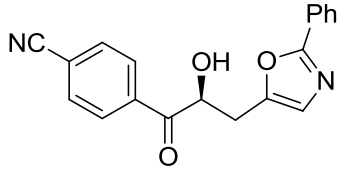


	Retention Time	Area	% Area	Height
1	19.066	6139556	50.19	120157
2	23.212	6093577	49.81	110436



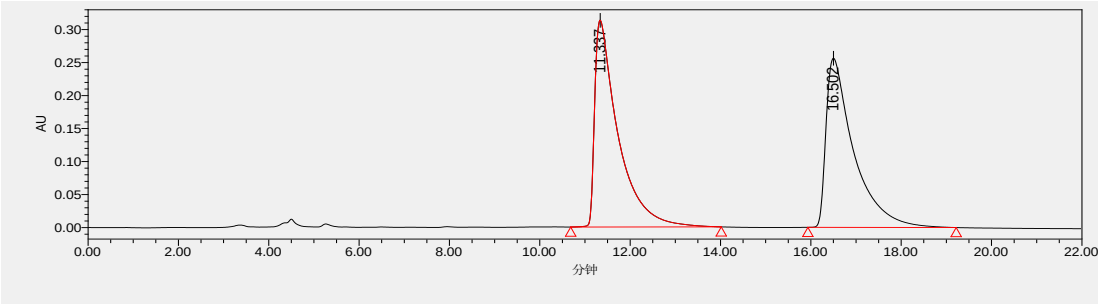
	Retention Time	Area	% Area	Height
1	18.941	7424933	99.15	144369
2	23.523	63463	0.85	1027

4-(2-hydroxy-3-(2-phenyloxazol-5-yl)propanoyl)benzonitrile 5q

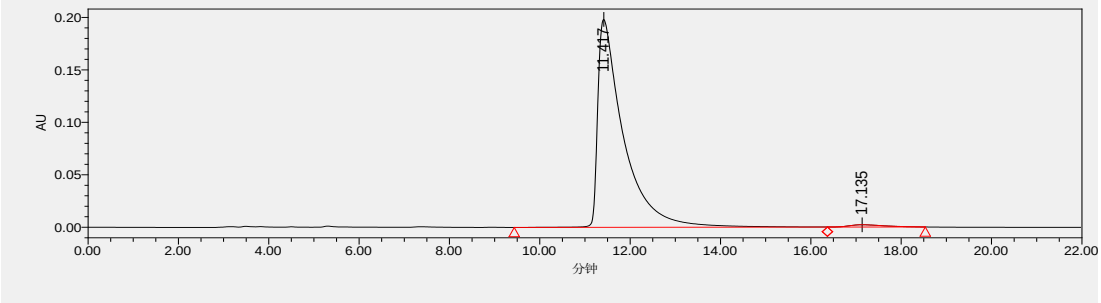


($C_{19}H_{14}N_2O_3$) a yellow amorphous solid; 60% yield, 97% ee. $[\alpha]_D^{20}$ = −60.5 (*c* 0.660 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB，n-hexane/2-propanol = 70/30, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 11.42 min (major), 17.14 min (minor). ^{1}H NMR (400 MHz, DMSO) δ = 8.27 – 8.11 (m, 2H), 8.09 – 7.96 (m, 2H), 7.93 – 7.80 (m, 2H), 7.61 – 7.40 (m, 3H), 7.08 (s, 1H), 6.08 (d, *J* = 7.2 Hz, 1H), 5.34 (dd, *J* = 12.4, 7.2 Hz, 1H), 3.24 (dd, *J* = 15.6, 4.8 Hz, 1H), 3.12

(dd, *J* = 15.6, 7.6 Hz, 1H). ^{13}C NMR (100 MHz, DMSO) δ = 199.27, 159.72, 149.28, 138.44, 132.62, 130.18, 129.33, 129.01, 127.07, 125.76, 125.52, 118.11, 115.11, 71.00, 29.73. ESI-HRMS: calcd for $C_{19}H_{15}N_2O_3^+$ ([M+H$^+$]) 319.1077, found 319.1087.

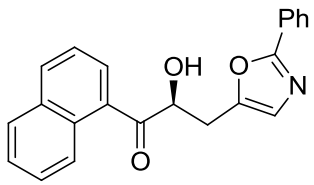


	Retention Time	Area	% Area	Height
1	11.337	11235777	50.82	313419
2	16.502	10871494	49.18	256333

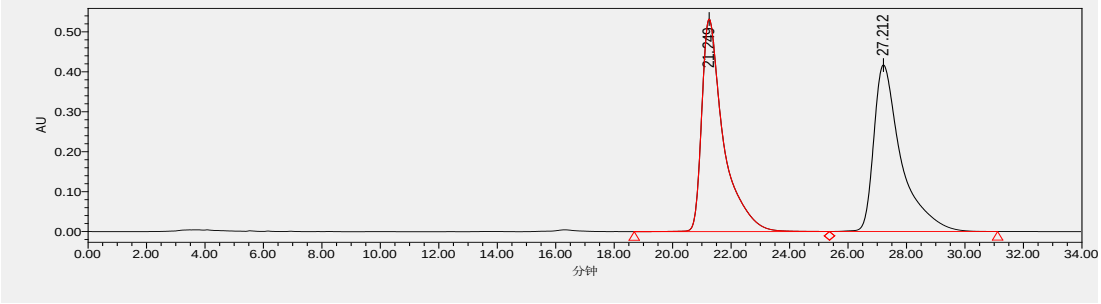


	Retention Time	Area	% Area	Height
1	11.417	7846573	98.50	198132
2	17.135	119718	1.50	2224

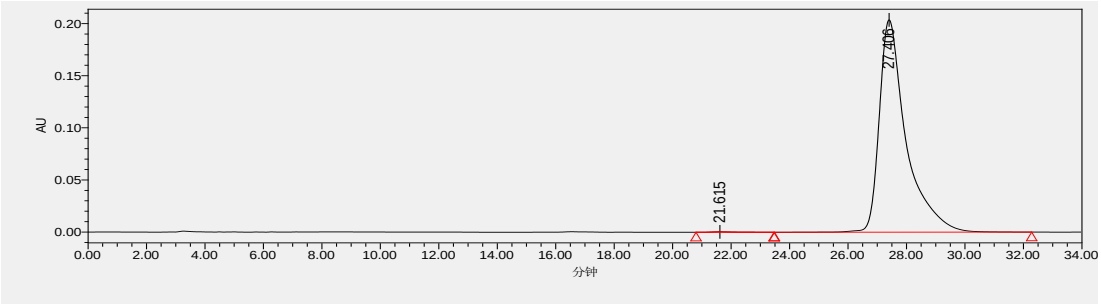
2-hydroxy-1-(naphthalen-1-yl)-3-(2-phenyloxazol-5-yl)propan-1-one 5r

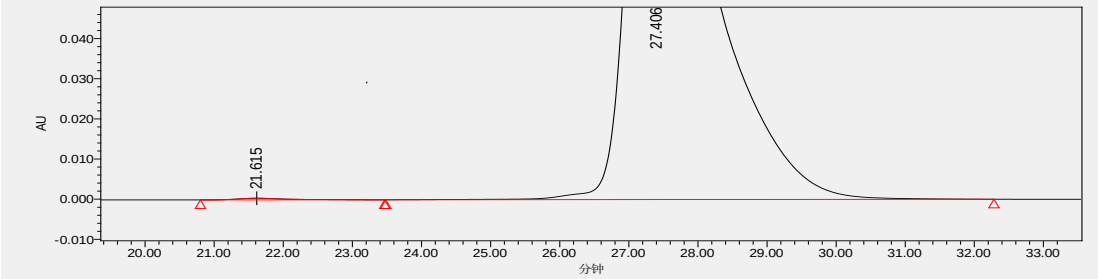


($C_{22}H_{17}NO_3$) a red viscous liquid; 99% yield, >99% ee. $[\alpha]_D^{20}$ = +43.7 (*c* 1.562 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IC, n-hexane/2-propanol = 75/25, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 21.62 min (minor), 27.41 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.52 – 8.24 (m, 1H), 8.03 – 7.86 (m, 1H), 7.86 – 7.71 (m, 2H), 7.71 – 7.53 (m, 2H), 7.53 – 7.35 (m, 3H), 7.34 – 7.18 (m, 3H), 6.76 (s, 1H), 5.39 (dd, *J* = 10.0 Hz, 5.2Hz, 1H), 4.18 (d, *J* = 5.6 Hz, 1H), 3.14 (dd, *J* = 15.6, 5.2 Hz, 1H), 3.00 (dd, *J* = 15.6, 5.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 209.44, 161.21, 147.27, 134.15, 134.06, 131.62, 130.43, 130.06, 128.68, 128.65, 128.58, 128.19, 127.25, 126.96, 126.52, 126.13, 125.46, 124.28, 72.67, 31.70. ESI-HRMS: calcd for $C_{22}H_{18}NO_3^+$ ([M+H$^+$]) 344.1281, found 344.1284.



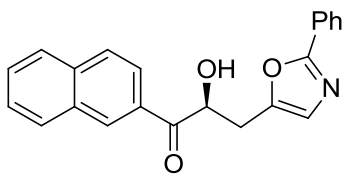
	Retention Time	Area	% Area	Height
1	21.249	27414728	50.29	532127
2	27.212	27094077	49.71	417093



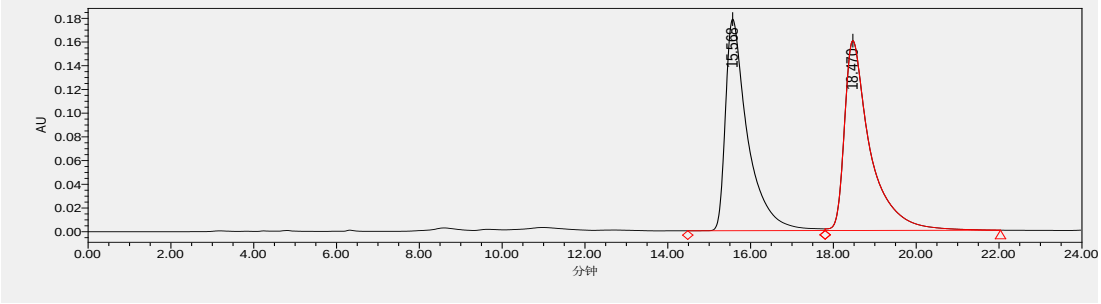


	Retention Time	Area	% Area	Height
1	21.615	20830	0.16	417
2	27.406	12953784	99.84	203694

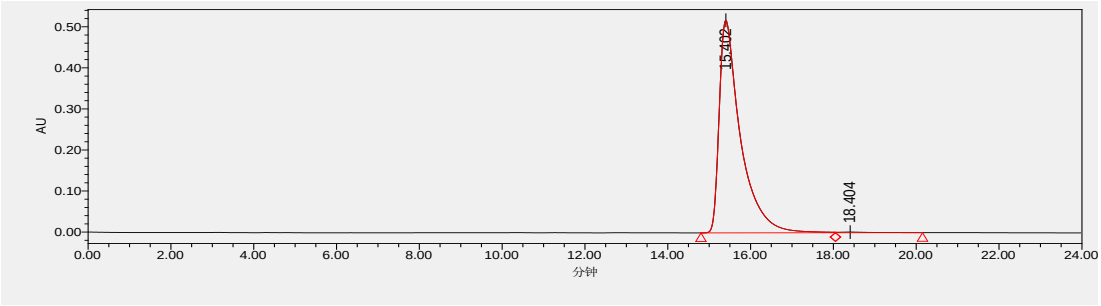
2-hydroxy-1-(naphthalen-2-yl)-3-(2-phenyloxazol-5-yl)propan-1-one 5s

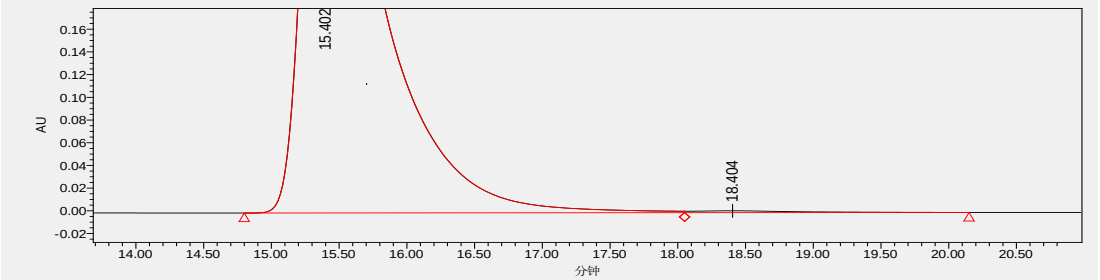


($C_{22}H_{17}NO_3$) a yellow amorphous solid; 99% yield, >99% ee. $[\alpha]_D^{20}$ = −75.5 (*c* 1.682 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB，n-hexane/2-propanol = 75/25, flow rate = 1.0 mL/min, λ = 254 nm, retention time:15.40 min (major), 18.40 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.44 (s, 1H), 8.07 – 7.76 (m, 6H), 7.68 – 7.30 (m, 5H), 6.92 (s, 1H), 5.54 (dd, *J* = 11.2, 6.4 Hz, 1H), 4.21 (d, *J* = 6.8 Hz, 1H), 3.36 (ddd, *J* = 15.6, 4.8, 0.8 Hz, 1H), 3.18 (ddd, *J* = 15.2, 6.0, 0.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 200.24, 161.29, 147.51, 136.03, 132.39, 130.87, 130.55, 130.15, 129.68, 129.22, 129.09, 128.70, 127.94, 127.36, 127.26, 126.43, 126.11, 123.80, 71.44, 32.69. ESI-HRMS: calcd for $C_{22}H_{18}NO_3^+$ ([M+H$^+$]) 344.1281, found 344.1290.



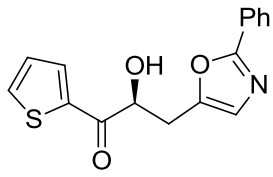
	Retention Time	Area	% Area	Height
1	15.568	6637289	49.04	178511
2	18.470	6897890	50.96	160135



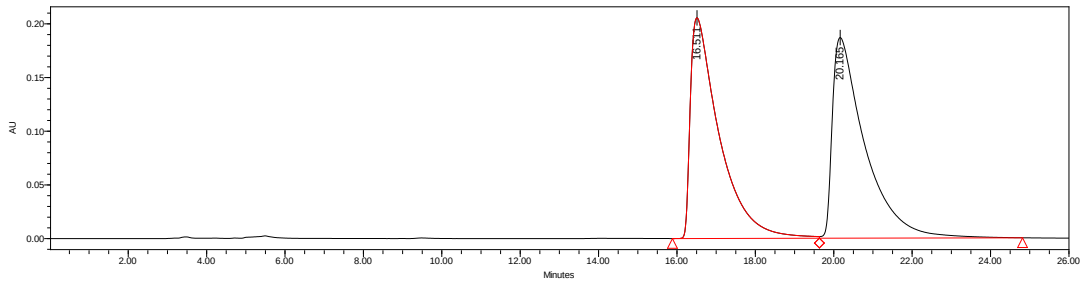


	Retention Time	Area	% Area	Height
1	15.402	18463513	99.52	517868
2	18.404	88480	0.48	1650

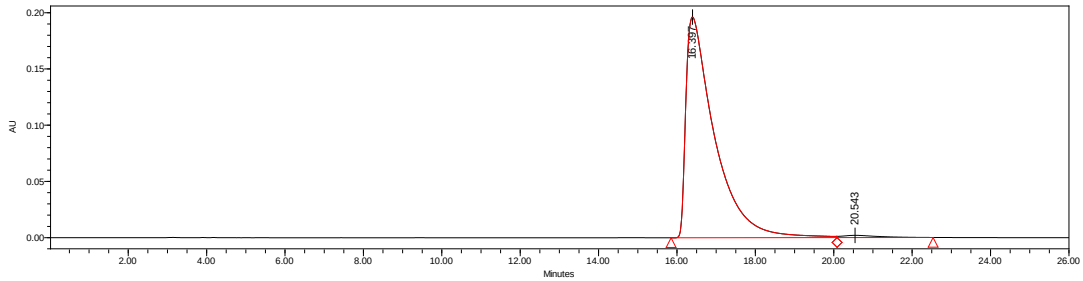
2-hydroxy-3-(2-phenyloxazol-5-yl)-1-(thiophen-2-yl)propan-1-one 5t



($C_{16}H_{13}NO_3S$) a yellow viscous liquid; 99% yield, 98% ee. $[\alpha]_D^{20}$ = +19.6 (*c* 1.288 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB, n-hexane/2-propanol = 85/15, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 16.40 min (major), 20.54 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.94 – 7.58 (m Hz, 4H), 7.41 – 7.25 (m, 3H), 7.14 – 7.01 (m, 1H), 6.86 (s, 1H), 5.09 (t, *J* = 5.2 Hz, 1H), 4.08 (s, 1H), 3.26 (dd, *J* = 15.2, 4.4 Hz, 1H), 3.10 (dd, *J* = 15.6, 6.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 192.68, 161.34, 147.53, 139.76, 135.38, 133.32, 130.22, 128.73, 128.56, 127.30, 126.37, 126.13, 72.44, 33.16. ESI-HRMS: calcd for $C_{16}H_{13}NNaO_3S^+$ ([M+Na^+]) 322.0508, found 322.0510.

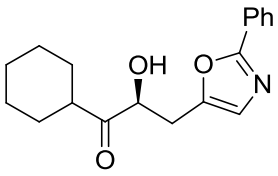


	Retention Time	Area	% Area	Height
1	16.511	10554011	49.44	205467
2	20.165	10792004	50.56	186832

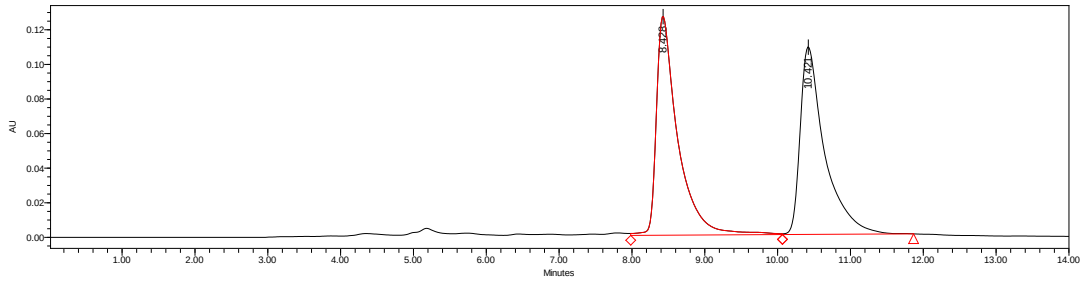


	Retention Time	Area	% Area	Height
1	16.397	9963175	98.77	196274
2	20.543	123761	1.23	1963

1-cyclohexyl-2-hydroxy-3-(2-phenyloxazol-5-yl)propan-1-one 5u

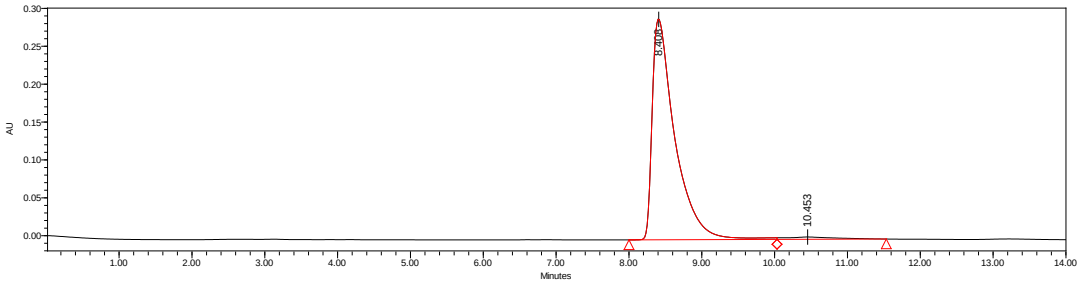


($C_{18}H_{21}NO_3$) a white amorphous solid; 84% yield, 96% ee. $[\alpha]_D^{20}$ = +51.6 (*c* 1.012 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB, n-hexane/2-propanol = 85/15, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 8.41 min (major), 10.45 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.18 – 7.69 (m, 2H), 7.54 – 7.23 (m, 3H), 6.88 (s, 1H), 4.52 (dd, *J* = 10.0 Hz, 5.2Hz, 1H), 3.86 (d, *J* = 5.2 Hz, 1H), 3.20 (dd, *J* = 15.6, 4.4 Hz, 1H), 2.98 (dd, *J* = 15.6, 6.4 Hz, 1H), 2.76 – 2.46 (m, 1H), 1.89 – 1.39 (m, 6H), 1.33 – 1.07 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 213.42, 161.25, 147.71, 130.21, 128.76, 127.36, 126.27, 126.10, 72.92, 46.28, 30.51, 29.77, 27.45, 25.83, 25.62, 25.15. ESI-HRMS: calcd for $C_{18}H_{21}NNaO_3^+$ ([M+Na$^+$]) 322.1414, found 322.1414.



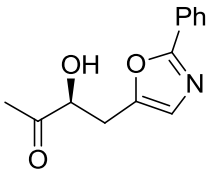
	Retention Time	Area	% Area	Height
1	8.428	2598919	50.77	126536

2	10.421	2519958	49.23	108521

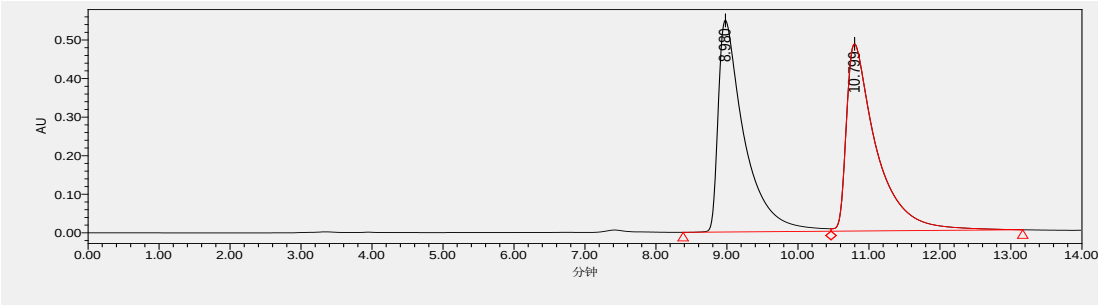


	Retention Time	Area	% Area	Height
1	8.408	6296400	97.77	292076
2	10.453	143676	2.23	3040

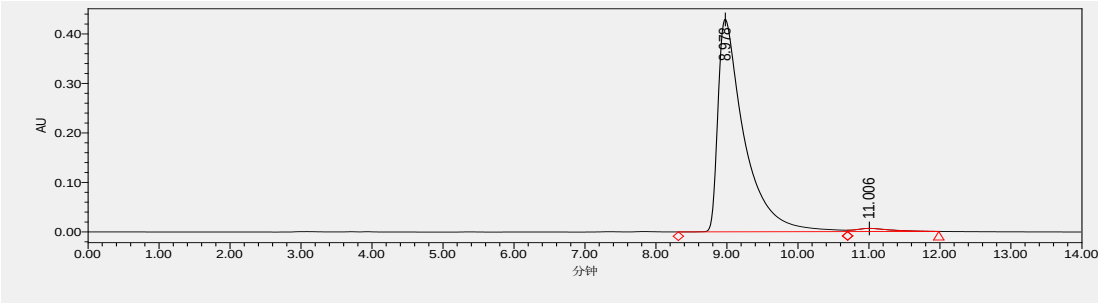
3-hydroxy-4-(2-phenyloxazol-5-yl)butan-2-one 5v



($C_{13}H_{13}NO_3$) a white amorphous solid; 97% yield, 96% ee. $[\alpha]_D^{20}$ = +84.6 (*c* 0.888 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 8.99 min (major), 11.01 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.96 – 7.81 (m, 2H), 7.47 – 7.34 (m, 3H), 6.94 (s, 1H), 4.46 (s, 1H), 4.32 (d, *J* = 2.8 Hz, 1H), 3.25 (dd, *J* = 15.6, 4.8 Hz, 1H), 3.07 (dd, *J* = 15.6, 6.4 Hz, 1H), 2.31 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 208.56, 161.23, 147.70, 130.31, 128.79, 127.15, 126.18, 126.05, 75.02, 30.24, 25.63. ESI-HRMS: calcd for $C_{13}H_{14}NO_3^+$ ([M+H$^+$]) 232.0968, found 232.0977.



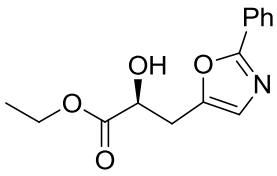
	Retention Time	Area	% Area	Height
1	8.980	13994143	49.61	549339
2	10.799	14214931	50.39	485621



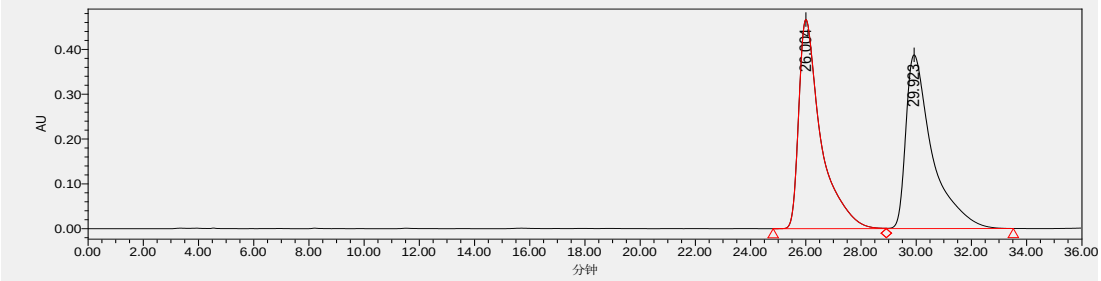
	Retention Time	Area	% Area	Height
1	8.978	11029101	98.05	429426

2	11.006	218973	1.95	6401

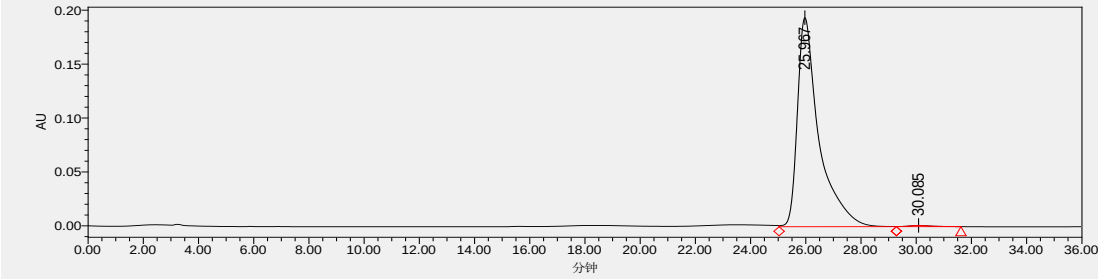
ethyl 2-hydroxy-3-(2-phenyloxazol-5-yl)propanoate 5w



($C_{14}H_{15}NO_4$) a colourless viscous liquid; 99% yield, 99% ee. $[\alpha]_D^{20}$ = −12.5 (*c* 1.172 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IC, n-hexane/2-propanol = 85/15, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 25.97 min (major), 30.09 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.98 – 7.79 (m, 2H), 7.46 – 7.25 (m, 3H), 6.89 (s, 1H), 4.44 (d, *J* = 4.4 Hz, 1H), 4.18 (q, *J* =6.8 Hz, 2H), 3.55 (d, *J* = 4.4 Hz, 1H), 3.17 (dd, *J* = 15.6, 4.8 Hz, 1H), 3.07 (dd, *J* = 15.6, 6.4 Hz, 1H), 1.21 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 172.49, 160.25, 146.83, 129.15, 127.71, 126.36, 125.06, 67.84, 61.06, 29.96, 13.16. ESI-HRMS: calcd for $C_{14}H_{16}NO_4^+$ ([M+H$^+$]) 262.1074, found 262.1078.

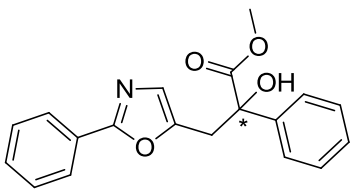


	Retention Time	Area	% Area	Height
1	26.004	25805306	50.23	466524
2	29.923	25572980	49.77	387614



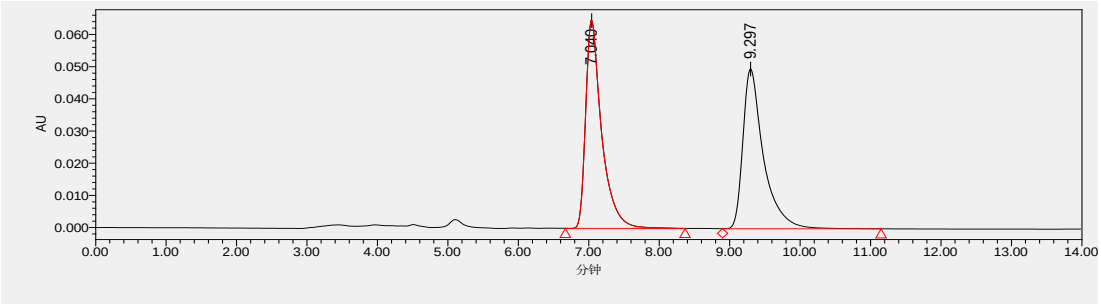
	Retention Time	Area	% Area	Height
1	25.967	10488604	99.35	193848
2	30.085	68461	0.65	1186

methyl 2-hydroxy-2-phenyl-3-(2-phenyloxazol-5-yl)propanoate 3a

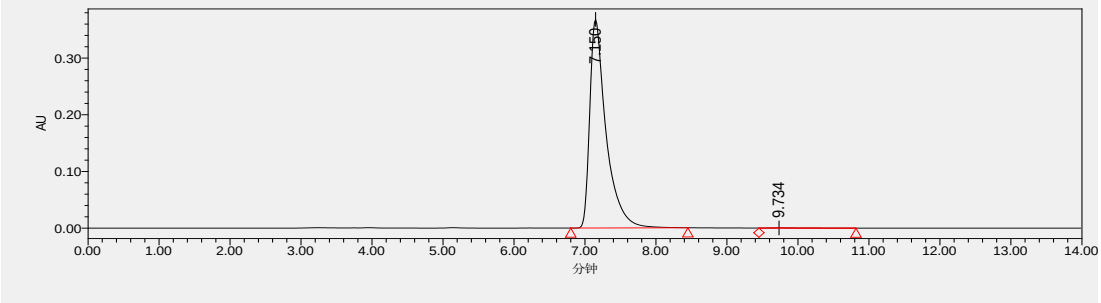


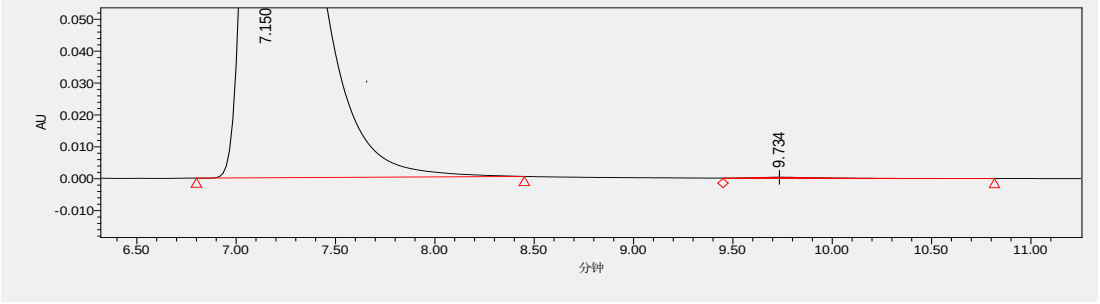
($C_{19}H_{17}NO_4$) a colourless viscous liquid; 97% yield, >99% ee. $[\alpha]_D^{20}$ = −6.7 (*c* 2.426 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 7.15 min (major), 9.13 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.03 – 7.84 (m, 2H), 7.74 – 7.58 (m, 2H), 7.52 – 7.28 (m, 6H), 6.93 (s, 1H), 4.02 (s, 1H), 3.83 (s, 3H), 3.73 (d, *J* = 15.6 Hz, 1H), 3.39 (d, *J* = 15.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ =

174.33, 161.20, 147.69, 140.54, 130.14, 128.76, 128.53, 128.32, 127.52, 126.75, 126.10, 125.45, 77.61, 53.58, 36.63. ESI-HRMS: calcd for $C_{19}H_{17}NNaO_4^+$ ([M+Na$^+$]) 346.1050, found 346.1060.



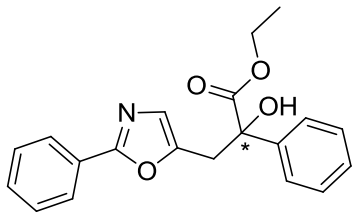
	Retention Time	Area	% Area	Height
1	7.040	1019680	50.35	64883
2	9.297	1005396	49.65	49714





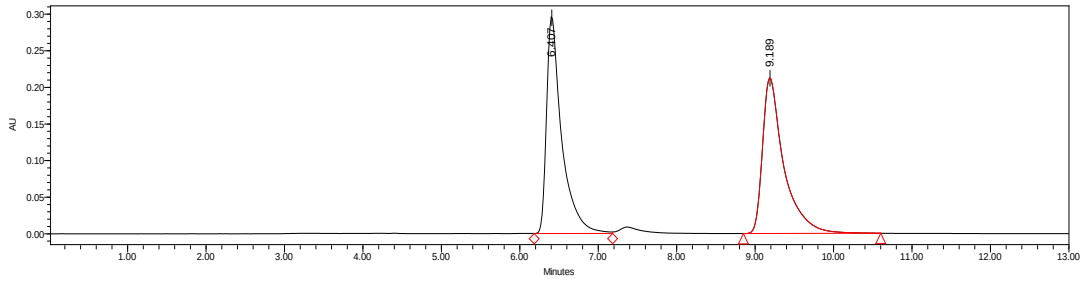
	Retention Time	Area	% Area	Height
1	7.150	5861012	99.80	367831
2	9.734	11878	0.20	408

ethyl 2-hydroxy-2-phenyl-3-(2-phenyloxazol-5-yl)propanoate 3a[2]

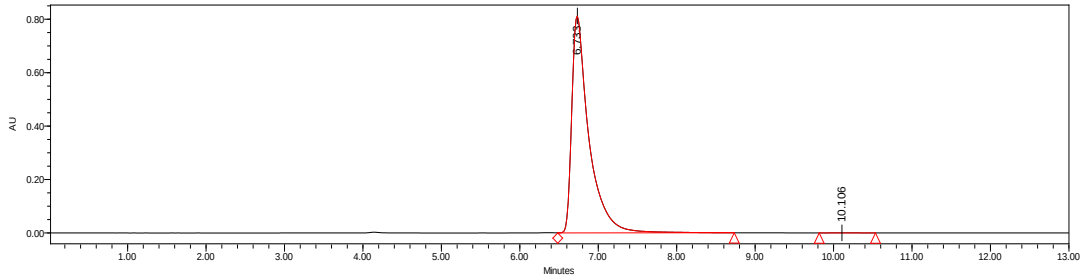


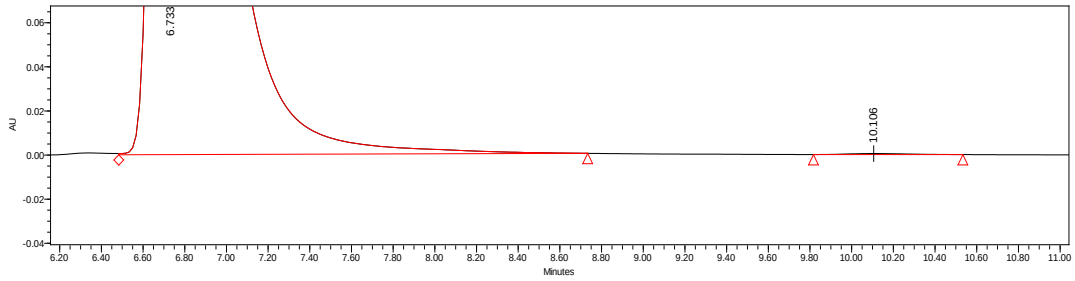
($C_{20}H_{19}NO_4$) a colourless viscous liquid; 99% yield, >99% ee. $[\alpha]_D^{20}$ = −10.3 (*c* 1.340 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 6.73 min (major), 10.11 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.94 – 7.75 (m, 2H), 7.65 – 7.51 (m, 2H), 7.41 – 7.19 (m, 6H), 6.85 (s, 1H), 4.18 (q, *J* = 8.0 Hz, 2H), 4.03 (d, *J* = 6.5 Hz, 1H), 3.64 (d, *J* = 16.0 Hz, 1H), 3.30 (d, *J* = 16.0 Hz, 1H), 1.18 (t, *J* = 8.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 172.75, 160.02, 146.77, 139.69, 129.02, 127.66, 127.40, 127.15, 126.48, 125.63, 125.01, 124.37, 75.39, 61.82,

35.53, 13.03. ESI-HRMS: calcd for $C_{20}H_{20}NO_4^+$ ([M+H$^+$]) 338.1387, found 338.1387.



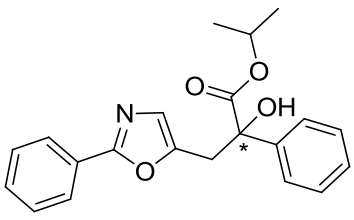
	Retention Time	Area	% Area	Height
1	6.407	3976331	49.89	297238
2	9.189	3994457	50.11	212820



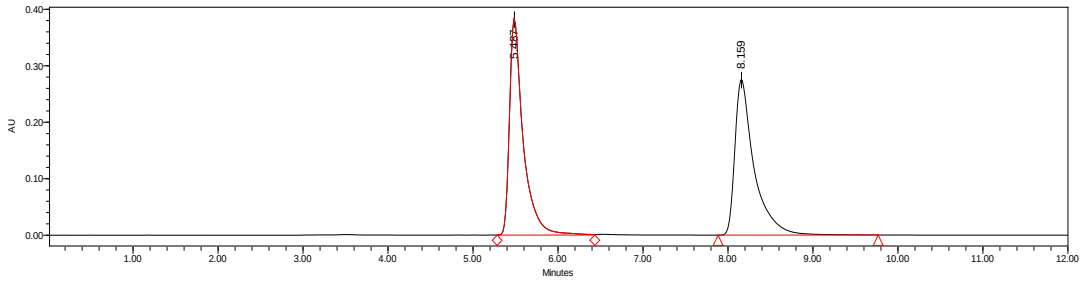


	Retention Time	Area	% Area	Height
1	6.733	12335739	99.93	812057
2	10.106	8709	0.07	452

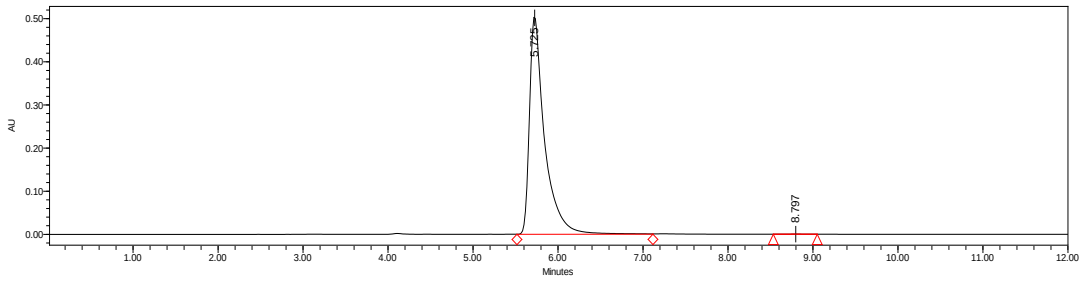
isopropyl 2-hydroxy-2-phenyl-3-(2-phenyloxazol-5-yl)propanoate 3a[3]

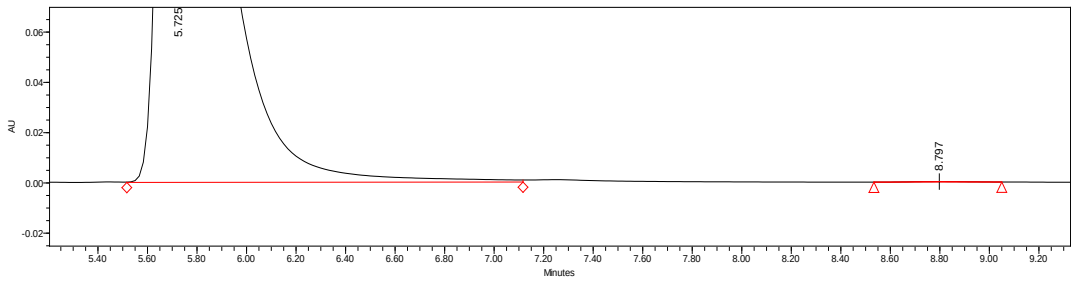


($C_{21}H_{21}NO_4$) a colourless viscous liquid; 98% yield, >99% ee. $[\alpha]_D^{20}$ = −16.0 (*c* 1.332 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 5.73 min (major), 8.80 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.95 – 7.79 (m, 2H), 7.64 – 7.54 (m, 2H), 7.39 – 7.19 (m, 6H), 6.87 (s, 1H), 4.98 (dt, *J* = 12.0, 4.0 Hz, 1H), 4.04 (s, 1H), 3.62 (d, *J* = 16.0 Hz, 1H), 3.28 (d, *J* = 16.0 Hz, 1H), 1.17 (d, *J* = 4.0 Hz, 3H), 1.11 (d, *J* = 4.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 173.33, 161.01, 147.98, 140.94, 130.07, 128.73, 128.41, 128.16, 127.58, 126.66, 126.10, 125.41, 77.45, 71.01, 36.51, 21.73, 21.52. ESI-HRMS: calcd for $C_{21}H_{22}NO_4^+$ ([M+H$^+$]) 352.1543, found 352.1544.



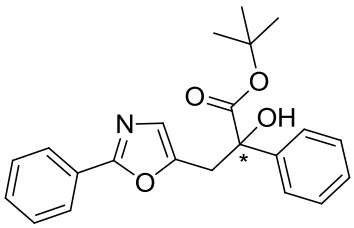
	Retention Time	Area	% Area	Height
1	5.487	4299866	49.93	384308
2	8.159	4312272	50.07	276233



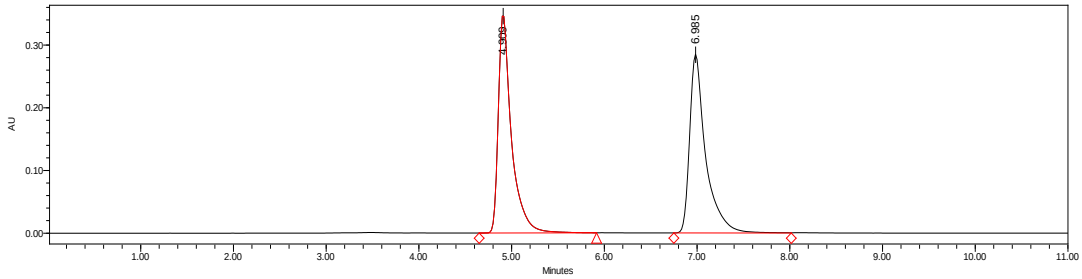


	Retention Time	Area	% Area	Height
1	5.725	6235597	99.95	506841
2	8.797	3146	0.05	220

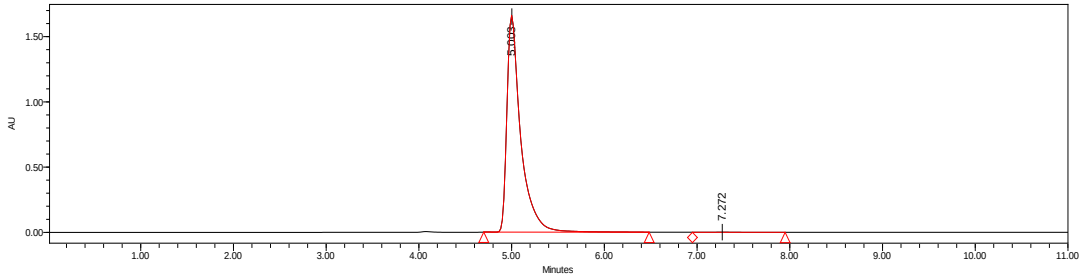
tert-butyl 2-hydroxy-2-phenyl-3-(2-phenyloxazol-5-yl)propanoate 3a[4]

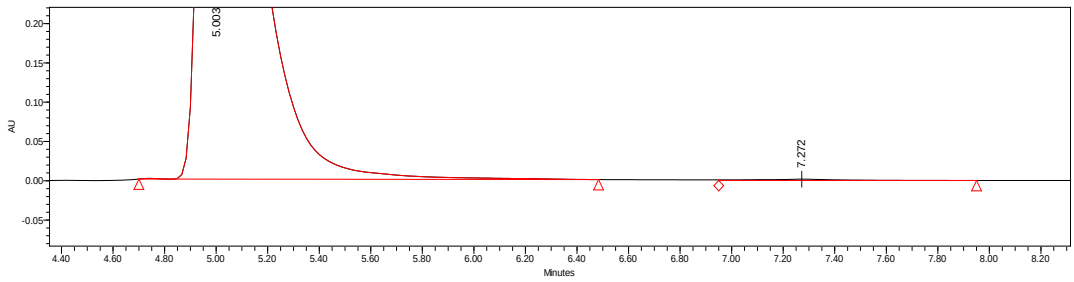


($C_{22}H_{23}NO_4$) a colourless viscous liquid; 98% yield, >99% ee. $[\alpha]_D^{20}$ = −15.2 (*c* 1.548 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 5.00 min (major), 7.27 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.03 – 7.92 (m, 2H), 7.71 – 7.63 (m, 2H), 7.58 – 7.26 (m, 6H), 6.97 (s, 1H), 4.09 (s, 1H), 3.67 (d, *J* = 15.2 Hz, 1H), 3.35 (d, *J* = 15.6 Hz, 1H), 1.42 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 172.87, 160.92, 148.24, 141.29, 130.04, 128.72, 128.36, 128.04, 127.62, 126.56, 126.12, 125.40, 83.95, 77.43, 36.47, 27.81. ESI-HRMS: calcd for $C_{22}H_{24}NO_4^+$ ([M+H$^+$]) 366.1700, found 366.1708.



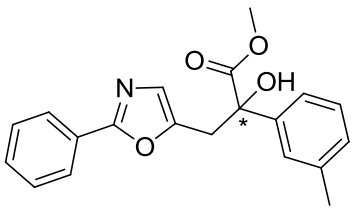
	Retention Time	Area	% Area	Height
1	4.909	3412739	49.96	349866
2	6.985	3417664	50.04	284985



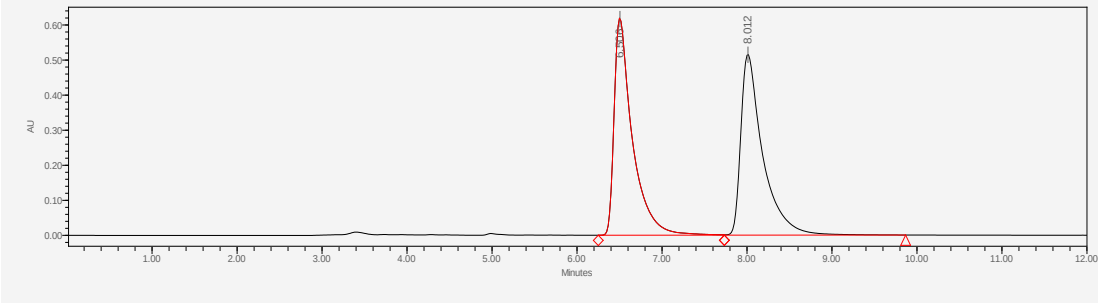


	Retention Time	Area	% Area	Height
1	5.003	17395024	99.78	1662989
2	7.272	39215	0.22	1683

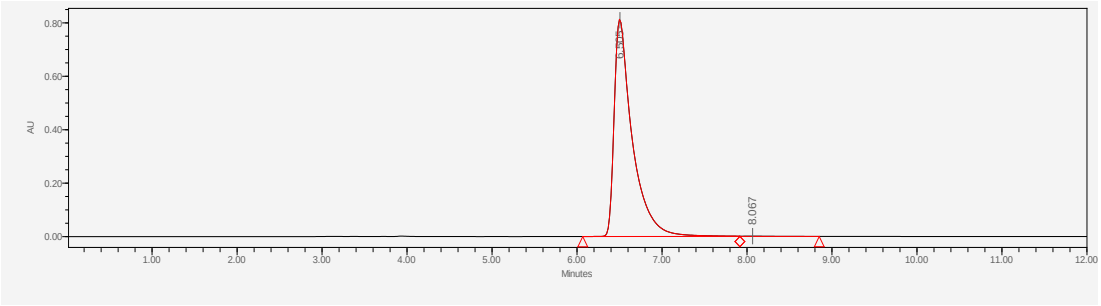
methyl 2-hydroxy-3-(2-phenyloxazol-5-yl)-2-(p-tolyl)propanoate 3b

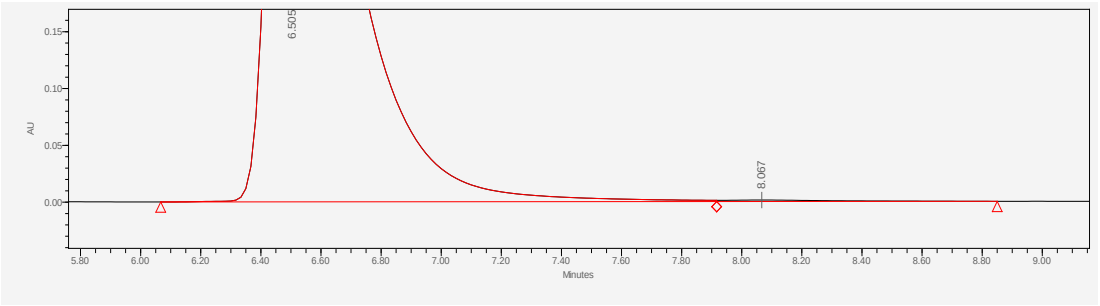


($C_{20}H_{19}NO_4$) a colourless viscous liquid; 95% yield, >99% ee. $[\alpha]_D^{20}$ = −5.7 (*c* 1.220 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 6.51 min (major), 8.07 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.10 – 7.68 (m, 2H), 7.54 – 7.25 (m, 5H), 7.23 – 7.13 (m, 1H), 7.10 – 7.02 (m, 1H), 6.83 (s, 1H), 4.00 (s, 1H), 3.73 (s, 3H), 3.64 (d, *J* = 14.8 Hz, 1H), 3.28 (d, *J* = 14.8 Hz, 1H), 2.28 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 173.30, 160.09, 146.75, 139.49, 137.16, 129.04, 127.98, 127.67, 127.35, 126.47, 125.64, 125.03, 124.98, 121.43, 76.58, 52.43, 35.50, 20.57. ESI-HRMS: calcd for $C_{20}H_{20}NO_4^+$ ([M+H$^+$]) 338.1387, found 338.1388.



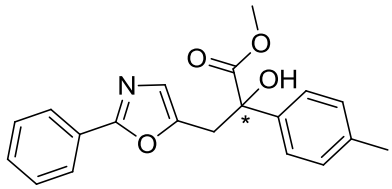
	Retention Time	Area	% Area	Height
1	6.506	9220809	50.06	620479
2	8.012	9197496	49.94	515331



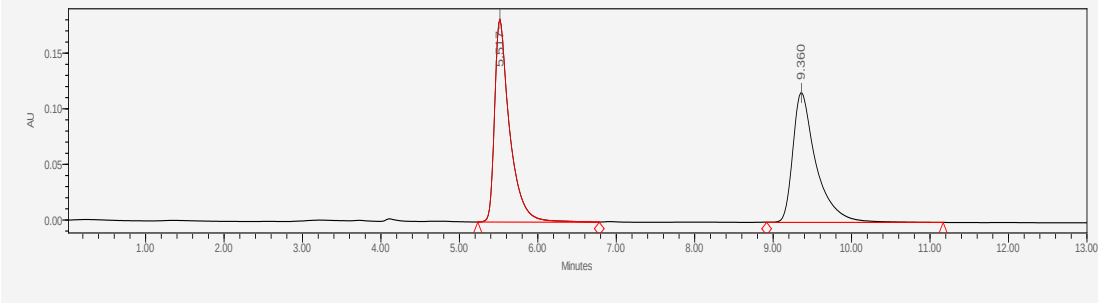


	Retention Time	Area	% Area	Height
1	6.505	12070019	99.72	814458
2	8.067	34250	0.28	1338

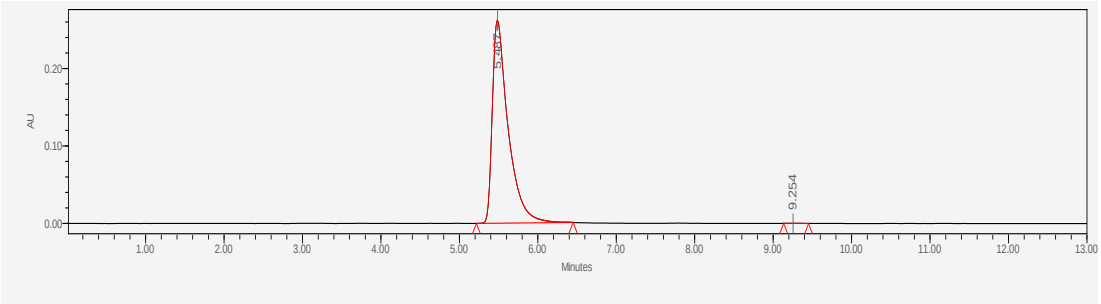
methyl 2-hydroxy-3-(2-phenyloxazol-5-yl)-2-(p-tolyl)propanoate 3c

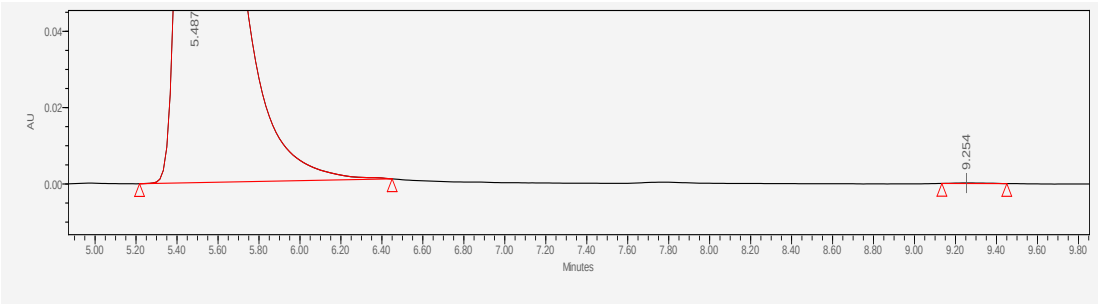


($C_{20}H_{19}NO_4$) a white amorphous solid; 77% yield, >99% ee. $[\alpha]_D^{20}$ = −6.5 (*c* 0.970 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB, n-hexane/2-propanol = 70/30, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 5.49 min (major), 9.25 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.00 – 7.87 (m, 2H), 7.60 – 7.48 (m, 2H), 7.46 – 7.36 (m, 3H), 7.23 – 7.10 (m, 2H), 6.92 (s, 1H), 4.03 (s, 1H), 3.81 (s, 3H), 3.72 (d, *J* = 15.2 Hz, 1H), 3.36 (d, *J* = 15.2 Hz, 1H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 174.47, 161.15, 147.81, 138.12, 137.67, 130.12, 129.21, 128.75, 127.54, 126.70, 126.09, 125.36, 77.53, 53.51, 36.58, 21.08. ESI-HRMS: calcd for $C_{20}H_{20}NO_4^+$ ([M+H$^+$]) 338.1387, found 338.1393.



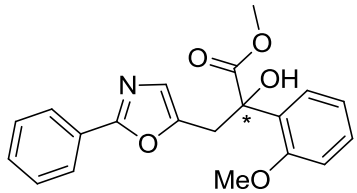
	Retention Time	Area	% Area	Height
1	5.517	2425905	50.21	182424
2	9.360	2405171	49.79	116718



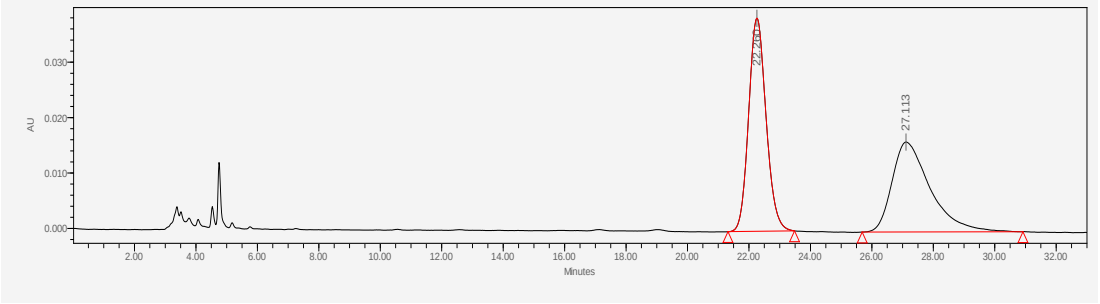


	Retention Time	Area	% Area	Height
1	5.487	3656803	99.95	262701
2	9.254	1647	0.05	145

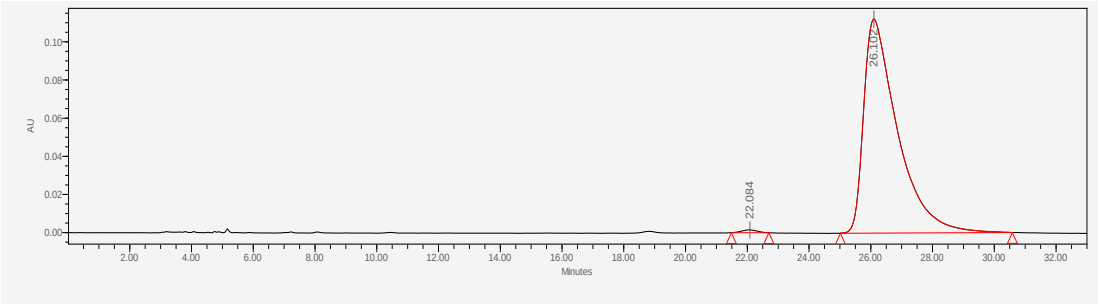
methyl 2-hydroxy-2-(2-methoxyphenyl)-3-(2-phenyloxazol-5-yl)propanoate 3d



($C_{20}H_{19}NO_5$) a yellow amorphous solid; 42% yield, 99% ee. $[\alpha]_D^{20}$ = +17.4 (*c* 0.494 in CH_2Cl_2). HPLC DAICEL CHIRALCEL ID, n-hexane/2-propanol = 70/30, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 22.08 min (minor), 26.10 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.98 – 7.85 (m, 2H), 7.50 – 7.37 (m, 4H), 7.35 – 7.28 (m, 1H), 7.04 – 6.82 (m, 3H), 4.21 (s, 1H), 3.80 (s, 3H), 3.72 (s, 3H), 3.65 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 174.08, 161.13, 156.55, 147.64, 130.00, 129.75, 129.38, 128.69, 127.61, 127.03, 126.43, 126.07, 120.92, 111.37, 76.15, 55.59, 52.79, 33.79. ESI-HRMS: calcd for $C_{20}H_{20}NO_5^+$ ([M+H$^+$]) 354.1336, found 354.1338.

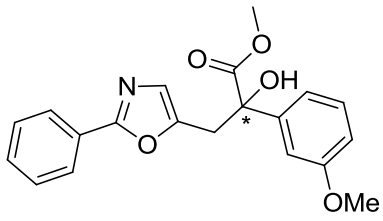


	Retention Time	Area	% Area	Height
1	22.260	1515197	52.03	38452
2	27.113	1397110	47.97	16229

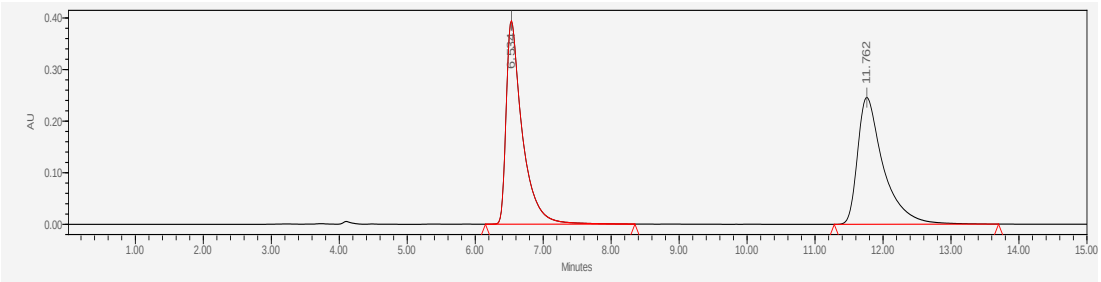


	Retention Time	Area	% Area	Height
1	22.084	51475	0.60	1473
2	26.102	8501323	99.40	112127

methyl 2-hydroxy-2-(3-methoxyphenyl)-3-(2-phenyloxazol-5-yl)propanoate 3e

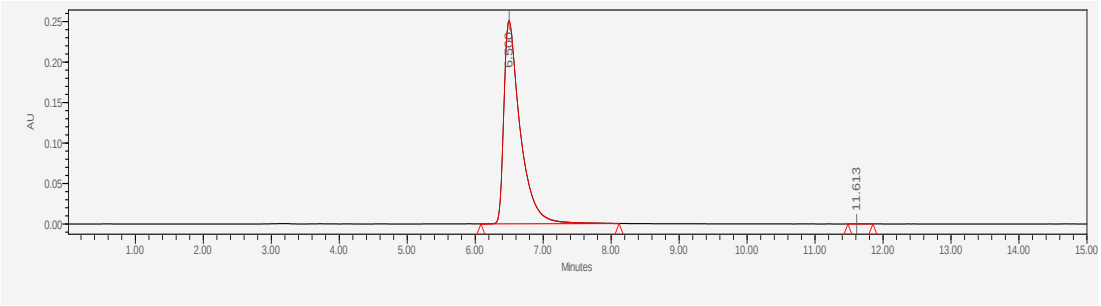


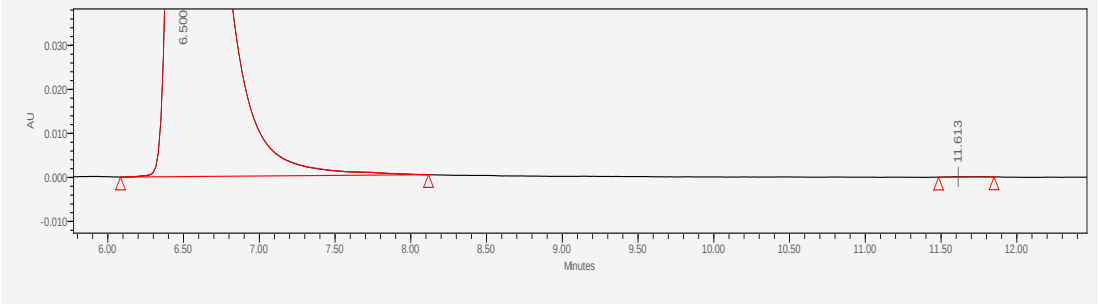
($C_{20}H_{19}NO_5$) a white amorphous solid; 97% yield, >99% ee. $[\alpha]_D^{20}$ = −1.3 (*c* 1.594 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB, n-hexane/2-propanol =70/30, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 6.50 min (major), 11.61 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.06 – 7.84 (m, 2H), 7.46 – 7.37 (m, 3H), 7.35 – 7.28 (m, 1H), 7.25 – 7.21 (m, 2H), 6.97 – 6.80 (m, 2H), 4.04 (s, 1H), 3.83 (s, 3H), 3.81 (s, 3H), 3.72 (d, *J* = 15.2 Hz, 1H), 3.37 (d, *J* = 15.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 174.22, 161.18, 159.73, 147.69, 142.21, 130.13, 129.55, 128.75, 127.52, 126.74, 126.09, 117.74, 113.63, 111.37, 77.58, 55.33, 53.60, 36.64. ESI-HRMS: calcd for $C_{20}H_{20}NO_5^+$ ([M+H$^+$]) 354.1336, found 354.1338.



	Retention Time	Area	% Area	Height

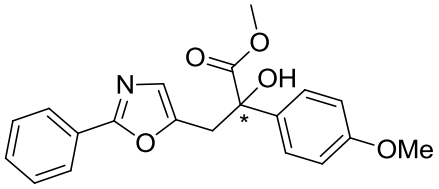
1	6.534	6482181	50.03	394550
2	11.762	6474184	49.97	245995



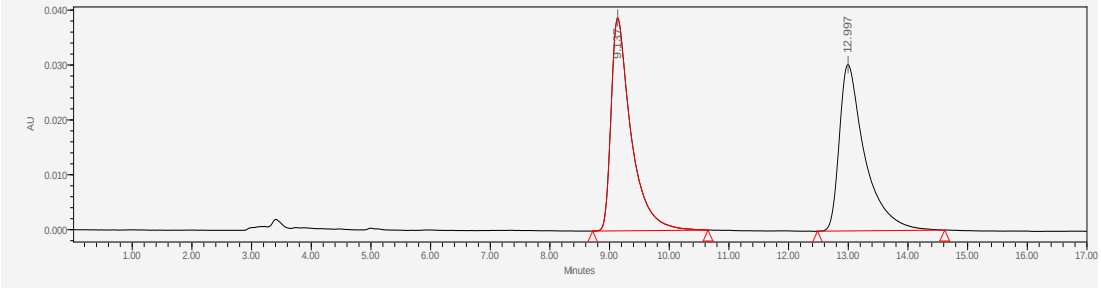


	Retention Time	Area	% Area	Height
1	6.500	4170284	99.97	251414
2	11.613	1144	0.03	83

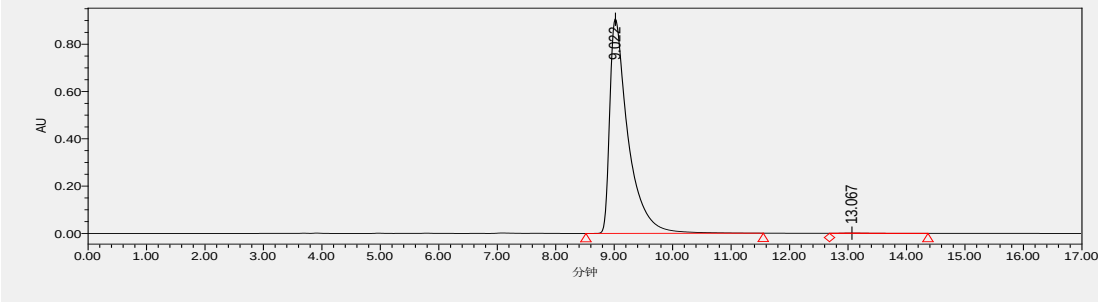
methyl 2-hydroxy-2-(4-methoxyphenyl)-3-(2-phenyloxazol-5-yl)propanoate 3f

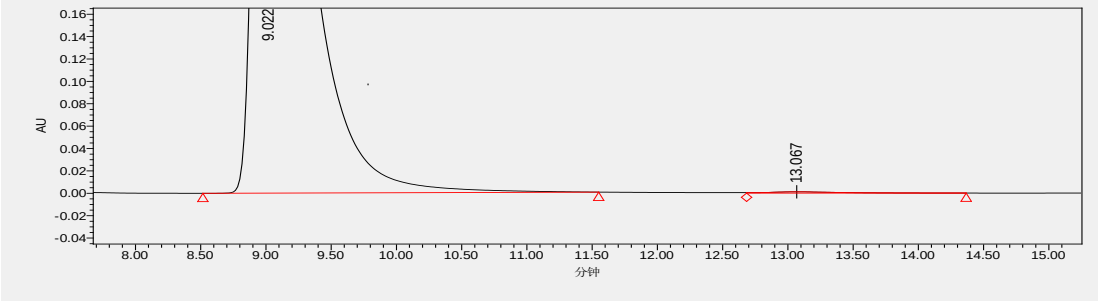


($C_{20}H_{19}NO_5$) a colourless viscous liquid; 63% yield, >99% ee. $[\alpha]_D^{20}$ = −7.5 (*c* 0.786 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 9.02 min (major), 13.07 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.05 – 7.84 (m, 2H), 7.64 – 7.54 (m, 2H), 7.48 – 7.35 (m, 3H), 7.03 – 6.79 (m, 3H), 4.00 (s, 1H), 3.82 (s, 3H), 3.80 (s, 3H), 3.70 (d, *J* = 15.6 Hz, 1H), 3.36 (d, *J* = 15.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ =174.53, 161.16, 159.50, 147.78, 132.62, 130.12, 128.75, 127.53, 126.76, 126.70, 126.09, 113.80, 77.30, 55.32, 53.50, 36.65. ESI-HRMS: calcd for $C_{20}H_{20}NO_5^+$ ([M+H$^+$]) 354.1336, found 354.1338.



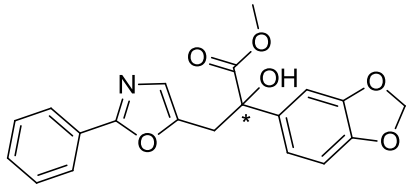
	Retention Time	Area	% Area	Height
1	9.137	899521	50.07	38850
2	12.997	896840	49.93	30342



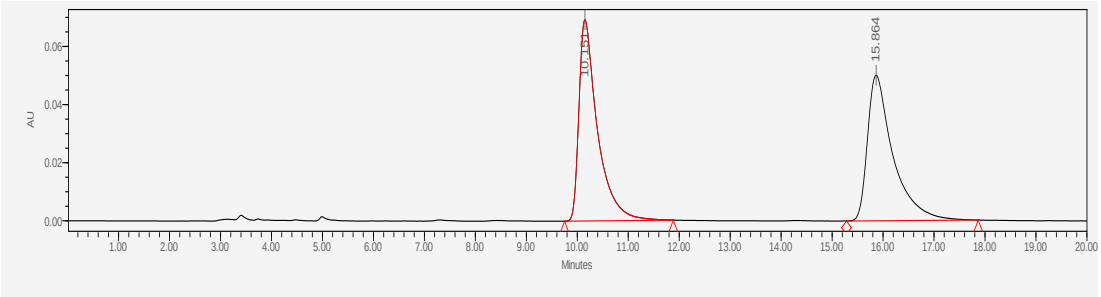


	Retention Time	Area	% Area	Height
1	9.022	19752096	99.77	907694
2	13.067	45381	0.23	1218

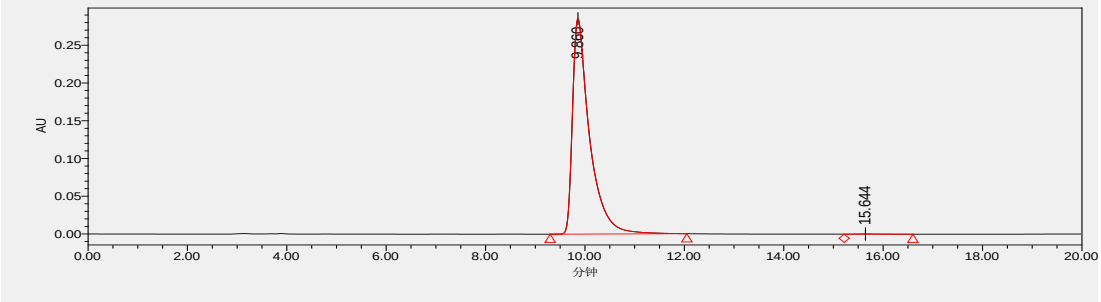
methyl 2-(benzo[d][1,3]dioxol-5-yl)-2-hydroxy-3-(2-phenyloxazol-5-yl)propanoate 3g

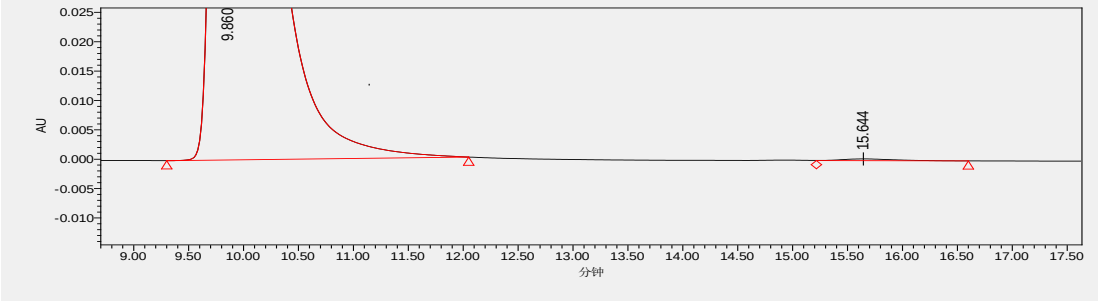


($C_{20}H_{17}NO_6$) a colourless viscous liquid; 66% yield, >99% ee. $[\alpha]_D^{20}$ = −3.8 (*c* 0.768 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 9.86 min (major), 15.64 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.01 – 7.74 (m, 2H), 7.45 – 7.25 (m, 3H), 7.13 – 7.00 (m, 2H), 6.85 (s, 1H), 6.76 – 6.57 (m, 1H), 5.89 (s, 2H), 3.90 (s, 1H), 3.76 (s, 3H), 3.59 (d, *J* = 15.2 Hz, 1H), 3.27 (d, *J* = 15.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 173.25, 160.14, 146.83, 146.58, 146.50, 133.43, 129.09, 127.70, 126.47, 125.68, 125.04, 117.94, 107.03, 105.31, 100.28, 76.34, 52.53, 35.69. ESI-HRMS: calcd for $C_{20}H_{18}NO_6^+$ ([M+H$^+$]) 368.1129, found 368.1133.



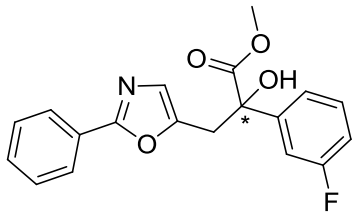
	Retention Time	Area	% Area	Height
1	10.151	1747227	50.09	69279
2	15.864	1741209	49.91	50082



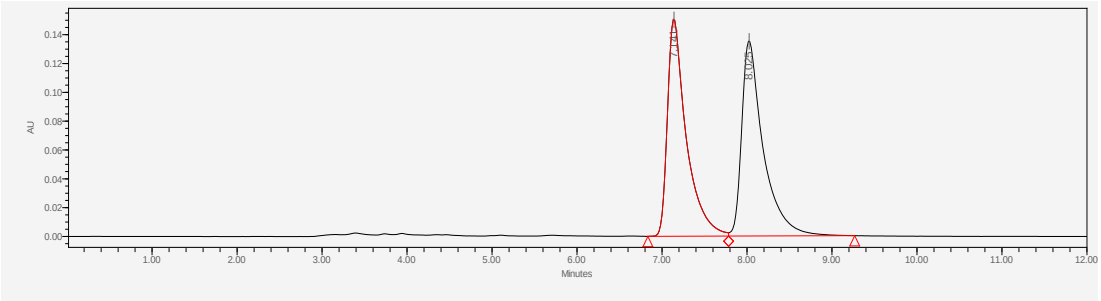


	Retention Time	Area	% Area	Height
1	9.860	6790296	99.85	285443
2	15.644	10035	0.15	302

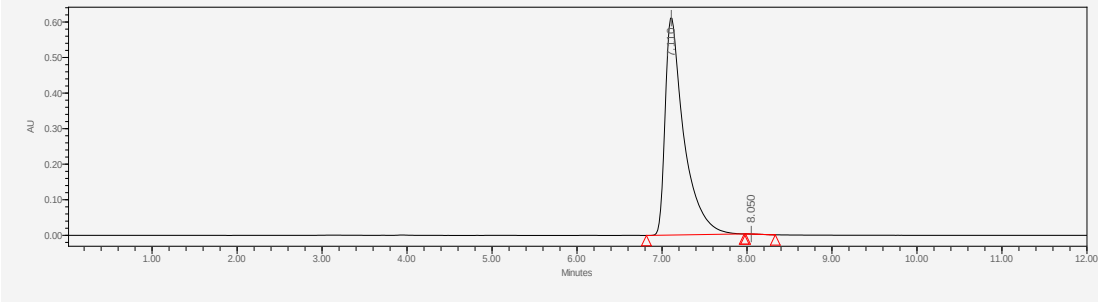
methyl 2-(3-fluorophenyl)-2-hydroxy-3-(2-phenyloxazol-5-yl)propanoate 3h

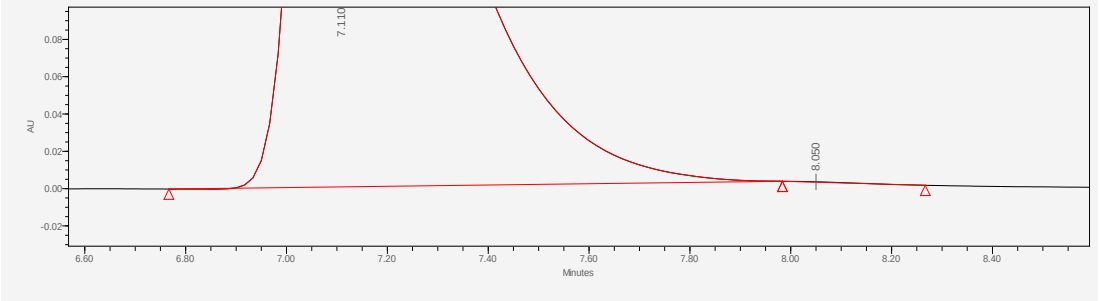


($C_{19}H_{16}FNO_4$) a colourless viscous liquid; 99% yield, >99% ee. $[\alpha]_D^{20}$ = −7.8 (*c* 1.530 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 7.11min (minor), 8.05 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.98 – 7.70 (m, 2H), 7.53 – 7.21 (m, 6H), 7.04 – 6.87 (m, 1H), 6.82 (s, 1H), 4.19 (s, 1H), 3.75 (s, 3H), 3.60 (d, *J* = 15.2 Hz, 1H), 3.26 (d, *J* = 15.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 172.79, 163.01, 160.38 (d, *J* = 6.1 Hz), 146.26, 142.12 (d, *J* = 7.0 Hz), 129.13, 128.97(d, *J* = 8.1 Hz) 127.70, 126.35, 125.76, 125.03, 120.15 (d, *J* = 2.9 Hz), 114.16 (d, *J* = 21.0 Hz), 111.94 (d, *J* = 23.4 Hz), 76.26(d, *J* = 1.6 Hz), 52.64, 35.72. ESI-HRMS: calcd for $C_{19}H_{17}FNO_4^+$ ([M+H$^+$]) 342.1136, found 342.1137.



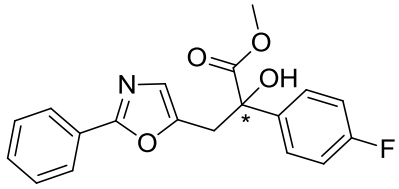
	Retention Time	Area	% Area	Height
1	7.141	2319432	49.45	151112
2	8.025	2371146	50.55	135758



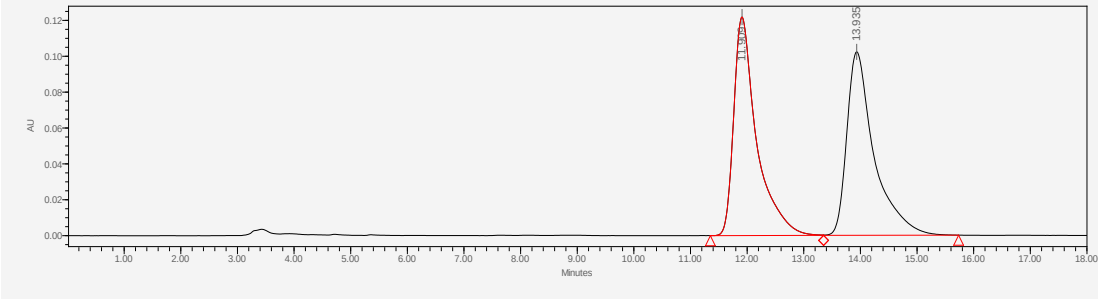


	Retention Time	Area	% Area	Height
1	7.110	9333283	99.98	614383
2	8.050	1740	0.02	231

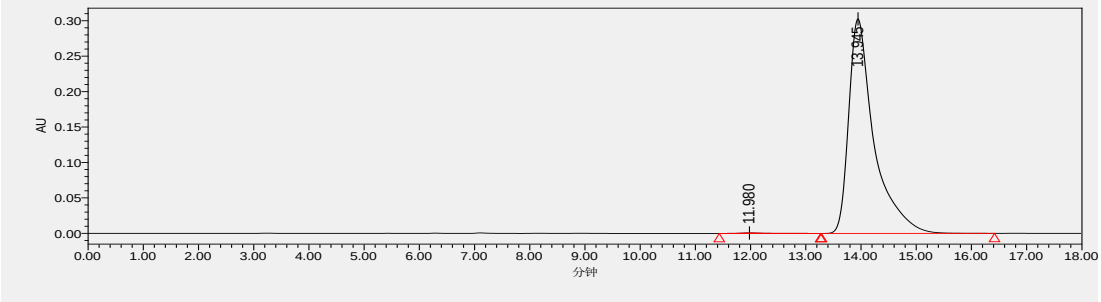
Methyl 2-(4-fluorophenyl)-2-hydroxy-3-(2-phenyloxazol-5-yl)propanoate 3i

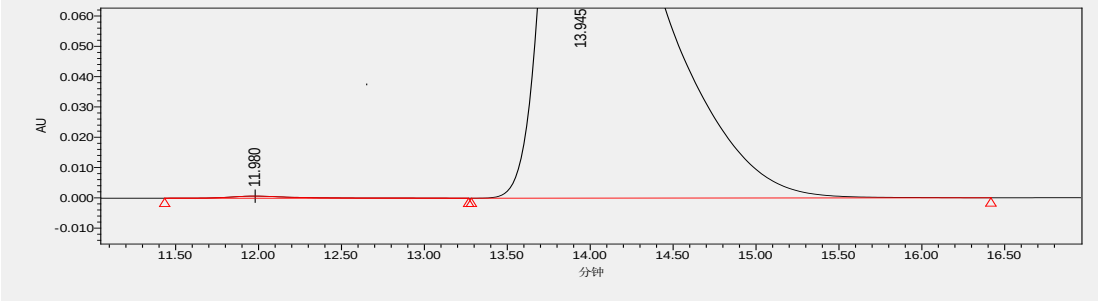


($C_{19}H_{16}FNO_4$) a colourless viscous liquid; 95% yield, >99% ee. $[\alpha]_D^{20} = -9.6$ (*c* 1.208 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IC, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 11.98 min (minor), 13.95 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ =7.98 – 7.73 (m, 2H), 7.66 – 7.47 (m, 2H), 7.42 – 7.23 (m, 3H), 7.06 – 6.90 (m, 2H), 6.82 (s, 1H), 4.10 (s, 1H), 3.74 (s, 3H), 3.60 (d, *J* = 15.6 Hz, 1H), 3.27 (d, *J* = 15.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 174.15, 163.85, 161.32 (d, *J* = 14.7 Hz), 147.43, 136.31 (d, *J* = 3.1 Hz), 130.19, 128.76, 127.49, 127.42 (d, *J* = 2.1 Hz), 126.80, 126.08, 115.33 (d, *J* = 21.4 Hz), 77.25, 53.62, 36.84. ESI-HRMS: calcd for $C_{19}H_{17}FNO_4^+$ ([M+H$^+$]) 342.1136, found 342.1135.



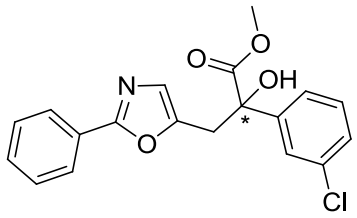
	Retention Time	Area	% Area	Height
1	11.909	3413272	50.01	121851
2	13.935	3412476	49.99	102329



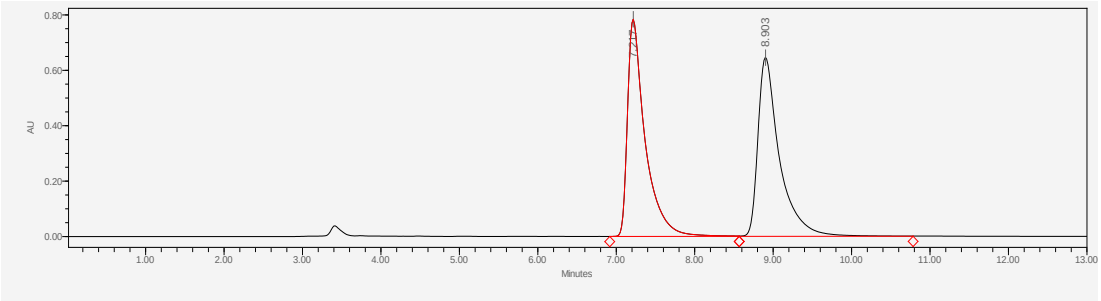


	Retention Time	Area	% Area	Height
1	11.980	18378	0.19	684
2	13.945	9595675	99.81	302810

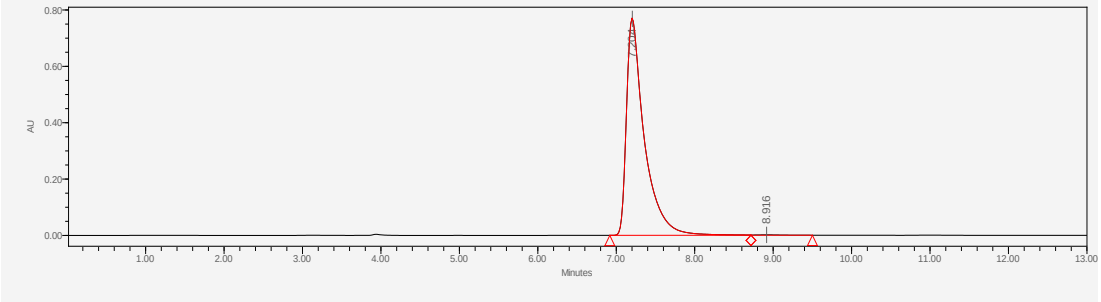
methyl 2-(3-chlorophenyl)-2-hydroxy-3-(2-phenyloxazol-5-yl)propanoate 3j

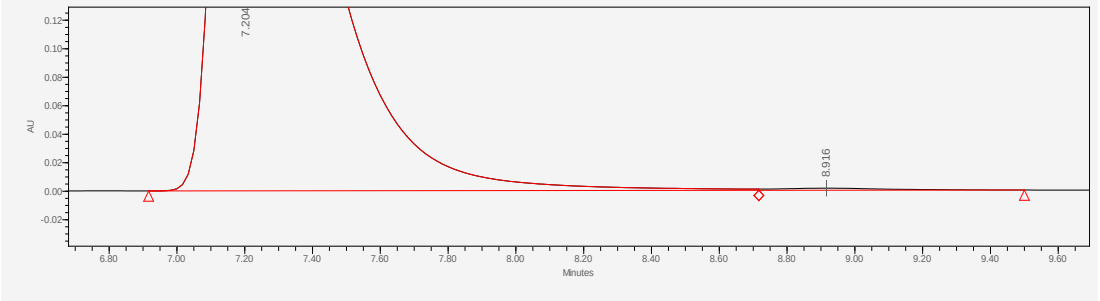


($C_{19}H_{16}ClNO_4$) a colourless viscous liquid; 98% yield, >99% ee. $[\alpha]_D^{20}$ = −8.9 (*c* 1.410 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 7.02 min (major), 8.92 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.03 – 7.85 (m, 2H), 7.70 (s, 1H), 7.60 – 7.51 (m, 1H), 7.45 – 7.38 (m, 3H), 7.35 – 7.28 (m, 2H), 6.92 (s, 1H), 4.23 (s, 1H), 3.84 (s, 3H), 3.69 (d, *J* = 15.2 Hz, 1H), 3.35 (d, *J* = 15.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 172.72, 160.22, 146.19, 141.53, 133.49, 129.14, 128.71, 127.70, 127.41, 126.33, 125.79, 125.03, 124.91, 122.74, 76.21, 52.68, 35.69. ESI-HRMS: calcd for $C_{19}H_{17}{}^{34.9689}ClNO_4^+$ ([M+H$^+$]) 358.0841, found 358.0848.



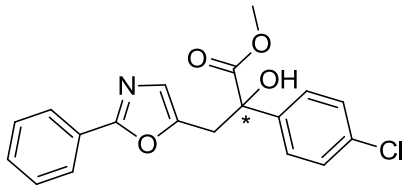
	Retention Time	Area	% Area	Height
1	7.217	12223451	49.83	783775
2	8.903	12305786	50.17	646768



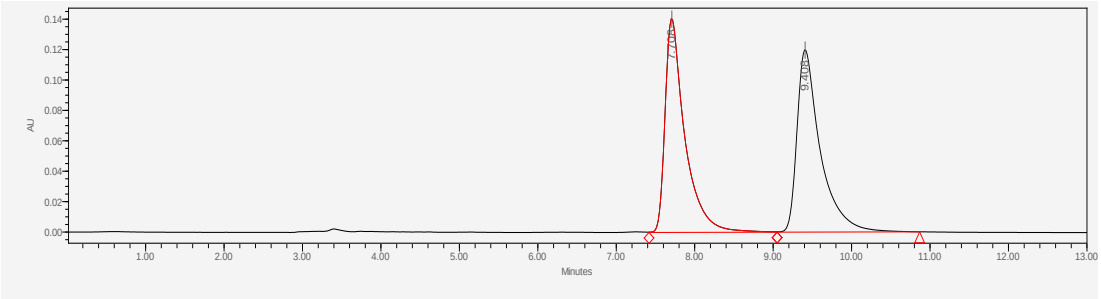


	Retention Time	Area	% Area	Height
1	7.204	12171318	99.73	771685
2	8.916	33123	0.27	1473

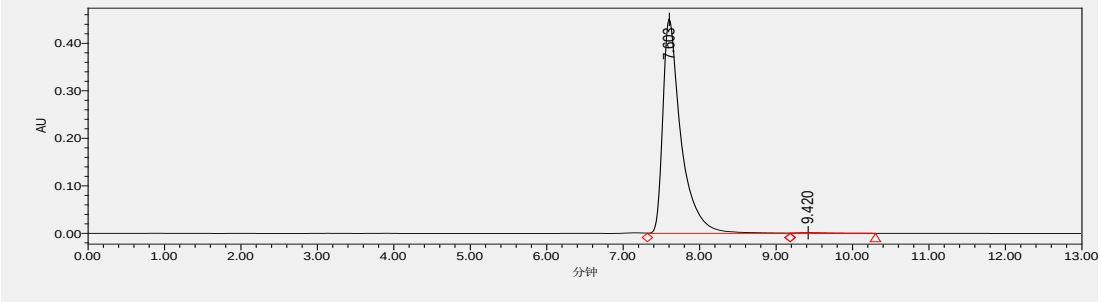
methyl 2-(4-chlorophenyl)-2-hydroxy-3-(2-phenyloxazol-5-yl)propanoate 3k

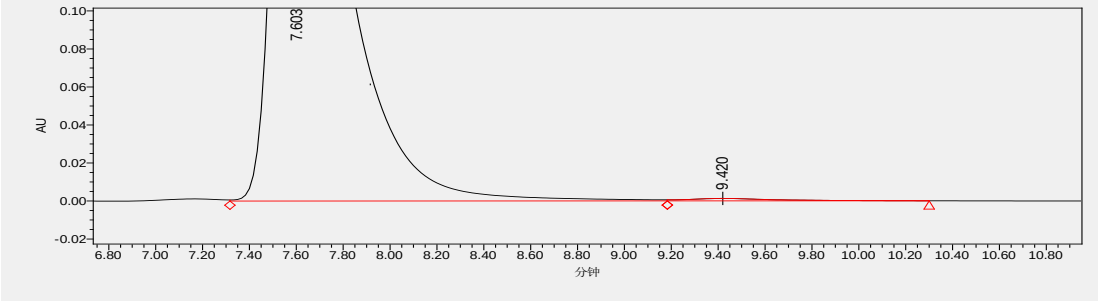


($C_{19}H_{16}ClNO_4$) a colourless viscous liquid; 99% yield, >99% ee. $[\alpha]_D^{20}$ = −4.60 (*c* 2.696 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 7.60 min (major), 9.42 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.00 – 7.85 (m, 2H), 7.67 – 7.54 (m, 2H), 7.49 – 7.29 (m, 5H), 6.91 (s, 1H), 4.19 (s, 1H), 3.83 (s, 3H), 3.67 (d, *J* = 15.2 Hz, 1H), 3.35 (d, *J* = 15.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 173.96, 161.27, 147.30, 139.05, 134.33, 130.21, 128.77, 128.63, 127.40, 127.08, 126.85, 126.09, 77.27, 53.69, 36.74. ESI-HRMS: calcd for $C_{19}H_{17}{}^{34.9689}ClNO_4{}^+$ ([M+H$^+$]) 358.0841, found 358.0840.



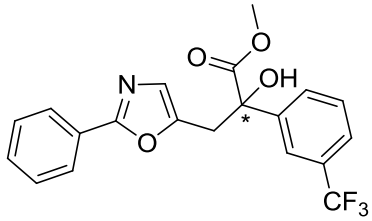
	Retention Time	Area	% Area	Height
1	7.708	2457605	49.94	140881
2	9.408	2463222	50.06	120064



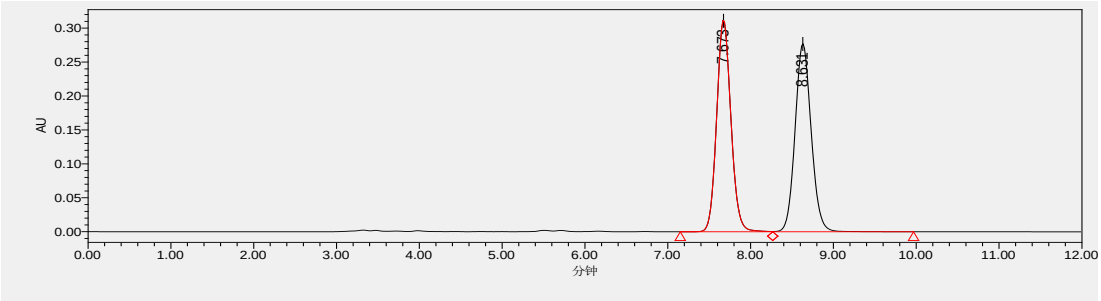


	Retention Time	Area	% Area	Height
1	7.603	7458156	99.56	451476
2	9.420	33037	0.44	1289

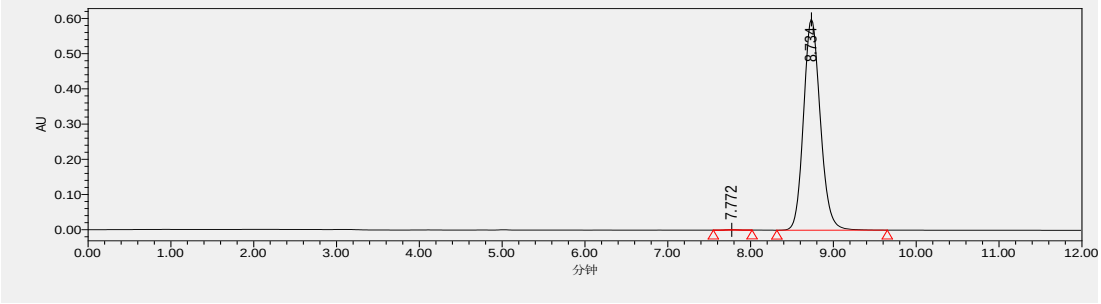
methyl 2-hydroxy-3-(2-phenyloxazol-5-yl)-2-(3-(trifluoromethyl)phenyl)propanoate 3l

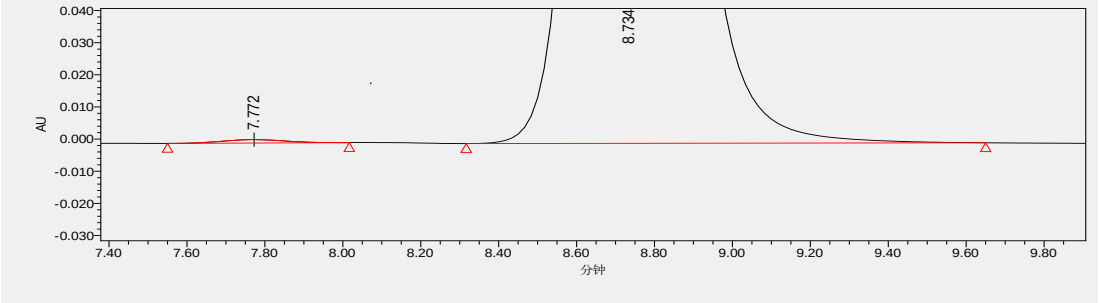


($C_{20}H_{16}F_3NO_4$) a colourless viscous liquid; 99% yield, >99% ee. $[\alpha]_D^{20}$ = −13.8 (*c* 1.774 in CH_2Cl_2). HPLC DAICEL CHIRALCEL ID, n-hexane/2-propanol = 70/30, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 7.78 min (minor), 8.73 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.96 – 7.88 (m, 1H), 7.86 – 7.74 (m, 3H), 7.55 – 7.48 (m, 1H), 7.45 – 7.38 (m, 1H), 7.38 – 7.28 (m, 3H), 6.84 (s, 1H), 4.29 (s, 1H), 3.77 (s, 3H), 3.64 (d, *J* = 15.2 Hz, 1H), 3.29 (d, *J* = 15.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 173.72, 161.36, 147.08, 141.57, 131.04, 130.72, 130.25, 129.08 (d, *J* = 9.3 Hz), 128.76, 127.32, 126.94, 126.08, 125.39, 125.18 (q, *J* = 3.7 Hz), 122.62 (q, *J* = 3.9 Hz), 77.41, 53.83, 36.92. ESI-HRMS: calcd for $C_{20}H_{17}F_3NO_4^+$ ([M+H$^+$]) 392.1104, found 392.1107.



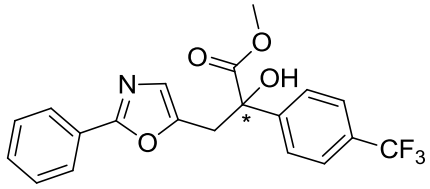
	Retention Time	Area	% Area	Height
1	7.673	3736883	49.93	312455
2	8.631	3746971	50.07	277216



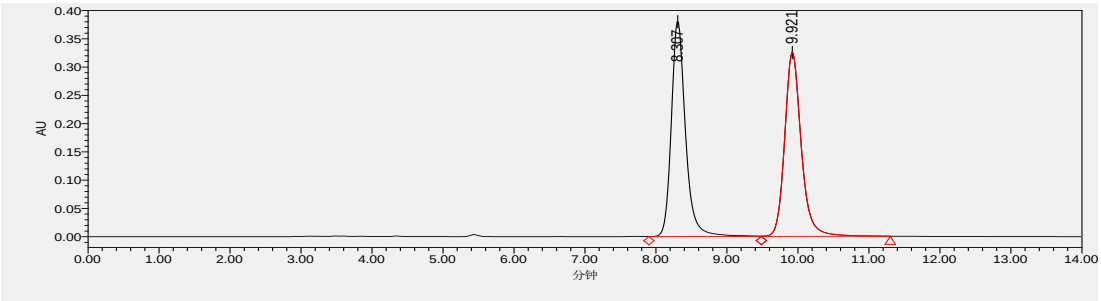


	Retention Time	Area	% Area	Height
1	7.772	11678	0.14	1050
2	8.734	8410791	99.86	599073

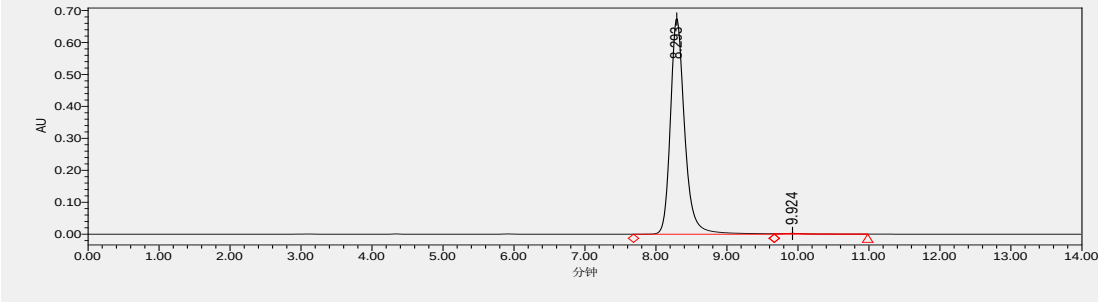
methyl 2-hydroxy-3-(2-phenyloxazol-5-yl)-2-(4-(trifluoromethyl)phenyl)propanoate 3m

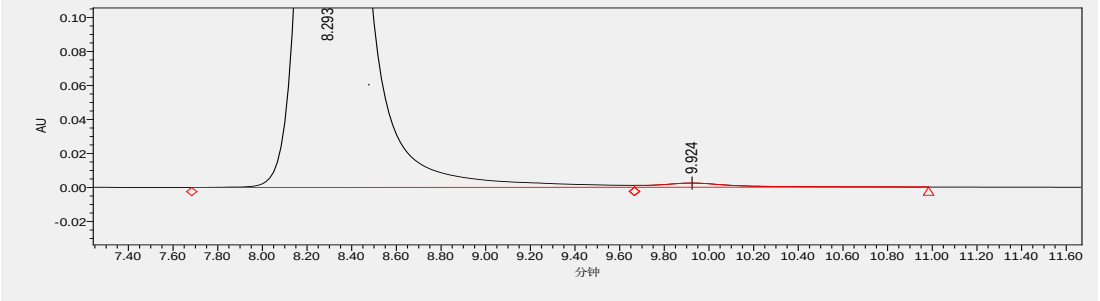


($C_{20}H_{16}F_3NO_4$) a colourless viscous liquid; 97% yield, 99% ee. $[\alpha]_D^{20}$ = −11.2 (*c* 1.250 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IA, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 8.29 min (major), 9.92 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.91 – 7.67 (m, 4H), 7.62 – 7.50 (m, 2H), 7.41 – 7.26 (m, 3H), 6.85 (s, 1H), 4.15 (s, 1H), 3.77 (s, 3H), 3.63 (d, *J* = 15.2 Hz, 1H), 3.31 (d, *J* = 15.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 173.67, 161.36, 147.03, 144.36, 130.68, 130.35, 130.26, 128.77, 127.35, 126.98, 126.11 (d, *J* = 7.8 Hz) , 125.41 (q, *J* = 3.6 Hz), 122.63, 77.38, 53.84, 36.83. ESI-HRMS: calcd for $C_{20}H_{17}F_3NO_4^+$ ([M+H$^+$]) 392.1104, found 392.1109.



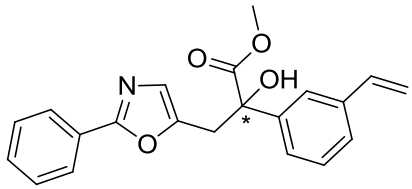
	Retention Time	Area	% Area	Height
1	8.307	5305638	50.11	381629
2	9.921	5281504	49.89	326108



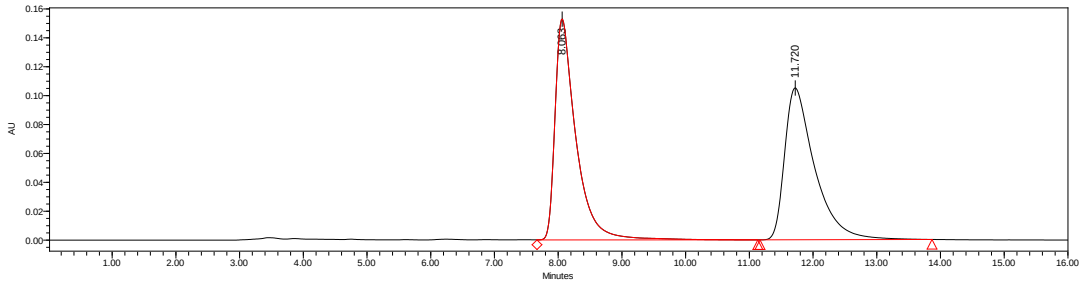


	Retention Time	Area	% Area	Height
1	8.293	9461496	99.38	675611
2	9.924	59501	0.62	2449

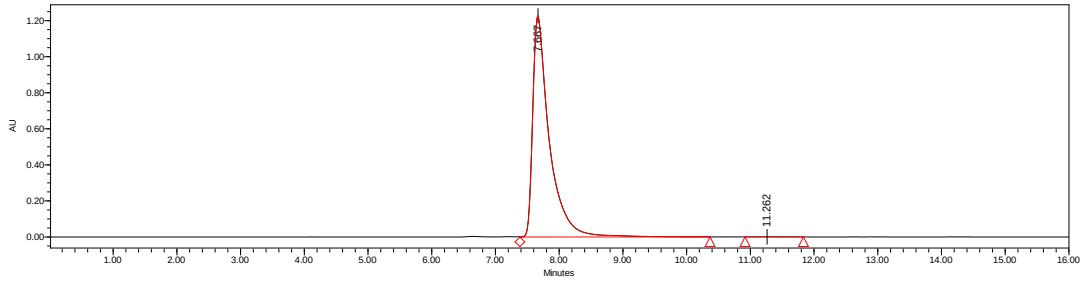
methyl 2-hydroxy-3-(2-phenyloxazol-5-yl)-2-(3-vinylphenyl)propanoate 3n

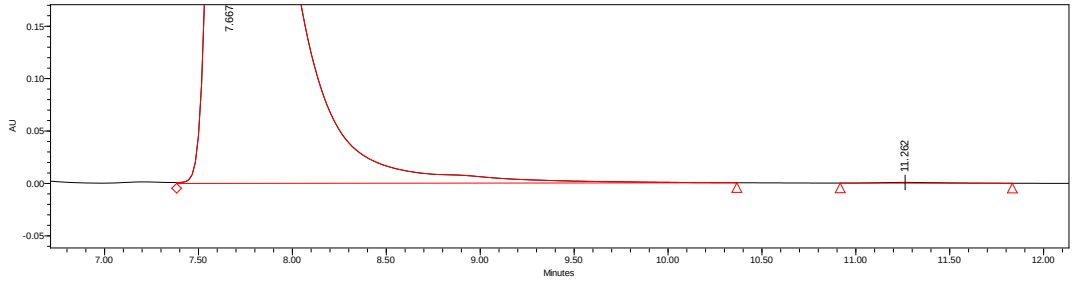


($C_{21}H_{19}NO_4$) a white amorphous solid; 97% yield, >99% ee. $[\alpha]_D^{20}$ = −7.5 (*c* 1.290 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 7.67 min (major), 11.26 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.00 – 7.84 (m, 2H), 7.79 – 7.66 (m, 1H), 7.63 – 7.50 (m, 1H), 7.48 – 7.30 (m, 5H), 6.94 (s, 1H), 6.74 (dd, *J* = 17.6, 10.8 Hz, 1H), 5.79 (d, *J* = 17.6 Hz, 1H), 5.29 (d, *J* = 10.8 Hz, 1H), 4.06 (s, 1H), 3.83 (s, 3H), 3.74 (d, *J* = 15.2 Hz, 1H), 3.38 (d, *J* = 15.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 174.23, 161.23, 147.63, 140.86, 137.87, 136.60, 130.15, 128.76, 128.74, 127.50, 126.78, 126.10, 126.01, 124.92, 123.47, 114.61, 77.58, 53.63, 36.66. ESI-HRMS: calcd for $C_{21}H_{20}NO_4$+ ([M+H$^+$]) 350.1387, found 350.1387.



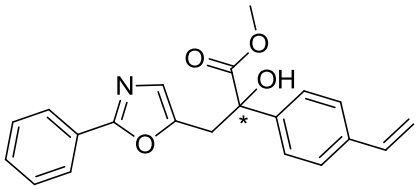
	Retention Time	Area	% Area	Height
1	8.063	3492300	50.40	152983
2	11.720	3436740	49.60	105187



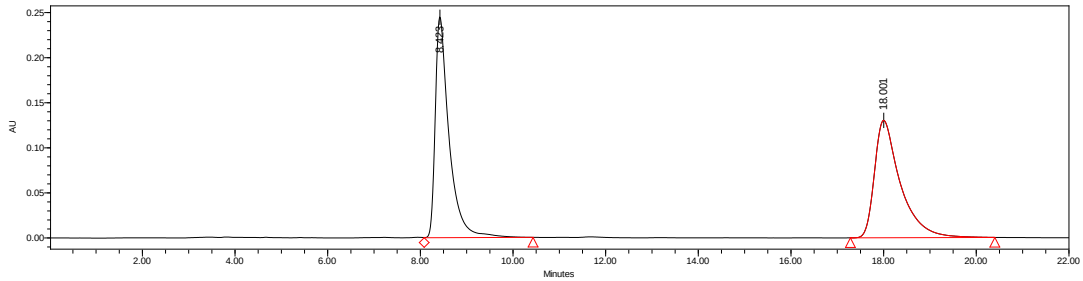


	Retention Time	Area	% Area	Height
1	7.667	22176913	99.93	1226431
2	11.262	16072	0.07	693

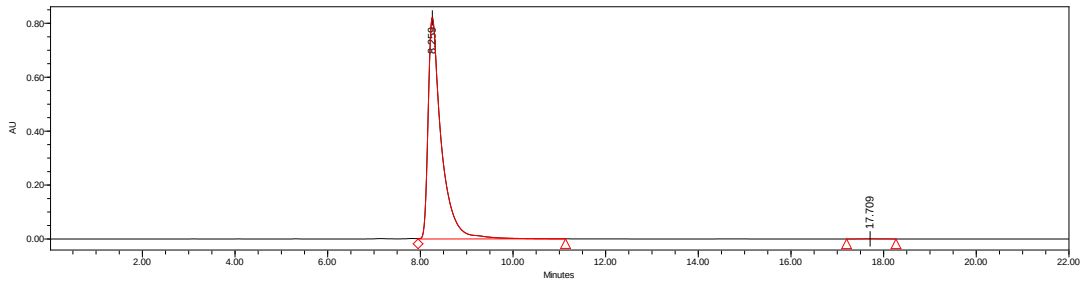
methyl 2-hydroxy-3-(2-phenyloxazol-5-yl)-2-(4-vinylphenyl)propanoate 3o

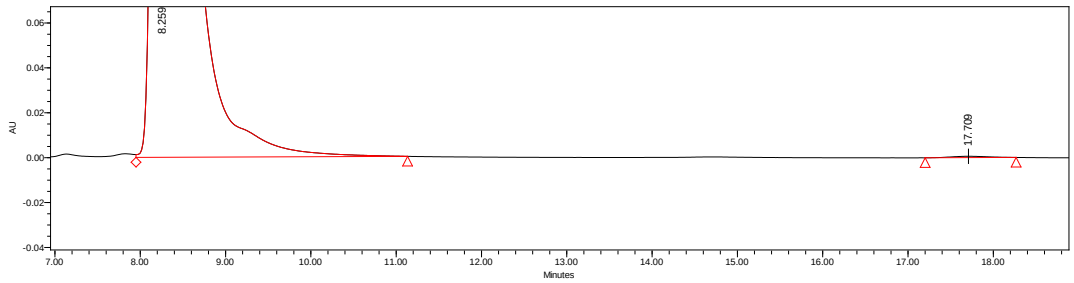


($C_{21}H_{19}NO_4$) a colourless viscous liquid; 95% yield, >99% ee. $[\alpha]_D^{20}$ = −3.9 (*c* 1.260 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 8.26 min (major), 17.71 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.93 – 7.77 (m, 2H), 7.61 – 7.47 (m, 2H), 7.42 – 7.25 (m, 5H), 6.84 (s, 1H), 6.63 (dd, *J* = 17.6, 10.8 Hz, 1H), 5.69 (d, *J* = 17.6 Hz, 1H), 5.20 (d, *J* = 11.2 Hz, 1H), 4.01 (s, 1H), 3.74 (s, 3H), 3.64 (d, *J* = 15.2 Hz, 1H), 3.29 (d, *J* = 15.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 173.17, 160.13, 146.55, 138.90, 136.52, 135.04, 129.07, 127.69, 126.41, 125.69, 125.24, 125.02, 124.65, 113.60, 76.49, 52.53, 35.51. ESI-HRMS: calcd for $C_{21}H_{20}NO_4$+ ([M+H$^+$]) 350.1387, found 350.1387.



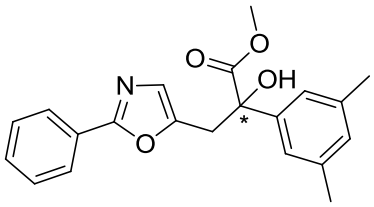
	Retention Time	Area	% Area	Height
1	8.423	5079731	50.18	245268
2	18.001	5043538	49.82	130292



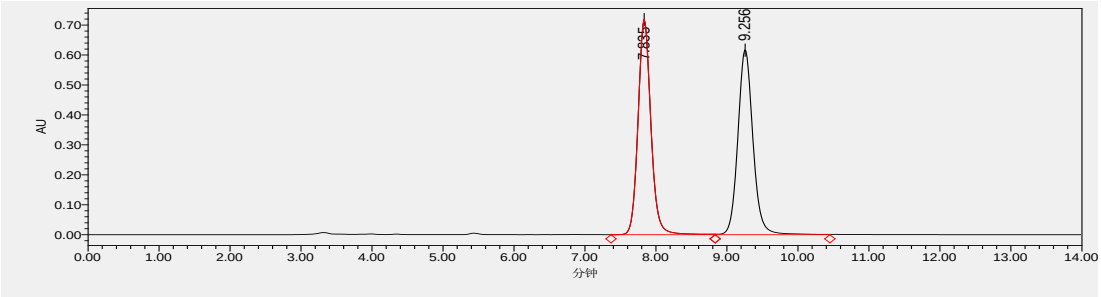


	Retention Time	Area	% Area	Height
1	8.259	16248691	99.88	823221
2	17.709	18907	0.12	614

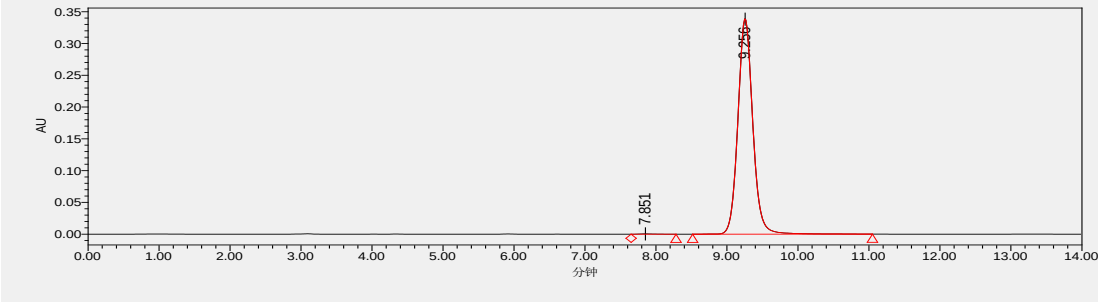
methyl 2-(3,5-dimethylphenyl)-2-hydroxy-3-(2-phenyloxazol-5-yl)propanoate 3p

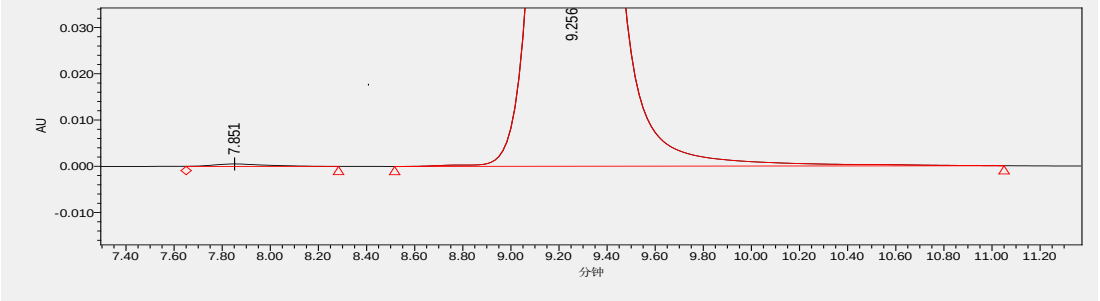


($C_{21}H_{21}NO_4$) a white amorphous solid; 93% yield, >99% ee. $[\alpha]_D^{20}$ = −6.7 (*c* 1.142 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IA, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 7.85 min (minor), 9.26 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.96 – 7.80 (m, 2H), 7.41 – 7.26 (m, 3H), 7.18 (s, 2H), 6.89 (s, 1H) , 6.85(s, 1H) , 3.90 (s, 1H), 3.74 (s, 3H), 3.65 (d, *J* = 15.2 Hz, 1H), 3.27 (d, *J* = 15.2 Hz, 1H), 2.25 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 174.41, 161.15, 147.89, 140.54, 138.12, 130.10, 129.96, 128.74, 127.58, 126.70, 126.09, 123.13, 77.64, 53.49, 36.51, 21.52. ESI-HRMS: calcd for $C_{21}H_{22}NO_4^+$ ([M+H$^+$]) 352.1543, found 352.1546.



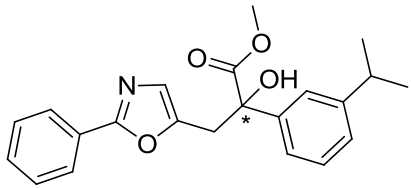
	Retention Time	Area	% Area	Height
1	7.835	9048493	49.80	718767
2	9.256	9120398	50.20	618384



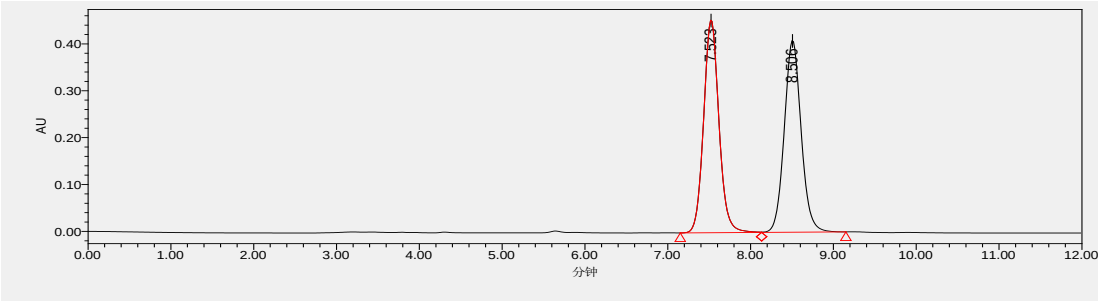


	Retention Time	Area	% Area	Height
1	7.851	8329	0.17	541
2	9.256	4930960	99.83	339287

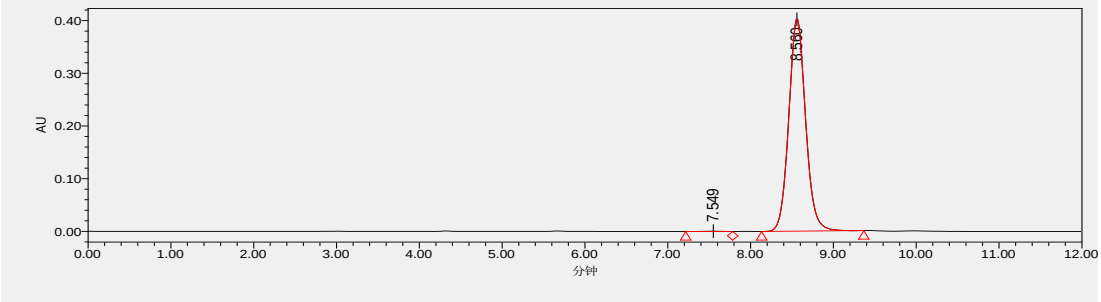
methyl 2-hydroxy-2-(3-isopropylphenyl)-3-(2-phenyloxazol-5-yl)propanoate 3q

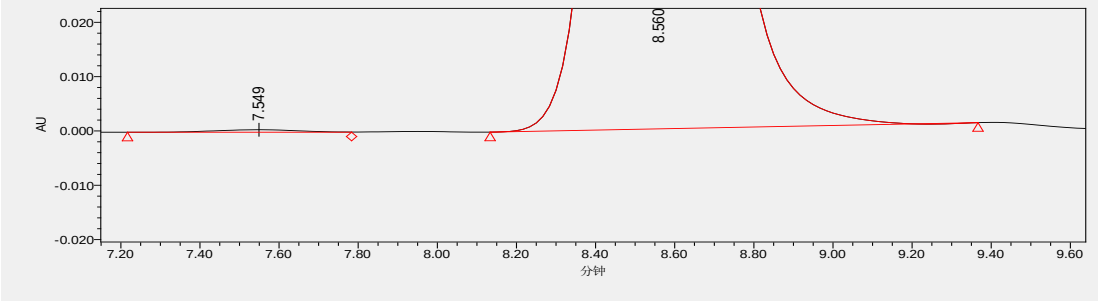


($C_{22}H_{23}NO_4$) a colourless viscous liquid; 95% yield, >99% ee. $[\alpha]_D^{20}$ = −3.3 (*c* 1.610 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IA, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 7.55 min (minor), 8.56 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.02 – 7.88 (m, 2H), 7.57 – 7.37 (m, 5H), 7.36 – 7.27 (m, 1H), 7.23 – 7.15 (m, 1H), 6.94 (s, 1H), 3.96 (s, 1H), 3.84 (s, 3H), 3.73 (d, *J* = 15.2 Hz, 1H), 3.39 (d, *J* = 15.2 Hz, 1H), 2.93 (dt, *J* = 14.0, 7.2 Hz, 1H), 1.25 (d, *J* = 7.2 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 174.41, 161.17, 149.26, 147.81, 140.48, 130.12, 128.75, 128.46, 127.55, 126.73, 126.32, 126.09, 123.56, 122.93, 77.75, 53.53, 36.70, 34.32, 24.06, 24.03. ESI-HRMS: calcd for $C_{22}H_{24}NO_4^+$ ([M+H$^+$]) 366.1700, found 366.1704.



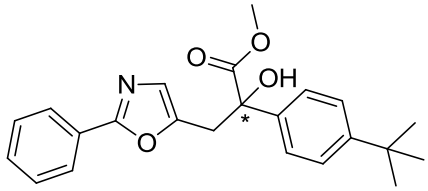
	Retention Time	Area	% Area	Height
1	7.523	5819334	50.15	454439
2	8.506	5785306	49.85	409373



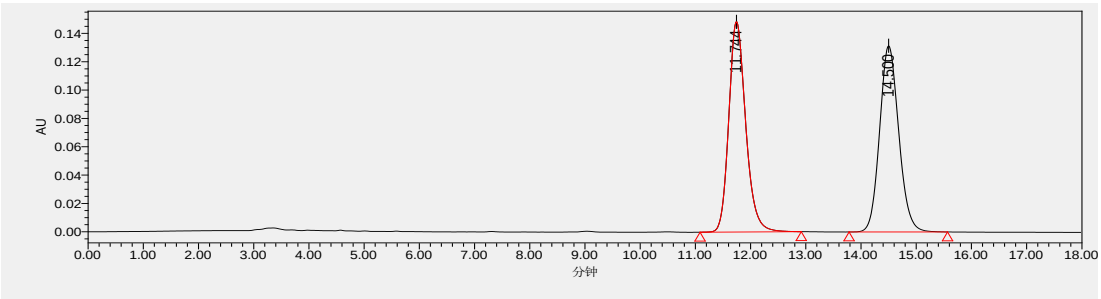


	Retention Time	Area	% Area	Height
1	7.549	6647	0.12	457
2	8.560	5688697	99.88	403439

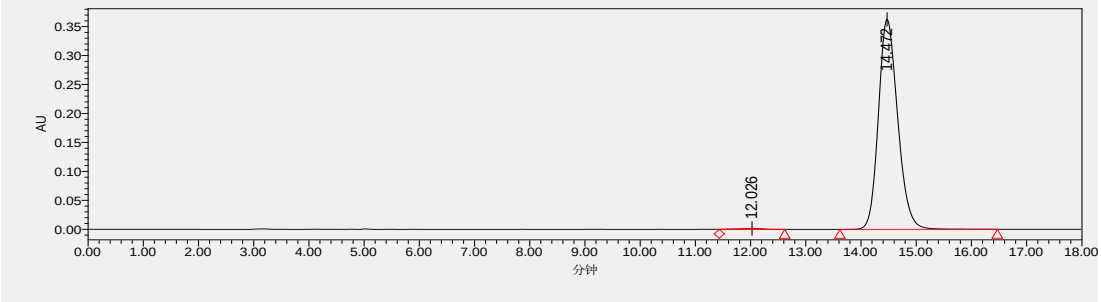
methyl 2-(4-(tert-butyl)phenyl)-2-hydroxy-3-(2-phenyloxazol-5-yl)propanoate 3r

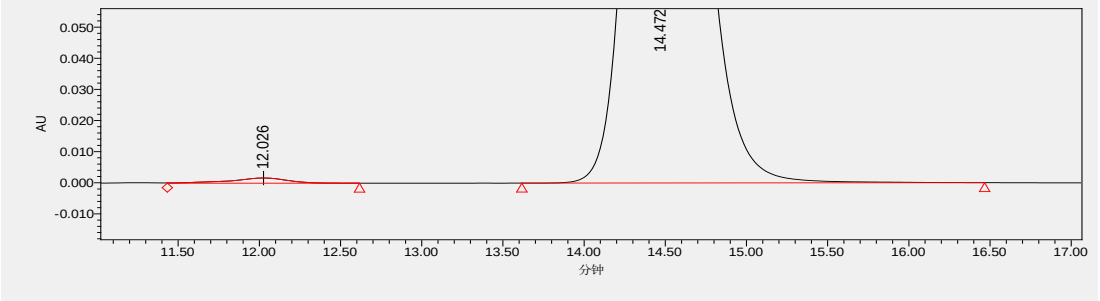


($C_{23}H_{25}NO_4$) a white amorphous solid; 96% yield, >99% ee. $[\alpha]_D^{20} = -7.9$ (*c* 1.404 in CH_2Cl_2). HPLC DAICEL CHIRALCEL ID, n-hexane/2-propanol = 70/30, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 12.03 min (minor), 14.47 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.92 – 7.75 (m, 2H), 7.55 – 7.43 (m, 2H), 7.39 – 7.25 (m, 5H), 6.85 (s, 1H), 3.93 (s, 1H), 3.74 (s, 3H), 3.63 (d, *J* = 15.2 Hz, 1H), 3.30 (d, *J* = 15.2 Hz, 1H), 1.24 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 174.44, 151.23, 147.84, 137.59, 130.10, 128.74, 127.55, 126.72, 126.08, 125.44, 125.16, 77.52, 53.49, 36.65, 34.56, 31.32. ESI-HRMS: calcd for $C_{23}H_{26}NO_4^+$ ([M+H$^+$]) 380.1856, found 380.1860.



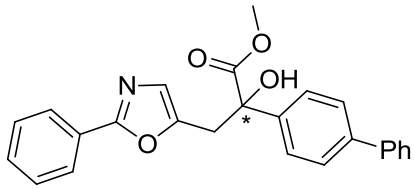
	Retention Time	Area	% Area	Height
1	11.744	3156417	49.98	148507
2	14.500	3159071	50.02	131364



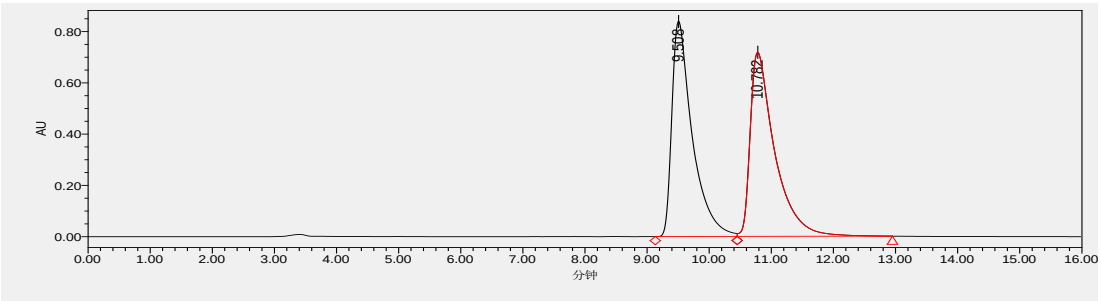


	Retention Time	Area	% Area	Height
1	12.026	40547	0.46	1677
2	14.472	8791702	99.54	362992

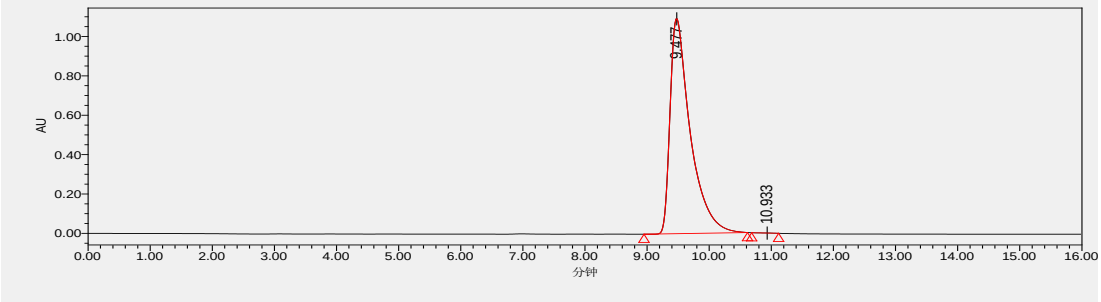
methyl 2-([1,1'-biphenyl]-4-yl)-2-hydroxy-3-(2-phenyloxazol-5-yl)propanoate 3s

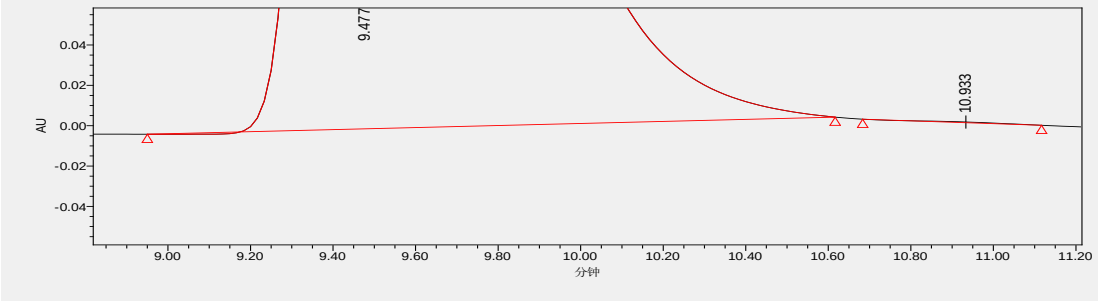


($C_{25}H_{21}NO_4$) a white amorphous solid; 95% yield, >99% ee. $[\alpha]_D^{20}$ = −0.7 (*c* 1.428 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 9.48 min (major), 10.93 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.94 – 7.76 (m, 2H), 7.72 – 7.58 (m, 2H), 7.55 – 7.45 (m, 4H), 7.42 – 7.24 (m, 6H), 6.88 (s, 1H), 3.95 (s, 1H), 3.78 (s, 3H), 3.68 (d, *J* = 15.2 Hz, 1H), 3.35 (d, *J* = 15.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 174.30, 161.25, 147.63, 141.23, 140.43, 139.53, 130.15, 128.86, 128.77, 127.57, 127.55, 127.23, 127.15, 126.85, 126.10, 125.98, 77.55, 53.65, 36.71. ESI-HRMS: calcd for $C_{25}H_{22}NO_4^+$ ([M+H$^+$]) 400.1543, found 400.1553.



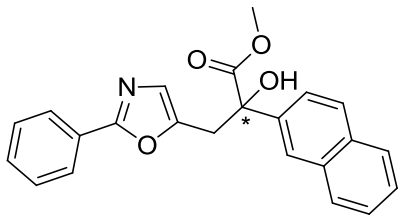
	Retention Time	Area	% Area	Height
1	9.508	19112697	49.39	840691
2	10.782	19587319	50.61	718042



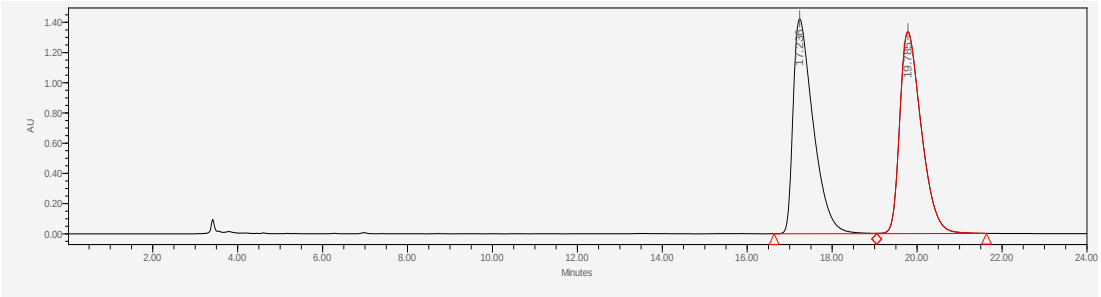


	Retention Time	Area	% Area	Height
1	9.477	24598525	99.98	1092342
2	10.933	4784	0.02	367

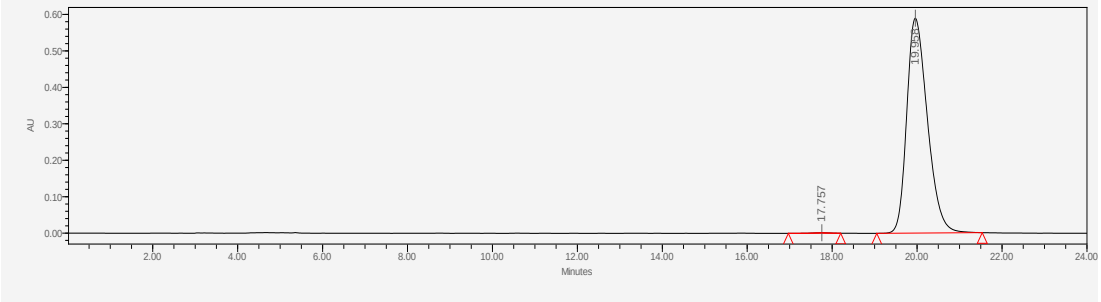
methyl 2-hydroxy-2-(naphthalen-2-yl)-3-(2-phenyloxazol-5-yl)propanoate 3t

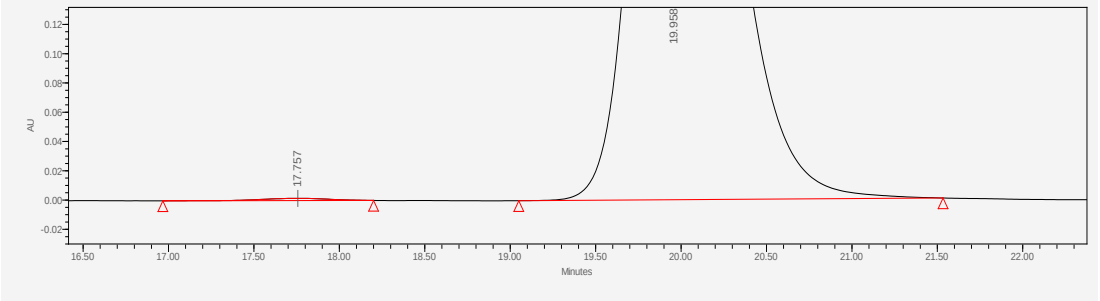


($C_{23}H_{19}NO_4$) a colourless viscous liquid; 98% yield, >99% ee. $[\alpha]_D^{20}$ = +0.7 (*c* 1.376 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IE, n-hexane/2-propanol = 70/30, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 17.76 min (minor), 19.96 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.27 – 8.12 (m, 1H), 8.08 – 7.76 (m, 6H), 7.66 – 7.37 (m, 5H), 6.99 (s, 1H), 4.33 (s, 1H), 3.95 – 3.80 (m, 4H), 3.51 (d, *J* = 15.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 174.30, 161.23, 147.68, 137.89, 133.02, 133.00, 130.13, 128.74, 128.46, 128.32, 127.56, 127.49, 126.81, 126.57, 126.45, 126.10, 124.78, 123.28, 77.84, 53.61, 36.59. ESI-HRMS: calcd for $C_{23}H_{20}NO_4^+$ ([M+H$^+$]) 374.1387, found 374.1390.



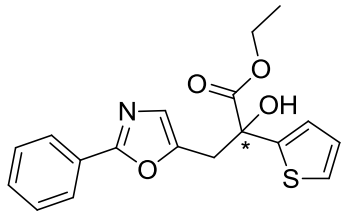
	Retention Time	Area	% Area	Height
1	17.236	46799868	49.99	1423002
2	19.785	46822465	50.01	1336157



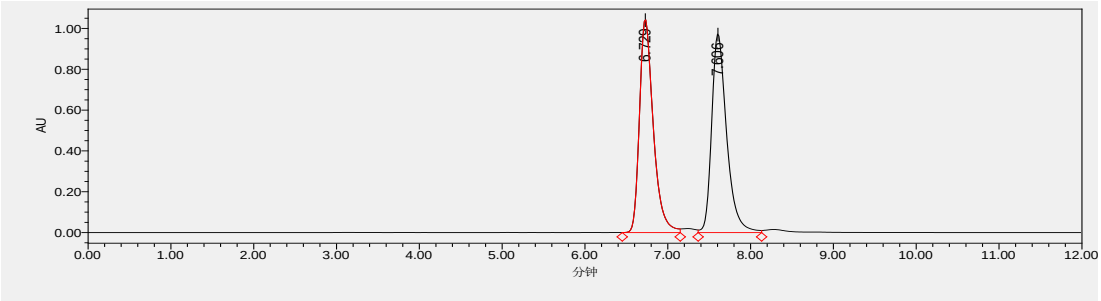


	Retention Time	Area	% Area	Height
1	17.757	42222	0.21	1534
2	19.958	19891642	99.79	589747

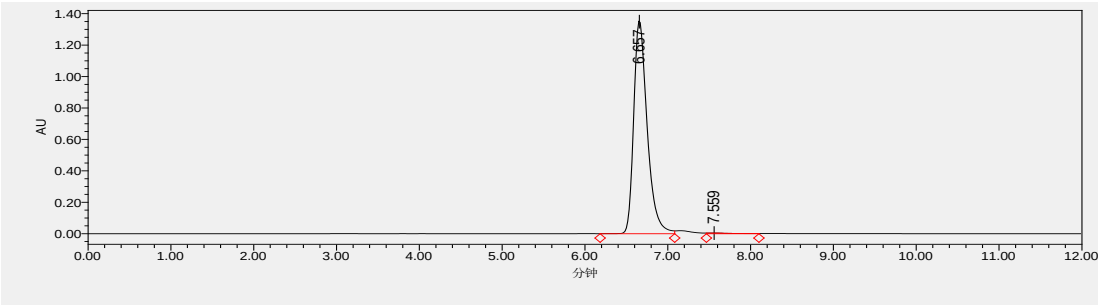
ethyl 2-hydroxy-3-(2-phenyloxazol-5-yl)-2-(thiophen-2-yl)propanoate 3u



($C_{18}H_{17}NO_4S$) a colourless viscous liquid; 98% yield, 99% ee. $[\alpha]_D^{20}$ = −9.7 (*c* 1.292 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 6.66 min (major), 7.56 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.12 – 7.82 (m, 2H), 7.50 – 7.35 (m, 3H), 7.33 – 7.14 (m, 2H), 7.04 – 6.98 (m, 1H), 6.96 (s, 1H), 4.39 (s, 1H), 4.31 (q, *J* = 7.2, 3.2 Hz, 2H), 3.69 (d, *J* = 15.2 Hz, 1H), 3.45 (d, *J* = 15.3 Hz, 1H), 1.31 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 172.87, 161.27, 147.17, 145.44, 130.18, 128.76, 127.49, 127.20, 126.90, 126.13, 125.56, 124.53, 76.36, 63.23, 37.95, 14.10. ESI-HRMS: calcd for $C_{18}H_{18}NO_4S^+$ ([M+H$^+$]) 344.0951, found 344.0960.

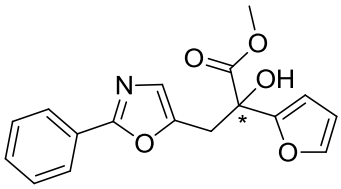


	Retention Time	Area	% Area	Height
1	6.729	12099168	49.66	1044155
2	7.606	12264017	50.34	975266

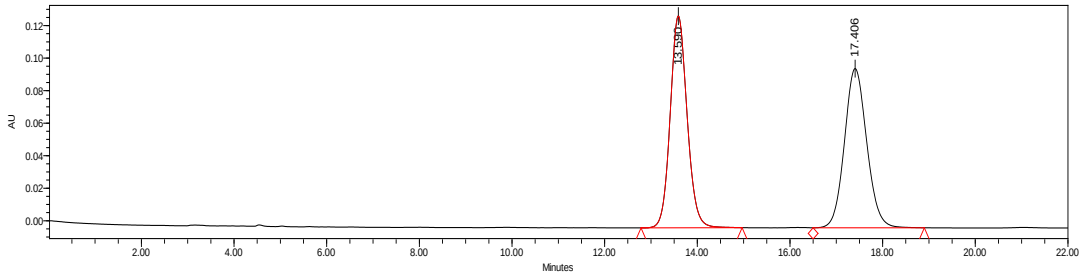


	Retention Time	Area	% Area	Height
1	6.657	15324320	99.44	1359154
2	7.559	86533	0.56	4393

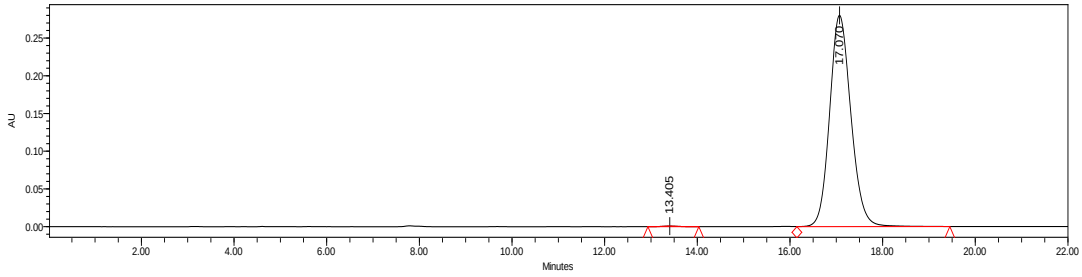
methyl 2-(furan-2-yl)-2-hydroxy-3-(2-phenyloxazol-5-yl)propanoate 3v

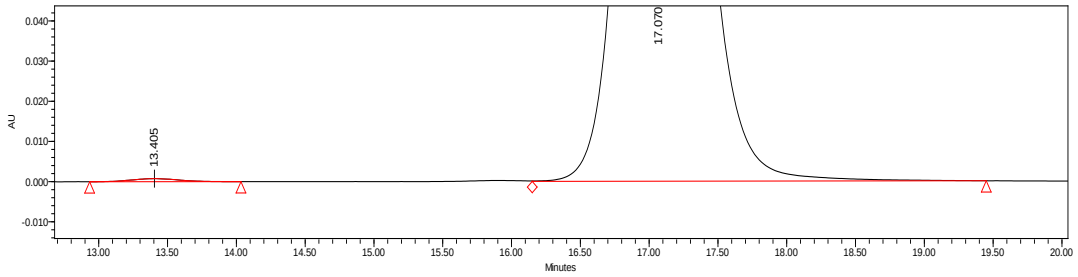


($C_{17}H_{15}NO_5$) a yellow amorphous solid; 96% yield, >99% ee. $[\alpha]_D^{20}$ = −23.2 (*c* 1.120 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IC, n-hexane/2-propanol = 70/30, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 13.41 min (minor), 17.07 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.94 – 7.77 (m, 2H), 7.46 – 7.23 (m, 4H), 6.87 (s, 1H), 6.37 – 6.25 (m, 2H), 4.17 (s, 1H), 3.76 (s, 3H), 3.60 (d, *J* = 15.6 Hz, 1H), 3.45 (d, *J* = 15.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 172.68, 161.38, 152.71, 146.84, 142.92, 130.19, 128.75, 127.44, 126.96, 126.11, 110.63, 107.49, 74.35, 53.72, 33.90. ESI-HRMS: calcd for $C_{17}H_{15}NNaO_5^+$ ([M+Na$^+$]) 336.0842, found 336.0851.



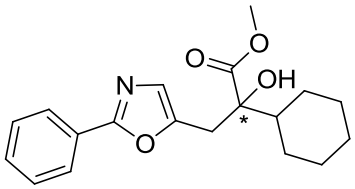
	Retention Time	Area	% Area	Height
1	13.590	3297917	50.20	130286
2	17.406	3271967	49.80	97945



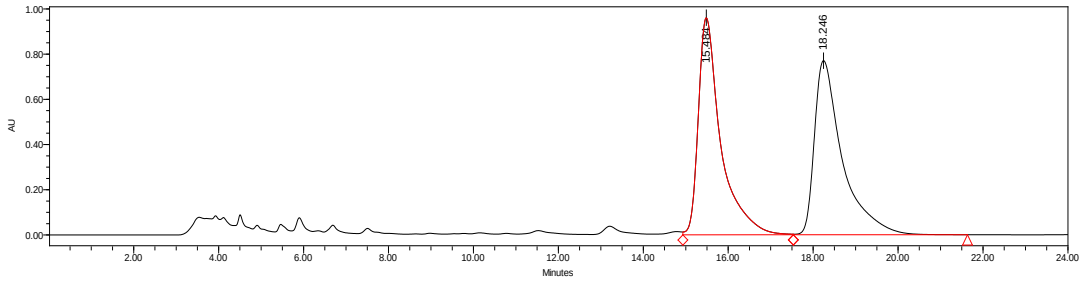


	Retention Time	Area	% Area	Height
1	13.405	18472	0.21	774
2	17.070	8921466	99.79	280148

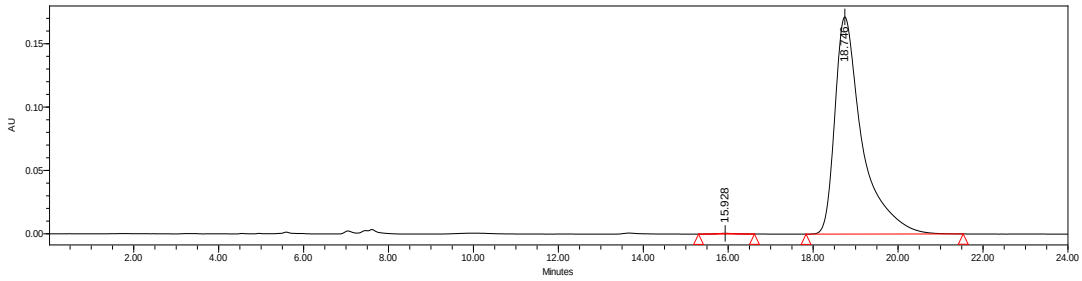
methyl 2-cyclohexyl-2-hydroxy-3-(2-phenyloxazol-5-yl)propanoate 3w

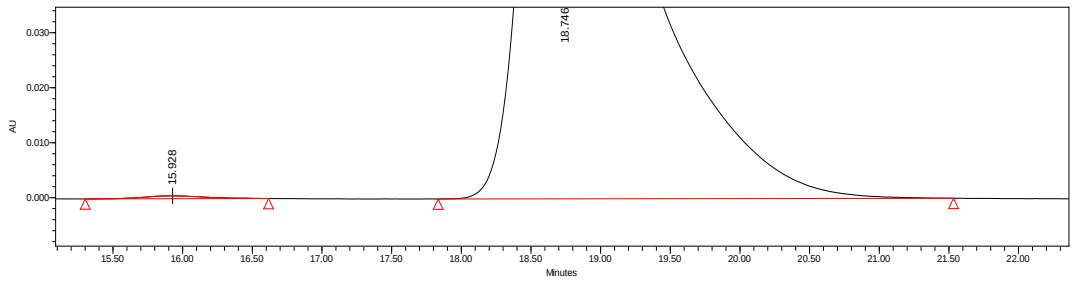


($C_{19}H_{23}NO_4$) a yellow amorphous solid; 40% yield, >99% ee. $[\alpha]_D^{20}$ = +2.0 (*c* 0.734 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IC, n-hexane/2-propanol = 70/30, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 15.93 min (minor), 18.75 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.01 – 7.83 (m, 2H), 7.43 – 7.30 (m, 3H), 6.85 (s, 1H), 3.73 (s, 3H), 3.22 (s, 1H), 3.15 (d, *J* = 14.8 Hz, 1H), 3.06 (d, *J* = 15.2 Hz, 1H), 1.90 – 1.55 (m, 5H), 1.37 – 1.01 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 174.91, 160.17, 147.29, 129.06, 127.72, 126.52, 125.30, 124.99, 78.33, 51.88, 43.90, 32.28, 26.45, 25.20, 25.18, 25.05, 24.82. ESI-HRMS: calcd for $C_{19}H_{24}NO_4^+$ ([M+H$^+$]) 330.1700, found 330.1704.



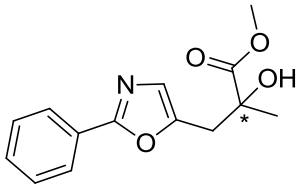
	Retention Time	Area	% Area	Height
1	15.484	35186858	50.09	960516
2	18.246	35064501	49.91	770679



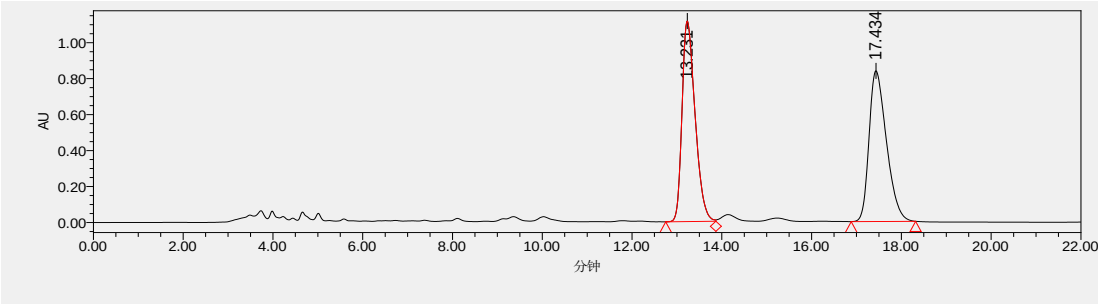


	Retention Time	Area	% Area	Height
1	15.928	16178	0.21	527
2	18.746	7615625	99.79	171387

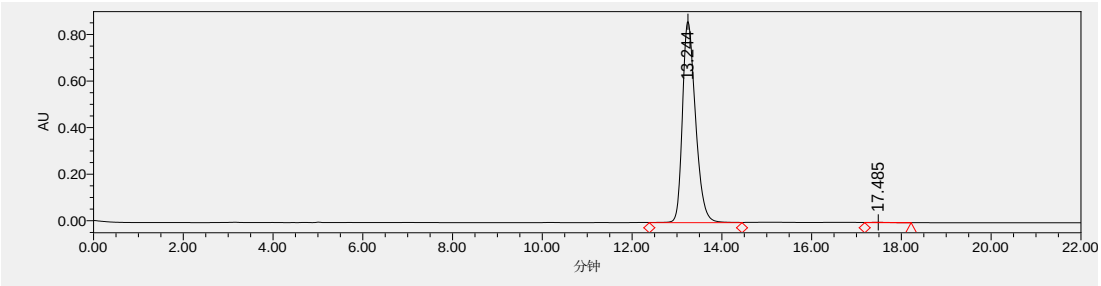
methyl 2-hydroxy-2-methyl-3-(2-phenyloxazol-5-yl)propanoate 3x

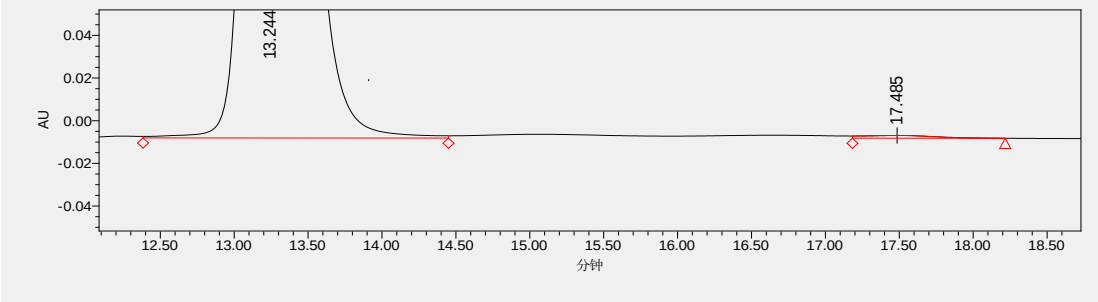


($C_{14}H_{15}NO_4$) a colourless amorphous solid; 84% yield, >99% ee. $[\alpha]_D^{20}$ = +9.0 (*c* 0.818 in CH_2Cl_2). HPLC DAICEL CHIRALCEL ID, n-hexane/2-propanol = 70/30, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 13.24 min (major), 17.49 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.18 – 7.78 (m, 2H), 7.54 – 7.32 (m, 3H), 6.96 (s, 1H), 3.81 (s, 3H), 3.60 (s, 1H), 3.24 (d, *J* = 15.2 Hz, 1H), 3.08 (d, *J* = 14.8 Hz, 1H), 1.54 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 176.09, 161.30, 147.75, 130.16, 128.75, 127.45, 126.49, 126.06, 73.95, 53.04, 36.79, 25.79. ESI-HRMS: calcd for $C_{14}H_{16}NO_4^+$ ([M+H$^+$]) 262.1074, found 262.1078.



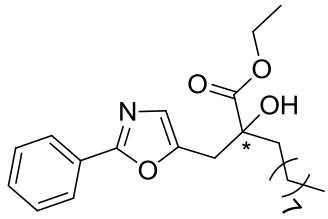
	Retention Time	Area	% Area	Height
1	13.231	22525910	49.99	1116137
2	17.434	22534179	50.01	838058



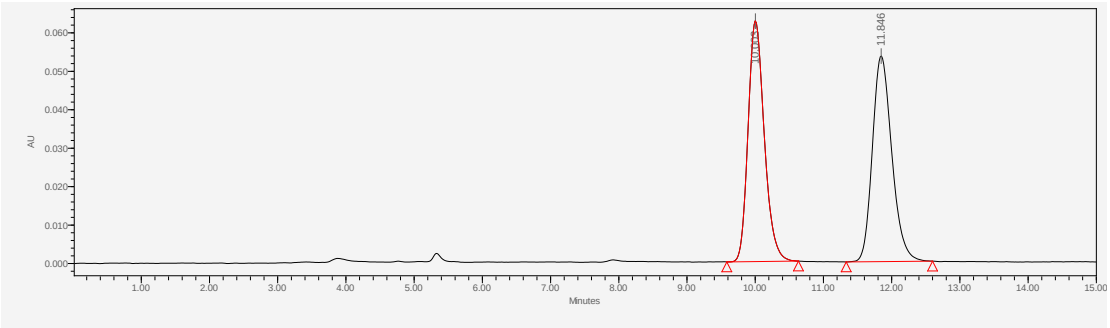


	Retention Time	Area	% Area	Height
1	13.244	17453835	99.75	863766
2	17.485	44207	0.25	1288

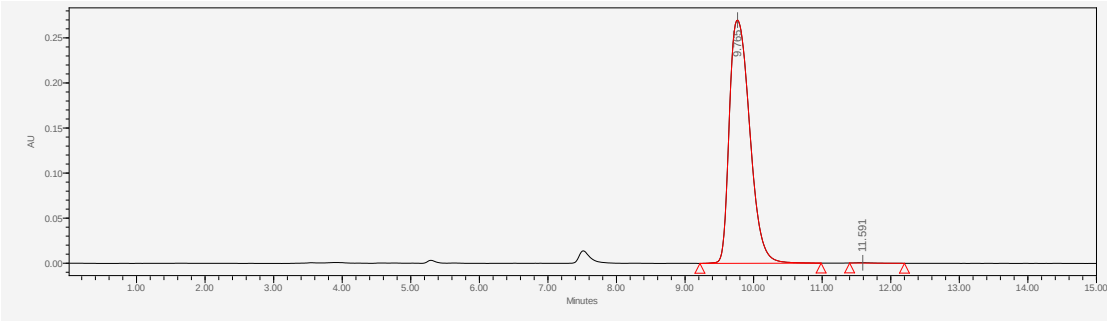
ethyl 2-hydroxy-2-((2-phenyloxazol-5-yl)methyl)undecanoate 3y

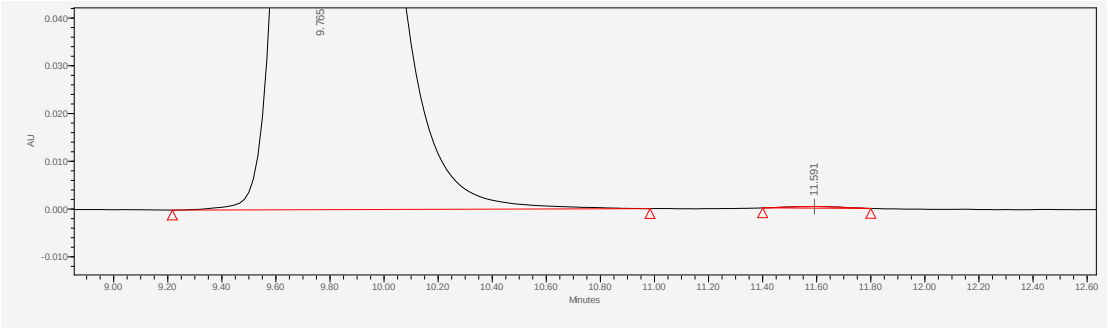


($C_{23}H_{33}NO_4$) a colourless viscous liquid; 75% yield, >99% ee. $[\alpha]_D^{20}$ = –1.8 (*c* 1.140 in CH_2Cl_2). HPLC DAICEL CHIRALCEL ID, n-hexane/2-propanol = 70/30, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 9.77 min (major), 11.59 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.04 – 7.90 (m, 2H), 7.50 – 7.38 (m, 3H), 6.94 (s, 1H), 4.26 (qd, *J* = 7.1, 1.2 Hz, 2H), 3.42 (s, 1H), 3.21 (d, *J* = 14.8 Hz, 1H), 3.08 (d, *J* = 15.2 Hz, 1H), 1.97 – 1.67 (m, 2H), 1.61 – 1.44 (m, 1H), 1.36 – 1.09 (m, 16H), 0.88 (t, *J* = 6.8 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 175.32, 161.19, 147.97, 130.07, 128.72, 127.59, 126.43, 126.06, 76.59, 62.19, 38.99, 36.02, 31.88, 29.58, 29.46, 29.43, 29.28, 23.43, 22.67, 14.25, 14.11. ESI-HRMS: calcd for $C_{23}H_{34}NO_4^+$ ([M+H$^+$]) 388.2482, found 388.2483.



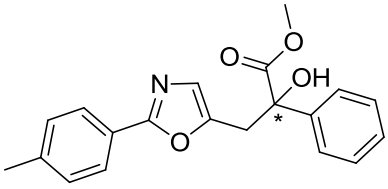
	Retention Time	Area	% Area	Height	Height
1	10.003	Unknown	1033183	49.43	62628
2	11.846	Unknown	1057202	50.57	53523



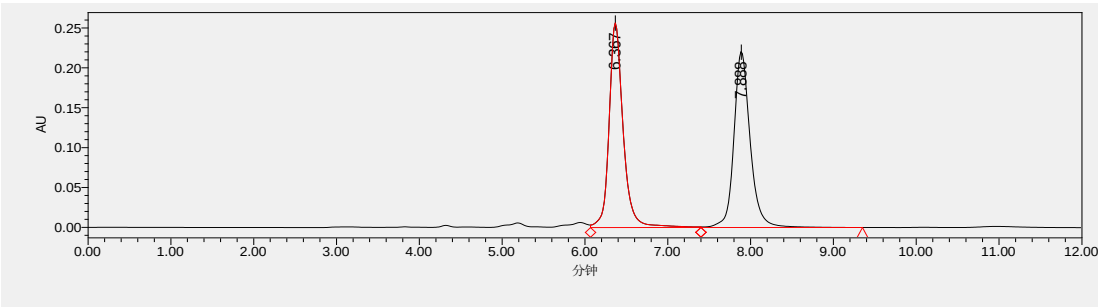


	Retention Time	Area	% Area	Height	Height
1	9.765	Unknown	5583247	99.91	269965
2	11.591	Unknown	4815	0.09	360

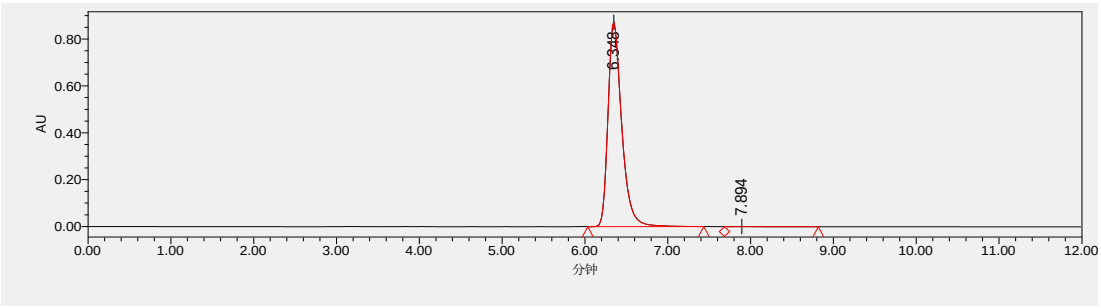
methyl 2-hydroxy-2-phenyl-3-(2-(p-tolyl)oxazol-5-yl)propanoate 3ba

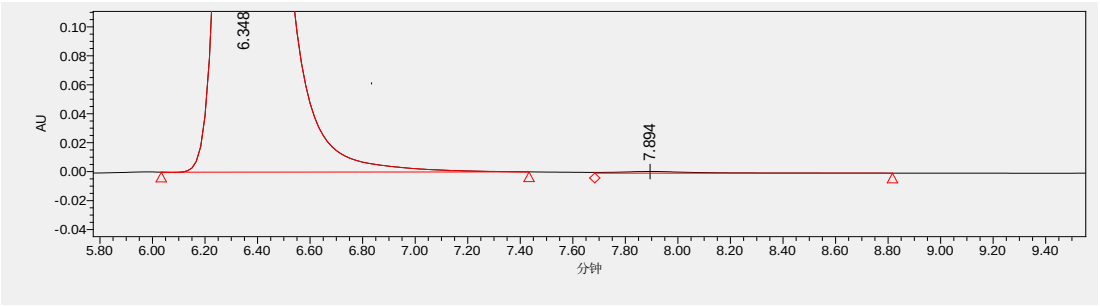


($C_{20}H_{19}NO_4$) a colourless viscous liquid; 98% yield, >99% ee. $[\alpha]_D^{20}$ = −5.2 (*c* 1.300 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB, n-hexane/2-propanol = 70/30, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 6.35 min (major), 7.89 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.81 – 7.67 (m, 2H), 7.61 – 7.54 (m, 2H), 7.36 – 7.21 (m, 3H), 7.15 – 7.07 (m, 2H), 6.80 (s, 1H), 4.08 (s, 1H), 3.72 (s, 3H), 3.63 (d, *J* = 15.2 Hz, 1H), 3.27 (d, *J* = 15.2 Hz, 1H), 2.28 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 173.25, 160.33, 146.26, 139.54, 139.28, 128.37, 127.43, 127.20, 125.49, 124.99, 124.39, 123.75, 76.57, 52.43, 35.58, 20.44. ESI-HRMS: calcd for $C_{20}H_{20}NO_4^+$ ([M+H$^+$]) 338.1387, found 338.1390.



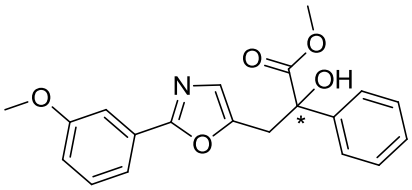
	Retention Time	Area	% Area	Height
1	6.367	3031351	50.14	256394
2	7.888	3014660	49.86	220694



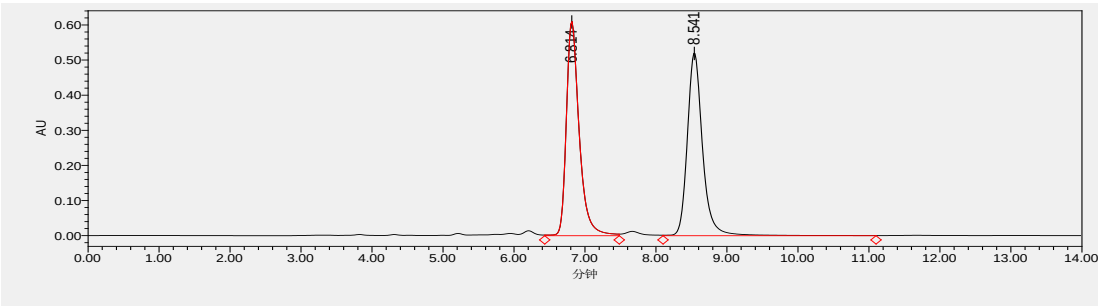


	Retention Time	Area	% Area	Height
1	6.348	10018961	99.77	872327
2	7.894	23347	0.23	1103

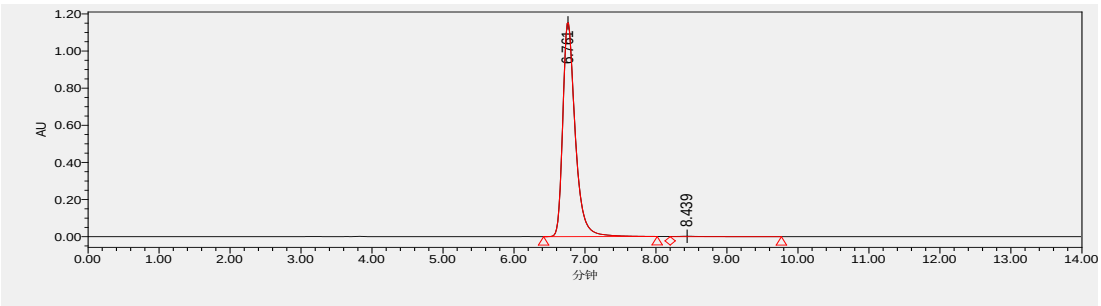
methyl 2-hydroxy-3-(2-(3-methoxyphenyl)oxazol-5-yl)-2-phenylpropanoate 3ca

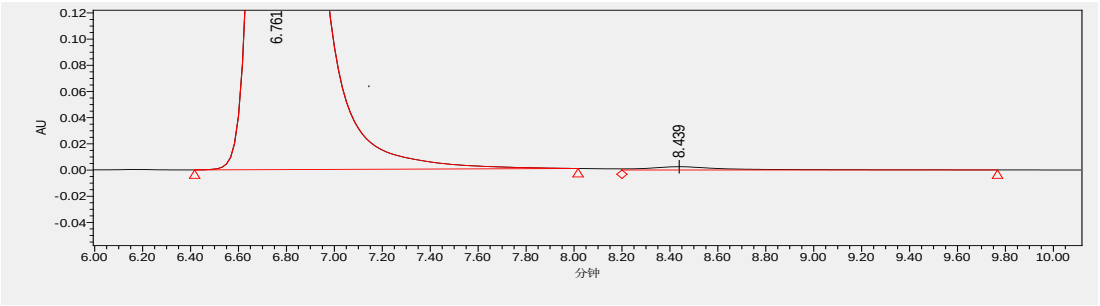


($C_{20}H_{19}NO_5$) a white amorphous solid; 91% yield, >99% ee. $[\alpha]_D^{20}$ = −8.2 (*c* 1.426 in CH_2Cl_2). HPLC DAICEL CHIRALCEL IB, n-hexane/2-propanol = 70/30, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 6.76 min (major), 8.44 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.68 – 7.52 (m, 2H), 7.46 – 7.35 (m, 2H), 7.34 – 7.18 (m, 4H), 6.92 – 6.83 (m, 1H), 6.82 (s, 1H), 4.12 (s, 1H), 3.74 (s, 3H), 3.73 (s, 3H), 3.64 (d, *J* = 15.2 Hz, 1H), 3.29 (d, *J* = 15.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 174.33, 161.05, 159.79, 147.79, 140.58, 129.85, 128.64, 128.52, 128.31, 126.70, 125.46, 118.54, 116.79, 110.57, 77.63, 55.41, 53.54, 36.64. ESI-HRMS: calcd for $C_{20}H_{20}NO_5^+$ ([M+H$^+$]) 354.1336, found 354.1344.



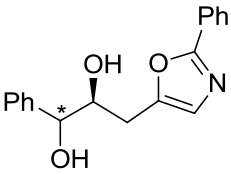
	Retention Time	Area	% Area	Height
1	6.814	7664485	49.70	609921
2	8.541	7756966	50.30	521146



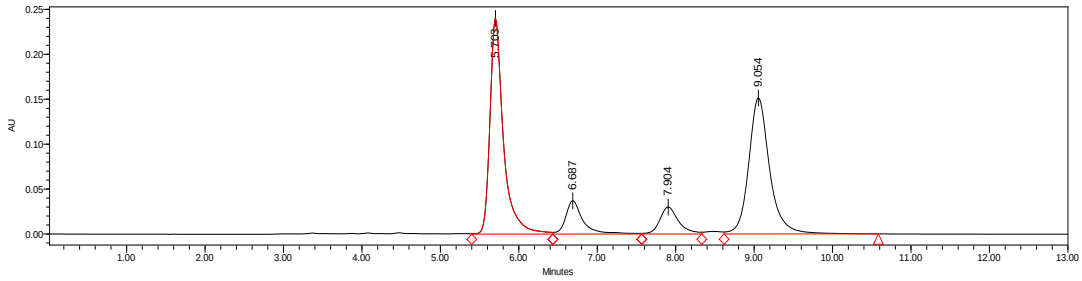


	Retention Time	Area	% Area	Height
1	6.761	14013349	99.61	1155152
2	8.439	55435	0.39	2490

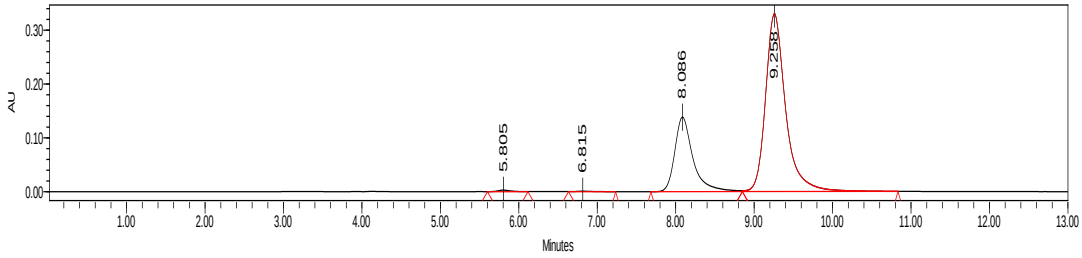
1-phenyl-3-(2-phenyloxazol-5-yl)propane-1,2-diol 6



($C_{18}H_{17}NO_3$) a white amorphous solid; 91% yield, d.r. = 72:28, 99% ee for major isomer. HPLC DAICEL CHIRALCEL IA, n-hexane/2-propanol = 70/30, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 5.81 min, t_2 = 6.82 min, t_3 = 8.09 min, t_4 = 9.26 min. ^{1}H NMR (400 MHz, DMSO) δ = 8.10 – 7.84 (m, 2H), 7.62 – 7.19 (m, 8H), 7.03 (s, 1H), 5.56 (d, *J* = 4.4Hz, 1H), 4.97 (d, *J* = 6.4 Hz, 1H), 4.52 (t, *J* = 5.2 Hz, 1H), 3.92 (m, 1H), 3.10 – 2.94 (m, 1H), 2.89 – 2.73 (m, 1H). ^{13}C NMR (100 MHz, DMSO) δ = 159.38, 151.42, 143.23, 129.98, 129.00, 127.65, 127.33, 127.05, 126.78, 125.46, 125.03, 75.86, 72.98, 29.11. ESI-HRMS: calcd for $C_{18}H_{17}NNaO_3^+$ ([M+Na$^+$]) 318.1101, found 318.1109.



	Retention Time	Area	% Area	Height
1	5.703	2872519	42.55	240739
2	6.687	570726	8.45	37153
3	7.904	498915	7.39	30069
4	9.054	2809147	41.61	151625



	Retention Time	Area	% Area	Height
1	5.805	33237	0.41	2870
2	6.815	13868	0.17	882
3	8.086	2237398	27.46	138887
4	9.258	5862610	71.96	330527

10. References:

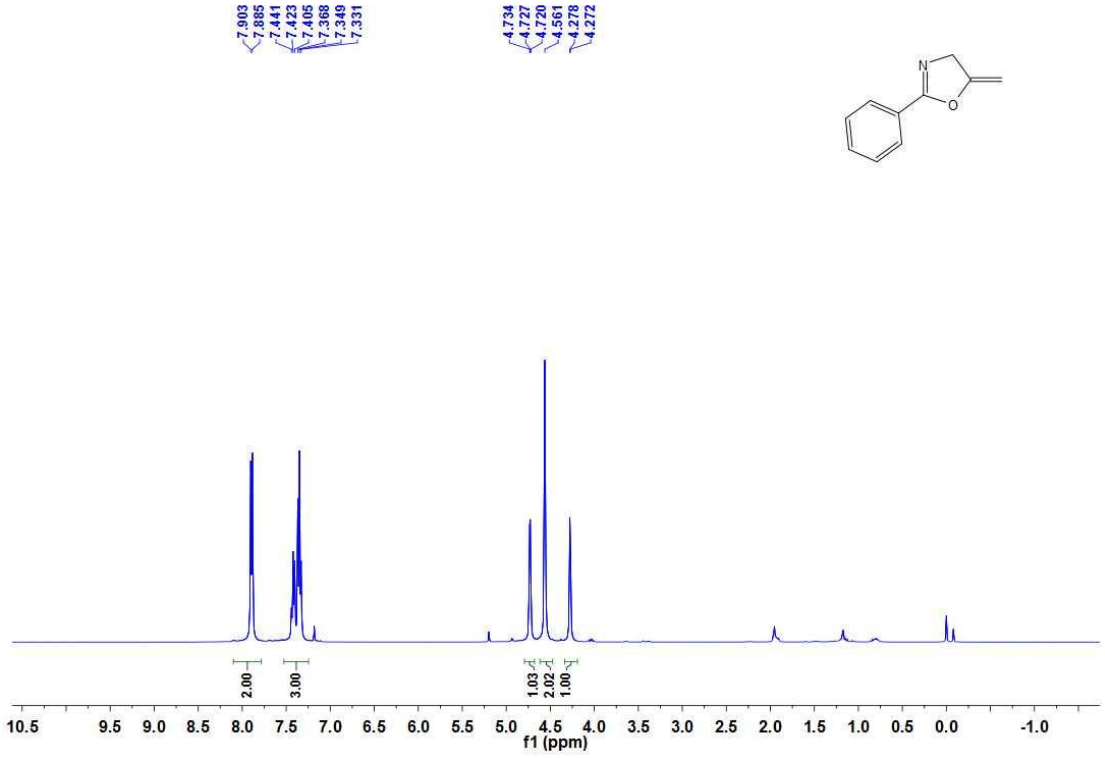
1. G. C. Senadi, W-P. Hu, J-S Hsiao, J. K. Vandavasi, C-Y. Chen and J-J. Wang, *Org. Lett.* **2012**, *14*, 4478–4481.

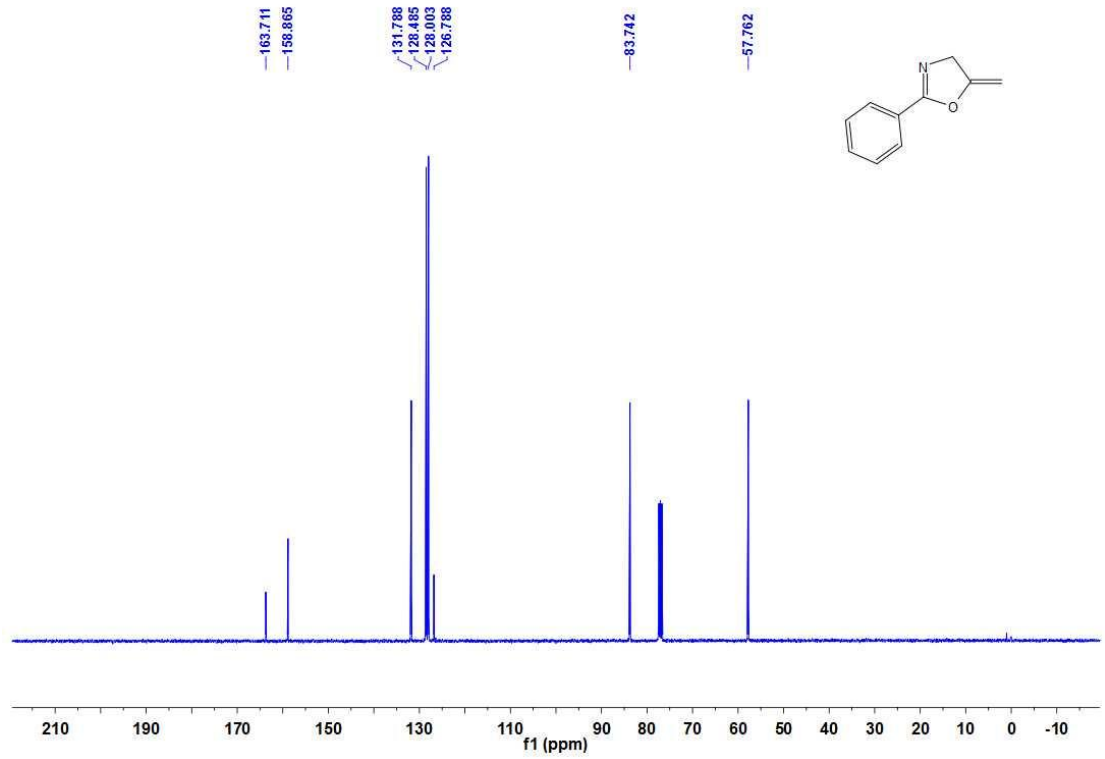
2. a) F. Wang, X. H. Liu, Y. L. Zhang, L. L. Lin , X. M. Feng, *Chem. Commun.* **2009**, 7297–7299; b) M. Rambaud, M. Bakasse, G. Duguay, J. Villieras, *Synthesis* **1988**, 564–566; c) J. S. Nimitz , H. S. Mosher, *J. Org. Chem.* **1981**, *46*, 211–213. d) J. M. Domagala, *Tetrahedron Letters* **1980**, *21*, 4997–5000.

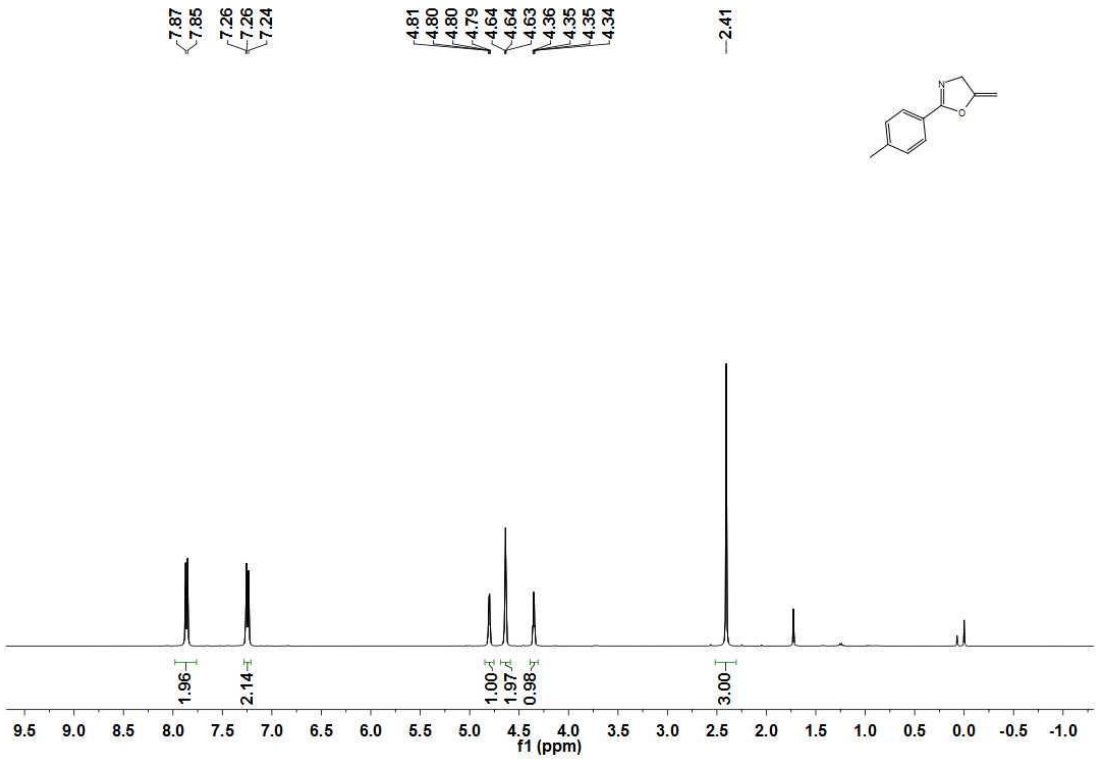
3. B. Qin, X. H. Liu, J. Shi, K. Zheng, H. T. Zhao, X. M. Feng, *J. Org. Chem.* **2007**, *72*, 2374–2378, and references therein.

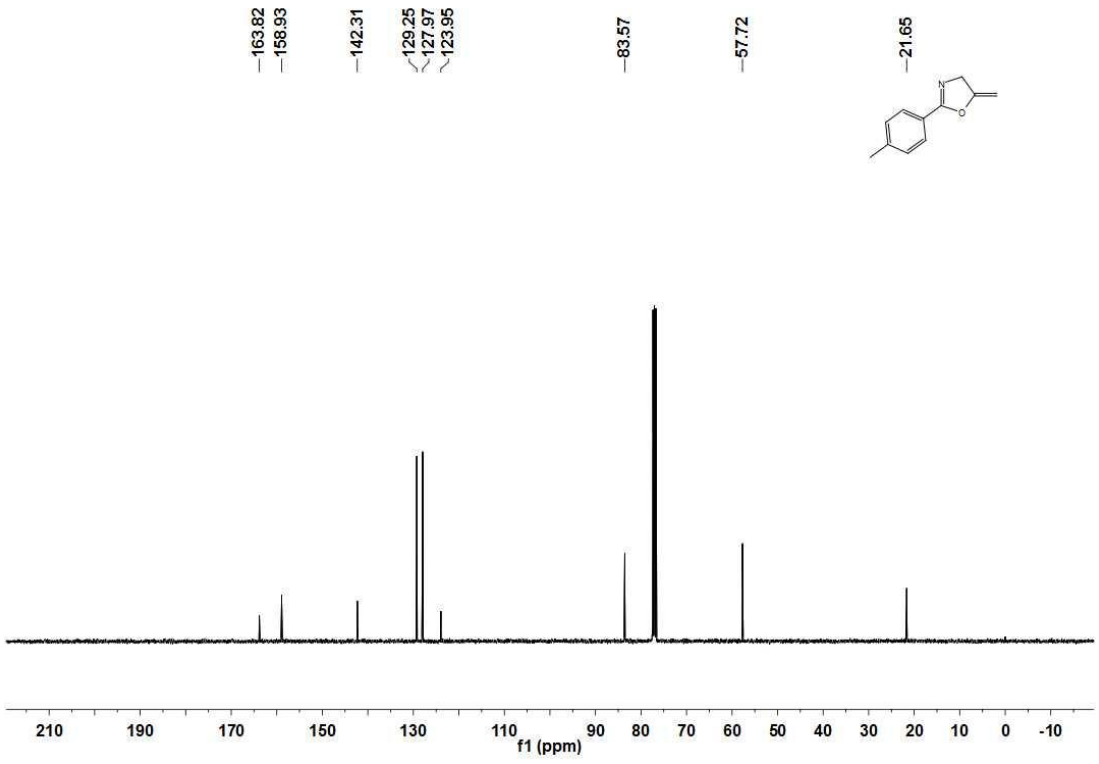
4. a) Y. H. Wen, X. Huang, J. L. Huang, Y. Xiong, B. Qin, X. M. Feng, *Synlett* **2005**, 2445; b) Z. P. Yu, X. H. Liu, Z. H. Dong, M. S. Xie, X. M. Feng, *Angew. Chem. Int. Ed.* **2008**, *47*, 1308; c) X. Zhou, D. J. Shang, Q. Zhang, L. L. Lin, X. H. Liu, X. M. Feng, *Org. Lett.* **2009**, *11*, 1401; d) K. Zheng, Y. Yang, J. N. Zhao, C, K. Yin, L.L. Lin, X. H. Liu, X. M. Feng, *Chem. Eur. J.* **2010**, *16*, 9969–9972, and references therein.

11. Copies of ^{1}H NMR and ^{13}C NMR spectra for the reactants and the products






7.87
7.85
7.26
7.26
7.24
4.81
4.80
4.80
4.79
4.64
4.64
4.63
4.36
4.35
4.35
4.34
2.41
1.96
2.14
1.00
1.97
0.98
3.00
f1 (ppm)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158.93
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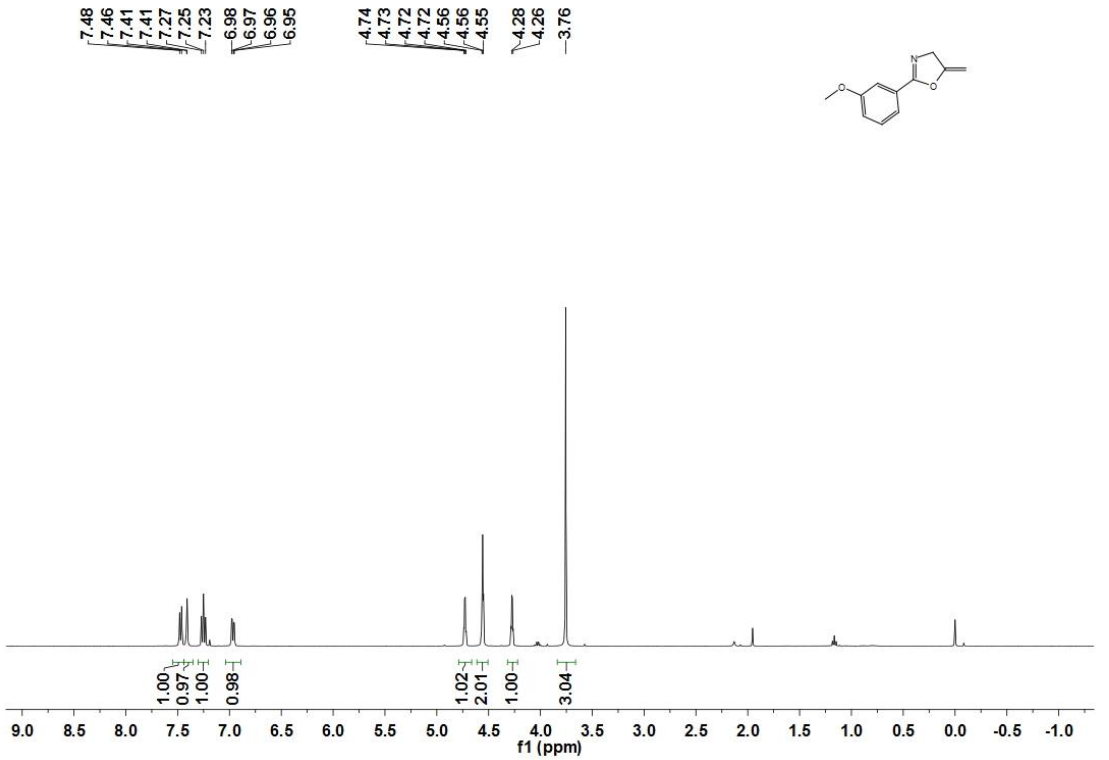
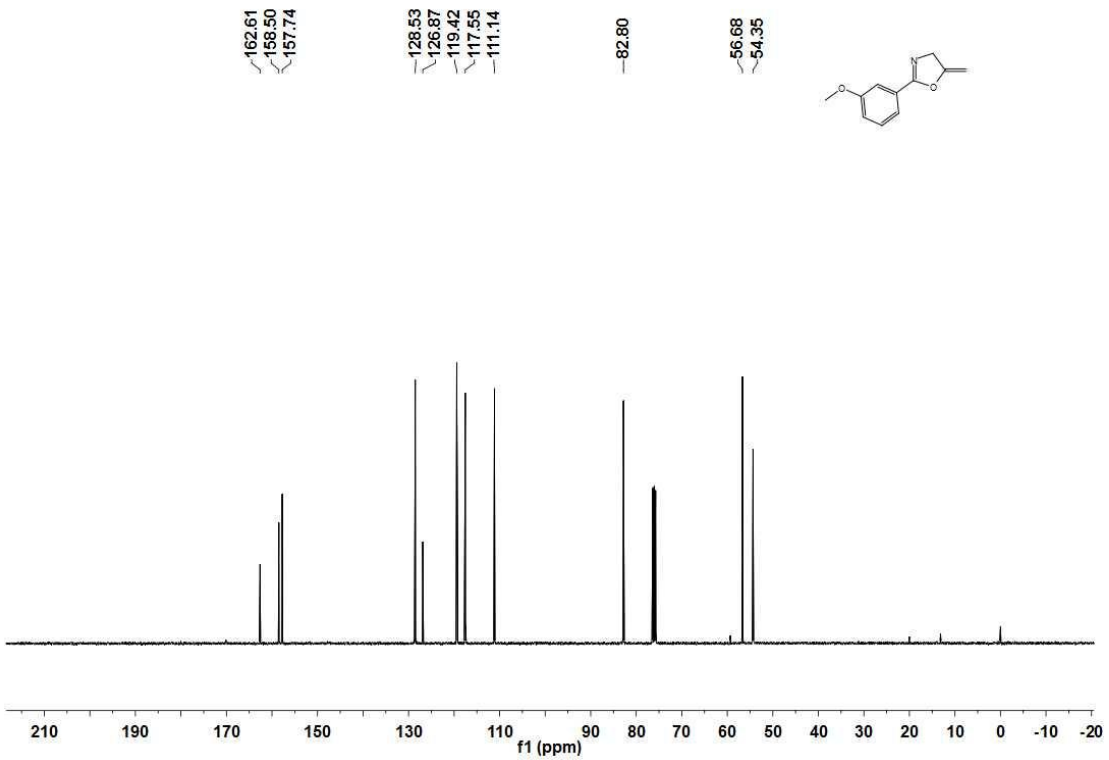
129.25
127.97
123.95
83.57
57.72
21.65
f1 (ppm)


7.48
7.46
7.41
7.41
7.27
7.25
7.23
6.98
6.97
6.96
6.95
4.74
4.73
4.72
4.72
4.56
4.56
4.55
4.28
4.26
3.76
1.00
0.97
1.00
0.98
1.02
2.01
1.00
3.04
f1 (ppm)


162.61
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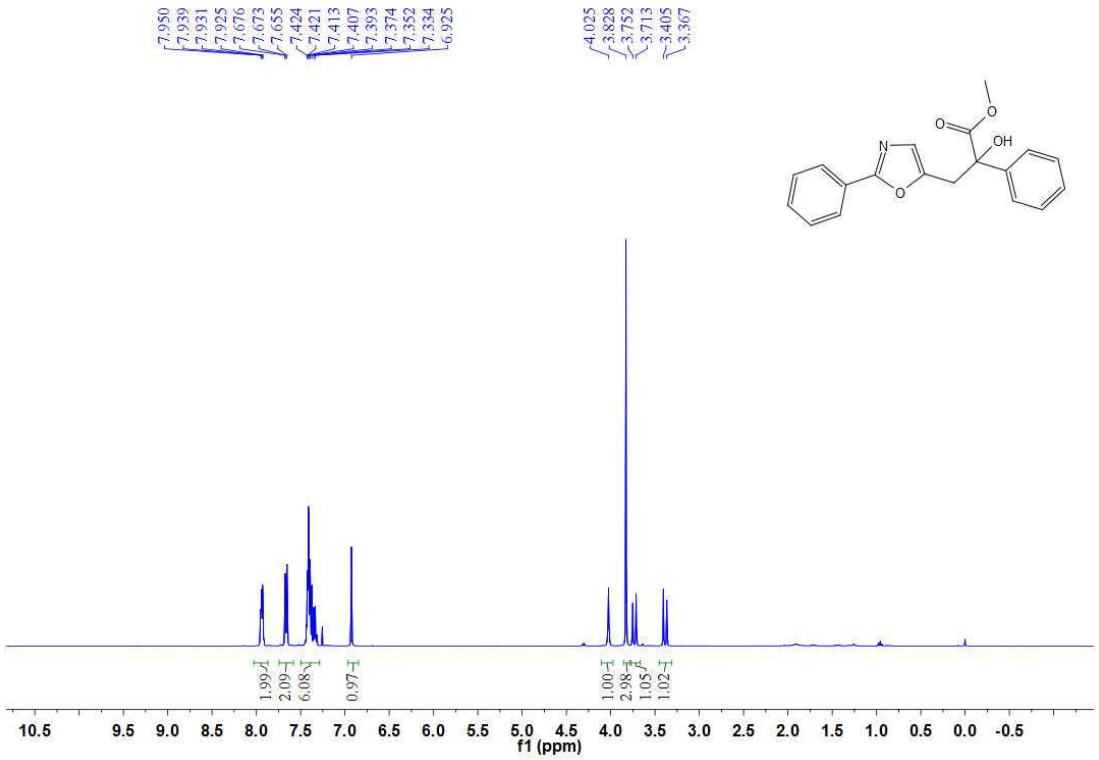
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7.939
7.931
7.925
7.676
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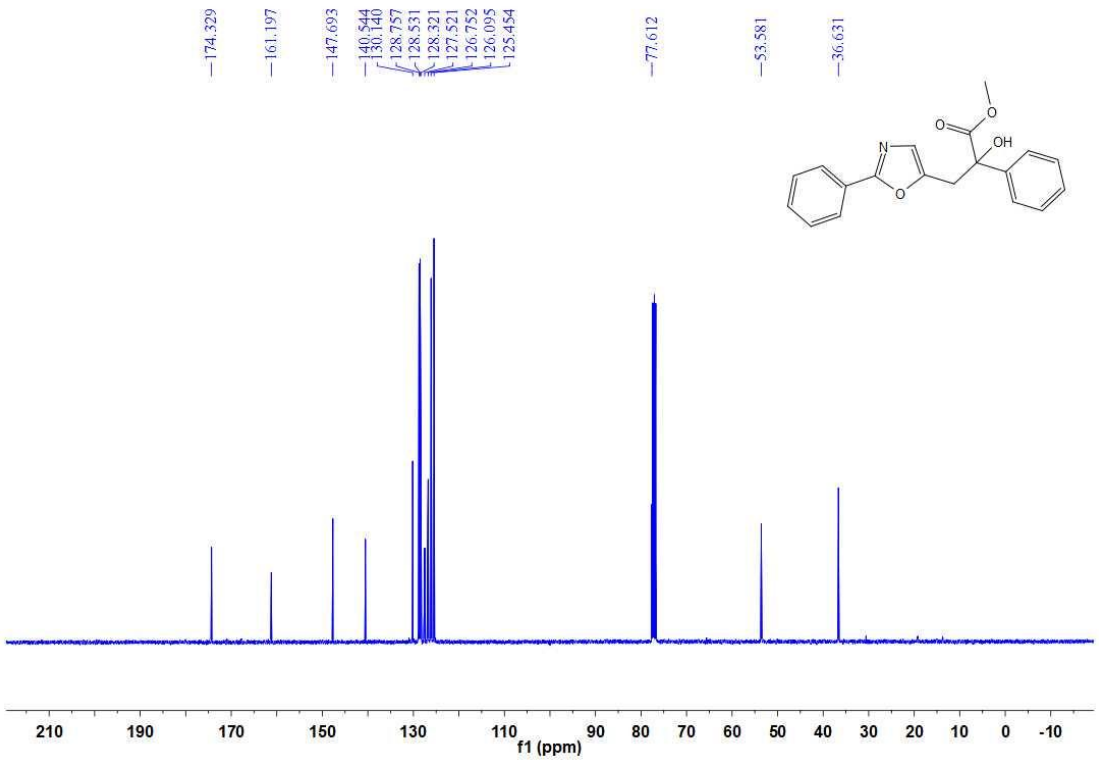
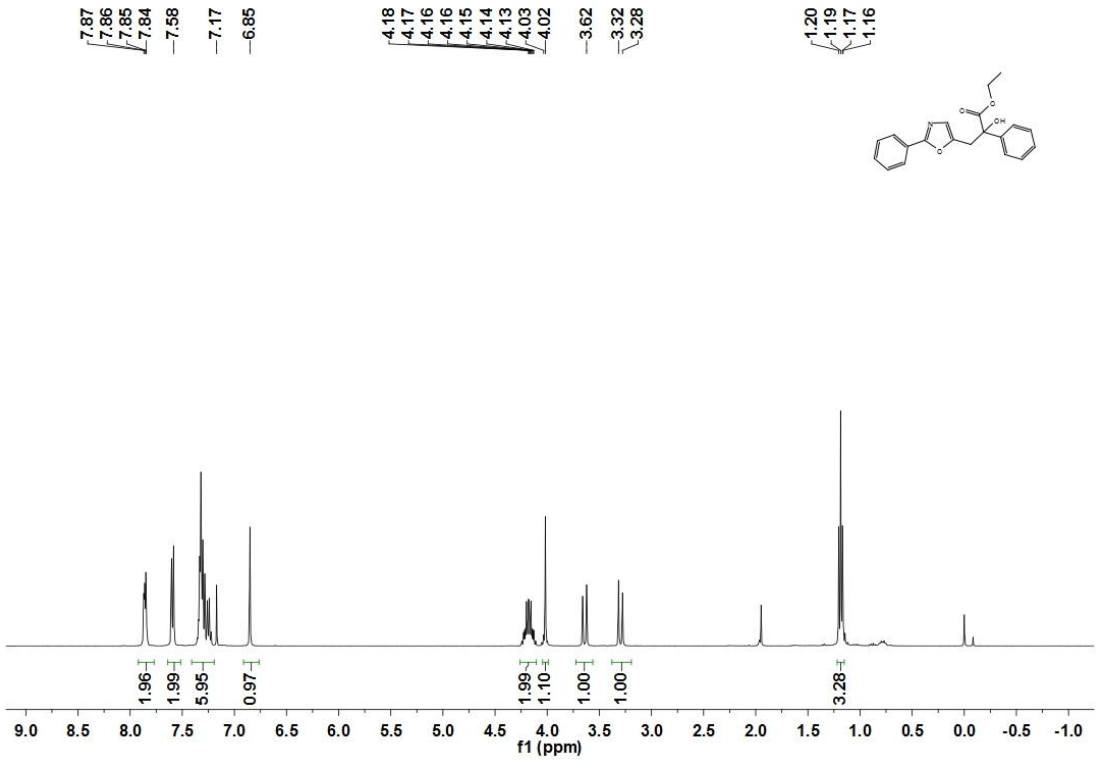
7.424
7.421
7.413
7.407
7.393
7.374
7.352
7.334
6.925
4.025
3.828
3.752
3.713
3.405
3.367
O
O
OH
N
O
1.99
2.09
6.08
0.97
1.00
2.98
1.05
1.02
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


174.329
161.197
147.693
140.544
130.140
128.757
128.531
128.321
127.521
126.752
126.095
125.454
77.612
53.581
36.631
O
O
OH
N
O
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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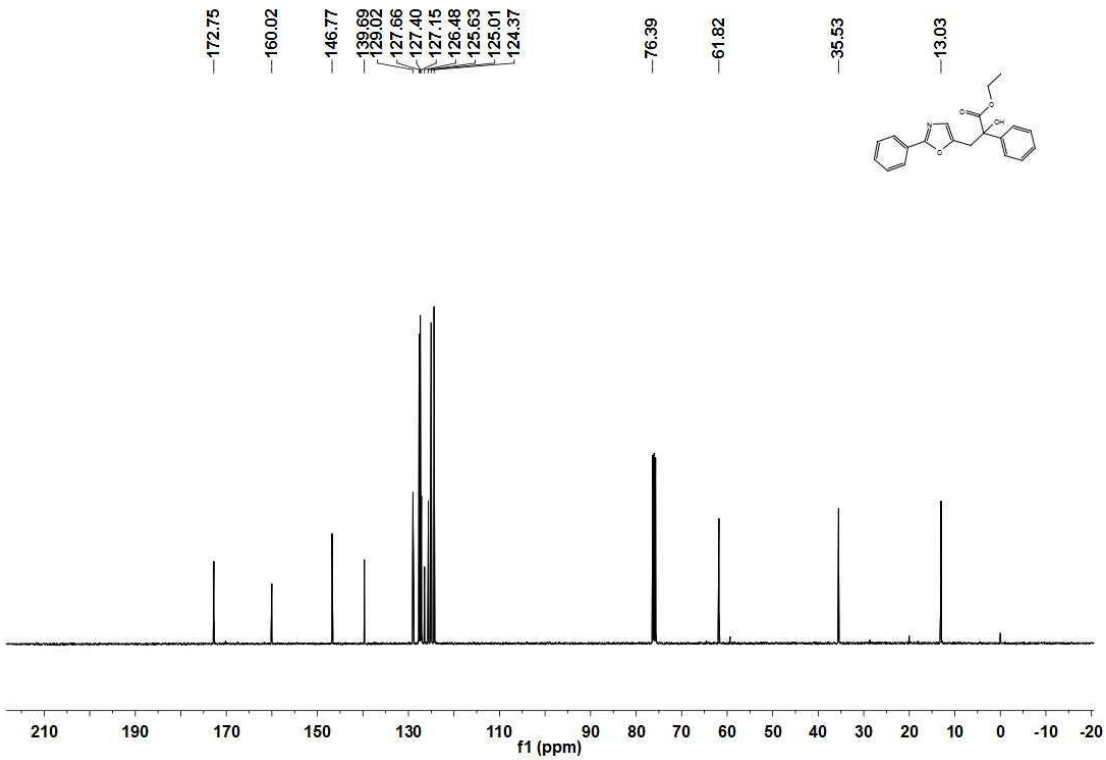
7.86
7.85
7.84
7.58
7.17
6.85
4.18
4.17
4.16
4.16
4.15
4.14
4.13
4.03
4.02
3.62
3.32
3.28
1.20
1.19
1.17
1.16
1.96
1.99
5.95
0.97
1.99
1.10
1.00
1.00
3.28
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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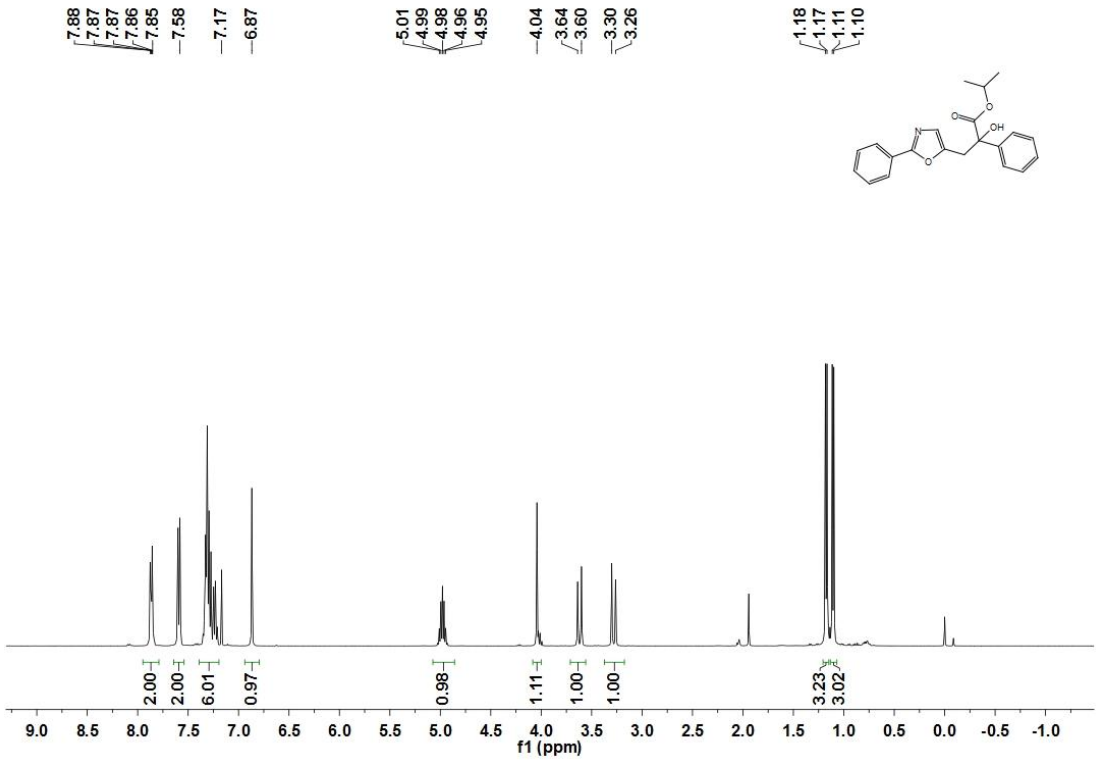
146.77
139.69
129.02
127.66
127.40
127.15
126.48
125.63
125.01
124.37
76.39
61.82
35.53
13.03
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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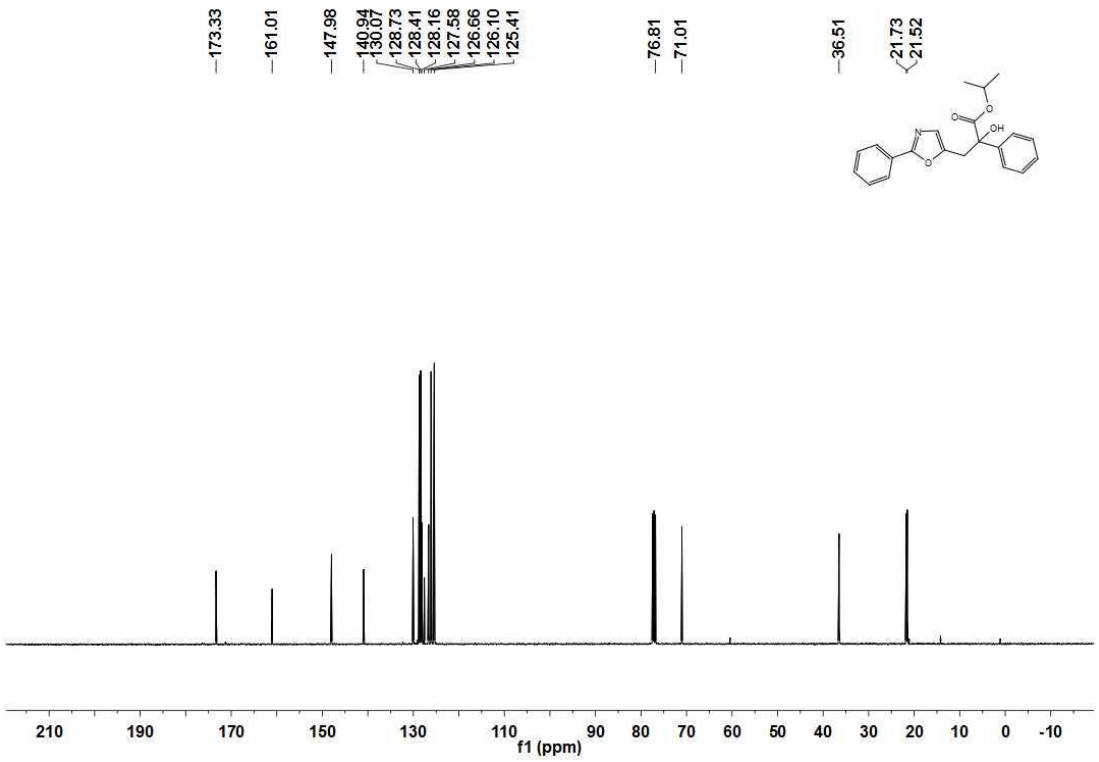
7.87
7.86
7.85
7.58
7.17
6.87
5.01
4.99
4.98
4.96
4.95
4.04
3.64
3.60
3.30
3.26
1.18
1.17
1.11
1.10
OH
2.00
2.00
6.01
0.97
0.98
1.11
1.00
1.00
3.23
3.02
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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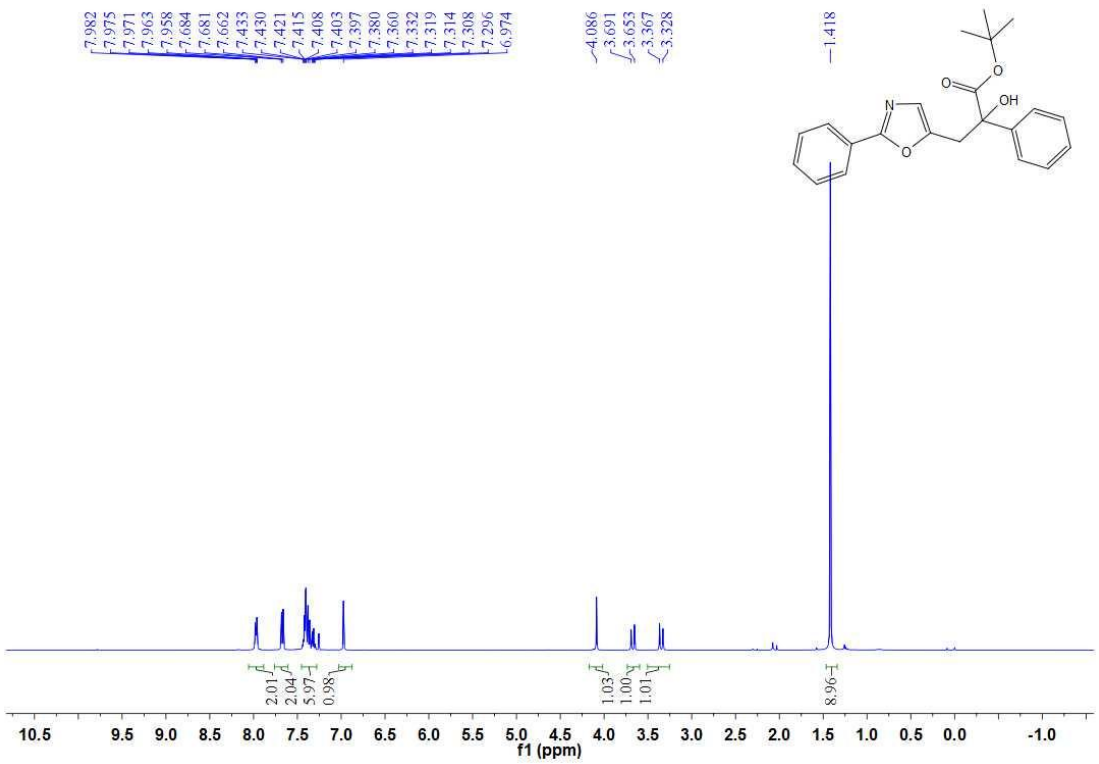
128.73
128.41
128.16
127.58
126.66
126.10
125.41
76.81
71.01
36.51
21.73
21.52
OH
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.971
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7.958
7.684
7.681
7.662
7.433
7.430
7.421
7.415
7.408
7.403
7.397
7.380
7.360
7.332
7.319
7.314
7.308
7.296
6.974
4.086
3.691
3.653
3.367
3.328
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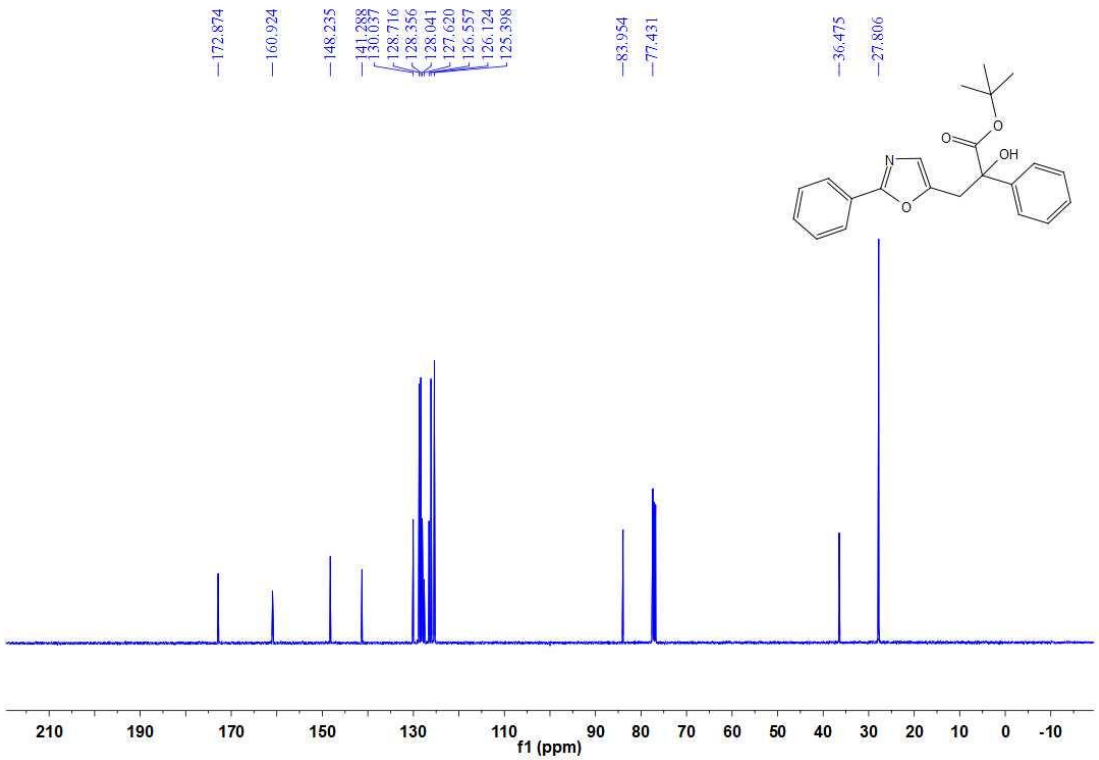
2.01
2.04
5.97
0.98
1.03
1.00
1.01
8.96
f1 (ppm)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148.235
141.288
130.037
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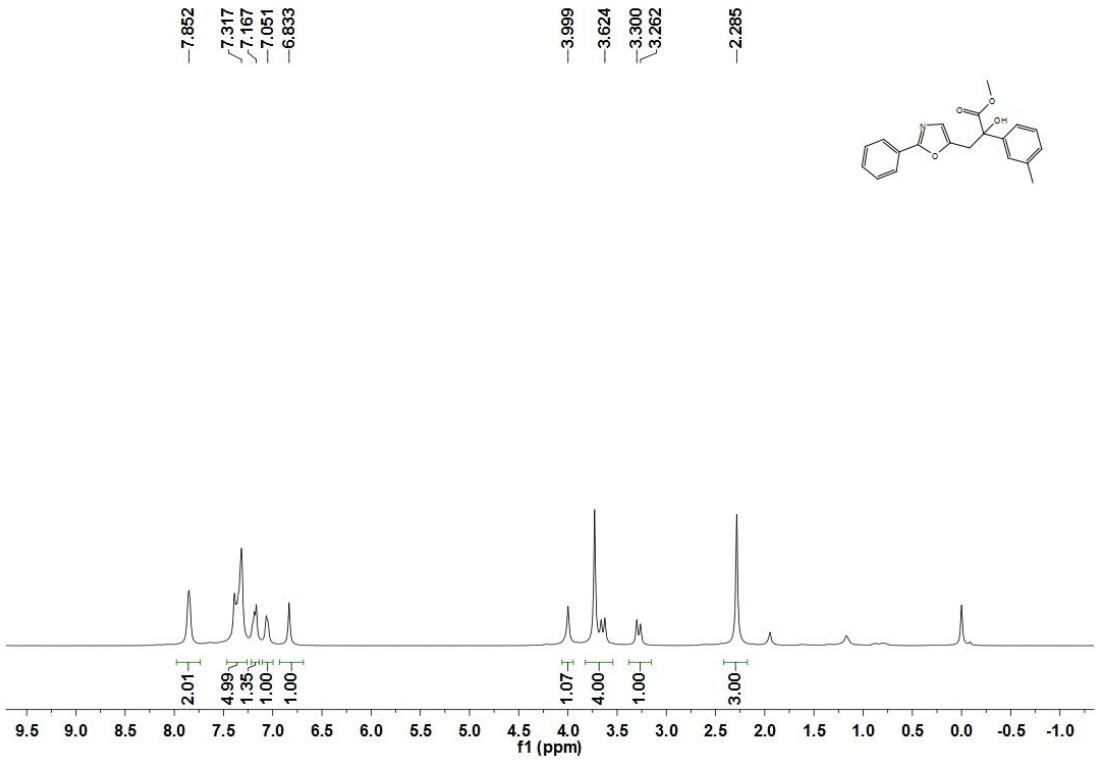
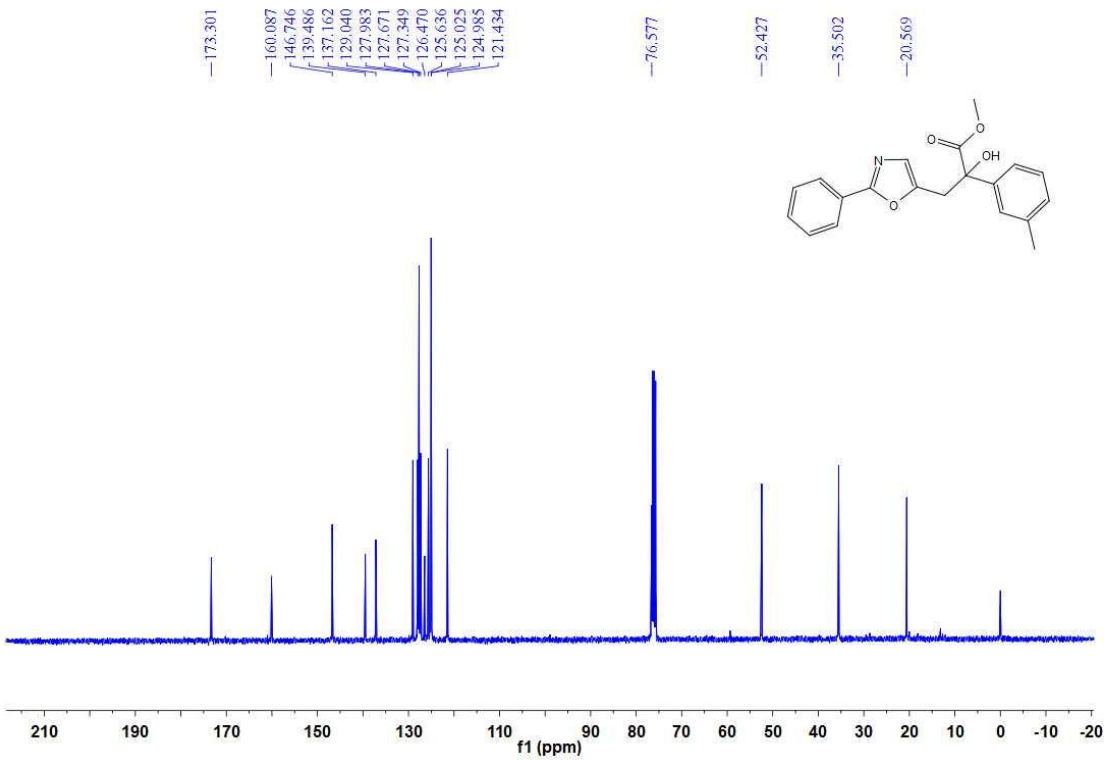
128.356
128.041
127.620
126.557
126.124
125.398
83.954
77.431
36.475
27.806
f1 (ppm)


7.852
7.317
7.167
7.051
6.833
3.999
3.624
3.300
3.262
2.285
2.01
4.99
1.35
1.00
1.00
1.07
4.00
1.00
3.00
f1 (ppm)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160.087
146.746
139.486
137.162
129.040
127.983
127.671
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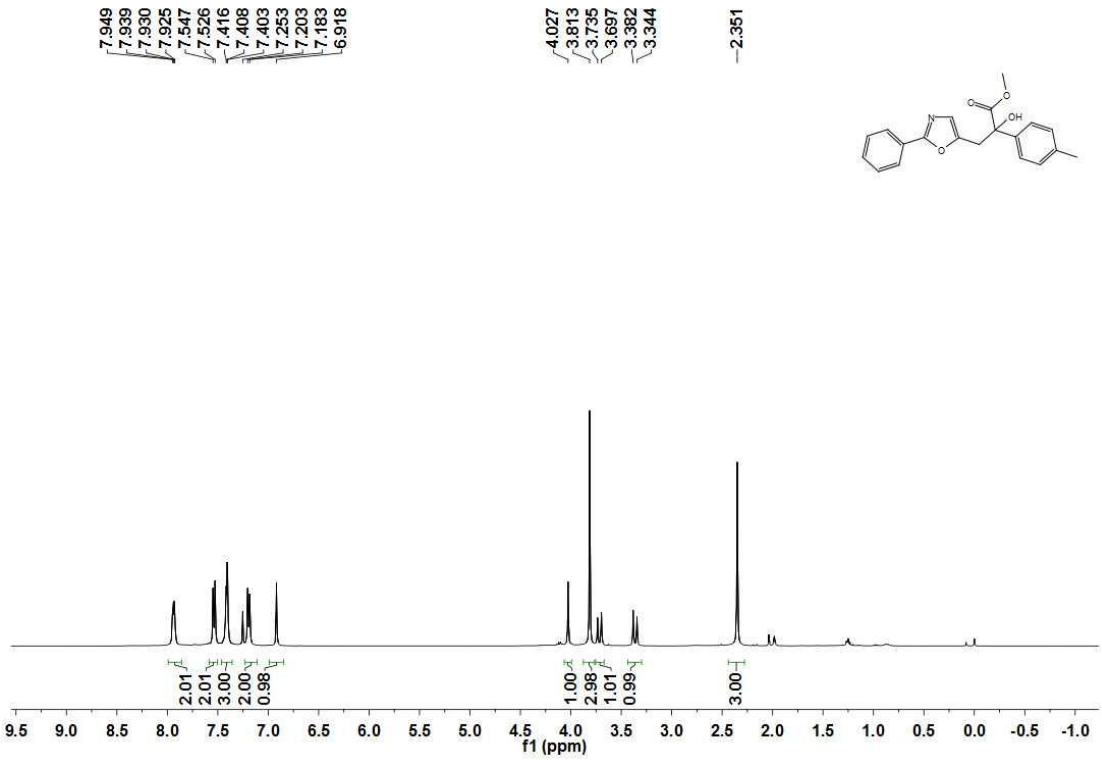
125.636
125.025
124.985
121.434
76.577
52.427
35.502
20.569
f1 (ppm)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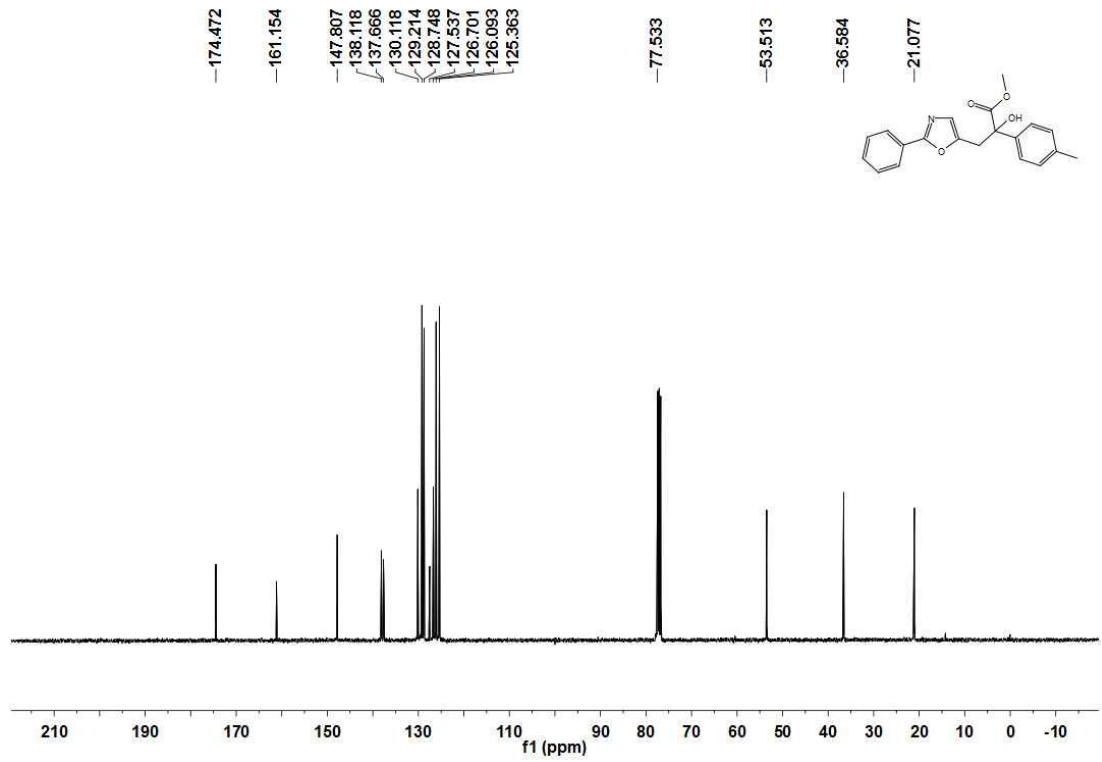
7.930
7.925
7.547
7.526
7.416
7.408
7.403
7.253
7.203
7.183
6.918
4.027
3.813
3.735
3.697
3.382
3.344
2.351
OH
2.01
2.01
3.00
2.00
0.98
1.00
2.98
1.01
0.99
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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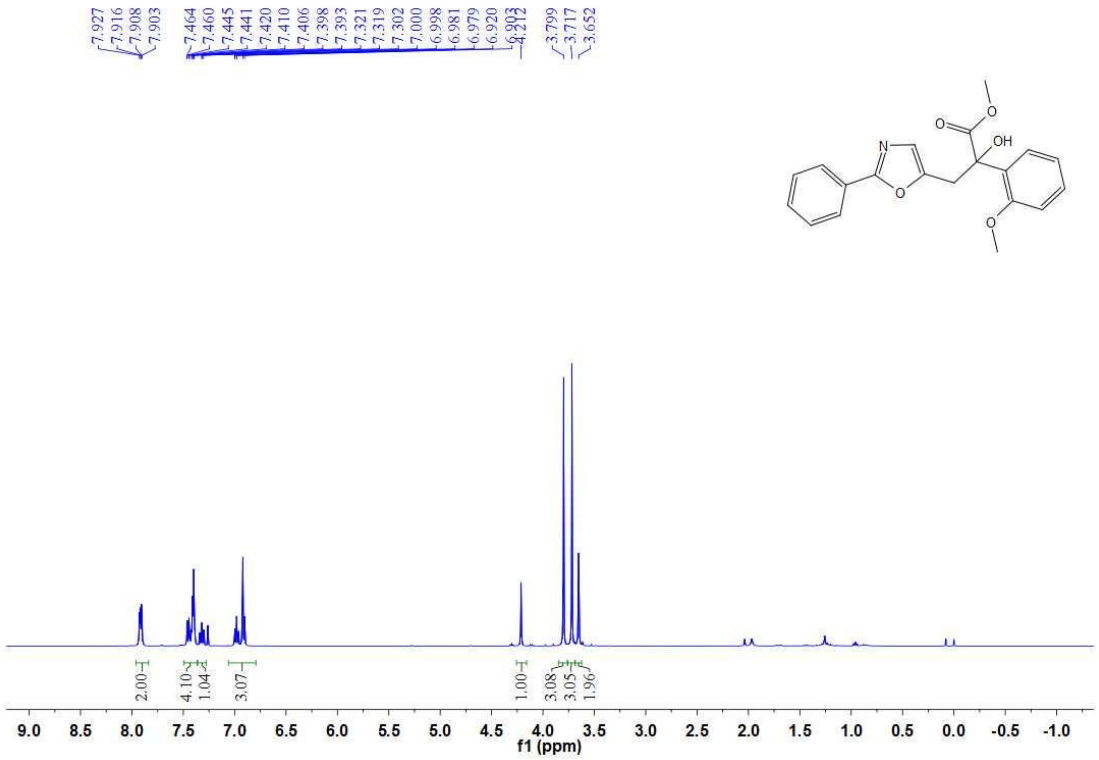
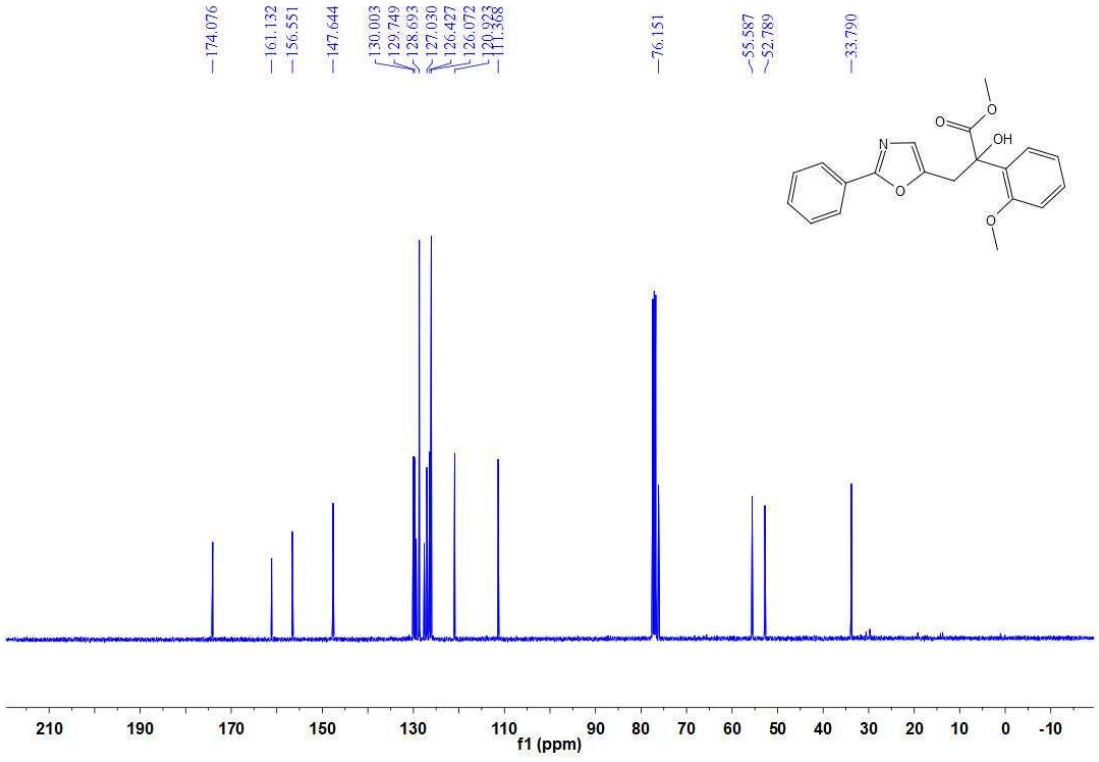
161.154
147.807
138.118
137.666
130.118
129.214
128.748
127.537
126.701
126.093
125.363
77.533
53.513
36.584
21.077
OH
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.927
7.916
7.908
7.903
7.464
7.460
7.445
7.441
7.420
7.410
7.406
7.398
7.393
7.321
7.319
7.302
7.000
6.998
6.981
6.979
6.920
6.903
4.212
3.799
3.717
3.652
O
O
OH
N
O
O
2.00
4.10
1.04
3.07
1.00
3.08
3.05
1.96
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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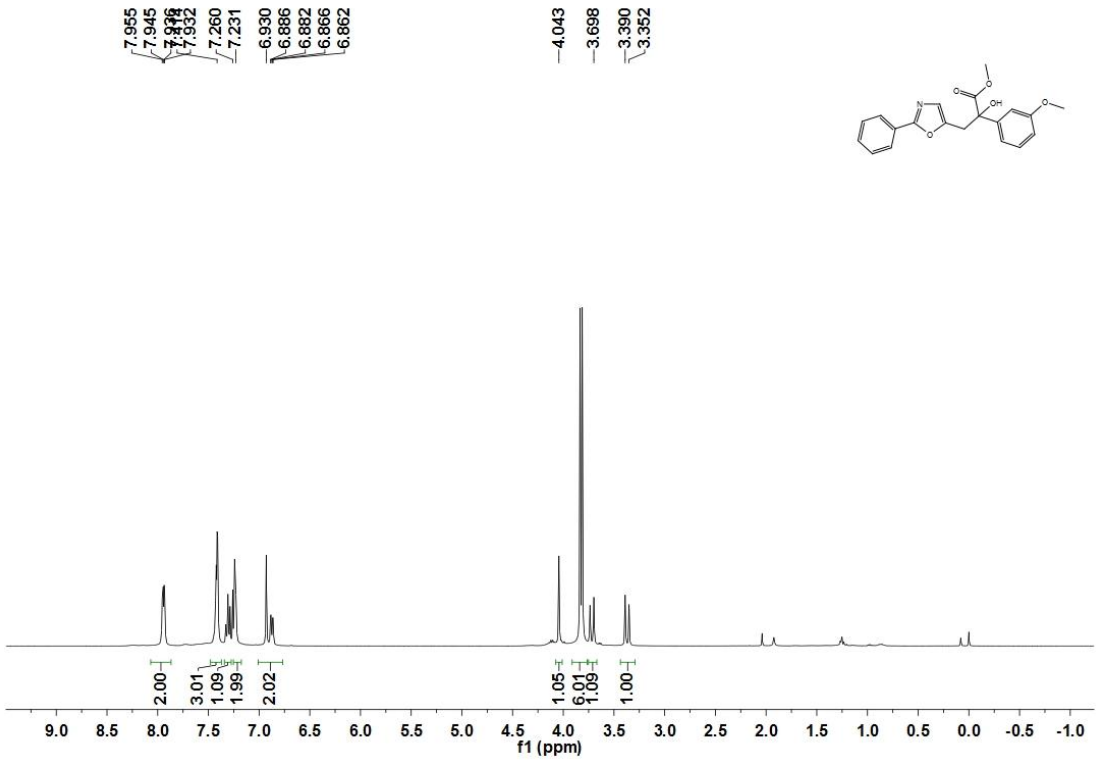
161.132
156.551
147.644
130.003
129.749
128.693
127.030
126.427
126.072
120.323
111.368
76.151
55.587
52.789
33.790
O
O
OH
N
O
O
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.955
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7.932
7.260
7.231
6.930
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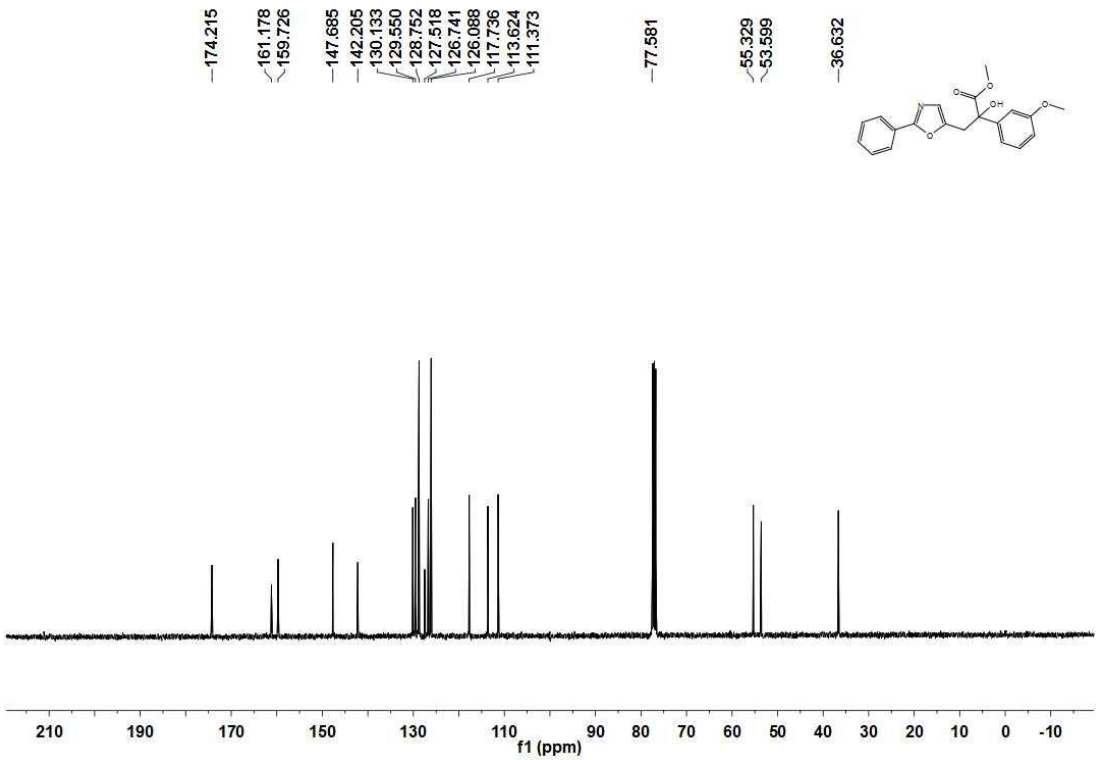
6.882
6.866
6.862
4.043
3.698
3.390
3.352
2.00
3.01
1.09
1.99
2.02
1.05
1.09
1.00
f1 (ppm)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130.133
129.550
128.752
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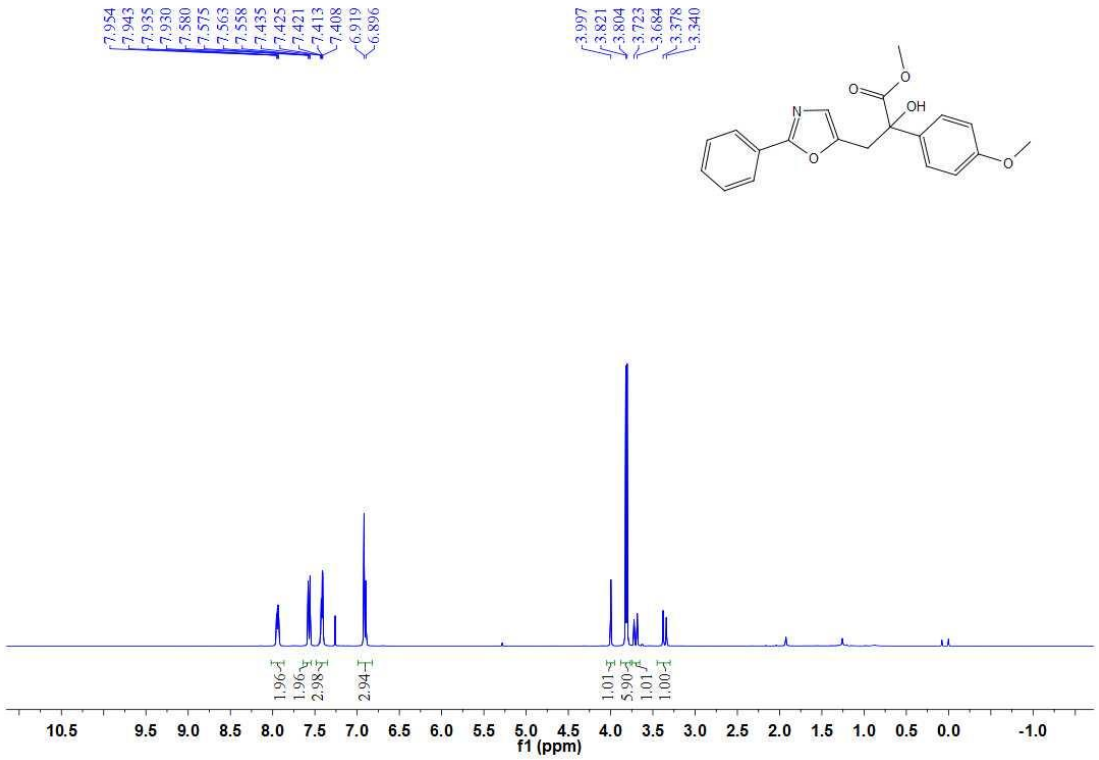
126.088
117.736
113.624
111.373
77.581
55.329
53.599
36.632
f1 (ppm)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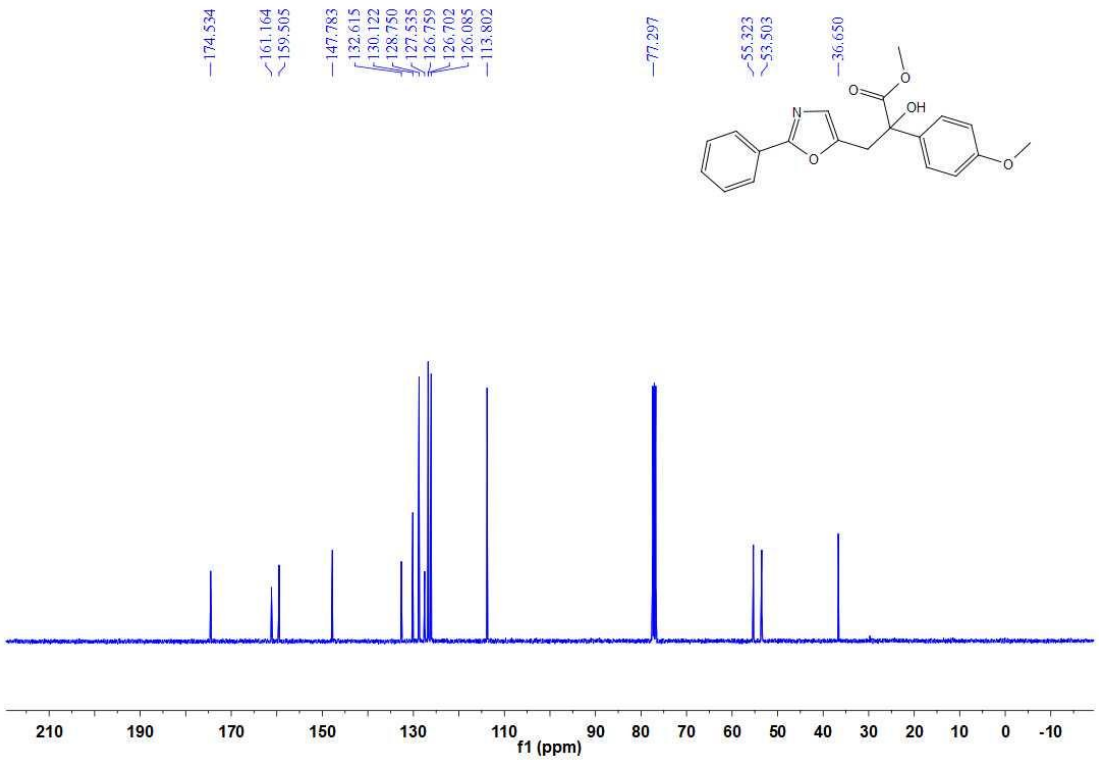
7.943
7.935
7.930
7.580
7.575
7.563
7.558
7.435
7.425
7.421
7.413
7.408
6.919
6.896
3.997
3.821
3.804
3.723
3.684
3.378
3.340
O
O
OH
N
O
O
1.96
1.96
2.98
2.94
1.01
5.90
1.01
1.00
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -1.0
f1 (ppm)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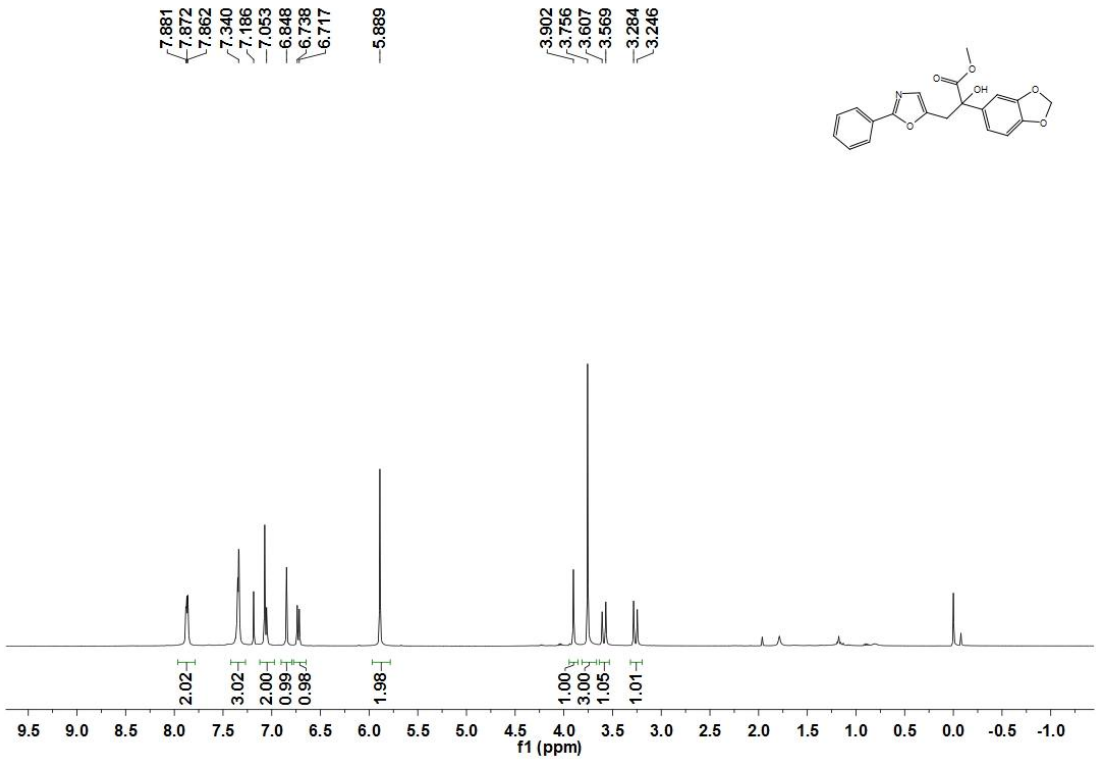
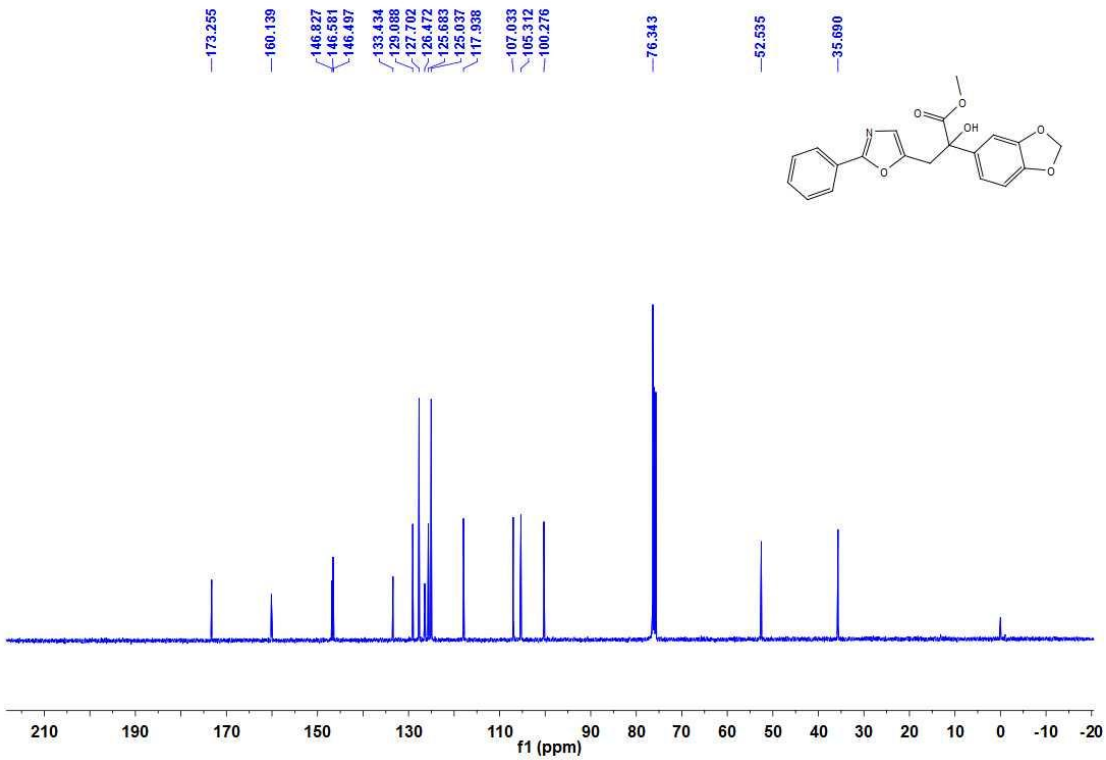
159.505
147.783
132.615
130.122
128.750
127.535
126.759
126.702
126.085
113.802
77.297
55.323
53.503
36.650
O
O
OH
N
O
O
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.881
7.872
7.862
7.340
7.186
7.053
6.848
6.738
6.717
5.889
3.902
3.756
3.607
3.569
3.284
3.246
2.02
3.02
2.00
0.99
0.98
1.98
1.00
3.00
1.05
1.01
f1 (ppm)


173.255
160.139
146.827
146.581
146.497
133.434
129.088
127.702
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125.683
125.037
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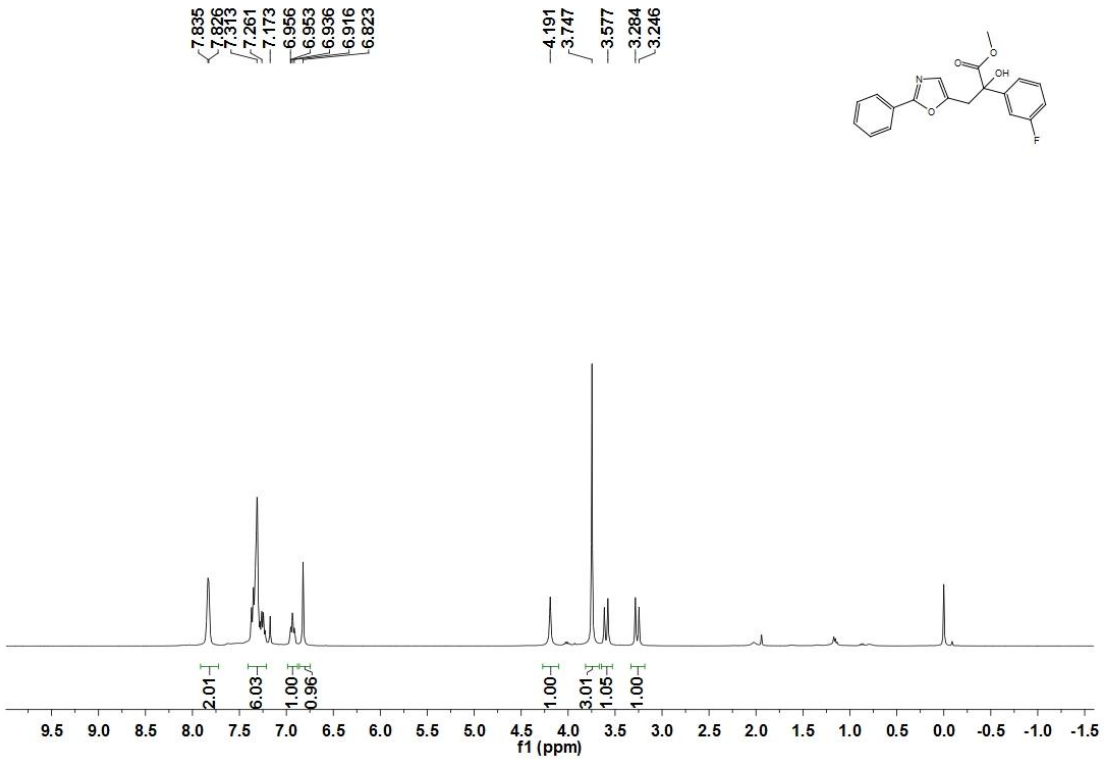
107.033
105.312
100.276
76.343
52.535
35.690
f1 (ppm)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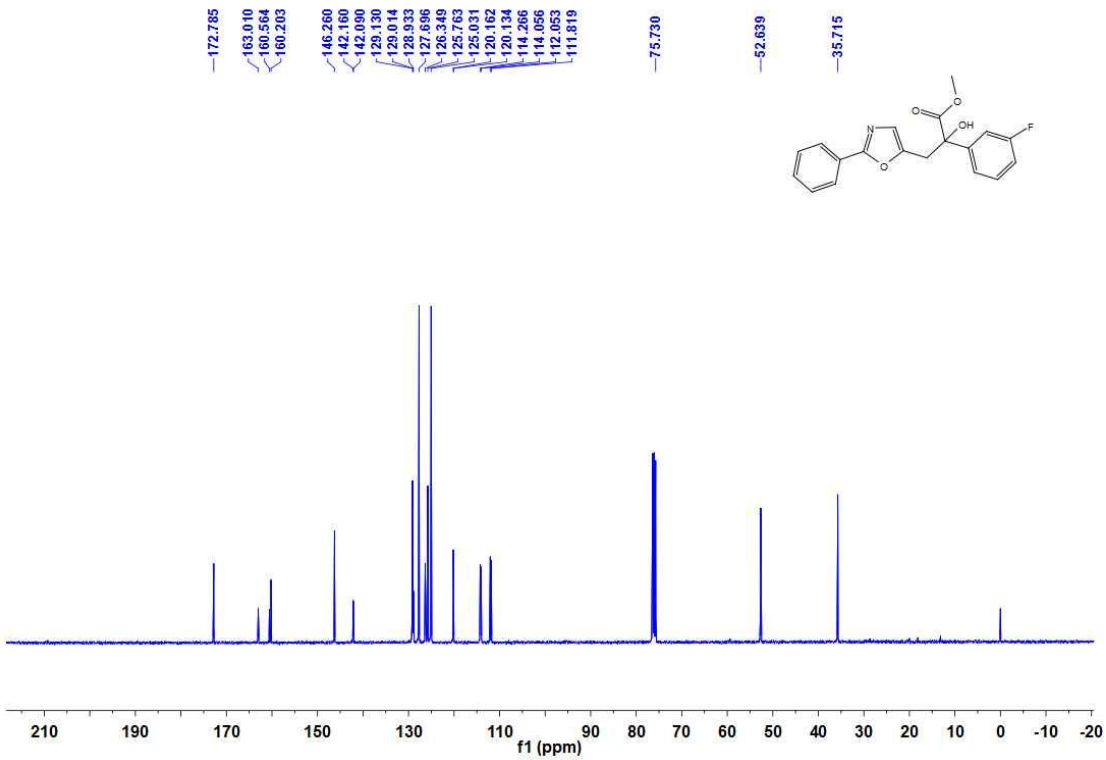
7.826
7.313
7.261
7.173
6.956
6.953
6.936
6.916
6.823
4.191
3.747
3.577
3.284
3.246
2.01
6.03
1.00
0.96
1.00
3.01
1.05
1.00
f1 (ppm)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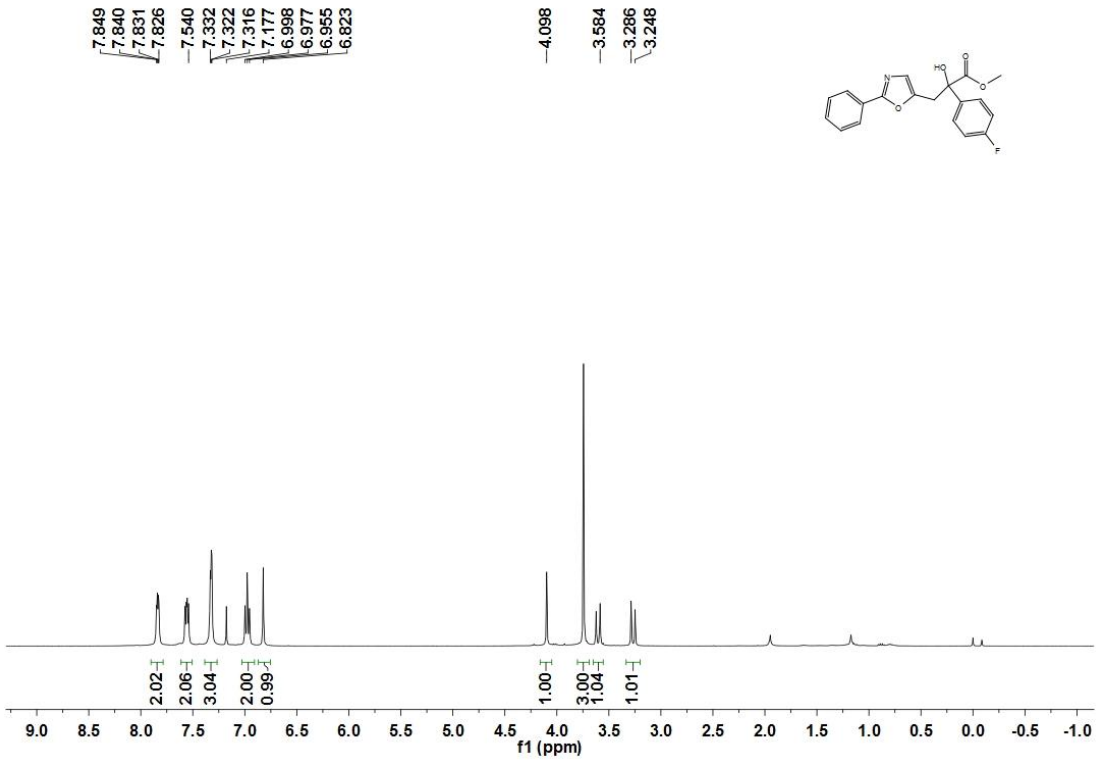
160.564
160.203
146.260
142.160
142.090
129.130
129.014
128.933
127.696
126.349
125.763
125.031
120.162
120.134
114.266
114.056
112.053
111.819
75.730
52.639
35.715
f1 (ppm)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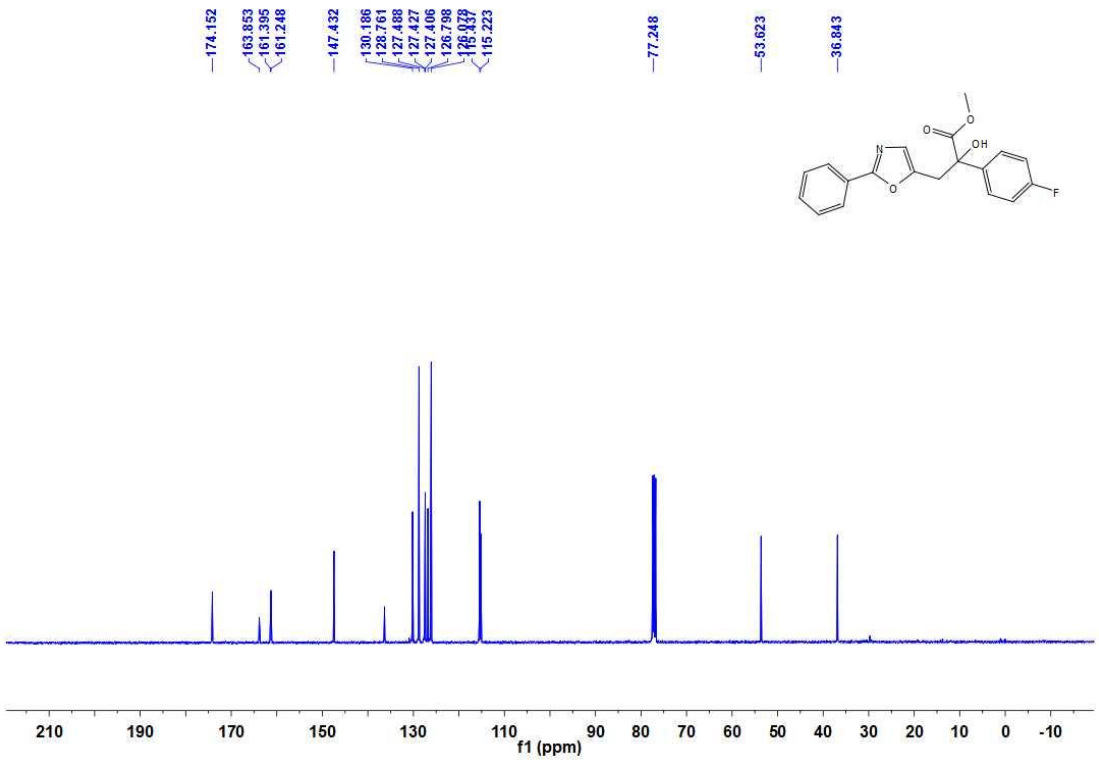
7.840
7.831
7.826
7.540
7.332
7.322
7.316
7.177
6.998
6.977
6.955
6.823
4.098
3.584
3.286
3.248
2.02
2.06
3.04
2.00
0.99
1.00
3.00
1.04
1.01
f1 (ppm)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161.395
161.248
147.432
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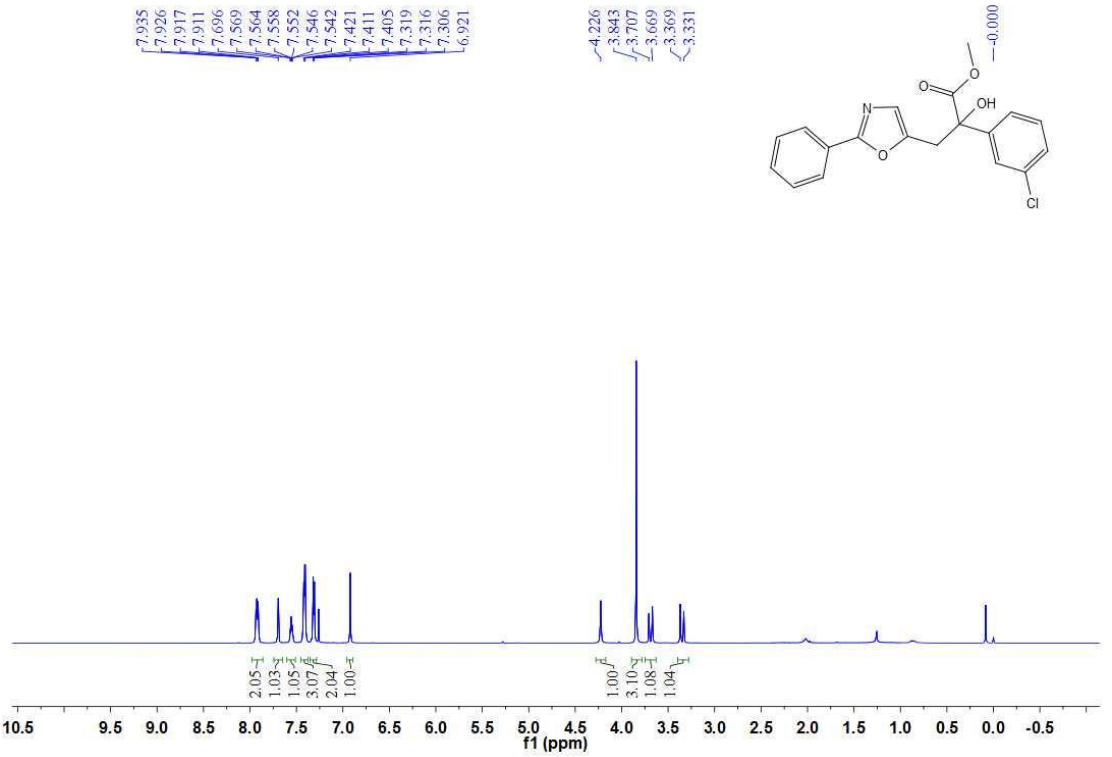
127.488
127.427
127.406
126.798
115.223
77.248
53.623
36.843
f1 (ppm)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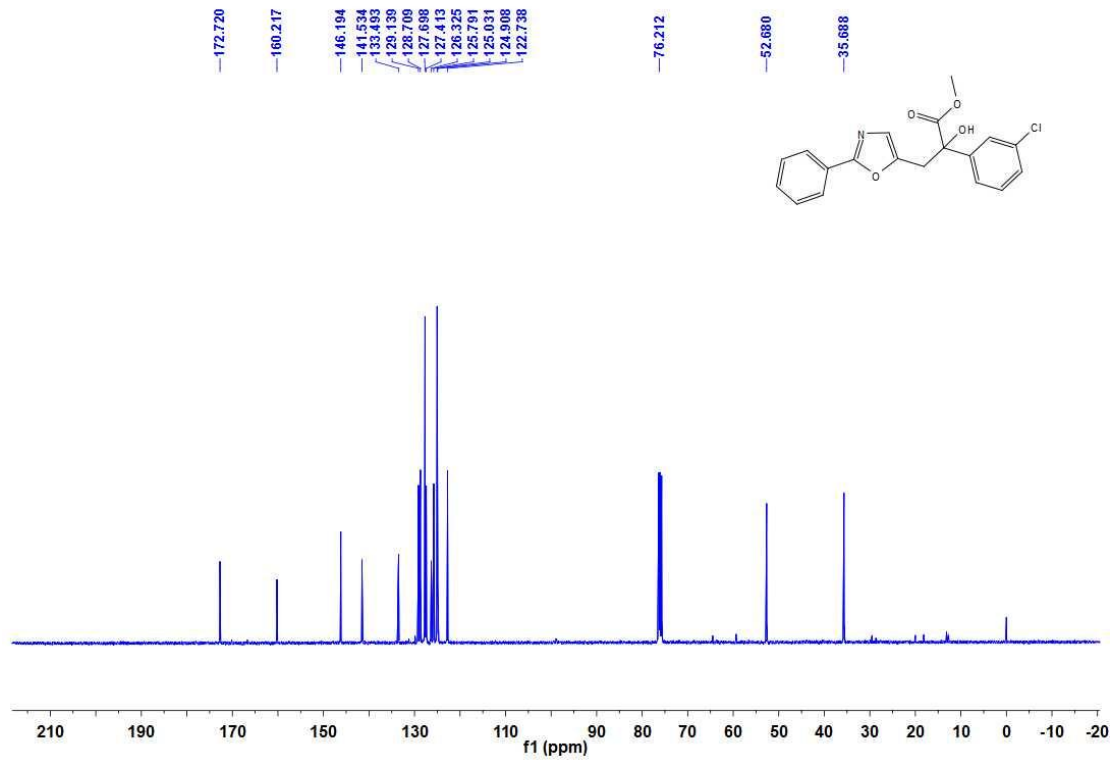
7.558
7.552
7.546
7.542
7.421
7.411
7.405
7.319
7.316
7.306
6.921
4.226
3.843
3.707
3.669
3.369
3.331
0.000
O
O
OH
N
O
Cl
2.05
1.03
1.05
3.07
2.04
1.00
1.00
3.10
1.08
1.04
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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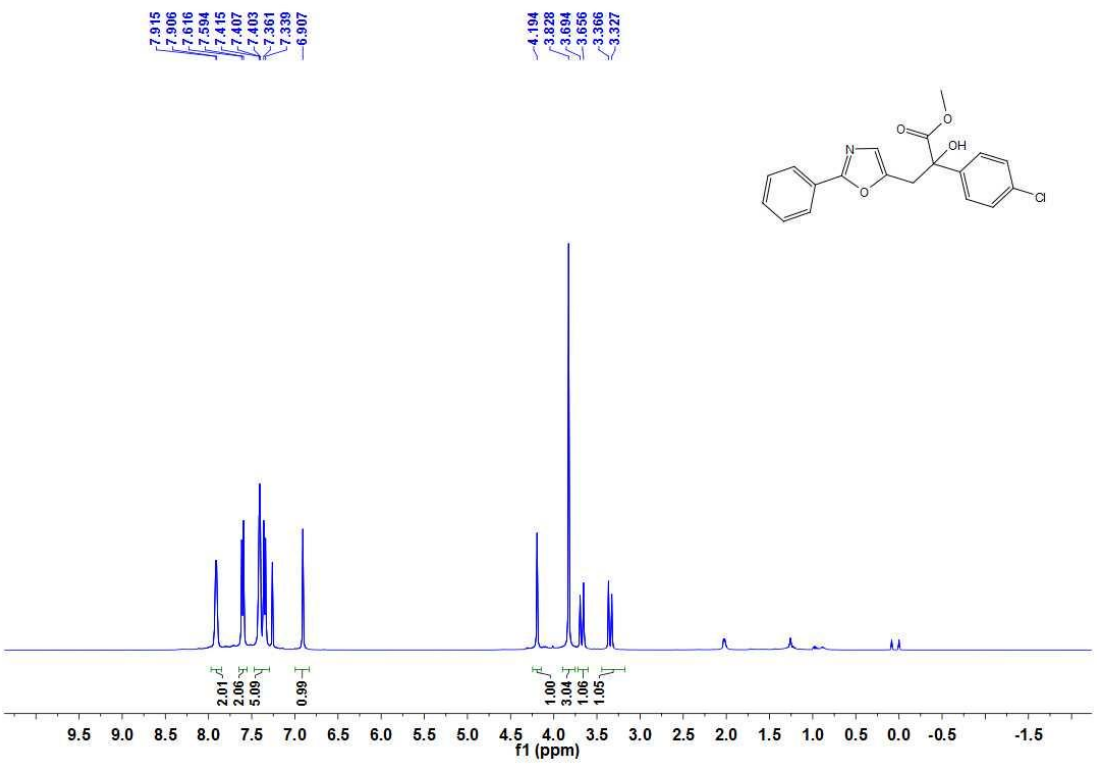
129.139
128.709
127.698
127.413
126.325
125.791
125.031
124.908
122.738
76.212
52.680
35.688
O
O
OH
N
O
Cl
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)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7.906
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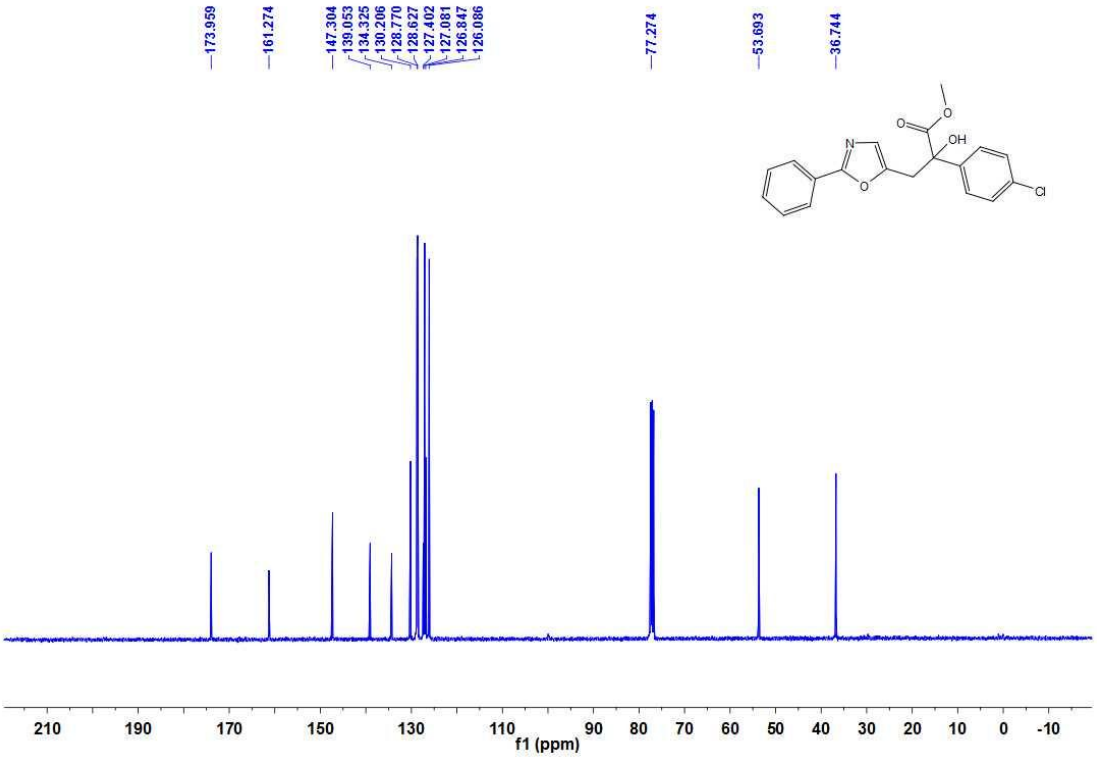
7.594
7.415
7.407
7.403
7.361
7.339
6.907
4.194
3.828
3.694
3.656
3.366
3.327
O
O
OH
N
O
Cl
2.01
2.06
5.09
0.99
1.00
3.04
1.06
1.05
f1 (ppm)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161.274
147.304
139.053
134.325
130.206
128.770
128.627
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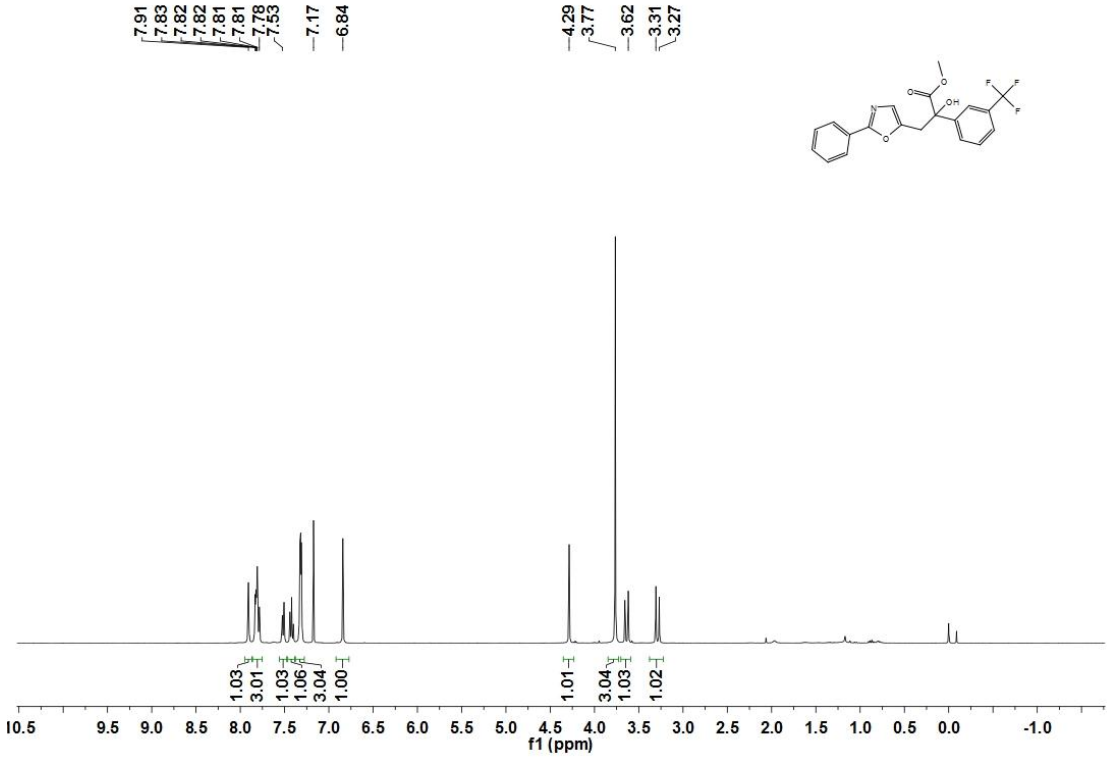
127.081
126.847
126.086
77.274
53.693
36.744
O
O
OH
N
O
Cl
f1 (ppm)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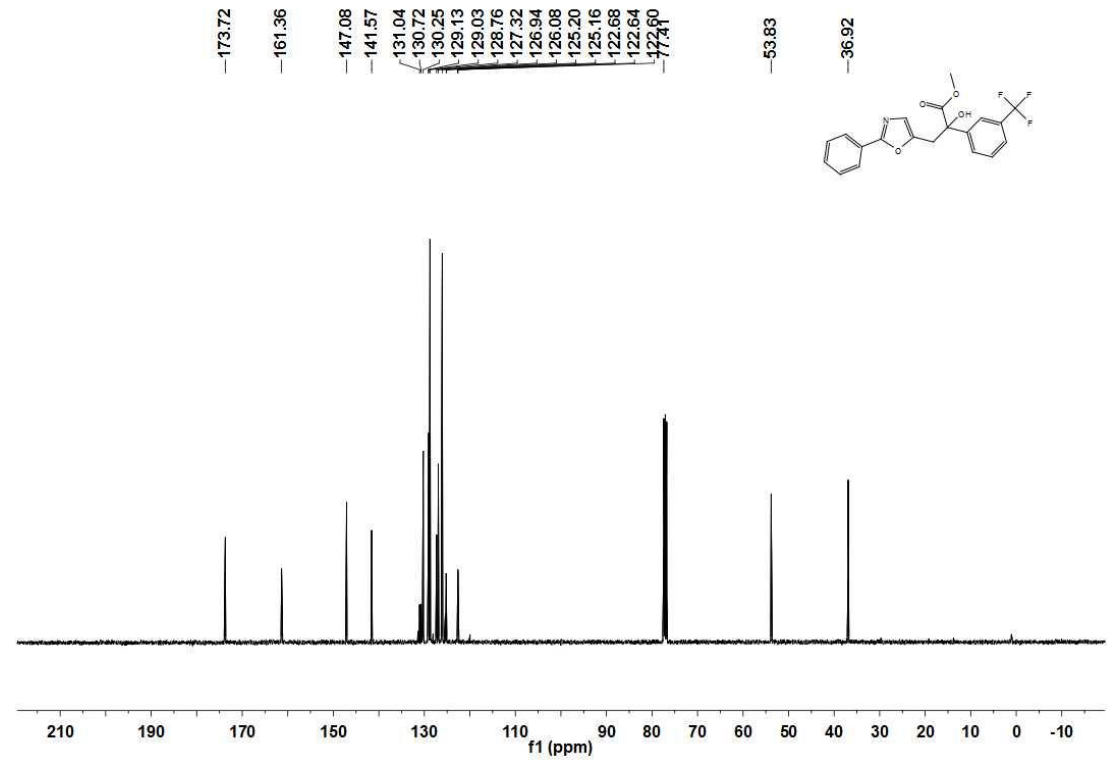
7.83
7.82
7.82
7.81
7.81
7.78
7.53
7.17
6.84
4.29
3.77
3.62
3.31
3.27
1.03
3.01
1.03
1.06
3.04
1.00
1.01
3.04
1.03
1.02
f1 (ppm)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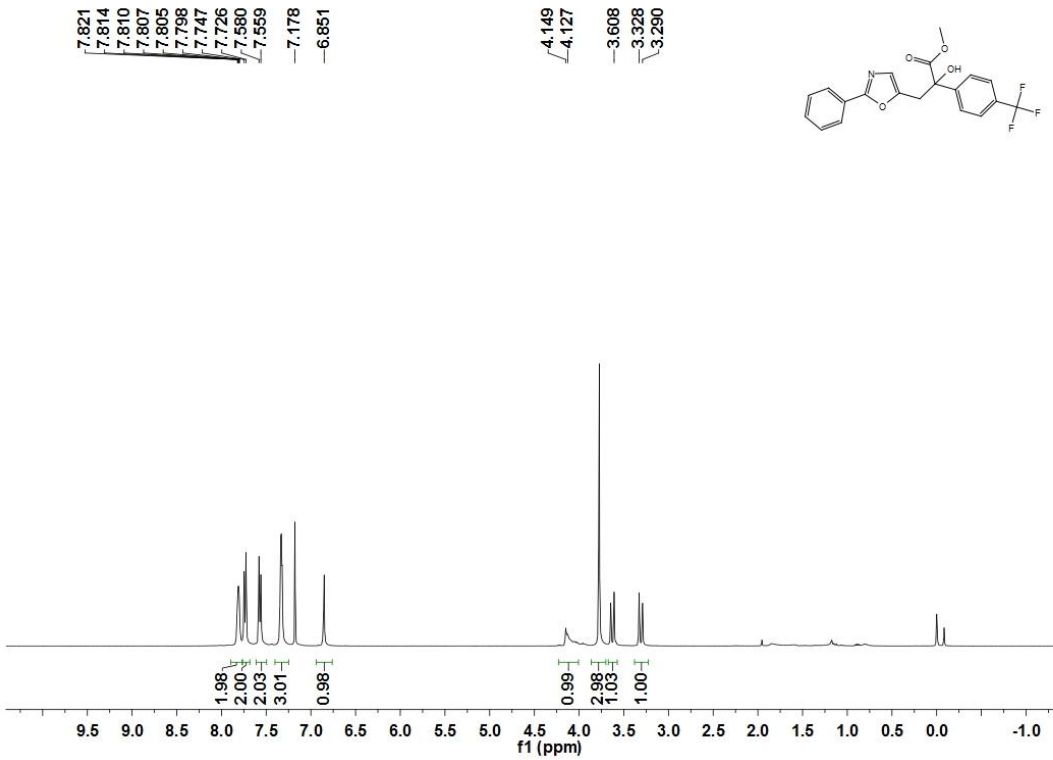
141.57
131.04
130.72
130.25
129.13
129.03
128.76
127.32
126.94
126.08
125.20
125.16
122.68
122.64
122.60
77.41
53.83
36.92
f1 (ppm)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7.810
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7.798
7.747
7.726
7.580
7.559
7.178
6.851
4.149
4.127
3.608
3.328
3.290
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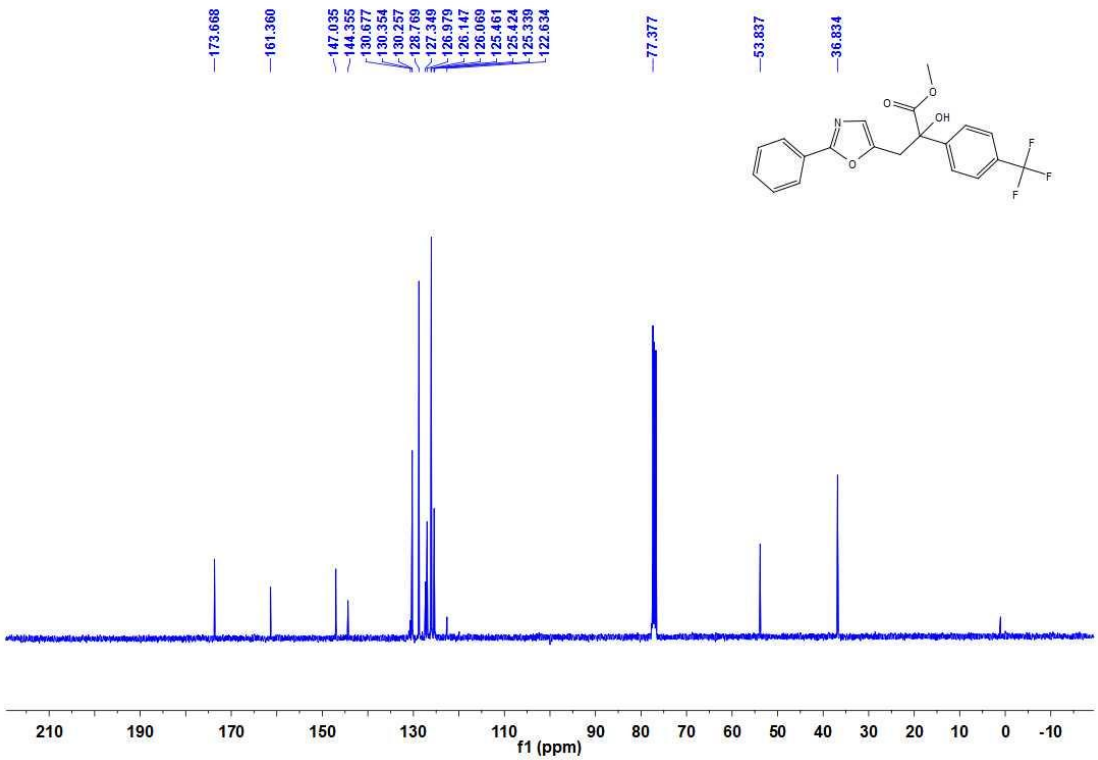
2.00
2.03
3.01
0.98
0.99
2.98
1.03
1.00
f1 (ppm)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125.339
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77.377
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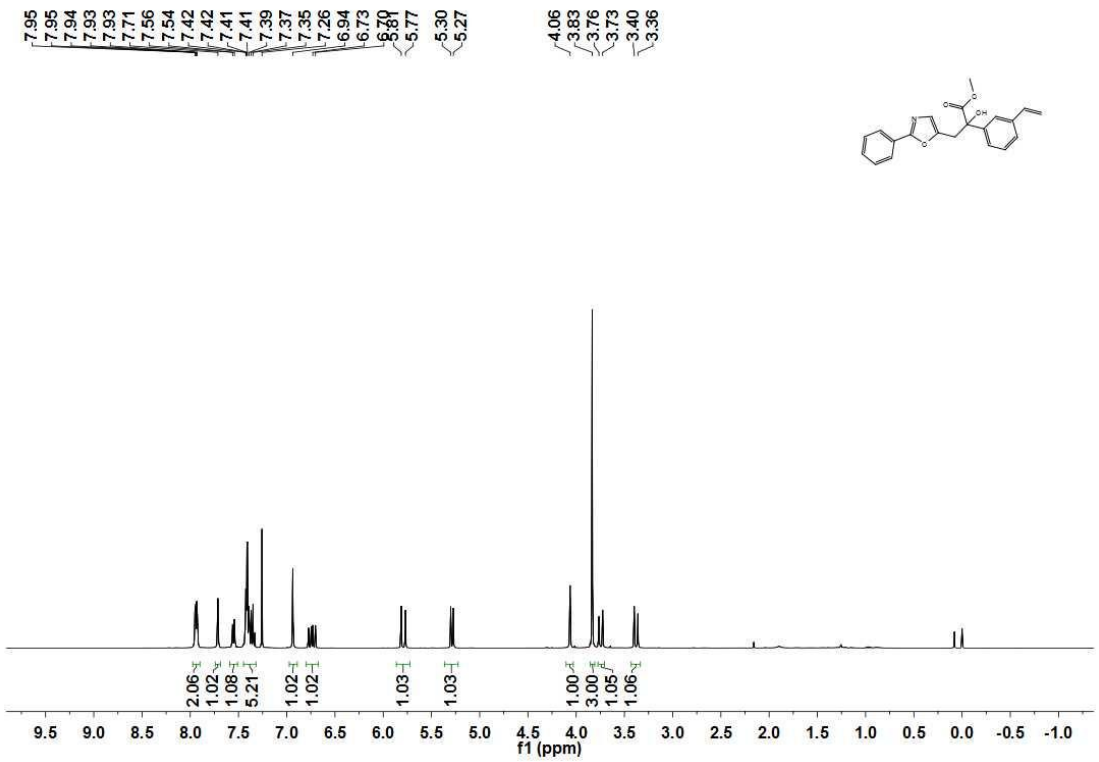
36.834
f1 (ppm)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7.93
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7.54
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7.41
7.41
7.39
7.37
7.35
7.26
6.94
6.73
6.70
5.81
5.77
5.30
5.27
4.06
3.83
3.76
3.73
3.40
3.36
2.06
1.02
1.08
5.21
1.02
1.02
1.03
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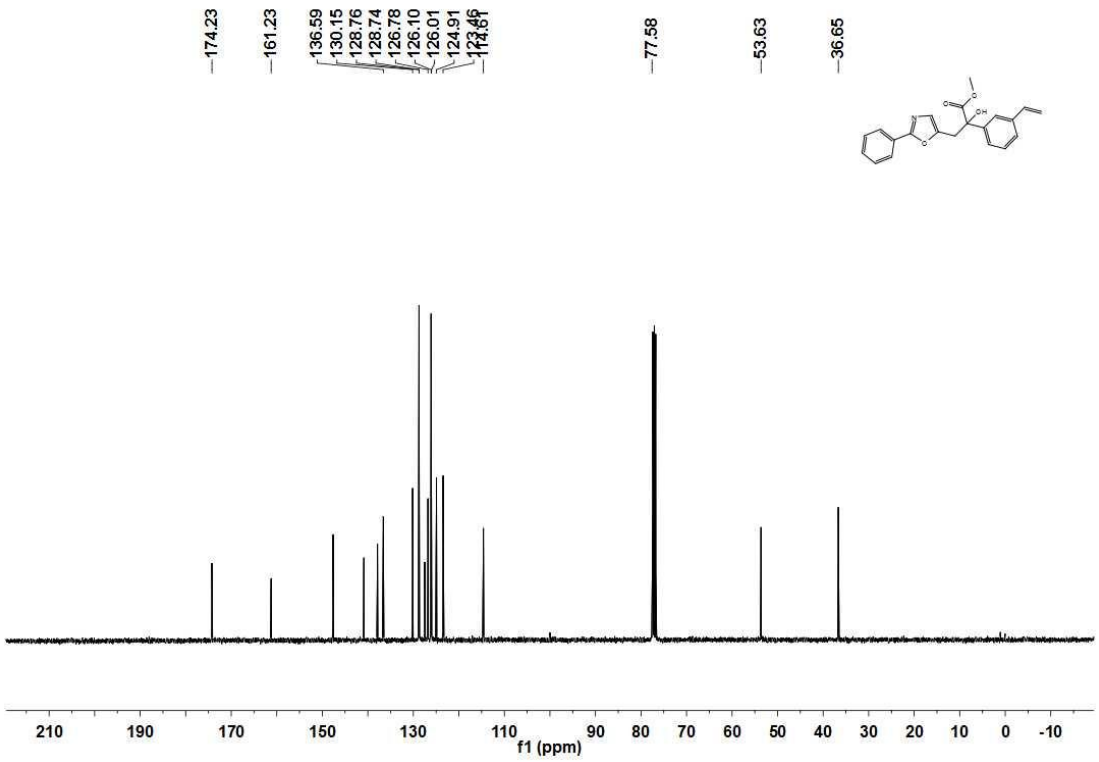
1.00
3.00
1.05
1.06
f1 (ppm)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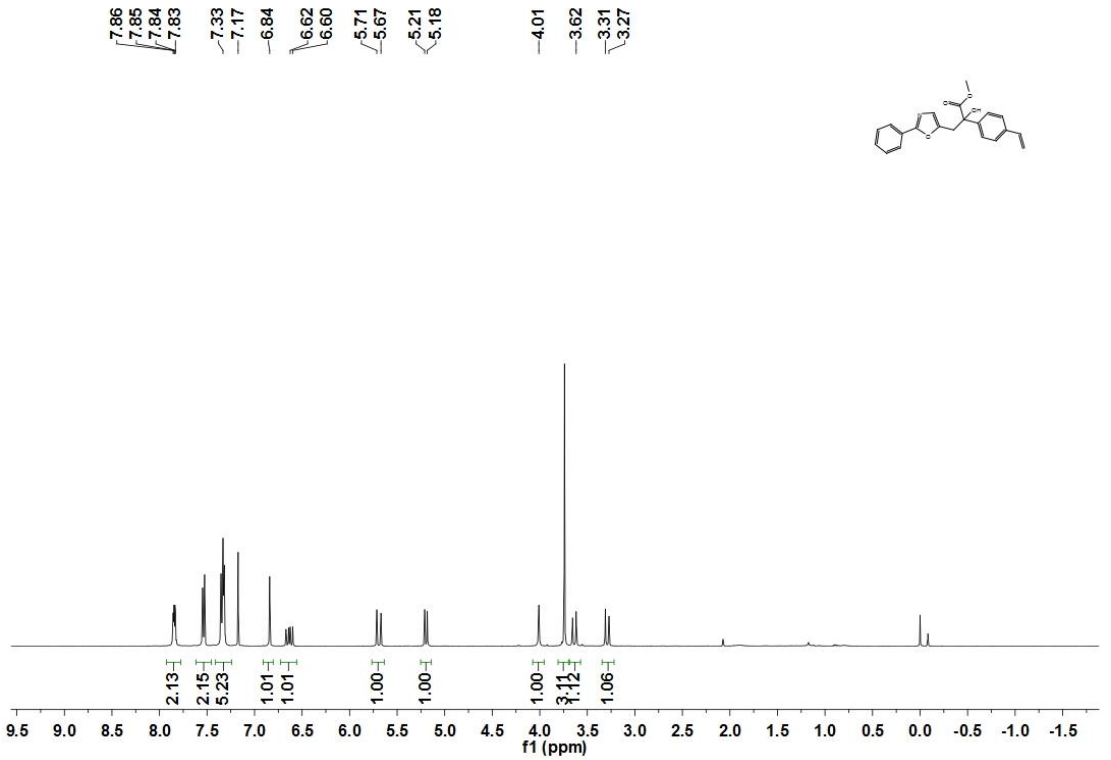
126.78
126.10
126.01
124.91
77.58
53.63
36.65
f1 (ppm)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7.85
7.84
7.83
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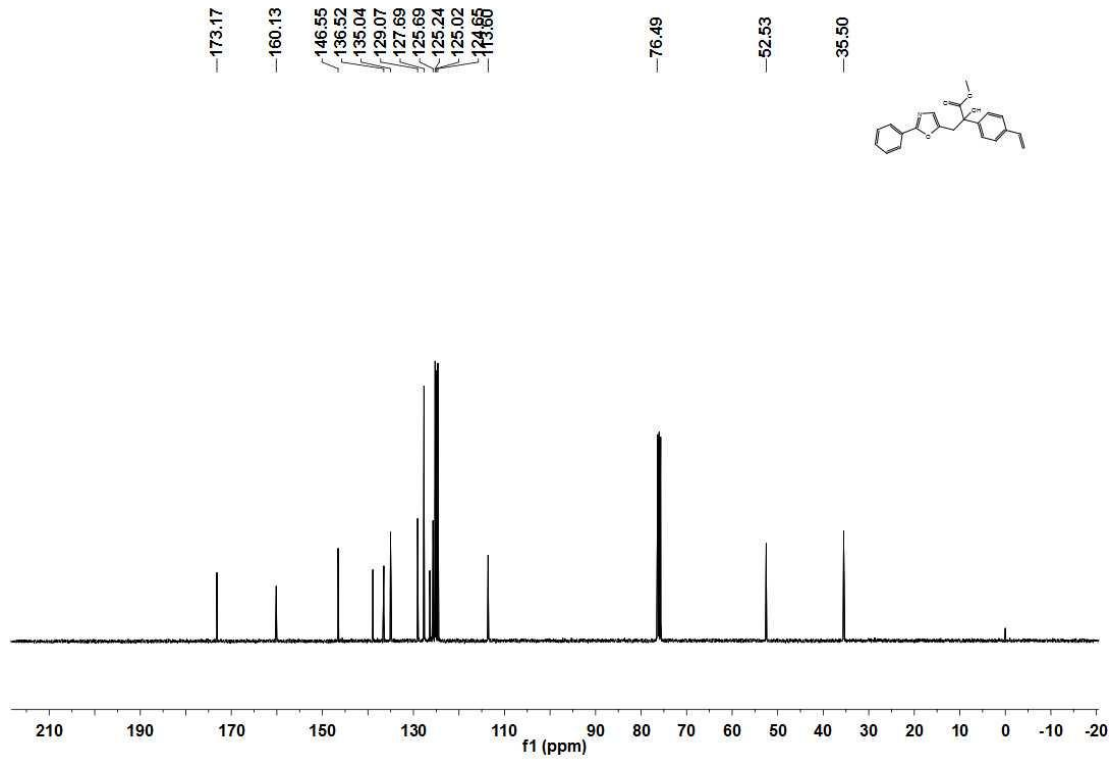
7.17
6.84
6.62
6.60
5.71
5.67
5.21
5.18
4.01
3.62
3.31
3.27
2.13
2.15
5.23
1.01
1.01
1.00
1.00
1.00
3.11
3.12
1.06
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)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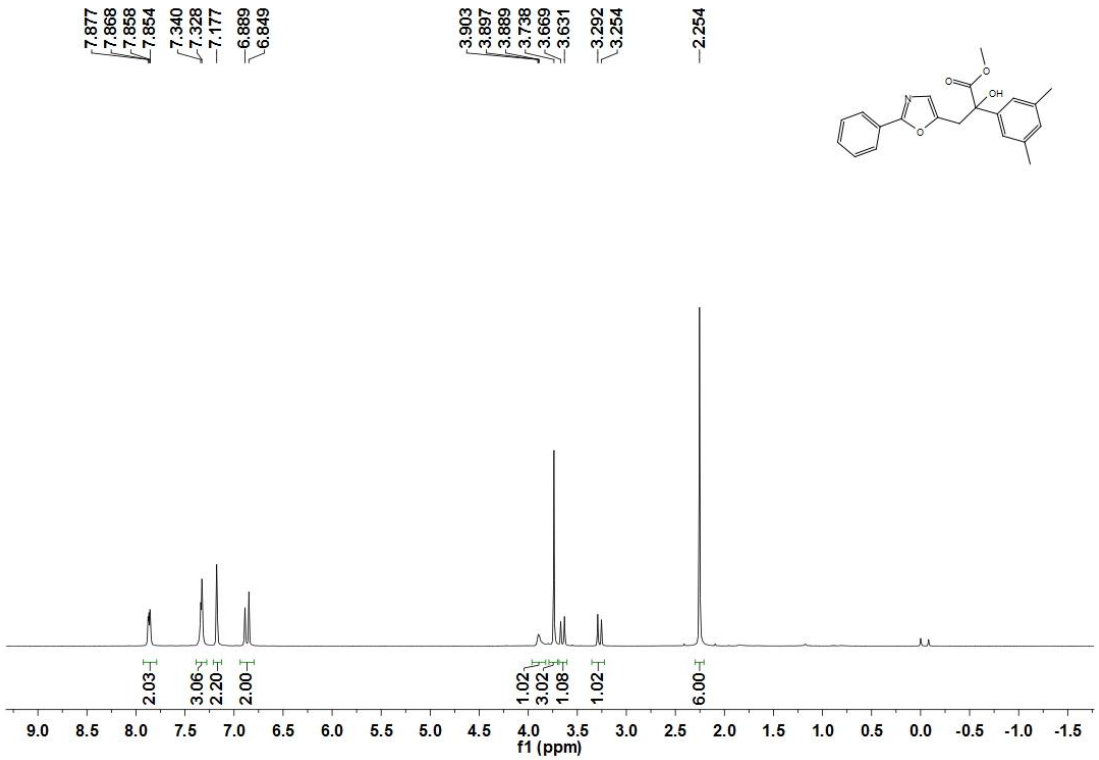
160.13
146.55
136.52
135.04
129.07
127.69
125.69
125.24
125.02
76.49
52.53
35.50
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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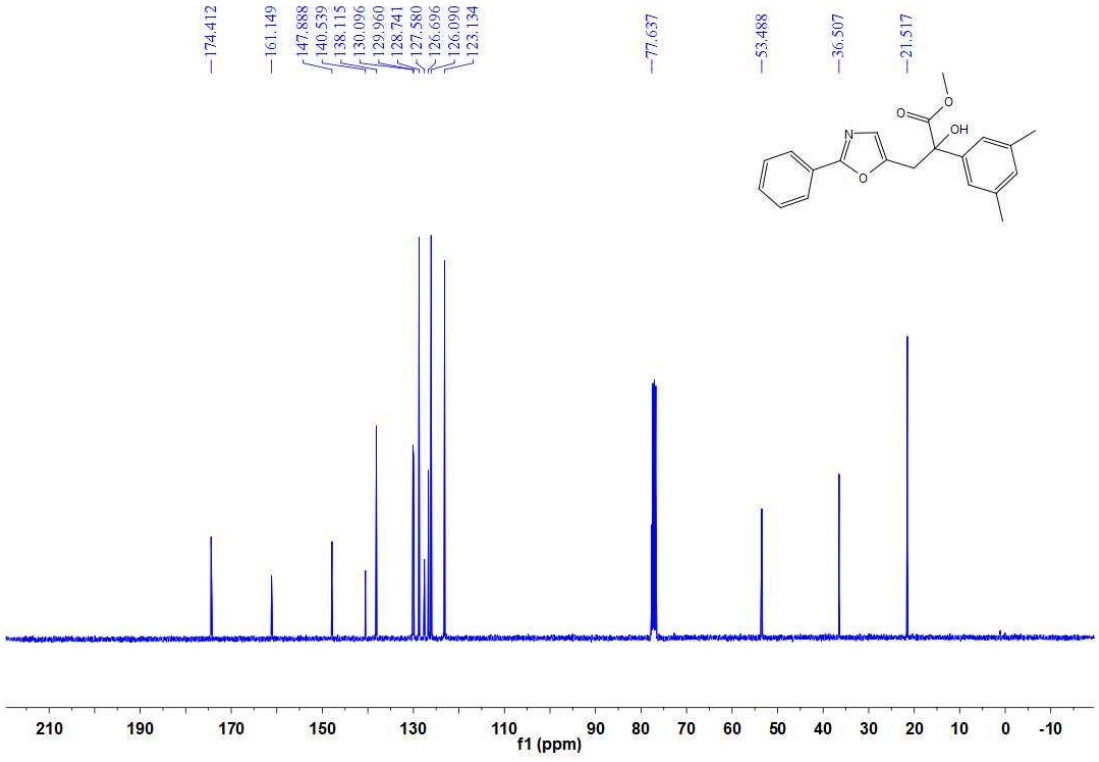
7.858
7.854
7.340
7.328
7.177
6.889
6.849
3.903
3.897
3.889
3.738
3.669
3.631
3.292
3.254
2.254
2.03
3.06
2.20
2.00
1.02
3.02
1.08
1.02
6.00
f1 (ppm)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127.580
126.696
126.090
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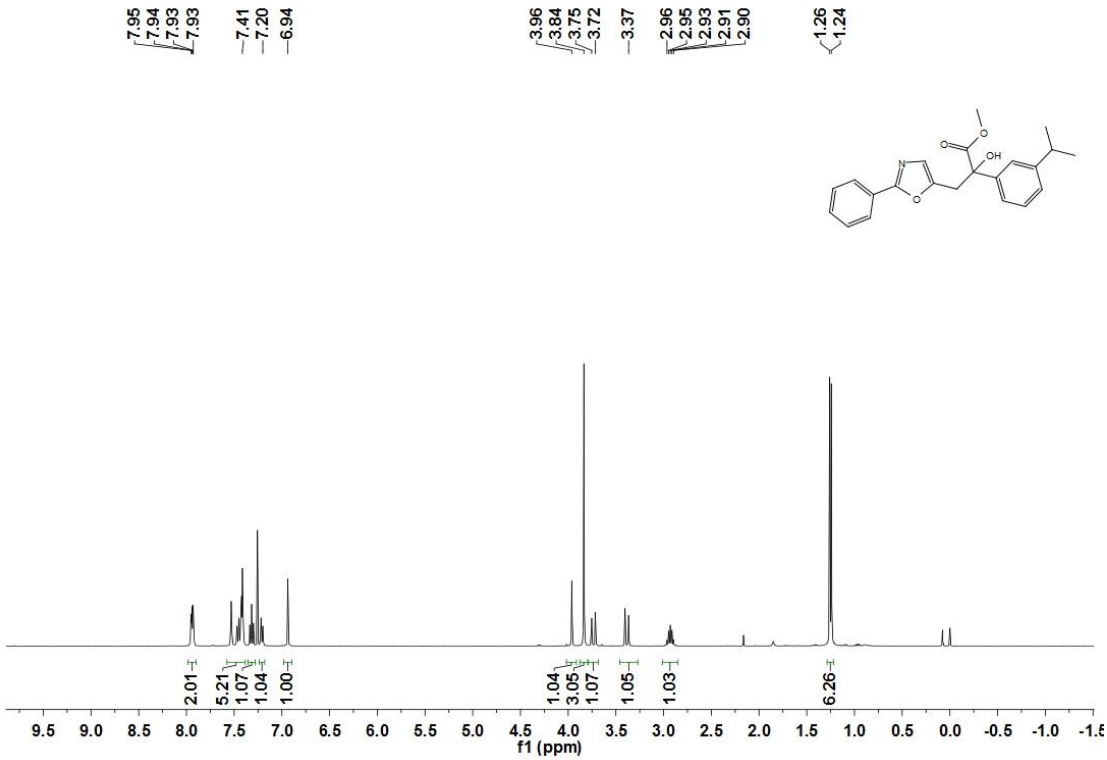
77.637
53.488
36.507
21.517
f1 (ppm)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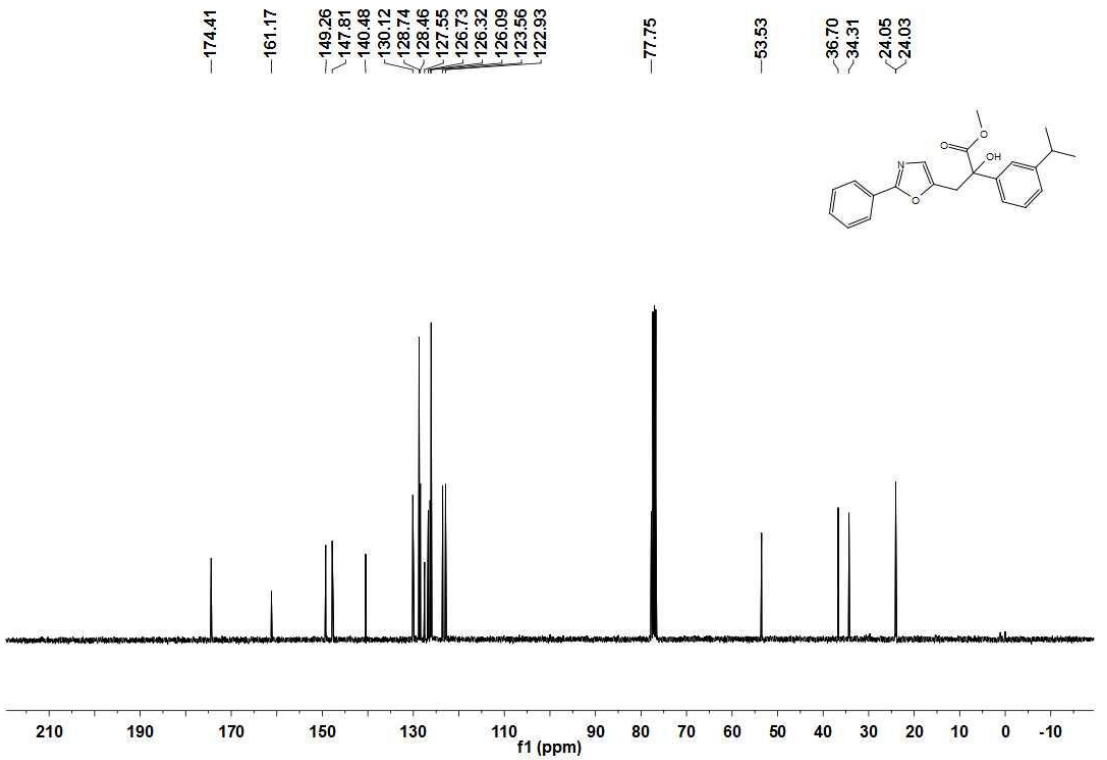
7.94
7.93
7.93
7.41
7.20
6.94
3.96
3.84
3.75
3.72
3.37
2.96
2.95
2.93
2.91
2.90
1.26
1.24
OH
2.01
5.21
1.07
1.04
1.00
1.04
3.05
1.07
1.05
1.03
6.26
f1 (ppm)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161.17
149.26
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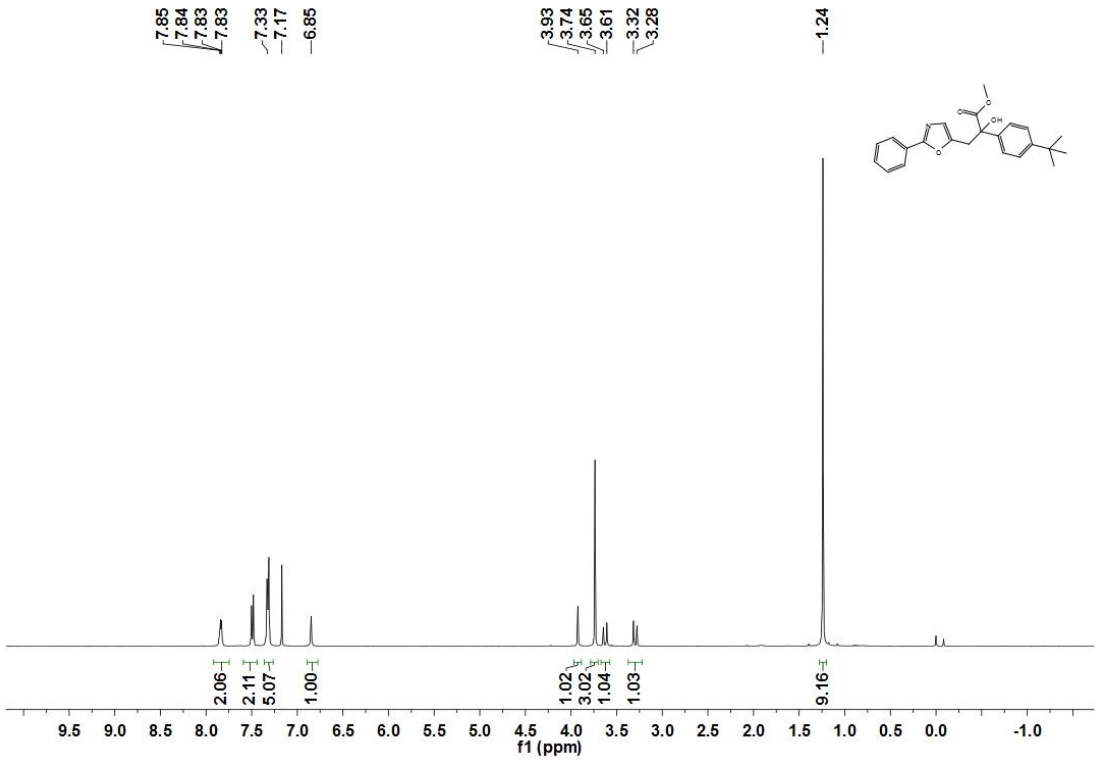
140.48
130.12
128.74
128.46
127.55
126.73
126.32
126.09
123.56
122.93
77.75
53.53
36.70
34.31
24.05
24.03
OH
f1 (ppm)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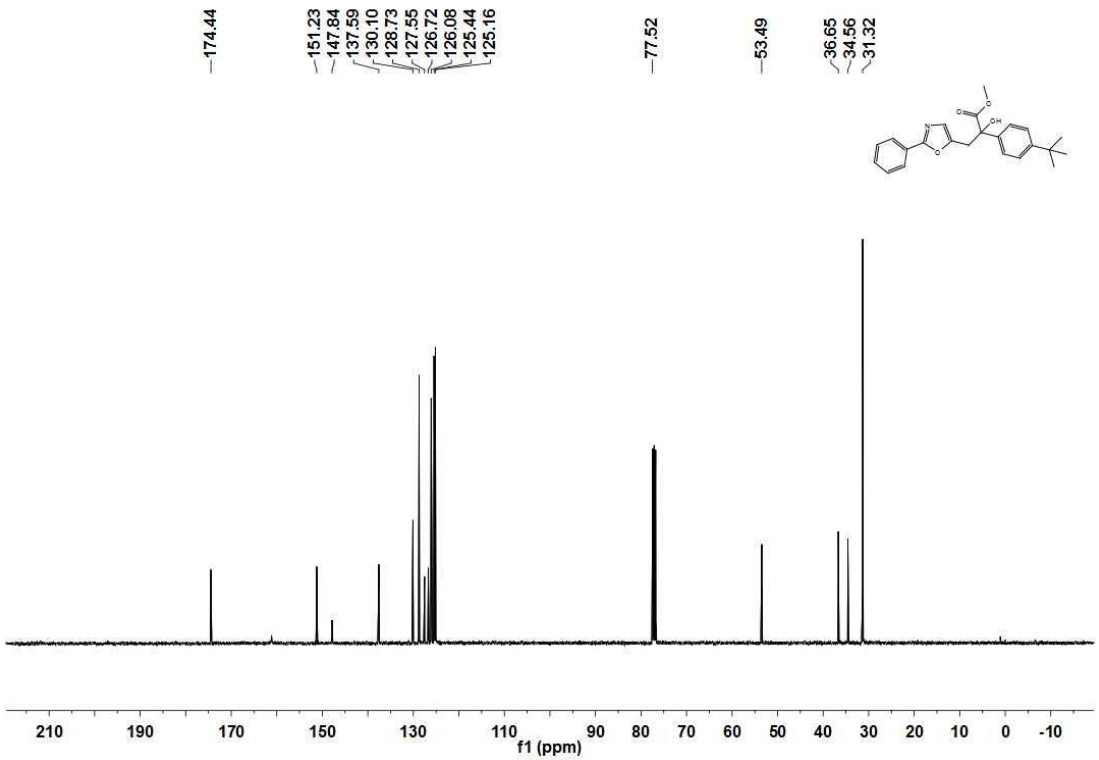
7.84
7.83
7.83
7.33
7.17
6.85
3.93
3.74
3.65
3.61
3.32
3.28
1.24
2.06
2.11
5.07
1.00
1.02
3.02
1.04
1.03
9.16
f1 (ppm)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130.10
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127.55
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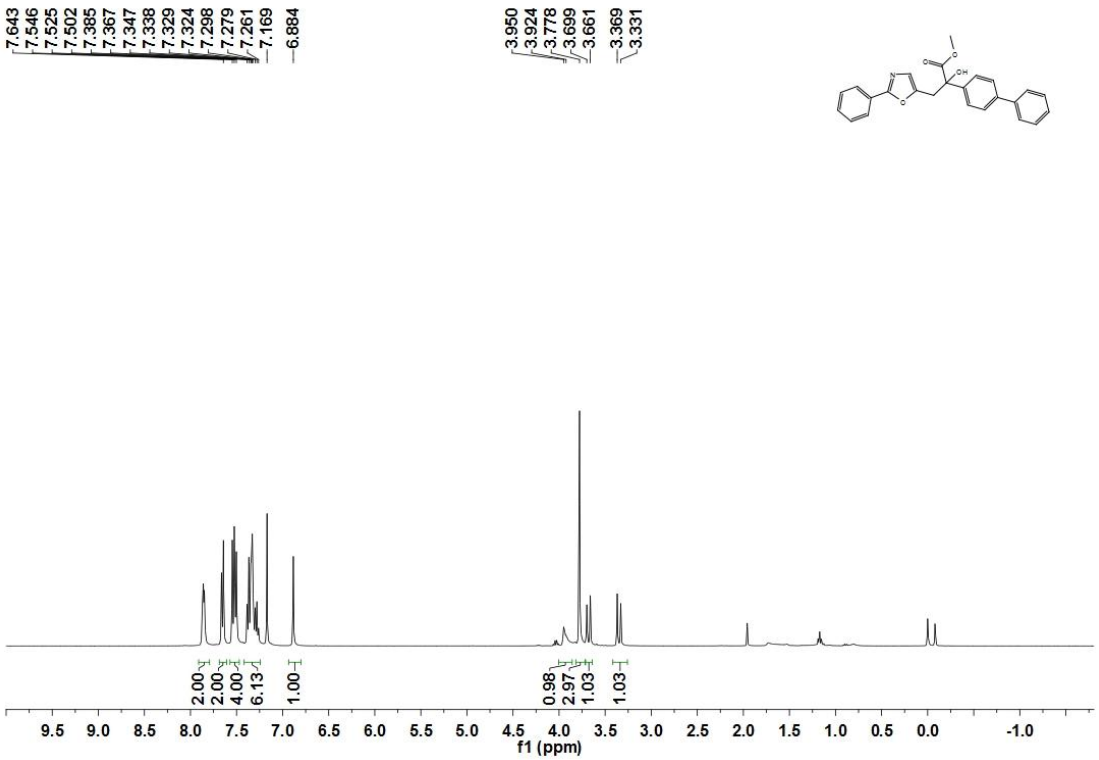
126.08
125.44
125.16
77.52
53.49
36.65
34.56
31.32
f1 (ppm)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7.525
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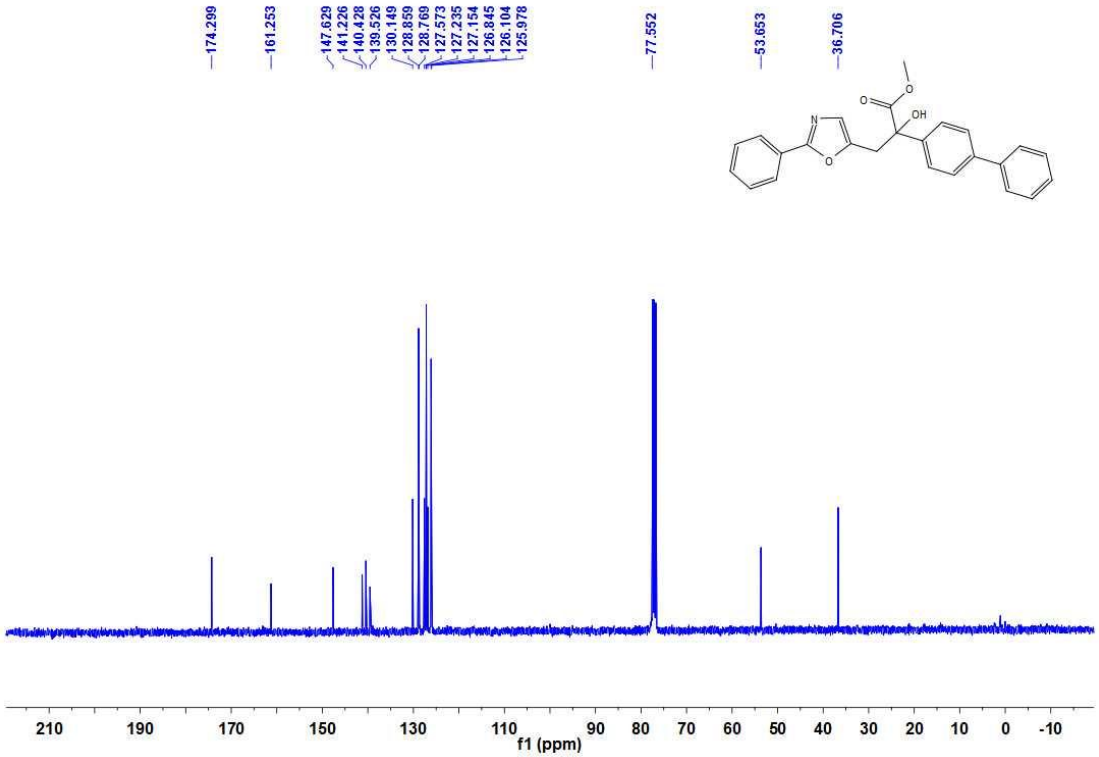
7.385
7.367
7.347
7.338
7.329
7.324
7.298
7.279
7.261
7.169
6.884
3.950
3.924
3.778
3.699
3.661
3.369
3.331
2.00
2.00
4.00
6.13
1.00
0.98
2.97
1.03
1.03
f1 (ppm)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140.428
139.526
130.149
128.859
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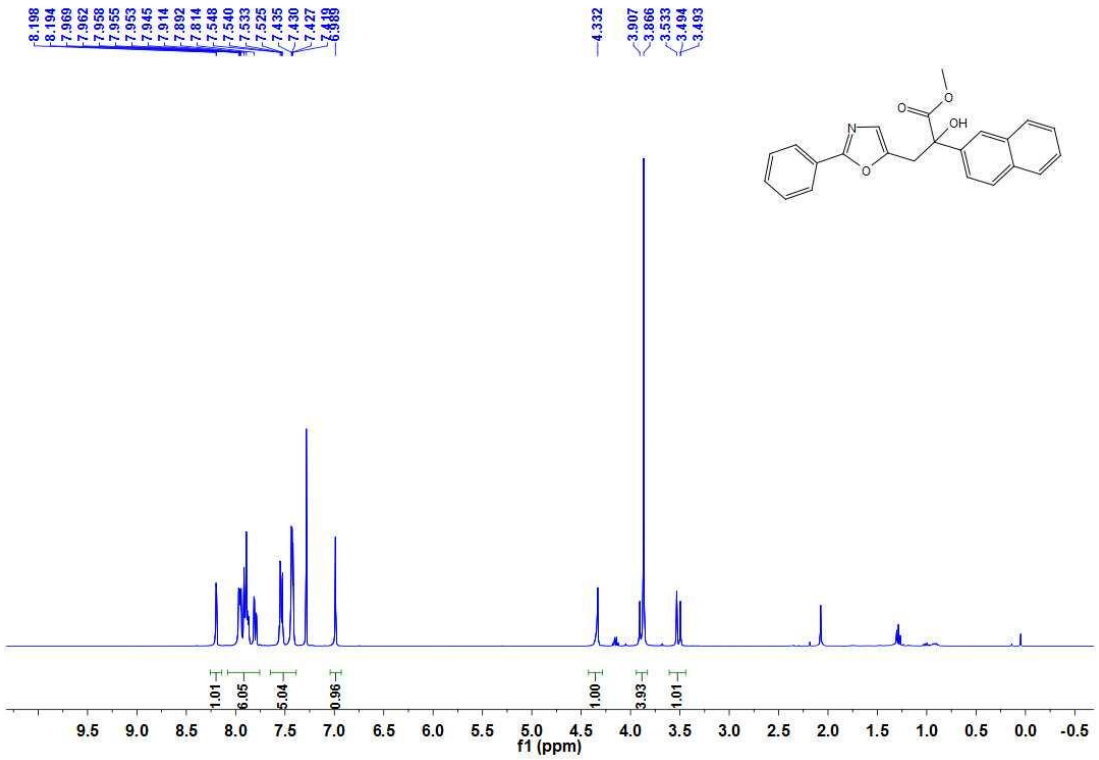
127.235
127.154
126.845
126.104
125.978
77.552
53.653
36.706
f1 (ppm)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8.194
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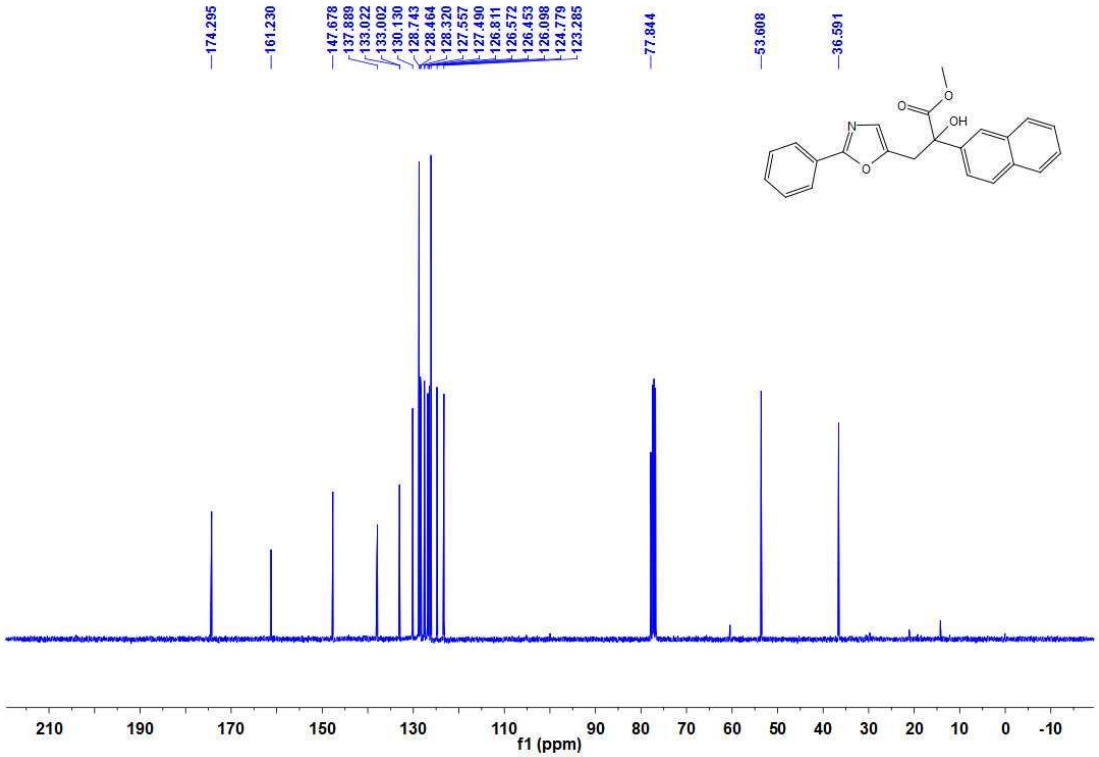
7.955
7.953
7.945
7.914
7.892
7.814
7.548
7.540
7.533
7.525
7.435
7.430
7.427
7.419
6.989
4.332
3.907
3.866
3.533
3.494
3.493
O
O
OH
N
O
1.01
6.05
5.04
0.96
1.00
3.93
1.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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133.002
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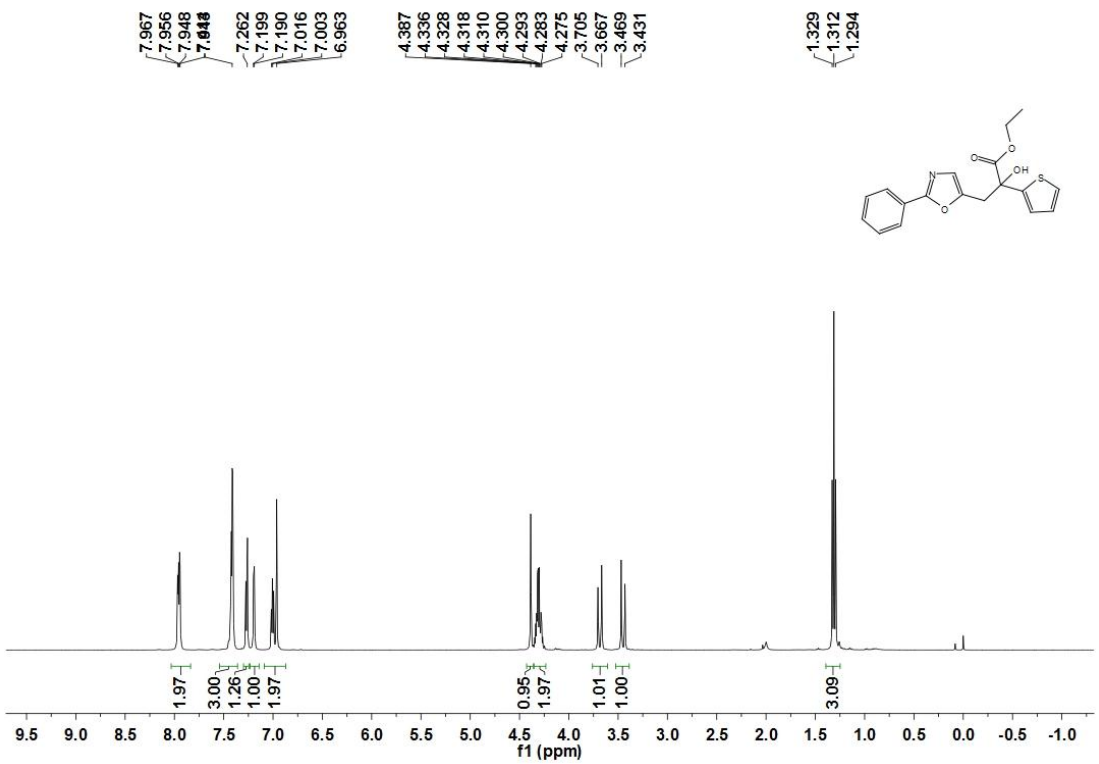
128.464
128.320
127.557
127.490
126.811
126.572
126.453
126.098
124.779
123.285
77.844
53.608
36.591
O
O
OH
N
O
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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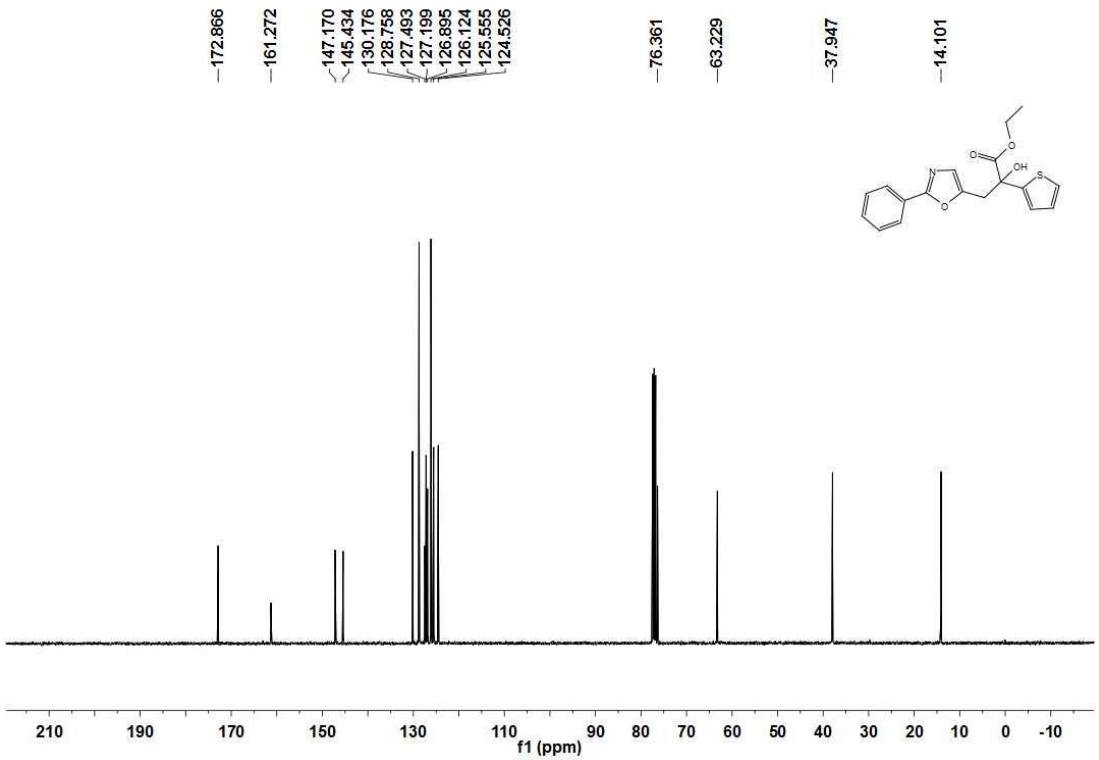
7.956
7.948
7.262
7.199
7.190
7.016
7.003
6.963
4.387
4.336
4.328
4.318
4.310
4.300
4.293
4.283
4.275
3.705
3.667
3.469
3.431
1.329
1.312
1.294
1.97
3.00
1.26
1.00
1.97
0.95
1.97
1.01
1.00
3.09
f1 (ppm)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130.176
128.758
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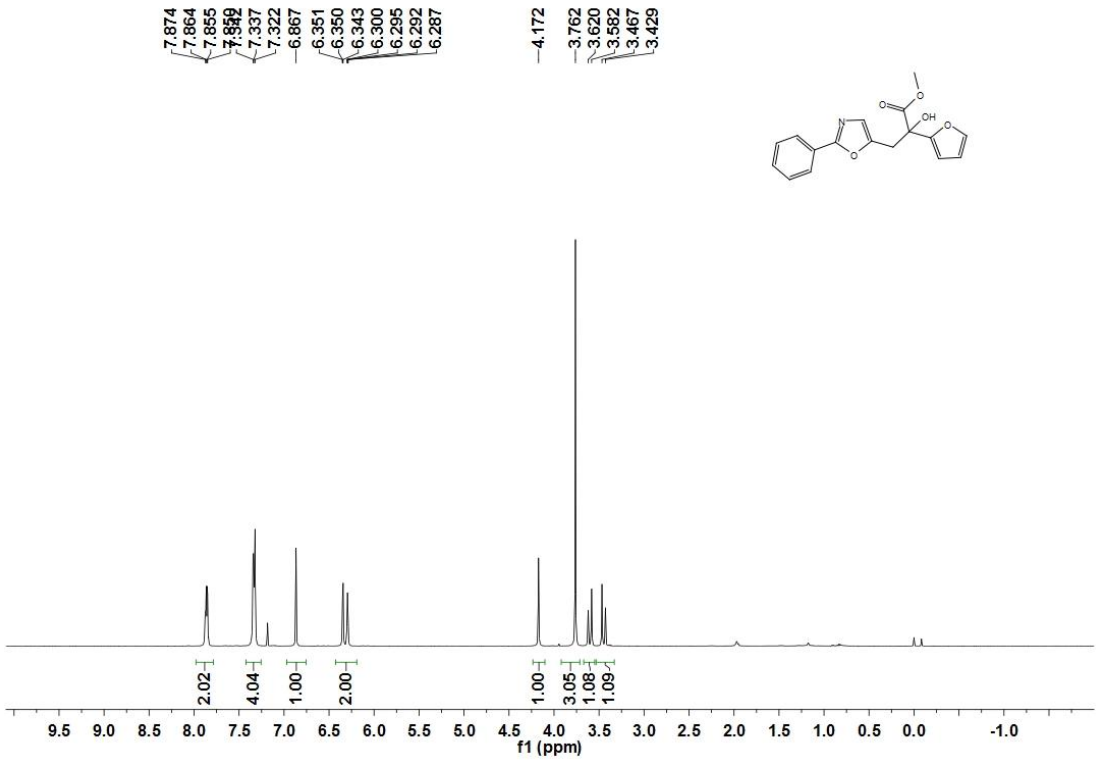
127.199
126.895
126.124
125.555
124.526
76.361
63.229
37.947
14.101
f1 (ppm)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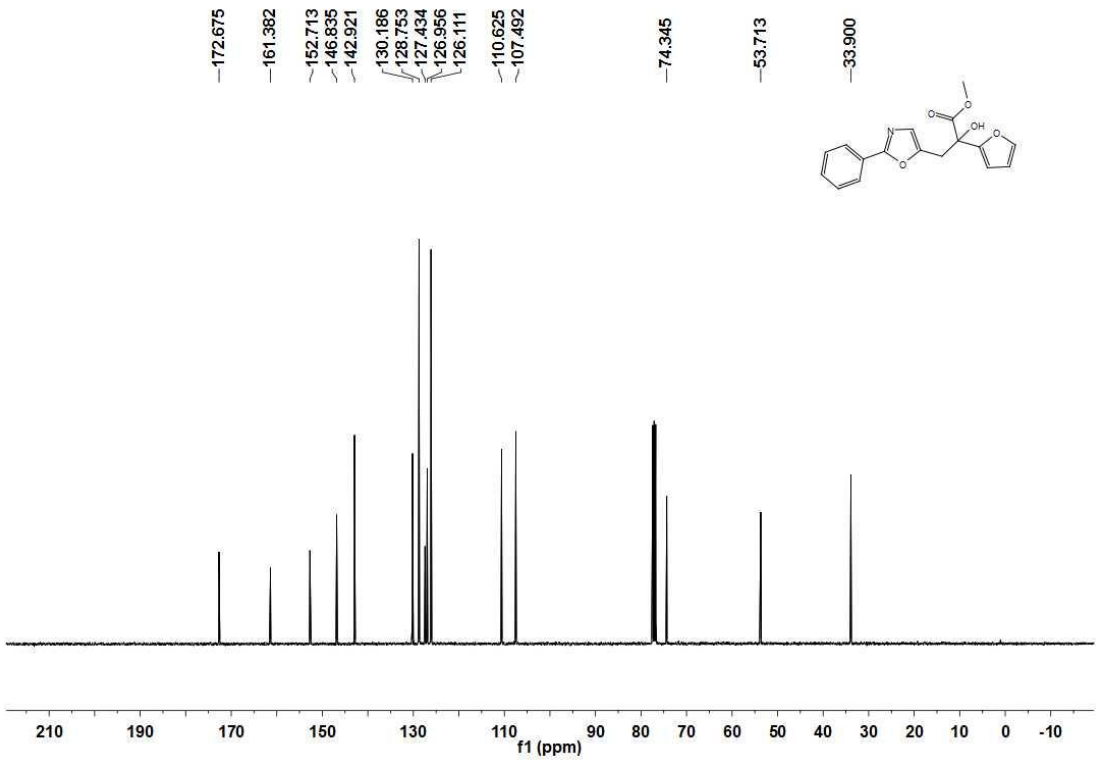
7.337
7.322
6.867
6.351
6.350
6.343
6.300
6.295
6.292
6.287
4.172
3.762
3.620
3.582
3.467
3.429
2.02
4.04
1.00
2.00
1.00
3.05
1.08
1.09
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -1.0
f1 (ppm)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127.434
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107.492
74.345
53.713
33.900
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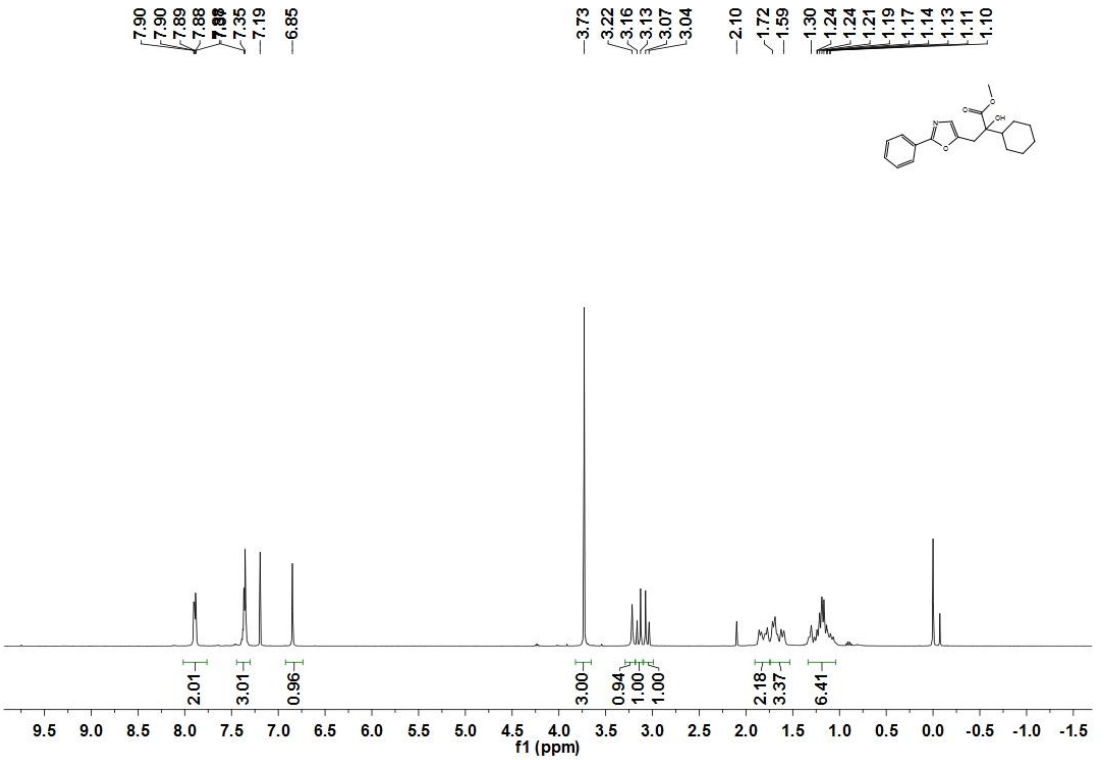
f1 (ppm)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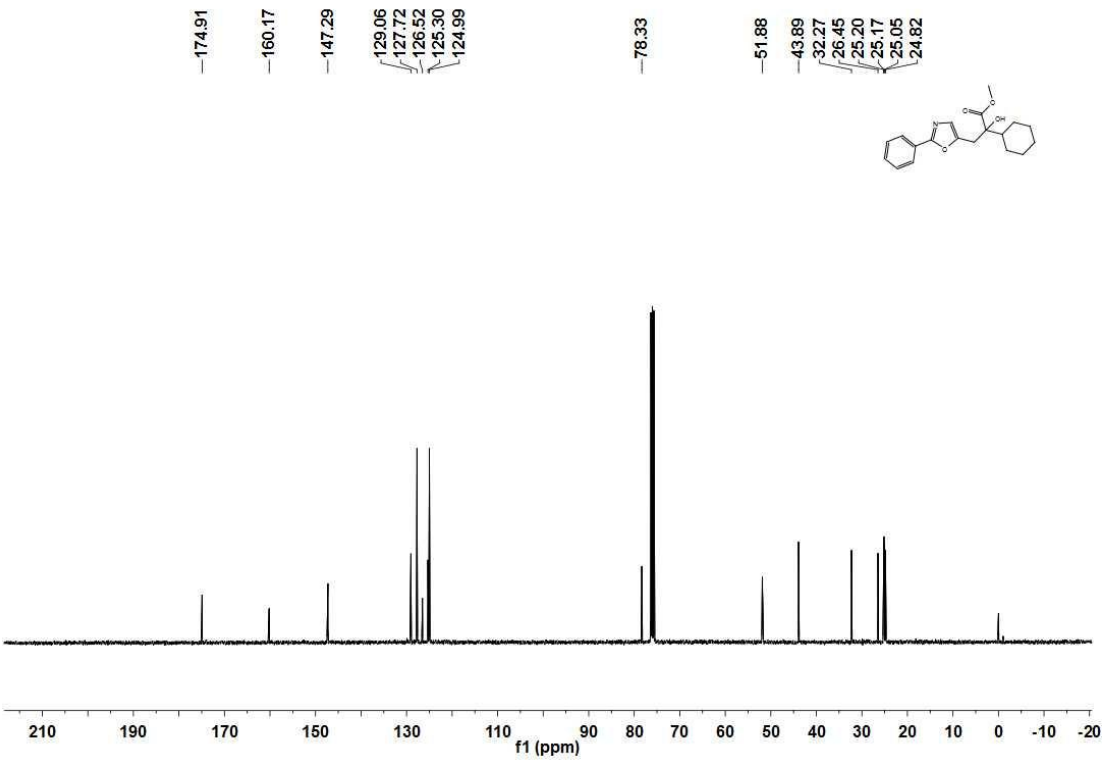
7.19
6.85
3.73
3.22
3.16
3.13
3.07
3.04
2.10
1.72
1.59
1.30
1.24
1.24
1.21
1.19
1.17
1.14
1.13
1.11
1.10
2.01
3.01
0.96
3.00
0.94
1.00
1.00
2.18
3.37
6.41
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)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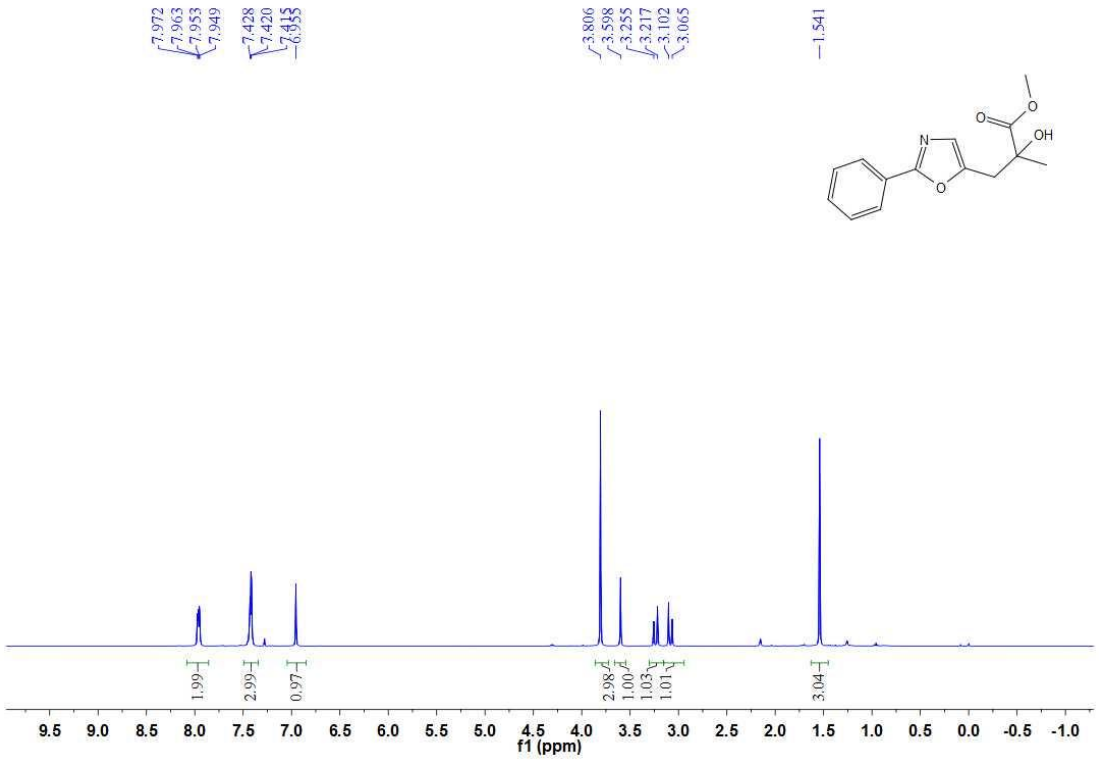
127.72
126.52
125.30
124.99
78.33
51.88
43.89
32.27
26.45
25.20
25.17
25.05
24.82
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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3.255
3.217
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1.99
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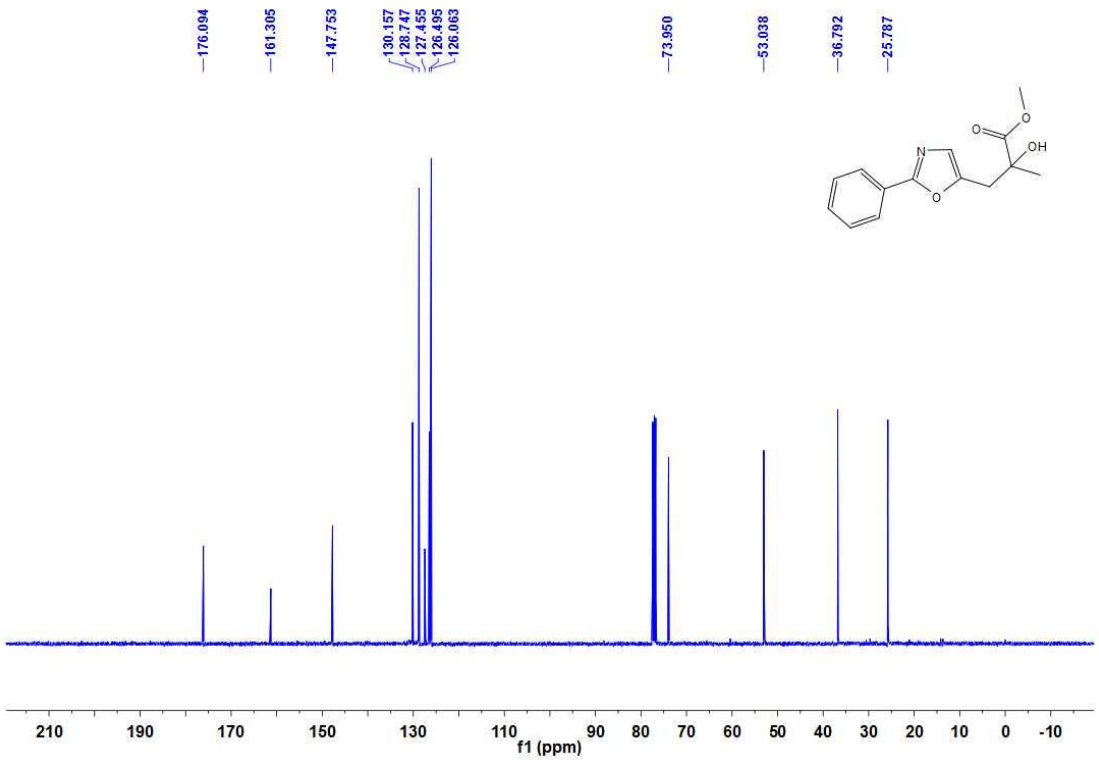
0.97
2.98
1.00
1.03
1.01
3.04
f1 (ppm)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126.063
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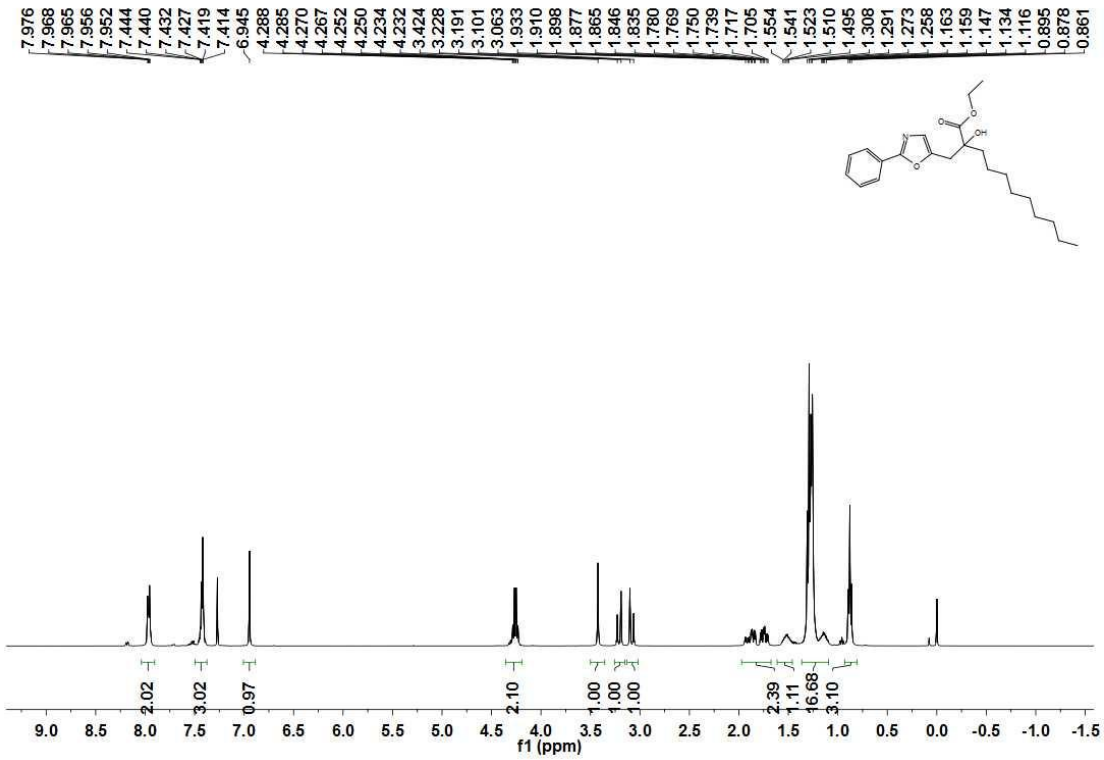
53.038
36.792
25.787
f1 (ppm)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4.285
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4.252
4.250
4.234
4.232
3.424
3.228
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3.101
3.063
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1.898
1.877
1.865
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1.835
1.780
1.769
1.750
1.739
1.717
1.705
1.554
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1.523
1.510
1.495
1.308
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1.273
1.258
1.163
1.159
1.147
1.134
1.116
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0.861
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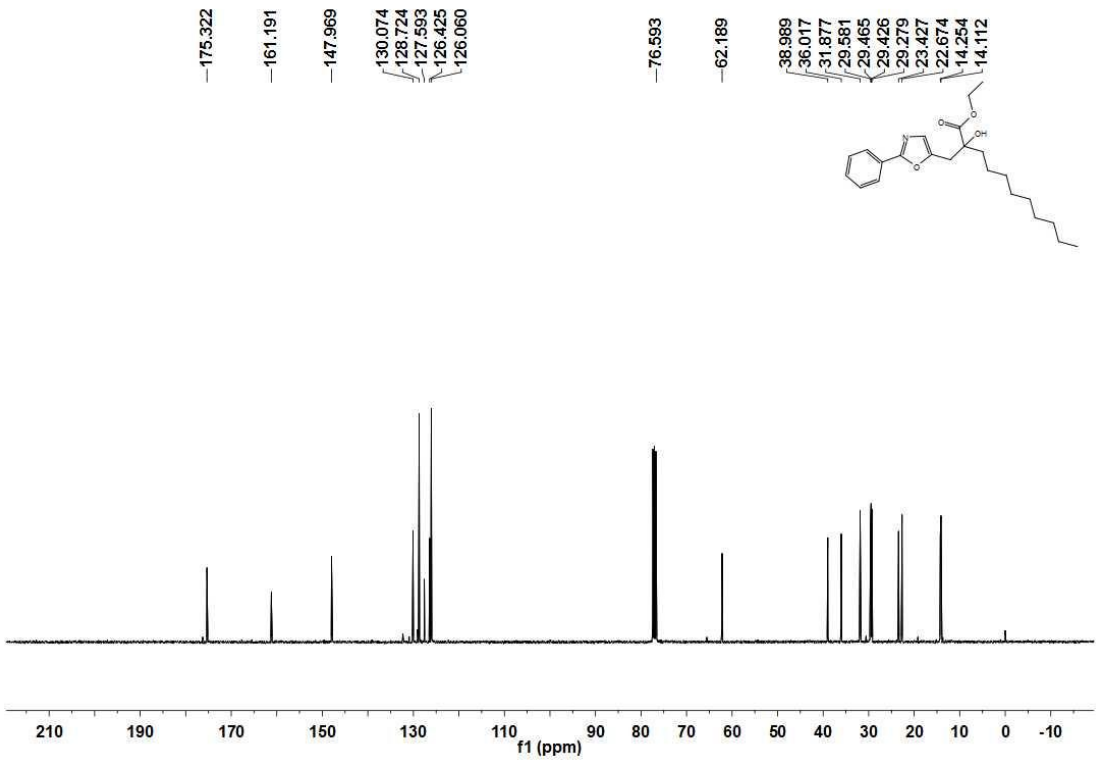
3.02
0.97
2.10
1.00
1.00
1.00
2.39
1.11
16.68
3.10
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)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126.060
76.593
62.189
38.989
36.017
31.877
29.581
29.465
29.426
29.279
23.427
22.674
14.254
14.112
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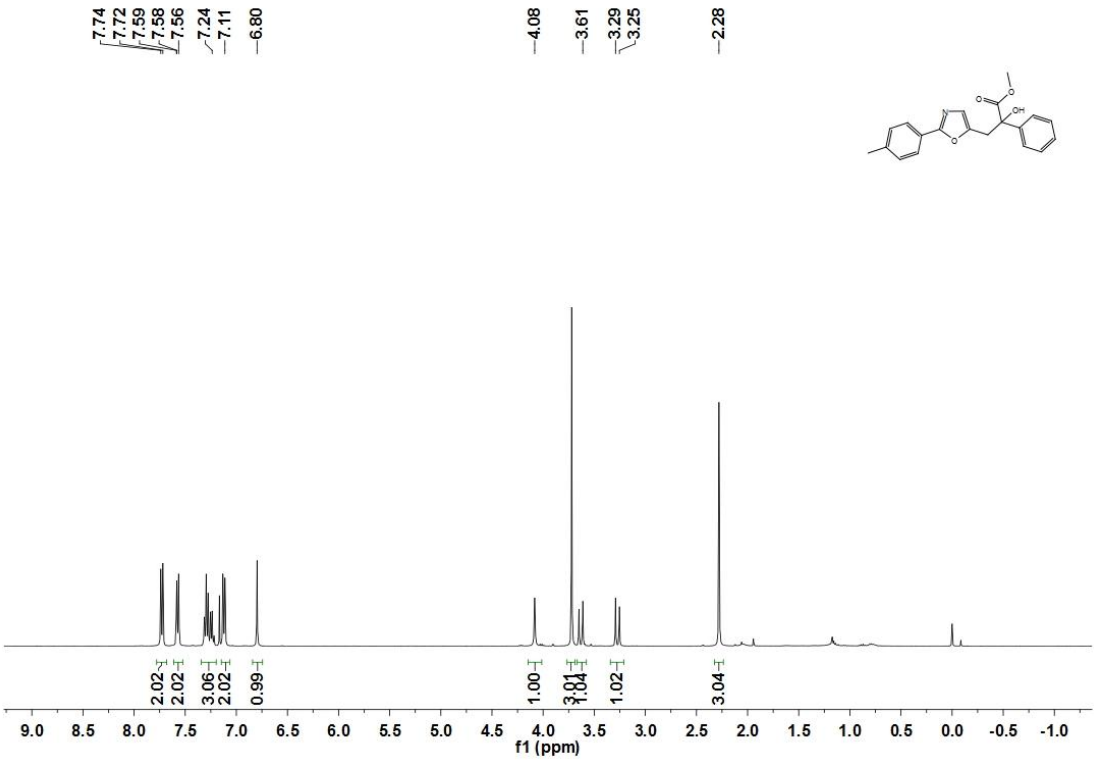
f1 (ppm)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7.72
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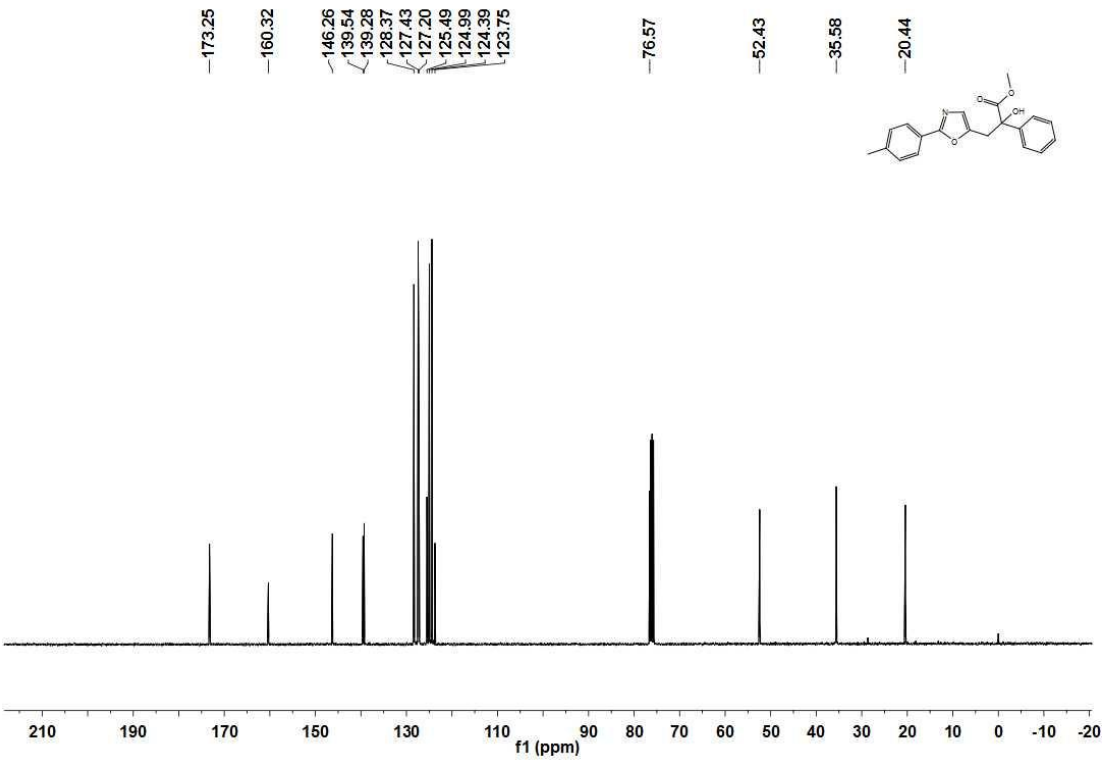
7.58
7.56
7.24
7.11
6.80
4.08
3.61
3.29
3.25
2.28
2.02
2.02
3.06
2.02
0.99
1.00
3.01
1.04
1.02
3.04
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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160.32
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139.54
139.28
128.37
127.43
127.20
125.49
124.99
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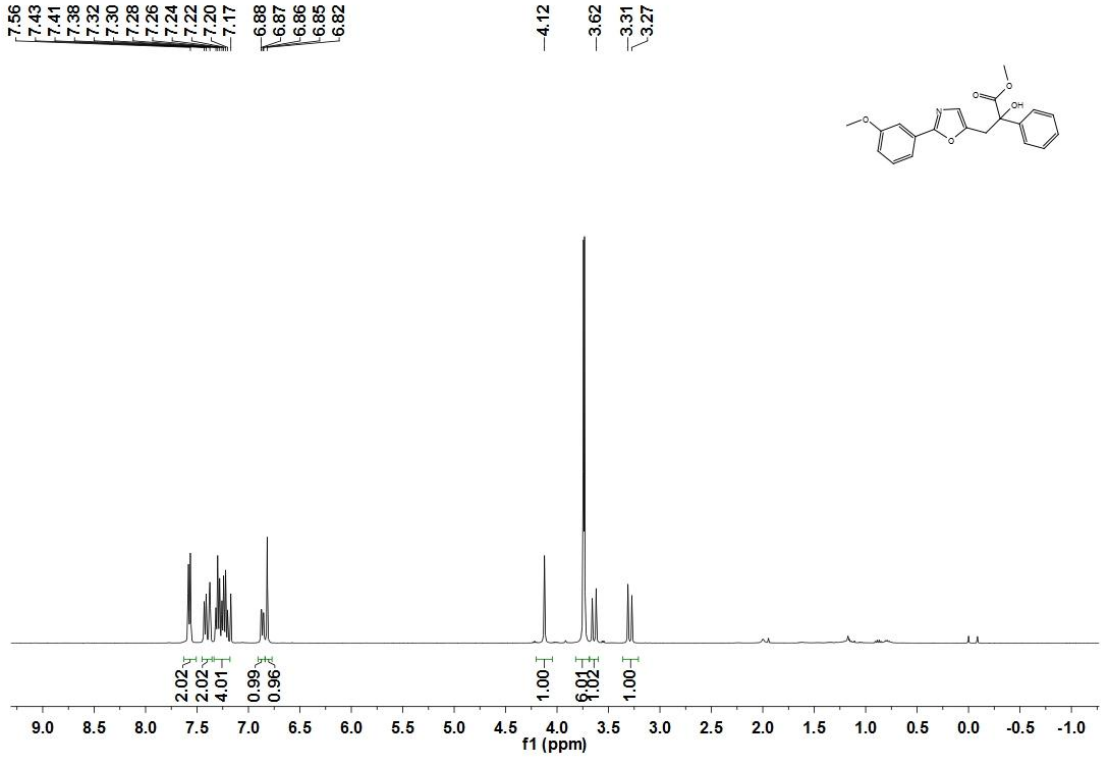
76.57
52.43
35.58
20.44
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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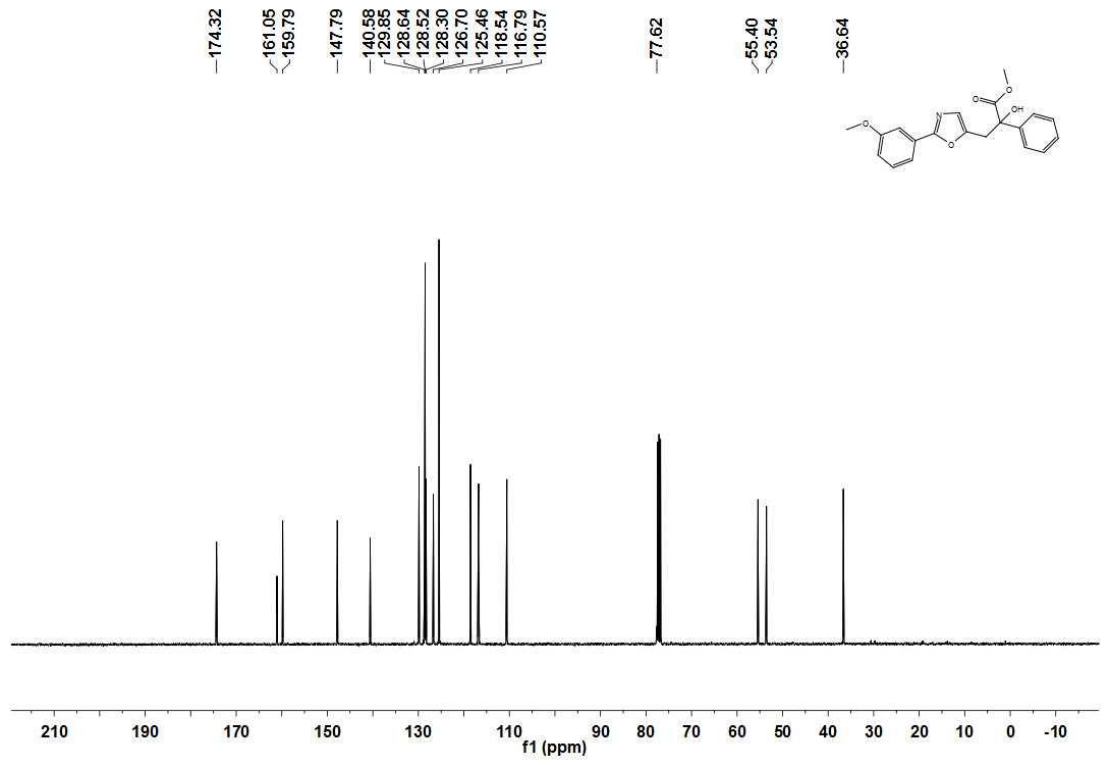
7.32
7.30
7.28
7.26
7.24
7.22
7.20
7.17
6.88
6.87
6.86
6.85
6.82
4.12
3.62
3.31
3.27
2.02
2.02
4.01
0.99
0.96
1.00
6.01
1.02
1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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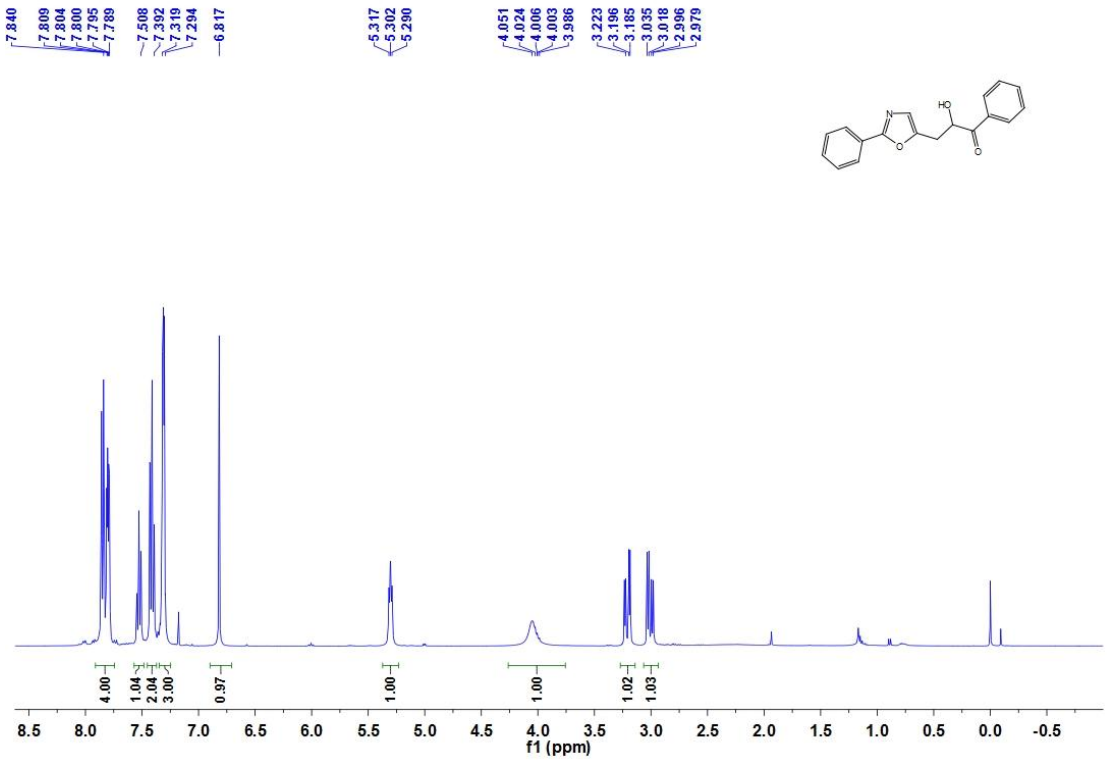
161.05
159.79
147.79
140.58
129.85
128.64
128.52
128.30
126.70
125.46
118.54
116.79
110.57
77.62
55.40
53.54
36.64
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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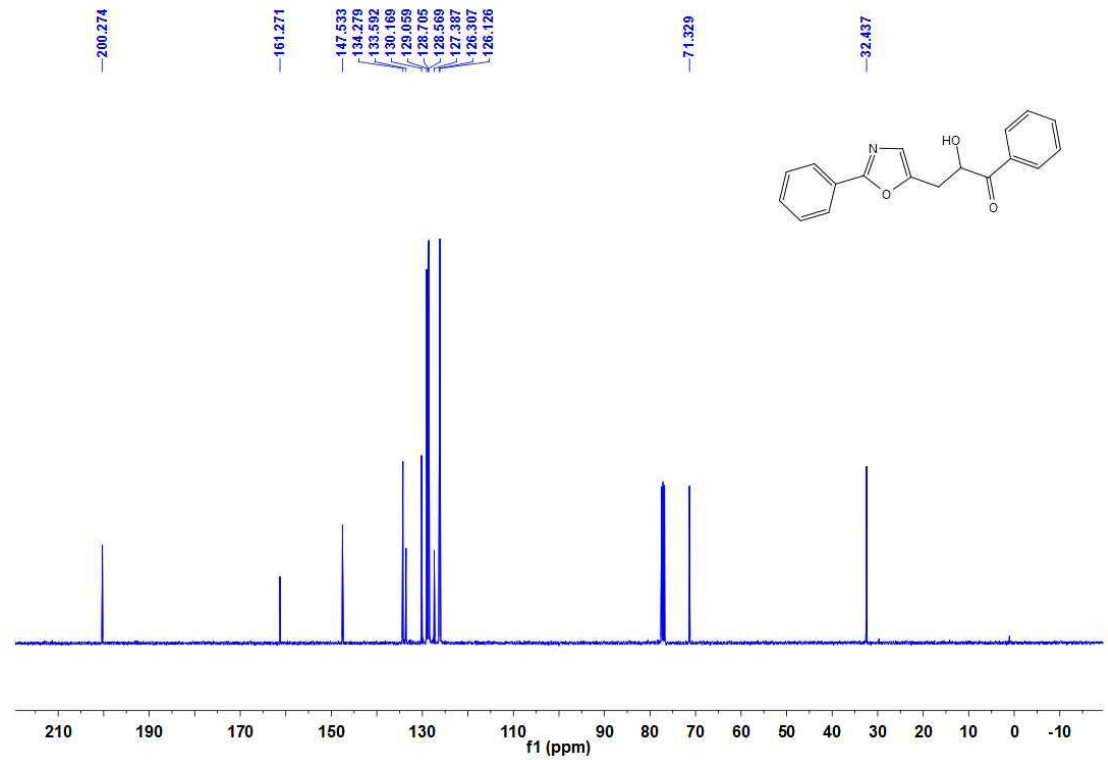
7.508
7.392
7.319
7.294
6.817
5.317
5.302
5.290
4.051
4.024
4.006
4.003
3.986
3.223
3.196
3.185
3.035
3.018
2.996
2.979
HO
N
O
O
4.00
1.04
2.04
3.00
0.97
1.00
1.00
1.02
1.03
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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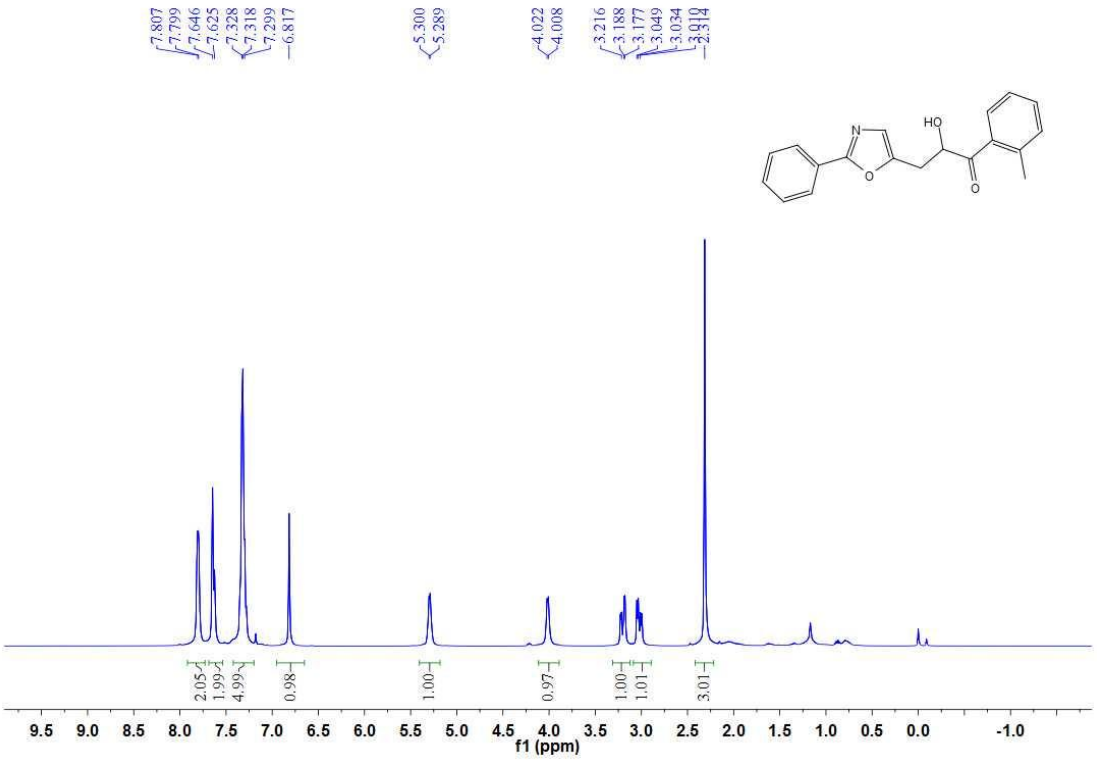
161.271
147.533
134.279
133.592
130.169
129.059
128.705
128.569
127.387
126.307
126.126
71.329
32.437
HO
N
O
O
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.799
7.646
7.625
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7.318
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6.817
5.300
5.289
4.022
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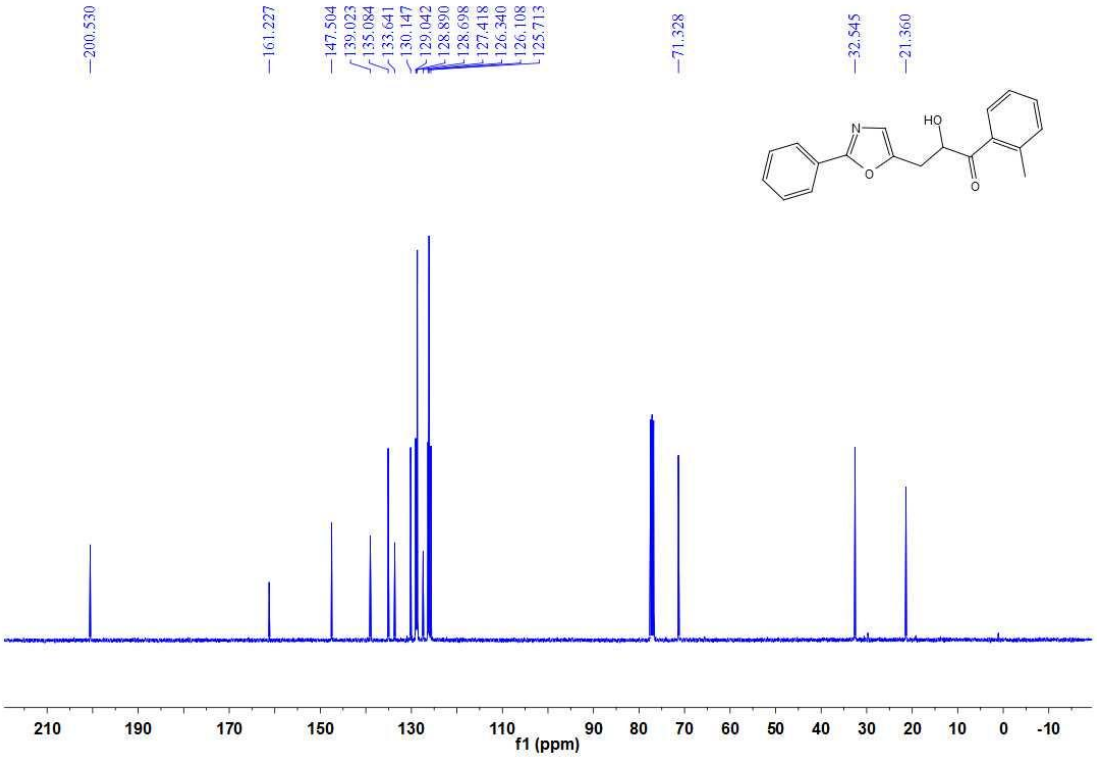
3.216
3.188
3.177
3.049
3.034
2.914
HO
N
O
O
2.05
1.99
4.99
0.98
1.00
0.97
1.00
1.01
3.01
f1 (ppm)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130.147
129.042
128.890
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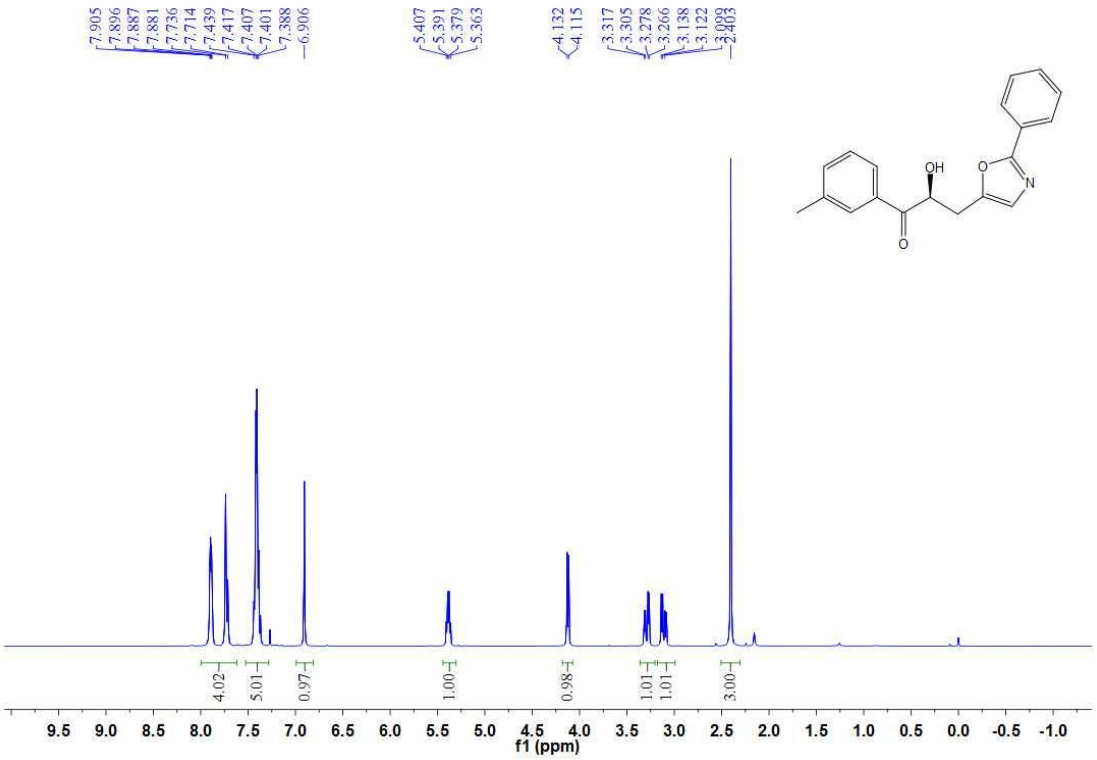
126.108
125.713
71.328
32.545
21.360
HO
N
O
O
f1 (ppm)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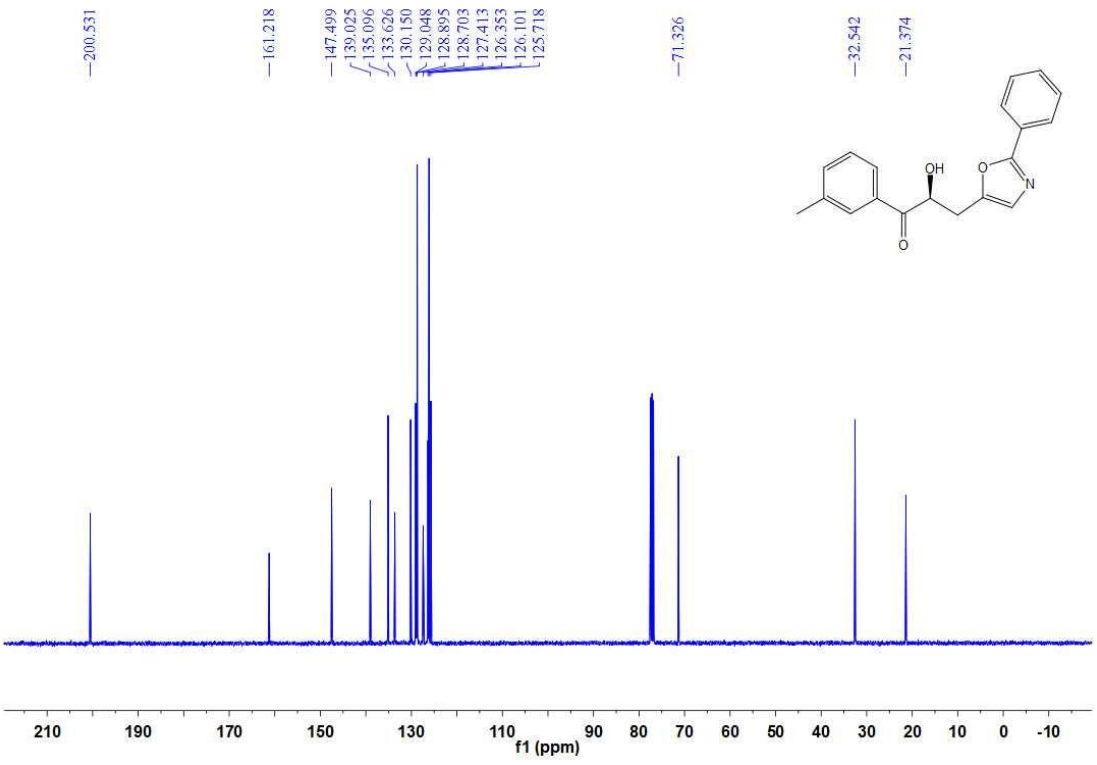
7.896
7.887
7.881
7.736
7.714
7.439
7.417
7.407
7.401
7.388
6.906
5.407
5.391
5.379
5.363
4.132
4.115
3.317
3.305
3.278
3.266
3.138
3.122
3.099
2.403
OH
O
N
O
4.02
5.01
0.97
1.00
0.98
1.01
1.01
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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135.096
133.626
130.150
129.048
128.895
128.703
127.413
126.353
126.101
125.718
71.326
32.542
21.374
OH
O
N
O
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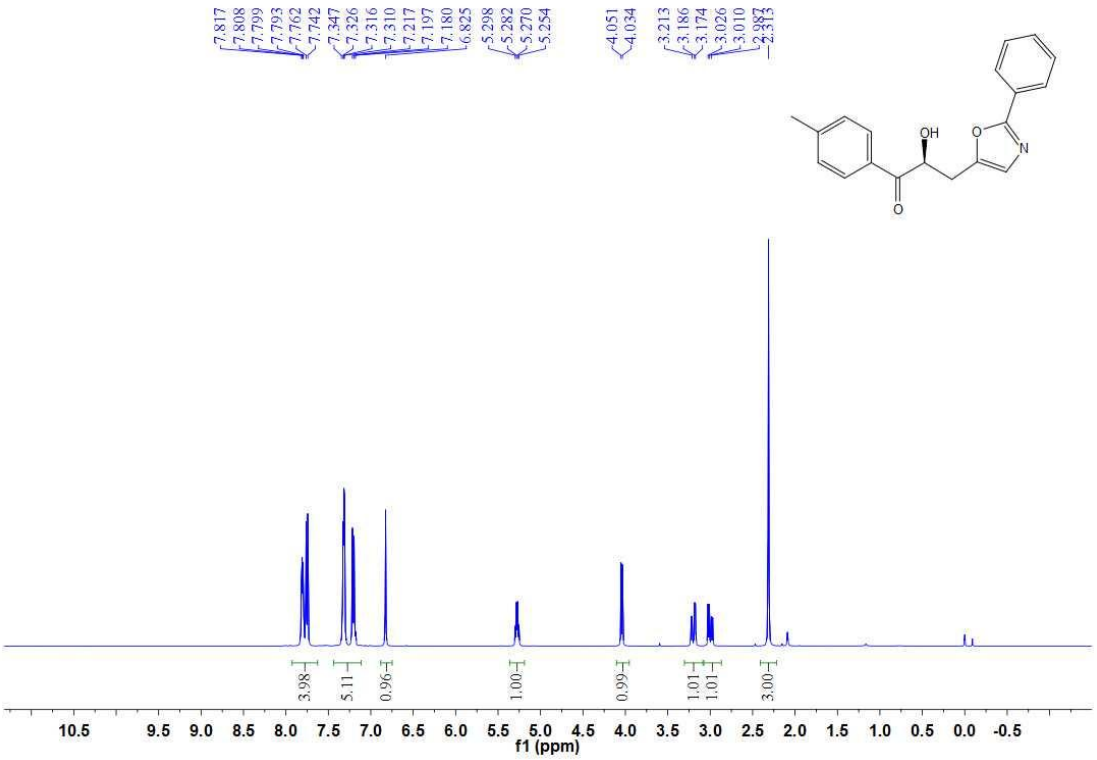
f1 (ppm)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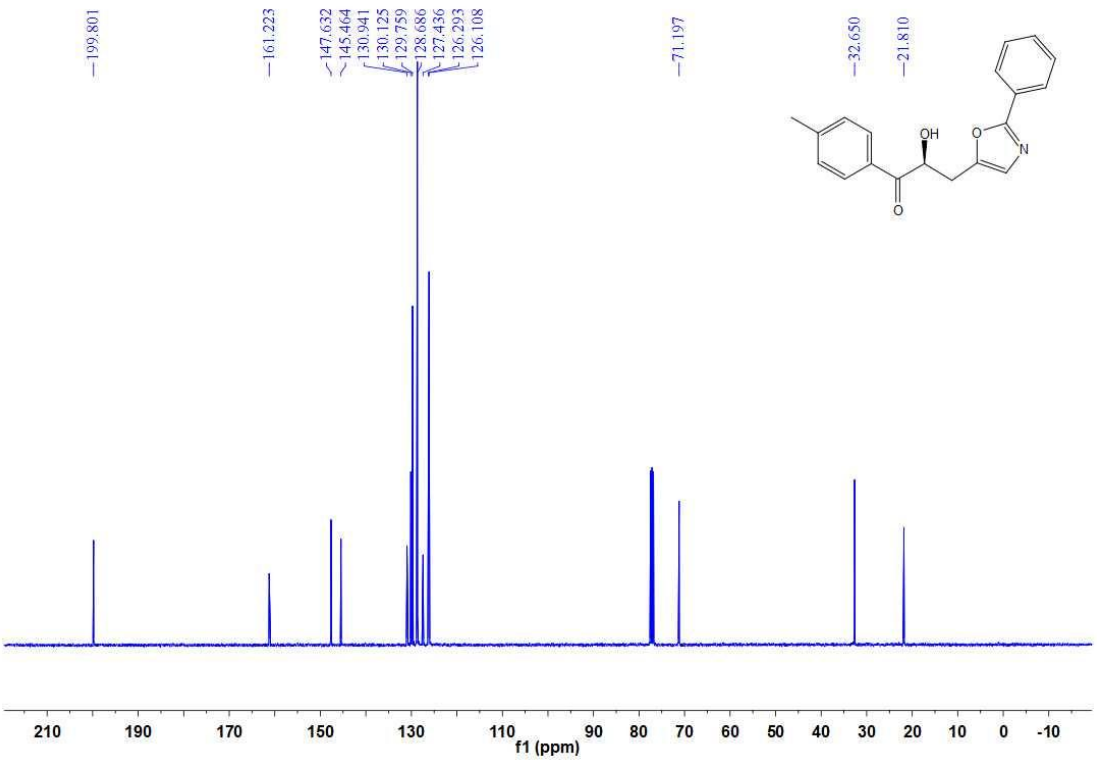
7.808
7.799
7.793
7.762
7.742
7.347
7.326
7.316
7.310
7.217
7.197
7.180
6.825
5.298
5.282
5.270
5.254
4.051
4.034
3.213
3.186
3.174
3.026
3.010
2.987
2.313
OH
O
N
O
3.98
5.11
0.96
1.00
0.99
1.01
1.01
3.00
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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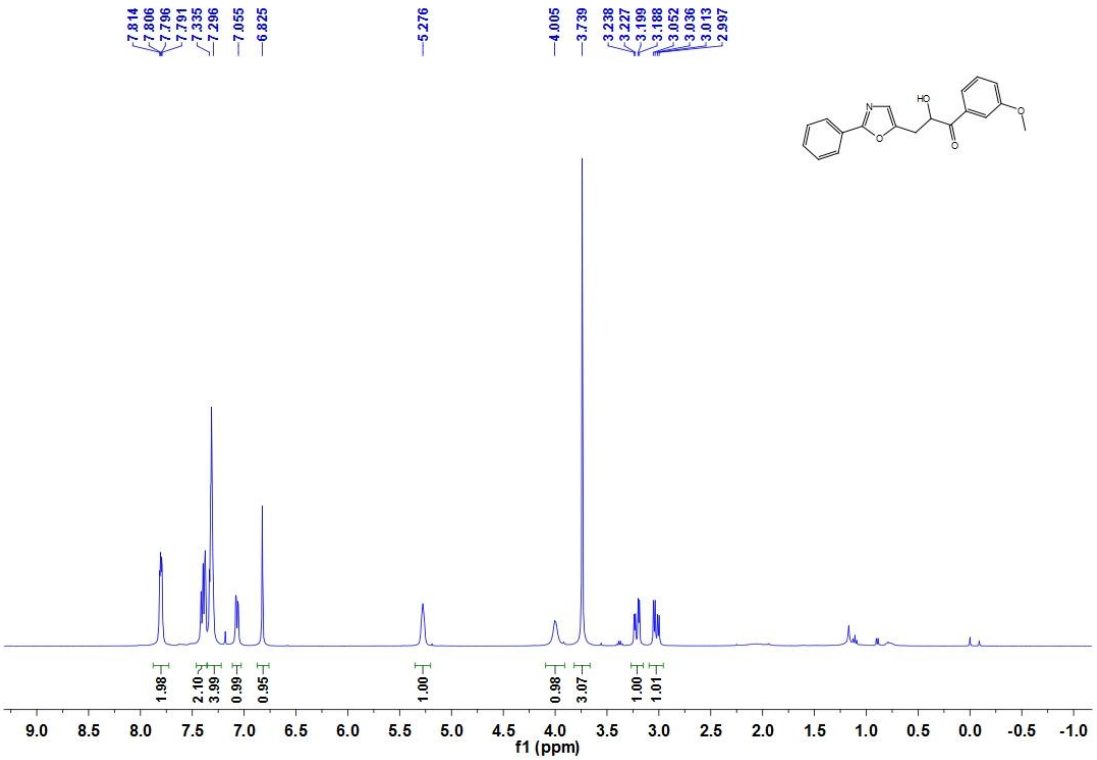
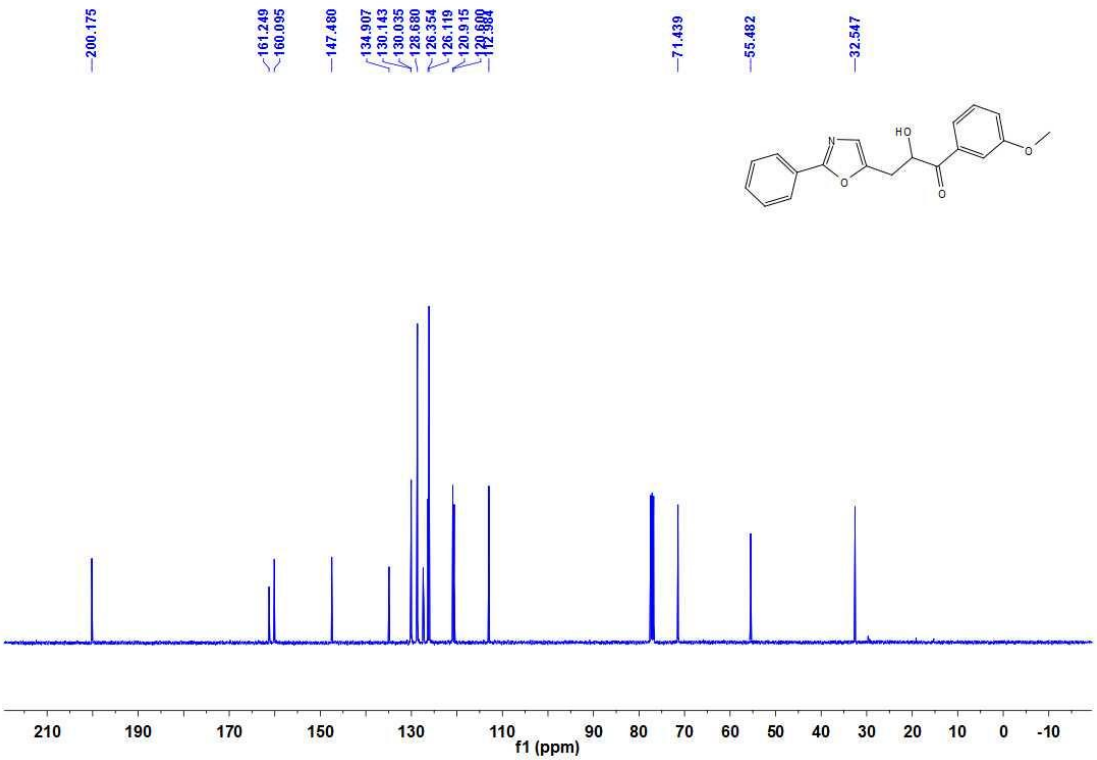
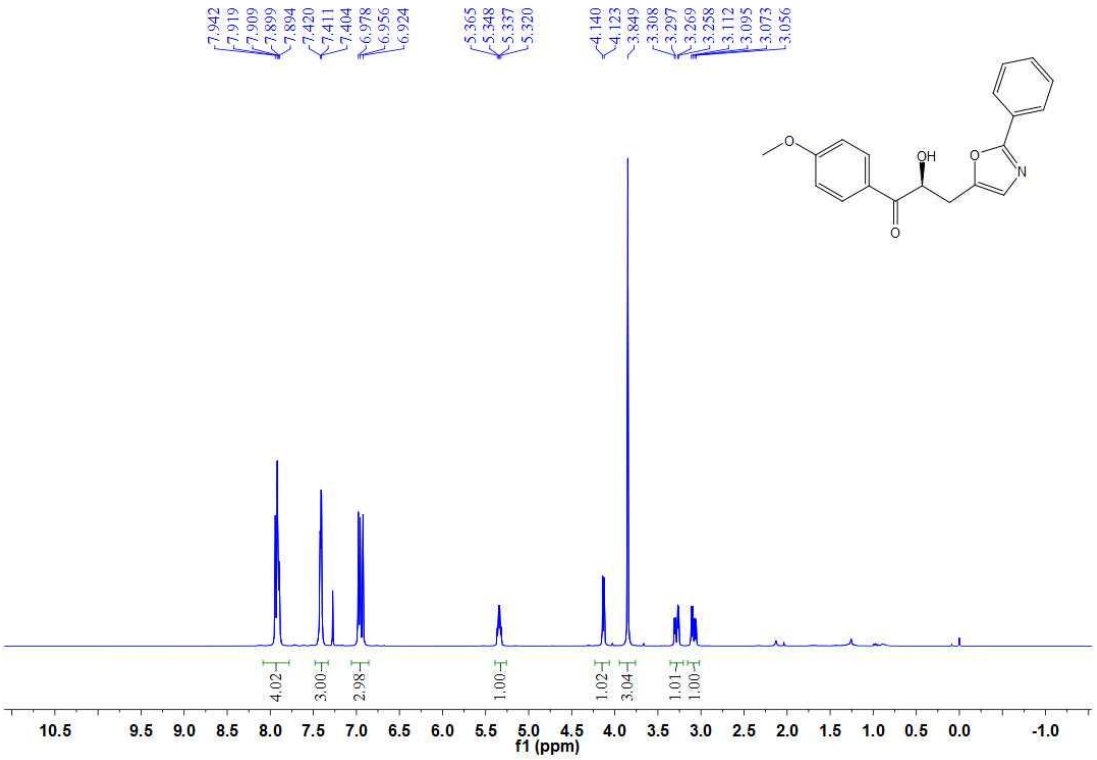
161.223
147.632
145.464
130.941
130.125
129.759
128.686
127.436
126.293
126.108
71.197
32.650
21.810
OH
O
N
O
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.814
7.806
7.796
7.791
7.335
7.296
7.055
6.825
5.276
4.005
3.739
3.238
3.227
3.199
3.188
3.052
3.036
3.013
2.997
HO
N
O
O
O
1.98
2.10
3.99
0.99
0.95
1.00
0.98
3.07
1.00
1.01
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


200.175
161.249
160.095
147.480
134.907
130.143
130.035
128.680
126.354
126.119
120.915
120.600
112.984
71.439
55.482
32.547
HO
N
O
O
O
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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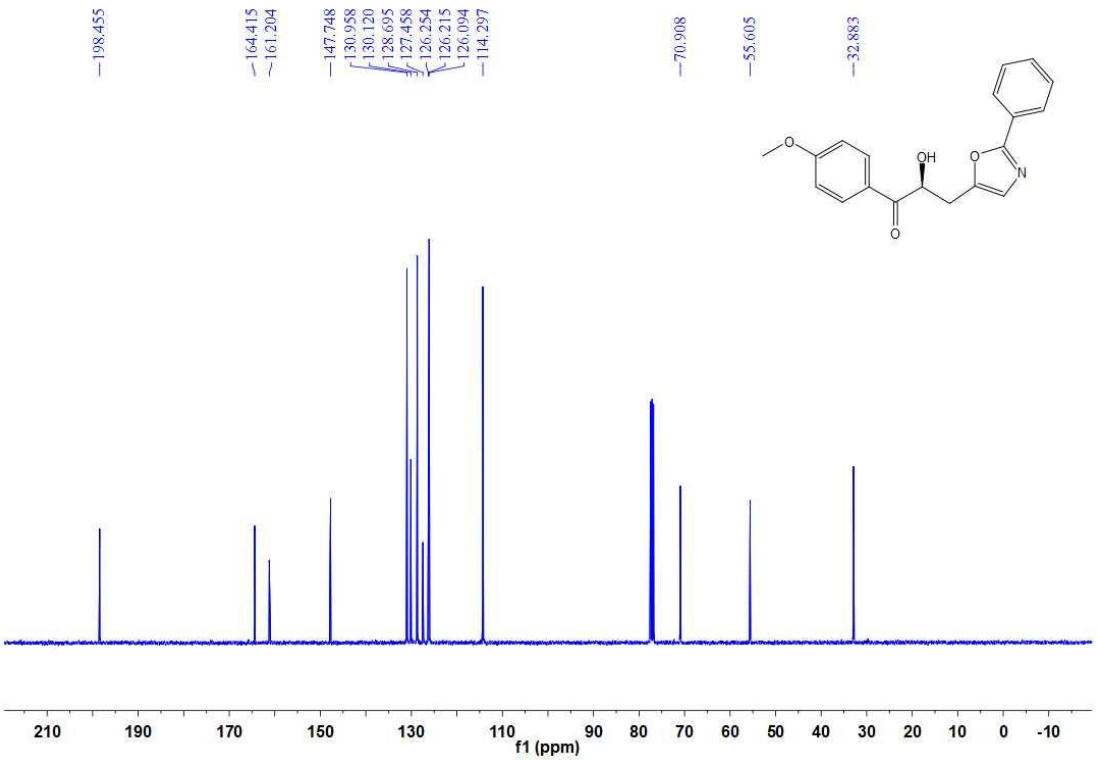
7.919
7.909
7.899
7.894
7.420
7.411
7.404
6.978
6.956
6.924
5.365
5.348
5.337
5.320
4.140
4.123
3.849
3.308
3.297
3.269
3.258
3.112
3.095
3.073
3.056
OH
O
N
4.02
3.00
2.98
1.00
1.02
3.04
1.01
1.00
f1 (ppm)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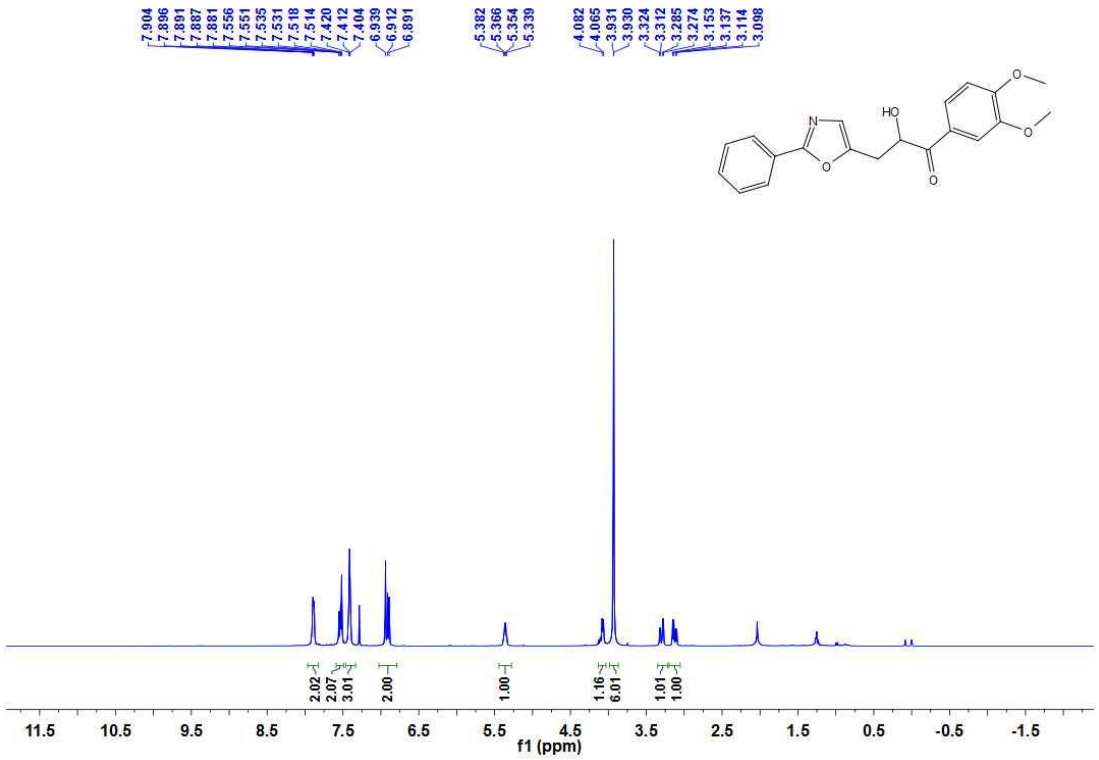
164.415
161.204
147.748
130.958
130.120
128.695
127.458
126.254
126.215
126.094
114.297
70.908
55.605
32.883
OH
O
N
f1 (ppm)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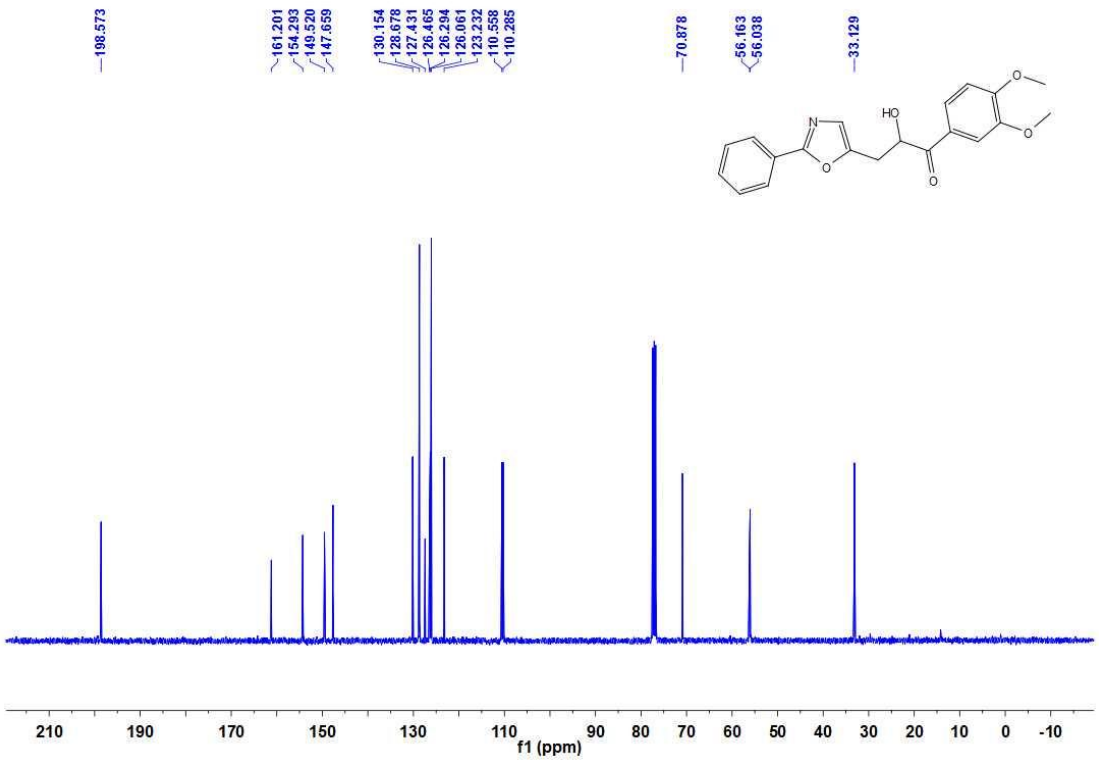
7.896
7.891
7.887
7.881
7.556
7.551
7.535
7.531
7.518
7.514
7.420
7.412
7.404
6.939
6.912
6.891
5.382
5.366
5.354
5.339
4.082
4.065
3.931
3.930
3.324
3.312
3.285
3.274
3.153
3.137
3.114
3.098
HO
N
O
O
O
O
2.02
2.07
3.01
2.00
1.00
1.16
6.01
1.01
1.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
f1 (ppm)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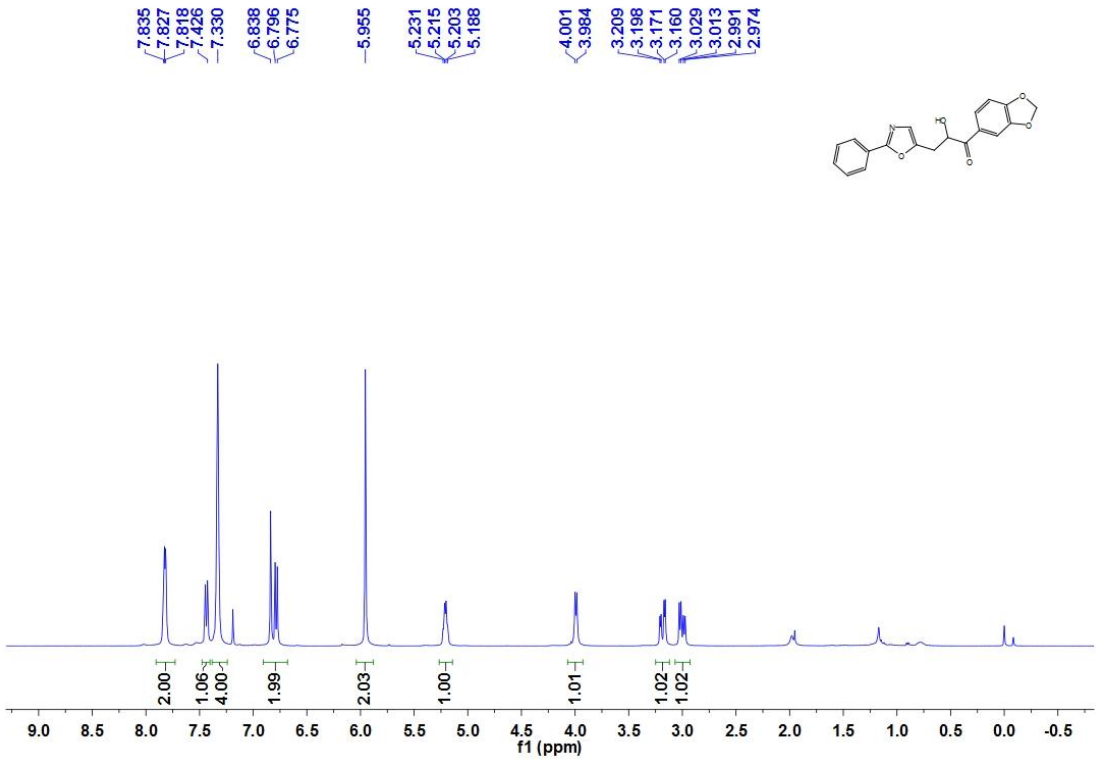
149.520
147.659
130.154
128.678
127.431
126.465
126.294
126.061
123.232
110.558
110.285
70.878
56.163
56.038
33.129
HO
N
O
O
O
O
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.827
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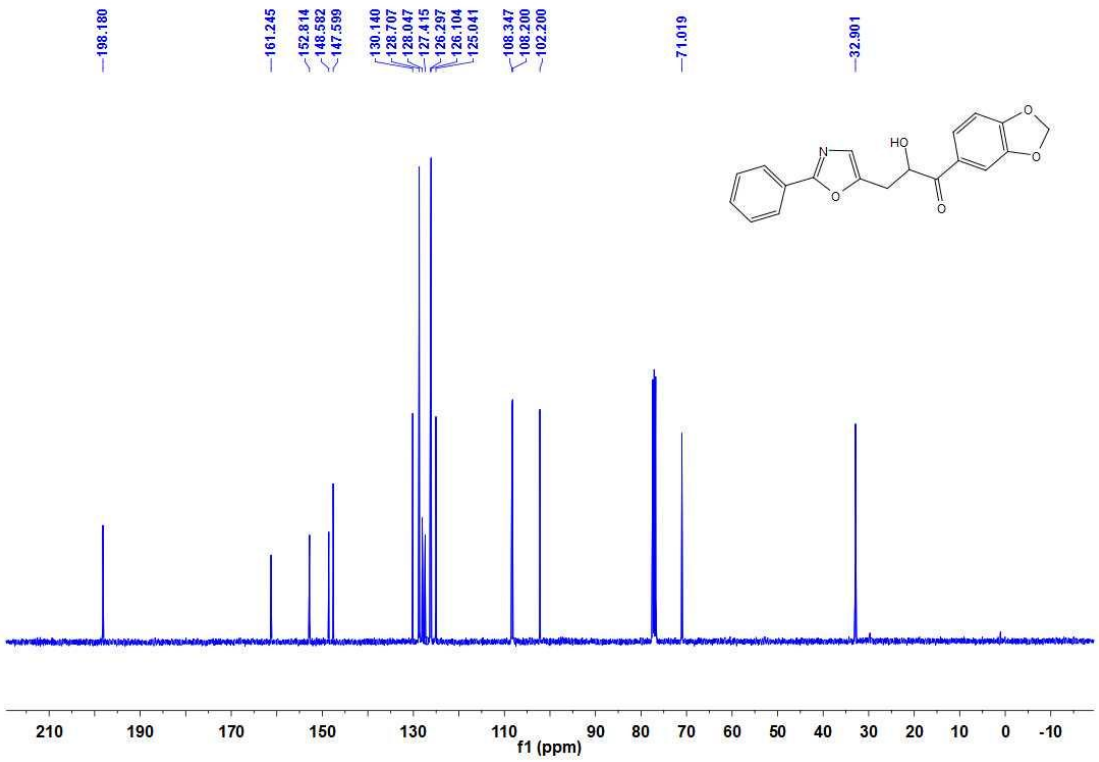
7.426
7.330
6.838
6.796
6.775
5.955
5.231
5.215
5.203
5.188
4.001
3.984
3.209
3.198
3.171
3.160
3.029
3.013
2.991
2.974
HO
O
O
O
N
O
2.00
1.06
4.00
1.99
2.03
1.00
1.01
1.02
1.02
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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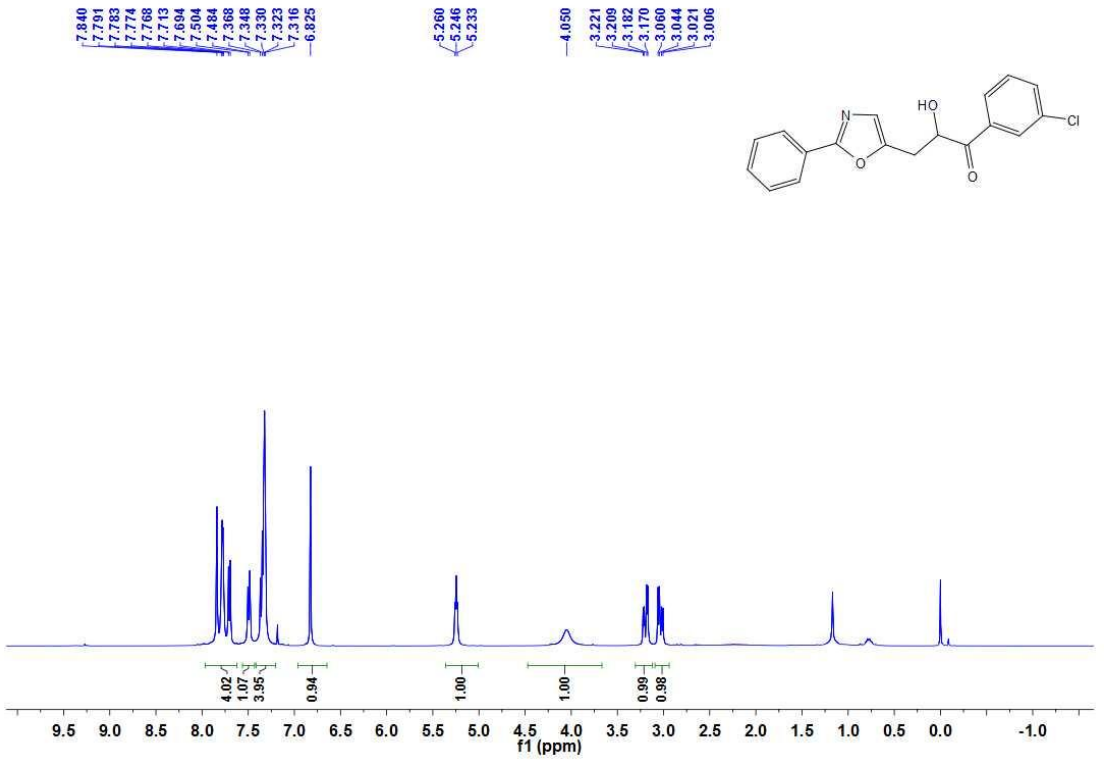
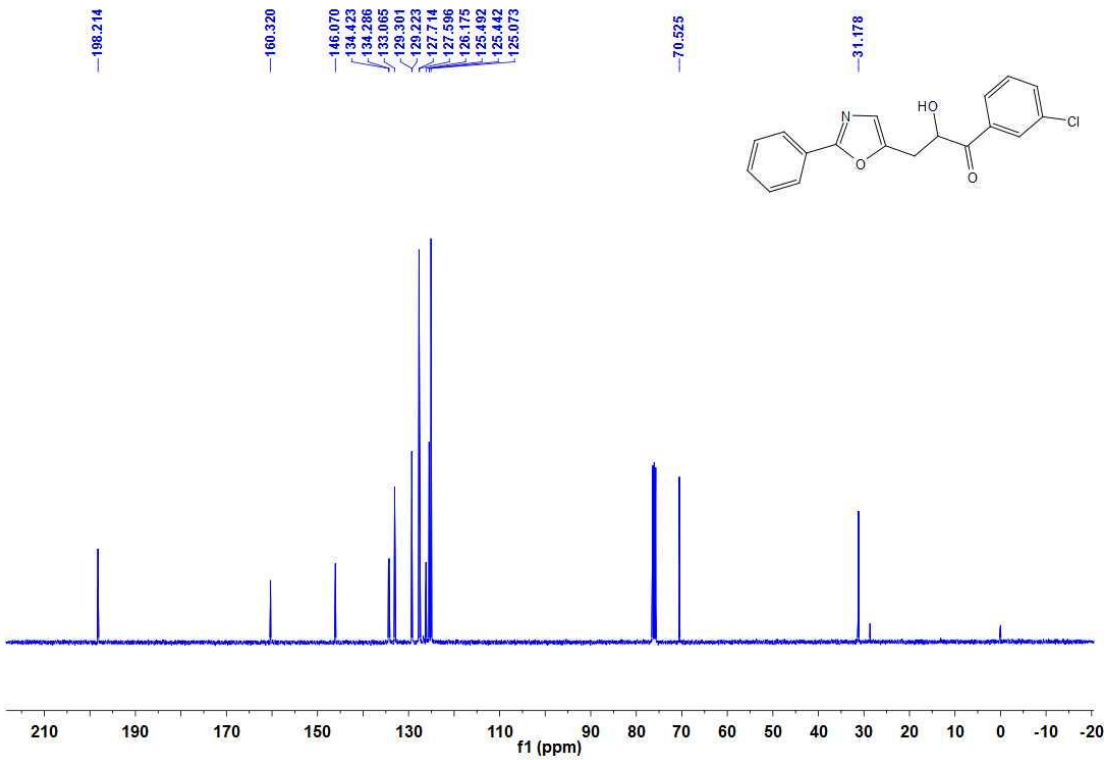
128.707
128.047
127.415
126.297
126.104
125.041
108.347
108.200
102.200
71.019
32.901
HO
N
O
O
O
O
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.840
7.791
7.783
7.774
7.768
7.713
7.694
7.504
7.484
7.368
7.348
7.330
7.323
7.316
6.825
5.260
5.246
5.233
4.050
3.221
3.209
3.182
3.170
3.060
3.044
3.021
3.006
HO
Cl
N
O
O
4.02
1.07
3.95
0.94
1.00
1.00
0.99
0.98
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -1.0
f1 (ppm)


198.214
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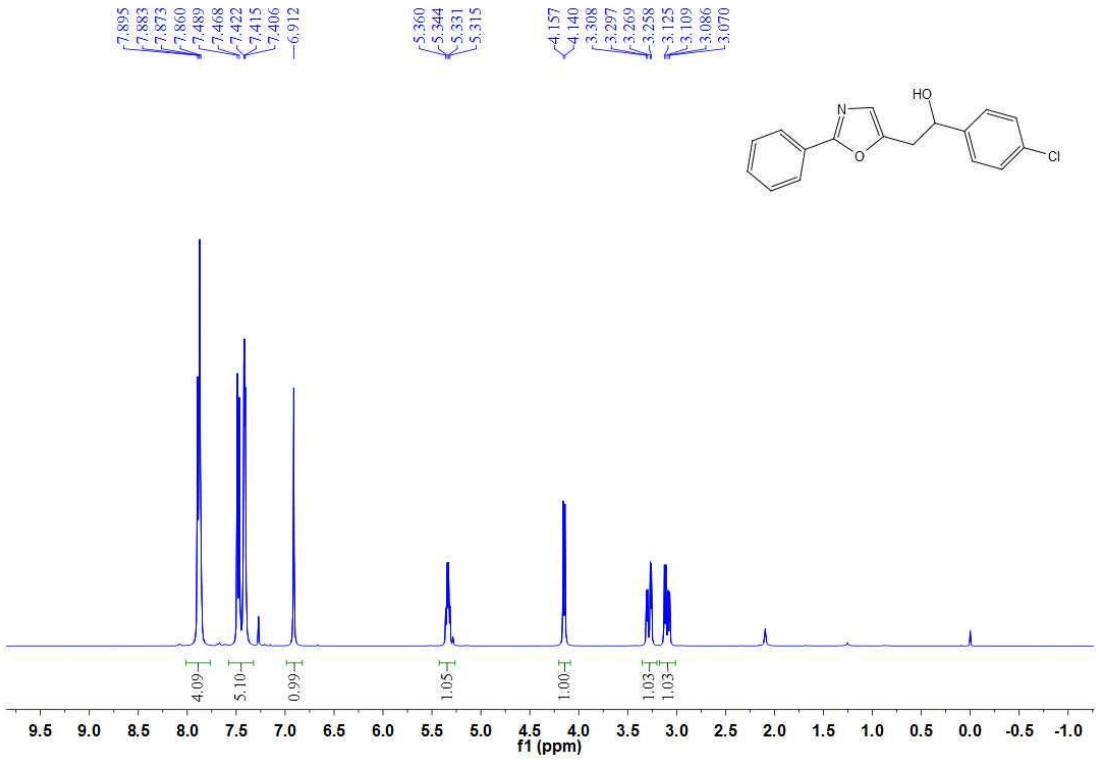
146.070
134.423
134.286
133.065
129.301
129.223
127.714
127.596
126.175
125.492
125.442
125.073
70.525
31.178
HO
Cl
N
O
O
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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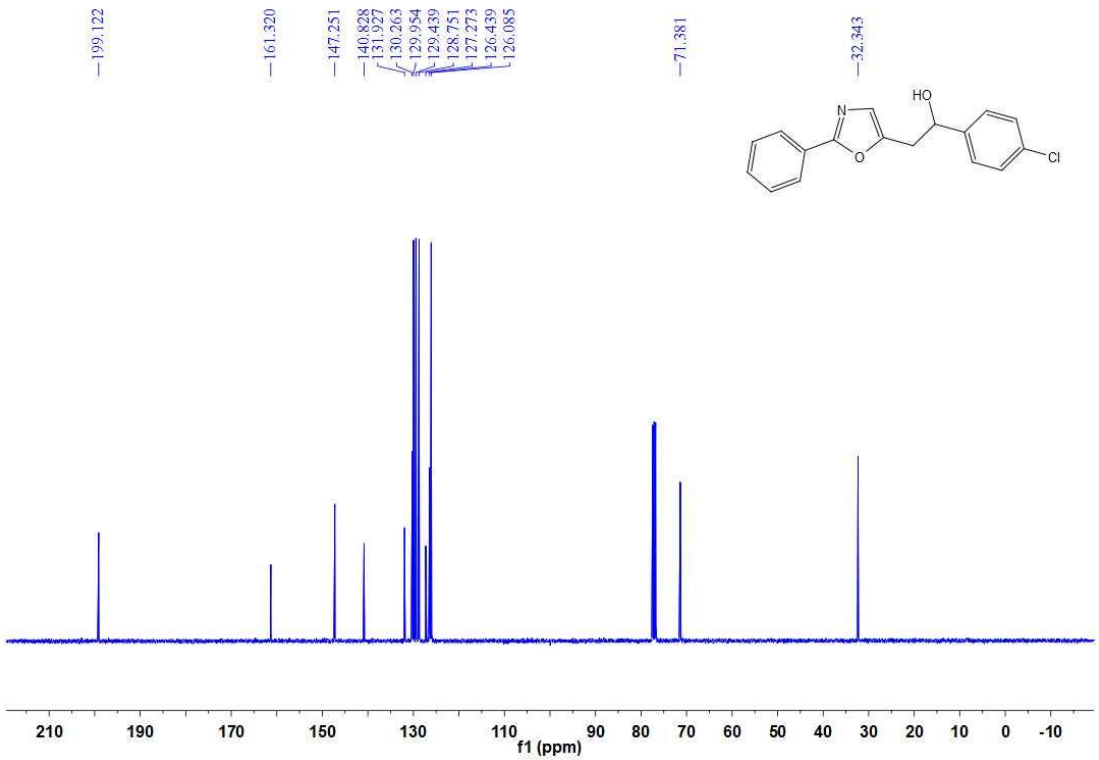
7.873
7.860
7.489
7.468
7.422
7.415
7.406
6.912
5.360
5.344
5.331
5.315
4.157
4.140
3.308
3.297
3.269
3.258
3.125
3.109
3.086
3.070
HO
N
O
Cl
4.09
5.10
0.99
1.05
1.00
1.03
1.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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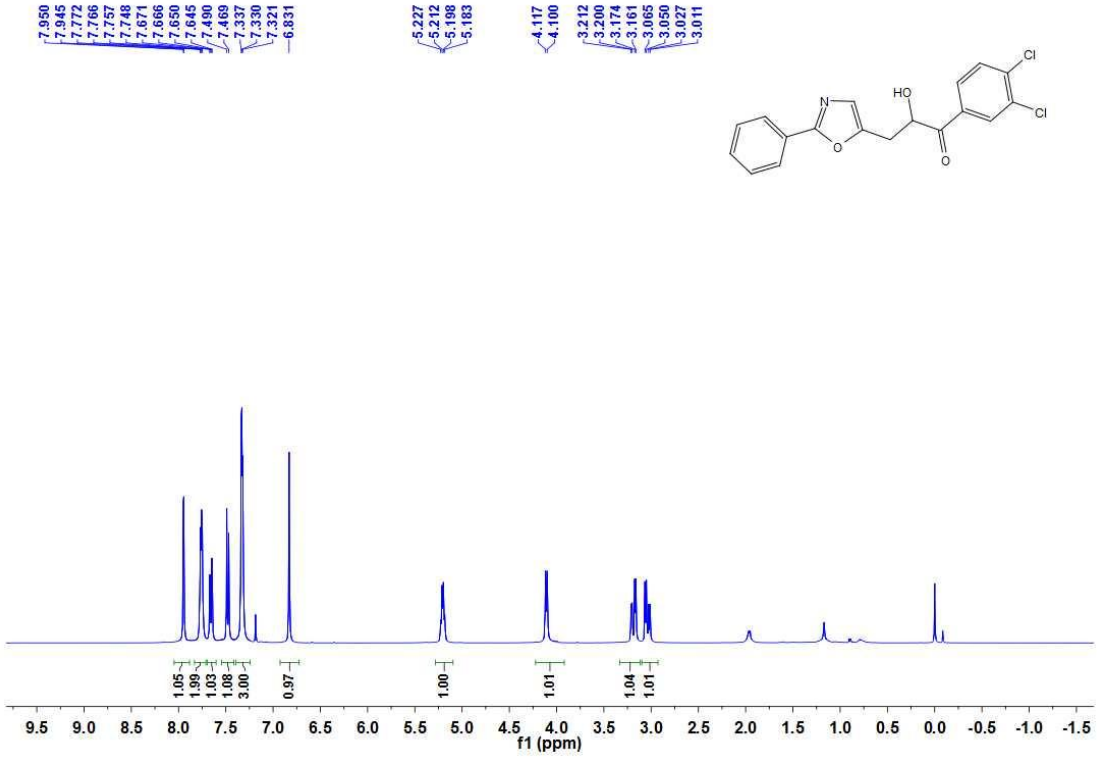
161.320
147.251
140.828
131.927
130.263
129.954
129.439
128.751
127.273
126.439
126.085
71.381
32.343
HO
N
O
Cl
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.772
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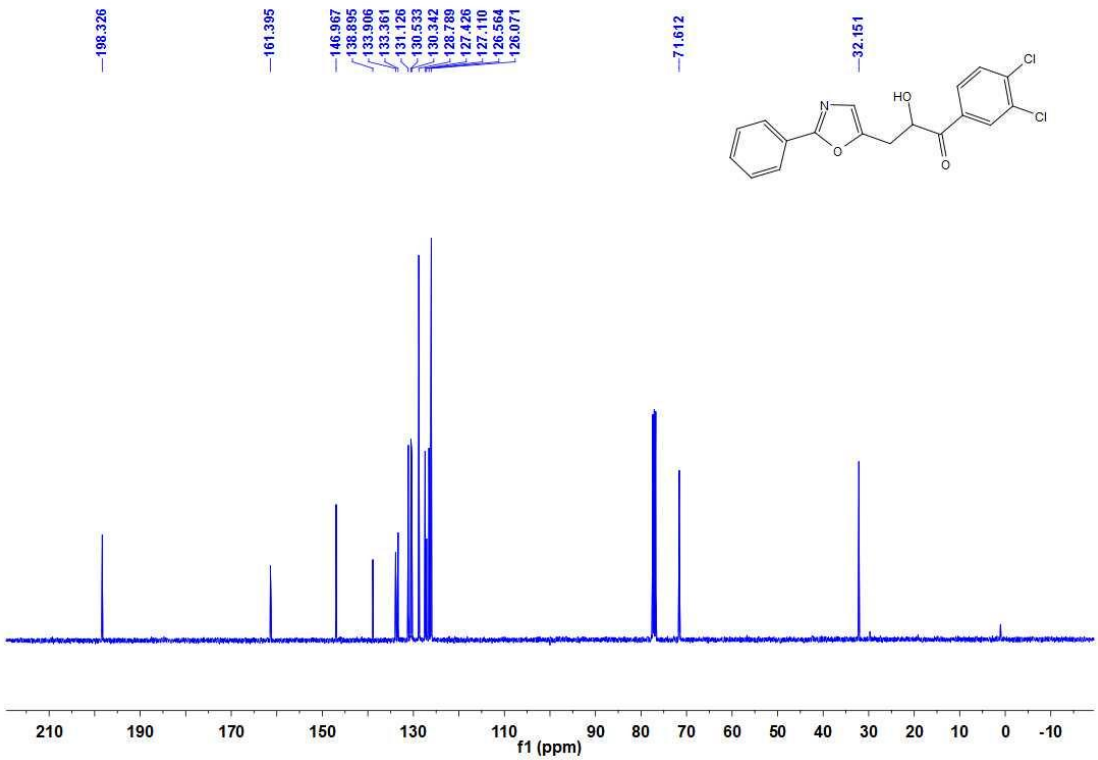
7.748
7.671
7.666
7.650
7.645
7.490
7.469
7.337
7.330
7.321
6.831
5.227
5.212
5.198
5.183
4.117
4.100
3.212
3.200
3.174
3.161
3.065
3.050
3.027
3.011
Cl
Cl
HO
N
O
O
1.05
1.99
1.03
1.08
3.00
0.97
1.00
1.01
1.04
1.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)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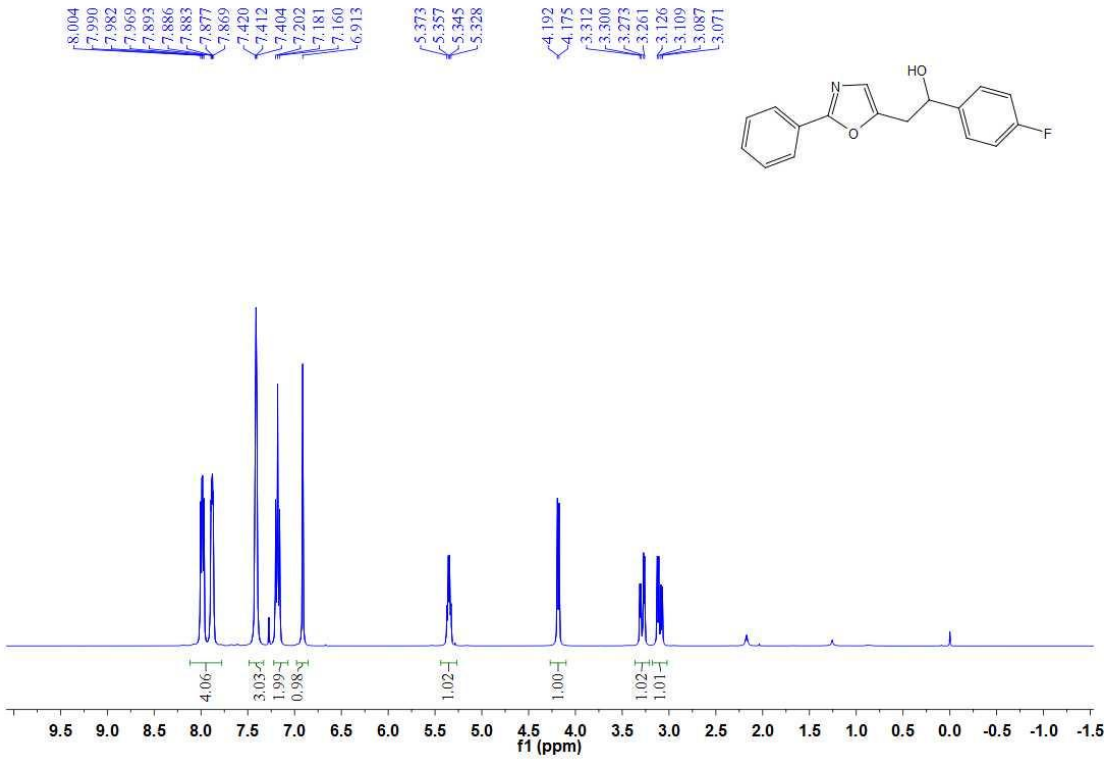
131.126
130.533
130.342
128.789
127.426
127.110
126.564
126.071
71.612
32.151
Cl
Cl
HO
N
O
O
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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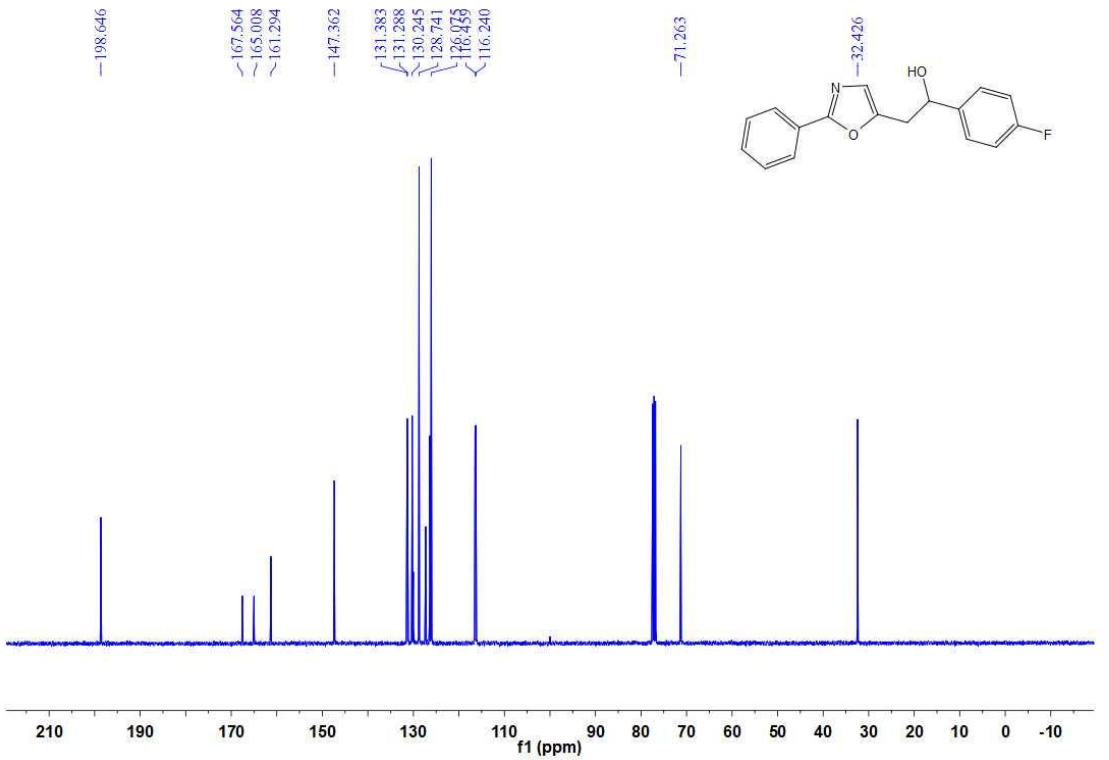
7.883
7.877
7.869
7.420
7.412
7.404
7.202
7.181
7.160
6.913
5.373
5.357
5.345
5.328
4.192
4.175
3.312
3.300
3.273
3.261
3.126
3.109
3.087
3.071
HO
N
O
F
4.06
3.03
1.99
0.98
1.02
1.00
1.02
1.01
f1 (ppm)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161.294
147.362
131.383
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130.245
128.741
126.075
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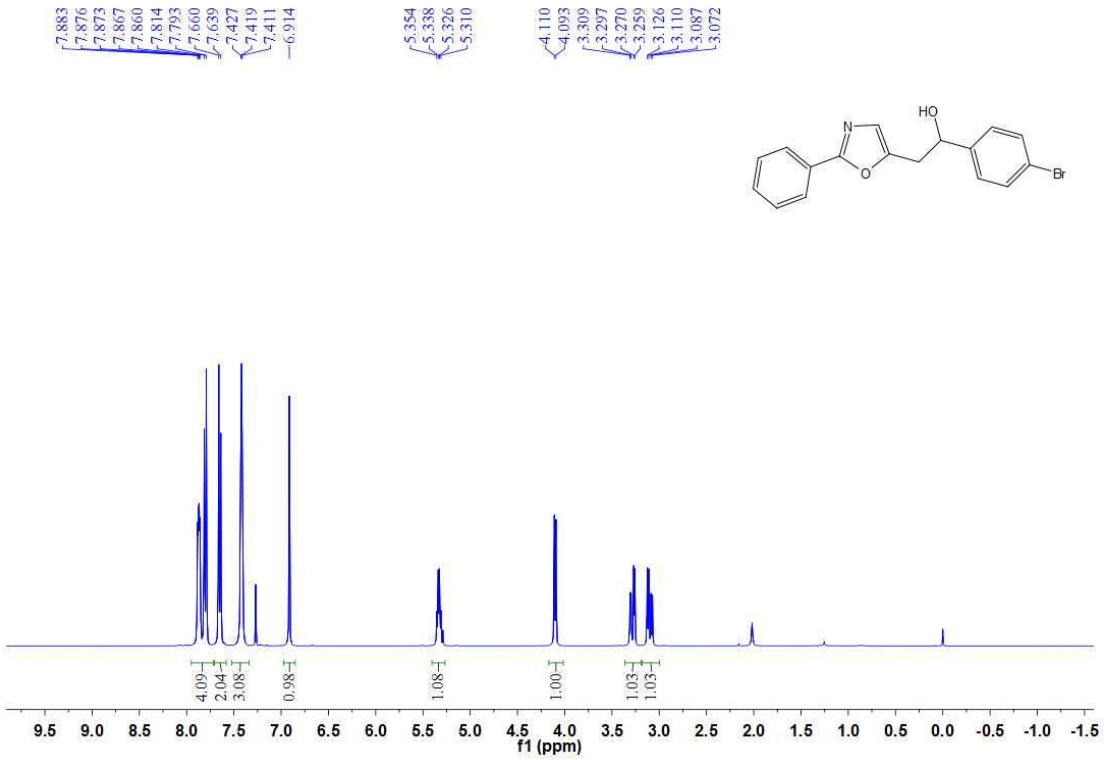
116.240
71.263
32.426
HO
N
O
F
f1 (ppm)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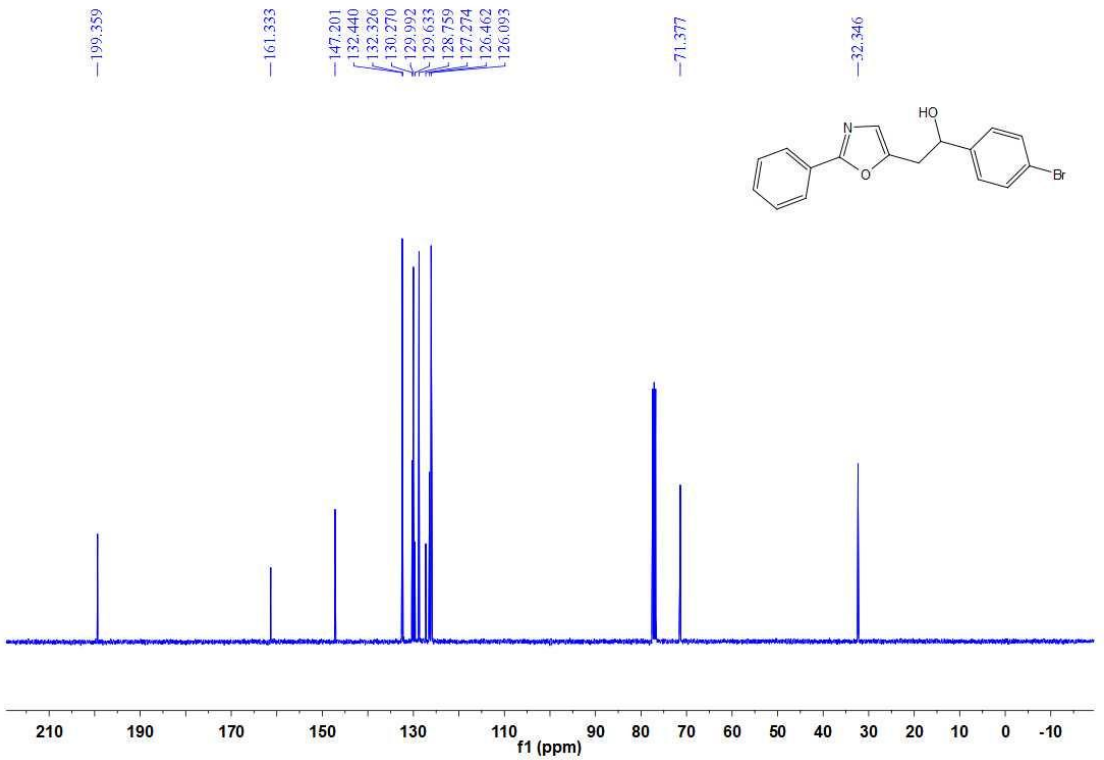
7.419
7.411
6.914
5.354
5.338
5.326
5.310
4.110
4.093
3.309
3.297
3.270
3.259
3.126
3.110
3.087
3.072
HO
N
O
Br
4.09
2.04
3.08
0.98
1.08
1.00
1.03
1.03
f1 (ppm)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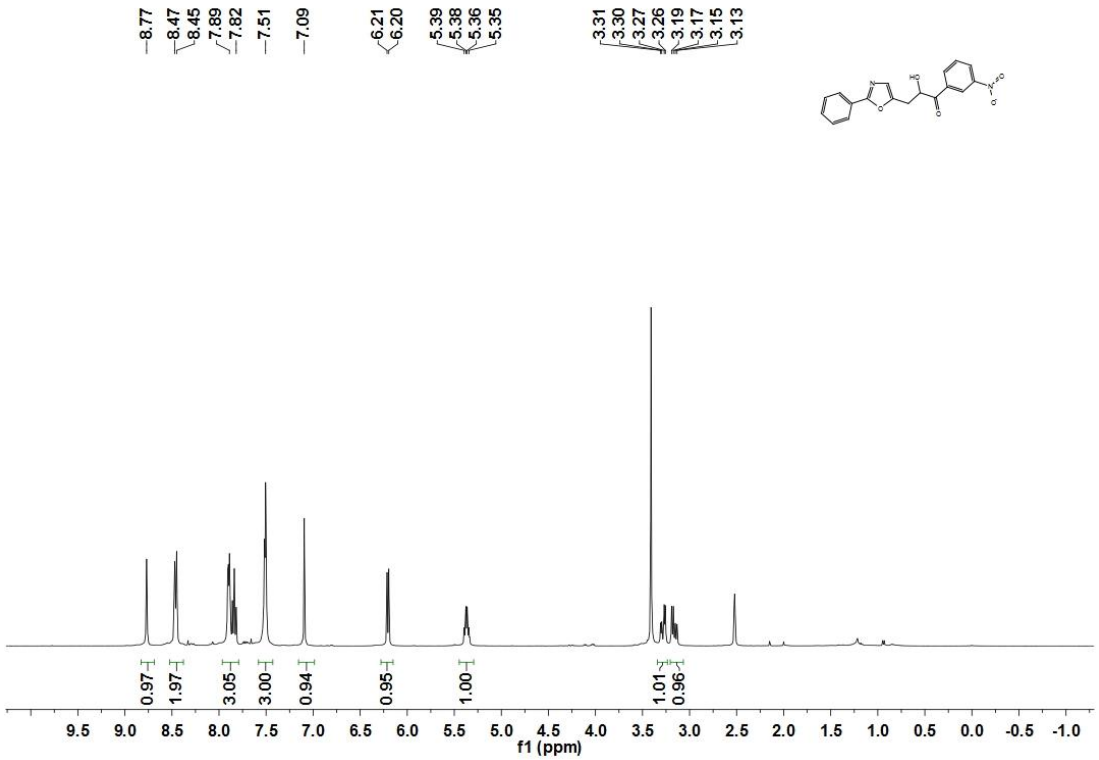
161.333
147.201
132.440
132.326
130.270
129.992
129.633
128.759
127.274
126.462
126.093
71.377
32.346
HO
N
O
Br
f1 (ppm)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8.47
8.45
7.89
7.82
7.51
7.09
6.21
6.20
5.39
5.38
5.36
5.35
3.31
3.30
3.27
3.26
3.19
3.17
3.15
3.13
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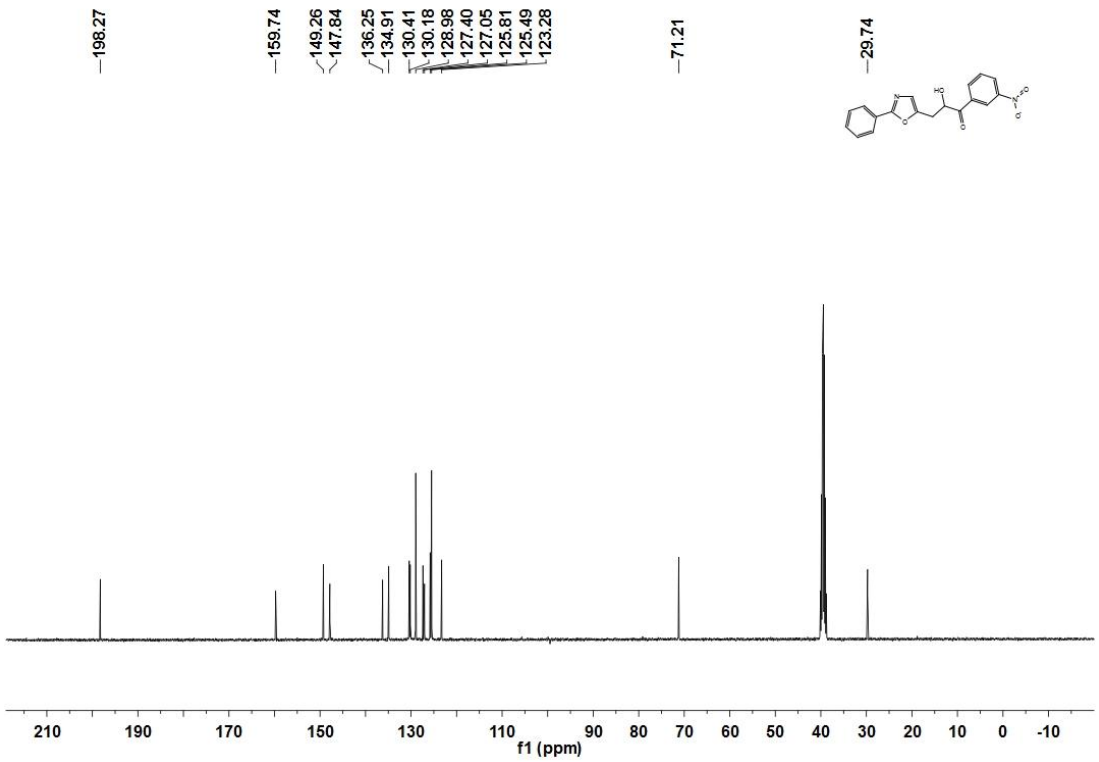
1.97
3.05
3.00
0.94
0.95
1.00
1.01
0.96
f1 (ppm)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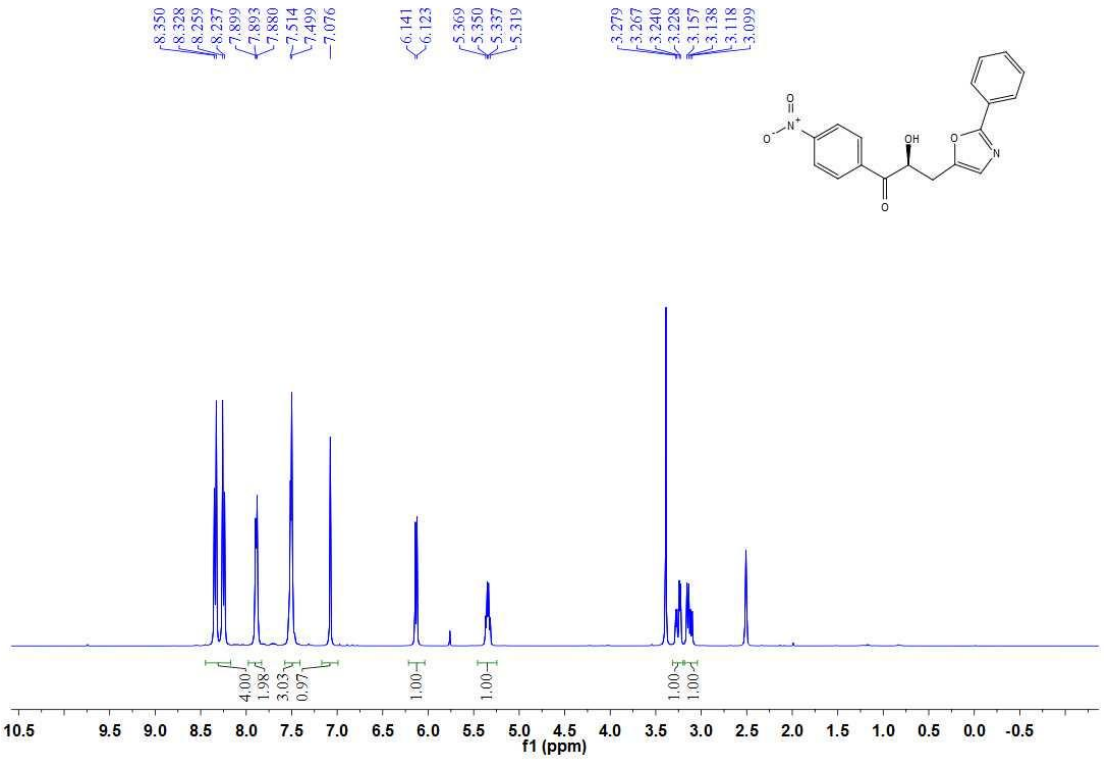
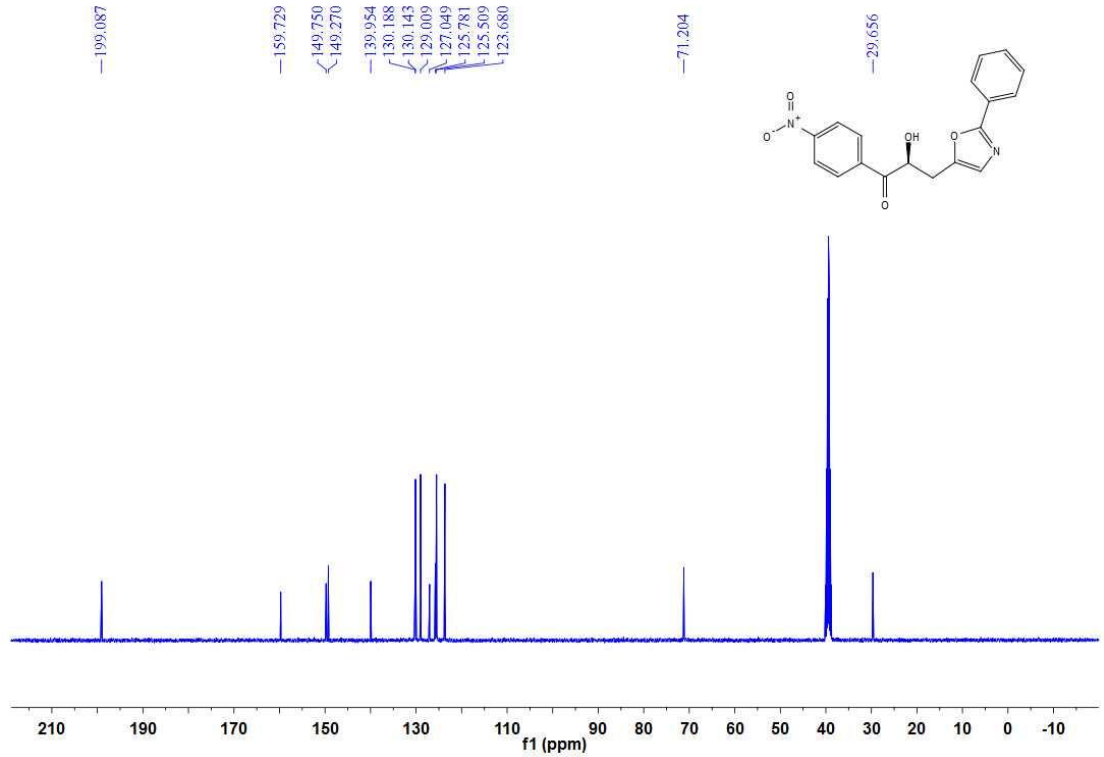
149.26
147.84
136.25
134.91
130.41
130.18
128.98
127.40
127.05
125.81
125.49
123.28
71.21
29.74
f1 (ppm)


8.350
8.328
8.259
8.237
7.899
7.893
7.880
7.514
7.499
7.076
6.141
6.123
5.369
5.350
5.337
5.319
3.279
3.267
3.240
3.228
3.157
3.138
3.118
3.099
OH
4.00
1.98
3.03
0.97
1.00
1.00
1.00
1.00
f1 (ppm)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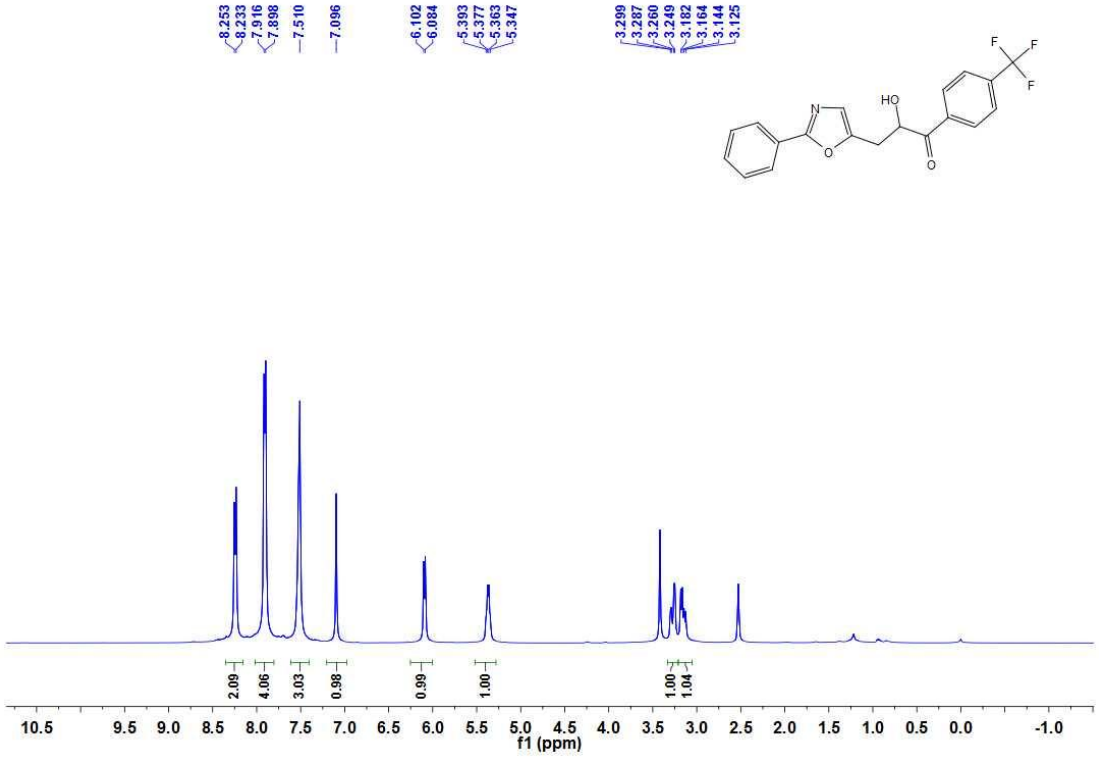
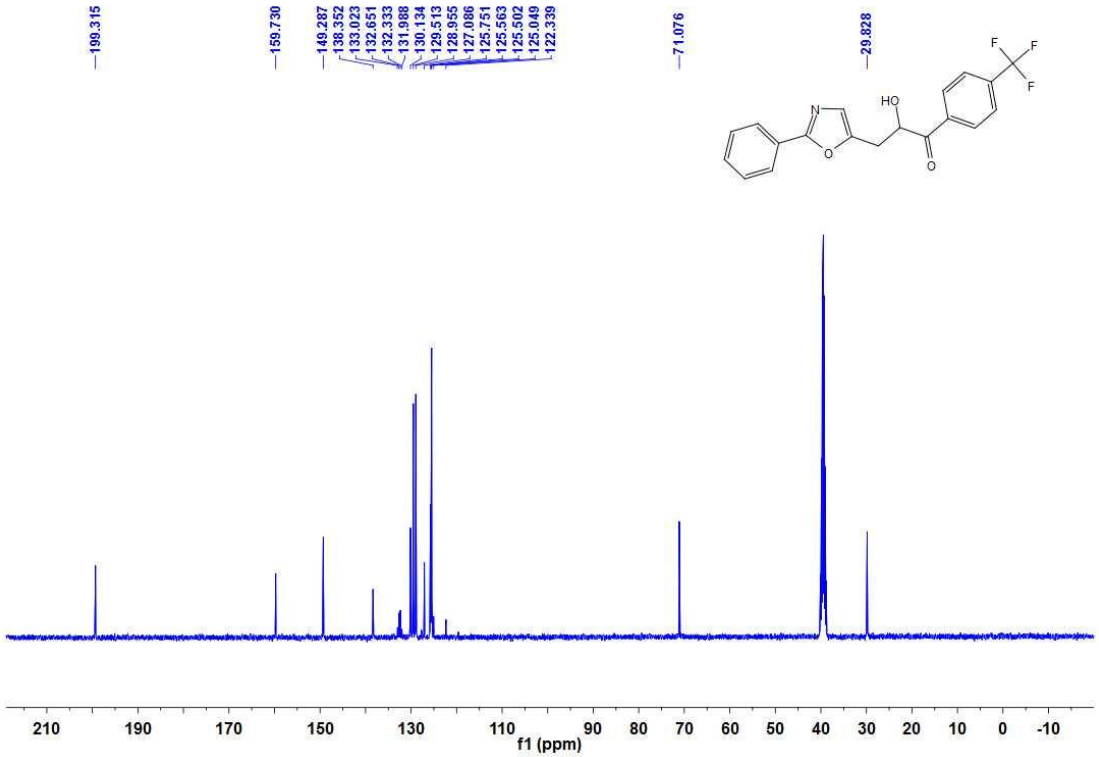
149.750
149.270
139.954
130.188
130.143
129.009
127.049
125.781
125.509
123.680
71.204
29.656
OH
f1 (ppm)


8.253
8.233
7.916
7.898
7.510
7.096
6.102
6.084
5.393
5.377
5.363
5.347
3.299
3.287
3.260
3.249
3.182
3.164
3.144
3.125
F
F
F
HO
N
O
O
2.09
4.06
3.03
0.98
0.99
1.00
1.00
1.04
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-1.0
f1 (ppm)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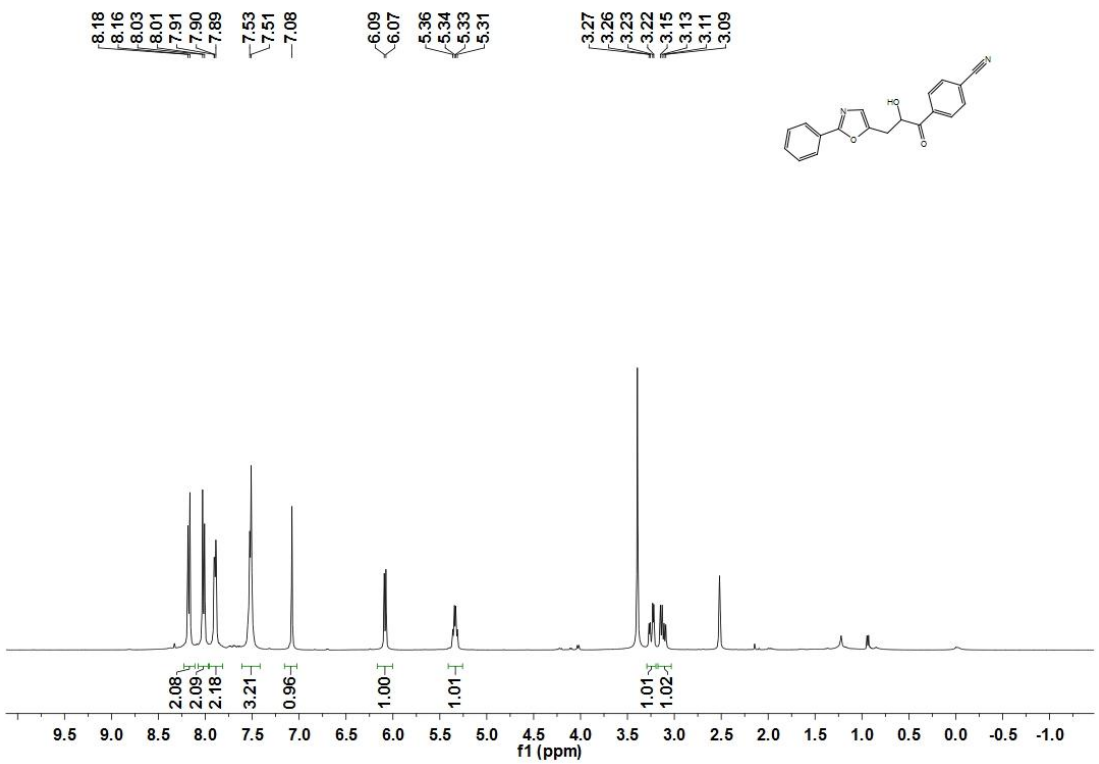
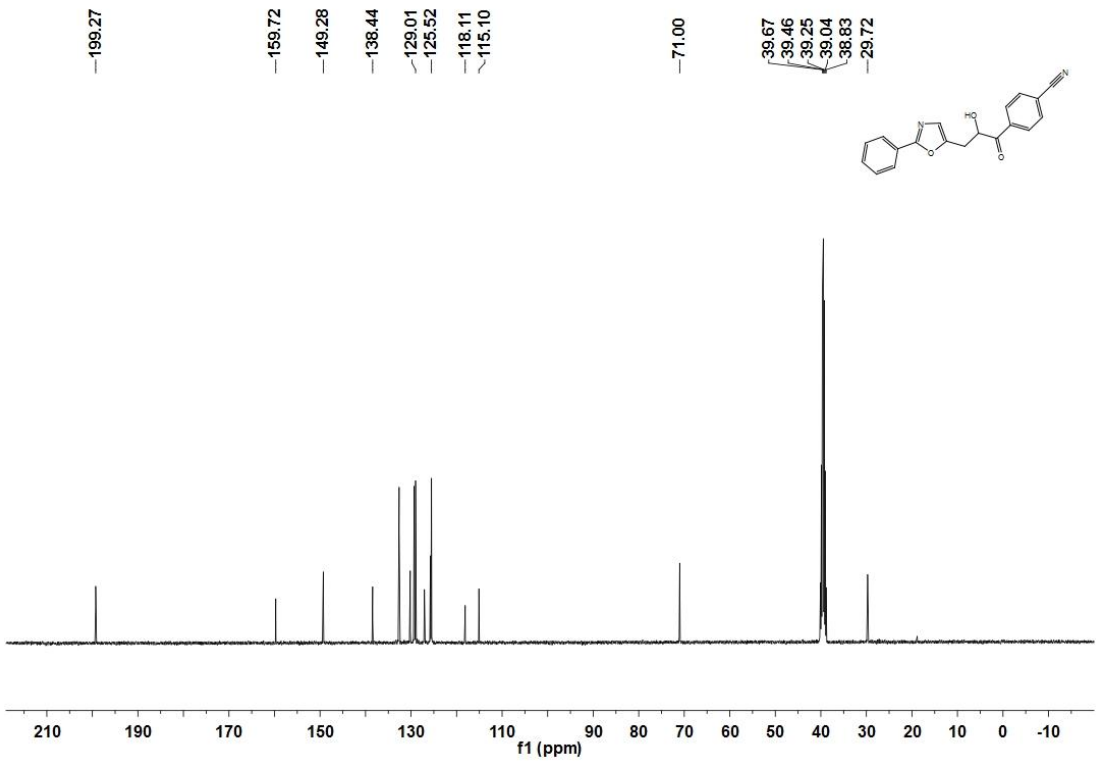
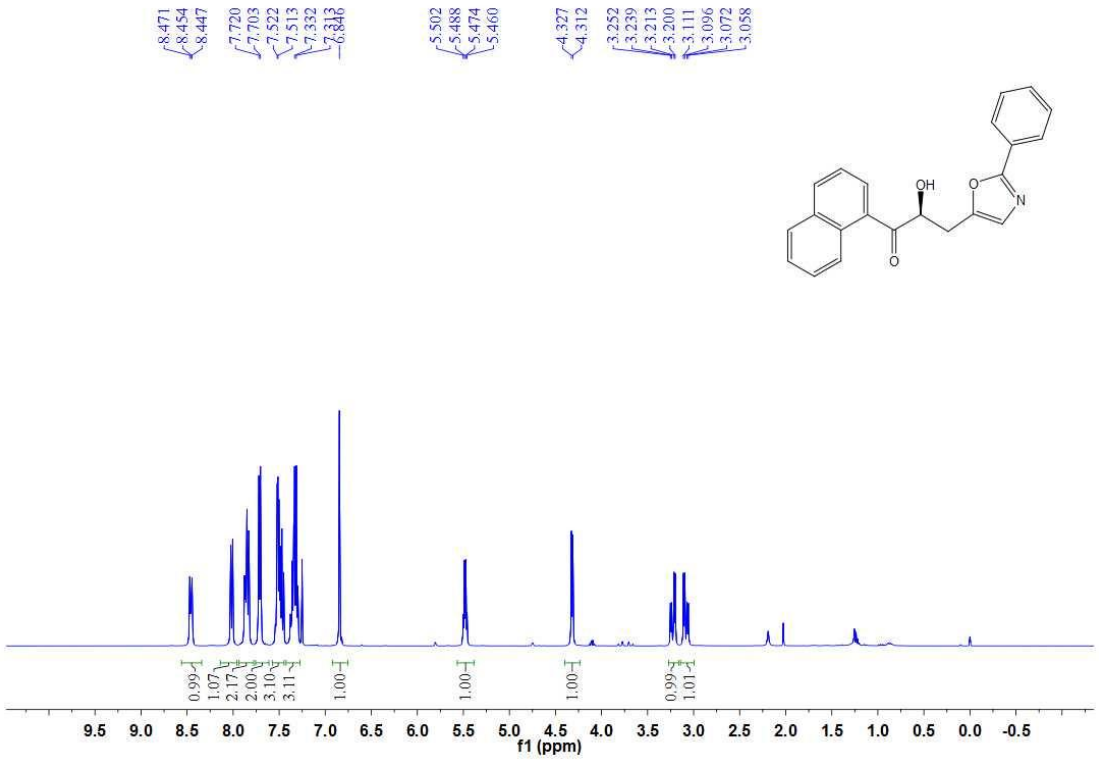
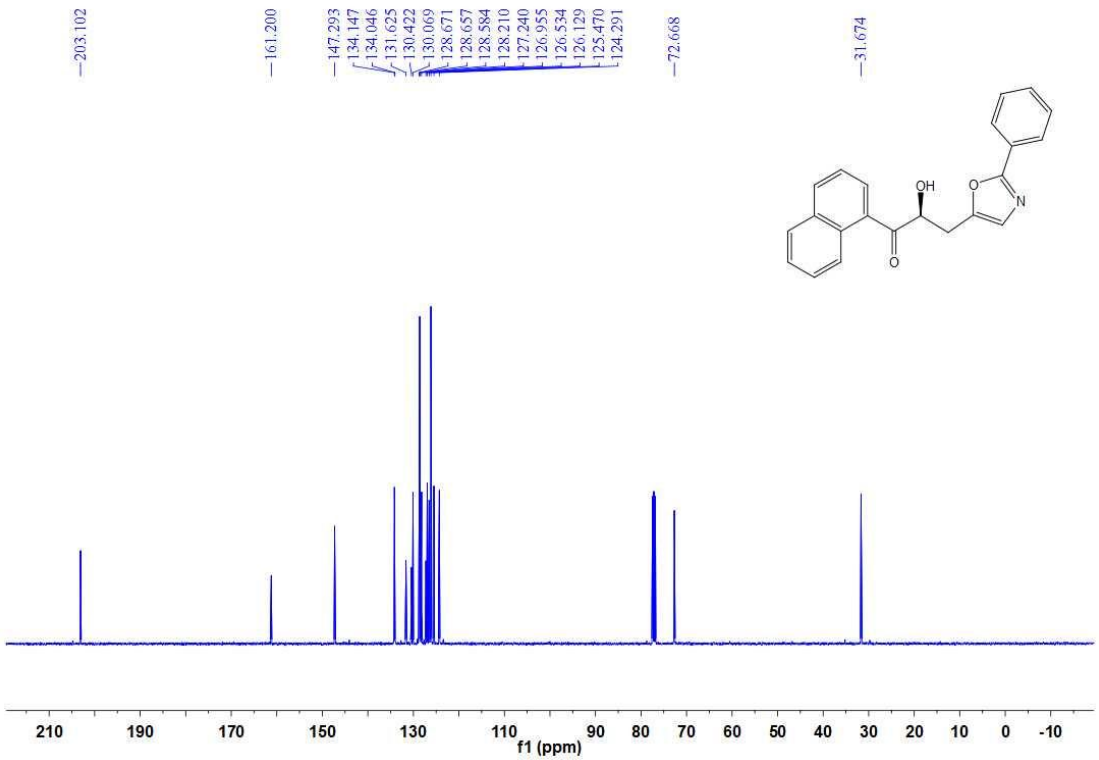
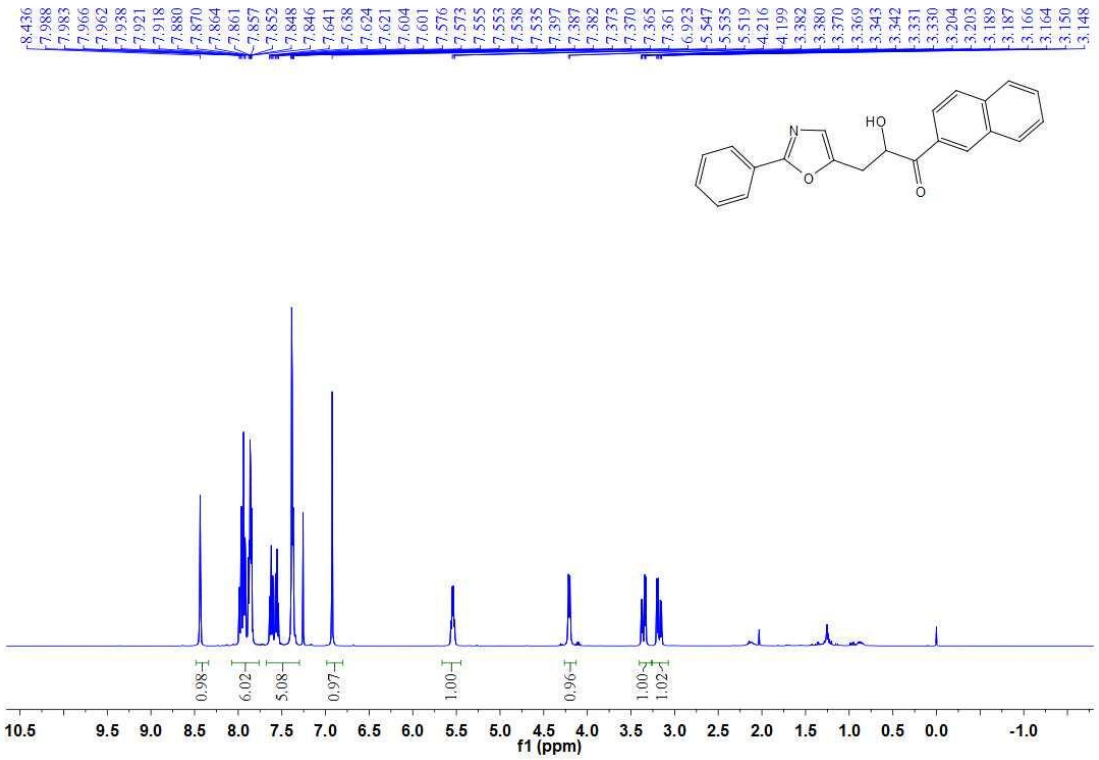
132.651
132.333
131.988
130.134
129.513
128.955
127.086
125.751
125.563
125.502
125.049
122.339
71.076
29.828
F
F
F
HO
N
O
O
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.18
8.16
8.03
8.01
7.91
7.90
7.89
7.53
7.51
7.08
6.09
6.07
5.36
5.34
5.33
5.31
3.27
3.26
3.23
3.22
3.15
3.13
3.11
3.09
2.08
2.09
2.18
3.21
0.96
1.00
1.01
1.01
1.02
f1 (ppm)


199.27
159.72
149.28
138.44
129.01
125.52
118.11
115.10
71.00
39.67
39.46
39.25
39.04
38.83
29.72
f1 (ppm)


8.471
8.454
8.447
7.720
7.703
7.522
7.513
7.332
7.313
6.846
5.502
5.488
5.474
5.460
4.327
4.312
3.252
3.239
3.213
3.200
3.111
3.096
3.072
3.058
OH
O
N
O
0.99
1.07
2.17
2.00
3.10
3.11
1.00
1.00
1.00
0.99
1.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


203.102
161.200
147.293
134.147
134.046
131.625
130.422
130.069
128.671
128.657
128.584
128.210
127.240
126.955
126.534
126.129
125.470
124.291
72.668
31.674
OH
O
N
O
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.988
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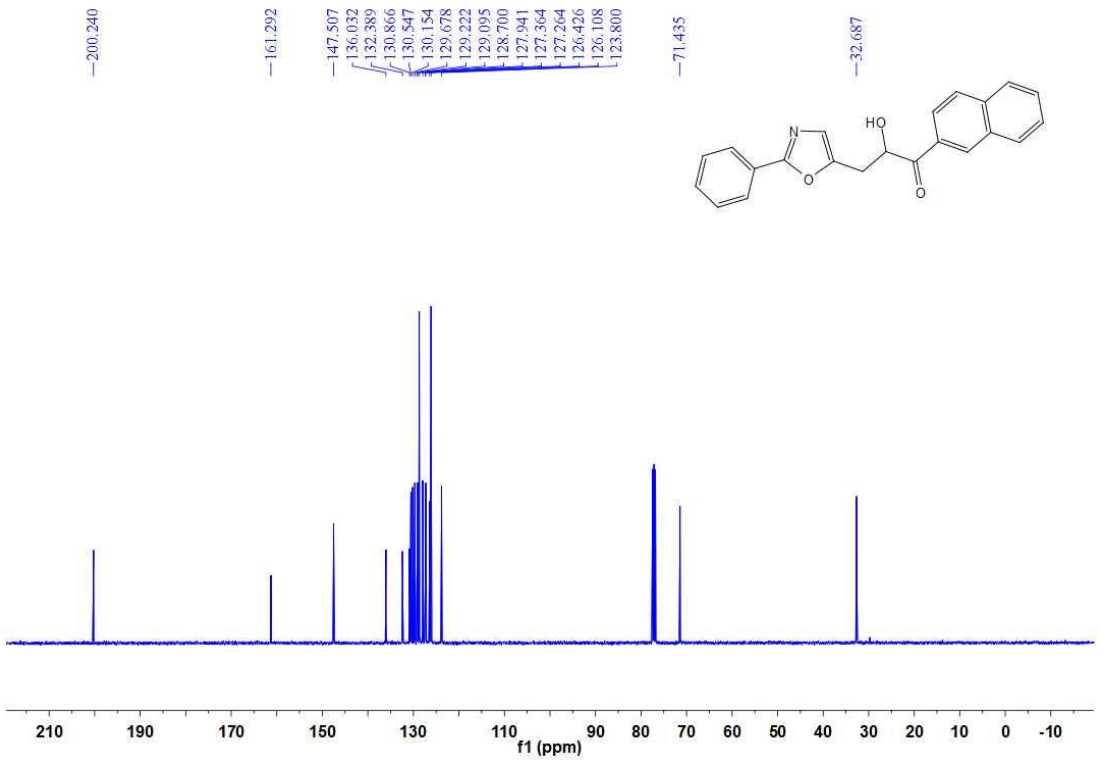
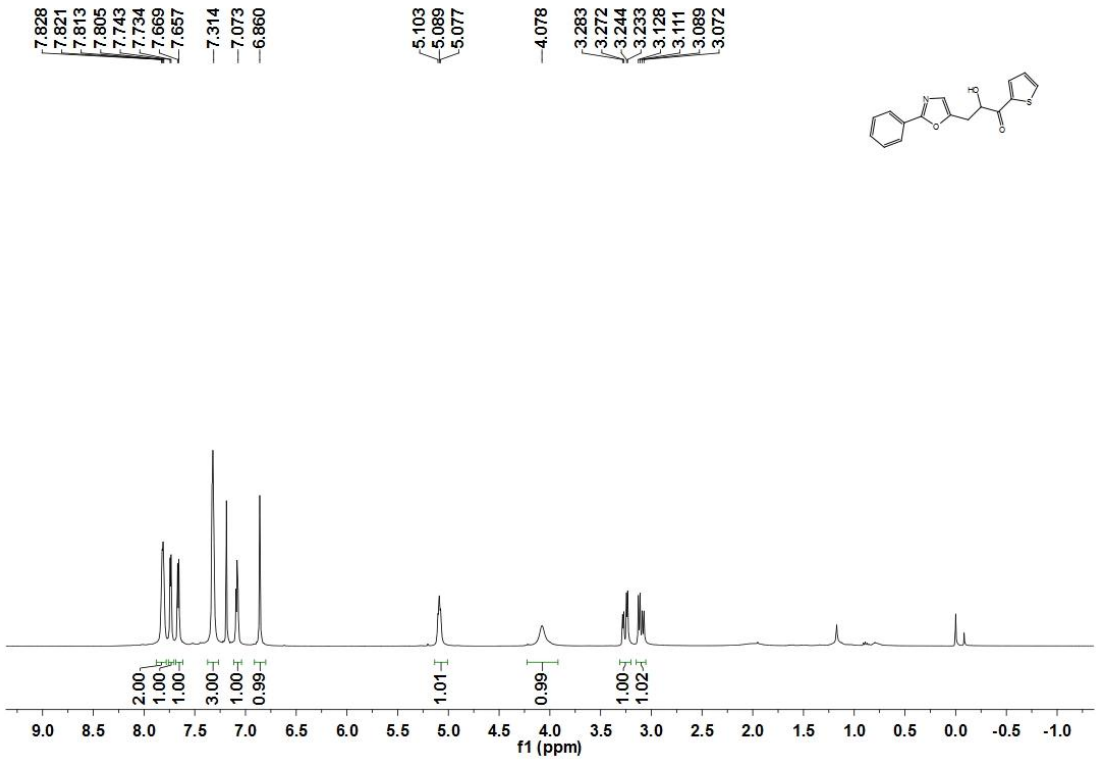
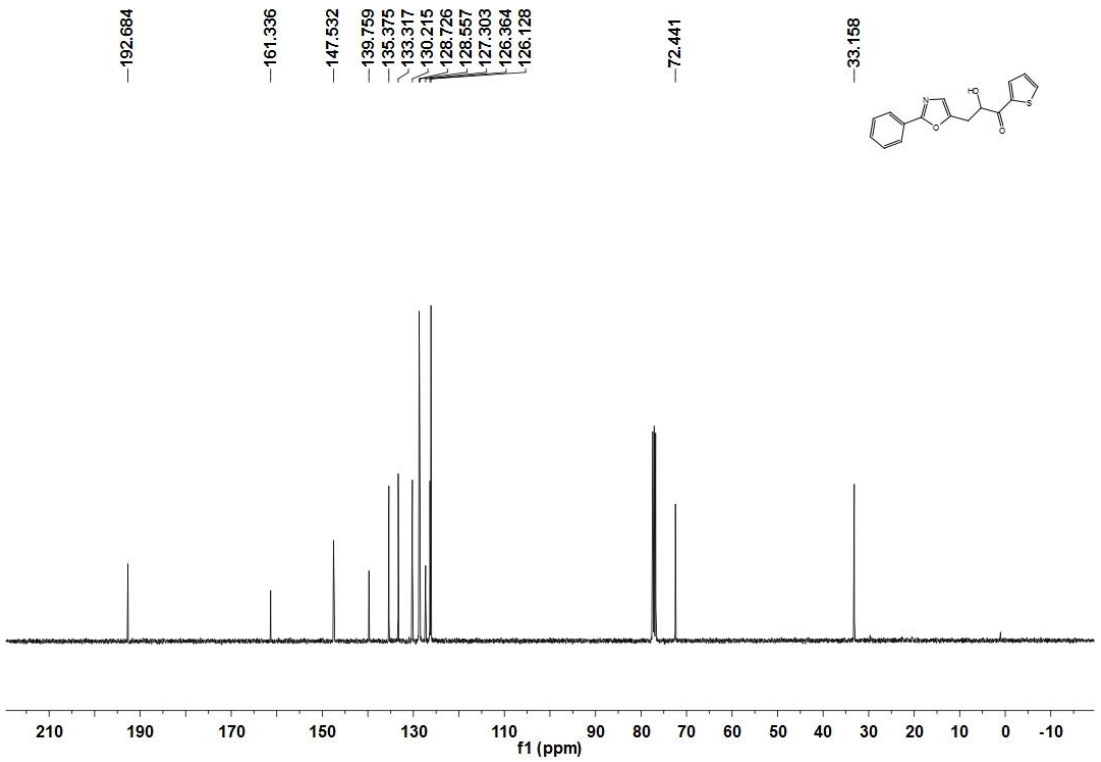
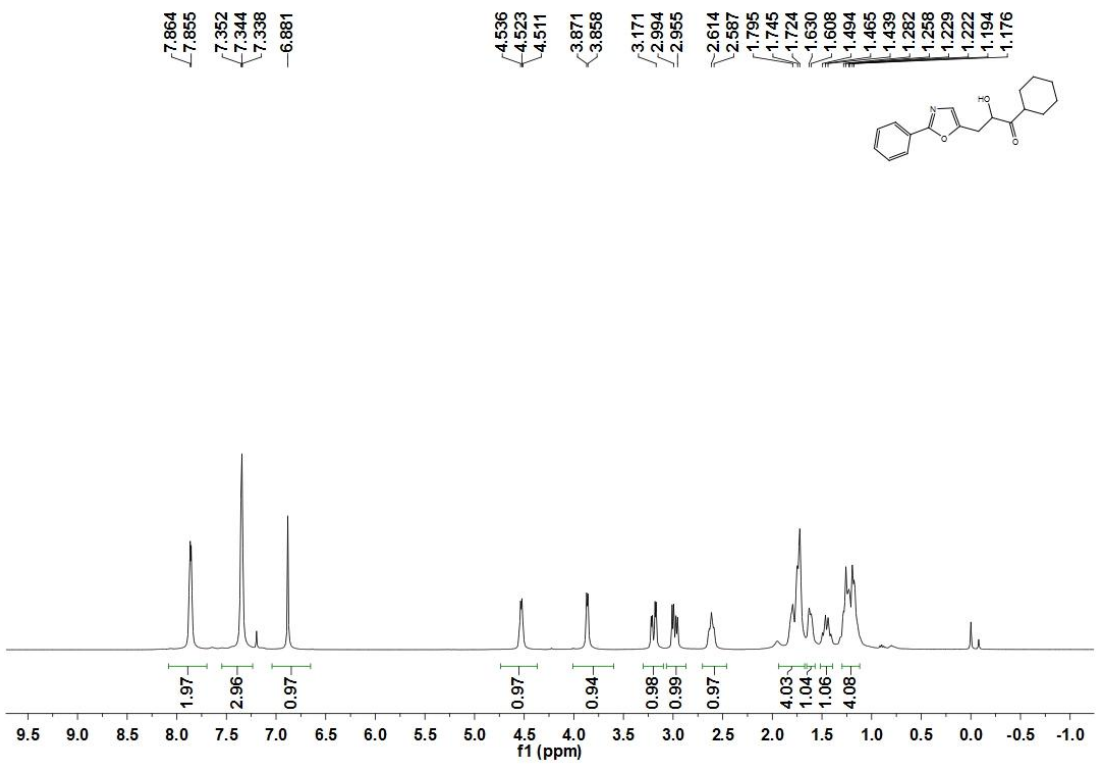
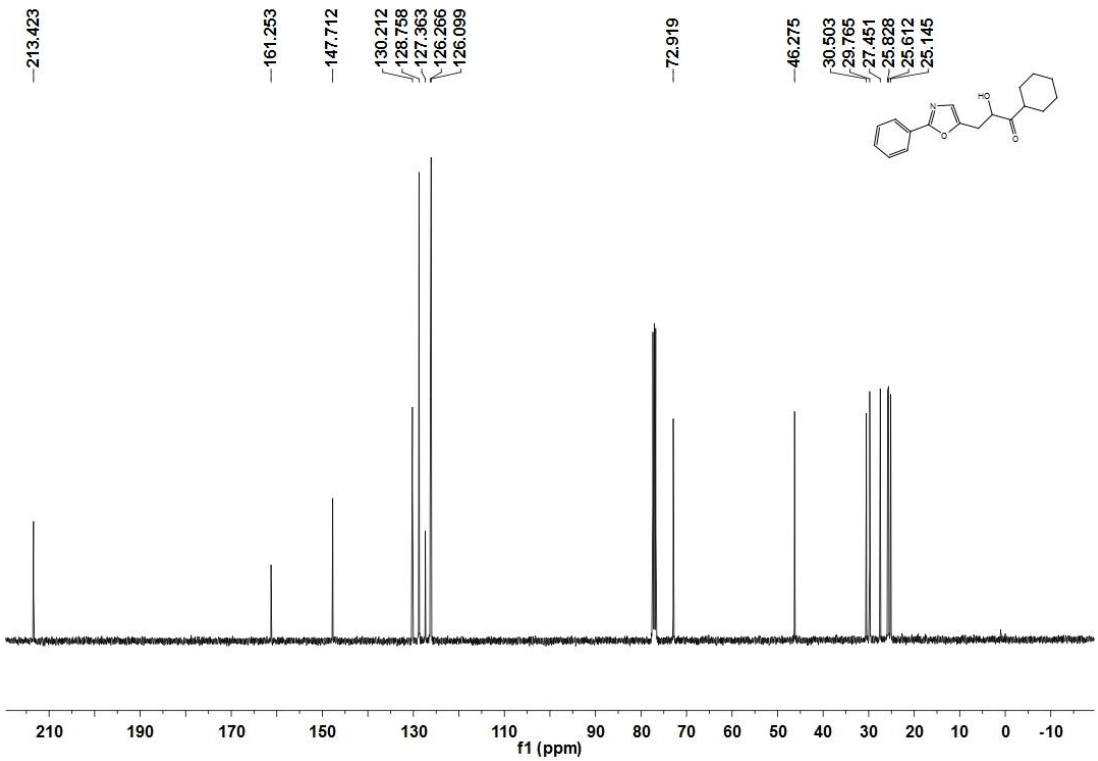
7.966
7.962
7.938
7.921
7.918
7.880
7.870
7.864
7.861
7.857
7.852
7.848
7.846
7.641
7.638
7.624
7.621
7.604
7.601
7.576
7.573
7.555
7.553
7.538
7.535
7.397
7.387
7.382
7.373
7.370
7.365
7.361
6.923
5.547
5.535
5.519
4.216
4.199
3.382
3.380
3.370
3.369
3.343
3.342
3.331
3.330
3.204
3.203
3.189
3.187
3.166
3.164
3.150
3.148
HO
N
O
O
0.98
6.02
5.08
0.97
1.00
0.96
1.00
1.02
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-1.0
f1 (ppm)

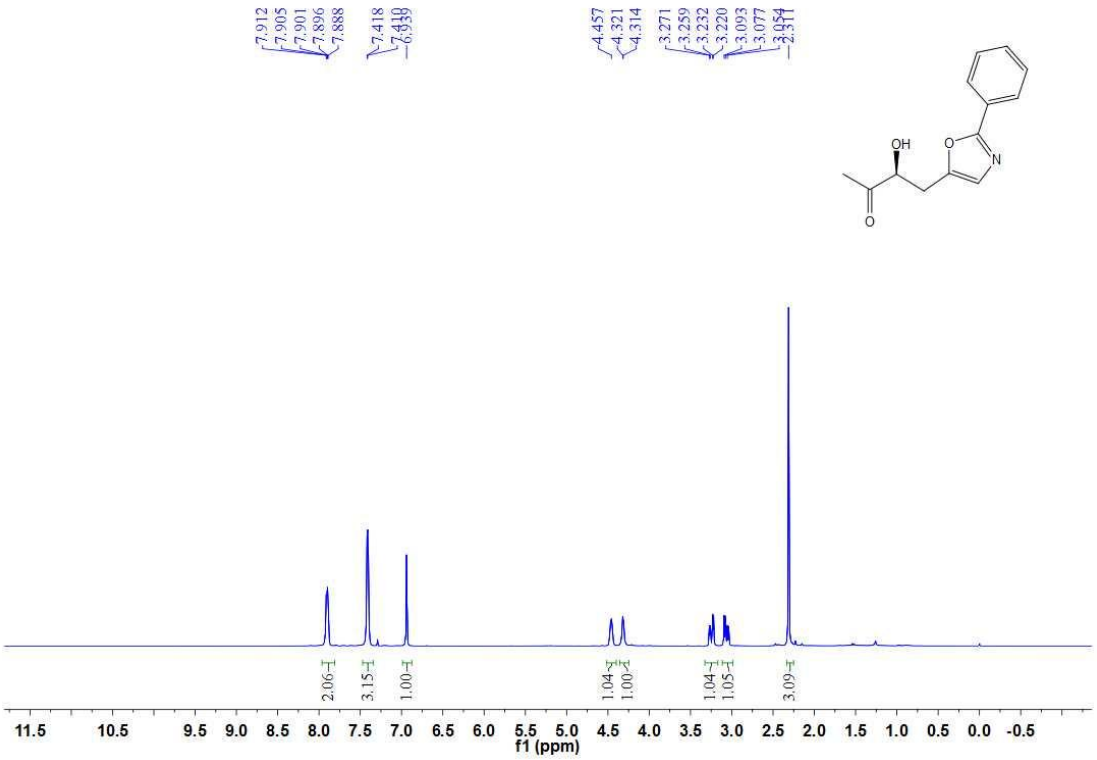

200.240
161.292
147.507
136.032
132.389
130.866
130.547
130.154
129.678
129.222
129.095
128.700
127.941
127.364
127.264
126.426
126.108
123.800
71.435
32.687
HO
N
O
O
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.828
7.821
7.813
7.805
7.743
7.734
7.669
7.657
7.314
7.073
6.860
5.103
5.089
5.077
4.078
3.283
3.272
3.244
3.233
3.128
3.111
3.089
3.072
2.00
1.00
1.00
3.00
1.00
0.99
1.01
0.99
1.00
1.02
f1 (ppm)


192.684
161.336
147.532
139.759
135.375
133.317
130.215
128.726
128.557
127.303
126.364
126.128
72.441
33.158
f1 (ppm)


7.864
7.855
7.352
7.344
7.338
6.881
4.536
4.523
4.511
3.871
3.858
3.171
2.994
2.955
2.614
2.587
1.795
1.745
1.724
1.630
1.608
1.494
1.465
1.439
1.282
1.258
1.229
1.222
1.194
1.176
1.97
2.96
0.97
0.97
0.94
0.98
0.99
0.97
4.03
1.04
1.06
4.08
f1 (ppm)


213.423
161.253
147.712
130.212
128.758
127.363
126.266
126.099
72.919
46.275
30.503
29.765
27.451
25.828
25.612
25.145
f1 (ppm)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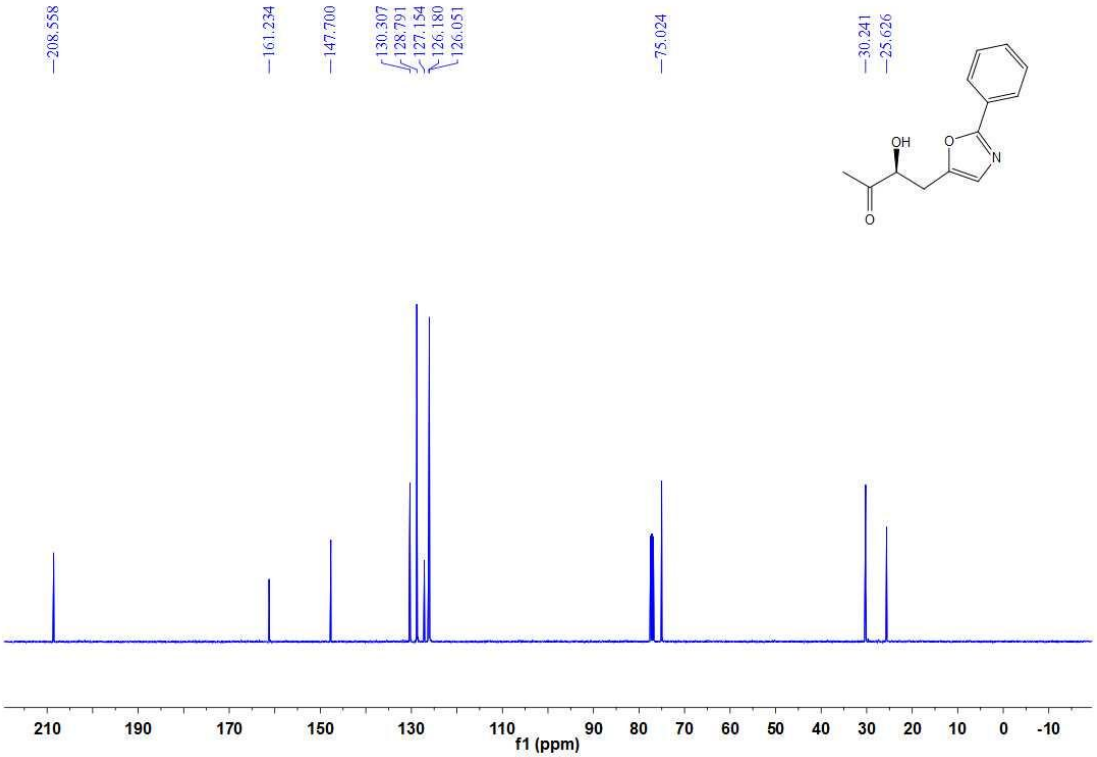
7.905
7.901
7.896
7.888
7.418
7.410
7.338
4.457
4.321
4.314
3.271
3.259
3.232
3.220
3.093
3.077
2.311
OH
O
N
O
2.06
3.15
1.00
1.04
1.00
1.04
1.05
3.09
11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


208.558
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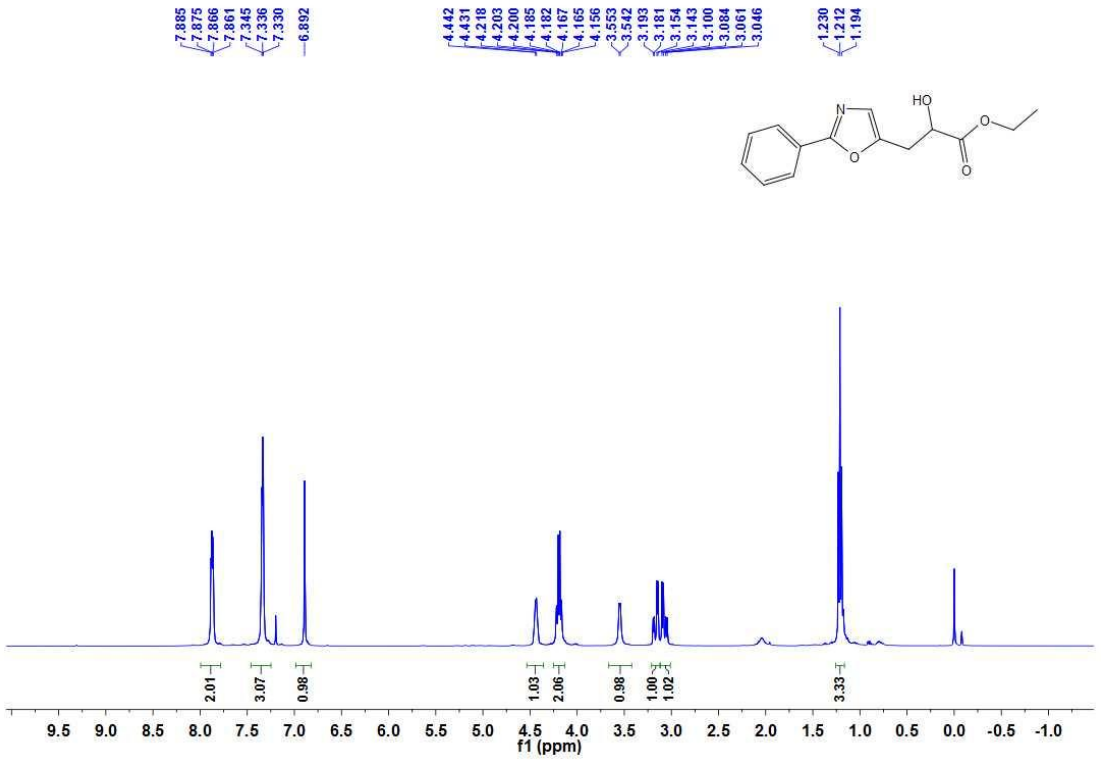
147.700
130.307
128.791
127.154
126.180
126.051
75.024
30.241
25.626
OH
O
N
O
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.875
7.866
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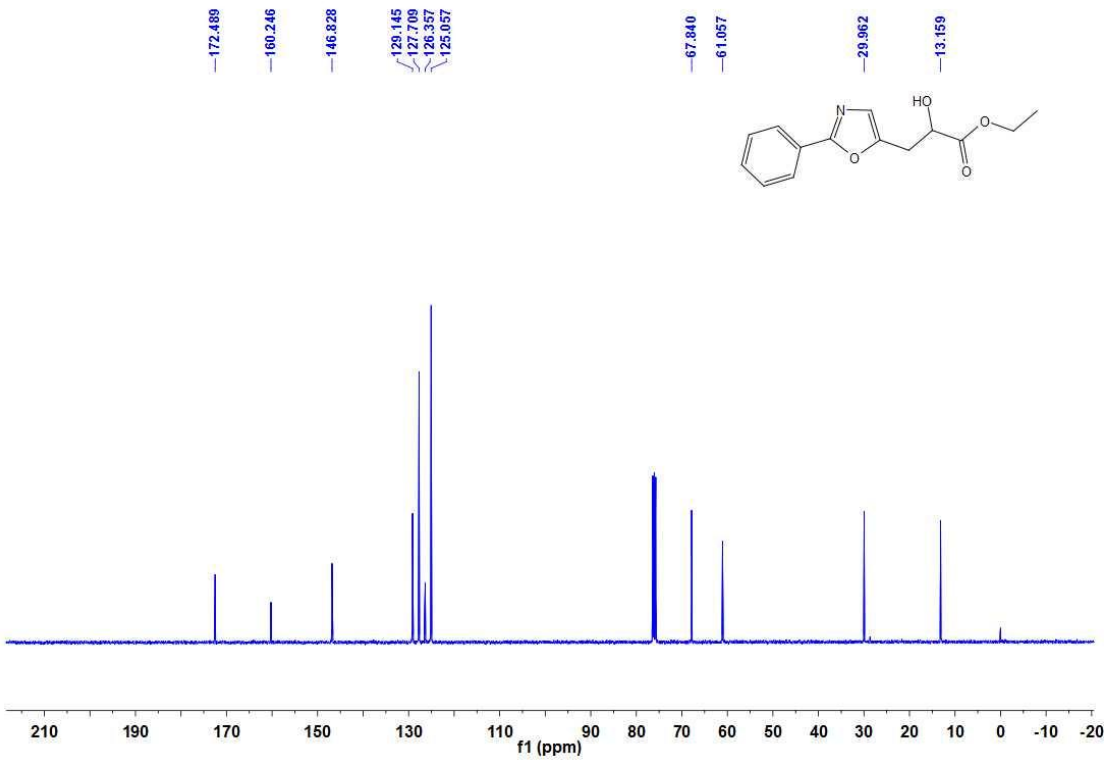
7.345
7.336
7.330
6.892
4.442
4.431
4.218
4.203
4.200
4.185
4.182
4.167
4.165
4.156
3.553
3.542
3.193
3.181
3.154
3.143
3.100
3.084
3.061
3.046
1.230
1.212
1.194
HO
N
O
O
O
2.01
3.07
0.98
1.03
2.06
0.98
1.00
1.02
3.33
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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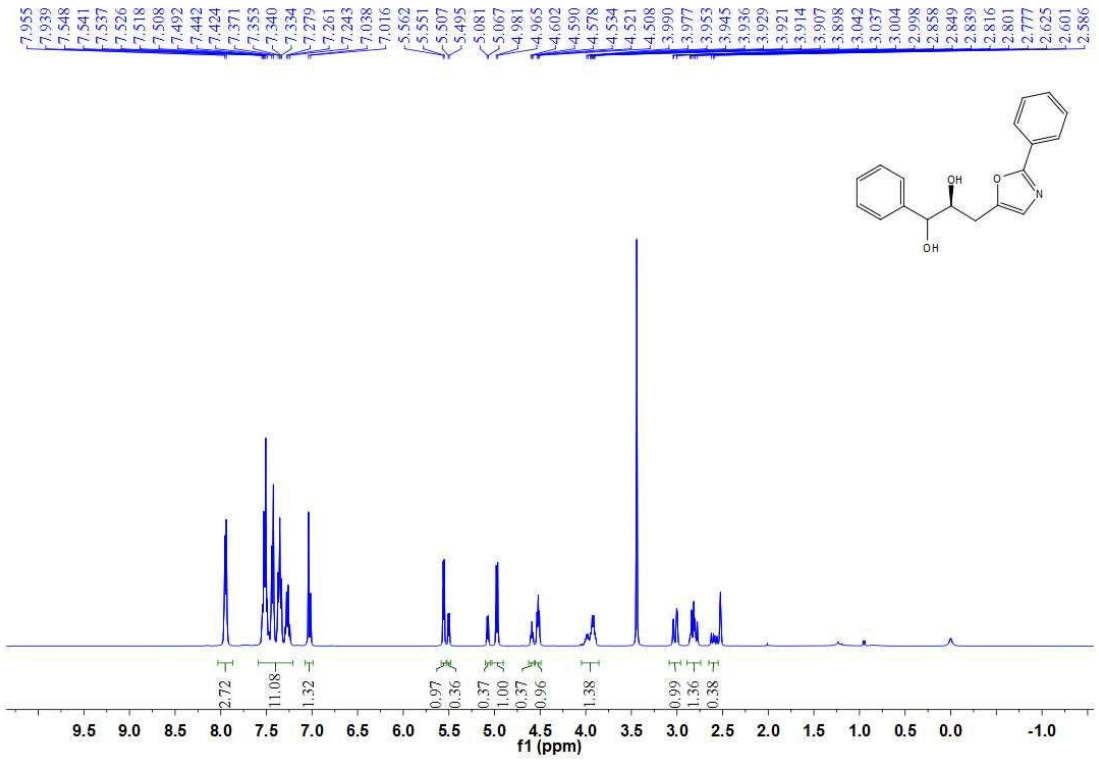
127.709
126.357
125.057
67.840
61.057
29.962
13.159
HO
N
O
O
O
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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7.548
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7.537
7.526
7.518
7.508
7.492
7.442
7.424
7.371
7.353
7.340
7.334
7.279
7.261
7.243
7.038
7.016
5.562
5.551
5.507
5.495
5.081
5.067
4.981
4.965
4.602
4.590
4.578
4.534
4.521
4.508
3.990
3.977
3.953
3.945
3.936
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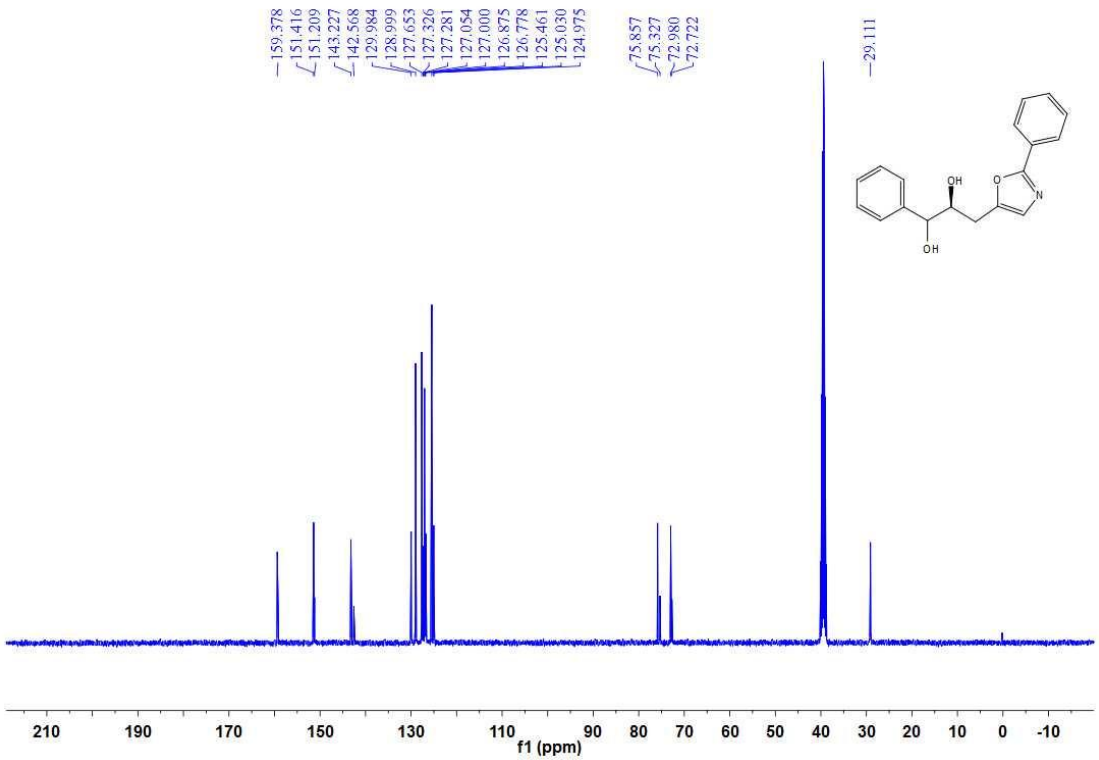
3.921
3.914
3.907
3.898
3.042
3.037
3.004
2.998
2.858
2.849
2.839
2.816
2.801
2.777
2.625
2.601
2.586
OH
O
N
OH
2.72
11.08
1.32
0.97
0.36
0.37
1.00
0.37
0.96
1.38
0.99
1.36
0.38
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -1.0
f1 (ppm)


159.378
151.416
151.209
143.227
142.568
129.984
128.999
127.653
127.326
127.281
127.054
127.000
126.875
126.778
125.461
125.030
124.975
75.857
75.327
72.980
72.722
29.111
OH
O
N
OH
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)