Polarity Effect of Water Enables an Asymmetric Cross Reaction of α-Keto acid to α-Keto ester for the Synthesis of Quaternary Isotetronic Acid

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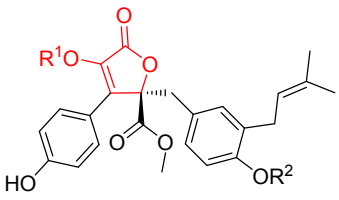
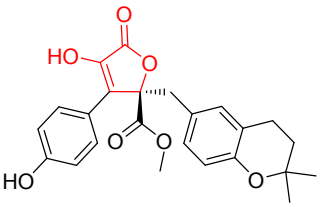
1. General information

Unless otherwise noted, all reactions were carried out in reaction tubes or flask with magnetic stirring and no special precautions were taken to exclude air or water from the reaction vessels. TLC was performed with silica gel GF_{254} precoated on glass plates and spots were visualized with UV. Column chromatography was performed on silica gel (300-400 mesh). NMR spectra were recorded with a Bruker Avance II 400 NMR spectrometer. Chemical shifts are reported in parts per million (ppm) down field from TMS with the solvent resonance as the internal standard. The following abbreviations were used to designate chemical shift multiplicities: s = singlet, d = doublet, t = triplet, q = quartert, m = multiplet, br = broad. HPLC analysis was performed on Agilent HPLC 1100 or 1260 equipped with Daicel chiral column. High resolution mass spectra for all the unknown compounds were done by an LTQ-Orbitrap instrument (ESI) (Thermo Fisher Scientific, USA). All solvents were purified by using standard methods prior to use. Substrates **1** were commercial available. Substrates **2** and catalysts were synthesized according to published procedures. All other reagents were purchased from commercial sources and used without further purification.

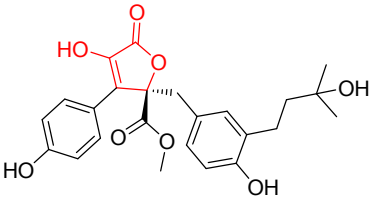
2. Representative QC-Isotetronic acid



$R^1 = R^2 = H$, **Butyrolactone I**
$R^1 = SO_3H$, $R^2 = H$
$R^1 = H$, $R^2 = SO_3H$



Aspernolides A



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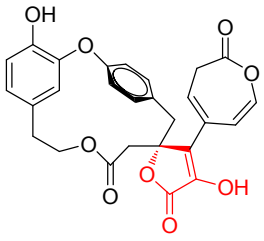
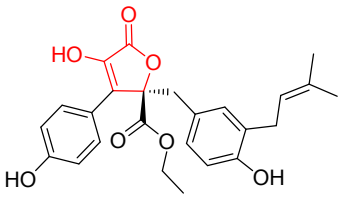
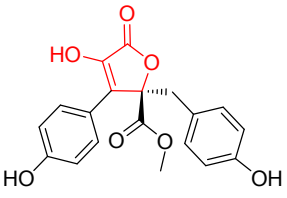


Retipolide C



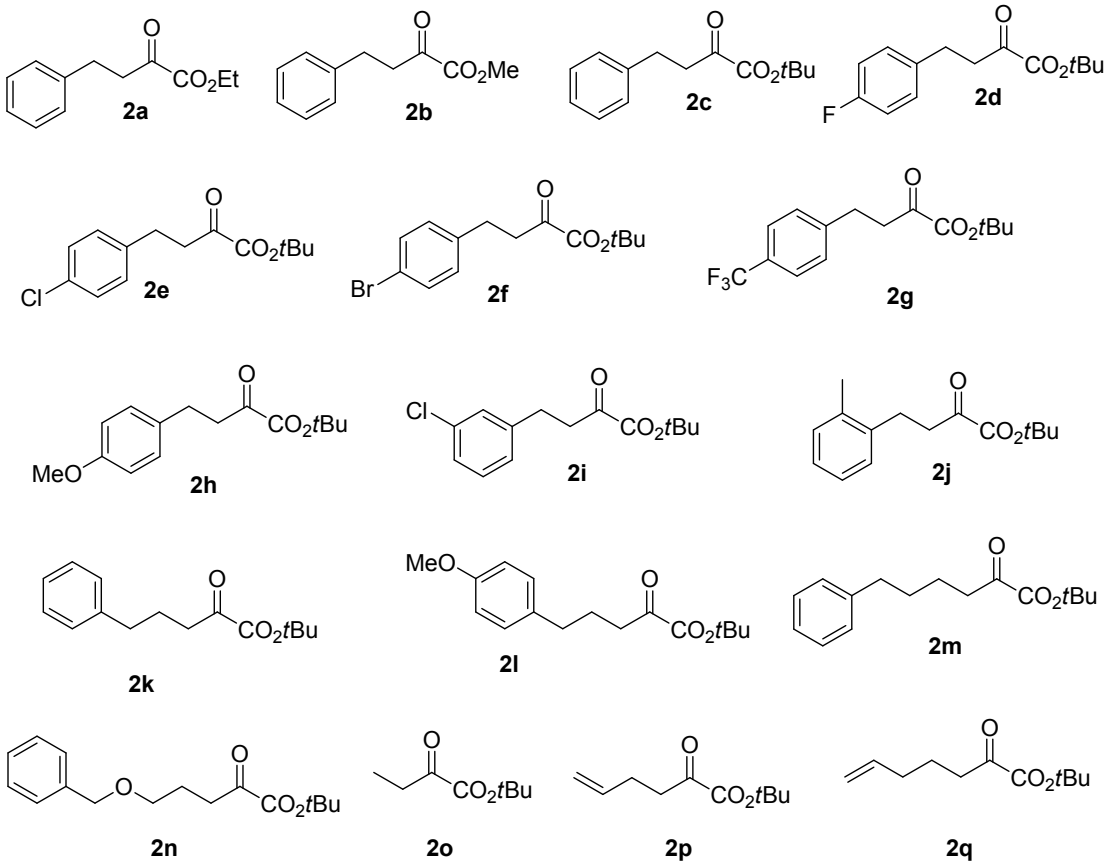
Butyrolactone VII



Butyrolactone II

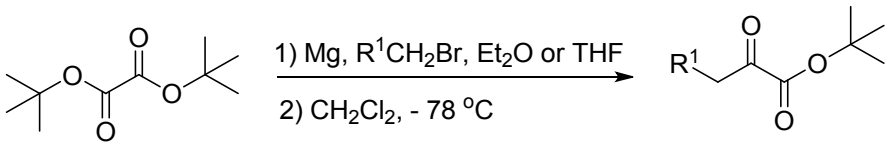
Supplementary Figure 1. Representative QC-Isotetronic acid (bearing an ester moiety and an alkyl substituent)

3. General procedure for synthesis of substrates 2



Supplementary Figure 2. Substrates were investigated in the manuscript

2 (α-Ketoesters) used in this work were prepared according to the reported procedure[1]. **2a**-**2e**, **2g**-**2i**, **2k**, **2m**-**2q** are known compounds[1-6].



In a 3-necked flask, magnesium turnings (0.29 g, 11.9 mmol), Et_2O or THF (2 mL) and a piece of iodine were added. When yellow color of iodine had faded out, alkyl bromide (16.4 mmol) in Et_2O or THF (3 mL) was added dropwise over 30 min at 0 °C and further stirred for 1 h. To a solution of di-*tert*-butyl oxalate (1.0 eq.) in dichloromethane (20 mL) was added the obtained Grignard solution by dropwise over 30 min at -78 °C and further stirred for 1 h at -78 °C. After that, the solution was quenched with saturated aqueous NH_4Cl (20 mL), extracted with dichloromethane (3

x 15 mL). The combined organic layers were washed with brine, dried over Na_2SO_4, concentrated in *vacuo*, purified by column chromatography[1].

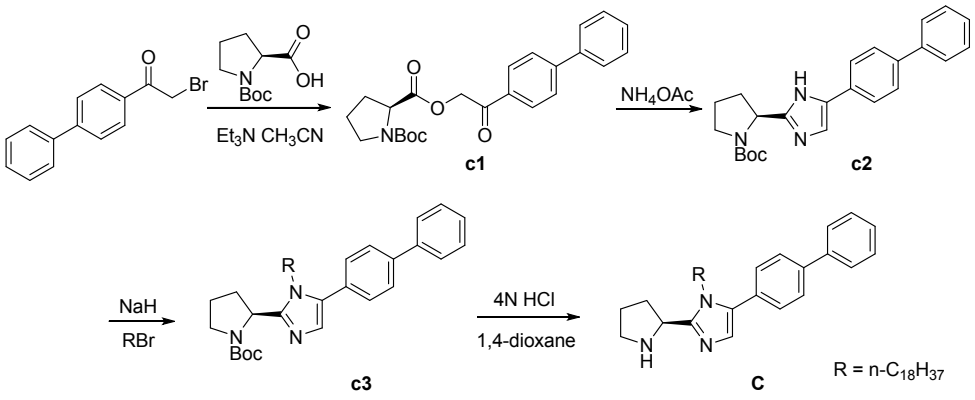
4. General procedure for synthesis of catalysts C-G

Catalyst **A** is known compound.

Catalyst **B** was synthesized according to PhD Thesis, Boyu Zhang, Oxidation reaction of thiophene and asymmetric emulsion catalysis in biphase system, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, **2013.**

Herein, we used catalyst **C** as an example to demonstrate how to synthesize the catalysts described in manuscript and other catalysts were prepared accordingly. Intermediate products **c2, d2, e3** are synthesized according to literature[7-11].

For catalyst **C**:



To a stirred solution of 1-([1,1'-biphenyl]-4-yl)-2-bromoethanone (30 mmol) in CH_3CN (50 mL), (S)-1-(tert-butoxycarbonyl)pyrrolidine-2-carboxylic acid (30 mmol) and then Et_3N (90 mmol) was added. The reaction was stirred and detected by TLC until the disappearance of starting materials. After the reaction completed, the solution was concentrated and diluted with CH_2Cl_2 (100 mL). The mixture was washed with water (20 mL), the organic phase was dried over Na_2SO_4, filtered, concentrated, purified by silica gel chromatography to afford **c1** (11.9 g, 97% yield).

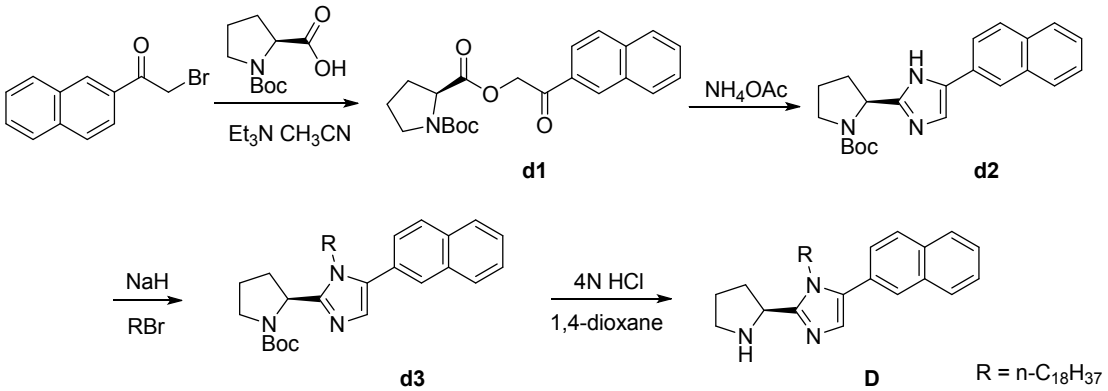
To a stirred solution of **c1** (10 mmol) in dimethylbenzene (20 mmol), NH_4OAc (100 mmol) was added and the mixture was stirred at 140°C overnight. After cooling down to room temperature, the solution was concentrated and diluted with CH_2Cl_2 (20 mL).

The mixture was washed with brine (20 mL), the organic phase was dried over Na_2SO_4, filtered, concentrated, purified by silica gel chromatography to afford **c2** (3.7 g, 96% yield, known compound).

Under N_2 atmosphere, to a solution of **c2** (3.0 mmol) in dry THF (15 mL), NaH (240 mg, 60% suspension in mineral oil, 6 mmol, 2 eq.) was added with in small portions and the resulting mixture was stirred at room temperature until no gas evolution (about 30 min), and then n-$C_{18}H_{37}Br$ (4.5 mmol, 1.5 eq.) was added dropwise. The mixture was stirred at room temperature until the disappearance of **c2**. After the reaction finished, water (10 mL) was added carefully and then the solution was extracted with EtOAc repeatedly. The collected organic layers were then dried over Na_2SO_4, filtered, concentrated, and the crude material was purified by flash silica gel chromatography to afford crude **c3**.

To a stirred solution of **c3** (obtained in previous step) in 1,4 dioxane (12 mL) concentrated hydrochloric acid (6 mL) was added dropwise and the reaction was detected by TLC until the disappearance of **c3**. After reaction, the solution was concentrated under vacuo and subsequently neutralized with saturated $NaHCO_3$ to ph about 7-8. And then the solution was extracted with CH_2Cl_2 repeatedly. The collected organic layers were dried over Na_2SO_4, filtered, concentrated, purified by flash silica gel chromatography to afford catalyst **C**.

For catalyst **D**:

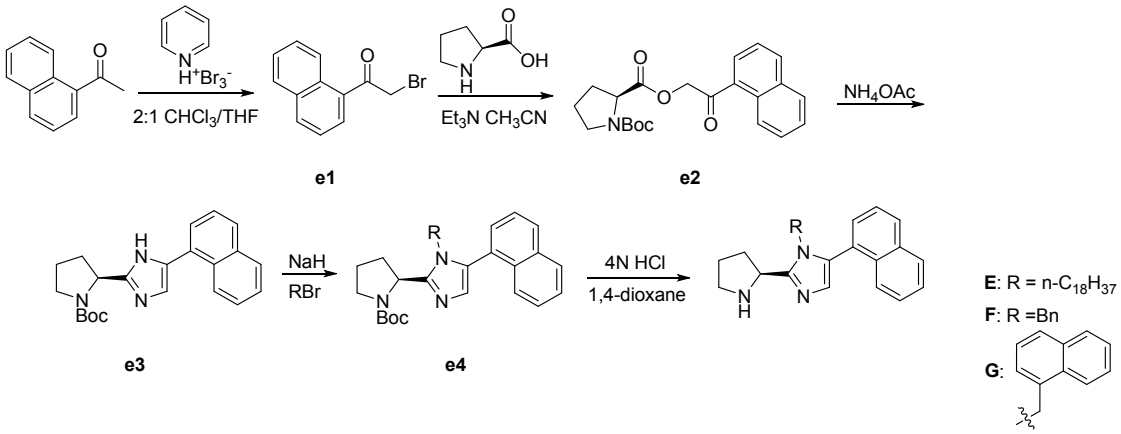


Catalyst **D** was synthesized similarly according to catalyst **C** with the starting material was 2-bromo-1-(naphthalen-2-yl)ethanone. **d2** is known compound and catalyst **D** was synthesized starting from 6 mmol **d2**.

For catalyst **E, F, G**:

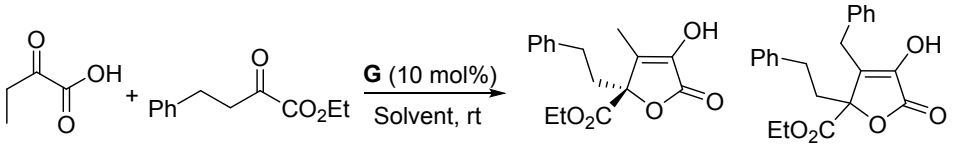
Catalyst **E, F, G** were prepared similarly with catalyst **C** with the starting material was 2-bromo-1-(naphthalen-1-yl)ethanone which is known compound.

e3 is known compound and catalyst **D, E, F** was synthesized starting from 2 mmol **e3**.



5. General procedure for the synthesis of isotetronic acids 3 and solvent screening

5.1 Solvent screening

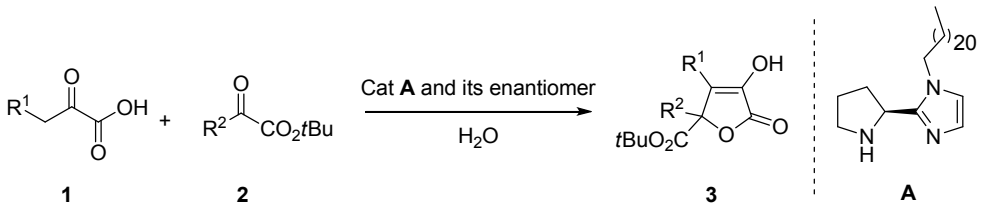


1a **2a** **3a** **4**

Entry	Solvent	Conv(%) [b]	**3a/4** [b]	ee (%) [c]
1	H_2O:DMSO=20:1	47	>15:1	63
2	H_2O:DMF=20:1	57	>15:1	62.
3	H_2O:THF=20:1	53	>15:1	63.
4	H_2O:1,4-dioxane=20:1	51	>15:1	63
5	H_2O:DCE=20:1	79	>15:1	73

[a]Unless noted otherwise, reactions were performed with **1a** (0.3 mmol), **2a** (0.1 mmol), **G** (10 mol%) in 0.5 mL solvent at rt for 3 days; [b]Determined by ^{1}H NMR spectroscopy of the crude mixture; [c]Determined by chiral HPLC analysis.

5.2 Preparation of racemic isotetronic acids 3



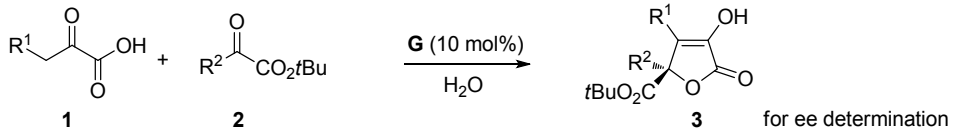
1 **2** **3** **A**

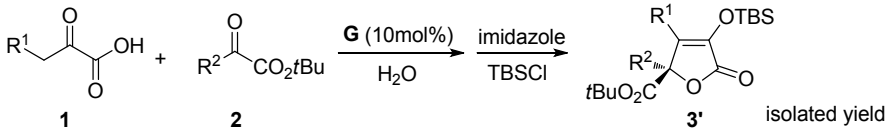
The racemic isotetronic acids were synthesized by using equal amount of **A** and its enantiomer as catalysts. To a mixture of α-ketoacid (0.3 mmol) and α-ketoester (0.1 mmol) in 0.5 mL H_2O, catalyst **A** and its enantiomer (0.02 mmol, 20 mol%) in an ordinary test tube was added. The reactions were performed at room temperature for 3 days. After that, the mixture was diluted with brine, extracted with EtOAc (3 x 10 mL). The combined organic solvents were dried over Na_2SO_4, filtered, concentrated

in *vacuo*, isolated by flash chromatograph on silica gel.

5.3 Preparation of chiral isotetronic acids 3

To a mixture of α-ketoacid **1** (1.2 mmol), α-ketoester **2** (0.4 mmol) and catalyst **G** (0.04 mmol), 2 mL H_2O was added (a few drops, about 100 μL CH_2Cl_2 was added to dissolve the substrates and catalyst). The reaction was performed at room temperature for 4-5 days. After that, the mixture was diluted with brine (10 mL), extracted 3 times with EtOAc (3 x 10 mL). The combined organic solvents were dried over Na_2SO_4, filtered, concentrated in *vacuo*, isolated by flash chromatograph on silica gel (SiO_2, PE:EA =5:1 to 3:1) to afford **3** for ee determination.





Because isotetronic acids are unstable for silica gel[12], TBS protecting group are introduced to get real isolated yields under standard conditions in a one-pot reaction immediately: the mixture (obtained before chromatography) was dissolved in CH_2Cl_2 (5 mL) was added imidazole (5 eq.), followed by tert-butyldimethylsilyl chloride (3.5 eq.) and stirred overnight. After that, the solution was diluted with CH_2Cl_2 (5 mL), washed with water (10 mL), and extracted with CH_2Cl_2 (3 x 10 mL). The combined organic layers were washed with brine, dried over Na_2SO_4, filtered, concentrated in vacuo, purified by silica gel chromatography (SiO_2, PE:EA =100:1 to 50:1) to afford **3'**.

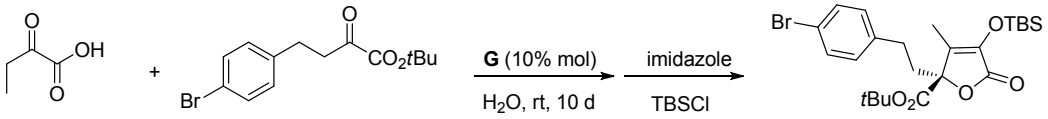
For pyruvic acid as substrate:

Because the TBS-protected products cannot be separated with α-ketoester, the isolated products were directly separated by flash chromatography.

To a mixture of pyruvic acid (5 mmol) and α-ketoester (1 mmol), catalyst **G** (0.1

mmol) in an ordinary test tube equipped with a magnetic stirring bar was added 2 mL H_2O and the reaction was performed at room temperature for 10 days. After that, the mixture was diluted with brine (10 mL), extracted 3 times with EtOAc (3 x 10 mL). The combined organic solvents were dried over Na_2SO_4, filtered, concentrated in *vacuo*, isolated by flash chromatograph on silica gel (SiO_2, PE:EA =5:1 to 3:1).

5.4 Gram-scale reaction



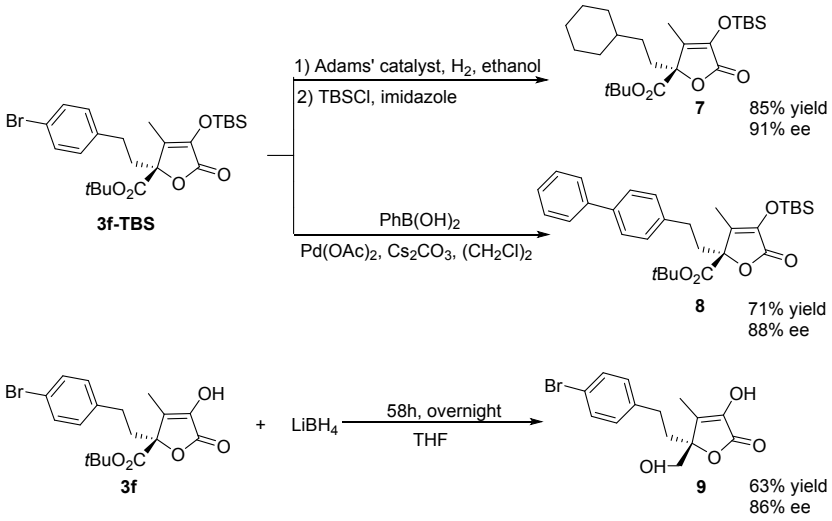
1a
9 mmol

2f
3 mmol

3f-TBS
1.08 g
70% yield
88% ee

To a mixture of **1a** (9 mmol), **2f** (3 mmol) and catalyst **G** (0.3 mmol), 15 mL H_2O (750 μL CH_2Cl_2 was added to dissolve the substrates) was added and the reactions were performed at room temperature for 10 days. After that, the mixture was diluted with brine (30 mL), extracted 3 times with EtOAc (3 x 30 mL). The combined organic solvents were dried over Na_2SO_4, filtered, concentrated in *vacuo*. The mixture was dissolved in CH_2Cl_2 (25 mL) was added imidazole (15 mmol), followed by tert-butyldimethylsilyl chloride (10.5 mmol) and stirred overnight. After that, the solution was diluted with CH_2Cl_2 (25 mL), washed with water (30 mL), and extracted with CH_2Cl_2 (3 x 30 mL). The combined organic layers were washed with brine, dried over Na_2SO_4, filtered, concentrated in vacuo, purified by silica gel chromatography (SiO_2, PE:EA =100:1 to 50:1) to afford **3f-TBS** (**3'f**) with 70% yield (1.08 g) and 88% ee.

6. Synthetic transformations



For **7**[13]:

To **3f-TBS** (0.1 mmol, 51.1 mg) in 2 mL ethanol, Admas' catalyst (20 wt %, 10 mg) was added. The reaction was performed at 50 °C under hydrogen gas (7 MPa) in a stainless autoclave for 48 h. After releasing the hydrogen carefully, the solution was filtrated and washed with CH_2Cl_2. The filtrate was concentrated under vacuum and dissolved in 5 mL CH_2Cl_2, imidazole (0.5 mmol), TBSCl (0.35 mmol) were added. The solution was stirred overnight. After that, the solution was diluted with CH_2Cl_2 (5 mL), washed with water (10 mL), and extracted with CH_2Cl_2 (3 x 10 mL). The combined organic layers were washed with brine, dried over Na_2SO_4, filtered, concentrated in vacuo, purified by silica gel chromatography to afford **7**.

For **8**[14,15]:

Under N_2 atmosphere, phenylboronic acid (0.25 mmol, 2.5 eq.), Cs_2CO_3 (0.2 mmol, 2.0 eq.), $Pd(OAc)_2$ (0.1 mmol, 1.0 eq.) were added to a solution of **3f-TBS** (0.1 mmol, 51.1 mg) in 3 mL DCE. The reaction was stirred at 80 °C and detected by TLC, and then filtrated and washed with CH_2Cl_2, concentrated in *vacuo*, purified by silica gel chromatography to afford **8**.

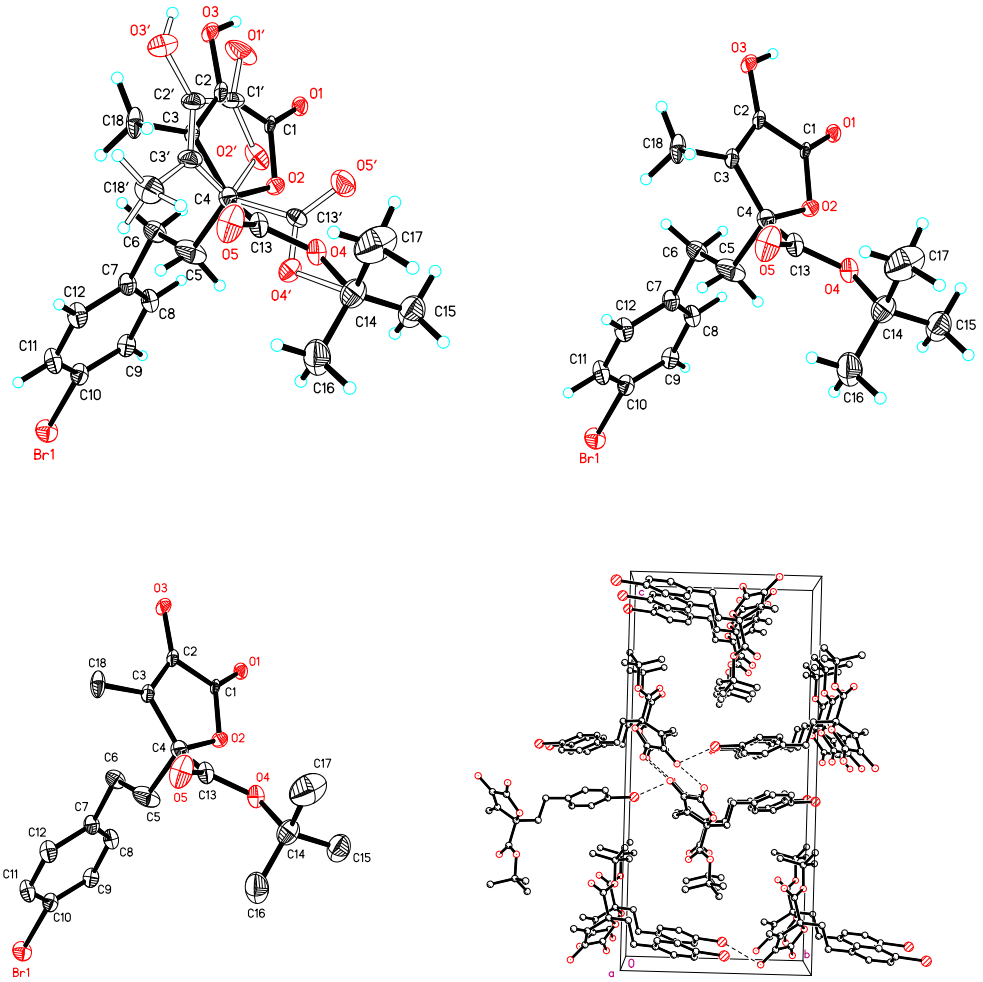
For **9**[16]:

To a solution of **3f** (0.20mmol, 79.7mg) in anhydrous tetrahydrofuran (THF, 4.0 mL),

a THF solution of $LiBH_4$ (0.6 mL, 1.2mmol, 2.0M) was added at room temperature under argon atmosphere. After stirring for 58 hours, 5ml saturated aq. NH_4Cl was added slowly to the solution to quench the reaction. The reaction mixture was then extracted with EtOAc (2 x 10 mL). The combined organic phase was dried over anhydrous Na_2SO_4, filtered, concentrated in *vacuo* and purified by silica gel chromatography (SiO_2, PE/EA=1:1) to give the product **9** with 63% yield and 86% ee.

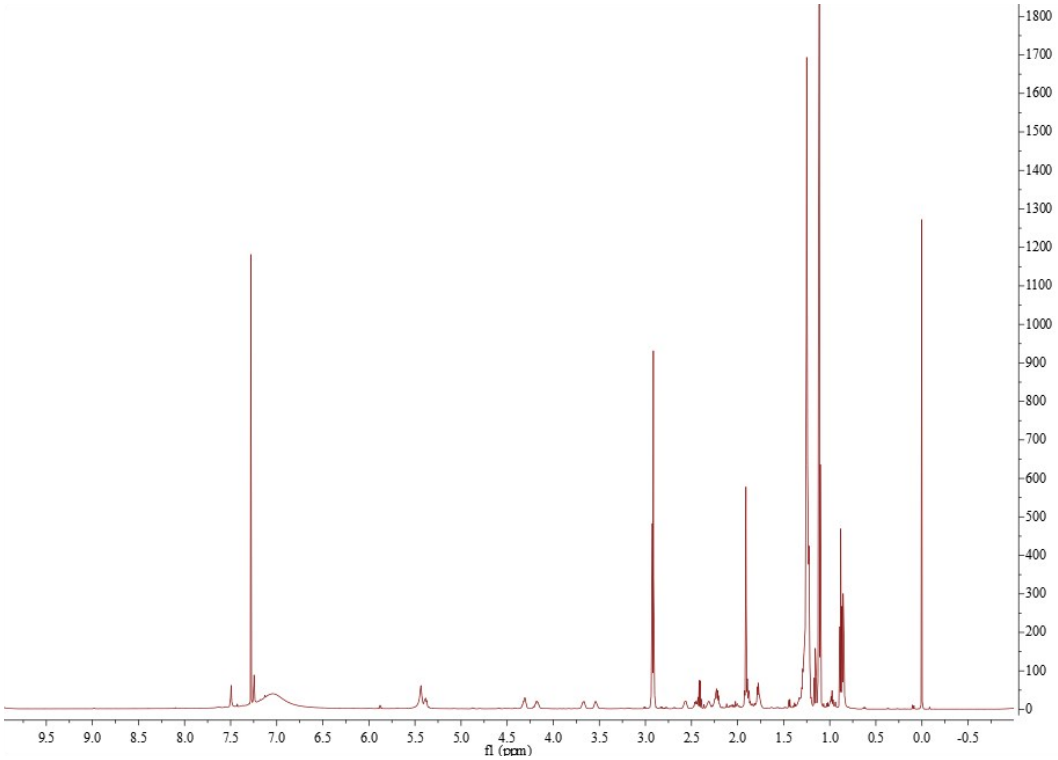
7. X-ray crystal structure of 3f

X-Ray diffraction for compounds **3f** was carried out on a SMART APEX diffractometer with graphite-monochromated Mo Kα radiation.

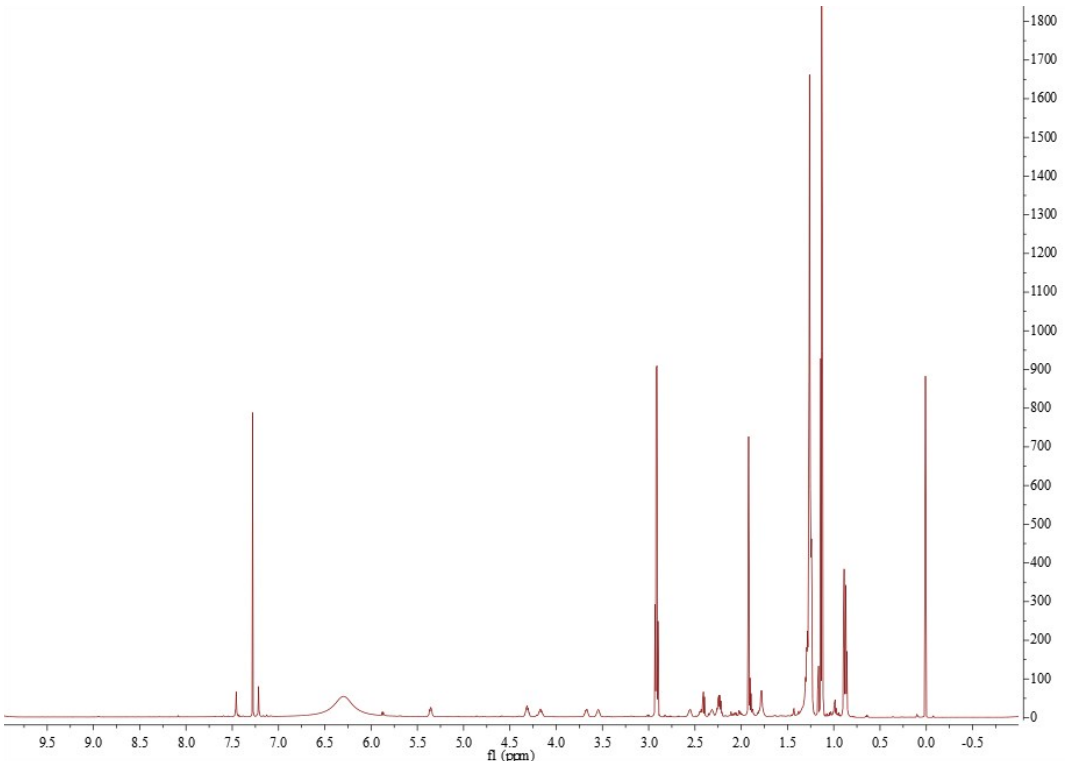


Supplementary Figure 3. X-ray Single Crystal Structure of **3f (**CCDC 1816205**)**

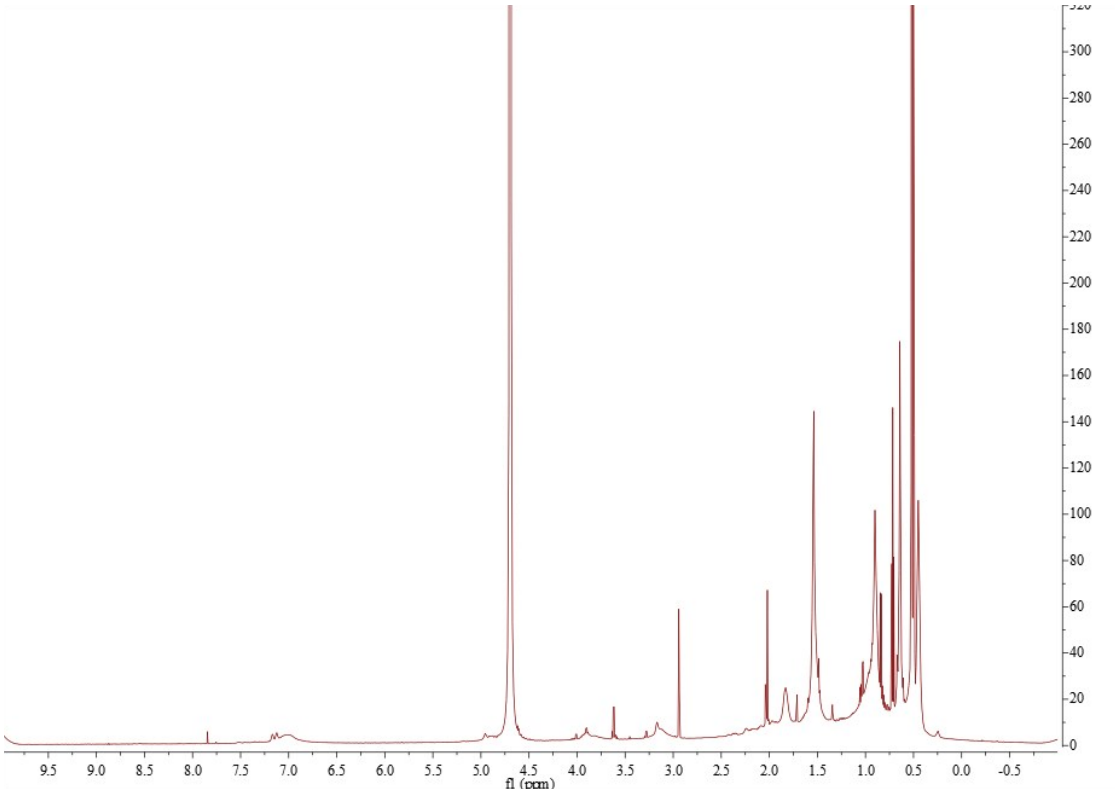
8. VT-HNMR spectra and IR spectrum of the mixture of 1a and catalyst A



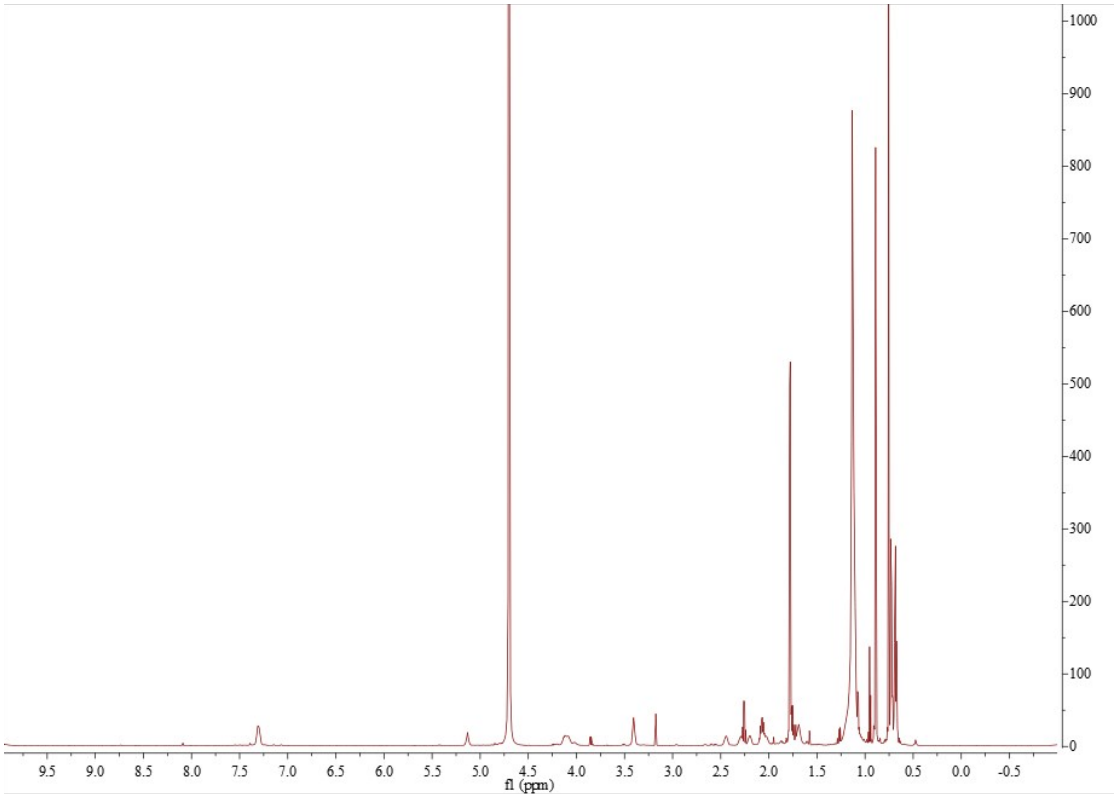
Supplementary Figure 4. The mixture of **1a** (0.10 mmol) and catalyst **A** (0.01 mmol) in 0.60 mL $CDCl_3$ at 5 ℃



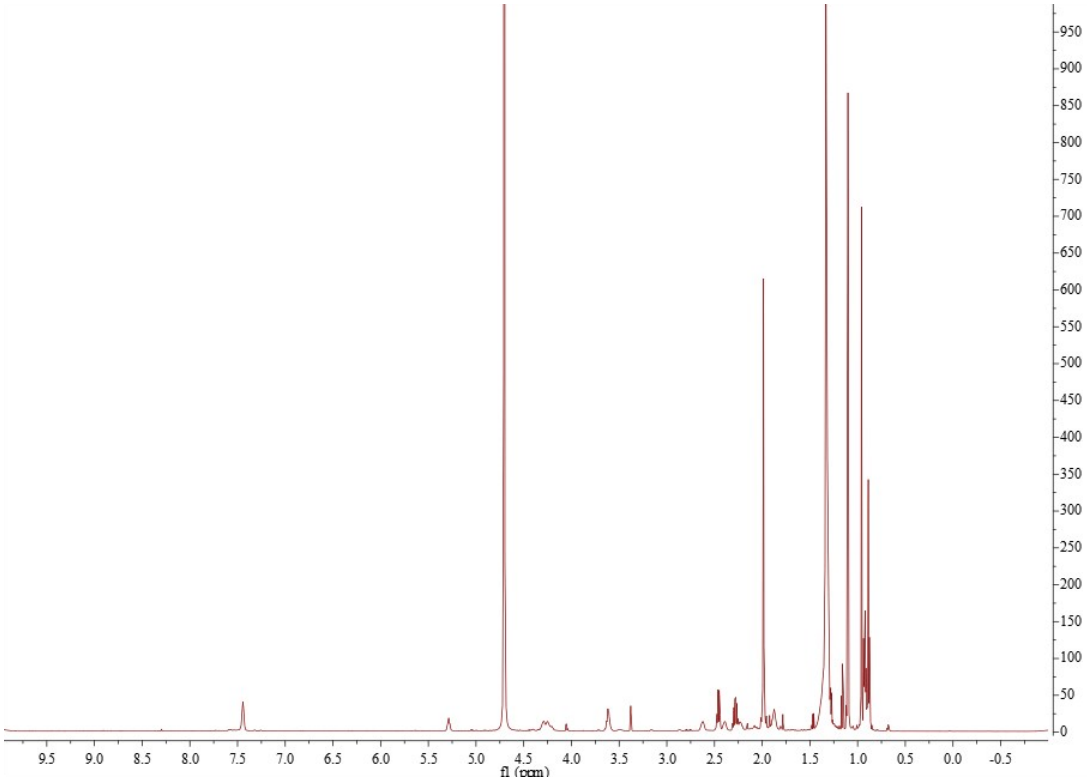
Supplementary Figure 5. The mixture of **1a** (0.10 mmol) and catalyst **A** (0.01 mmol) in 0.60 mL $CDCl_3$ at 25 ℃



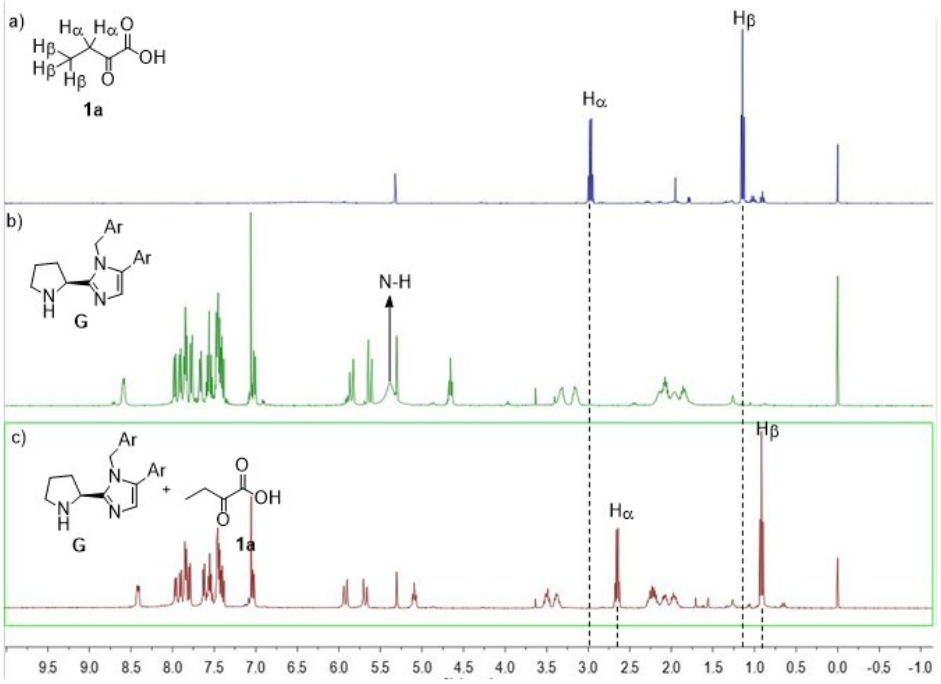
Supplementary Figure 6. The mixture of **1a** (0.10 mmol) and catalyst **A** (0.01 mmol) in 0.55 ml D_2O and 0.05 ml CD_3OD at 5 ℃



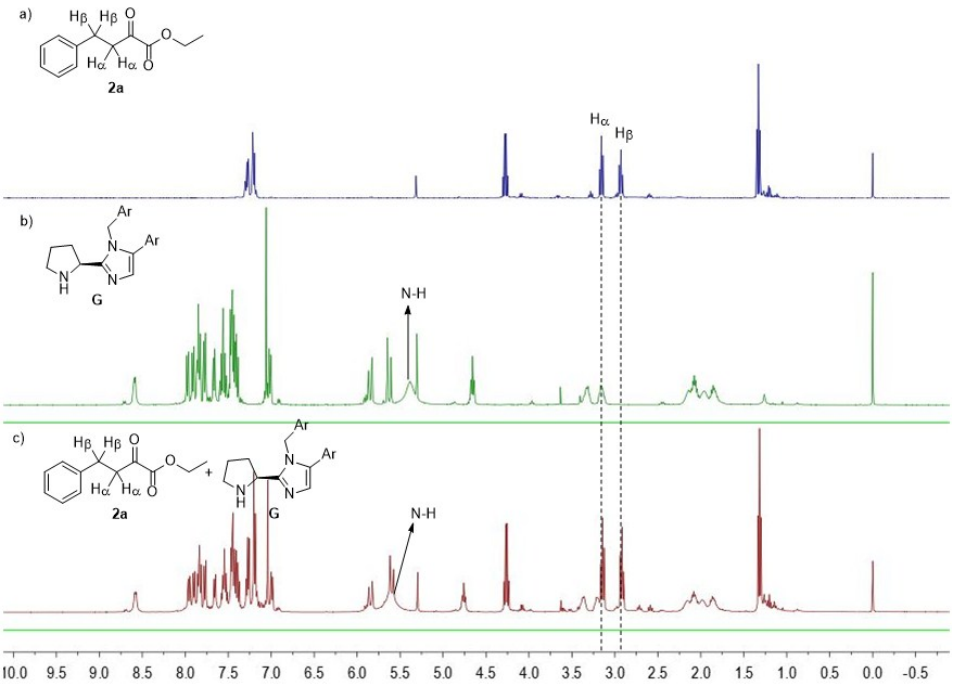
Supplementary Figure 7. The mixture of **1a** (0.10 mmol) and catalyst **A** (0.01 mmol) in 0.55 ml D_2O and 0.05 ml CD_3OD at 25 ℃



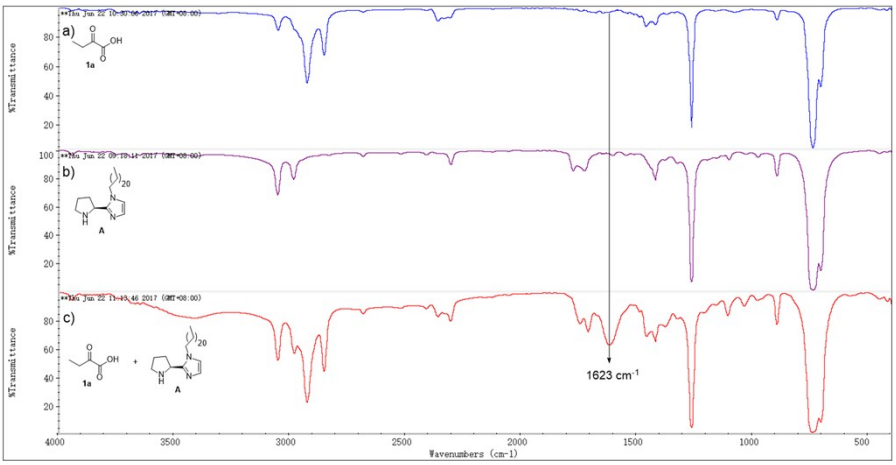
Supplementary Figure 8. The mixture of **1a** (0.10 mmol) and catalyst **A** (0.01 mmol) in 0.55 ml D_2O and 0.05 ml CD_3OD at 45 ℃



Supplementary Figure 9. a) 0.05 mmol **1a** in 0.5 ml CD_2Cl_2; b) 0.05 mmol **G** in 0.5 ml CD_2Cl_2; c) 0.05 mmol **1a**+ 0.05 mmol **G** in 0.5 ml CD_2Cl_2. (Ar= 1-naphthyl)



Supplementary Figure 10. a) 0.05 mmol **2a** in 0.5 ml CD_2Cl_2; b) 0.05 mmol **G** in 0.5 ml CD_2Cl_2; c) 0.05 mmol **2a**+ 0.05 mmol **G** in 0.5 ml CD_2Cl_2. (Ar= 1-naphthyl)



Supplementary Figure 11. IR spectrum. a) 0.1M **1a** in DCM; b) 0.1M **A** in DCM; c) 0.1M **1a** + 0.1M **A** in DCM.

9. DFT studies

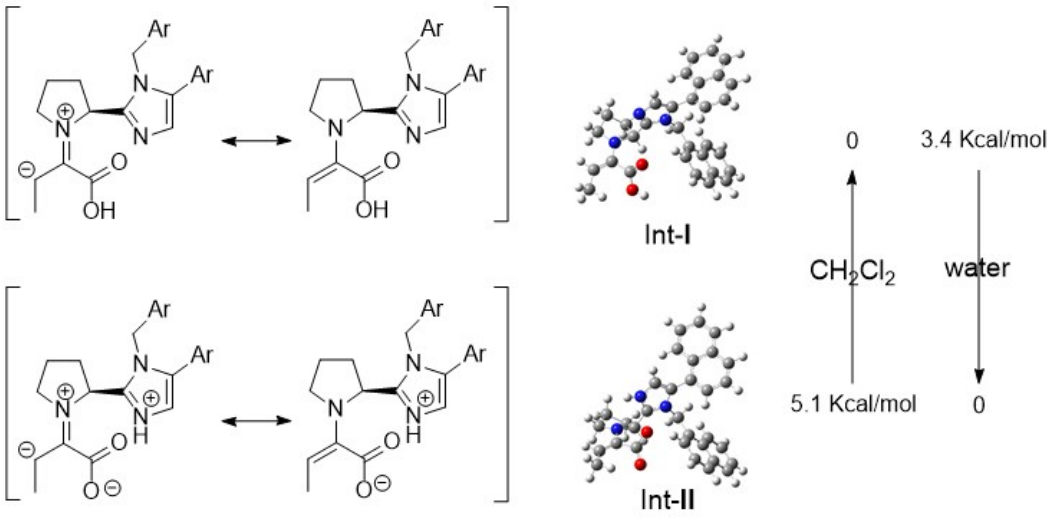
All quantum mechanical calculations were carried out with the Gaussian 09 program[17]. Int-**I** and Int-**II** was calculated with B3LYP/def2-TZVPP-CPCM//B3LYP/ 6-311G(d)-CPCM level of theory. For other structures, geometry optimization and frequency analysis were calculated with the B3LYP[18-20]/6-31G(d,p)[21,22] method within SMD model and each transition structure was confirmed with only one imaginary frequency. Intrinsic reaction coordinates (IRC) was conducted at the same level which further authenticate our computational results. Gibbs free energy was obtained by combining single point energy evaluated with the B3LYP/def2-TZVPP-SMD[25,26] method and thermal corrections from frequency analysis. The final activation energies were the difference between Gibbs free energy of transition states and that of the corresponding reactants.

To improve our understanding of mechanism and figure out the role of water played in this reaction, density functional theory (DFT) calculations for the key step-aldol reaction in the cascade reaction were carried out. All these substrates, intermediates and transition states were located at the B3LYP/def2-TZVPP-SMD//B3LYP/6-31G(d, p)-SMD level of theory using Gaussian 09. The α-keto acid **1a** and α-keto ester **2a** were chosen as the substrates for our theoretical studies, and catalyst **G** was used to model the catalyst. Initially, two plausible intermediates, Int-**I** and Int-**II** were found through the full optimization of geometries. The energy of each structure was further evaluated in both CH_2Cl_2 and water. As shown in Supplementary Figure 12, the Int-**I** was predicted to be more favorable than Int-**II** in dichloromethane with a lower energy of about 5.1 Kcal/mol. While the zwitterionic Int-**II** could be stabilized by the high polarity of water, which was proven by the calculated results in which a inverted energy difference of about 3.4 Kcal/mol was obtained. These results suggest that the Int-**I** may dominate in low polar solvent, while the Int-**II** may dominate in water.

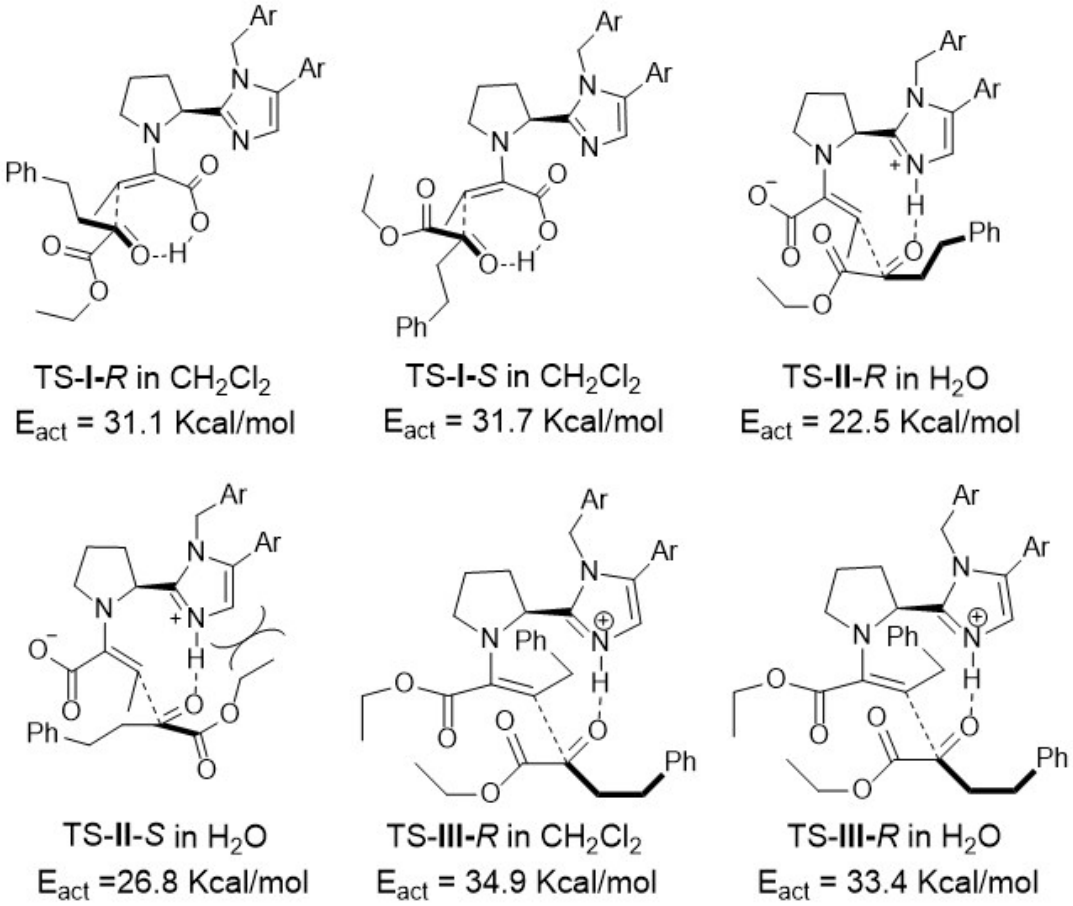
Further calculations were performed on the reaction of Int-**I** and Int-**II** with α-keto ester **2a**, and the transition structures towards (*R*)- and (*S*)-aldol products were located as TS-**I**-*R*, TS-**I**-*S*, TS-**II**-*R* and TS-**II**-*S*, respectively (Supplementary Figure 13). In TS-**I**, the carbonyl moiety of α-ketoester **2a** is activated by the hydrogen bond formation with an acidic proton from carboxylic acid of Int-**I**. However, **2a** is activated by the proton on N atom of imidazole ring in TS-**II**. It was found that TS-**I** had high activation barriers (31.1 Kcal/mol, 31.7 Kcal/mol) and the relatively small energy difference between TS-**I**-*R* and TS-**I**-*S* (0.6 Kcal/mol), which suggests that the asymmetric aldol reaction of **1a** and **2a** catalyzed by **A** in dichloromethane should have low reactivity and poor enantioselectivity. On the other hand, TS-**II** from the water-stabilized intermediate Int-**II** has the lower activation energies (22.5 Kcal/mol, 26.8 Kcal/mol). Moreover, Int-**II** prefers to attack the **2a** from the *Re* face (TS-**II**-*R*) because of the steric hindrance between ester group and imidazole ring, thus showing higher energy difference between TS-**II**-*R* and TS-**II**-*S* (4.3 Kcal/mol). These calculated results suggest that the asymmetric reaction of **1a** with **2a** should exhibit the higher reactivity and enantioselectivity in the presence of water which agrees well with the experimental results.

To investigate the water effect on chemoselectivity in this reaction, the homo-aldol reaction of **2a** was also studied by theoretical calculations (Supplementary Figure 13). In view of the absolute configuration of products, the corresponding transition states (TS-**III**-*R*) were received in both dichloromethane and water. Differing from the switch of active models of cross aldol reaction from dichloromethane to water, the homo aldol reaction of **2a** has almost the same transition states with similar activation energies in both

dichloromethane and water. The higher energy difference between cross and homo aldol reactions in water is the main reason that water can increase the chemoselectivity of cross aldol reaction.



Supplementary Figure 12. Model enamine intermediates with optimized geometries and relative energies (Ar = 1-naphthyl).



Supplementary Figure 13. Model transition states of TS-**I**, TS-**II** and TS-**III** with optimized geometries, and relative energies (Ar = 1-naphthyl). Unimportant hydrogens are omitted for clarity.

Supplementary Table 5. Activation energy of all transition states (unit: kcal/mol)

Transition states	In DCM	In water
TS-**I**-*R*	31.1	28.0
TS-**I**-*S*	31.7	31.3
TS-**II**-*R*	21.2	22.5
TS-**II**-*S*	25.5	26.8
TS-**III**-*R*	34.9	33.4
TS-**III**-*S*	44.0	40.2

Supplementary Table 6. Calculated energy of all structures (unit : hartree)

Geometry	Thermal correction to G[a]	$E_{single\text{-}point}$[b]	G_{corr}
Int-**I**-DCM	0.239033	-782.518387	-782.279354
Int-**II**-DCM	0.240783	-782.514440	-782.273657
Int-**I**-water	0.239309	-782.520791	-782.281482
Int-**II**-water	0.240602	-782.520212	-782.279610
Int-**III**-DCM	0.477196	-1552.212171	-1551.734975
Int-**IV**-DCM	0.479870	-1552.206647	-1551.726777
Int-**III**-water	0.478743	-1552.193924	-1551.715181
Int-**IV**-water	0.479271	-1552.199844	-1551.720573
TS-**I**-*R*-DCM	0.695725	-2243.873848	-2243.178123
TS-**I**-*S*-DCM	0.696326	-2243.873560	-2243.177234
TS-**II**-*R*-DCM	0.696625	-2243.882359	-2243.185734
TS-**II**-*S*-DCM	0.697662	-2243.876550	-2243.178888
TS-**III**-*R*-DCM	0.837888	-2554.120981	-2553.283093
TS-**III**-*S*-DCM	0.838783	-2554.107360	-2553.268577
TS-**I**-*R*-water	0.696984	-2243.850166	-2243.153182
TS-**I**-*S*-water	0.699978	-2243.847832	-2243.147854
TS-**II**-*R*-water	0.698265	-2243.865610	-2243.167345
TS-**II**-*S*-water	0.700974	-2243.861412	-2243.160438
TS-**III**-*R*-water	0.837269	-2554.086305	-2553.249036
TS-**III**-*S*-water	0.839415	-2554.077546	-2553.238131

[a] The thermal correction to Gibbs free energy calculated by B3LYP/6-31G(d,p)-SMD. [b] The single point energy calculated by B3LYP/def2-TZVPP-SMD.

Optimized geometry coordinates for all the compounds and transition structures.

Int-**I**-DCM

N	-0.60787700	0.93936900	0.10769500
C	-0.70469300	2.39890400	0.18269200
C	0.56877100	0.50535900	-0.66957700
H	-0.86935900	2.72708100	1.21412800
H	-1.55730200	2.75337600	-0.41557700

C	0.61950500	2.90164600	-0.39892100
C	0.99104400	1.80225000	-1.40045000
H	0.28422400	-0.25716800	-1.39729000
H	1.37520500	2.96545300	0.38545200
H	0.51678800	3.88442100	-0.86227400
H	2.04723800	1.79970500	-1.67443400
H	0.40229600	1.90493500	-2.31717200
C	-1.73123000	0.15831600	0.31727900
C	-2.92444500	0.63725000	0.75004700
H	-3.00003100	1.70532500	0.92389400
C	-4.15323400	-0.14333600	1.13635900
H	-4.99502500	0.07184000	0.46687500
H	-4.00907500	-1.22434600	1.14546300
H	-4.48172000	0.14564900	2.14022600
C	-1.53262700	-1.32435500	0.12288600
O	-0.63475200	-1.96779500	0.60512200
O	-2.44653900	-1.93759200	-0.66351100
C	1.67698400	-0.03316100	0.20677000
C	3.14252600	-0.26132500	1.76406400
C	3.37756800	-1.27354100	0.87327000
H	3.66997300	-0.04296300	2.68154100
H	4.10028600	-2.07362600	0.85245900
N	2.43886100	-1.12009700	-0.12713500
N	2.08387800	0.50899700	1.34096600
C	2.26698700	-2.01233700	-1.26891600
H	3.05395200	-2.76335200	-1.24528300
H	1.30085700	-2.51526600	-1.21604000
H	2.34308800	-1.46425000	-2.20888100
H	-3.06425900	-1.28929800	-1.03141500

Int-**II**-DCM

N	1.02102400	0.89931400	-0.15776200
C	1.78256800	2.12520900	-0.43889900
C	-0.34245800	1.20731400	0.27449000
H	2.07813800	2.16885700	-1.49440000
H	2.70100200	2.14369000	0.15659900
C	0.83373200	3.27084300	-0.06149500
C	-0.56203500	2.65707800	-0.21311900
H	-0.44163700	1.14440100	1.36109100
H	0.97193400	4.15538600	-0.68561700
H	0.99971900	3.56656200	0.97806500
H	-0.87383700	2.66573300	-1.26125300
H	-1.33038600	3.16546500	0.37082500
C	1.65954400	-0.30154600	0.19642300
C	2.95684300	-0.53703300	-0.08641600

H	3.53463200	0.23259800	-0.59407200
C	3.70861300	-1.79808700	0.24269300
H	4.17671000	-2.22618100	-0.65308000
H	4.52353700	-1.61548100	0.95522400
H	3.05453200	-2.56166500	0.66344600
C	0.78305600	-1.32275800	0.95898100
O	0.56600700	-2.42130400	0.40668600
O	0.35754800	-0.91959500	2.07581600
C	-1.31874500	0.23929900	-0.32608000
C	-2.32379400	-1.07501200	-1.82011300
C	-3.02092300	-1.14775400	-0.65706000
H	-2.47150400	-1.55944200	-2.76920900
H	-3.90090300	-1.71008300	-0.39748600
N	-2.38491800	-0.32494500	0.25846400
N	-1.28036300	-0.20635600	-1.58902200
H	-0.53525800	0.01879500	-2.23297900
C	-2.74292500	-0.19614600	1.67732500
H	-3.00966100	0.83436200	1.90621700
H	-3.59810900	-0.83864000	1.86970400
H	-1.88552200	-0.51843800	2.26889000

Int-**I**-water

N	-0.60280800	0.94529000	0.14826000
C	-0.71001900	2.40670900	0.18329500
C	0.56232200	0.50205400	-0.64419000
H	-0.89330700	2.75962400	1.20313500
H	-1.55362400	2.74198300	-0.43817500
C	0.61856200	2.90077900	-0.39310700
C	0.98778600	1.79258700	-1.38533200
H	0.26313800	-0.25943500	-1.36754300
H	1.37120700	2.96810300	0.39438900
H	0.52194900	3.88061100	-0.86372900
H	2.04354500	1.78463500	-1.66062100
H	0.39869200	1.88999400	-2.30215400
C	-1.73263800	0.16666900	0.34396400
C	-2.93841300	0.65014500	0.73203200
H	-3.02531300	1.72232300	0.87249200
C	-4.17308600	-0.12722700	1.10453500
H	-4.99700000	0.07066000	0.40842100
H	-4.02511000	-1.20720900	1.13913700
H	-4.52860100	0.18179700	2.09314000
C	-1.52050700	-1.31969400	0.20124100
O	-0.64023500	-1.94308000	0.74069400
O	-2.39745500	-1.96285800	-0.60157000

C	1.67647200	-0.04551000	0.21839400
C	3.15468700	-0.29823600	1.76055400
C	3.38724300	-1.29176000	0.84825300
H	3.68866800	-0.09574100	2.67796700
H	4.11381400	-2.08747700	0.80572500
N	2.44012700	-1.12272100	-0.14154000
N	2.08931700	0.47623100	1.36036700
C	2.26822200	-1.98867900	-1.30394900
H	3.05718600	-2.73773600	-1.29975200
H	1.30392400	-2.49651100	-1.26238800
H	2.33963300	-1.41826000	-2.23062900
H	-3.00051200	-1.33198900	-1.02100300

Int-**II**-water

N	1.02385100	0.89354300	-0.13662600
C	1.77820600	2.11654600	-0.44676000
C	-0.34480100	1.19947600	0.28089600
H	2.04809600	2.15339100	-1.50946800
H	2.71020100	2.13908300	0.12681100
C	0.83657600	3.26259800	-0.05620900
C	-0.56108800	2.65233200	-0.20156000
H	-0.45372000	1.13299100	1.36604400
H	0.97225100	4.14932700	-0.67760900
H	1.01156400	3.55236200	0.98362100
H	-0.87839000	2.66578400	-1.24774400
H	-1.32528800	3.15981300	0.38820100
C	1.66508500	-0.30448000	0.21138500
C	2.95726800	-0.54449700	-0.09535800
H	3.52253300	0.21931200	-0.62514600
C	3.72106800	-1.79796800	0.23581900
H	4.16187500	-2.24426100	-0.66505100
H	4.55849400	-1.59950600	0.91741600
H	3.08303600	-2.55403700	0.69317200
C	0.81123700	-1.31741900	1.00812800
O	0.60518200	-2.43513300	0.48841900
O	0.39455400	-0.89723000	2.12184100
C	-1.32016700	0.23738000	-0.33098800
C	-2.33665400	-1.05353000	-1.83819800
C	-3.03075000	-1.13773100	-0.67401600
H	-2.49118900	-1.52216700	-2.79411800
H	-3.91449000	-1.69653900	-0.41974000
N	-2.38674000	-0.33064800	0.25005100
N	-1.28685300	-0.19456000	-1.59903100
H	-0.55386900	0.04637000	-2.25126400

C	-2.75438700	-0.20070900	1.66636900
H	-3.04437400	0.82519300	1.88723600
H	-3.59619500	-0.86041600	1.85887300
H	-1.89596100	-0.50022600	2.26748200

Int-**III**-DCM

C	-2.23266500	-0.93855500	0.95812500
C	-4.03396400	-2.49428500	1.45227500
C	-2.81117800	-2.85030300	2.30142600
C	-2.07127400	-1.51042600	2.39034100
H	-2.21696200	0.15629300	0.97841800
H	-4.84895000	-2.11741500	2.09058300
H	-4.42702700	-3.34442600	0.88263900
H	-3.09258000	-3.25135200	3.27836200
H	-2.19326700	-3.59380300	1.78879900
H	-2.57339600	-0.84408400	3.10063900
H	-1.02513000	-1.60659900	2.69187600
C	-1.13204700	-1.43465600	0.03811400
N	0.12471800	-0.87499200	0.00653100
C	0.02517500	-2.60011400	-1.34932300
C	0.88169200	-1.62602000	-0.89684000
H	0.24794600	-3.38565100	-2.05946700
N	-1.21435300	-2.48133000	-0.76278000
C	0.60736400	0.28283300	0.75683600
H	0.10632700	0.29061100	1.72881000
H	1.66652600	0.11191300	0.96518700
C	2.30361200	-1.35896000	-1.21937500
C	3.35580500	-1.80020100	-0.34475900
C	2.62929200	-0.70760900	-2.39676600
C	3.10386600	-2.50624400	0.86471600
C	4.71901300	-1.53397500	-0.70721600
C	3.97494200	-0.45347500	-2.75199700
H	1.83307600	-0.38104000	-3.05823400
C	4.13910100	-2.91497400	1.67731800
H	2.07803500	-2.73049800	1.13909100
C	5.76296400	-1.96785700	0.15571500
C	4.99727000	-0.85184700	-1.92266600
H	4.19199100	0.06314500	-3.68224300
C	5.48251500	-2.64162500	1.32297600
H	3.92533100	-3.45595900	2.59476400
H	6.79117000	-1.75868500	-0.12787600
H	6.03315600	-0.65575200	-2.18672400
H	6.28886500	-2.96953700	1.97260400
C	0.43176900	1.62854300	0.06746300

C	0.97222100	2.80165300	0.69546700
C	-0.22653800	1.74647500	-1.13824200
C	1.65815100	2.76790200	1.94271600
C	0.81411400	4.07231500	0.04500000
C	-0.38193500	3.00370600	-1.77364700
H	-0.64718300	0.86764200	-1.61143600
C	2.16519000	3.91838200	2.50939800
H	1.78989200	1.82461800	2.46189600
C	1.35109700	5.23764900	0.65621100
C	0.12902600	4.14200100	-1.19932000
H	-0.90731400	3.05438700	-2.72302000
C	2.01231900	5.16669400	1.86193700
H	2.68638200	3.86636900	3.46099000
H	1.22697000	6.19150300	0.14998600
H	0.01819900	5.10913800	-1.68257800
H	2.41793100	6.06509100	2.31802400
N	-3.56102200	-1.43488500	0.55359600
C	-4.49534100	-0.64575400	-0.11229700
C	-5.83026500	-0.88465400	-0.12012700
H	-6.18944600	-1.74312600	0.43974900
C	-6.89063200	-0.15301000	-0.89374800
H	-7.44763700	-0.84827900	-1.53588500
H	-7.62977000	0.29926800	-0.21804200
H	-6.49630400	0.64385000	-1.52620500
C	-3.91253200	0.44063500	-0.97183000
O	-3.05457500	0.27103600	-1.81614700
O	-4.44502900	1.65337700	-0.71521200
H	-4.04415600	2.28003600	-1.34854600

Int-**IV**-DCM

C	-2.28318100	-0.80005400	1.08477100
C	-3.97406200	-2.38306100	1.78253000
C	-2.82651900	-2.43736000	2.78841000
C	-2.17686200	-1.06018700	2.61362300
H	-2.42785100	0.26484900	0.88120800
H	-4.84766600	-1.87214100	2.21848400
H	-4.30444200	-3.37392300	1.45284600
H	-3.17520800	-2.61419900	3.80899300
H	-2.12219200	-3.23510600	2.52767600
H	-2.76131800	-0.29495900	3.13352300
H	-1.14977200	-1.01143200	2.98377400
C	-1.03485100	-1.23943200	0.35491800
N	0.15245500	-0.60931900	0.26321600
C	0.35044600	-2.55000200	-0.79016400

C	1.04782000	-1.42154400	-0.46607000
H	0.64859200	-3.41471000	-1.36024100
N	-0.90872900	-2.41766800	-0.25492600
C	0.50323800	0.66414500	0.91246200
H	0.04703100	0.66280500	1.90611100
H	1.58340500	0.63243300	1.06617500
C	2.44232100	-1.04923800	-0.78133400
C	3.54127500	-1.87290100	-0.35036200
C	2.69059100	0.09116100	-1.52943000
C	3.38341300	-3.04012500	0.44781700
C	4.87239300	-1.48877800	-0.73127800
C	4.00519400	0.46716400	-1.88288900
H	1.85740800	0.69943200	-1.86562100
C	4.47175800	-3.79519200	0.82755000
H	2.39001300	-3.33688600	0.76419900
C	5.97217900	-2.29415200	-0.32568300
C	5.07255400	-0.31016000	-1.49819900
H	4.16120800	1.36629500	-2.47079200
C	5.77971900	-3.42542300	0.43331600
H	4.32490300	-4.68158300	1.43787100
H	6.97205600	-1.99374400	-0.62745800
H	6.08650900	-0.03494300	-1.77550300
H	6.62746000	-4.03255500	0.73682700
C	0.11421600	1.92296800	0.15179800
C	0.60843100	3.18146300	0.63822400
C	-0.70257100	1.88935000	-0.95980900
C	1.43604000	3.30206100	1.79044700
C	0.25636700	4.38081400	-0.06899600
C	-1.05890600	3.08257400	-1.63797900
H	-1.11184300	0.95234300	-1.33277400
C	1.89667300	4.53113100	2.21375100
H	1.70973400	2.41718500	2.35479900
C	0.75068800	5.63034800	0.39339900
C	-0.58787100	4.29920900	-1.21052600
H	-1.71917900	3.01481300	-2.49730100
C	1.55568000	5.70827800	1.50788600
H	2.52682800	4.59630900	3.09607300
H	0.47808400	6.52888800	-0.15419700
H	-0.85462700	5.21548800	-1.73052700
H	1.92637700	6.67021400	1.84973600
N	-3.43128500	-1.61604300	0.65027000
C	-4.31651600	-1.12161100	-0.34019500
C	-5.60421500	-1.53001000	-0.40480600
H	-5.96896800	-2.23825500	0.33638400

C	-6.60887700	-1.14619200	-1.45601200
H	-6.99037800	-2.03225400	-1.98420300
H	-7.48744100	-0.66125600	-1.00577500
H	-6.18427500	-0.45288900	-2.18230400
C	-3.66817600	-0.20042200	-1.39603500
O	-4.30744900	0.81069800	-1.76303400
O	-2.52422200	-0.57888300	-1.78888400
H	-1.71849700	-3.00244200	-0.42934600

Int-**III**-water

C	-2.24657100	-0.65069900	1.35227800
C	-4.13725200	-2.12192700	1.65823100
C	-3.07956700	-2.46489500	2.72621600
C	-2.15481300	-1.23715700	2.77778900
H	-2.04516300	0.42141000	1.36979100
H	-5.13558200	-1.96306600	2.08294400
H	-4.22357000	-2.93351900	0.92434200
H	-3.53179300	-2.67890500	3.69748200
H	-2.51716600	-3.35177700	2.42348000
H	-2.53195800	-0.49435200	3.48730700
H	-1.12830100	-1.48362600	3.05840900
C	-1.27952300	-1.30606700	0.38825900
N	0.02980300	-0.90280300	0.26778300
C	-0.36359800	-2.60198000	-1.06537700
C	0.62862800	-1.73394100	-0.68049200
H	-0.28098600	-3.41201700	-1.77713600
N	-1.53994500	-2.33979700	-0.39788500
C	0.64529000	0.27617800	0.87435200
H	0.22723800	0.40037600	1.87661600
H	1.70559200	0.05652600	1.01783000
C	2.02348800	-1.61351300	-1.15667200
C	3.14638000	-1.92480000	-0.31481400
C	2.24506200	-1.23180400	-2.46992900
C	3.00375100	-2.38267300	1.02471600
C	4.47164700	-1.78960100	-0.84970800
C	3.55282300	-1.12037900	-2.99637000
H	1.39289100	-1.00259800	-3.10199900
C	4.10691800	-2.66253700	1.80180700
H	2.00846400	-2.52141700	1.43320000
C	5.58804400	-2.08345300	-0.01940100
C	4.64348000	-1.38136200	-2.20002300
H	3.68756000	-0.81561900	-4.02959000
C	5.41318700	-2.50595300	1.27901200
H	3.97450600	-3.01246400	2.82118800

H	6.58583800	-1.97099700	-0.43475700
H	5.65242000	-1.28614700	-2.59187400
H	6.27371100	-2.72793600	1.90286500
C	0.48316800	1.55849700	0.07252100
C	1.08435600	2.76357900	0.56902000
C	-0.22787100	1.59262100	-1.10866300
C	1.83322900	2.81254500	1.77880900
C	0.93001900	3.97731900	-0.18250400
C	-0.38589000	2.79523800	-1.84187400
H	-0.68435700	0.68664700	-1.49112800
C	2.40071000	3.99046900	2.21715300
H	1.96531800	1.91228900	2.36926500
C	1.52808400	5.17332000	0.29860400
C	0.18204300	3.96261800	-1.39203700
H	-0.96208600	2.78162900	-2.76188800
C	2.24933300	5.18325500	1.47156100
H	2.96988900	4.00352400	3.14182700
H	1.40385400	6.08368800	-0.28164600
H	0.06882600	4.88854300	-1.94899700
H	2.70239600	6.10351800	1.82770400
N	-3.66817600	-0.87497000	1.03098400
C	-4.22576200	-0.48427700	-0.19320000
C	-5.26462200	-1.11632400	-0.79305800
H	-5.64206800	-2.01612600	-0.31748400
C	-6.02580600	-0.69216100	-2.01536700
H	-5.84522700	-1.38478000	-2.84873100
H	-7.10440500	-0.72558600	-1.81829100
H	-5.77201800	0.31032100	-2.36152600
C	-3.70971100	0.78763600	-0.79154200
O	-3.48932300	0.95497900	-1.98240500
O	-3.53055900	1.77101800	0.11533300
H	-3.15846100	2.54083800	-0.35457600

Int-**IV**-water

C	-2.07156600	-1.09072300	1.05013700
C	-3.59849000	-2.83729900	1.73990800
C	-2.45447500	-2.77308500	2.74723000
C	-1.95778000	-1.33349000	2.58012500
H	-2.33464200	-0.04959800	0.84281900
H	-4.51386000	-2.40506600	2.17212700
H	-3.83409600	-3.85493500	1.41389500
H	-2.78742900	-2.98863600	3.76500600
H	-1.66731700	-3.48830500	2.48629900
H	-2.63150900	-0.63630700	3.08658300

H	-0.94700000	-1.16802200	2.95945800
C	-0.77136500	-1.38909600	0.34308300
N	0.32402800	-0.60883500	0.25039400
C	0.78556700	-2.51444900	-0.78094900
C	1.32101400	-1.29891800	-0.46551400
H	1.20298600	-3.34217700	-1.33014800
N	-0.48901200	-2.54266600	-0.26491300
C	0.48135100	0.72250500	0.85734100
H	0.04864600	0.67853600	1.85942100
H	1.55544100	0.86801500	0.98972300
C	2.65892400	-0.75455500	-0.77123400
C	3.84292100	-1.41684100	-0.29397200
C	2.77223500	0.38342500	-1.55342100
C	3.81498800	-2.56883500	0.54026100
C	5.12143300	-0.87956500	-0.66766800
C	4.03535700	0.91170300	-1.90027300
H	1.87423000	0.87061300	-1.91835100
C	4.98224100	-3.16778700	0.96148100
H	2.86020100	-2.97674000	0.85237300
C	6.30565400	-1.52525000	-0.21739600
C	5.18488600	0.28892100	-1.47284200
H	4.08798500	1.80349000	-2.51653200
C	6.24087600	-2.64748900	0.57605000
H	4.93696600	-4.04547900	1.59917400
H	7.26506600	-1.10994800	-0.51306900
H	6.16083600	0.68140800	-1.74436400
H	7.15144200	-3.13294400	0.91360400
C	-0.11923500	1.87585800	0.07326200
C	0.00613500	3.19675200	0.62242600
C	-0.78046300	1.69438700	-1.12275300
C	0.67381900	3.46726400	1.85028600
C	-0.56764000	4.30008700	-0.09480700
C	-1.35269800	2.78756000	-1.82015800
H	-0.88980400	0.70258600	-1.54626300
C	0.76892500	4.75295500	2.33995700
H	1.11931800	2.65648300	2.41656400
C	-0.44935200	5.61194700	0.43810200
C	-1.24736600	4.06228400	-1.32143800
H	-1.88343900	2.59840000	-2.74779100
C	0.20382800	5.83741500	1.62923900
H	1.28298900	4.93494300	3.27895600
H	-0.88838400	6.43691600	-0.11632300
H	-1.68363300	4.90561000	-1.84941400
H	0.28720100	6.84466600	2.02602100

N	-3.12834700	-2.02435600	0.60201700
C	-4.07388400	-1.58112100	-0.35032900
C	-5.34277900	-2.03900600	-0.39606500
H	-5.66967400	-2.76589900	0.34303600
C	-6.36819800	-1.67774700	-1.43540700
H	-6.69992500	-2.56332900	-1.99468900
H	-7.27021000	-1.25588000	-0.97160400
H	-5.99536100	-0.94503700	-2.15426800
C	-3.52474100	-0.62433000	-1.41376800
O	-4.03669000	0.52821000	-1.48261400
O	-2.59111100	-1.07672800	-2.13803700
H	-1.18201300	-3.27508300	-0.37489000

TS-**I**-*R*-DCM

N	0.00165700	-2.75058600	1.60535700
C	-1.03845200	-2.17125600	2.49271000
C	0.35213900	-1.80768000	0.50538500
H	-0.63688000	-2.07668300	3.50572700
H	-1.89813500	-2.84369700	2.52493700
C	-1.39538900	-0.82168900	1.85355000
C	-0.94066900	-0.97105500	0.39487100
H	0.53474700	-2.37281000	-0.40848100
H	-0.83944800	-0.01853100	2.34116400
H	-2.46311600	-0.60804600	1.93878000
H	-0.76577500	-0.01840600	-0.10767300
H	-1.67722800	-1.53636100	-0.18551200
C	0.50382900	-3.97285500	1.77492500
C	0.02039400	-4.89678500	2.73069100
H	-0.68425000	-4.48721300	3.44791300
C	0.97494500	-5.93096800	3.30267700
H	1.36406700	-6.60006400	2.53068900
H	1.82625400	-5.45272200	3.80097700
H	0.46509900	-6.54714700	4.04604700
C	1.64098700	-4.38889600	0.84003900
O	2.65479600	-3.71150900	0.78375900
O	1.46674900	-5.47577400	0.13043400
H	0.59939800	-6.06097600	0.35716000
C	-1.24073600	-6.11075500	1.48016000
O	-0.42999800	-6.86427100	0.83668300
C	-1.98344900	-6.71829300	2.68256800
O	-2.88287800	-6.14947700	3.27761000
O	-1.54625700	-7.94623700	2.97883900
C	-2.10388600	-5.12683700	0.69551800
C	-3.07445400	-5.89364900	-0.23841100

H	-1.46141700	-4.49069000	0.08122500
H	-2.67679100	-4.49195800	1.37299000
H	-2.48351300	-6.54177800	-0.89325300
H	-3.72091900	-6.54226900	0.36379800
C	-2.20308700	-8.60932500	4.09427500
H	-2.06363400	-8.00247100	4.99410200
H	-3.27554300	-8.66266000	3.88501700
C	-1.58416900	-9.98314100	4.23467100
H	-0.51199200	-9.91450900	4.44208800
H	-2.06122000	-10.51308000	5.06528300
H	-1.72644800	-10.57353500	3.32455100
C	-3.92645600	-4.95460600	-1.06406900
C	-5.17099200	-4.50992300	-0.59405100
C	-3.47583700	-4.48101800	-2.30546200
C	-5.94369700	-3.61861800	-1.34129200
H	-5.53816000	-4.86982700	0.36426100
C	-4.24501700	-3.58913700	-3.05571600
H	-2.51697000	-4.82091300	-2.68987900
C	-5.48265100	-3.15417900	-2.57549700
H	-6.90749300	-3.29028300	-0.96162500
H	-3.88010100	-3.23876600	-4.01741900
H	-6.08400200	-2.46326300	-3.15951500
C	1.56520100	-0.97948100	0.86269300
C	2.95529000	0.24759600	1.94347900
C	3.48365300	0.12844600	0.67681200
N	2.56898400	-0.66727300	-0.01816900
N	1.77230200	-0.44041500	2.05189900
C	2.64468500	-1.05933400	-1.42383200
H	3.69771700	-1.04644000	-1.71268400
H	2.32782200	-2.10216000	-1.49316100
C	1.84301700	-0.18578400	-2.37807400
C	1.69617300	-0.60447900	-3.74379200
C	1.27773300	1.00506200	-1.97087400
C	2.26633800	-1.80586400	-4.25303300
C	0.94372000	0.22215600	-4.64616400
C	0.54131700	1.81930300	-2.86619100
H	1.39582000	1.33179500	-0.94351200
C	2.09743400	-2.17247800	-5.57148200
H	2.84912500	-2.44735500	-3.60109900
C	0.78697300	-0.18799200	-5.99800400
C	0.37293700	1.43590600	-4.17440600
H	0.11166000	2.74944700	-2.50602500
C	1.34929600	-1.35888900	-6.45439000
H	2.54277000	-3.09358100	-5.93618700

H	0.21307000	0.44672300	-6.66822900
H	-0.19246400	2.05296400	-4.86744100
H	1.22285800	-1.65977100	-7.49028500
H	3.38959500	0.77211800	2.78394400
C	4.76623000	0.60817900	0.11988900
C	5.06920900	2.01245700	0.04295200
C	5.71346900	-0.31324600	-0.30365200
C	4.15764500	3.02796000	0.44655000
C	6.34869400	2.41638100	-0.47110100
C	6.96328100	0.09361700	-0.82202900
H	5.49745400	-1.37389100	-0.21503700
C	4.49230500	4.36166500	0.35917600
H	3.18524100	2.73882700	0.82904400
C	6.66222600	3.80173200	-0.54459500
C	7.27616400	1.43053400	-0.90216500
H	7.67704300	-0.65882600	-1.14382200
C	5.75818200	4.75575300	-0.13706100
H	3.77859800	5.11837200	0.67217000
H	7.63572900	4.09185900	-0.93125900
H	8.23811100	1.75330800	-1.29138800
H	6.01025300	5.81048000	-0.19791700

TS-**I**-*S*-DCM

N	5.20407200	-2.99204600	1.73221000
C	5.87545500	-2.50238000	2.96311900
C	3.78046400	-3.33402100	1.99297000
H	6.30057600	-1.51205600	2.78104300
H	6.68012300	-3.19805600	3.21041700
C	4.77554100	-2.50618700	4.02930900
C	3.78493800	-3.56239300	3.52157800
H	3.51643000	-4.24452000	1.45196400
H	4.29393900	-1.52627200	4.08074800
H	5.17458700	-2.74526800	5.01746000
H	2.78774700	-3.46072700	3.95411100
H	4.15341900	-4.57262700	3.72630600
C	5.81231900	-3.09390400	0.56130400
C	7.20532700	-2.91614600	0.37558000
H	7.71370900	-2.44699300	1.21452600
C	7.73092500	-2.44322700	-0.96575500
H	8.81705400	-2.55641000	-1.00958000
H	7.29525100	-2.97661200	-1.81388400
H	7.51152600	-1.37705300	-1.10502700
C	5.00344800	-3.70261100	-0.58160100
O	4.46031400	-2.99722800	-1.41617900

O	4.98267600	-5.01091300	-0.55854500
H	5.70303400	-5.41550100	0.21088100
C	7.69685200	-5.02177500	0.65911700
O	6.64690300	-5.63833400	1.09571200
C	8.80392600	-4.72173000	1.67005500
O	9.92000700	-4.35154400	1.34995500
O	8.42227100	-4.93769400	2.93710300
C	8.23466400	-5.41254800	-0.71293900
C	8.69869700	-6.89343100	-0.69260600
H	9.07170500	-4.77720100	-0.99992200
H	7.44213700	-5.30414300	-1.45736300
H	9.48493800	-7.01527300	0.06121000
H	7.85342900	-7.51751900	-0.38568500
C	9.43055200	-4.70189500	3.95872600
H	10.33518400	-5.25387300	3.68955200
H	9.67519600	-3.63494300	3.96759000
C	8.86055900	-5.16431900	5.28258300
H	8.61371200	-6.22994800	5.25307200
H	9.60326300	-5.00647800	6.07128300
H	7.95820500	-4.60494200	5.54805900
C	9.21675300	-7.34290300	-2.04118200
C	8.34217900	-7.85532400	-3.01109300
C	10.57658400	-7.22768900	-2.36465500
C	8.81180400	-8.24146600	-4.26790200
H	7.28507900	-7.95529300	-2.77610500
C	11.05068500	-7.61324500	-3.62033500
H	11.26877500	-6.83554000	-1.62320900
C	10.16889600	-8.12110600	-4.57734800
H	8.11858900	-8.63962900	-5.00391400
H	12.10880600	-7.51998100	-3.84974200
H	10.53597600	-8.42404900	-5.55394800
C	2.88525000	-2.18878700	1.57284300
N	1.53269500	-2.31235600	1.36670800
N	3.29192900	-0.93967000	1.43489300
C	1.05097200	-1.02765200	1.09093500
C	0.71709900	-3.51450600	1.55597400
C	2.16374500	-0.21660300	1.13806600
C	-0.35940200	-0.70463700	0.79562900
H	1.08638900	-4.03901400	2.44243000
H	-0.29088000	-3.17253200	1.80311200
C	0.65889000	-4.47121200	0.37396300
H	2.20260700	0.84788000	0.95108500
C	-1.06097100	0.29983500	1.55485600
C	-1.01623300	-1.34426400	-0.24588300

C	-0.19019600	-5.62587500	0.47000100
C	1.38528500	-4.25748300	-0.77846700
C	-0.48956500	0.97945500	2.66715000
C	-2.41253700	0.62377200	1.18916700
C	-2.35176000	-1.03248500	-0.58413700
H	-0.48644200	-2.08882500	-0.83042800
C	-0.96600900	-5.92402000	1.62575300
C	-0.26481200	-6.52691600	-0.64551800
C	1.31279200	-5.15431800	-1.87338200
H	2.03623200	-3.39497000	-0.86031800
C	-1.19784000	1.93748400	3.35969200
H	0.52029900	0.73229300	2.97303700
C	-3.11193900	1.62296100	1.92099900
C	-3.03388900	-0.06204200	0.11160800
H	-2.82710800	-1.55539200	-1.40866000
C	-1.77321600	-7.04114400	1.67448200
H	-0.92787100	-5.26547100	2.48673600
C	-1.10879400	-7.66711600	-0.56248300
C	0.50230600	-6.26095400	-1.81354800
H	1.90968700	-4.95302500	-2.75772100
C	-2.51988800	2.27099800	2.98064600
H	-0.73855500	2.43875800	4.20693500
H	-4.13036700	1.86215400	1.62588100
H	-4.05697600	0.19420700	-0.15047000
C	-1.84762700	-7.92291900	0.57121800
H	-2.35637600	-7.24697900	2.56749400
H	-1.15695100	-8.33888800	-1.41566400
H	0.43903000	-6.95170000	-2.65012400
H	-3.06504600	3.03184400	3.53172500
H	-2.48793500	-8.79880500	0.62162000

TS-**II**-*R*-DCM

N	2.87739900	-0.78109800	0.45649000
C	3.84331900	0.28516700	0.07405100
C	1.69876400	-0.22736500	1.15356800
H	4.15496200	0.15550000	-0.95980000
H	4.71569500	0.21216000	0.73508700
C	3.06550200	1.58161900	0.30621400
C	2.11027900	1.23169700	1.45542700
H	1.52812700	-0.79160200	2.07391100
H	2.50160800	1.84647700	-0.59423900
H	3.72664900	2.41633100	0.54957600
H	1.25117300	1.89952200	1.53088200
H	2.63981000	1.24593200	2.41306500

C	3.09785800	-2.09502200	0.36708500
C	4.12997500	-2.61091000	-0.45394100
H	4.96033900	-1.92616500	-0.61691500
C	4.55705200	-4.05352300	-0.27983900
H	5.12947400	-4.39232400	-1.14817800
H	5.19860600	-4.17123500	0.60305900
H	3.70033600	-4.72106200	-0.15517600
C	2.13694100	-3.01889700	1.14364200
O	1.15705100	-3.48846300	0.52535200
O	2.48310800	-3.15200100	2.33898400
C	0.48104600	-0.36271400	0.26598500
C	-0.76961200	-0.69453400	-1.51310300
C	-1.62989600	-0.49964500	-0.46741700
N	-0.81314000	-0.28131800	0.65464600
N	0.51759900	-0.60627500	-1.04293300
H	1.44647900	-0.86104600	-1.62207700
C	-1.27730400	-0.03029400	2.02384300
H	-2.14493700	-0.67058000	2.19178100
H	-0.49792400	-0.38783000	2.70065200
C	3.22342600	-2.27385300	-2.31906000
O	2.65242900	-1.11686600	-2.32368800
C	4.57187900	-2.34054400	-3.04340900
O	5.05535100	-3.36542900	-3.49516100
O	5.16942500	-1.14014800	-3.13372800
C	2.36456600	-3.51861500	-2.52361000
C	1.65674200	-3.47374200	-3.90026400
H	1.62815200	-3.56778600	-1.71642000
H	2.98307400	-4.41600300	-2.47157200
H	1.02343000	-2.58061600	-3.94016200
H	2.40889200	-3.36606200	-4.69013700
C	6.46180500	-1.11949200	-3.79407300
H	7.14727100	-1.77559700	-3.24842700
H	6.34624300	-1.52188800	-4.80498500
C	6.94616700	0.31492700	-3.81128300
H	7.06545000	0.70526800	-2.79579200
H	7.91755000	0.36498600	-4.31369100
H	6.24739800	0.96003500	-4.35279700
C	0.82728000	-4.71133400	-4.16737800
C	1.32880300	-5.75478500	-4.95895600
C	-0.45207900	-4.85895000	-3.60889200
C	0.57715500	-6.90909600	-5.19041200
H	2.31855500	-5.65886000	-5.39927100
C	-1.20656000	-6.01110800	-3.83622800
H	-0.86086200	-4.06353100	-2.99025500

C	-0.69485800	-7.04138600	-4.62958000
H	0.98497300	-7.70296800	-5.81051900
H	-2.19586500	-6.10322800	-3.39591100
H	-1.28235400	-7.93736700	-4.80968000
C	-1.62866300	1.41608300	2.33075300
C	-2.08919300	1.73400100	3.65272500
C	-1.52193600	2.41752700	1.38863100
C	-2.23563400	0.75780400	4.67853100
C	-2.42221900	3.09626900	3.95993100
C	-1.85181600	3.76045200	1.69797000
H	-1.18563800	2.18343600	0.38476100
C	-2.68166300	1.10797000	5.93539400
H	-1.99553100	-0.28063300	4.47690300
C	-2.87723300	3.42187900	5.26620000
C	-2.29015600	4.09440100	2.95573900
H	-1.75564400	4.52057400	0.92849100
C	-3.00569300	2.45182100	6.23497300
H	-2.78511400	0.34575800	6.70221000
H	-3.12466300	4.45730100	5.48522100
H	-2.54524700	5.12151200	3.20179800
H	-3.35461500	2.71446400	7.22934600
H	-0.98767000	-0.91127400	-2.54699900
C	-3.10729600	-0.57146400	-0.42532600
C	-3.92042400	0.37862000	-1.13269900
C	-3.70918600	-1.60179100	0.27976800
C	-3.38314700	1.46099900	-1.88353000
C	-5.34821800	0.23230600	-1.07722500
C	-5.11477100	-1.73124900	0.33577400
H	-3.08844400	-2.33666300	0.78400200
C	-4.20760000	2.34405600	-2.54574800
H	-2.30724100	1.58642100	-1.93452100
C	-6.16906900	1.16174400	-1.77354600
C	-5.91660800	-0.83304900	-0.32887300
H	-5.55260100	-2.55042600	0.89768100
C	-5.61437800	2.19469100	-2.49381300
H	-3.77512900	3.16346900	-3.11257700
H	-7.24761500	1.03813300	-1.72468800
H	-6.99848000	-0.92843100	-0.29619900
H	-6.25146200	2.89815200	-3.02172100

TS-**II**-*S*-DCM

N	-4.51041800	-0.51368100	-2.47903400
C	-5.37538000	-1.69142600	-2.73946900
C	-4.32490500	-0.32046000	-1.02027200

H	-4.75753600	-2.57625100	-2.90969800
H	-5.98542700	-1.51000600	-3.62427100
C	-6.20113100	-1.80122200	-1.45891600
C	-5.19825200	-1.42437500	-0.36254900
H	-4.68755900	0.67931900	-0.76686600
H	-6.61636600	-2.80244800	-1.32038700
H	-7.02868500	-1.08480300	-1.48663500
H	-4.58219800	-2.28921900	-0.10122500
H	-5.67057000	-1.05827100	0.55003600
C	-4.15038200	0.40337100	-3.38384600
C	-4.13848500	0.08606600	-4.76698600
H	-4.78105200	-0.74639000	-5.04282300
C	-4.15793700	1.20765700	-5.78664900
H	-3.87420200	0.84305900	-6.77676600
H	-5.16856300	1.62984700	-5.87177300
H	-3.47275500	2.01047000	-5.51379500
C	-3.68471800	1.79595800	-2.88072200
O	-2.54059100	2.16312900	-3.21673900
O	-4.56031500	2.39625500	-2.21116600
C	-2.86401900	-0.42365900	-0.66822600
C	-0.72907700	-0.93301800	-0.78131000
C	-0.91738600	-0.32591300	0.43085600
N	-2.28526500	-0.01103400	0.48438900
N	-1.93268400	-0.98022300	-1.44029900
H	-2.09317500	-1.32163900	-2.50173100
C	-2.98704800	0.64578700	1.59342600
H	-2.30161000	1.38021600	2.02025000
H	-3.81334200	1.21156600	1.15725400
C	-2.45353000	-1.12676600	-4.85155000
O	-2.38907800	-1.84371400	-3.78268100
C	-1.39127600	-0.04423900	-5.08344000
O	-1.27147100	0.56199700	-6.13440300
O	-0.55253600	0.09420700	-4.04735200
C	-2.73824200	-1.88585800	-6.16192200
C	-3.65802700	-3.10570600	-5.99617100
H	-1.76257300	-2.23340600	-6.53122000
H	-3.11963900	-1.20827300	-6.92891800
H	-3.22585400	-3.76833300	-5.24089200
H	-4.63376500	-2.78464700	-5.61441700
C	0.41861600	1.16421600	-4.18690000
H	0.98621800	1.00370000	-5.10847000
H	-0.13323200	2.10258000	-4.27647300
C	1.31841100	1.15776100	-2.97035000
H	1.85291000	0.20727200	-2.87283600

H	2.06309500	1.95472500	-3.07005100
H	0.74781400	1.33744900	-2.05532200
C	-3.85357500	-3.85805700	-7.29599800
C	-4.84810400	-3.47184000	-8.20732100
C	-3.03178700	-4.94368500	-7.63275800
C	-5.01685200	-4.14680300	-9.41760700
H	-5.49906000	-2.63542100	-7.96309800
C	-3.19640300	-5.62244100	-8.84243800
H	-2.25844500	-5.26208500	-6.93740500
C	-4.19018800	-5.22592300	-9.74019000
H	-5.79630700	-3.83222700	-10.10645900
H	-2.55133900	-6.46375400	-9.08148600
H	-4.32217800	-5.75464600	-10.68002100
C	-3.49275700	-0.28901100	2.68040700
C	-4.28720900	0.27034700	3.73761200
C	-3.20661900	-1.63795500	2.68596700
C	-4.61847000	1.65311700	3.81113400
C	-4.77453400	-0.59903800	4.77120300
C	-3.68469400	-2.48961400	3.71222900
H	-2.60382700	-2.06860700	1.89406400
C	-5.39184700	2.14584500	4.84081000
H	-4.25792600	2.33855000	3.05169000
C	-5.57021600	-0.05750600	5.81678700
C	-4.45382100	-1.98384200	4.73121200
H	-3.43615500	-3.54623400	3.68261900
C	-5.87512700	1.28469100	5.85354700
H	-5.63198900	3.20448700	4.87517100
H	-5.93361800	-0.72824500	6.59096400
H	-4.82675500	-2.63030700	5.52092100
H	-6.48437100	1.68603900	6.65803400
H	0.17892900	-1.30472500	-1.22718400
C	0.06680200	0.03121400	1.47592700
C	0.79668300	-0.98427600	2.18407400
C	0.31595400	1.36869000	1.74150700
C	0.60086400	-2.37787400	1.97461900
C	1.76978200	-0.57411200	3.15779500
C	1.26732800	1.76117800	2.70935400
H	-0.21681300	2.13190700	1.18186700
C	1.32950900	-3.31167100	2.67840600
H	-0.13275200	-2.70598000	1.24671200
C	2.50542100	-1.56512900	3.86430800
C	1.98018500	0.80965400	3.40074400
H	1.43714000	2.81779700	2.89161400
C	2.29401800	-2.90460900	3.63116200

H	1.16221900	-4.37027200	2.50202200
H	3.24080400	-1.24022000	4.59549600
H	2.71901100	1.10246800	4.14171900
H	2.86234900	-3.65185200	4.17709000

TS-**III**-*R*-DCM

N	4.45846700	0.85058900	-0.78532400
C	4.63184300	2.08337700	0.03444800
C	4.30484200	1.18387500	-2.23393700
H	5.67764600	2.18021400	0.33310800
H	4.00956900	2.00578100	0.92883800
C	4.19818300	3.20294100	-0.91077800
C	4.64574100	2.69186500	-2.28155800
H	3.26089900	1.03394200	-2.51975400
H	4.66082700	4.15585500	-0.64561700
H	3.11097600	3.32671200	-0.88059000
H	5.72616400	2.81882600	-2.39978200
H	4.14515700	3.17868300	-3.11916300
C	4.35023500	-0.37318600	-0.25770600
C	4.81510800	-0.67663700	1.03472800
H	4.97745400	0.19295400	1.66413300
C	4.40392300	-1.91755100	1.80847900
H	4.13021100	-2.72500100	1.12509400
H	5.26603700	-2.26584000	2.38525200
C	3.77370800	-1.48253900	-1.12216400
O	4.32967600	-2.53763700	-1.34423100
C	5.20265500	0.33195000	-3.09363500
C	6.94507500	-0.76454700	-3.78972000
C	6.05526500	-0.76793000	-4.83510000
H	7.91990200	-1.22619400	-3.74393400
N	4.94002800	-0.06015600	-4.37155100
N	6.40938500	-0.08605200	-2.72398800
H	6.91491700	0.03921200	-1.38408000
C	3.72116600	0.22333500	-5.13582000
H	3.55737100	-0.62430300	-5.80369800
H	2.88639300	0.22635900	-4.43019200
C	3.26359800	-1.63777100	2.77892600
C	3.51297600	-1.53673900	4.15391500
C	1.94903800	-1.46436200	2.32123200
C	2.47535700	-1.27644300	5.05273900
H	4.52738800	-1.66789900	4.52246900
C	0.91002600	-1.20615500	3.21625800
H	1.73832500	-1.53220700	1.25702900
C	1.17014600	-1.11113000	4.58648100

H	2.68798500	-1.20653500	6.11591200
H	-0.10355800	-1.08135300	2.84521500
H	0.36118200	-0.91189000	5.28339100
O	2.54720100	-1.15752400	-1.54099400
C	1.81747400	-2.18286100	-2.29456200
C	0.39518200	-1.69854900	-2.46236800
H	1.87137900	-3.11828000	-1.73311700
H	2.32620100	-2.32483200	-3.25192700
H	-0.16979800	-2.44757000	-3.02595800
H	-0.09221900	-1.56227900	-1.49253100
H	0.35304100	-0.75365400	-3.01240400
C	6.98628900	-0.74621300	0.48879800
O	7.18061000	0.23618400	-0.33904000
C	7.37039400	-0.44271600	1.93378300
O	7.53397300	-1.32261900	2.75979900
O	7.50755300	0.86146500	2.16711300
C	7.20557000	-2.17384000	0.05146900
C	8.72205400	-2.44656200	-0.16968000
H	6.65333100	-2.37029600	-0.86792500
H	6.83382500	-2.85170100	0.81986900
H	9.08898200	-1.80468400	-0.97706700
H	9.27222600	-2.17573500	0.73729800
C	7.89026100	1.23809700	3.52506400
H	7.14353700	0.83817800	4.21674000
H	8.85239500	0.77018300	3.75045400
C	7.96533300	2.74786800	3.57472200
H	6.99554600	3.20067900	3.34732800
H	8.26001300	3.05869300	4.58196000
H	8.70698100	3.13087300	2.86742300
C	8.97905600	-3.90020100	-0.50281600
C	9.12067000	-4.85041400	0.51957200
C	9.05322800	-4.33376300	-1.83364000
C	9.33123800	-6.19718500	0.21986600
H	9.06903100	-4.52907100	1.55726100
C	9.26399000	-5.68043800	-2.13759000
H	8.95086000	-3.60928900	-2.63803500
C	9.40335100	-6.61690500	-1.11101800
H	9.44322200	-6.91830800	1.02486800
H	9.32329800	-5.99642900	-3.17549400
H	9.57043700	-7.66431600	-1.34555700
C	6.14265500	-1.41420100	-6.16315400
C	7.11030200	-0.98220000	-7.13386100
C	5.29668700	-2.47135700	-6.46035100
C	8.01759300	0.09000100	-6.90807100

C	7.16335800	-1.66270500	-8.39766700
C	5.35202000	-3.12973200	-7.70935500
H	4.58839000	-2.81386500	-5.71148100
C	8.92752500	0.46546400	-7.87184200
H	7.98967700	0.61555100	-5.96023400
C	8.11531100	-1.24850700	-9.36963100
C	6.26612000	-2.73283600	-8.65737900
H	4.67525500	-3.95495200	-7.90837900
C	8.98044000	-0.20927000	-9.11520800
H	9.61005600	1.28775900	-7.67766300
H	8.14495700	-1.77300300	-10.32094200
H	6.32004500	-3.23631400	-9.61874100
H	9.70300100	0.09786200	-9.86542400
C	3.74566400	1.51354100	-5.93779400
C	2.57746000	1.85635600	-6.69785400
C	4.84662100	2.34320800	-5.96696000
C	1.40564200	1.04818800	-6.72515700
C	2.58627200	3.06571500	-7.47096000
C	4.84930800	3.53567700	-6.73277800
H	5.73718500	2.08222100	-5.40522000
C	0.30603300	1.41506000	-7.47193000
H	1.36956700	0.12436200	-6.15708200
C	1.43484200	3.41380300	-8.22774300
C	3.74476800	3.89064900	-7.46798100
H	5.73569900	4.16281600	-6.73415300
C	0.31776500	2.60864900	-8.23074900
H	-0.57651900	0.78210500	-7.47956300
H	1.45489700	4.33220300	-8.80822700
H	3.73964300	4.80244900	-8.05900200
H	-0.55491500	2.88507900	-8.81499300

TS-**III**-*S*-DCM

N	2.81594400	-1.32755000	-5.39081500
C	1.75213000	-2.27426200	-5.83426300
C	3.93602500	-1.28071400	-6.38160000
H	0.93854300	-1.71340500	-6.29845700
H	1.36981500	-2.81815700	-4.96896500
C	2.47651700	-3.16482300	-6.84020800
C	3.43746100	-2.19467500	-7.53066800
H	4.82858600	-1.72024500	-5.92833700
H	1.78019100	-3.63307600	-7.53906500
H	3.02737200	-3.95514500	-6.32012600
H	2.90091100	-1.59109100	-8.26834700
H	4.27390000	-2.68397200	-8.02949100

C	2.80800700	-0.71120400	-4.20628500
C	1.62459400	-0.51797400	-3.46158100
H	0.80976500	-1.17785400	-3.73944600
C	1.65366800	-0.18433900	-1.97554900
H	2.51819300	0.43891100	-1.73552900
H	0.77466900	0.42225000	-1.74415700
C	4.09259700	-0.04449800	-3.73362400
O	4.17929100	1.16238300	-3.66211200
C	4.23182700	0.12964100	-6.81943800
C	3.95374500	2.20545300	-7.39972400
C	5.26949900	1.91373100	-7.65916400
H	3.43800900	3.14352100	-7.52864500
N	5.43242500	0.57485100	-7.28105300
N	3.32849800	1.10111600	-6.87961000
H	2.08812400	1.03929300	-6.30443700
C	6.67280900	-0.20415800	-7.36810500
H	7.49932000	0.49850100	-7.24521600
H	6.70438300	-0.86601900	-6.49937100
C	1.65254200	-1.42223400	-1.08883300
C	2.76839600	-1.74023600	-0.30300300
C	0.52988100	-2.26212400	-1.02607700
C	2.76757800	-2.86967800	0.52101700
H	3.63932200	-1.09007100	-0.32511600
C	0.52643700	-3.39134300	-0.20633200
H	-0.35309200	-2.02373400	-1.61442800
C	1.64782400	-3.70125700	0.56859100
H	3.64049300	-3.09495000	1.12739700
H	-0.35427900	-4.02641900	-0.16774700
H	1.64382900	-4.57831500	1.20932200
O	5.12850900	-0.81781600	-3.39289500
C	5.01641600	-2.26227800	-3.16556900
C	6.15110600	-2.65329400	-2.24381000
H	5.10060100	-2.77415300	-4.12742500
H	4.04491000	-2.48292600	-2.72019500
H	6.11107400	-3.73231400	-2.06503700
H	7.12012500	-2.41464000	-2.69153200
H	6.07304600	-2.14041200	-1.28140400
C	0.72894200	1.03983700	-4.67241400
O	1.05056100	0.80708800	-5.90871000
C	1.27724100	2.28136900	-3.96161200
O	0.94423200	2.57961500	-2.82944300
O	2.05813400	3.02362200	-4.74561600
C	-0.72556100	0.75018700	-4.33778900
C	-1.65426800	1.81936200	-4.97488400

H	-0.87403400	0.74097700	-3.25707000
H	-0.98475100	-0.23359000	-4.73764400
H	-1.38131300	2.80888300	-4.59190600
H	-1.48781600	1.82774900	-6.05656800
C	2.59532100	4.23467300	-4.12844900
H	1.78002400	4.74072200	-3.60640700
H	3.33956800	3.92488900	-3.38997900
C	3.19432400	5.10436400	-5.21102100
H	2.44550600	5.37017300	-5.96358300
H	3.55917000	6.03066800	-4.75521400
H	4.03717200	4.61377100	-5.70419700
C	-3.11163200	1.54407500	-4.67390400
C	-3.90058300	0.79790500	-5.56094800
C	-3.69656100	2.00781500	-3.48625200
C	-5.23874000	0.52262600	-5.27103600
H	-3.46409200	0.43681000	-6.48936000
C	-5.03352100	1.73426800	-3.19274600
H	-3.09952400	2.59287500	-2.79064000
C	-5.80938000	0.98984300	-4.08492500
H	-5.83616600	-0.05197200	-5.97357400
H	-5.47057400	2.10705700	-2.27047500
H	-6.85092500	0.77954400	-3.85924800
C	6.36741800	2.78010300	-8.14123500
C	6.34849900	3.34224500	-9.46362100
C	7.41757100	3.07491500	-7.28510500
C	5.30800100	3.09657900	-10.40245400
C	7.43689900	4.19063100	-9.86289000
C	8.48739900	3.90411300	-7.69012700
H	7.40960200	2.67472800	-6.27536000
C	5.33625000	3.66180700	-11.65857800
H	4.47962900	2.45723500	-10.11818200
C	7.43350100	4.75729100	-11.16717100
C	8.49624100	4.44990400	-8.95256100
H	9.29350400	4.11312900	-6.99369600
C	6.40732000	4.50178900	-12.04748400
H	4.53077400	3.46019000	-12.35872700
H	8.26229000	5.39852600	-11.45470000
H	9.31221000	5.09262200	-9.27190700
H	6.41583500	4.94077600	-13.04069000
C	6.85136300	-0.99405100	-8.65467700
C	7.96973200	-1.88879100	-8.75508100
C	5.98593100	-0.86454200	-9.72069400
C	8.91721800	-2.06871600	-7.70790400
C	8.15257500	-2.63347700	-9.96893200

C	6.17324800	-1.59994500	-10.91688300
H	5.14438800	-0.18384800	-9.65350700
C	9.97491700	-2.94230100	-7.84665400
H	8.81570200	-1.50990300	-6.78379100
C	9.25172400	-3.52766400	-10.07660200
C	7.22994200	-2.46869900	-11.03824500
H	5.47110700	-1.46949800	-11.73482300
C	10.14581300	-3.68092600	-9.04075900
H	10.68603300	-3.06208600	-7.03447100
H	9.37461100	-4.08734000	-11.00008800
H	7.38076300	-3.03688600	-11.95202200
H	10.98260300	-4.36641300	-9.13673300

TS-**I**-*R*-water

N	0.25145800	1.22315200	1.53991700
C	0.67867700	2.53746600	2.09088700
C	1.08534800	0.83340200	0.36973000
H	0.94260100	2.41951700	3.14527800
H	-0.14517300	3.25005800	2.02184600
C	1.85433100	2.96245500	1.20465700
C	1.60773600	2.20902300	-0.10854200
H	0.44914600	0.36588100	-0.38431100
H	2.80297300	2.65161700	1.64871900
H	1.87940000	4.04529800	1.06855400
H	2.50350200	2.11601700	-0.72510900
H	0.82710700	2.69805100	-0.69965800
C	-0.85875700	0.60079300	1.93406600
C	-1.82231200	1.15844700	2.80130200
H	-1.53724400	2.09173500	3.27544000
C	-2.67113400	0.23782600	3.65725800
H	-3.28192700	-0.43796000	3.05101300
H	-2.04607900	-0.37444300	4.31706700
H	-3.34354000	0.82002100	4.29044000
C	-1.09554100	-0.80821900	1.40256100
O	-0.32186400	-1.70380100	1.71119900
O	-2.14945700	-1.01295100	0.64482000
H	-2.85740600	-0.22465300	0.64205800
C	-3.24364500	1.82386900	1.28493300
O	-3.85521000	0.75762300	0.91214100
C	-3.95970500	2.72873800	2.29437900
O	-3.55490400	3.83566100	2.62174100
O	-5.08565100	2.17624100	2.75317800
C	-2.41845500	2.58821400	0.26092300
C	-3.34008800	3.19648000	-0.82741100

H	-1.72235900	1.89872400	-0.22222000
H	-1.84757900	3.38561900	0.73771100
H	-3.91935900	2.38675000	-1.28316400
H	-4.05114900	3.88665900	-0.36089700
C	-5.83908200	2.95441300	3.73201600
H	-5.20432100	3.10255900	4.60980900
H	-6.06165100	3.93114900	3.29508900
C	-7.09481700	2.17943700	4.06082100
H	-6.85523400	1.19810800	4.48044800
H	-7.67601500	2.73668100	4.80176300
H	-7.71601000	2.04024100	3.17133500
C	-2.54369100	3.92547100	-1.88701000
C	-2.40667800	5.32020900	-1.85606600
C	-1.89728000	3.21380900	-2.90986100
C	-1.64846700	5.98810800	-2.82090000
H	-2.90229400	5.88672000	-1.07170300
C	-1.13749200	3.87736400	-3.87485800
H	-1.99852000	2.13212200	-2.95342700
C	-1.01073100	5.26861000	-3.83365100
H	-1.55888300	7.07006500	-2.78224100
H	-0.64982000	3.30937000	-4.66204500
H	-0.42319000	5.78646300	-4.58605500
C	2.20892000	-0.10463600	0.74908800
C	3.76170000	-1.13097800	1.81641700
C	3.90754100	-1.52107800	0.50530300
N	2.89282600	-0.84771900	-0.18239000
N	2.71117000	-0.25611500	1.96285900
C	2.66817500	-0.86834300	-1.63010800
H	2.48389600	0.15862900	-1.95667800
H	3.61185500	-1.16833200	-2.09268400
C	1.54202800	-1.76934100	-2.11225800
C	1.23311800	-1.78830100	-3.51429200
C	0.81392600	-2.55835400	-1.24678300
C	1.94718800	-1.01808500	-4.47515100
C	0.16082000	-2.62394100	-3.97656700
C	-0.24846200	-3.37518600	-1.70737900
H	1.04466100	-2.55165600	-0.18846500
C	1.62060900	-1.07007400	-5.81388800
H	2.76508600	-0.38066000	-4.15765100
C	-0.15030800	-2.65148100	-5.36295200
C	-0.57010900	-3.40854000	-3.04218800
H	-0.80541400	-3.97118400	-0.99099400
C	0.56192500	-1.89277900	-6.26487600
H	2.18103400	-0.47507900	-6.52877500

H	-0.96510100	-3.28773400	-5.69790000
H	-1.38317000	-4.03116500	-3.40498600
H	0.31520700	-1.92355800	-7.32184200
H	4.35165900	-1.45448600	2.66240800
C	4.88071100	-2.43985400	-0.11677000
C	6.29692600	-2.22478000	0.04042200
C	4.44047800	-3.54268400	-0.83403900
C	6.84491100	-1.10073700	0.71978200
C	7.20795400	-3.17719900	-0.53233400
C	5.34517400	-4.46315600	-1.40832900
H	3.37494800	-3.71644000	-0.94149900
C	8.20747100	-0.93964400	0.84825600
H	6.17405600	-0.35829400	1.13623200
C	8.60816200	-2.98335900	-0.37542400
C	6.70075400	-4.29082800	-1.25361200
H	4.95860000	-5.31530300	-1.95880100
C	9.10091200	-1.89242400	0.30324200
H	8.59994800	-0.07086300	1.36834200
H	9.28305200	-3.71680800	-0.80824600
H	7.40372700	-5.00096400	-1.68018800
H	10.17209800	-1.75474700	0.41578500

TS-**I**-*S*-water

N	5.34829000	-2.28637700	1.61531200
C	6.06485900	-1.70563400	2.78525100
C	3.87149500	-2.17162600	1.77814700
H	6.79419300	-0.97097300	2.43335400
H	6.59356100	-2.49996600	3.31485800
C	4.95543700	-1.10865000	3.65244300
C	3.73950100	-1.97541800	3.30837100
H	3.40119700	-3.10200800	1.45308700
H	4.77159500	-0.06685100	3.37863400
H	5.21279300	-1.14570400	4.71282200
H	2.78740000	-1.51650800	3.58182100
H	3.81386300	-2.94884300	3.80144000
C	5.98623700	-2.97644700	0.66579300
C	7.34151600	-3.35939500	0.75772600
H	7.88143400	-2.96352100	1.61102800
C	8.17742000	-3.49539300	-0.49799300
H	9.14786400	-3.94096500	-0.26850300
H	7.69713300	-4.11016500	-1.26242800
H	8.36832400	-2.50772100	-0.93399900
C	5.21503000	-3.35115500	-0.59704100
O	4.70060400	-2.47394900	-1.27598000

O	5.15784500	-4.62072200	-0.94052600
H	5.78758700	-5.27312100	-0.40624100
C	7.12013600	-5.44802700	1.31758600
O	6.85780700	-6.03926200	0.21108500
C	5.98298100	-5.36137900	2.35332100
O	6.10386900	-4.90016800	3.47874100
O	4.86179400	-5.91531500	1.88536100
C	8.48632000	-5.65461200	1.95502800
C	8.66435700	-7.13962700	2.36822600
H	8.59671700	-5.01132600	2.83014700
H	9.26300300	-5.39583300	1.23224000
H	7.88144900	-7.41321800	3.08424900
H	8.53009500	-7.76461100	1.47981000
C	3.71844000	-6.00275900	2.78860000
H	4.06839200	-6.38666300	3.74962000
H	3.32181300	-4.99513800	2.93644900
C	2.70481700	-6.91987100	2.14105700
H	3.11442000	-7.92514900	2.00616900
H	1.82254900	-6.99169500	2.78414100
H	2.38770000	-6.53493000	1.16741000
C	10.02499500	-7.39084300	2.97831600
C	11.12962500	-7.68418800	2.16483900
C	10.22087000	-7.30296800	4.36410400
C	12.39523200	-7.88256300	2.71953100
H	10.99345700	-7.76132200	1.08890600
C	11.48514300	-7.50225900	4.92310800
H	9.37430800	-7.08013800	5.00886600
C	12.57748000	-7.79137300	4.10179600
H	13.23748100	-8.11274100	2.07313600
H	11.61618400	-7.43463700	5.99939800
H	13.56109300	-7.94821500	4.53479800
C	3.29112500	-1.00383100	1.01346300
N	1.95813600	-0.92728200	0.68767600
N	3.94731500	0.08775700	0.65811200
C	1.76421300	0.31562800	0.07560200
C	0.90145600	-1.86904700	1.07308500
C	3.00748000	0.90535500	0.07681500
C	0.47943100	0.79166700	-0.46949900
H	1.08090800	-2.16629600	2.11013400
H	-0.03409700	-1.30444400	1.07841100
C	0.75281500	-3.10968900	0.20782000
H	3.27264300	1.86823400	-0.33667400
C	-0.04873700	2.08067000	-0.10055700
C	-0.21809500	0.01207100	-1.38139700

C	-0.24015200	-4.08011100	0.57496500
C	1.54323200	-3.33361100	-0.89938600
C	0.56563500	2.93041900	0.86169700
C	-1.26816600	2.52851200	-0.71517600
C	-1.42642800	0.45353600	-1.96418600
H	0.18480200	-0.95191800	-1.67375200
C	-1.10744100	-3.91612200	1.69200300
C	-0.37203800	-5.27061500	-0.21701600
C	1.41386000	-4.51368700	-1.67361700
H	2.29268700	-2.60403200	-1.18047400
C	0.02524400	4.15827400	1.17758500
H	1.46990200	2.59772800	1.35787900
C	-1.79387100	3.80457400	-0.37160300
C	-1.93689600	1.69053700	-1.64697300
H	-1.93715800	-0.18642100	-2.67710500
C	-2.04803400	-4.87341400	2.00928400
H	-1.03490500	-3.02540200	2.30608000
C	-1.35156600	-6.23689200	0.13921600
C	0.47908200	-5.46385800	-1.34073100
H	2.06629100	-4.65816700	-2.52921300
C	-1.16134000	4.60700300	0.55005800
H	0.51109100	4.78584400	1.91882600
H	-2.71199500	4.13080300	-0.85266900
H	-2.85743400	2.04545600	-2.10197400
C	-2.17293500	-6.04600800	1.22798100
H	-2.69946700	-4.72576000	2.86541600
H	-1.43931100	-7.13334700	-0.46858700
H	0.37249800	-6.37215100	-1.92722100
H	-1.57349100	5.57871400	0.80493800
H	-2.91773900	-6.79161200	1.48921800

TS-**II**-*R*-water

N	-3.70822500	-0.85129600	-1.78633800
C	-4.34088000	-2.18240600	-2.02104600
C	-3.22356400	-0.72078200	-0.39252400
H	-3.95625600	-2.63199000	-2.93246900
H	-5.42111700	-2.02840900	-2.12124300
C	-3.99579600	-2.98097300	-0.76511700
C	-3.89633900	-1.91067000	0.32725500
H	-3.55692600	0.23034700	0.02985000
H	-3.03471000	-3.48885200	-0.89210700
H	-4.75417300	-3.73524200	-0.54664400
H	-3.33602300	-2.23119200	1.20582000
H	-4.89267600	-1.59240400	0.64733700

C	-3.73118700	0.16432900	-2.65006900
C	-4.02058200	-0.03009100	-4.02234900
H	-4.60453100	-0.92306900	-4.23423900
C	-4.40340800	1.16403200	-4.87132700
H	-4.36123200	0.90875900	-5.93303200
H	-5.42899500	1.48478800	-4.65194600
H	-3.74762500	2.02260700	-4.70358300
C	-3.40364000	1.56101000	-2.10021800
O	-2.20125100	1.87869500	-1.93225400
O	-4.43456700	2.23757500	-1.85873700
C	-1.71220300	-0.74946000	-0.36407000
C	0.38850100	-0.97767100	-1.00346500
C	0.41954600	-0.50833800	0.27937400
N	-0.92350800	-0.36988200	0.66629400
N	-0.92709900	-1.12339300	-1.37507400
H	-1.28048500	-1.36111900	-2.37350800
C	-1.38698600	0.03508200	1.99982100
H	-0.75856000	0.86806700	2.31899700
H	-2.39643800	0.43698200	1.88767500
C	-2.18367000	-0.86214700	-4.59802100
O	-1.82232100	-1.75012000	-3.73428800
C	-2.77721800	-1.42001700	-5.89526500
O	-2.80884100	-0.80937400	-6.95597400
O	-3.24595400	-2.66648300	-5.74821400
C	-1.28437800	0.35249600	-4.81131900
C	0.11891000	-0.08592800	-5.29540600
H	-1.19060600	0.88600400	-3.86279200
H	-1.72179000	1.03721700	-5.54028600
H	0.53234800	-0.79247200	-4.56767400
H	0.02421100	-0.61788100	-6.24873800
C	-3.82794800	-3.28951700	-6.93046400
H	-4.69148300	-2.69629800	-7.24417700
H	-3.08419000	-3.26805700	-7.73129100
C	-4.21557200	-4.70243200	-6.55339500
H	-4.95573000	-4.70695900	-5.74785300
H	-4.65271200	-5.20140400	-7.42350400
H	-3.34175500	-5.27682300	-6.23212400
C	1.05446900	1.09078600	-5.45750100
C	1.21450100	1.72056100	-6.70008300
C	1.75574300	1.60347600	-4.35528900
C	2.05070300	2.83068700	-6.84018900
H	0.68077600	1.33457400	-7.56513300
C	2.59222200	2.71294300	-4.49066000
H	1.64379300	1.12665300	-3.38409700

C	2.74272500	3.33112500	-5.73486800
H	2.16381600	3.30161700	-7.81268500
H	3.12918000	3.09268800	-3.62590700
H	3.39514400	4.19279600	-5.84194700
C	-1.36578100	-1.07148600	3.04114900
C	-1.74159200	-0.73921800	4.38598600
C	-1.00555500	-2.36762600	2.73575600
C	-2.13411100	0.57113200	4.77961200
C	-1.72644400	-1.77115400	5.38385500
C	-0.99361100	-3.38170000	3.72561900
H	-0.72208900	-2.62975400	1.72236100
C	-2.48762800	0.84575900	6.08375800
H	-2.15917400	1.37200100	4.04879100
C	-2.09655000	-1.45286400	6.71841200
C	-1.34411200	-3.09167100	5.02133900
H	-0.70234000	-4.38960800	3.44680100
C	-2.46954200	-0.17341200	7.06462800
H	-2.78317300	1.85320600	6.36074500
H	-2.07968800	-2.24450200	7.46254500
H	-1.33647200	-3.86272700	5.78660300
H	-2.75027800	0.05705300	8.08783000
H	1.20052700	-1.20362100	-1.67589800
C	1.57436100	-0.14697700	1.12857300
C	2.52935300	-1.13929700	1.53822400
C	1.75372300	1.17640500	1.49799500
C	2.41528900	-2.51893000	1.20909300
C	3.65336400	-0.71954800	2.32769200
C	2.85742400	1.57609100	2.28386000
H	1.04371900	1.92561900	1.16193300
C	3.36213200	-3.42820400	1.62755900
H	1.56943500	-2.85622000	0.62059500
C	4.61294800	-1.68476200	2.73942700
C	3.78881200	0.64792900	2.68717500
H	2.96768300	2.62128500	2.55440700
C	4.47438200	-3.01013500	2.39715400
H	3.25412900	-4.47656000	1.36620400
H	5.45951400	-1.35098000	3.33306800
H	4.64509200	0.94686000	3.28528000
H	5.21280200	-3.73859200	2.71776700

TS-**II**-*S*-water

N	-0.69475400	2.38491400	-1.88576300
C	-1.42724200	3.07126200	-2.98538300
C	-1.62030900	2.04602000	-0.77323200

H	-1.71639900	2.34463400	-3.74630500
H	-0.78220900	3.82594200	-3.43512600
C	-2.63996300	3.66487700	-2.27320500
C	-2.99847700	2.59569100	-1.23699300
H	-1.28631000	2.55025100	0.13706800
H	-3.45993000	3.86425900	-2.96631400
H	-2.36609300	4.60315100	-1.78116000
H	-3.57695200	1.79352000	-1.70359800
H	-3.56747200	2.98377000	-0.39083100
C	0.62856800	2.25220100	-1.80633700
C	1.46146100	2.35209500	-2.95165800
H	1.02696100	2.92389500	-3.76722800
C	2.93358200	2.65139400	-2.73993400
H	3.49493500	2.52408400	-3.66824200
H	3.07078700	3.69095900	-2.41738600
H	3.38573600	2.00444600	-1.98469000
C	1.24957300	1.95982100	-0.43019700
O	1.66446100	0.79845100	-0.19537900
O	1.29117000	2.97177700	0.31362300
C	-1.64805600	0.56053100	-0.54126000
C	-1.52397400	-1.60947100	-0.91536200
C	-2.06251700	-1.45582900	0.33178800
N	-2.13717500	-0.07081900	0.54772600
N	-1.28497000	-0.35976000	-1.43571000
H	-0.78139300	-0.14646700	-2.36713200
C	-2.70181400	0.57926500	1.74054800
H	-3.31829800	1.41414400	1.39872400
H	-3.38471900	-0.14607500	2.18823100
C	1.06645700	0.56829700	-3.91501600
O	-0.16625000	0.23748100	-3.73259300
C	2.14562200	-0.30289900	-3.25903300
O	3.34170200	-0.20840400	-3.50222000
O	1.63648800	-1.22958500	-2.43842900
C	1.48442000	0.94319500	-5.35041000
C	0.39676000	1.66682300	-6.15979900
H	1.71962200	-0.00461900	-5.85521100
H	2.41203600	1.52024700	-5.34833200
H	-0.50539600	1.04871800	-6.17396000
H	0.13014700	2.60941000	-5.66886200
C	2.60565700	-2.07492400	-1.75057000
H	3.21823900	-2.57909900	-2.50248200
H	3.25355100	-1.42868700	-1.15293300
C	1.84385100	-3.05784800	-0.89017000
H	1.20231900	-3.70372800	-1.49701800

H	2.55927900	-3.69143100	-0.35671000
H	1.22692700	-2.53937900	-0.15117200
C	0.84547200	1.94999000	-7.57791800
C	1.61351000	3.08627900	-7.87400700
C	0.52882700	1.07081400	-8.62349200
C	2.05359100	3.33686400	-9.17492900
H	1.86390500	3.78218500	-7.07691800
C	0.96656600	1.31747800	-9.92701700
H	-0.06978500	0.18765700	-8.41399700
C	1.73240200	2.45129400	-10.20710200
H	2.64420300	4.22457500	-9.38334100
H	0.70717200	0.62538600	-10.72323900
H	2.07193700	2.64569600	-11.22026100
C	-1.68302200	1.05569100	2.76183600
C	-2.16790700	1.70082900	3.94906700
C	-0.32575200	0.90018100	2.57734300
C	-3.55257600	1.89130700	4.21798000
C	-1.21717000	2.17728000	4.91362400
C	0.60731600	1.37975600	3.52980900
H	0.05479400	0.41575400	1.68589400
C	-3.97308600	2.51682100	5.37284800
H	-4.29482000	1.53968500	3.50979300
C	-1.68569300	2.81793000	6.09219300
C	0.17408300	2.00391900	4.67350100
H	1.66759200	1.25127300	3.33612600
C	-3.03336100	2.98597900	6.32024100
H	-5.03477500	2.65052300	5.55742000
H	-0.95448800	3.17429200	6.81263300
H	0.88201400	2.37624300	5.40869500
H	-3.37837800	3.47753400	7.22481400
H	-1.29036100	-2.50906100	-1.46072600
C	-2.50025300	-2.47476000	1.30783100
C	-3.58617500	-3.36357700	0.99657400
C	-1.83883400	-2.59099900	2.51958400
C	-4.33698100	-3.28800400	-0.20942000
C	-3.94329600	-4.36811500	1.95872200
C	-2.20575400	-3.57670900	3.46283400
H	-1.01635300	-1.91975400	2.74316000
C	-5.37088100	-4.16458400	-0.45654900
H	-4.09234900	-2.52467900	-0.93956300
C	-5.01192200	-5.25994700	1.66789200
C	-3.23136500	-4.45028200	3.18532700
H	-1.66379300	-3.64354400	4.40072900
C	-5.71089700	-5.16435100	0.48639600

H	-5.93295000	-4.08672900	-1.38230100
H	-5.26671600	-6.01824500	2.40299500
H	-3.51444100	-5.21712400	3.90091700
H	-6.52619700	-5.84958600	0.27555200

TS-**III**-*R*-water

N	4.41119200	0.84874700	-0.70069400
C	4.65473200	2.08061700	0.10966400
C	4.22496300	1.19359000	-2.14866900
H	5.71957000	2.16518600	0.32415900
H	4.09977200	2.00002500	1.04580500
C	4.15749800	3.19967300	-0.80201800
C	4.53412300	2.70812400	-2.20170300
H	3.18286800	1.01651100	-2.41852500
H	4.62650400	4.15348100	-0.55313100
H	3.07278300	3.30982100	-0.71014900
H	5.60075200	2.86124100	-2.38679300
H	3.97002900	3.18654000	-3.00275100
C	4.33606200	-0.37460000	-0.20269200
C	4.92713600	-0.70689700	1.05719600
H	5.00263900	0.16475200	1.70369900
C	4.46831000	-1.94467800	1.82995300
H	4.22211700	-2.75767300	1.14342700
H	5.30329000	-2.28662200	2.44584200
C	3.71950400	-1.46366800	-1.06803700
O	4.27546500	-2.50580500	-1.35819000
C	5.13301100	0.35133100	-3.00182100
C	6.89606700	-0.76482500	-3.66493300
C	6.00274700	-0.79956700	-4.70319700
H	7.87482600	-1.21348500	-3.59528500
N	4.88012800	-0.08983700	-4.25815100
N	6.35061000	-0.04592600	-2.63076000
H	6.77052800	0.03859600	-1.49717000
C	3.68699100	0.20889600	-5.05970600
H	3.50223900	-0.66235100	-5.68983800
H	2.83759600	0.27936800	-4.37645700
C	3.28811900	-1.64780000	2.73998200
C	3.50306500	-1.29285000	4.07895300
C	1.97045400	-1.70497400	2.26416100
C	2.42930800	-1.00426600	4.92424800
H	4.52049200	-1.24822000	4.45992400
C	0.89472300	-1.41910400	3.10702700
H	1.78602500	-1.97361000	1.22725700
C	1.12067200	-1.06790400	4.44049100

H	2.61529800	-0.73547000	5.96017500
H	-0.12009500	-1.47376700	2.72330700
H	0.28383700	-0.84787300	5.09680100
O	2.47918500	-1.13377600	-1.41317700
C	1.73789700	-2.10590300	-2.22852300
C	0.39166700	-1.49541900	-2.54091300
H	1.65448400	-3.02787200	-1.64874400
H	2.32499100	-2.30442600	-3.12789700
H	-0.18394600	-2.20057700	-3.14783500
H	-0.17251200	-1.29007300	-1.62687500
H	0.50031200	-0.56563900	-3.10680200
C	6.84148000	-0.76932400	0.56846900
O	7.11243200	0.20205000	-0.27419400
C	7.34327400	-0.48967500	1.99615500
O	7.55785200	-1.36714600	2.81980600
O	7.50986400	0.81246600	2.23524200
C	7.13450200	-2.19615300	0.10784600
C	8.63957200	-2.37993100	-0.20479500
H	6.55244700	-2.40083400	-0.79144300
H	6.83249100	-2.91546300	0.87085100
H	8.92543600	-1.66135200	-0.98005200
H	9.23179500	-2.14876500	0.68684500
C	7.95642000	1.17711400	3.57706900
H	7.23811900	0.77636600	4.29694700
H	8.92641700	0.70522700	3.75359100
C	8.03833800	2.68573900	3.63503400
H	7.06096600	3.14228600	3.45383600
H	8.37723100	2.98670900	4.63100000
H	8.75029500	3.07242700	2.90011600
C	8.94830200	-3.78719600	-0.66585400
C	9.45135300	-4.74380700	0.22714900
C	8.70775400	-4.17484400	-1.99306700
C	9.71102000	-6.05080600	-0.19210000
H	9.64494500	-4.45941400	1.25843700
C	8.96484300	-5.48008900	-2.41582800
H	8.31647000	-3.44591700	-2.69909700
C	9.46834300	-6.42337400	-1.51595900
H	10.10555500	-6.77564700	0.51442500
H	8.77622100	-5.75987900	-3.44848400
H	9.67171200	-7.43824200	-1.84489700
C	6.10107100	-1.47133900	-6.01646200
C	7.07304400	-1.04867200	-6.98608400
C	5.27070800	-2.54491100	-6.29563300
C	7.95342400	0.04986700	-6.78057300

C	7.15609000	-1.76527400	-8.22785200
C	5.35391500	-3.23642700	-7.52491300
H	4.55433300	-2.87397600	-5.54933500
C	8.87040000	0.41217600	-7.74296500
H	7.89920600	0.60570700	-5.85134000
C	8.11690900	-1.36574800	-9.19713800
C	6.27947800	-2.85662700	-8.46893700
H	4.68950300	-4.07420100	-7.71070800
C	8.95801200	-0.30240900	-8.96204700
H	9.53256100	1.25428700	-7.56578100
H	8.17163800	-1.92027400	-10.12981400
H	6.35667800	-3.38745000	-9.41366800
H	9.68774200	-0.00625300	-9.70934900
C	3.79877000	1.46242400	-5.91127800
C	2.69085600	1.80740100	-6.75589100
C	4.92016600	2.26524400	-5.89756300
C	1.50094700	1.02942800	-6.82917100
C	2.78118200	2.98778600	-7.56765600
C	5.00220900	3.43010800	-6.70007800
H	5.76537700	2.01039300	-5.26793300
C	0.46128500	1.39675700	-7.65717300
H	1.40415800	0.13106900	-6.22913100
C	1.69063900	3.33712100	-8.40882600
C	3.95736500	3.78509800	-7.51754400
H	5.90202900	4.03622900	-6.66175800
C	0.55411500	2.56118900	-8.45505400
H	-0.43689300	0.78792300	-7.69786700
H	1.77308200	4.23369600	-9.01713700
H	4.01234100	4.67631600	-8.13638200
H	-0.27196100	2.83915700	-9.10254400

TS-**III**-*S*-water

N	2.78615900	-1.29432900	-5.34662400
C	1.69385700	-2.12107800	-5.94781600
C	3.98739200	-1.29633700	-6.24393000
H	1.04197100	-1.47180800	-6.53147900
H	1.12214400	-2.59427700	-5.15044800
C	2.46585400	-3.10622600	-6.81857800
C	3.59337500	-2.25094300	-7.40347600
H	4.84298500	-1.70018600	-5.69852000
H	1.82738900	-3.53689800	-7.59237900
H	2.86820000	-3.91801700	-6.20531800
H	3.22611800	-1.66604900	-8.25015300
H	4.45685500	-2.82965900	-7.73134400

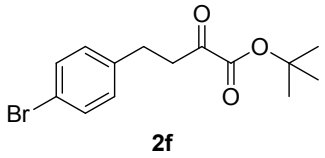
C	2.74892400	-0.75092700	-4.14595400
C	1.49815300	-0.45763900	-3.48795700
H	0.73394900	-1.17513500	-3.77608300
C	1.50729800	-0.22261600	-1.97343400
H	2.30757900	0.46990100	-1.69890800
H	0.57449500	0.28478400	-1.71390500
C	4.04905800	-0.22755300	-3.54673700
O	4.30990100	0.96101000	-3.57235300
C	4.29833500	0.10454000	-6.69538700
C	4.05627800	2.21703600	-7.23644700
C	5.35120100	1.88706500	-7.52936000
H	3.55100500	3.16343700	-7.33872900
N	5.48819900	0.53757300	-7.17014000
N	3.42290400	1.10741900	-6.73117600
H	2.38689900	1.07199200	-6.25508400
C	6.67810700	-0.29271600	-7.39238100
H	7.54761000	0.32192400	-7.15397600
H	6.65970200	-1.09686600	-6.65280200
C	1.62285900	-1.47897400	-1.12425000
C	2.55927300	-1.53367400	-0.08242800
C	0.77910900	-2.58324900	-1.32094400
C	2.65839200	-2.66143000	0.73688300
H	3.21665400	-0.68492300	0.08674900
C	0.87884800	-3.71295400	-0.50705500
H	0.03462600	-2.56236800	-2.11224700
C	1.82060800	-3.75756600	0.52453100
H	3.39129300	-2.68124800	1.53833900
H	0.21732900	-4.55774200	-0.67632600
H	1.89742200	-4.63643600	1.15771300
O	4.88196100	-1.08428900	-2.96566300
C	4.63220700	-2.53202300	-2.85128300
C	5.58655800	-3.05670900	-1.80329800
H	4.82742300	-2.98110300	-3.82728600
H	3.59043300	-2.69386900	-2.57117000
H	5.43734700	-4.13567600	-1.70070600
H	6.62540900	-2.87848300	-2.09454800
H	5.40306000	-2.58921300	-0.83270800
C	0.76838300	0.96907500	-4.49085300
O	1.11073500	0.88351700	-5.75836000
C	1.25217000	2.23266500	-3.74258100
O	0.79580300	2.60083500	-2.66875500
O	2.18452900	2.91401900	-4.41278900
C	-0.74207800	0.74912500	-4.26147100
C	-1.58605600	1.85906400	-4.92637600

H	-0.98011000	0.69734700	-3.19679600
H	-1.00116900	-0.21340900	-4.71309600
H	-1.33476500	2.82653400	-4.47787900
H	-1.32114600	1.90911100	-5.98704500
C	2.70422900	4.10889100	-3.75202900
H	1.86840500	4.78960800	-3.57158300
H	3.12147400	3.80896500	-2.78731700
C	3.75117500	4.72294200	-4.65364800
H	3.32182300	5.02039800	-5.61463800
H	4.15566700	5.61723900	-4.16964900
H	4.57537100	4.02713700	-4.83372800
C	-3.06983200	1.60519800	-4.77682500
C	-3.76686200	2.06388700	-3.64921000
C	-3.77548900	0.87697100	-5.74586700
C	-5.12982800	1.80354100	-3.49369400
H	-3.23593300	2.63410400	-2.89084000
C	-5.13877800	0.61449400	-5.59462700
H	-3.25160600	0.51906800	-6.62885300
C	-5.82083300	1.07660600	-4.46641700
H	-5.65279100	2.17120700	-2.61530100
H	-5.66838300	0.05328900	-6.35937700
H	-6.88163500	0.87592600	-4.34799200
C	6.45088800	2.72170600	-8.05671100
C	6.37194000	3.30183900	-9.36895100
C	7.55622600	2.97005000	-7.25861200
C	5.27754800	3.09025600	-10.25311300
C	7.45718800	4.12959300	-9.81583100
C	8.62209200	3.77877100	-7.71212300
H	7.59881200	2.55000100	-6.25858800
C	5.25395900	3.66926700	-11.50308500
H	4.45173200	2.46416500	-9.93485200
C	7.39777100	4.71409600	-11.11087600
C	8.57203000	4.34789900	-8.96320300
H	9.47218400	3.95375300	-7.06058600
C	6.32107900	4.49141600	-11.93823200
H	4.40971800	3.49204900	-12.16250900
H	8.22498900	5.34008800	-11.43381900
H	9.38395300	4.97617100	-9.31861000
H	6.28687700	4.94136600	-12.92569100
C	6.79796200	-0.86151600	-8.79634600
C	7.95130800	-1.65858400	-9.10450300
C	5.84307400	-0.64187800	-9.76692300
C	8.98011800	-1.93131500	-8.15924800
C	8.07725200	-2.21205500	-10.42301100

C	5.97551100	-1.18841000	-11.06749800
H	4.96797700	-0.04085900	-9.54542800
C	10.06840900	-2.70765900	-8.49727300
H	8.91432100	-1.52701300	-7.15510100
C	9.21252500	-3.00670100	-10.73730000
C	7.06661200	-1.95737600	-11.39005700
H	5.20321600	-0.99181700	-11.80461600
C	10.18832200	-3.25214300	-9.79739500
H	10.84111000	-2.90288800	-7.75979400
H	9.29455400	-3.41796100	-11.73971500
H	7.17572100	-2.38064200	-12.38463100
H	11.05074600	-3.86151900	-10.05002500

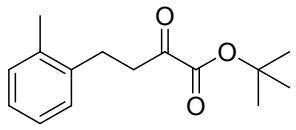
10.Compound characterization data

For unknown substrates 2



2f

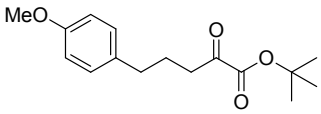
tert-butyl 4-(4-bromophenyl)-2-oxobutanoate (2f), (performed with 6 g di-tert-butyl oxalate), 3.15 g, 34% yield, light yellow solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, *J* = 8.3 Hz, 2H), 7.08 (d, *J* = 8.3 Hz, 2H), 3.09 (t, *J* = 7.4 Hz, 2H), 2.89 (t, *J* = 7.4 Hz, 2H), 1.53 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.4, 160.4, 139.4, 131.7, 130.3, 120.2, 84.2, 40.6, 28.6, 27.9. HRMS m/z $[M+NH_4]^+$ calcd. for $C_{14}H_{21}BrNO_3$: 330.0705, found: 330.0705.



2j

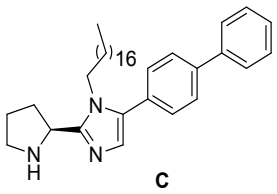
tert-butyl 2-oxo-4-(o-tolyl)butanoate (2j), 1.57 g, 53% yield, light yellow solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18-7.10 (m, 4H), 3.09-3.02 (m, 2H), 2.95-2.89 (m, 2H), 2.32 (s, 3H), 1.53 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.9, 157.9, 138.4, 136.0, 130.4, 128.8, 126.6, 126.3, 84.3, 39.6, 27.8, 26.6, 19.3. HRMS m/z $[M+Na]^+$ calcd. for $C_{15}H_{20}NaO_3$: 271.1310, found: 271.1309.

tert-butyl 5-(4-methoxyphenyl)-2-oxopentanoate (2l), 1.35 g, 41% yield, light yellow solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.09 (d, *J* = 8.6 Hz, 2H), 6.83 (d, *J* = 8.6 Hz, 2H), 3.78 (s, 3H), 2.77 (t, *J* = 7.3 Hz, 2H), 2.59 (t, *J* = 7.6 Hz, 2H), 1.97-1.86 (m, 2H), 1.53 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.6, 160.8, 158.1, 133.4, 129.4, 113.9, 83.9, 55.3, 38.4, 34.1, 27.9, 25.0. HRMS m/z $[M+Na]^+$ calcd. for $C_{16}H_{22}NaO_4$: 301.1416, found: 301.1439.



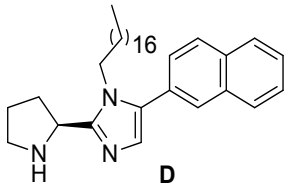
2l

For catalysts C-G



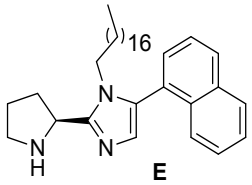
C

(*S*)-5-([1,1'-biphenyl]-4-yl)-1-octadecyl-2-(pyrrolidin-2-yl)-1H-imidazole (C), 1.47 g, 91% yield (over 2 steps starting from 3 mmol **c2)**, yellow solid, $[\alpha]^{20}_{D}$ = -36.11 (*c* 0.54, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.2 Hz, 2H), 7.65-7.57(m, 4H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.32 (t, *J* = 7.3 Hz, 1H), 7.16 (s, 1H), 4.24 (t, *J* = 7.4 Hz, 1H), 4.10-3.76 (m, 2H), 3.32-3.25 (m, 1H), 3.02-2.90 (m, 2H), 2.25-1.77 (m, 5H), 1.35-1.20 (m, 30H), 0.88 (t, *J* = 6.7 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.4, 141.2, 139.7, 139.2, 133.6, 128.8, 127.3, 127.1, 126.9, 125.2, 115.7, 55.1, 47.4, 46.0, 32.3, 32.0, 31.2, 29.8, 29.8, 29.7, 29.7, 29.6, 29.5, 29.3, 26.9, 26.3, 22.8, 14.2. HRMS m/z $[M+H]^+$ calcd. for$C_{37}H_{56}N_3$: 542.4474, found: 542.4501.



D

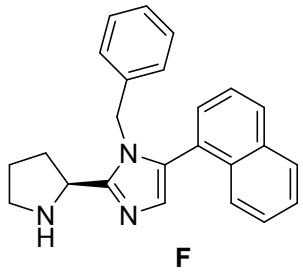
(*S*)-5-(naphthalen-2-yl)-1-octadecyl-2-(pyrrolidin-2-yl)-1H-imidazole (D), 2.39 g, 77% yield (over 2 steps starting from 6 mmol **d2)**, white solid, $[\alpha]^{20}_{D}$ = - 69.29 (*c* 0.71, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (s, 1H), 7.87 (d, *J* = 7.6 Hz, 1H), 7.83-7.76 (m, 3H), 7.48-7.38 (m, 2H), 7.15 (s, 1H), 4.85 (t, *J* = 7.3 Hz, 1H), 3.95-3.85 (m, 1H), 3.75-3.65 (m, 1H), 3.56-3.38 (m, 2H), 2.42-2.29 (m, 1H), 2.21-1.99 (m, 3H), 1.72-1.58 (m, 2H), 1.35-1.05 (m, 30H), 0.88 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.7, 140.3, 133.8, 132.7, 131.1, 128.3, 128.1, 127.8, 126.3, 125.6, 123.6, 123.0, 117.1, 54.2, 46.4, 46.0, 32.0, 31.4, 31.0, 29.8, 29.7, 29.6, 29.5, 29.4, 29.2, 26.7, 24.8, 22.8, 14.2. HRMS m/z $[M+H]^+$ calcd. for $C_{35}H_{54}N_3$: 516.4318, found: 516.4326.



E

(*S*)-5-(naphthalen-1-yl)-1-octadecyl-2-(pyrrolidin-2-yl)-1H-imidazole (E), 0.72 g, 70% yield (over 2 steps starting from 2 mmol **e2**), dark yellow viscous liquid, $[\alpha]^{20}_{D}$ = - 26.40 (*c* 1.00, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52-8.45 (m, 1H), 7.87-7.82(m, 1H), 7.77 (d, *J* = 8.2 Hz, 1H), 7.66 (d, *J* = 6.4 Hz, 1H), 7.48-7.44 (m, 3H), 7.11 (s, 1H), 4.53 (t, *J* = 7.6 Hz, 1H), 4.10-4.02 (m, 1H),

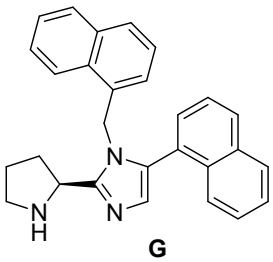
3.96-3.87 (m, 1H), 3.30-3.23 (m, 1H), 3.11-3.05 (m, 1H), 2.30-2.20 (m, 1H), 2.15-2.07 (m, 1H), 2.00-7.92 (m, 2H), 1.86-1.74 (m, 2H), 1.35-1.20 (m, 30H), 0.88 (t, J = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.4, 139.5, 134.1, 131.9, 131.4, 128.4, 127.7, 126.6, 126.2, 126.1, 125.7, 125.5, 119.1, 54.6, 46.6, 46.3, 32.2, 32.0, 31.3, 29.8, 29.8, 29.7, 29.6, 29.5, 29.3, 26.9, 25.6, 22.8, 14.2. HRMS m/z $[M+H]^+$ calcd. for $C_{35}H_{54}N_3$: 516.4318, found: 516.4332.



F

(*S*)-1-benzyl-5-(naphthalen-1-yl)-2-(pyrrolidin-2-yl)-1H-imidazole (F), 0.42 g, 59% yield (over 2 steps starting from 2 mmol **e2**), dark yellow viscous liquid, $[\alpha]^{20}_D$ = - 56.74 (*c* 0.46, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58-8.48 (m, 1H), 7.88-7.82 (m, 1H), 7.80-7.74(m, 1H), 7.70-7.64 (m, 1H), 7.50-7.35 (m, 3H), 7.34-7.27 (m, 4H), 7.18 (d, J = 7.1 Hz, 1H), 7.12 (s, 1H), 5.35-5.18 (AB, J = 15.9 Hz, 2H), 4.40 (t, J = 7.5 Hz, 1H), 3.72 (brs, 1H), 3.29-3.19 (m, 1H), 3.01 (m, 1H), 2.15-1.97 (m, 2H), 1.97-1.88 (m, 1H), 1.88-1.81 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.9, 139.7, 136.4, 134.1, 131.8, 131.4, 129.1, 128.4, 128.2, 127.0, 126.8, 126.6, 126.2, 126.1, 125.7, 125.5, 119.8, 55.0, 49.7, 46.9, 32.0, 25.9. HRMS(ESI) m/z $[M+H]^+$ calcd. for $C_{24}H_{24}N_3$: 354.1970, found: 354.1976.

(*S*)-5-(naphthalen-1-yl)-1-(naphthalen-1-ylmethyl)-2-(pyrrolidin-2-yl)-1H-imidazole (G), 0.65 g, 80% yield (over 2 steps starting from 2 mmol **e2**), yellow foam solid, $[\alpha]^{20}_D$ = - 73.33 (*c* 0.45, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63-8.49 (m, 1H), 7.87-7.77 (m, 5H), 7.70 (d, J = 6.7 Hz, 1H), 7.61 (s, 1H), 7.48 (m, 5H), 7.31 (dd, J = 8.5, 1.3 Hz, 1H), 7.17 (s, 1H), 5.52-5.34 (AB, J = 15.8 Hz, 2H), 4.45 (t, J = 7.5 Hz, 1H), 3.81 (brs, 1H), 3.26 (dt, J = 11.1, 7.2 Hz, 1H), 3.00 (dt, J = 11.1, 7.2 Hz, 1H), 2.13-1.98 (m, 2H), 1.98-1.90 (m, 1H), 1.87-1.79 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.2, 139.8, 134.2, 133.9, 133.4, 133.1, 131.9, 131.4, 129.1, 128.4, 128.0, 127.9, 127.8, 126.7, 126.6, 126.5, 126.2, 126.1, 126.0,

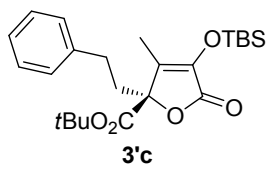


G

125.7, 125.5, 124.7, 119.8, 55.2, 49.9, 47.0, 32.0, 26.0. HRMS m/z $[M+H]^+$ calcd. for $C_{28}H_{26}N_3$: 404.2127, found: 404.2162.

For isotetronic acids and derivates

(*R*)-tert-butyl 4-((tert-butyldimethylsilyl)oxy)-3-methyl-5-oxo-2-phenethyl-2,5-di

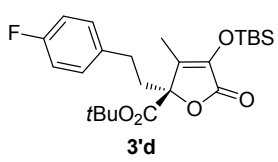


3'c

hydrofuran-2-carboxylate (3'c): 121 mg, 70% yield, light yellow solid, $[\alpha]^{20}_D$ = + 76.83 (*c* 0.60, $CHCl_3$). ^1H NMR (400 MHz, $CDCl_3$) δ 7.31-7.26 (m, 2H), 7.22-7.15 (m, 3H), 2.62-2.54 (m, 2H), 2.53-2.44 (m, 1H), 2.10-2.01 (m, 1H), 1.85 (s, 3H), 1.47 (s, 9H), 0.99 (s, 9H), 0.27 (s, 3H), 0.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.6, 167.3, 140.8, 139.1, 136.5, 128.6, 128.5, 126.3, 86.5, 83.5, 35.9, 29.4, 28.0, 25.6, 18.3, 9.3, -4.2, -4.2. HRMS m/z $[M+H]^+$ calcd. for $C_{24}H_{37}O_5Si$: 433.2410, found: 433.2431.

For **3c**: HPLC: 91% ee, Chiralcel AD-H column, 254 nm, 25 °C, *n*-hexane/*i*-propanol = 90/10, flow = 1 mL/min, retention time 6.7 min (maj) and 7.8 min.

(*R*)-tert-butyl 4-((tert-butyldimethylsilyl)oxy)-2-(4-fluorophenethyl)-3-methyl-5-o

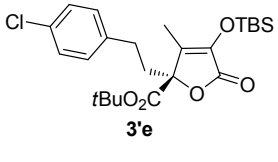


3'd

xo-2,5-dihydrofuran-2-carboxylate (3'd): 147 mg, 81% yield, light yellow solid, $[\alpha]^{20}_D$ = + 62.42 (*c* 0.99, $CHCl_3$). ^1H NMR (400 MHz, $CDCl_3$) δ 7.15-7.09 (m, 2H), 6.99-6.93 (m, 2H), 2.60-2.52 (m, 2H), 2.50-2.40 (m, 1H), 2.06-1.97 (m, 1H), 1.85 (s, 3H), 1.46 (s, 9H), 0.98 (s, 9H), 0.27 (s, 3H), 0.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.6, 167.3, 161.5 (d, *J* = 242.5 Hz), 139.1, 136.4, 136.4 (d, *J* = 2.9 Hz), 129.85 (d, *J* = 7.8 Hz), 115.4 (d, *J* = 21.1Hz), 86.3, 83.6, 36.0, 28.7, 27.9, 25.6, 18.3, 9.3, -4.2, -4.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -117.02. HRMS m/z $[M+H]^+$ calcd for $C_{24}H_{36}FO_5Si$: 451.2316, found: 451.2330.

For **3d**: HPLC: 92% ee, Chiralcel AD-H column, 254 nm, 25 °C, *n*-hexane/*i*-propanol = 90/10, flow = 1.0 mL/min, retention time 8.1 min (maj) and 9.8 min.

(*R*)-tert-butyl 4-((tert-butyldimethylsilyl)oxy)-2-(4-chlorophenethyl)-3-methyl-5-oxo-2,5-dihydrofuran-2-carboxylate (3'e): 134 mg, 72% yield, light yellow solid,

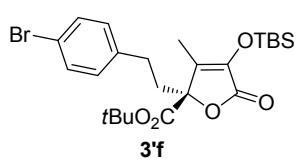


3'e

$[\alpha]^{20}_D$ = + 67.21 (*c* 1.15, $CHCl_3$). ^1H NMR (400 MHz, $CDCl_3$) δ 7.25 (d, *J* = 8.3 Hz, 2H), 7.10 (d, *J* = 8.2 Hz, 2H), 2.62-2.52 (m, 2H), 2.51-2.42 (m, 1H), 2.07-1.97 (m, 1H), 1.85 (s, 3H), 1.46 (s, 9H), 0.98 (s, 9H), 0.27 (s, 3H), 0.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.5, 167.2, 139.2, 139.1, 136.4, 132.1, 129.8, 128.7, 86.3, 83.6, 35.7, 28.8, 27.9, 25.6, 18.3, 9.3, -4.2, -4.3. HRMS m/z $[M+H]^+$ calcd for $C_{24}H_{36}ClO_5Si$: 467.2021, found: 467.2007.

For **3e**: HPLC: 95% ee, Chiralcel AD-H column, 254 nm, 25 ^{0}C, *n*-hexane/*i*-propanol = 90/10, flow = 1.0 mL/min, retention time 9.0 (maj) min and 10.9 min.

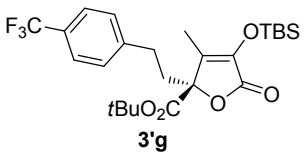
(*R*)-tert-butyl 2-(4-bromophenethyl)-4-((tert-butyldimethylsilyl)oxy)-3-methyl-5-oxo-2,5-dihydrofuran-2-carboxylate (3'f): 127 mg, 62% yield, light yellow solid, $[\alpha]^{20}_D$ = + 81.79 (*c* = 0.50, $CHCl_3$). ^1H NMR (400 MHz, $CDCl_3$) δ 7.39 (d, *J* = 8.0 Hz, 2H), 7.05 (d, *J* = 8.0 Hz, 2H), 2.60-2.50 (m, 2H), 2.50-2.39 (m, 1H), 2.07-1.95 (m, 1H), 1.85 (s, 3H), 1.46 (s, 9H), 0.98 (s, 9H), 0.27 (s, 3H), 0.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.6, 167.2, 139.7, 139.1, 136.4, 131.7, 130.2, 120.1, 86.3, 83.6, 35.6, 28.9, 27.9, 25.6, 18.3, 9.3, -4.2, -4.3. HRMS m/z $[M+H]^+$ calcd. for $C_{24}H_{36}BrO_5Si$: 511.1515, found: 511.1514.



3'f

For **3f**: HPLC: 92% ee Chiralcel AD-H column, 254 nm, 25 ^{0}C, *n*-hexane/*i*-propanol = 90/10, flow = 1.0 mL/min, retention time 9.8 min (maj) and 11.7 min.

(*R*)-tert-butyl 4-((tert-butyldimethylsilyl)oxy)-3-methyl-5-oxo-2-(4-(trifluorometh-yl)phenethyl)-2,5-dihydrofran-2-carboxylate (3'g): 150 mg, 75% yield, light yellow solid, $[\alpha]^{20}_D$ = + 61.61 (*c* 0.99, $CHCl_3$). ^1H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 7.9 Hz, 2H), 2.70-2.62 (m, 2H), 2.55-2.45(m, 1H), 2.09-2.00 (m, 1H), 1.85 (s, 3H), 1.47 (s, 9H), 0.99 (s, 9H), 0.27 (s, 3H), 0.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.4, 167.1, 144.8, 139.1, 136.2, 128.8, 128.7 (q, *J* = 32.3 Hz), 125.5 (q, *J* = 3.8 Hz), 124.2 (q, *J* = 270.2 Hz), 86.1, 83.6, 35.4,

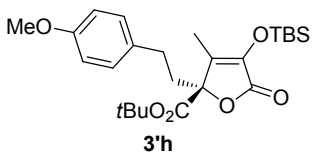


3'g

29.3, 27.8, 25.5, 18.2, 9.2, -4.2, -4.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.40. HRMS m/z $[M+H]^+$ calcd. for $C_{25}H_{36}F_3O_5Si$: 501.2284, found: 501.2293.

For **3g**: HPLC: 90% ee, Chiralcel AD-H column, 254 nm, 25 ^{0}C, *n*-hexane/*i*-propanol = 90/10, flow = 1.0 mL/min, retention time 7.4 min (maj) and 8.4 min.

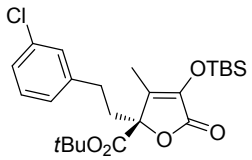
(*R*)-tert-butyl 4-((tert-butyldimethylsilyl)oxy)-2-(4-methoxyphenethyl)-3-methyl -5-oxo-2,5-dihydrofuran-2-carboxylate (3'h): 132 mg, 71% yield, light yellow solid, $[\alpha]^{20}_D$ = + 48.98 (*c* 0.49, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.08 (d, *J* = 8.6 Hz, 2H), 6.82 (d, *J* = 8.6 Hz, 2H), 3.78 (s, 3H), 2.57-2.49 (m, 2H), 2.48-2.40 (m, 1H), 2.06-1.98 (m, 1H), 1.85 (s, 3H), 1.46 (s, 9H), 0.98 (s, 9H), 0.26 (s, 3H), 0.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.5, 167.3, 158.1, 139.0, 136.5, 132.8, 129.3, 114.0, 86.4, 83.4, 55.3, 36.1, 28.4, 27.9, 25.6, 18.2, 9.2, -4.3, -4.3. HRMS m/z $[M+H]^+$ calcd. for $C_{25}H_{39}O_6Si$: 463.2516, found: 463.2532.



3'h

For **3h**: HPLC: 90% ee, Chiralcel AD-H column, 254 nm, 25 ^{0}C, *n*-hexane/*i*-propanol = 90/10, flow = 1.0 mL/min, retention time 10.1 min (maj) and 12.4 min.

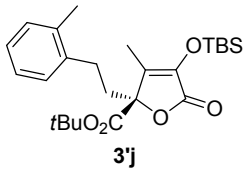
(*R*)-tert-butyl 4-((tert-butyldimethylsilyl)oxy)-2-(3-chlorophenethyl)-3-methyl-5-oxo-2,5-dihydrofuran-2-carboxylate (3'i): 136 mg, 73% yield, light yellow solid, $[\alpha]^{20}_D$ = + 37.81 (*c* 0.32, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24-7.14 (m, 3H), 7.07-7.03 (m, 1H), 2.60-2.54 (m, 2H), 2.51-2.44 (m, 1H), 2.06-1.97 (m, 1H), 1.85 (s, 3H), 1.46 (s, 9H), 0.98 (s, 9H), 0.27 (s, 3H), 0.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.4, 167.1, 142.7, 139.1, 136.2, 134.3, 129.8, 128.5, 126.6, 126.5, 86.2, 83.6, 35.5, 29.1, 27.9, 25.5, 18.2, 9.2, -4.3, -4.3. HRMS m/z $[M+H]^+$ calcd. for $C_{24}H_{36}ClO_5Si$: 467.2021, found: 467.2036.



3'i

For **3i**: HPLC: 89% ee, Chiralcel AS-H column, 254 nm, 25 ^{0}C, *n*-hexane/*i*-propanol = 90/10, flow = 1.0 mL/min, retention time 6.1 min and 7.6 min (maj).

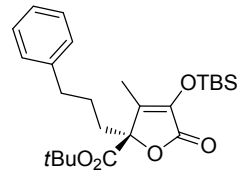
(*R*)-tert-butyl 4-((tert-butyldimethylsilyl)oxy)-3-methyl-2-(2-methylphenethyl)-5-oxo-2,5-dihydrofuran-2-carbocylate (3'j): 130 mg, 73% yield, light yellow solid, $[\alpha]^{20}_D$ = + 63.75 (*c* 1.12, $CHCl_3$). ^1H NMR (400 MHz, $CDCl_3$) δ 7.18-7.06 (m, 4H), 2.62-2.52 (m, 2H), 2.47-2.36 (m, 1H), 2.31 (s, 3H), 1.92-2.02 (m, 1H), 1.88 (s, 3H), 1.48 (s, 9H), 0.99 (s, 9H), 0.27 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.6, 167.3, 139.1, 138.9, 136.5, 136.0, 130.4, 129.0, 126.5, 126.3, 86.5, 83.5, 34.7, 27.9, 27.8, 26.9, 25.6, 19.3, 9.3, -4.2, -4.2. HRMS m/z $[M+H]^+$ calcd. for $C_{25}H_{39}O_5Si$: 447.2567, found: 447.2586.



3'j

Note: (**3j**) was characterized with TBS-protected product (**3j'**) for both ee and yield. HPLC: 90% ee, Chiralcel AD-H column, 254 nm, 25 ^{0}C, *n*-hexane/*i*-propanol = 90/10, flow = 0.5 mL/min, retention time 6.8 min (maj) and 7.9 min.

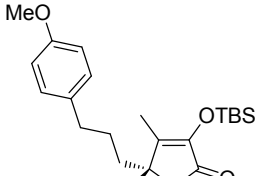
(*R*)-tert-butyl 4-((tert-butyldimethylsilyl)oxy)-3-methyl-5-oxo-2-(3-phenylpropyl)-2,5-dihydrofuran-2-carboxylate (3'k): 127 mg, 71% yield, light yellow viscous liquid, $[\alpha]^{20}_D$ = + 67.38 (*c* 0.42, $CHCl_3$). ^1H NMR (400 MHz, $CDCl_3$) δ 7.29-7.26 (m, 2H), 7.20-7.14 (m, 3H), 2.67-2.61 (m, 2H), 2.23-2.15 (m, 1H), 2.00-1.92 (m, 1H), 1.86-1.81 (m, 1H), 1.79 (s, 3H), 1.61-1.58 (m, 1H), 1.43 (s, 9H), 0.97 (s, 9H), 0.24 (s, 3H), 0.23 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.7, 167.5, 141.5, 139.0, 136.6, 128.5, 128.5, 126.1, 86.7, 83.3, 35.5, 33.0, 27.9, 25.6, 24.5, 18.3, 9.3, -4.2, -4.3. HRMS m/z $[M+H]^+$ calcd. for $C_{25}H_{39}O_5Si$: 447.2567, found: 447.2558.



3'k

For **3k**: HPLC: 93% ee, Chiralcel AD-H column, 254 nm, 25 ^{0}C, *n*-hexane/*i*-propanol = 90/10, flow = 1.0 mL/min, retention time 5.8 min and 6.4 min (maj).

(*R*)-tert-butyl 4-((tert-butyldimethylsilyl)oxy)-2-(3-(4-methoxyphenyl)propyl)-3-methyl-5-oxo-2,5-dihydrofuran-2-carboxylate (3'l): 131 mg, 69% yield, light yellow solid, $[\alpha]^{20}_D$ = + 63.73 (*c* 1.07, $CHCl_3$). ^1H NMR (400 MHz, $CDCl_3$) δ 7.04 (d, *J* = 8.1 Hz, 2H), 6.80 (d, *J* = 8.1 Hz, 2H), 3.76 (s, 3H), 2.60-2.50 (m, 2H), 2.20-2.10 (m,

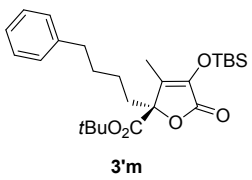


3'l

1H), 1.83-1.74 (m, 1H), 1.77 (s, 3H), 1.57-1.49 (m, 2H), 1.41 (s, 9H), 0.95 (s, 9H), 0.22 (s, 3H), 0.21 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.7, 167.5, 158.0, 139.0, 136.6, 133.6, 129.3, 113.9, 86.7, 83.3, 55.3, 34.6, 32.9, 27.9, 25.6, 24.7, 18.3, 9.3, -4.2, -4.3. HRMS m/z $[M+Na]^+$ calcd. for $C_{26}H_{40}NaO_6Si$: 499.2492, found: 499.2494.

For **3l**: HPLC: 89% ee, Chiralcel AD-H column, 254 nm, 25 ^{0}C, *n*-hexane/*i*-propanol = 90/10, flow = 0.5 mL/min, retention time 14.4 min and 15.4 min (maj).

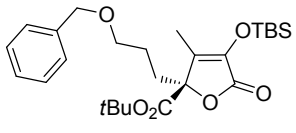
(*R*)-tert-butyl 4-((tert-butyldimethylsilyl)oxy)-3-methyl-5-oxo-2-(4-phenylbutyl) -2,5-dihydrofuran-2-carboxylate (3'm): 120 mg, 65% yield, light yellow viscous liquid, $[\alpha]^{20}_D$ = + 64.76 (*c* 1.07, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28-7.23 (m, 2H), 7.19-7.12 (m, 3H), 2.62-2.57 (m, 2H), 2.22-2.13 (m, 1H), 1.82 (s, 3H), 1.68-1.57 (m, 3H), 1.43 (s, 9H), 1.34-1.27 (m, 2H), 0.97 (s, 9H), 0.23 (s, 3H), 0.23(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.7, 167.6, 142.2, 138.9, 136.6, 128.4, 128.4, 125.8, 86.7, 83.3, 35.7, 33.5, 31.2, 27.9, 25.6, 22.5, 18.3, 9.3, -4.2, -4.3. HRMS m/z $[M+H]^+$ calcd. for $C_{26}H_{41}O_5Si$: 461.2723, found: 461.2726.



3'm

For **3m**: HPLC: 89% ee, Chiralcel AS-H column, 254 nm, 25 ^{0}C, *n*-hexane/*i*-propanol = 90/10, flow = 1 mL/min, retention time 5.7 min and 7.3 min (maj).

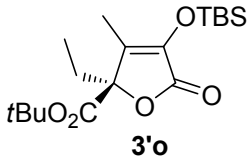
(*R*)-tert-butyl 2-(3-(benzyloxy)propyl)-4-((tert-butyldimethylsilyl)oxy)-3-methyl-5-oxo-2,5-dihydrofuran-2-carboxylate (3'n): 108 mg, 57% yield, light yellow viscous liquid, $[\alpha]^{20}_D$ = + 33.66 (*c* 0.30, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.26 (m, 5H), 4.48 (s, 2H), 3.53-3.43 (m, 2H), 2.30 -2.18 (m, 1H), 2.00-1.89 (m, 1H), 1.84 (s, 3H), 1.60-1.52 (m, 2H), 1.45 (s, 9H), 0.97 (s, 9H), 0.24 (s, 3H), 0.24 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.6, 167.5, 139.0, 138.5, 136.6, 128.4, 127.7, 127.6, 86.7, 83.3, 72.9, 69.6, 30.5, 27.9, 25.6, 23.3, 18.3, 9.3, -4.2, -4.3. HRMS m/z $[M+Na]^+$ calcd. for $C_{26}H_{40}NaO_6Si$: 499.2492, found: 499.2520.



3'n

For **3n**: HPLC: 91% ee, Chiralcel AS-H column, 254 nm, 25 ^{0}C, *n*-hexane/*i*-propanol = 90/10, flow = 1 mL/min, retention time 7.4 min and 8.7 min (maj).

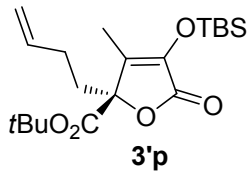
(*R*)-tert-butyl 4-((tert-butyldimethylsilyl)oxy)-2-ethyl-3-methyl-5-oxo-2,5-dihydrofuran-2-carboxylate (3'o): 87 mg, 61% yield, light yellow viscous liquid, $[\alpha]^{20}_D$ = + 62.32 (*c* 0.56, $CHCl_3$). ^1H NMR (400 MHz, $CDCl_3$) δ 2.19 (dq, *J* = 14.7, 7.3 Hz, 1H), 1.90-1.81 (m, 1H), 1.84 (s, 3H), 1.45 (s, 9H), 0.97 (s, 9H), 0.85 (t, *J* = 7.4 Hz, 3H), 0.24 (s, 6H (overlap)). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.8, 167.6, 139.1, 136.4, 87.1, 83.2, 27.9, 26.8, 25.6, 18.3, 9.3, 7.1, -4.3, -4.3. HRMS m/z $[M+H]^+$ calcd. for $C_{18}H_{33}O_5Si$: 357.2097, found: 357.2101.



3'o

For **3o**: HPLC: 90% ee, Chiralcel AS-H column, 254 nm, 25 ^0C, *n*-hexane/*i*-propanol = 95/5, flow = 0.5 mL/min, retention time 16.4 min and 17.1 min (maj).

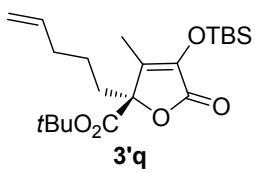
(*R*)-tert-butyl 2-(but-3-en-1-yl)-4-((tert-butyldimethylsilyl)oxy)-3-methyl-5-oxo-2,5-dihydrofuran-2-carboxylate (3'p): 113 mg, 74% yield, light yellow solid, $[\alpha]^{20}_D$ = + 65.85 (*c* 0.41, $CHCl_3$). ^1H NMR (400 MHz, $CDCl_3$) δ 5.85-5.70 (m, 1H), 5.08-4.94 (m, 2H), 2.31-2.21 (m, 1H), 2.01 (dd, *J* = 15.3, 7.2 Hz, 2H), 1.92-1.86 (m, 1H), 1.84 (s, 3H), 1.44 (s, 9H), 0.24 (s, 3H), 0.23 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.6, 167.4, 139.0, 136.9, 136.4, 115.6, 86.4, 83.4, 33.0, 27.9, 27.2, 25.6, 18.3, 9.3, -4.2, -4.3. HRMS m/z $[M+H]^+$ calcd. for $C_{20}H_{35}O_5Si$: 383.2254, found: 383.2260.



3'p

For **3p**: HPLC: 92% ee, Chiralcel AS-H column, 254 nm, 25 ^0C, *n*-hexane/*i*-propanol = 95/5, flow = 0.5 mL/min, retention time 15.1 min and 19.9 min (maj).

(*R*)-tert-butyl 4-((tert-butyldimethylsilyl)oxy)-3-methyl-5-oxo-2-(pent-4-en-1-yl)-2,5-dihydrofuran-2-carboxylate (3'q): 114 mg, 72% yield, light yellow solid, $[\alpha]^{20}_D$ = + 68.70 (*c* 0.62, $CHCl_3$). ^1H NMR (400 MHz, $CDCl_3$) δ 5.79-5.68 (m, 1H), 5.02-4.91 (m, 2H), 2.18-2.08 (m, 1H), 2.07-2.01 (m, 2H), 1.82 (s, 3H), 1.80-1.72 (m, 1H), 1.43 (s, 9H), 1.36-1.28 (m, 2H), 0.96 (s, 9H), 0.22 (s, 3H), 0.22 (s, 3H); ^{13}C

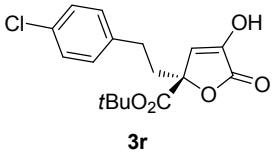


3'q

NMR (100 MHz, $CDCl_3$) δ 168.7, 167.5, 138.9, 137.8, 136.7, 115.3, 86.7, 83.3, 33.3, 33.0, 27.9, 25.6, 22.0, 18.3, 9.3, -4.2, -4.3. HRMS m/z $[M+Na]^+$ calcd. for $C_{21}H_{36}NaO_5Si$: 419.2230, found: 419.2235.

For **3q**: HPLC: 89% ee, Chiralcel AS-H column, 254 nm, 25 ^{0}C, *n*-hexane/*i*-propanol = 90/10, flow = 1.0 mL/min, retention time 5.3 min and 6.2 min (maj).

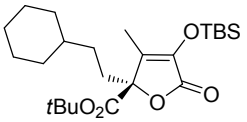
(*R*)-tert-butyl 2-(4-chlorophenethyl)-4-hydroxy-5-oxo-2,5-dihydrofuran-2-carboxylate (3s): 118 mg, 70% yield, white solid, $[\alpha]^{20}_D$ = + 34.89 (*c* = 0.47, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (d, *J* = 8.2 Hz, 2H), 7.09 (d, *J* = 8.2 Hz, 2H), 6.20 (s, 1H), 2.77-2.65 (m, 1H), 2.62-2.52 (m, 1H), 2.48-2.32 (m, 1H), 2.21-1.89 (m, 1H), 1.48 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.3, 166.9, 142.7, 138.8, 132.1, 129.7, 128.7, 118.2, 85.8, 84.2, 37.8, 29.2, 27.9. HRMS m/z $[M+Na]^+$ calcd. for $C_{17}H_{19}ClNaO_5$: 361.0819, found: 361.0814.



3r

HPLC: 72% ee, Chiralcel AD-H column, 254 nm, 25 ^{0}C, *n*-hexane/*i*-propanol = 90/10, flow = 1.0 mL/min, retention time 10.0 min (maj) and 11.4 min.

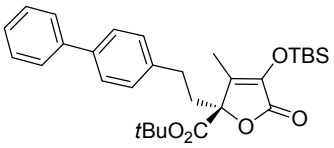
(R)-tert-butyl 4-((tert-butyldimethylsilyl)oxy)-2-(2-cyclohexylethyl)-3-methyl-5-oxo-2,5-dihydrofuran-2-carboxylate (7), 37 mg, 85% yield, light yellow viscous liquid, $[\alpha]^{20}_D$ = + 79.33 (*c* 0.60, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.20-2.10 (m, 1H), 1.83 (s, 3H), 1.82-1.76 (m, 1H), 1.72-1.63 (m, 5H), 1.45 (s, 9H), 1.23-1.07 (m, 6H), 0.98 (s, 9H), 0.91-0.85 (m, 2H), 0.27 (s, 3H), 0.26 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.8, 167.7, 139.0, 136.7, 86.9, 83.2, 37.6, 33.2, 31.1, 30.1, 27.9, 26.6, 26.3, 25.6, 18.3, 9.3, -4.2, -4.3. HRMS m/z $[M+H]^+$ calcd. for $C_{24}H_{43}O_5Si$: 439.2880, found: 439.2893.



7

HPLC: 91% ee, Chiralcel AD-H column, 254 nm, 25 ^{0}C, *n*-hexane/*i*-propanol = 95/5, flow = 0.3 mL/min, retention time 11.8 min (maj) and 13.6 min.

(R)-tert-butyl 2-(2-([1,1'-biphenyl]-4-yl)ethyl)-4-((tert-butyldimethylsilyl)oxy)-3-methyl-5-oxo-2,5-dihydrofuran-2-carboxylate (8), 36

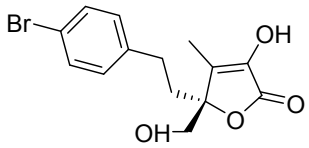


8

mg, 71% yield, light yellow solid, $[\alpha]^{20}_D$ = + 39.89 (*c* 0.61, $CHCl_3$). ^1H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 7.3 Hz, 2H), 7.52 (d, *J* = 7.6 Hz, 2H), 7.45-7.40 (m, 2H), 7.35-7.31 (m, 1H), 7.25 (d, *J* = 6.3 Hz, 2H), 2.67-2.50 (m, 3H), 2.14-2.04 (m, 1H), 1.47 (s, 9H), 0.99 (s, 9H), 0.27 (s, 3H), 0.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.7, 167.3, 141.0, 139.9, 139.4, 139.1, 136.5, 128.9, 128.8, 127.4, 127.2, 127.1, 86.5, 83.6, 35.9, 29.1, 28.0, 25.7, 18.3, 9.3, -4.1, -4.2. HRMS m/z $[M+H]^+$ calcd. for $C_{30}H_{41}O_5Si$: 509.2723, found: 509.2718.

HPLC: 88% ee, Chiralcel OD-H column, 254 nm, 25 ^{0}C, *n*-hexane/*i*-propanol = 97/3, flow = 0.3 mL/min, retention time 6.4 min (maj) and 7.0 min.

(R)-5-(4-bromophenethyl)-3-hydroxy-5-(hydroxymethyl)-4-methylfuran-2(5H)-

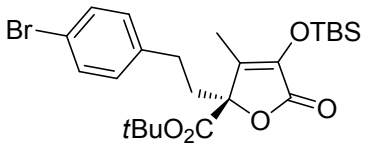


9

one (9), 41.1mg, 63% yield, white solid, $[\alpha]^{20}_D$ = - 4.07 (*c* 0.64, CH_3OH). ^1H NMR (400 MHz, DMSO) δ 9.31 (s, 1H), 7.44 (d, *J* = 8.3 Hz, 2H), 7.15 (d, *J* = 8.4 Hz, 2H), 5.00 (brs, 1H), 3.62 – 3.42 (m, 2H), 2.37 – 2.20 (m, 2H), 1.98 (ddd, *J* = 16.4, 11.8, 6.2 Hz, 1H), 1.86 (ddd, *J* = 14.3, 11.4, 5.7 Hz, 1H), 1.75 (s, 3H); ^{13}C NMR (**101** MHz, DMSO) δ 169.23, 141.16, 139.43, 131.58, 131.04, 130.95, 119.33, 88.14, 64.14, 33.43, 27.99, 9.27. HRMS m/z $[M+H]^+$ calcd. for $C_{14}H_{15}O_4Br$: 327.0226, found: 327.0225.

HPLC: 86% ee, Chiralcel AS-H column, 235 nm, 25 ^{o}C, *n*-hexane/*i*-propanol = 95/5, flow = 1.0 mL/min, retention time 54.8 min (maj) and 65.6 min.

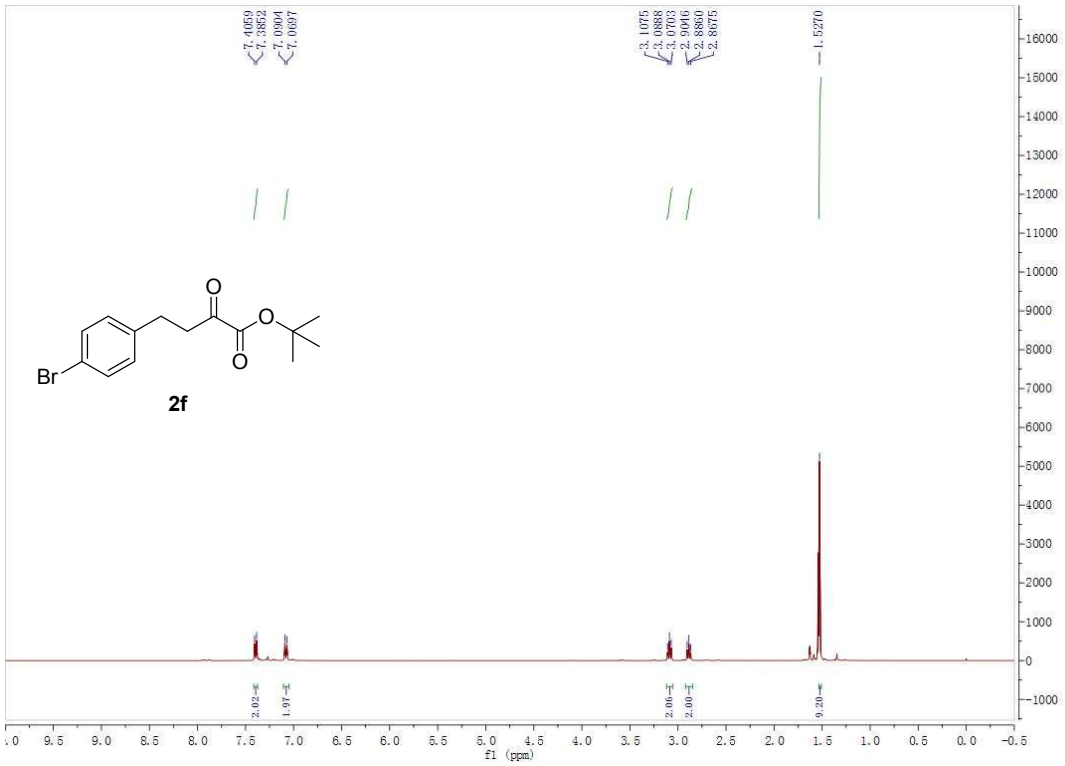
For gram scale (**3f-TBS** = **3'f**)

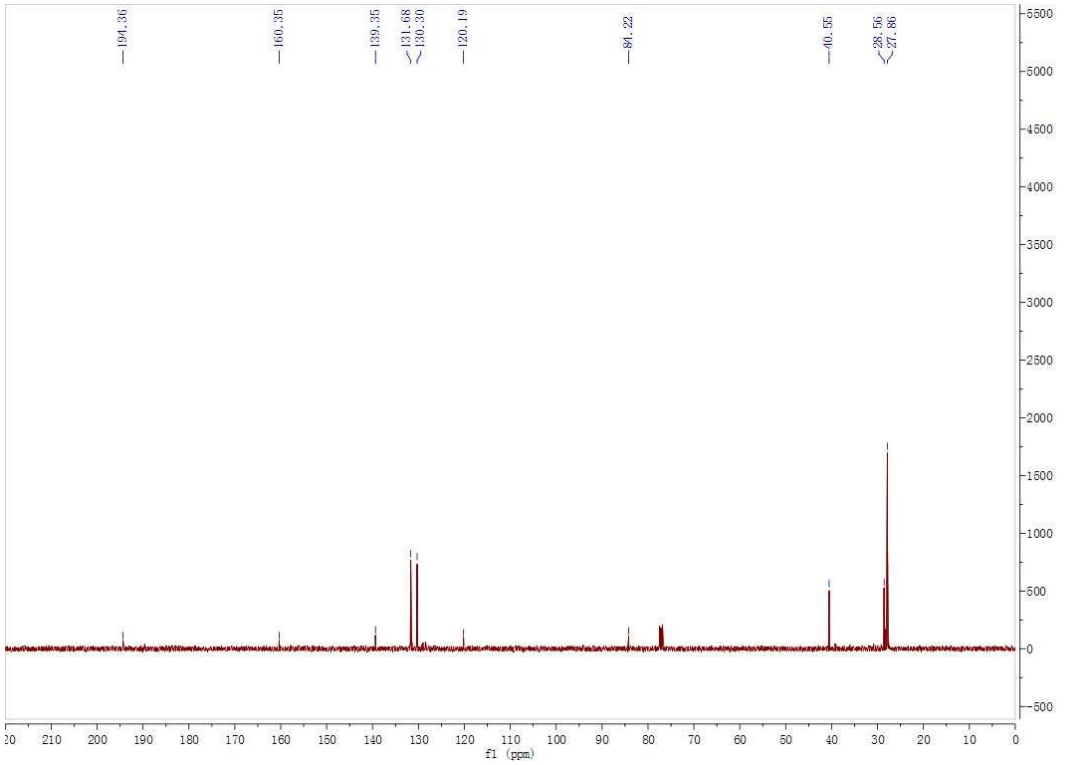


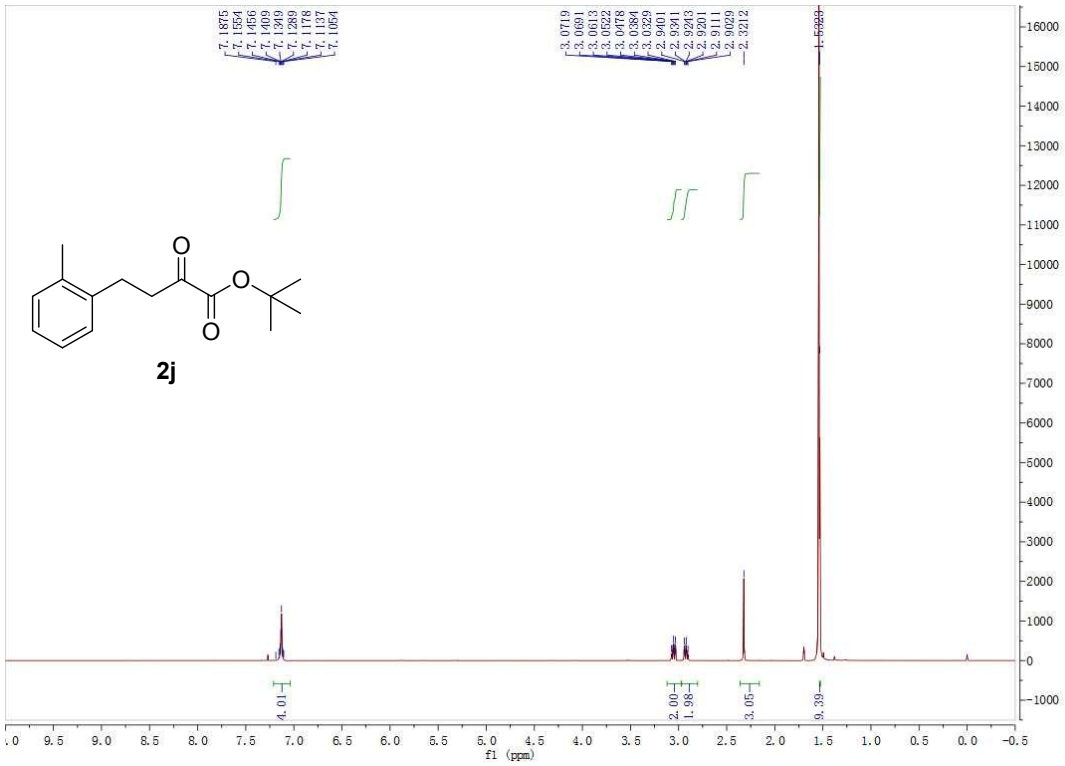
3f-TBS **= 3'f**

HPLC: 88% ee, Chiralcel AD-H column, 254 nm, 25 ^{0}C, *n*-hexane/*i*-propanol = 95/5, flow = 0.3 mL/min, retention time 15.0 min (maj) and 22.3 min.

11. Copy of NMR spectra and HPLC chromatograms






7.1875
7.1554
7.1456
7.1409
7.1289
7.1178
7.1137
7.1054
3.0719
3.0691
3.0613
3.0522
3.0478
3.0384
3.0329
2.9401
2.9341
2.9243
2.9201
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2.3212
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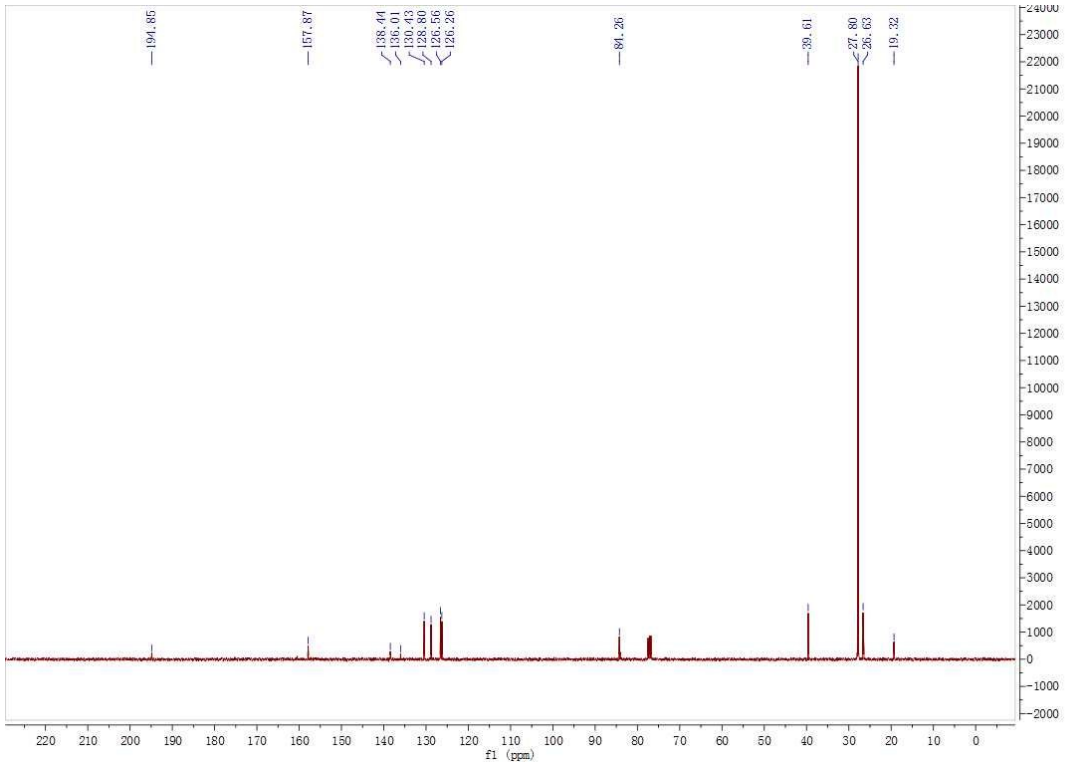
4.01
2.00
1.98
3.05
9.39
f1 (ppm)

2j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27.80
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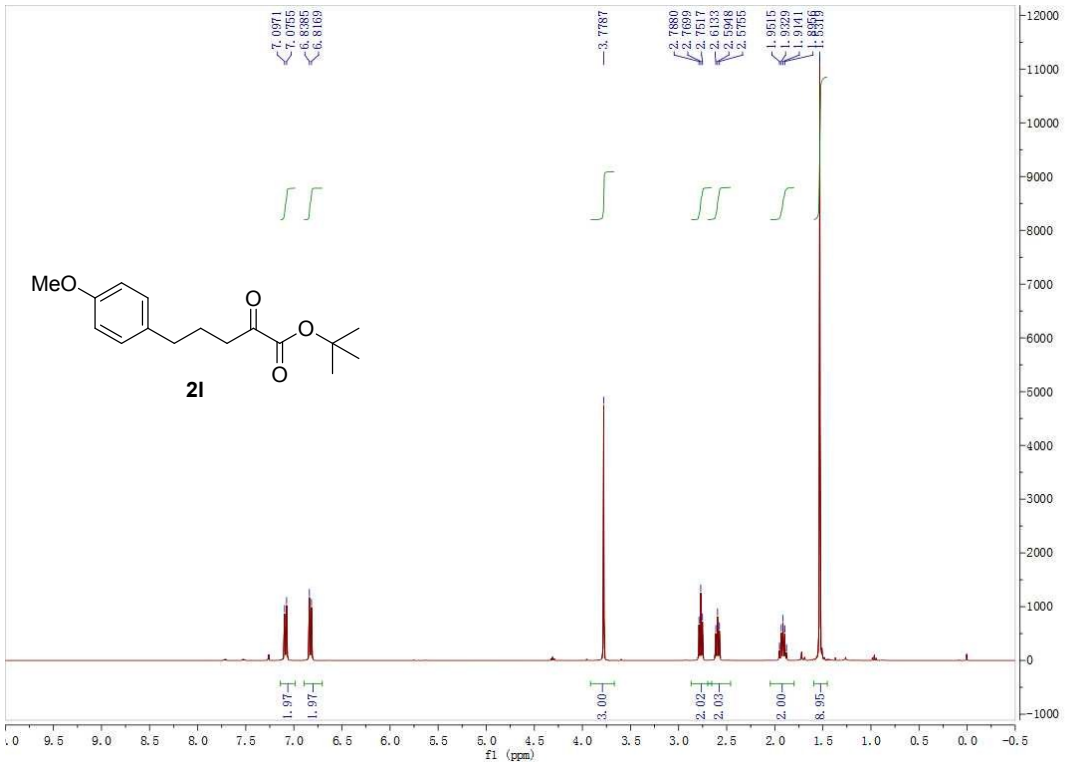
19.32
f1 (ppm)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2.5755
1.9515
1.9329
1.9141
1.8956
MeO
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O
2l
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1.97
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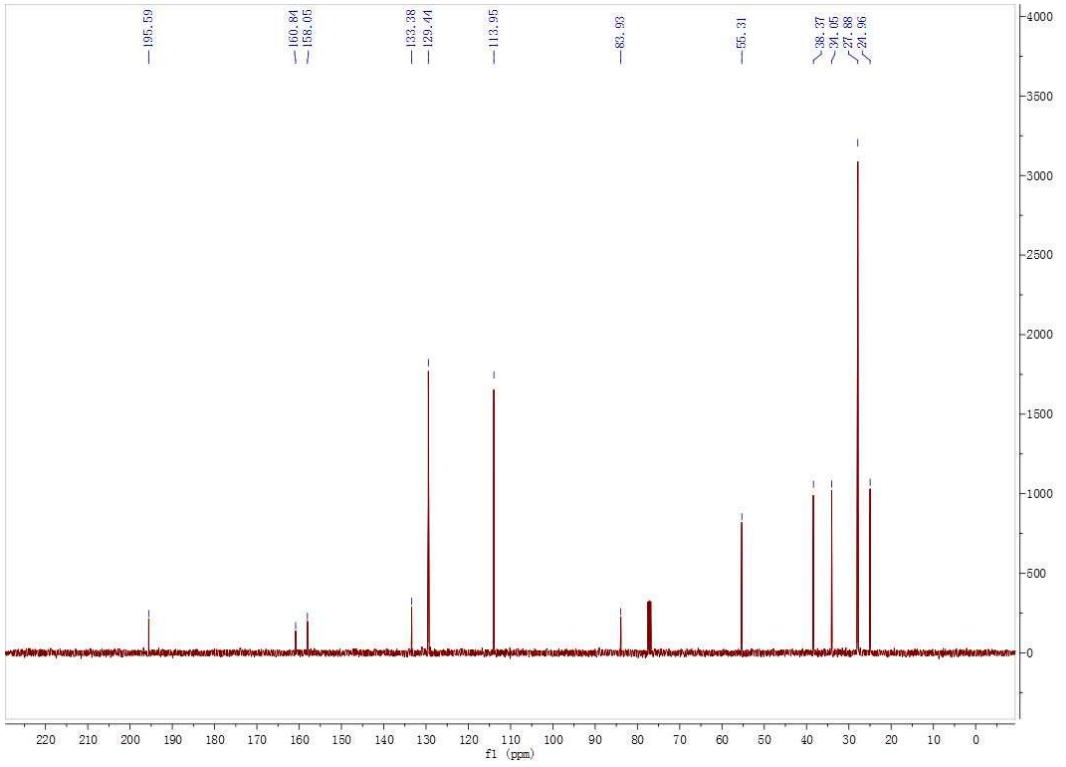
2.03
2.00
8.95
f1 (ppm)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55.31
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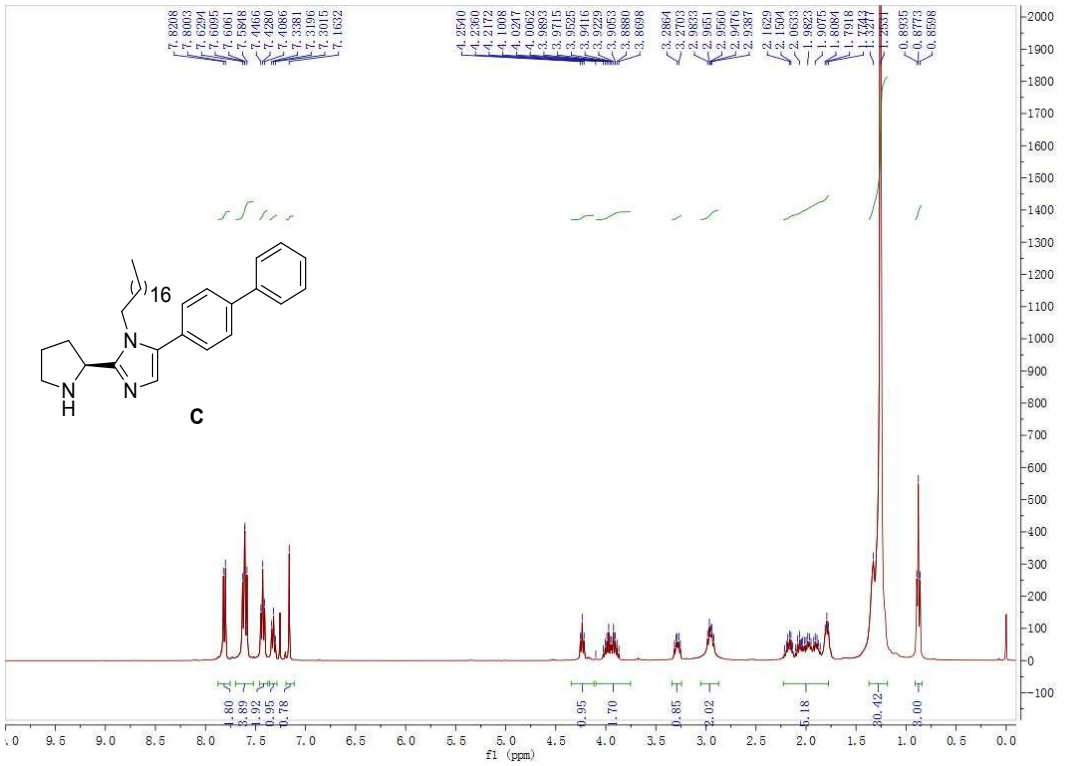
27.88
24.96
f1 (ppm)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7.3015
7.1632
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4.2360
4.2172
4.1008
4.0267
4.0062
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3.9715
3.9525
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3.9229
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3.8880
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2.0633
1.9823
1.9075
1.8084
1.7918
1.7443
1.3277
1.2651
0.8935
0.8773
0.8598
16
N
N
H
C
4.80
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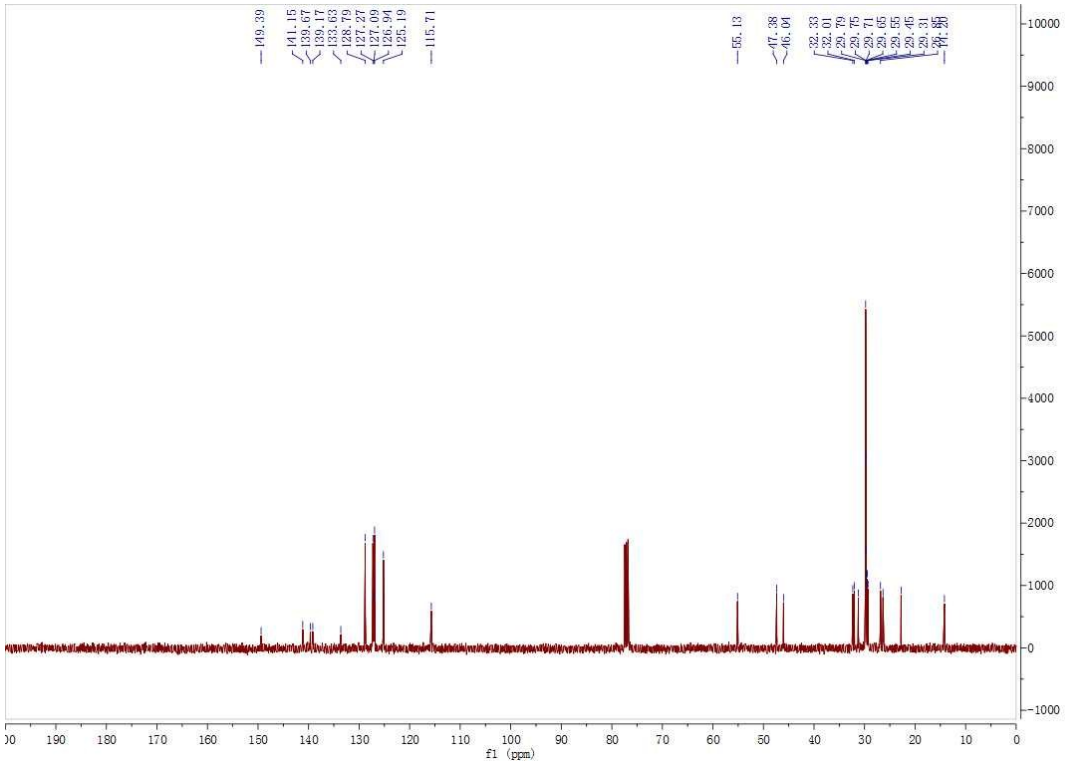
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127.09
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115.71
55.13
47.38
46.04
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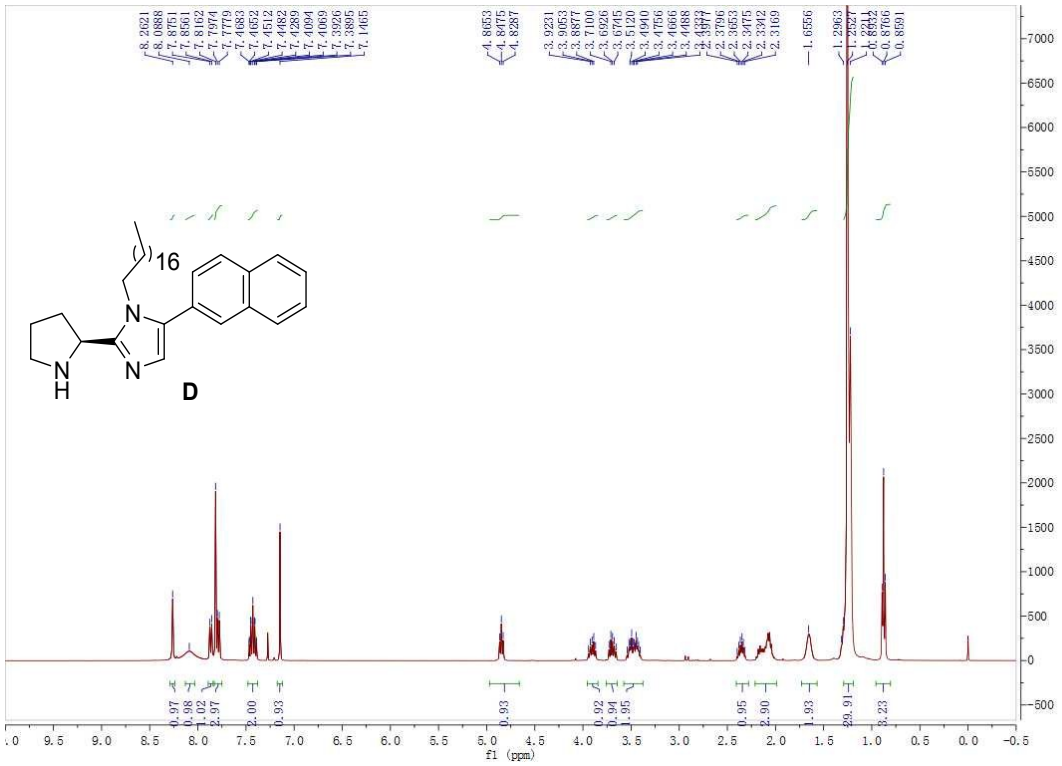
29.65
29.55
29.46
29.31
24.55
24.50
f1 (ppm)


16
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N
N
H
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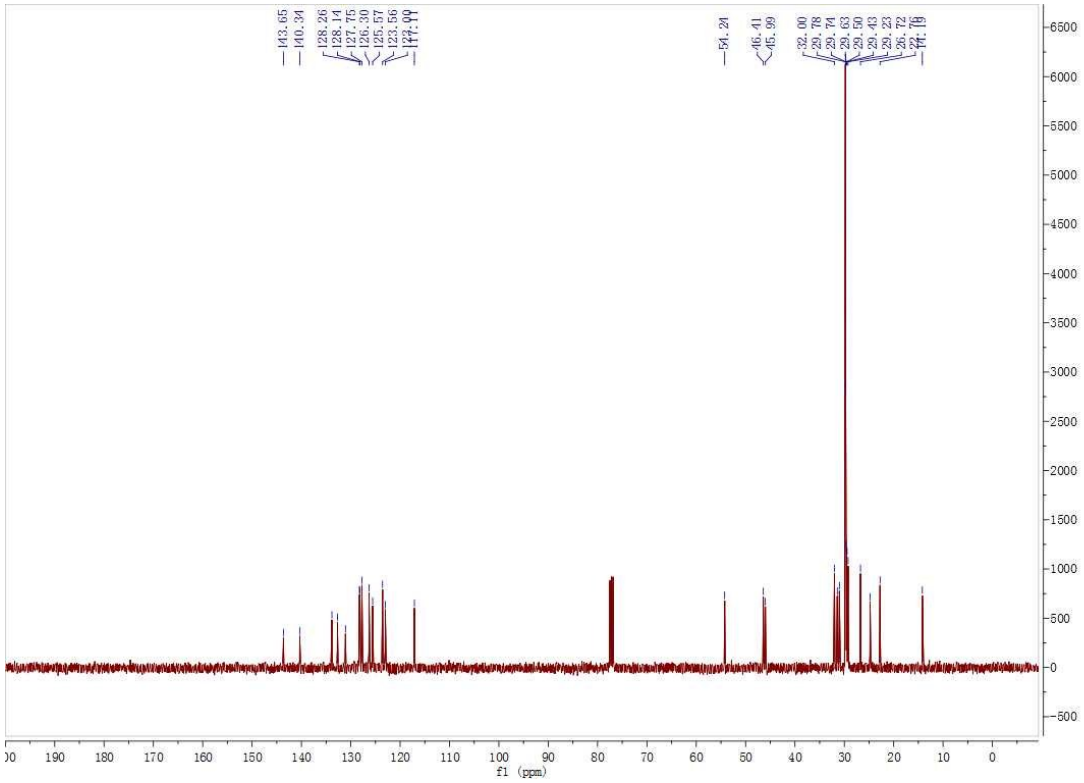
f1 (ppm)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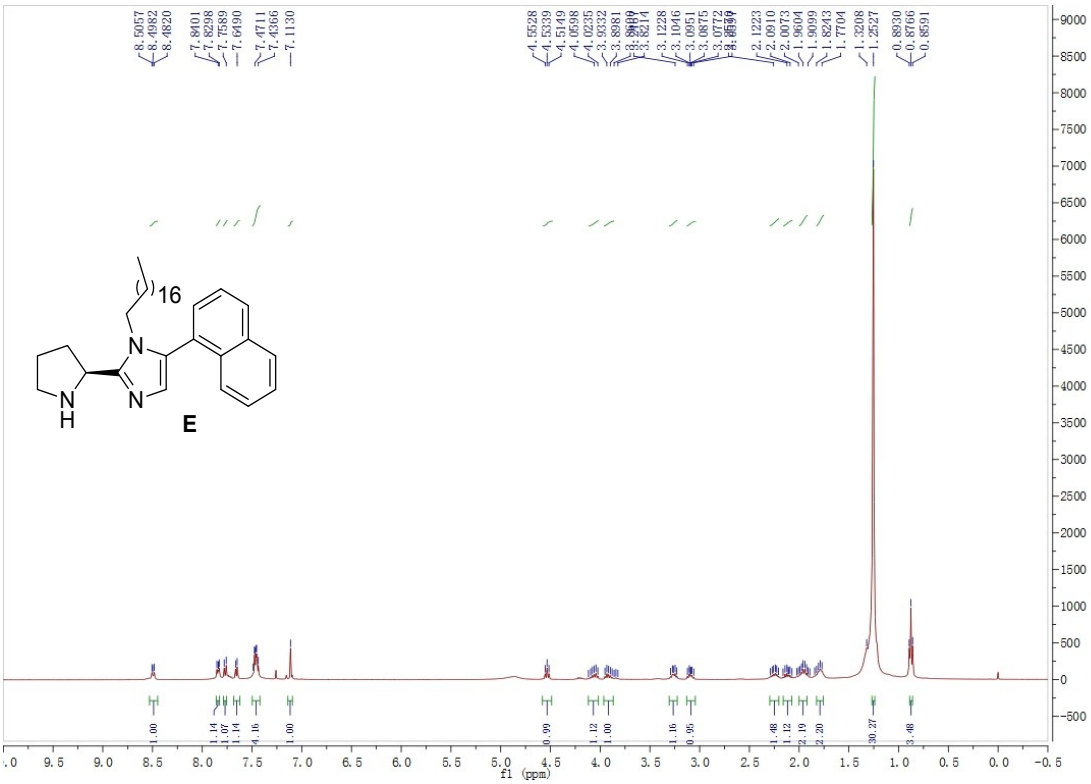
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7.1130
4.5528
4.5339
4.5149
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3.8214
3.1228
3.1046
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3.0875
3.0772
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2.0910
2.0073
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1.9099
1.8243
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16
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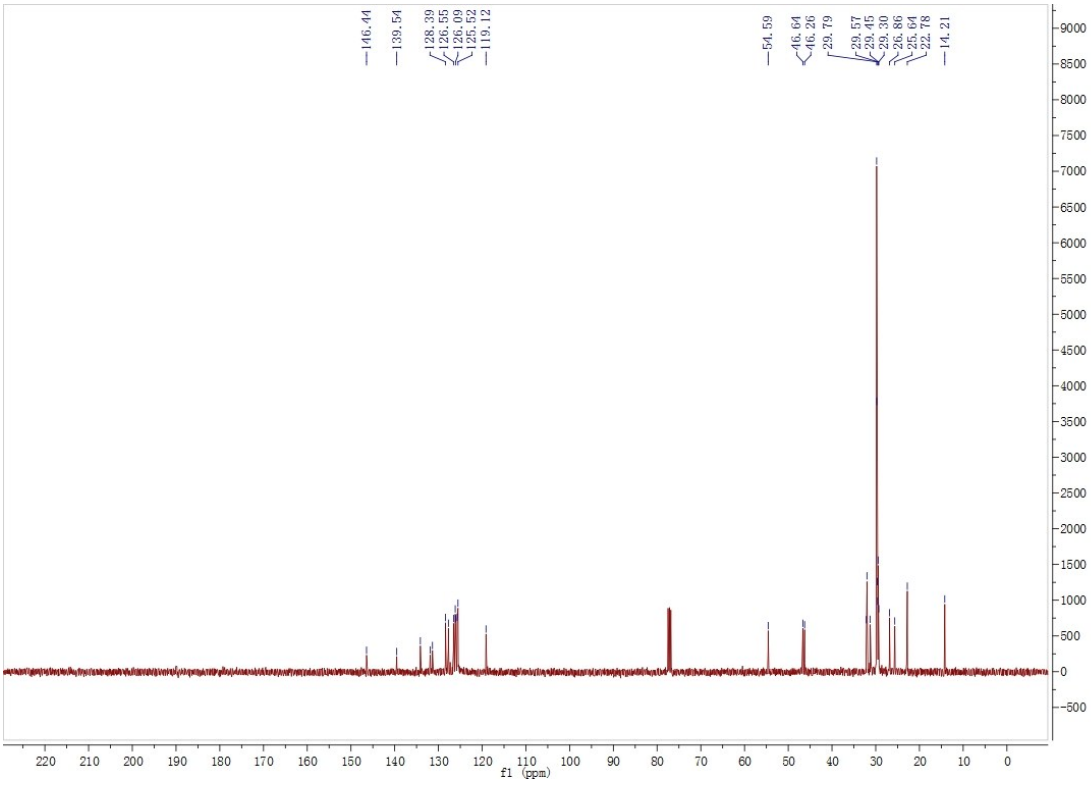
N
H
E
f1 (ppm)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139.54
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126.09
125.52
119.12
54.59
46.64
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29.79
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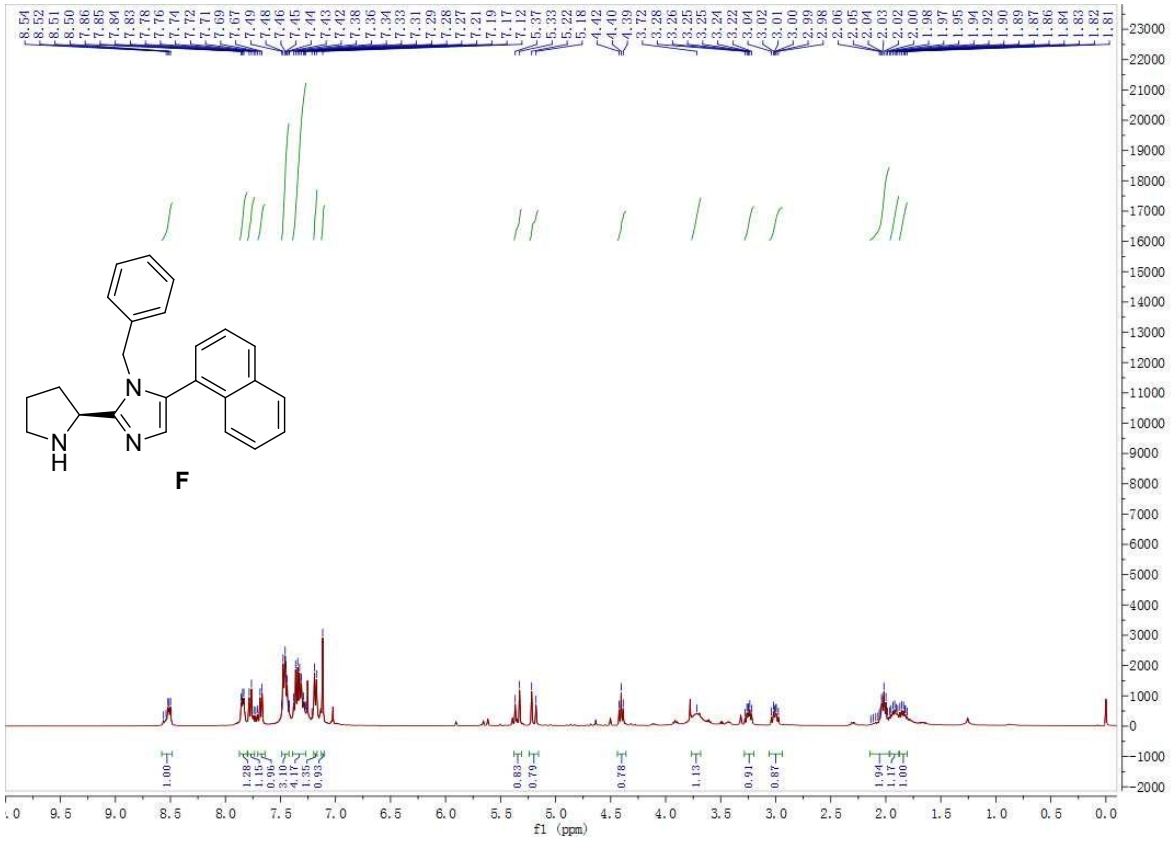
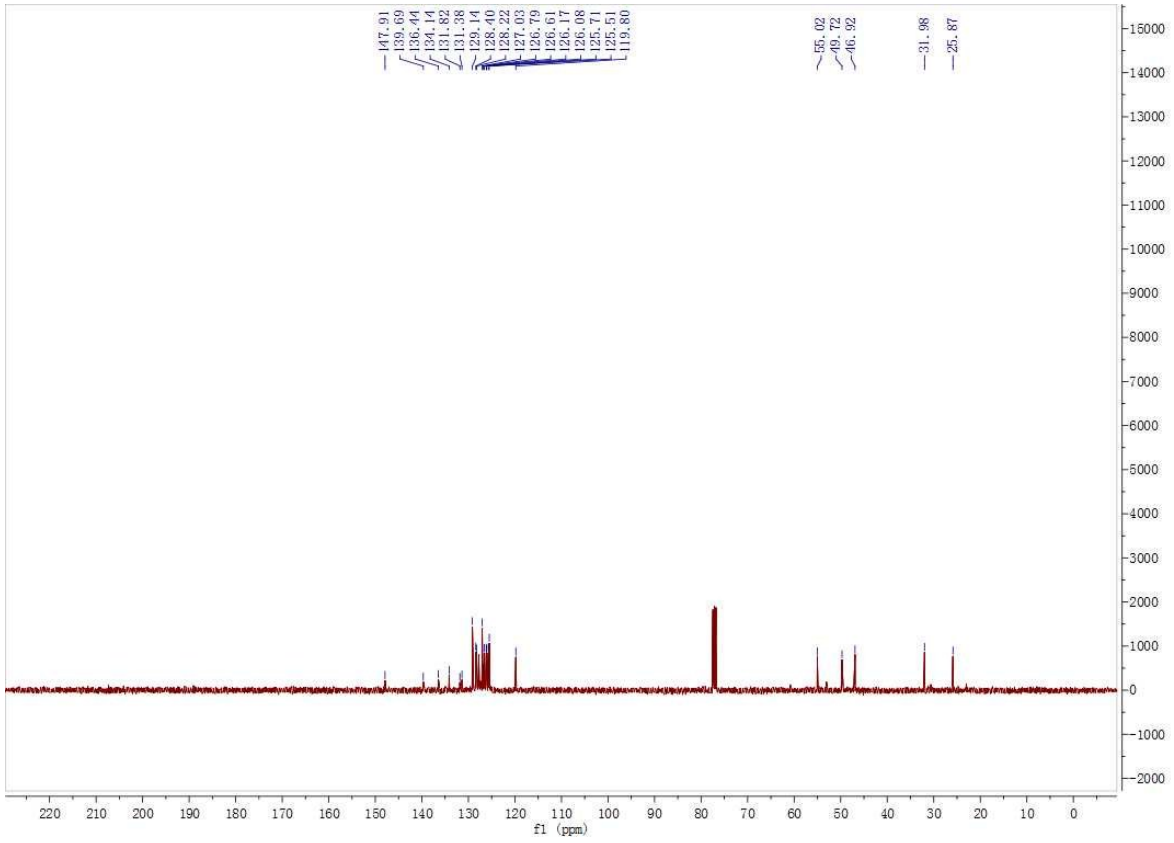
29.45
29.30
26.86
25.64
22.78
14.21
f1 (ppm)


F
f1 (ppm)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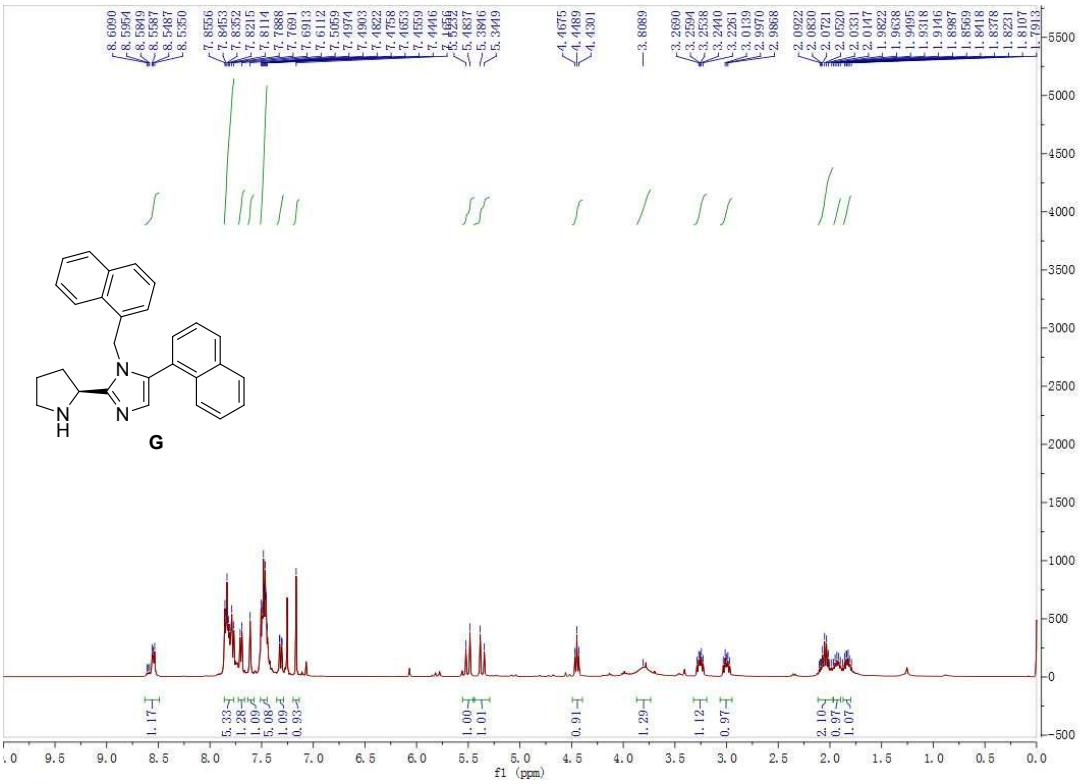
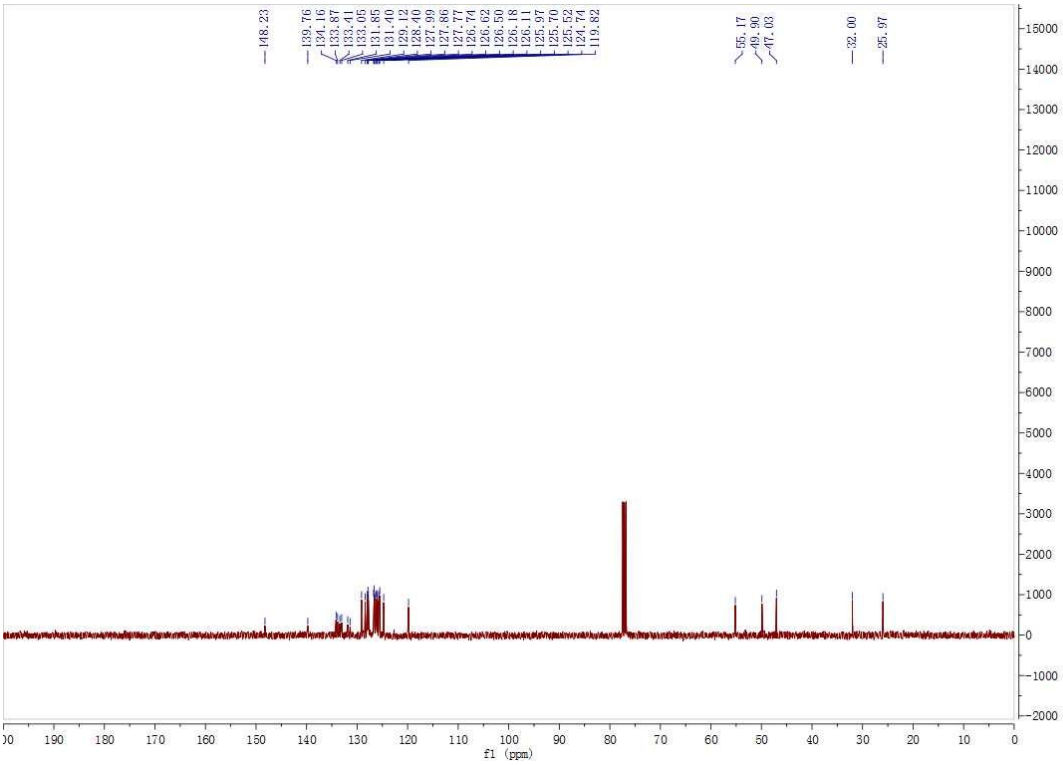

G
f1 (ppm)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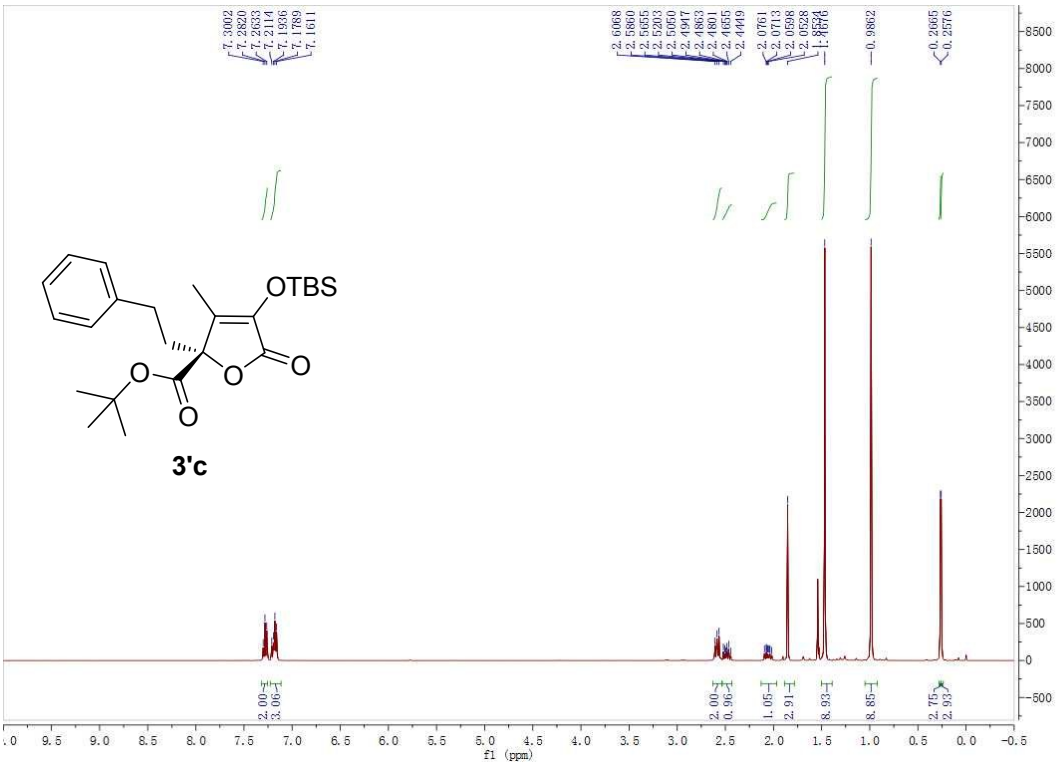
OTBS
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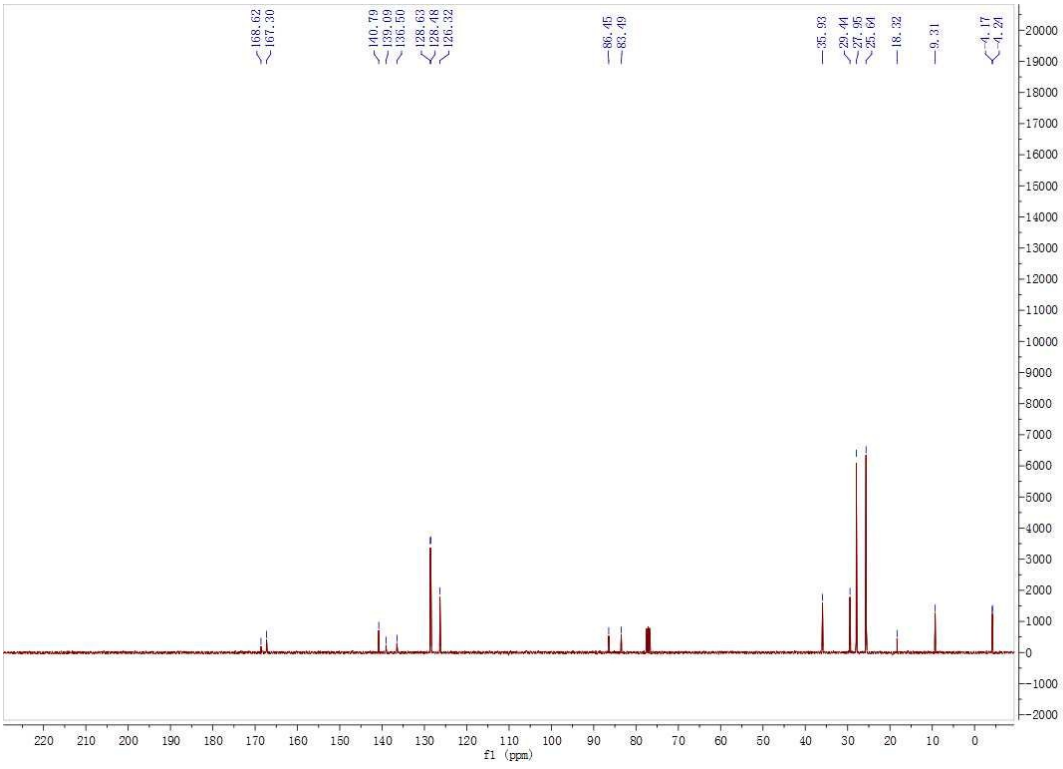
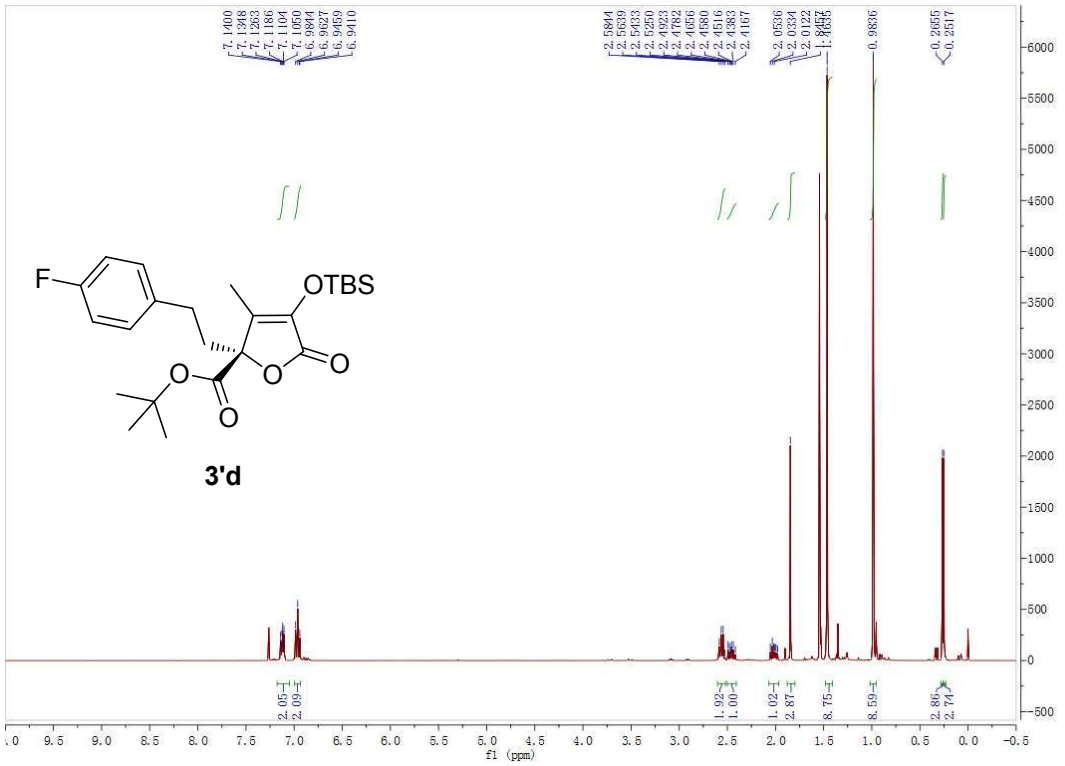
O
O
3'c
f1 (ppm)


f1 (ppm)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OTBS
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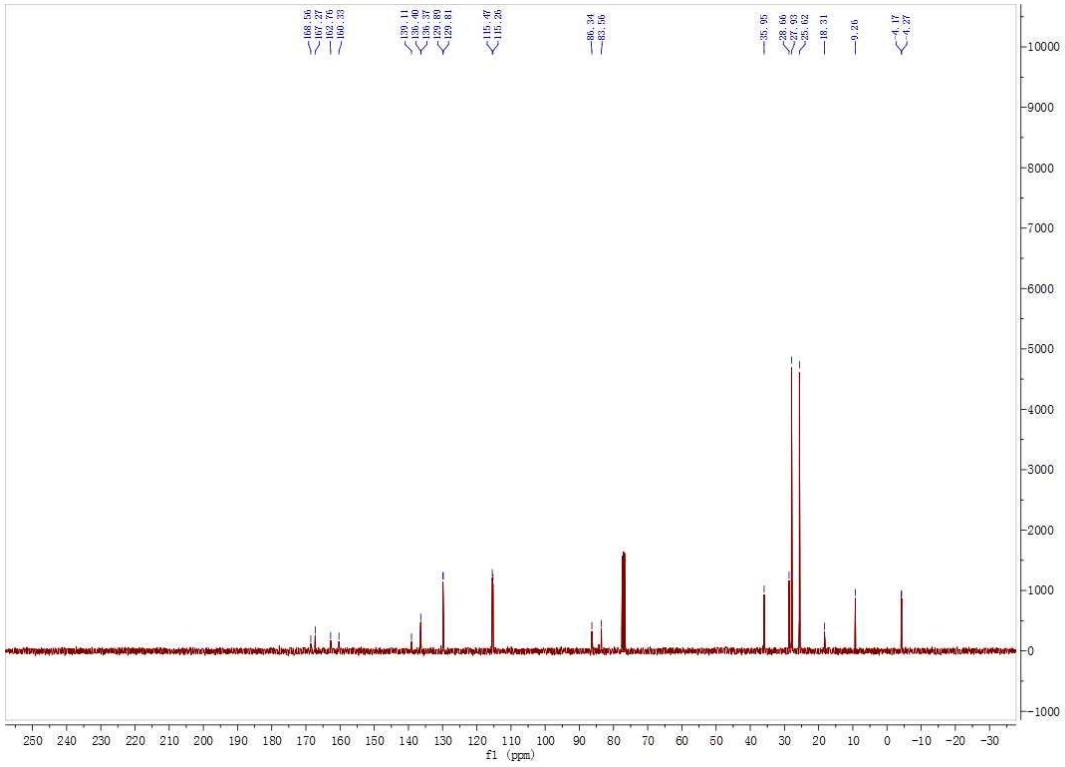
O
O
O
3'd
f1 (ppm)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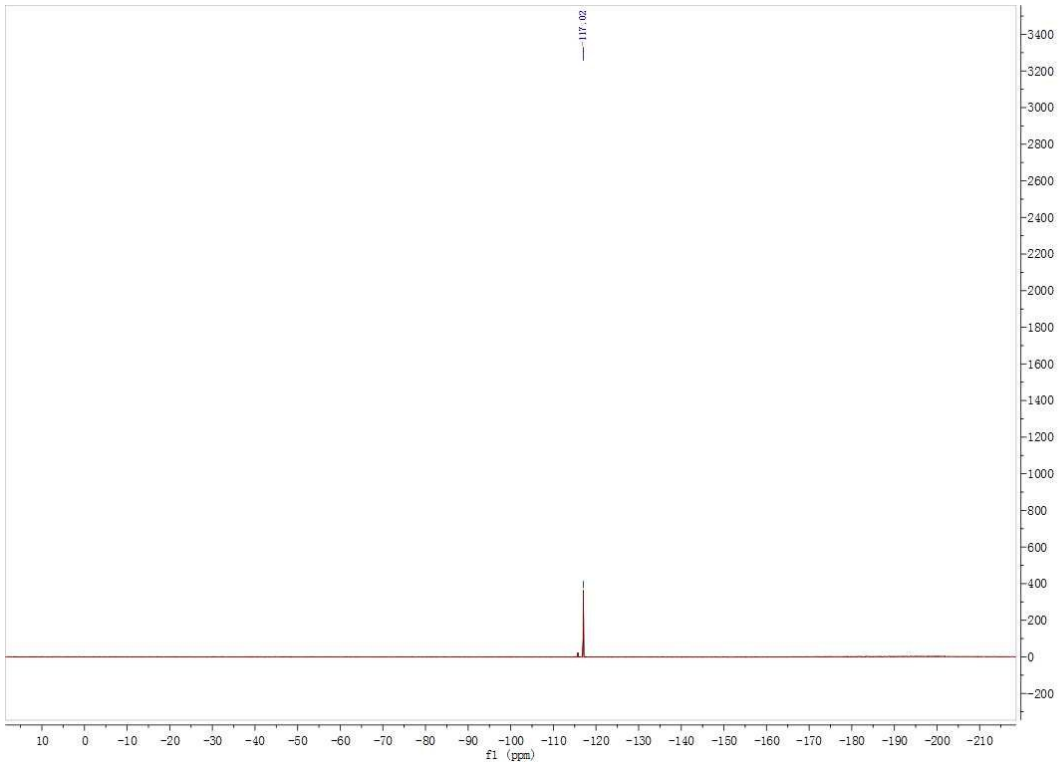
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3200
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2800
2600
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2200
2000
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1600
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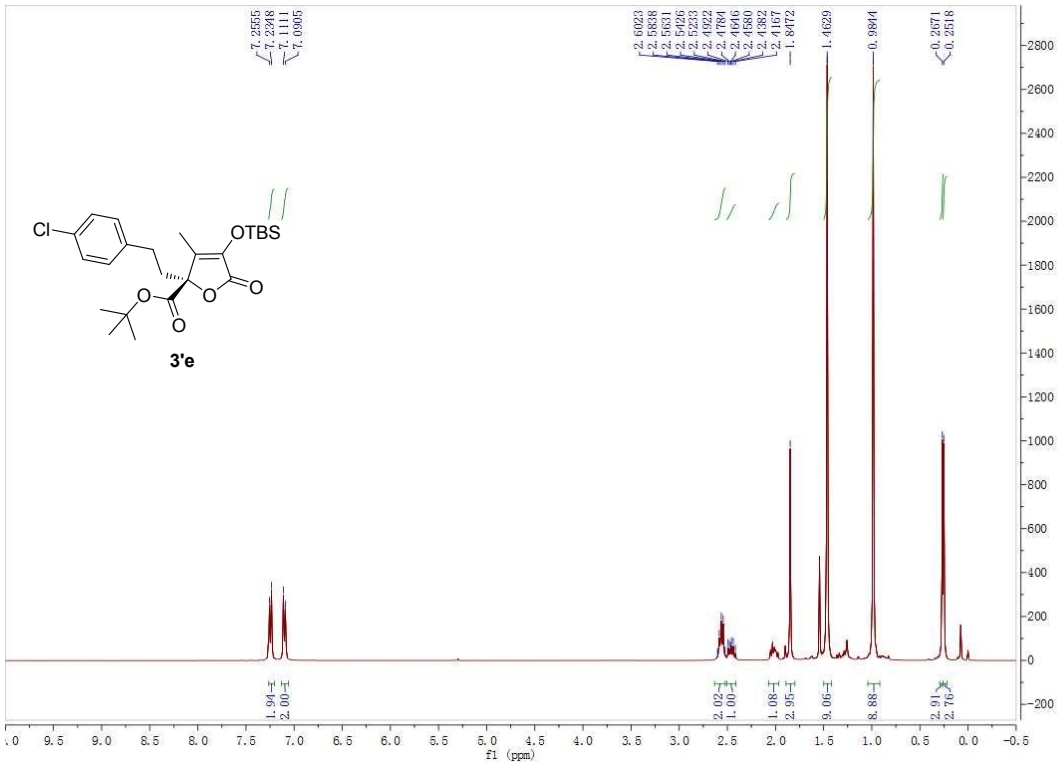
1200
1000
800
600
400
200
0
-200
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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7.1111
7.0905
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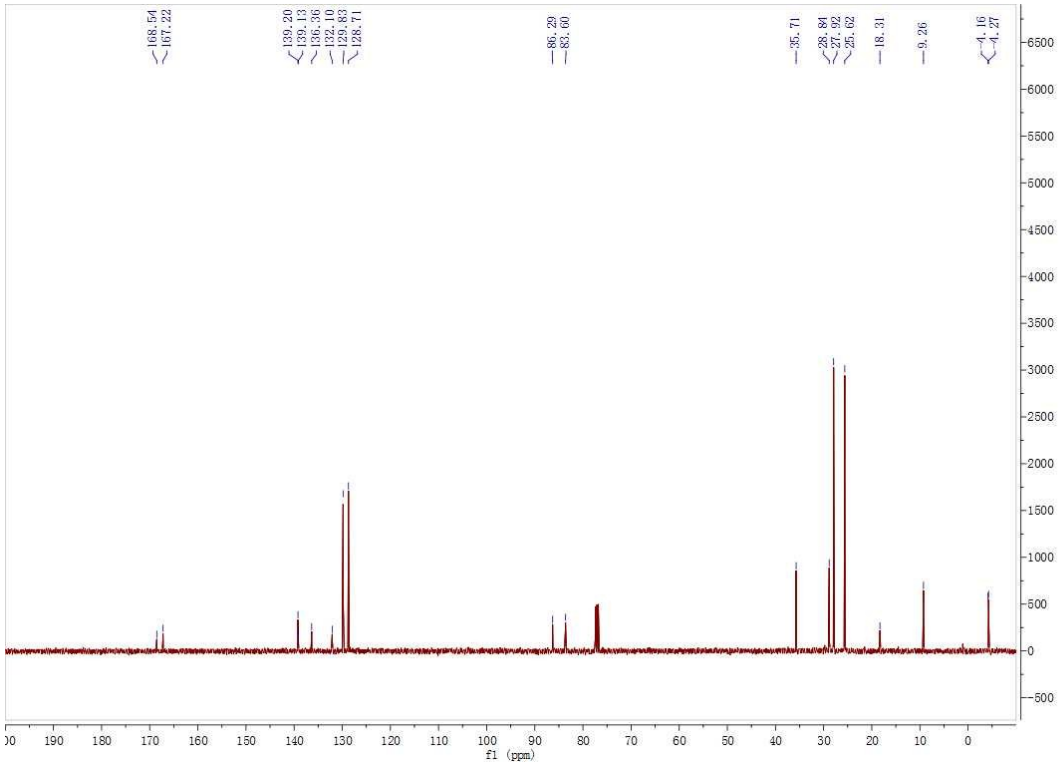
2.5838
2.5631
2.5426
2.5233
2.4922
2.4784
2.4646
2.4580
2.4382
2.4167
1.8472
1.4629
0.9804
0.2671
0.2518
Cl
OTBS
O
O
O
O
3'e
1.94
2.00
2.02
1.00
1.08
2.95
9.06
8.88
2.91
2.76
f1 (ppm)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139.13
136.36
132.10
129.83
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86.29
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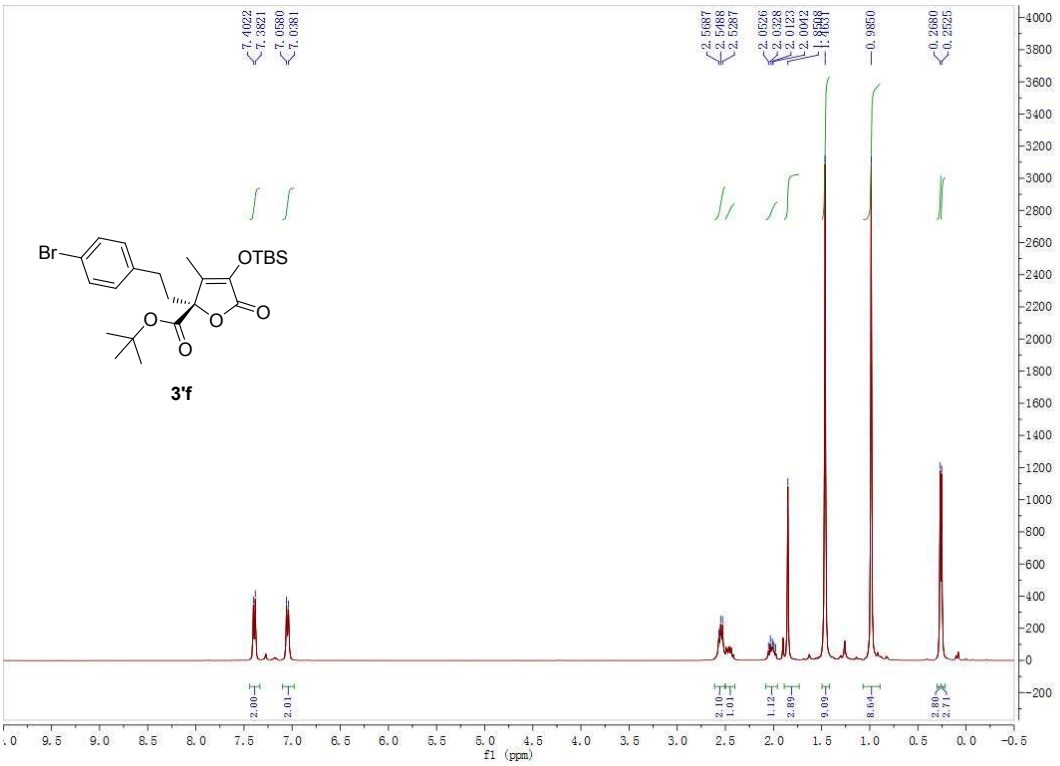
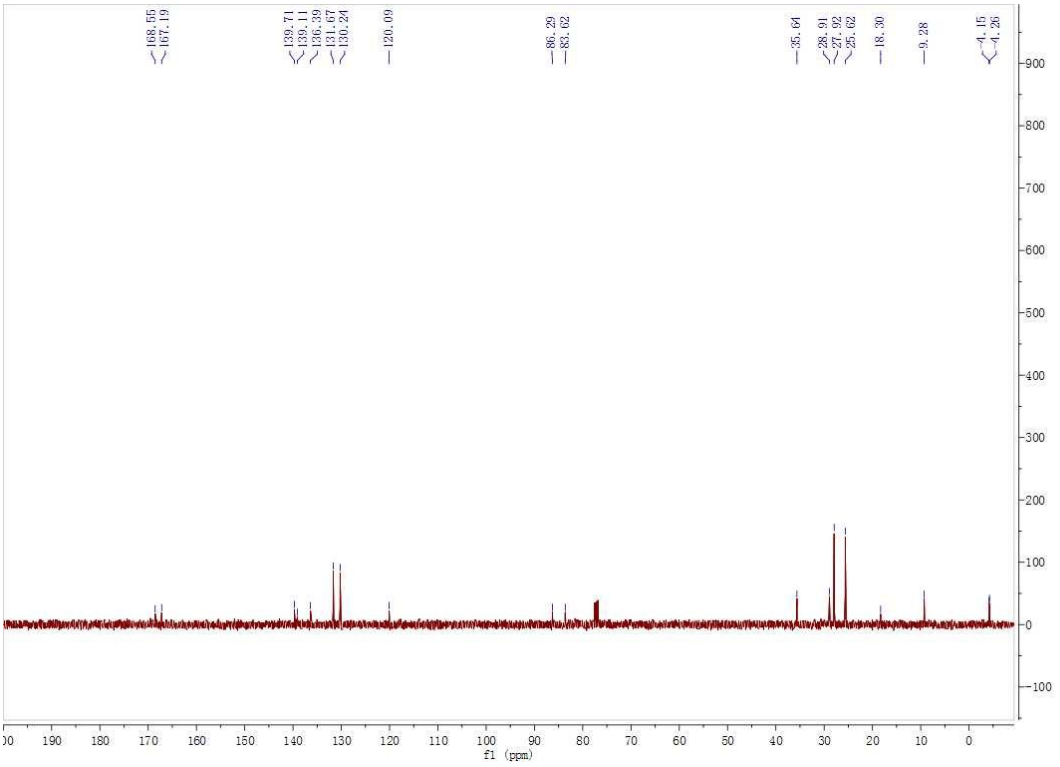
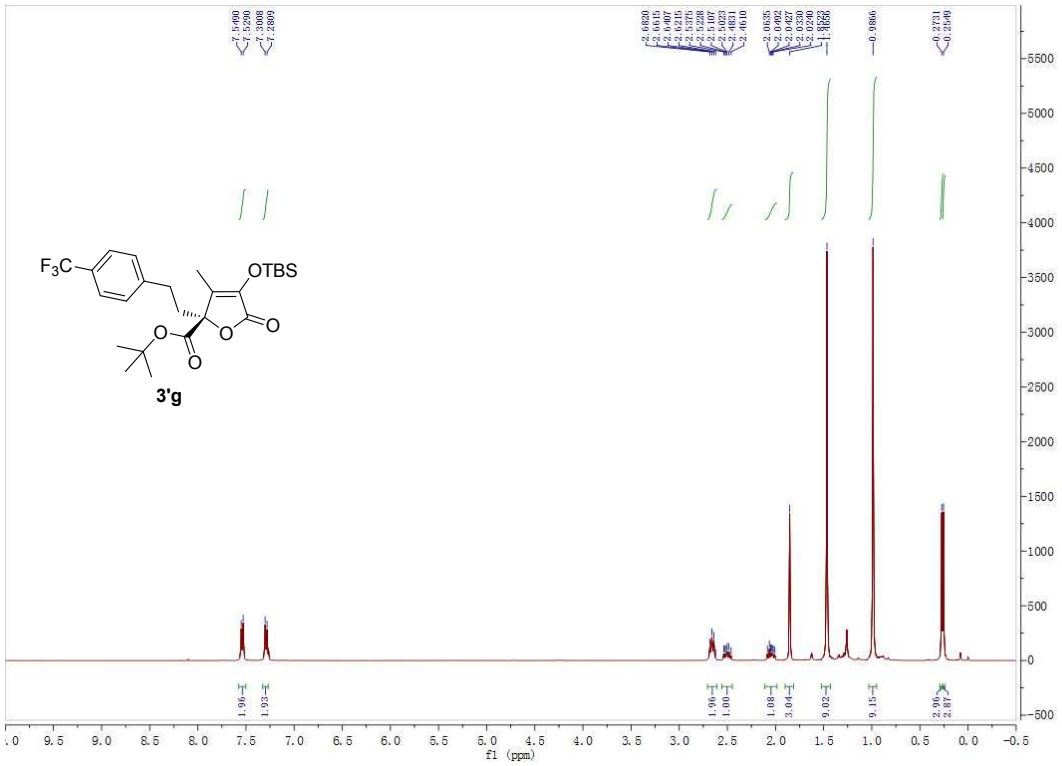
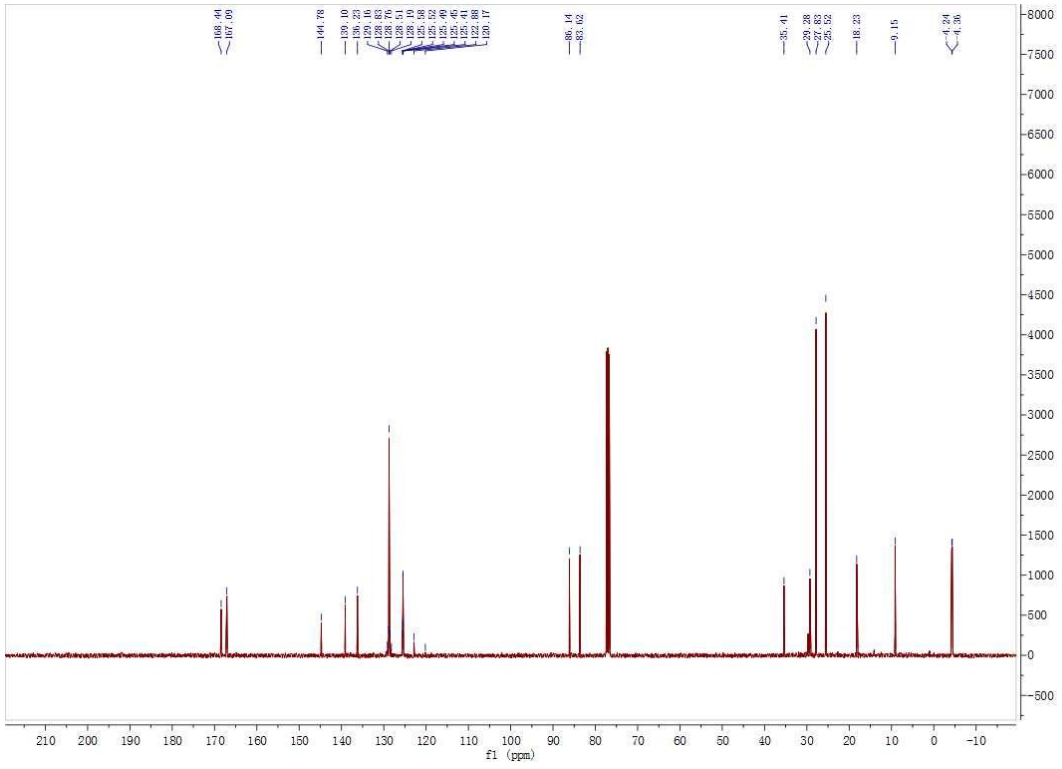
35.71
28.89
27.92
25.62
18.31
9.26
4.16
4.27
f1 (ppm)


Br
OTBS
O
O
O
O
3'f
f1 (ppm)


f1 (ppm)


F3C
OTBS
O
O
O
O
3'g
f1 (ppm)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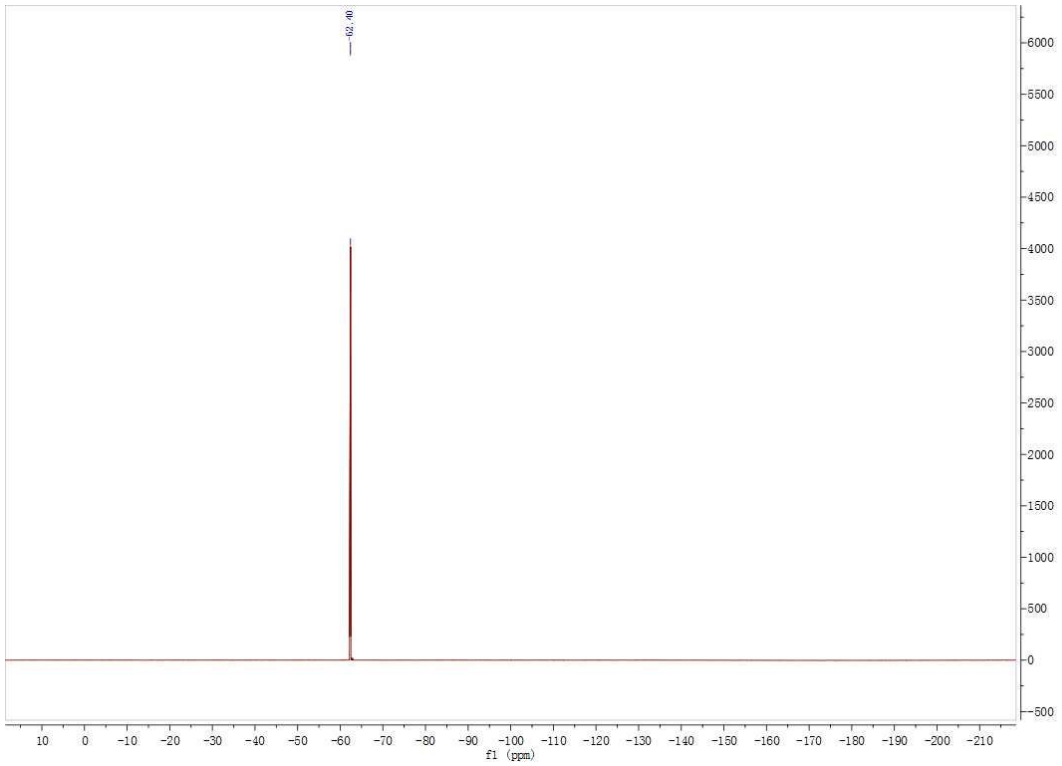
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5000
4500
4000
3500
3000
2500
2000
1500
1000
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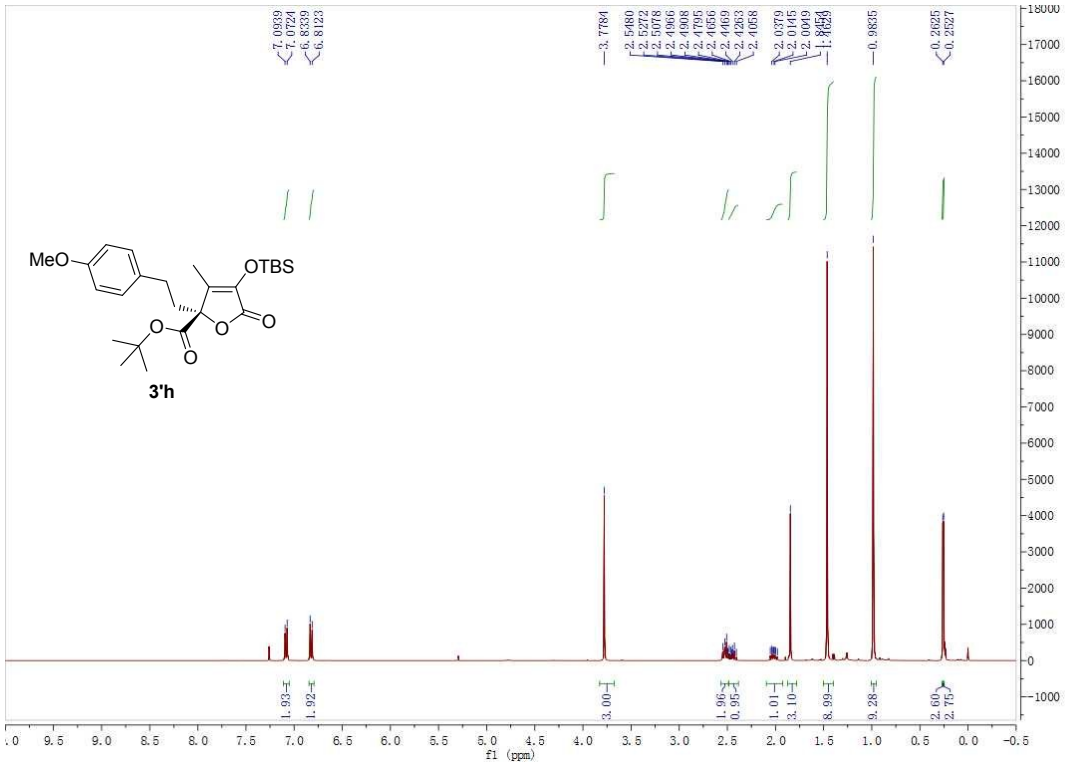
0
-500
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


MeO
OTBS
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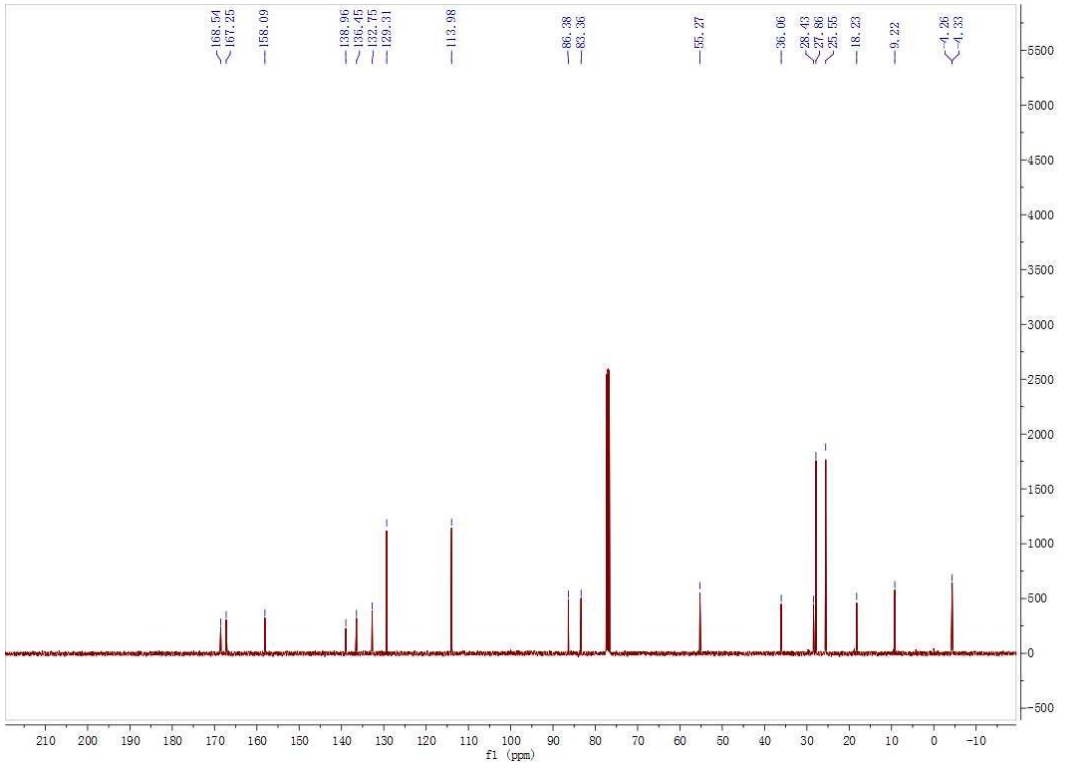
O
O
O
3'h
f1 (ppm)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9.22
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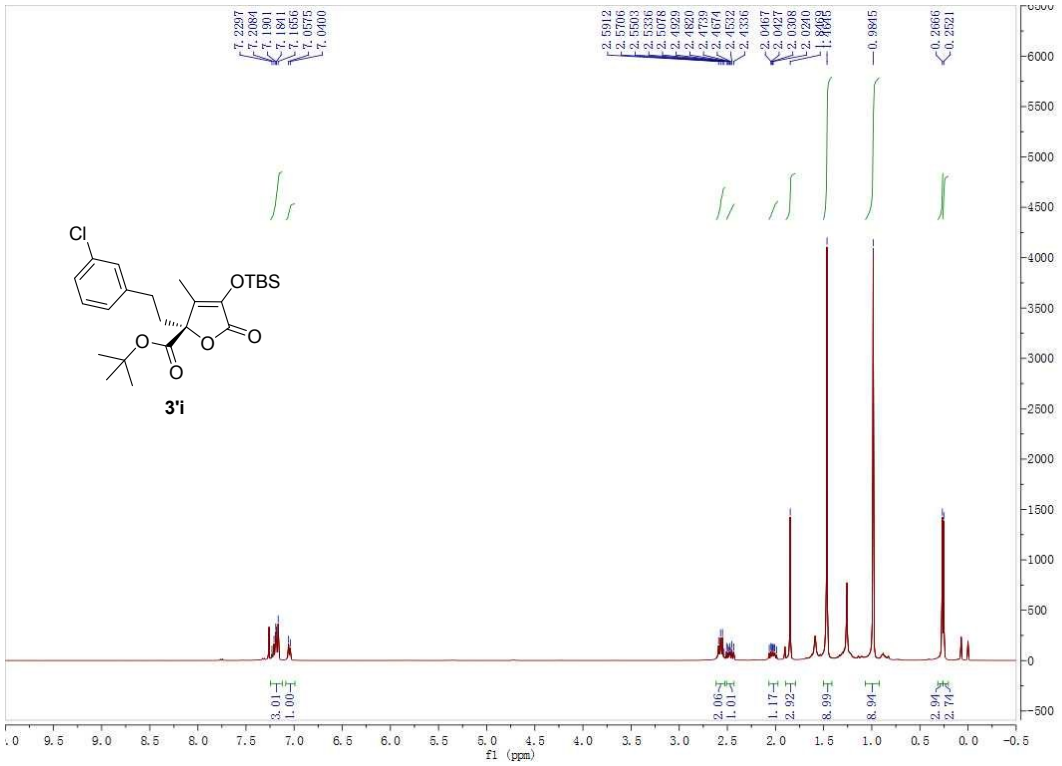
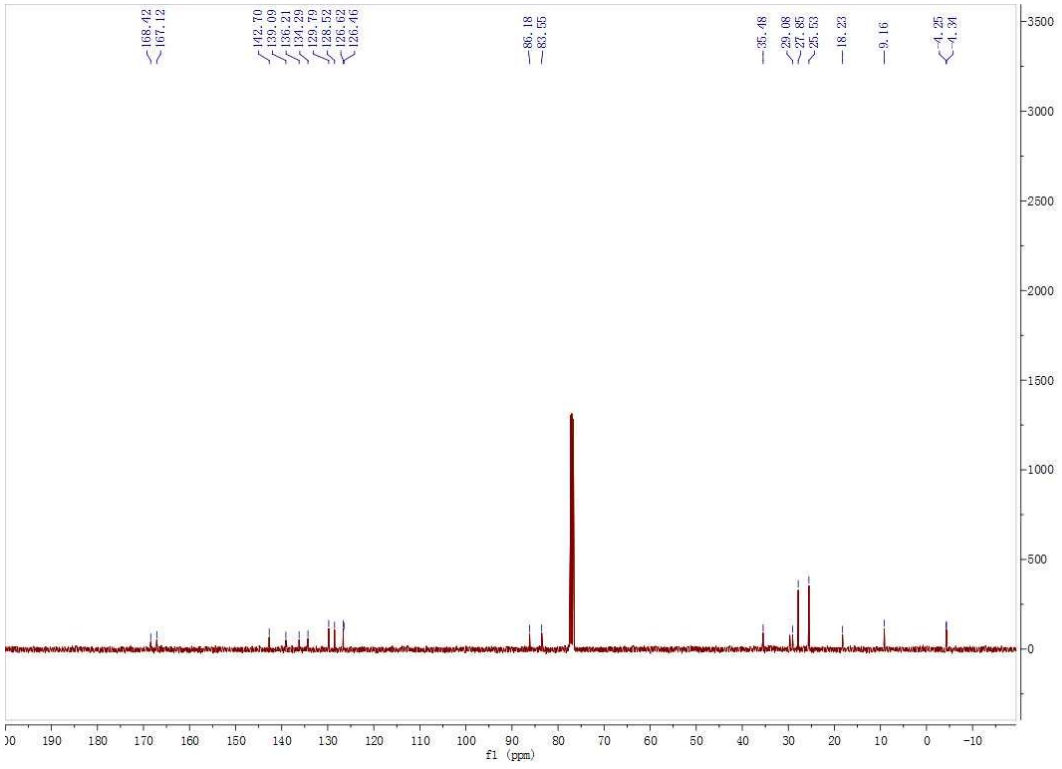
-4.33
f1 (ppm)


Cl
OTBS
O
O
O
O
3'i
f1 (ppm)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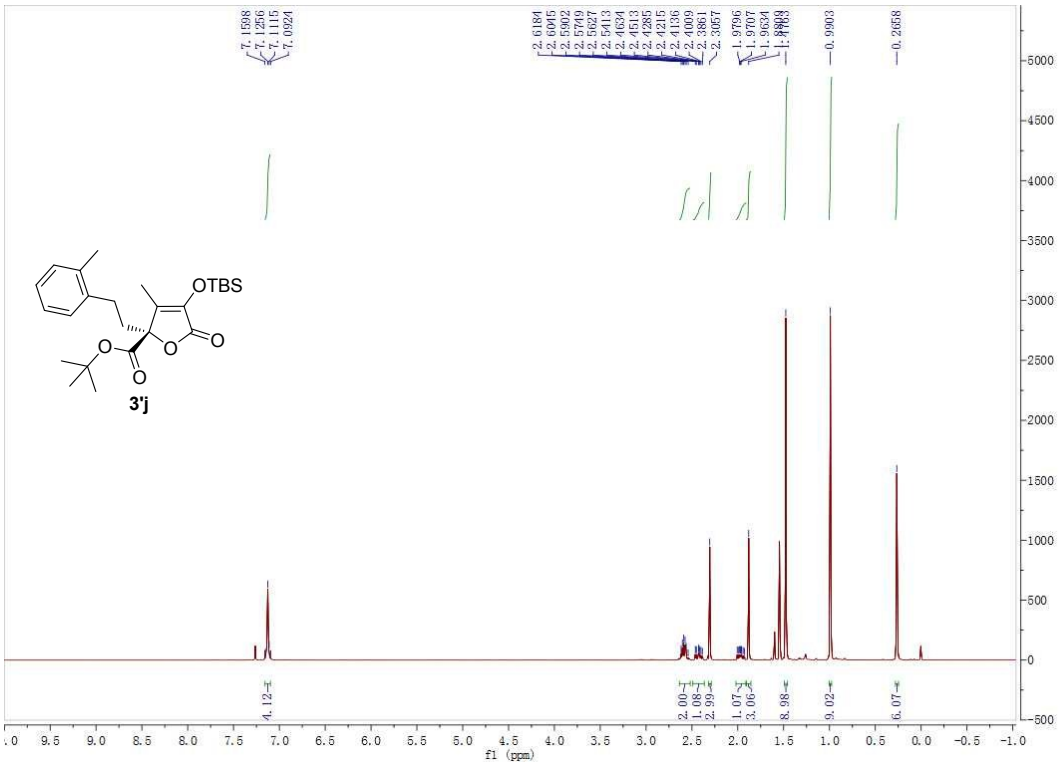
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O
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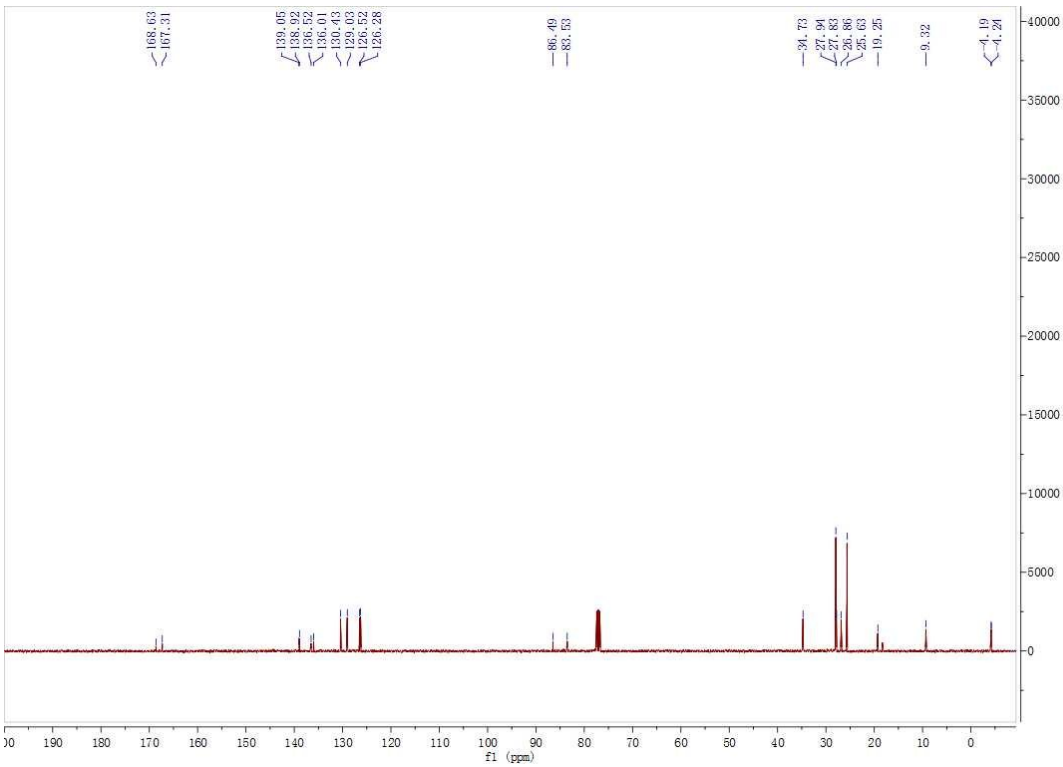
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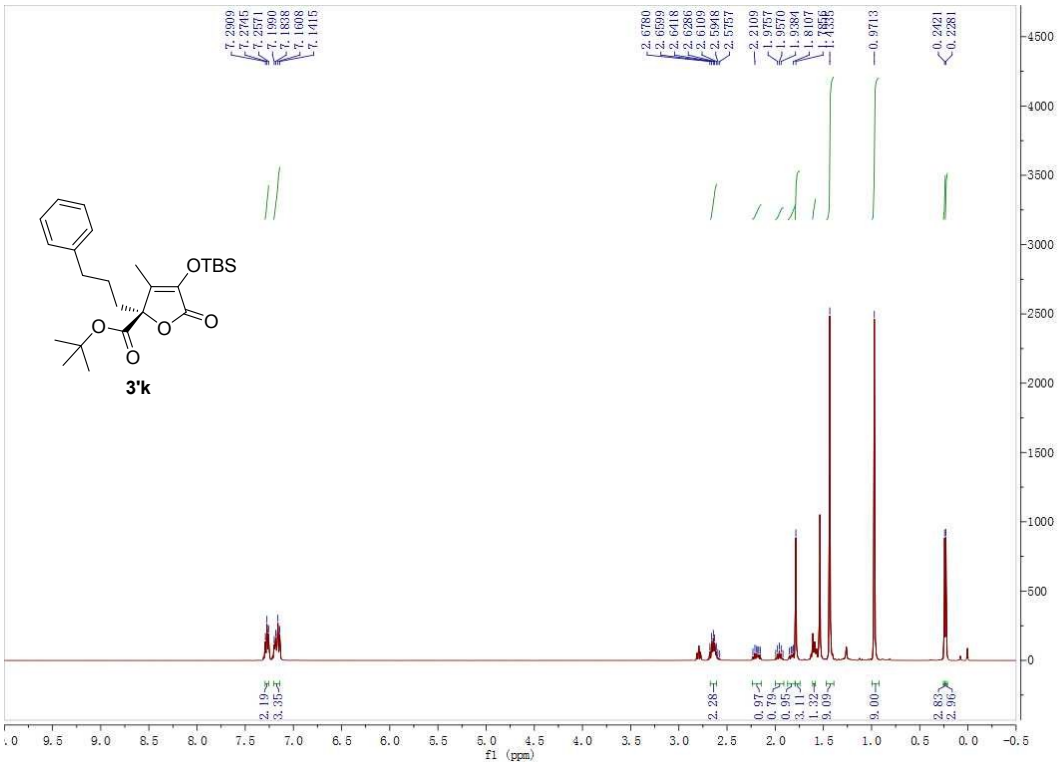
OTBS
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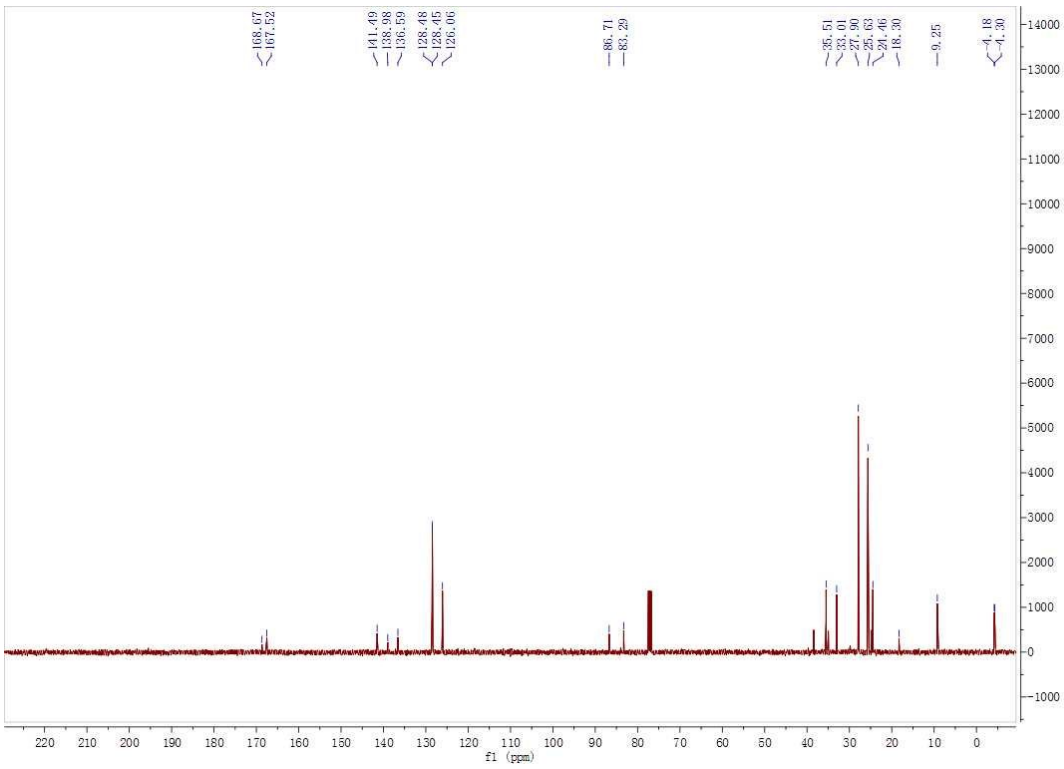
f1 (ppm)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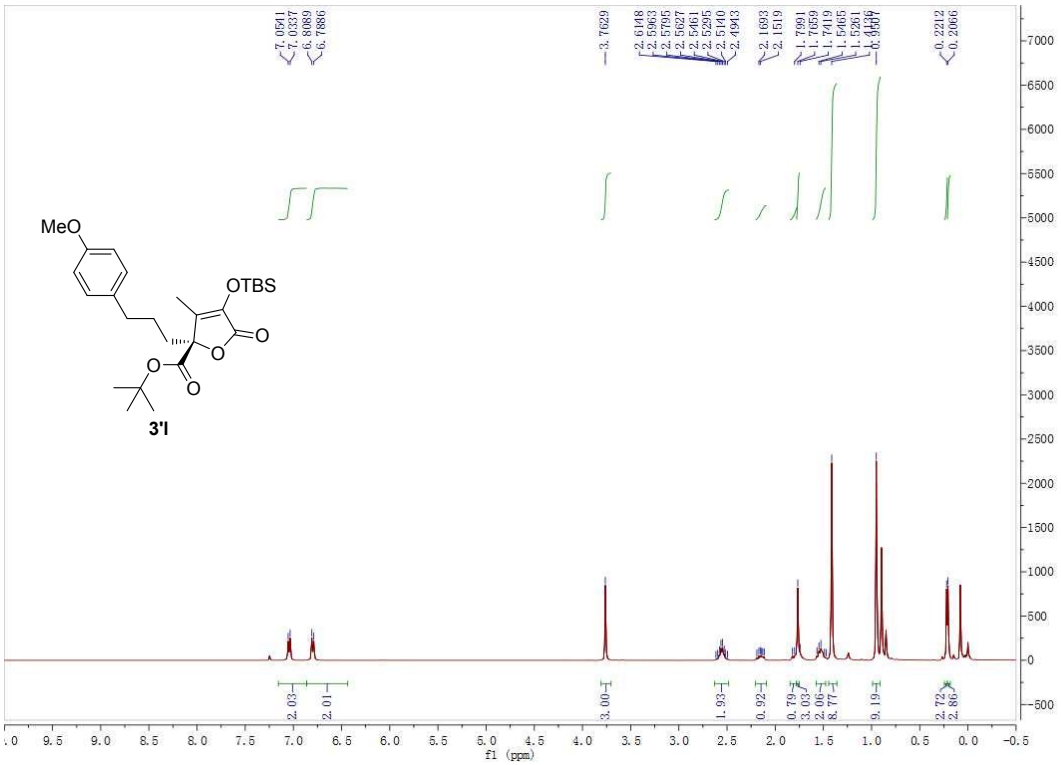
MeO
OTBS
O
O
O
O
3'l
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2.5963
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2.5627
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2.5295
2.5140
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1.7991
1.7659
1.7419
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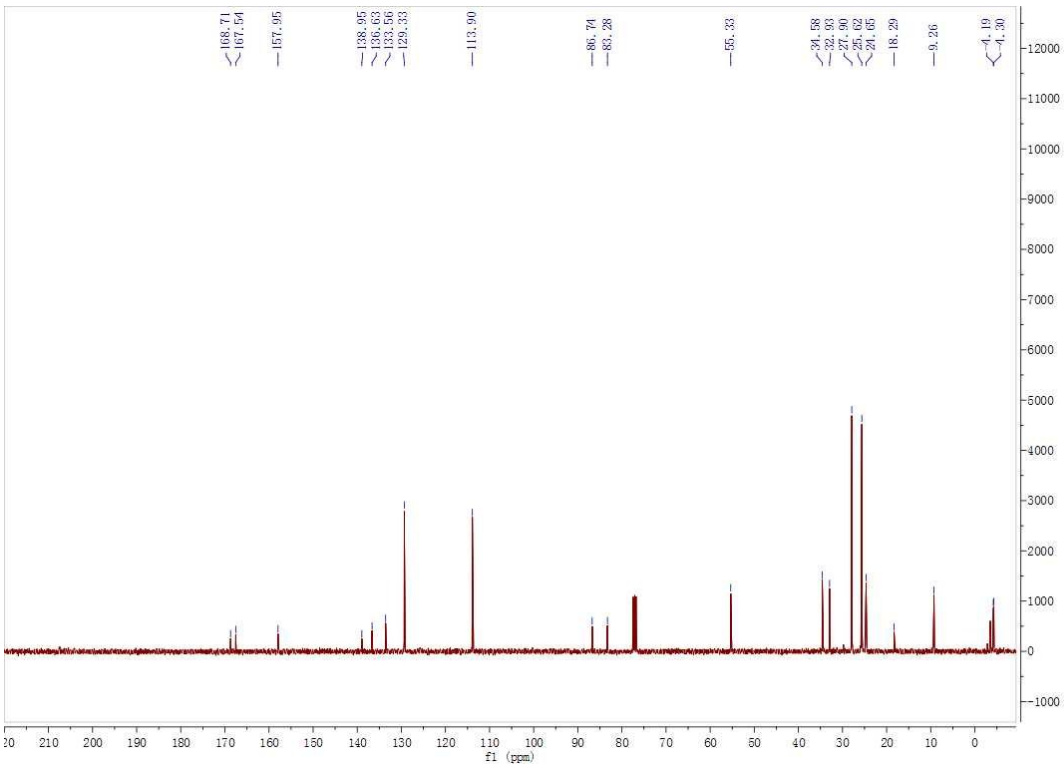
f1 (ppm)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25.02
21.65
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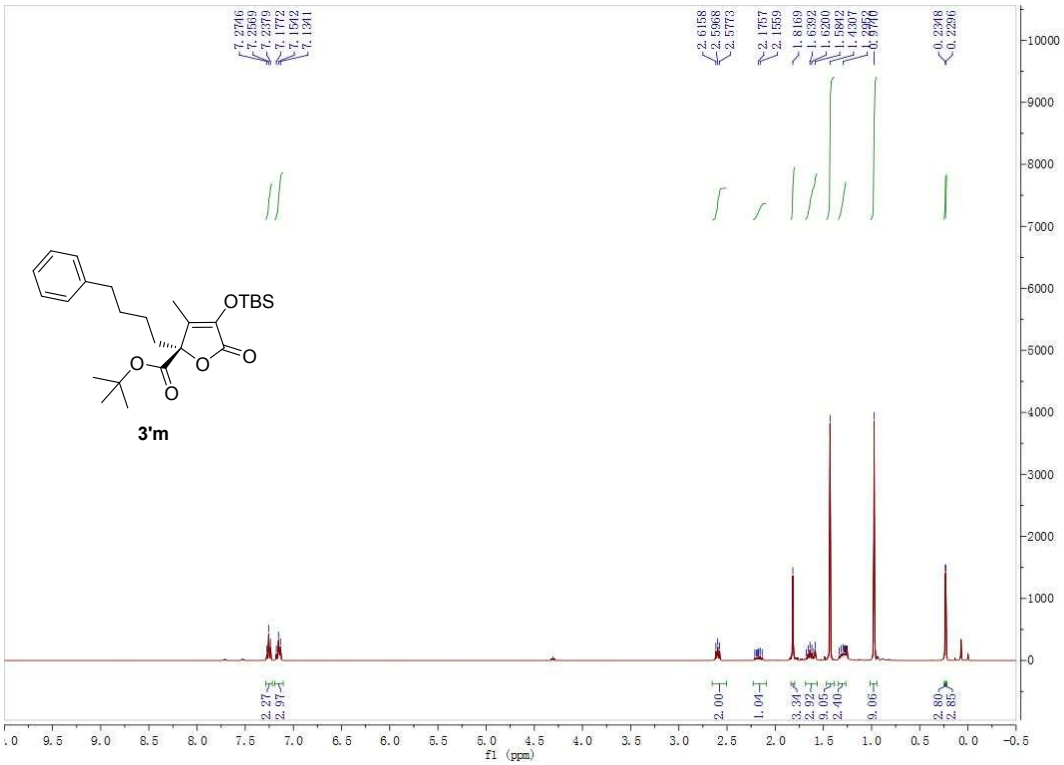
4.19
4.30
f1 (ppm)


OTBS
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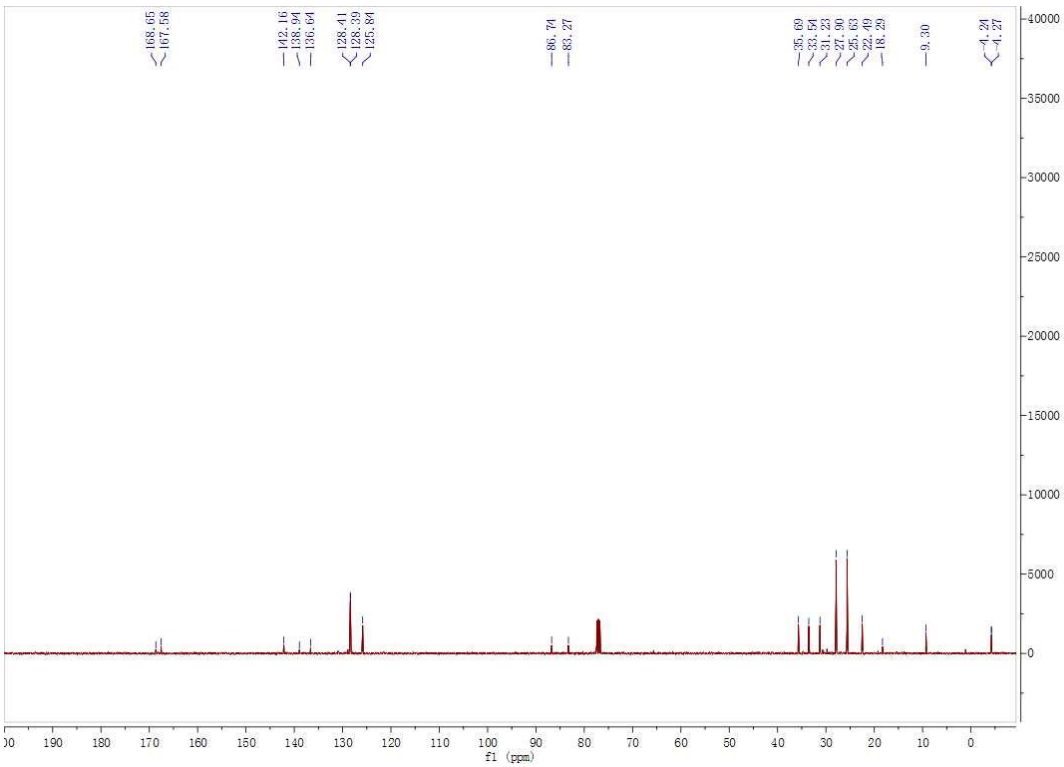
3'm
f1 (ppm)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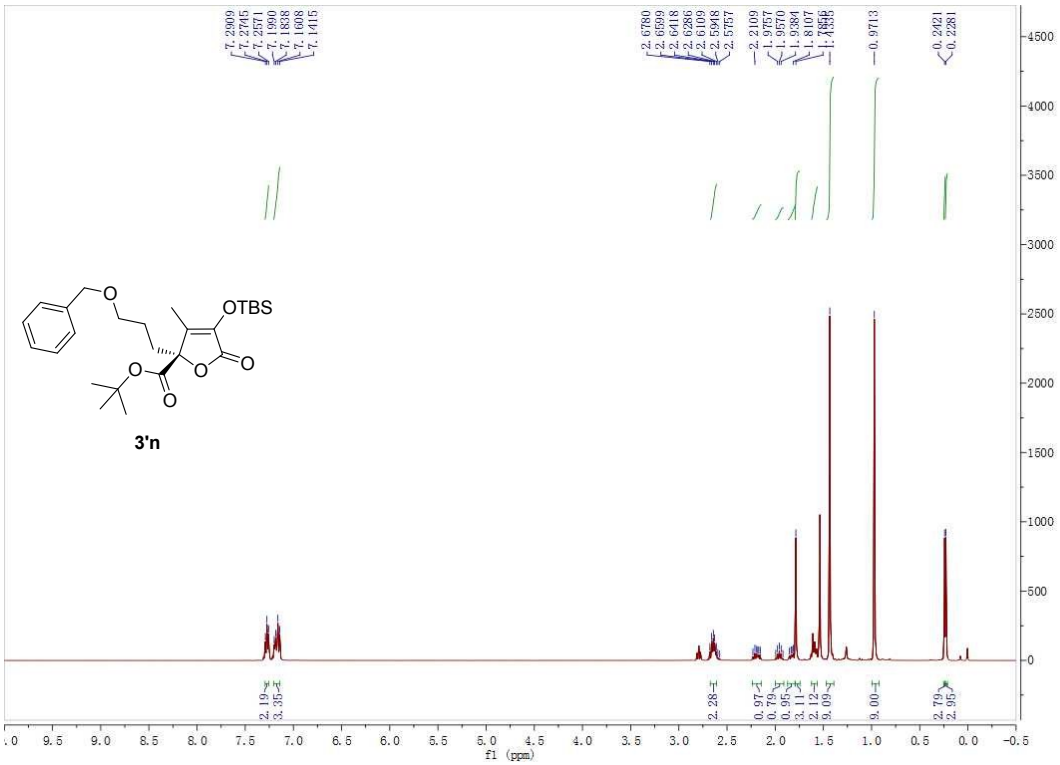
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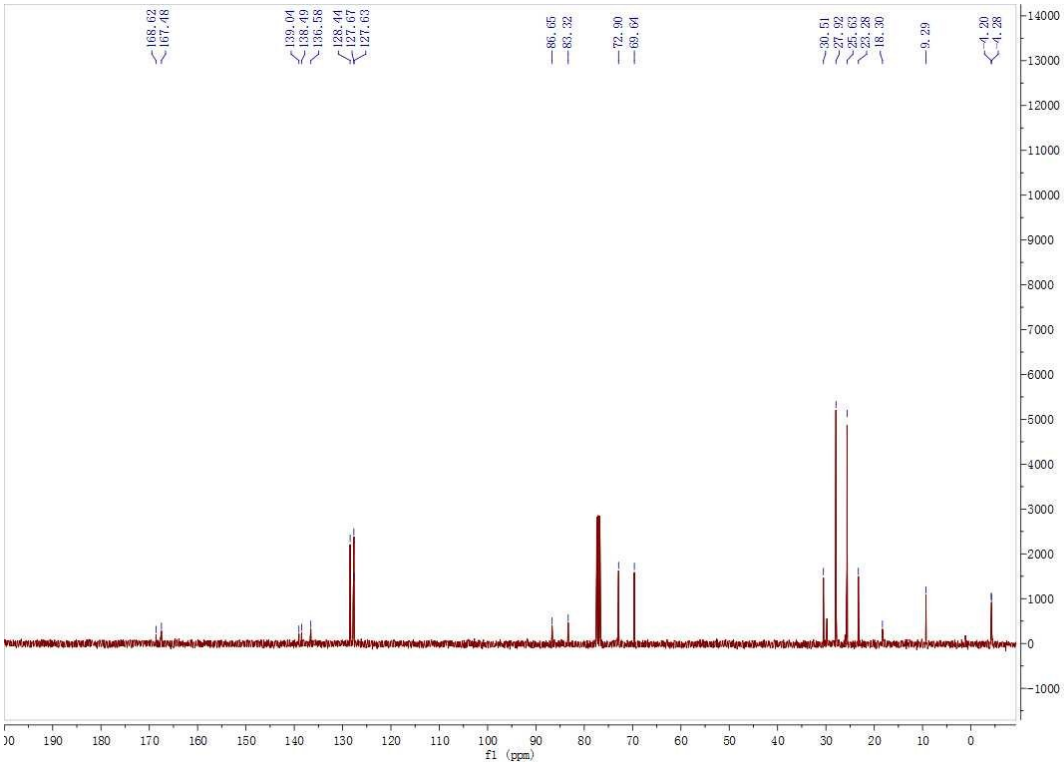
f1 (ppm)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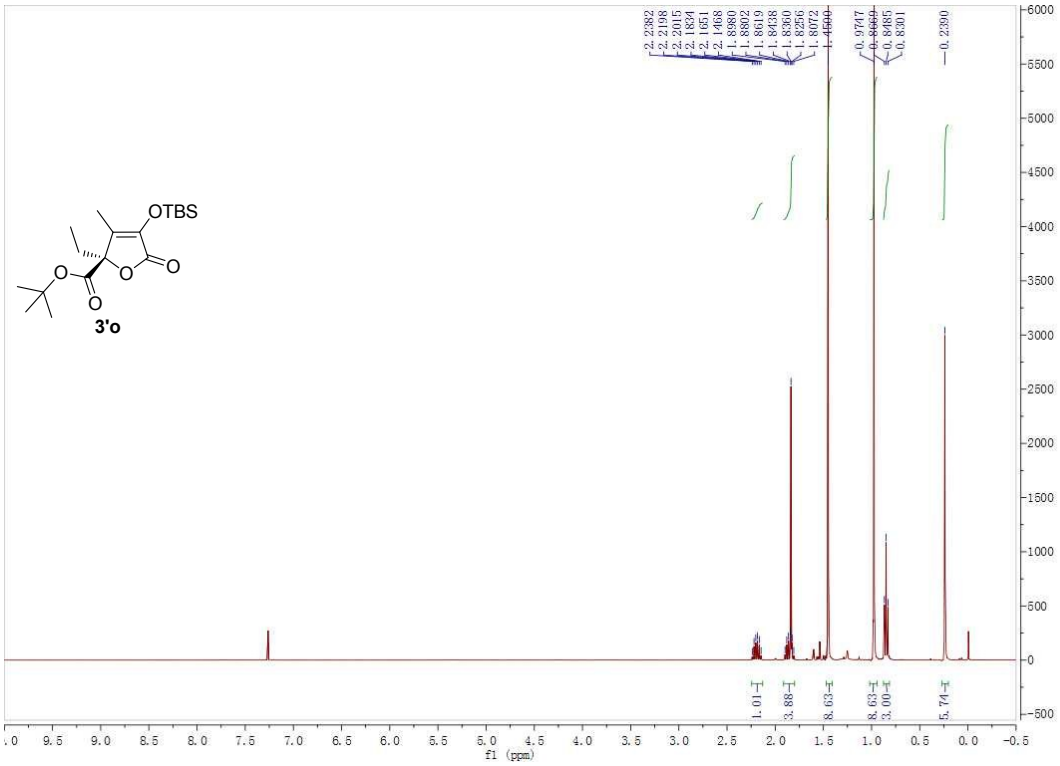
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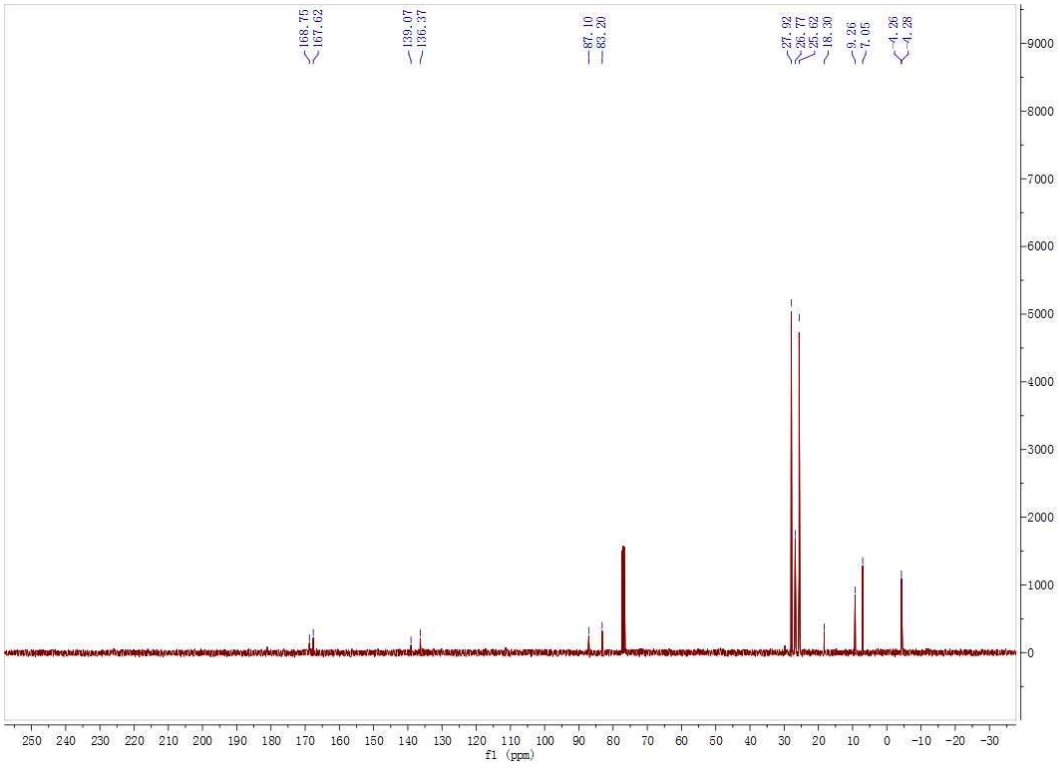
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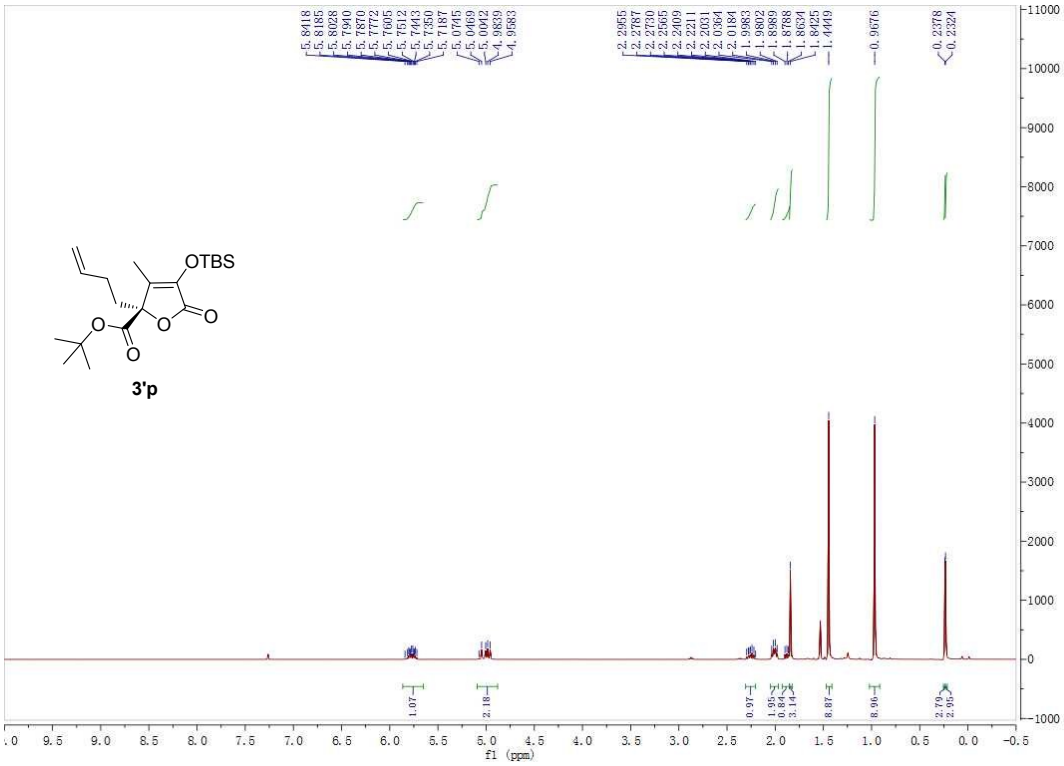
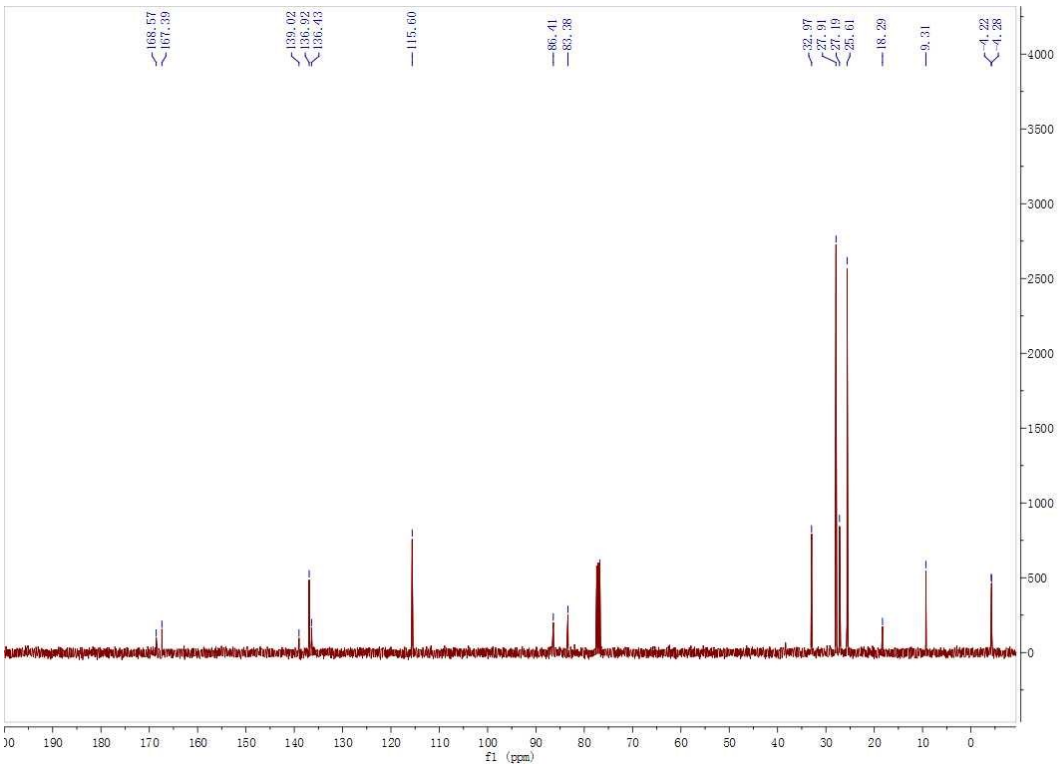

OTBS
O
O
O
O
3'p
f1 (ppm)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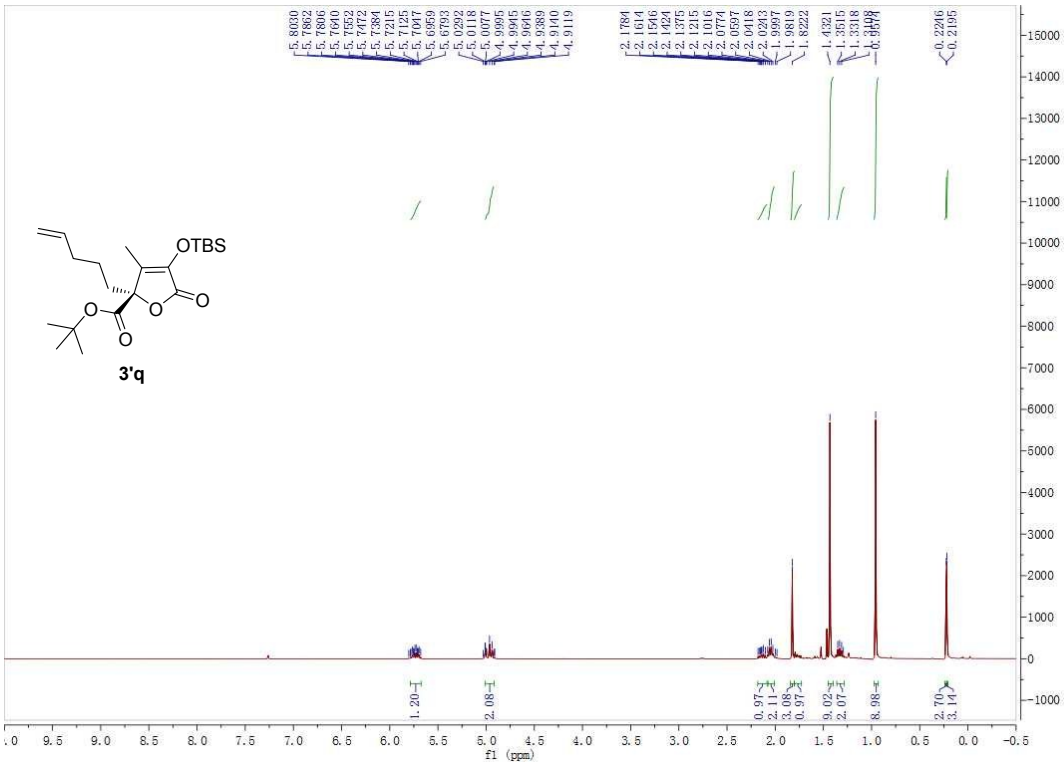
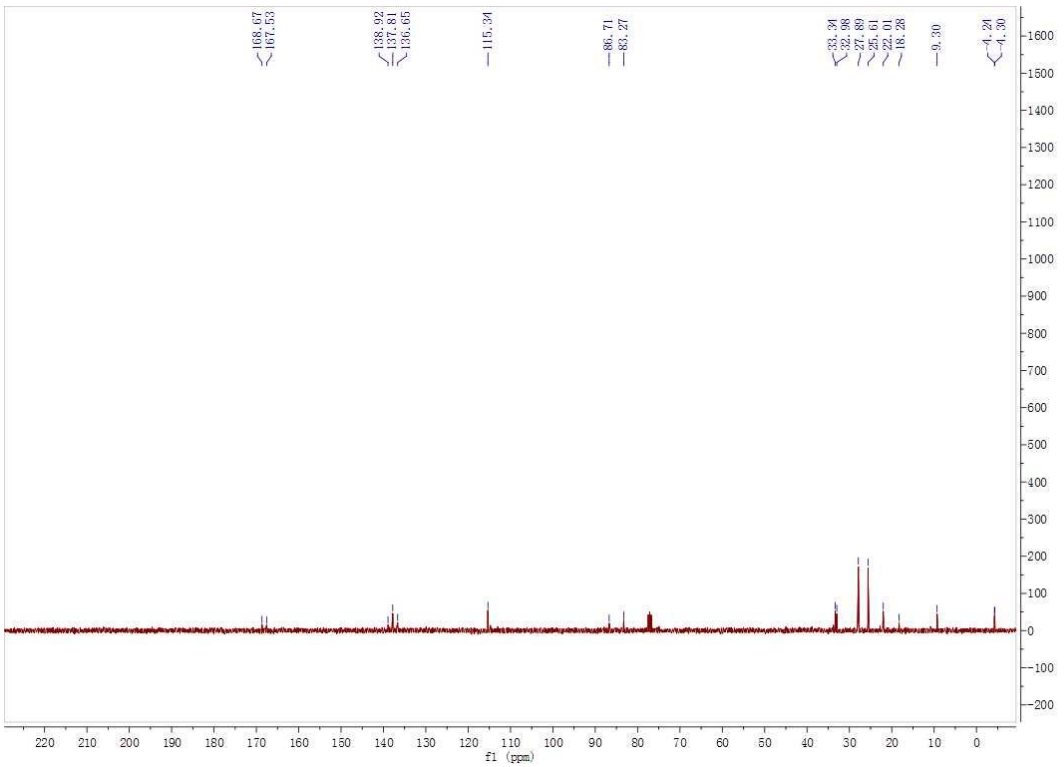

OTBS
O
O
O
O
3'q
f1 (ppm)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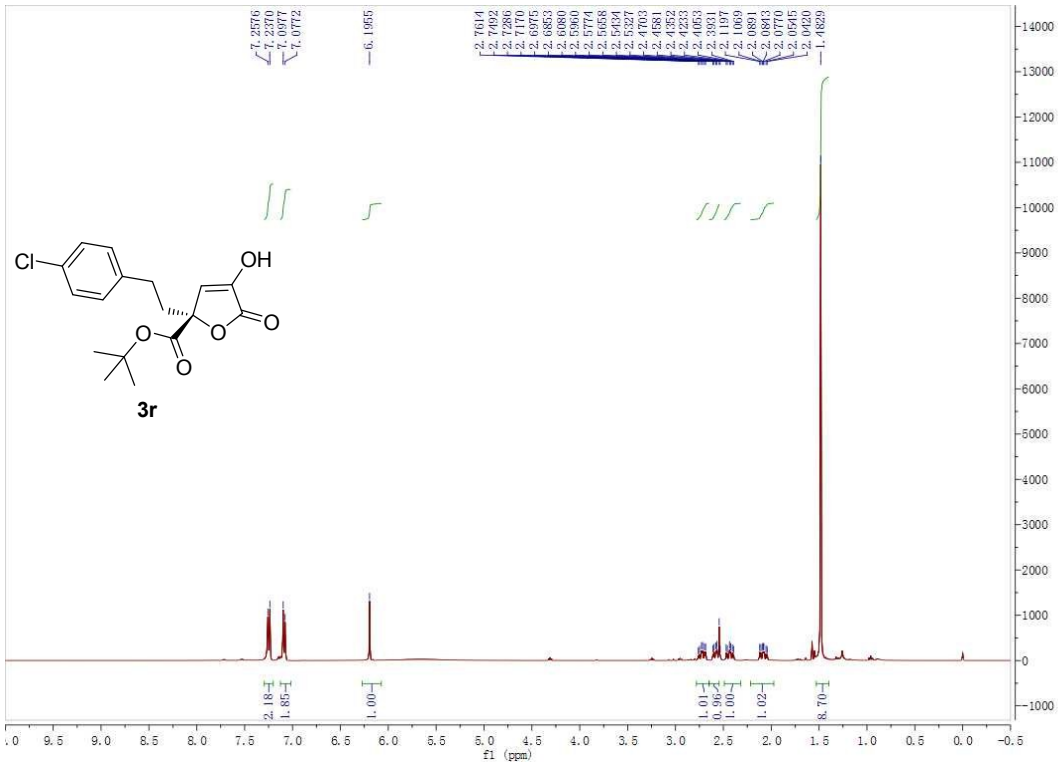
Cl
OH
O
O
O
O
3r
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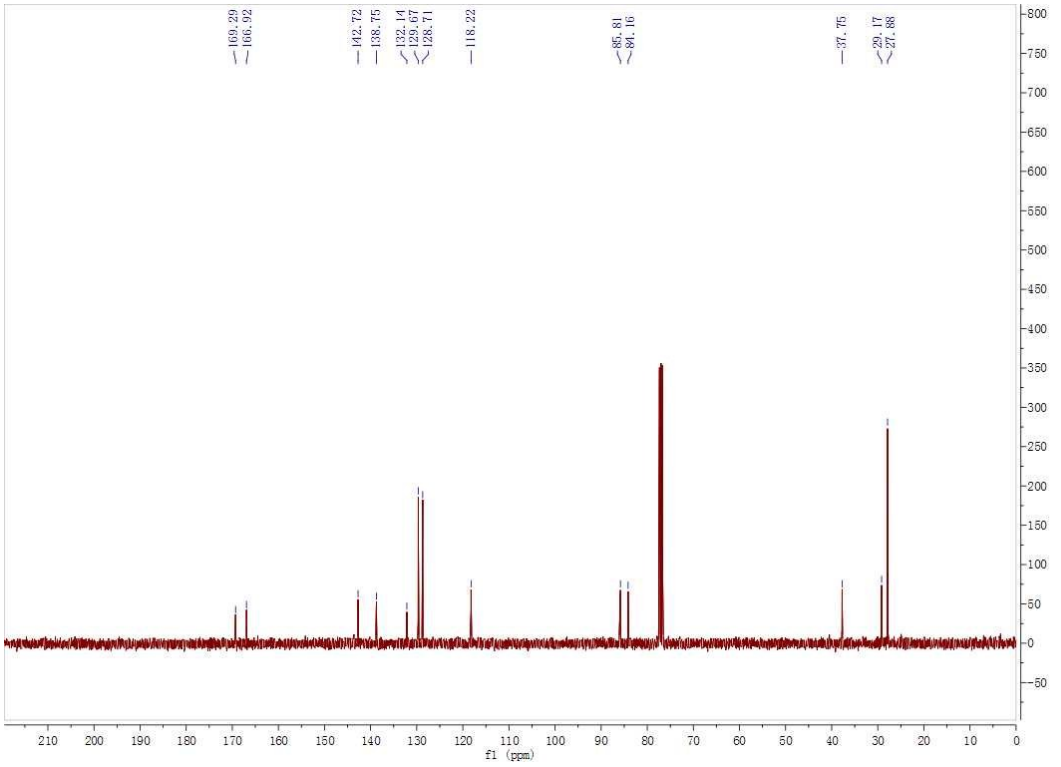
7.2370
7.0977
7.0772
6.1955
2.7614
2.7492
2.7286
2.7170
2.6975
2.6853
2.6080
2.5960
2.5774
2.5658
2.5474
2.5327
2.4703
2.4681
2.4352
2.4233
2.4053
2.3931
2.1197
2.1069
2.0891
2.0843
2.0770
2.0545
2.0420
1.4829
2.18
1.85
1.00
1.01
0.96
1.00
1.02
8.70
f1 (ppm)


169.29
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37.75
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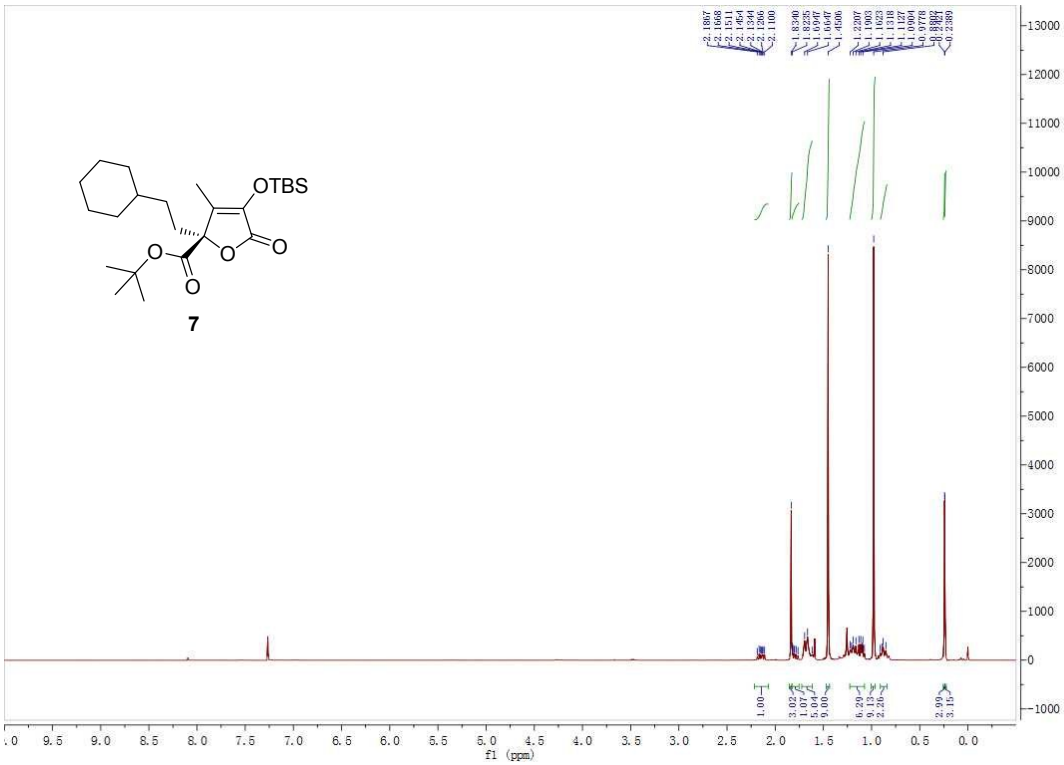
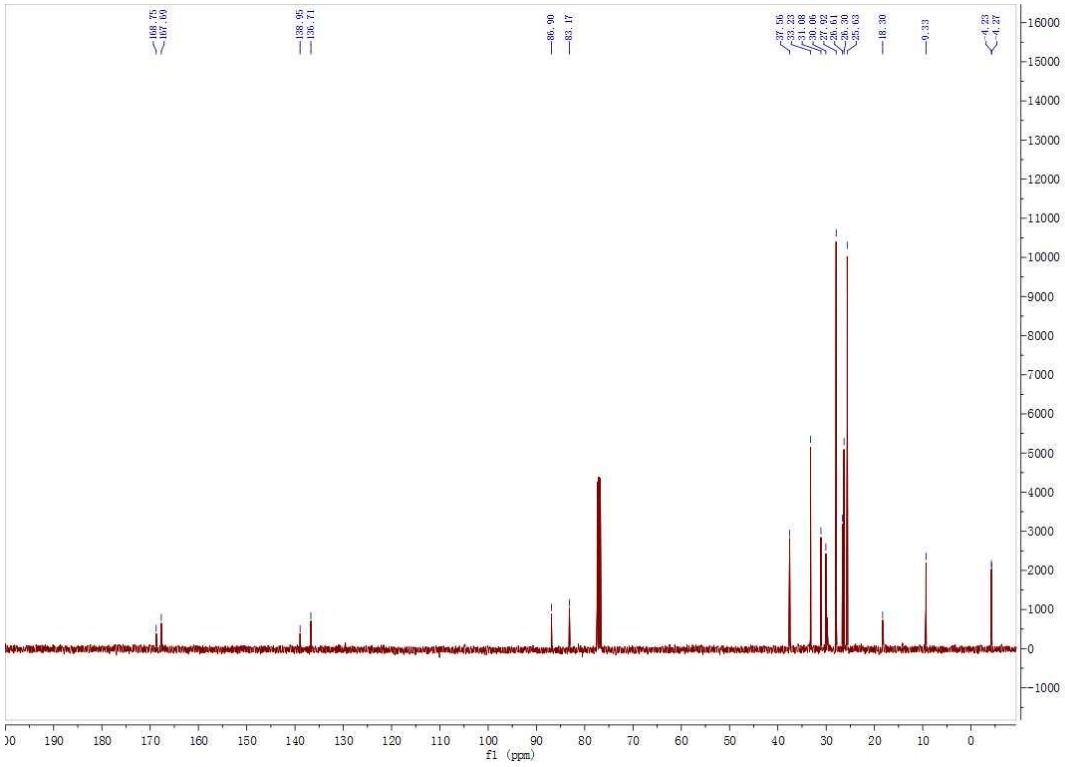
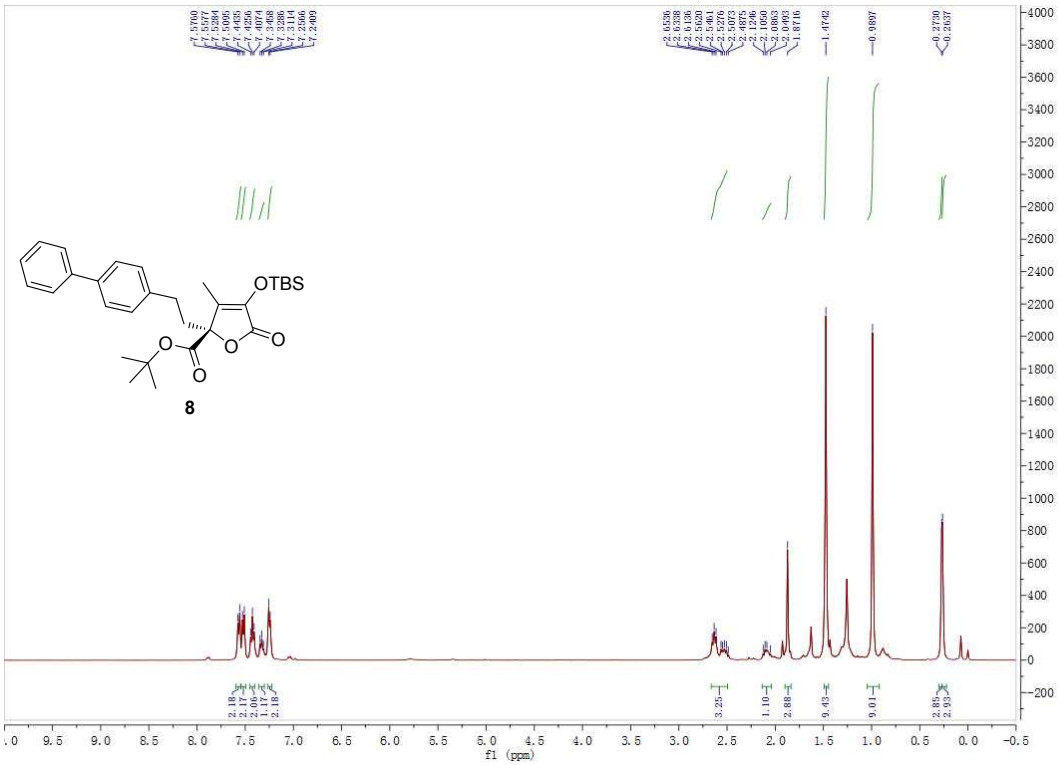
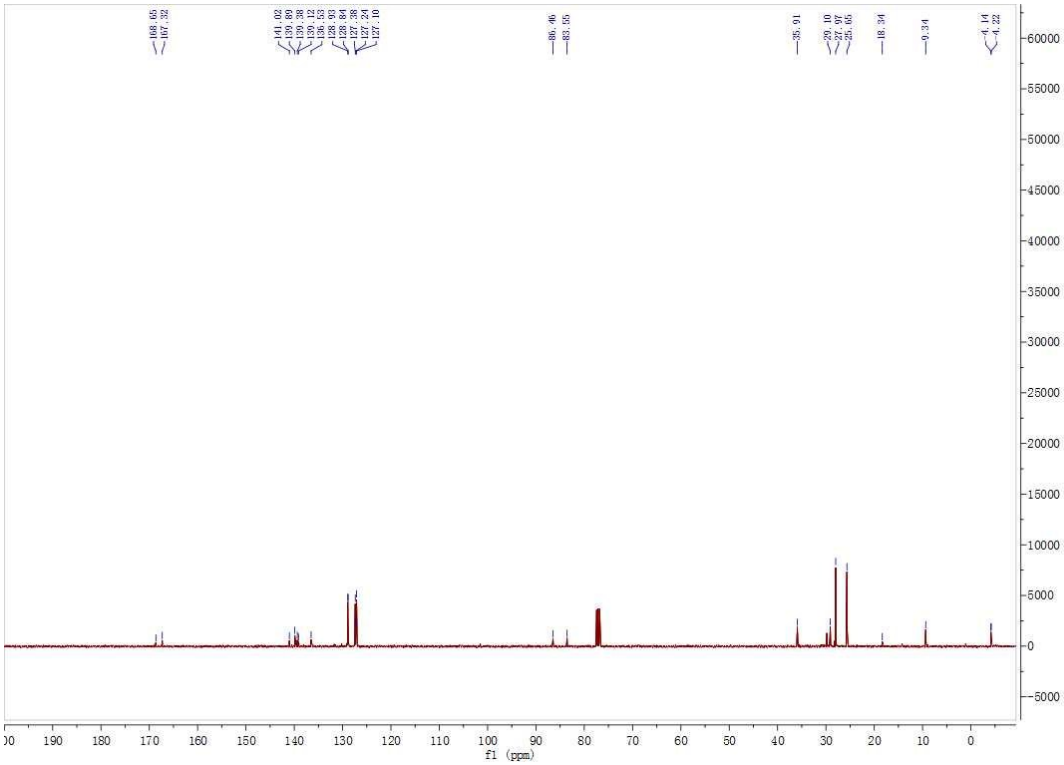
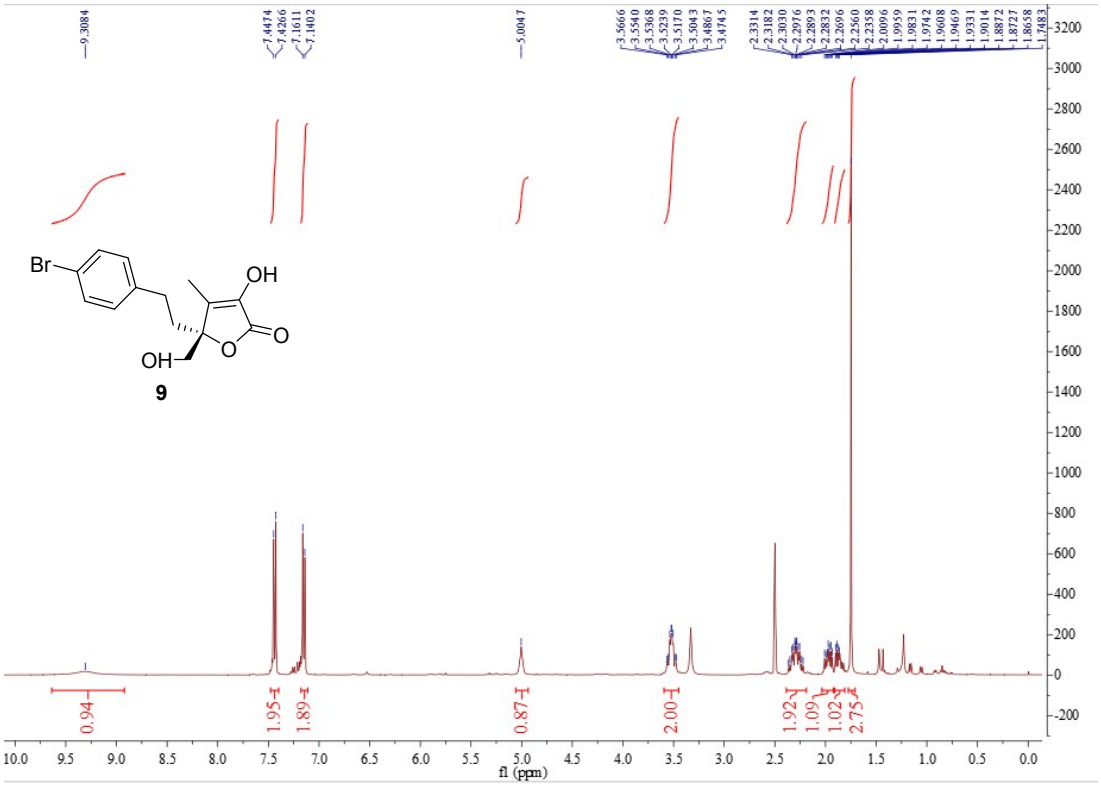
27.88
f1 (ppm)


OTBS
O
O
O
O
7
f1 (ppm)


f1 (ppm)


OTBS
O
O
O
O
8
f1 (ppm)


f1 (ppm)


Br
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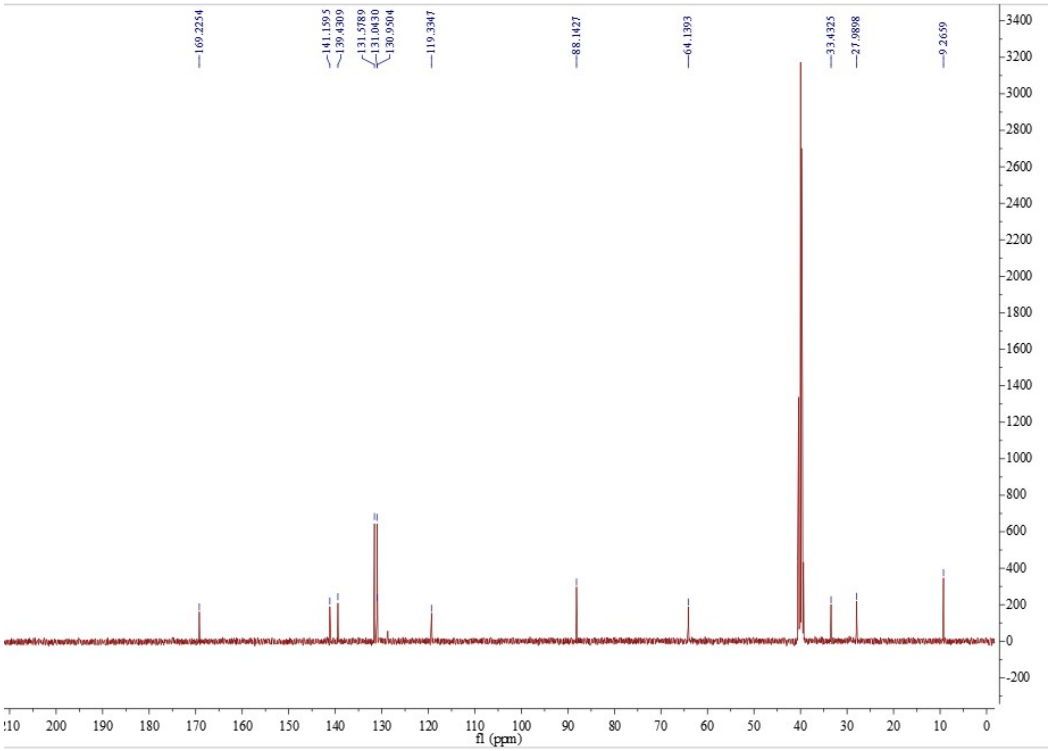
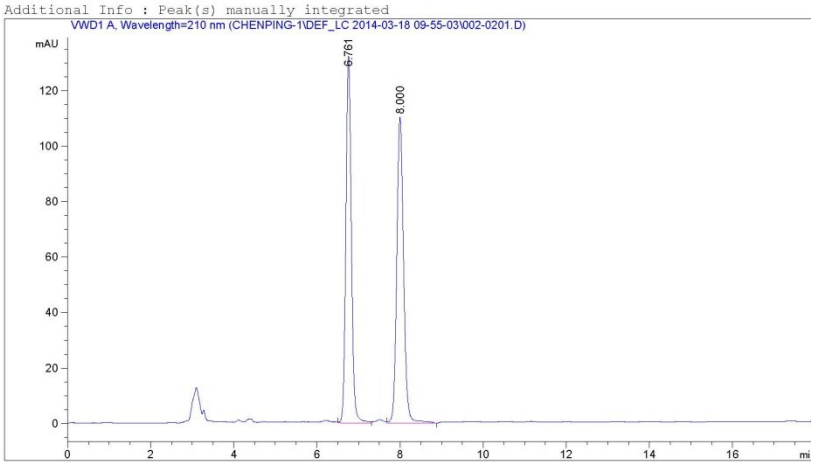
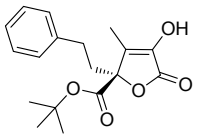
OH
O
O
9
fl (ppm)


fl (ppm)

Additional Info : Peak(s) manually integrated

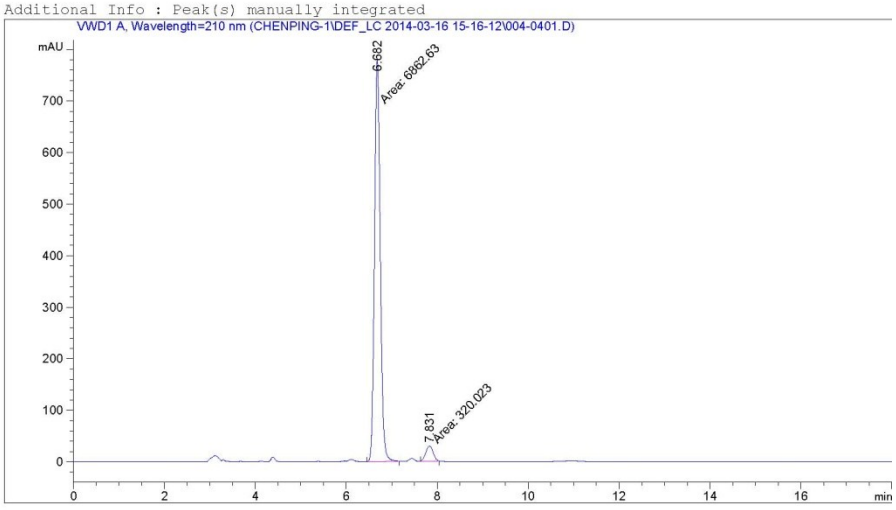




3c

```
=====================================================================
                      Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=210 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.761 VB    0.1415 1208.27039  132.35884  49.1092
   2   8.000 VV    0.1762 1252.10352  110.28090  50.8908

Totals :                  2460.37390  242.63974
```

Additional Info : Peak(s) manually integrated

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=====================================================================
                      Area Percent Report
=====================================================================

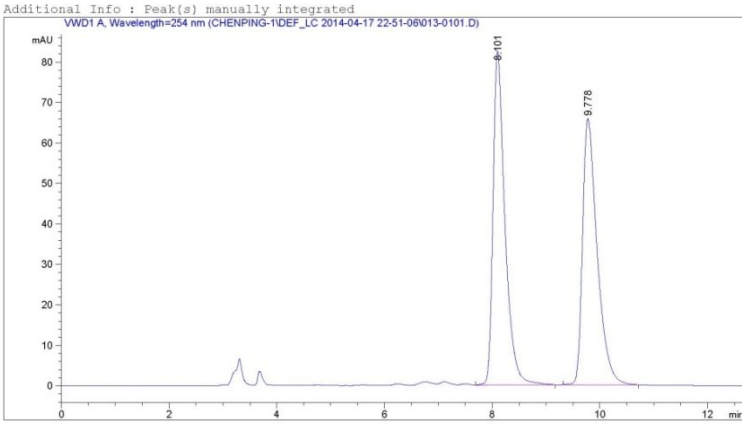
Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs

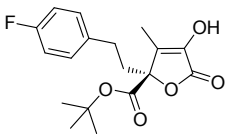

Signal 1: VWD1 A, Wavelength=210 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.682 MM    0.1467 6862.62500  779.72766  95.5445
   2   7.831 MM    0.1810  320.02280   29.46056   4.4555

Totals :                  7182.64780  809.18822
```

Additional Info : Peak(s) manually integrated





3d

```
=====================================================================
                        Area Percent Report
=====================================================================

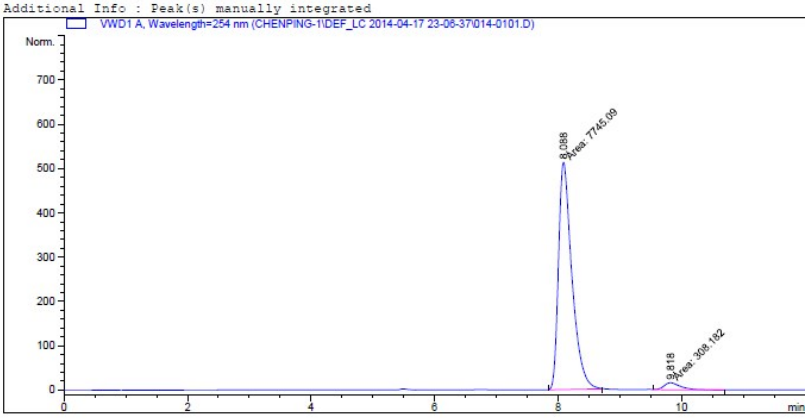
Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1   8.101 VB    0.2254 1263.78479   82.49129  50.5391
   2   9.778 BB    0.2807 1236.82141   65.75828  49.4609

Totals :                   2500.60620  148.24957
```

Additional Info : Peak(s) manually integrated




```
=====================================================================
                        Area Percent Report
=====================================================================

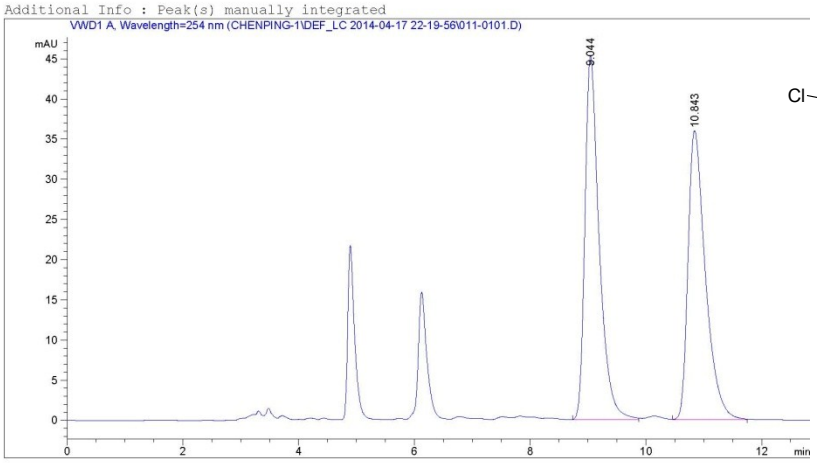
Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs

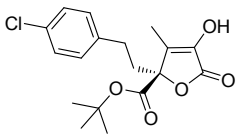

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1   8.088 MM    0.2516 7745.09277  513.13025  96.1732
   2   9.818 MM    0.3255  308.18161   15.77939   3.8268

Totals :                   8053.27438  528.90964
```

Additional Info : Peak(s) manually integrated





3e

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Area Percent Report

==========

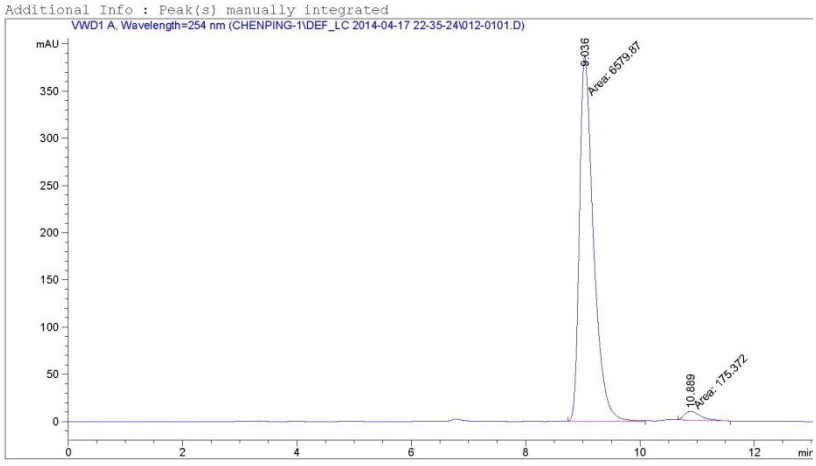
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.044	BB	0.2535	774.10028	45.25930	50.8352
2	10.843	VB	0.3129	748.66467	35.95360	49.1648

Totals : 1522.76495 81.21290

Additional Info : Peak(s) manually integrated



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Area Percent Report

==========

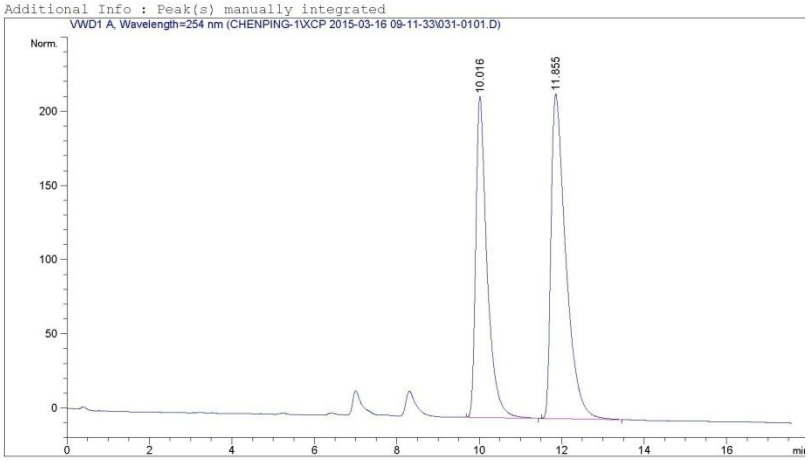
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

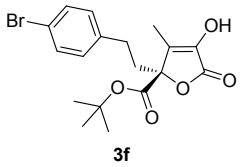
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.036	MM	0.2835	6579.87354	386.86435	97.4039
2	10.889	MM	0.3156	175.37206	9.26213	2.5961

Totals : 6755.24559 396.12648

Additional Info : Peak(s) manually integrated





3f

```
=====================================================================
                       Area Percent Report
=====================================================================

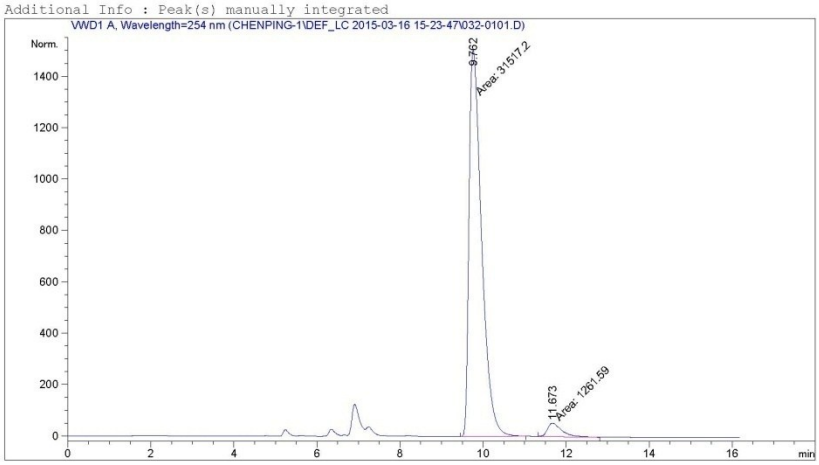
Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.016 BB    0.2791 4096.22998  216.40433  42.9419
   2  11.855 BB    0.3689 5442.77734  218.80510  57.0581

Totals :                  9539.00732  435.20943
```

Additional Info : Peak(s) manually integrated




```
=====================================================================
                       Area Percent Report
=====================================================================

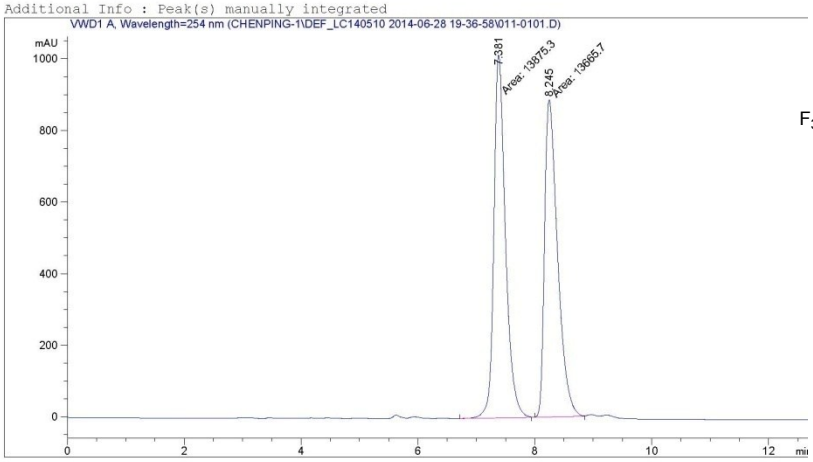
Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs

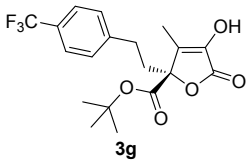

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.762 MM    0.3494 3.15172e4  1503.25098  96.1512
   2  11.673 MM    0.4002 1261.58545   52.54119   3.8488

Totals :                  3.27788e4  1555.79217
```

Additional Info : Peak(s) manually integrated





3g

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Area Percent Report

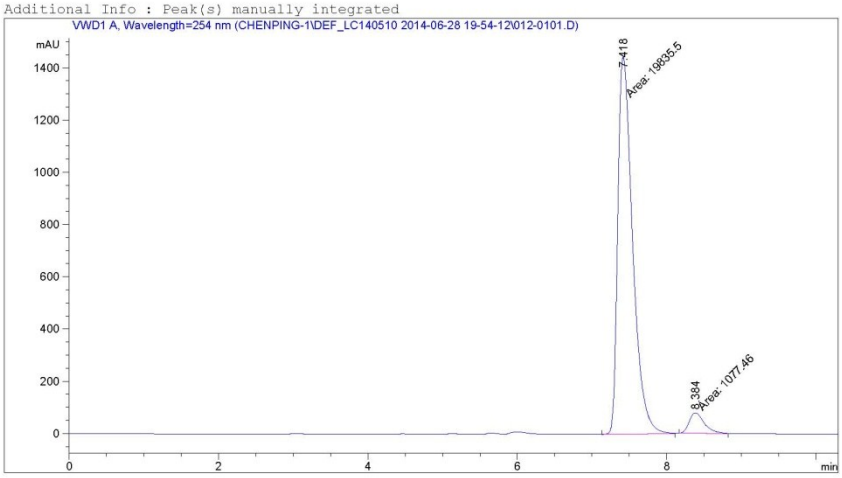
==========

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.381	MM	0.2281	1.38753e4	1013.64734	50.3805
2	8.245	MM	0.2571	1.36657e4	886.01923	49.6195
Totals :				2.75410e4	1899.66656	

Additional Info : Peak(s) manually integrated



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Area Percent Report

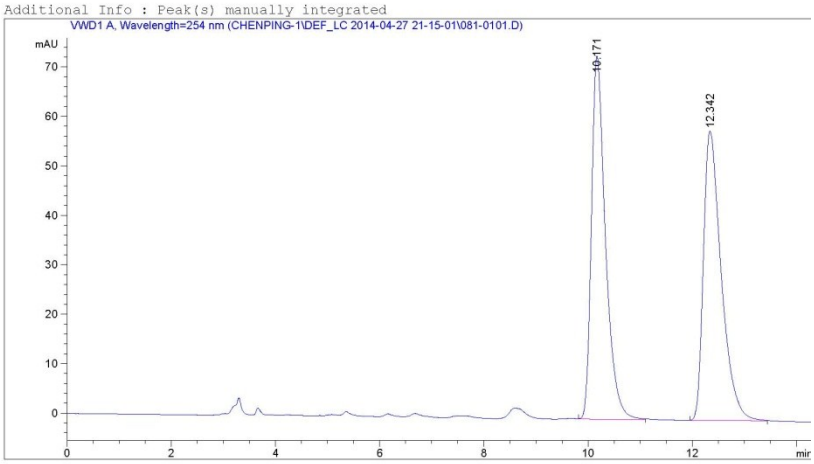
==========

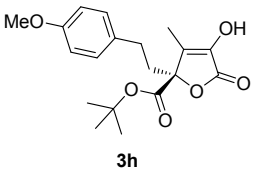
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.418	MM	0.2289	1.98355e4	1444.06348	94.8479
2	8.384	MM	0.2290	1077.45728	78.40644	5.1521
Totals :				2.09130e4	1522.46992	

Additional Info : Peak(s) manually integrated





3h

```
================================================================================
                              Area Percent Report
================================================================================

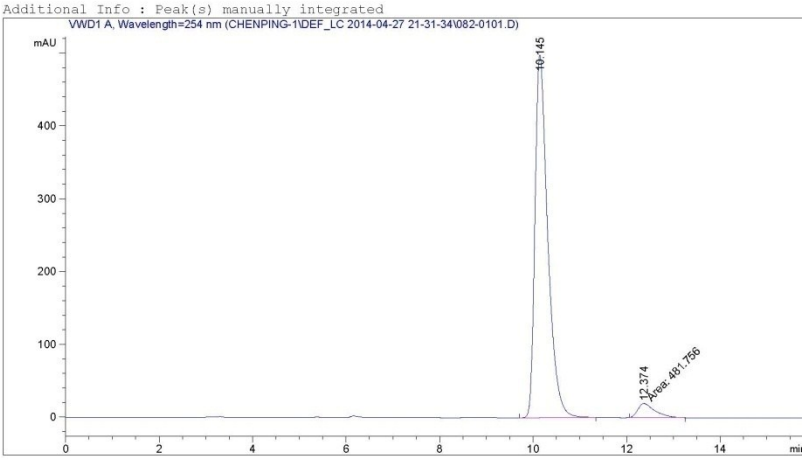
Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.171 BB    0.2778 1371.95129   73.41895  49.6204
   2  12.342 BB    0.3594 1392.94482   58.51374  50.3796

Totals :                  2764.89612  131.93270
```

Additional Info : Peak(s) manually integrated




```
================================================================================
                              Area Percent Report
================================================================================

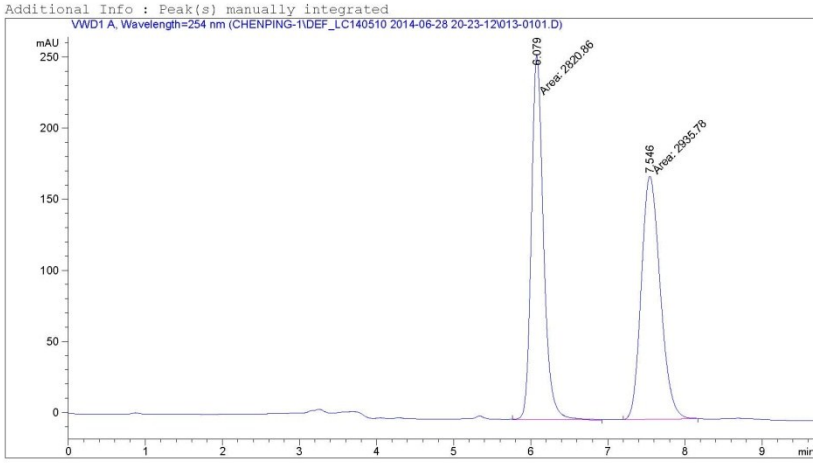
Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs

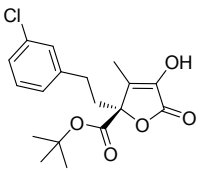

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.145 BB    0.2831 9409.86816  498.05588  95.1297
   2  12.374 MM    0.4157  481.75583   19.31502   4.8703

Totals :                  9891.62399  517.37090
```

Additional Info : Peak(s) manually integrated





3i

```
================================================================
                    Area Percent Report
================================================================

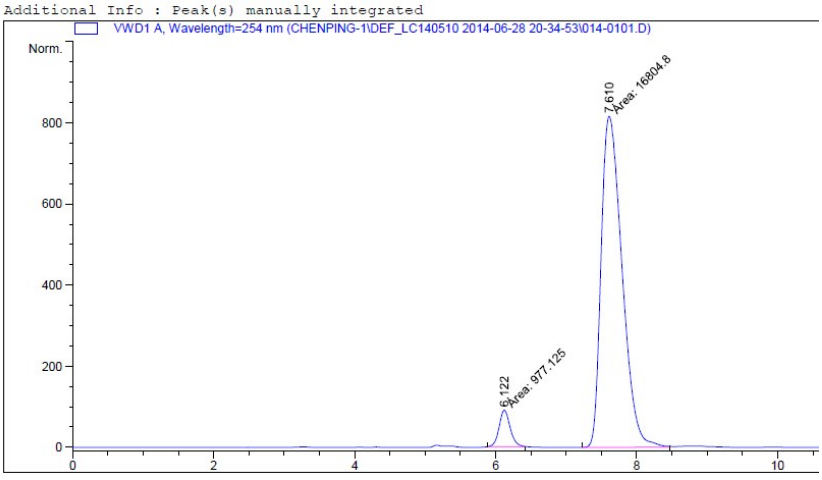
Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.079 MM    0.1832 2820.86011  256.63297  49.0018
   2   7.546 MM    0.2862 2935.78296  170.97847  50.9982

Totals :                  5756.64307  427.61143
```

Additional Info : Peak(s) manually integrated



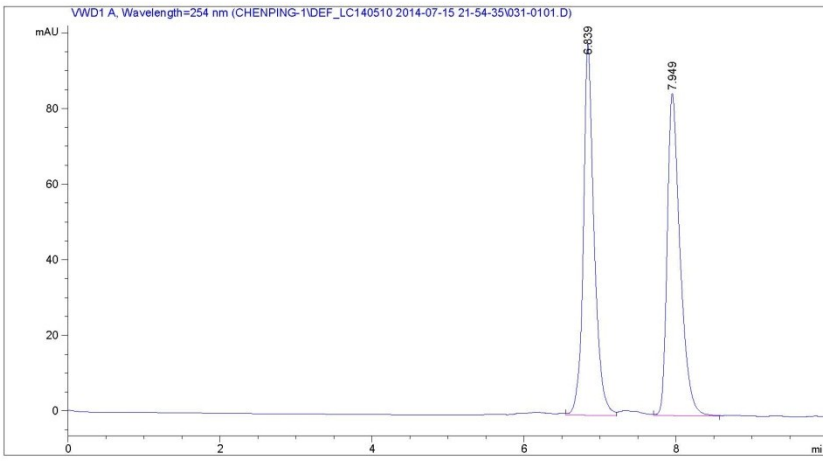

```
================================================================
                    Area Percent Report
================================================================

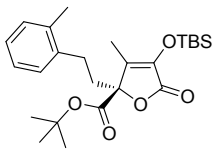
Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.122 MM    0.1814  977.12463   89.80032   5.4950
   2   7.610 MM    0.3432 1.68048e4   815.99213  94.5050

Totals :                  1.77819e4   905.79244
```





3'j

```
=====================================================================
                        Area Percent Report
=====================================================================

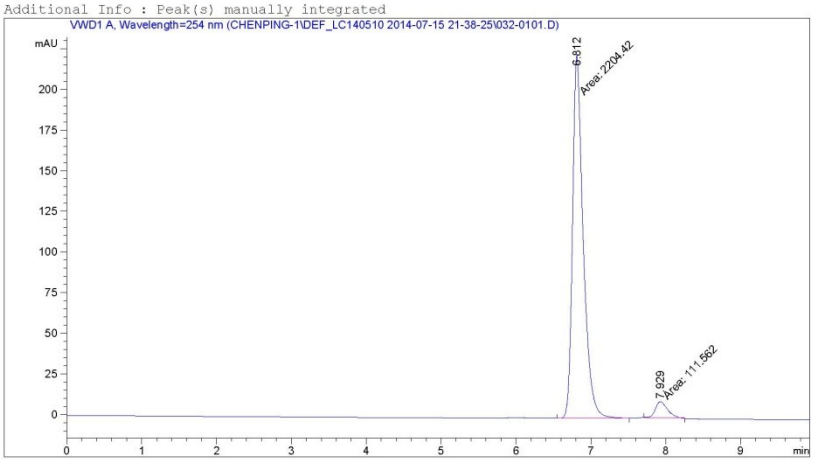
Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.839 VV    0.1407  963.61243   98.21481  49.0303
   2   7.949 VB    0.1750 1001.72888   85.23269  50.9697

Totals :                  1965.34131  183.44749
```

Additional Info : Peak(s) manually integrated




```
=====================================================================
                        Area Percent Report
=====================================================================

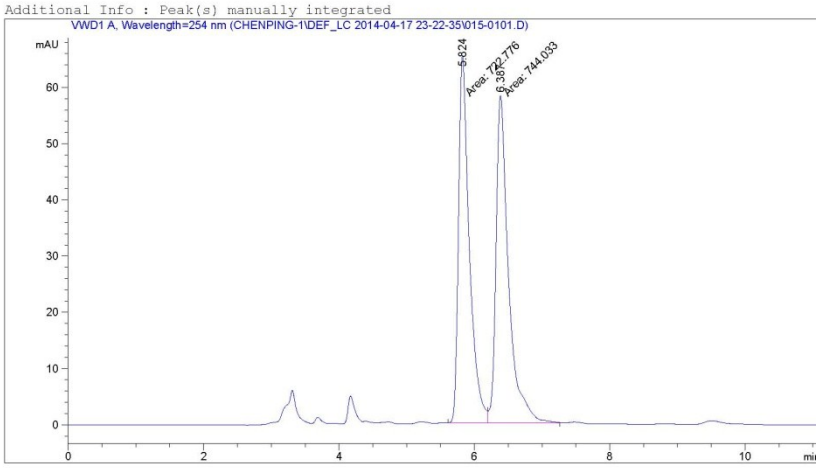
Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs

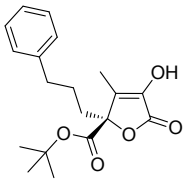

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.812 MM    0.1647 2204.41626  223.11368  95.1829
   2   7.929 MM    0.1858  111.56219   10.00721   4.8171

Totals :                  2315.97845  233.12088
```

Additional Info : Peak(s) manually integrated





3k

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Area Percent Report

==========

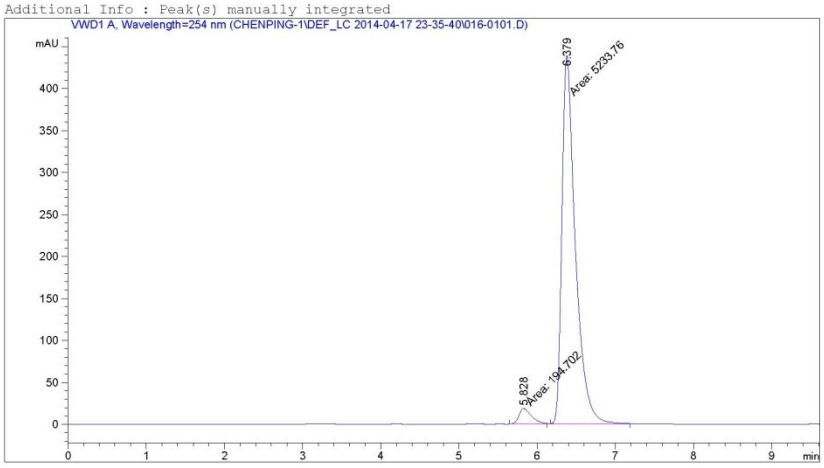
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.824	MF	0.1847	722.77557	65.22751	49.2754
2	6.387	FM	0.2130	744.03253	58.22231	50.7246

Totals : 1466.80811 123.44982

Additional Info : Peak(s) manually integrated



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Area Percent Report

==========

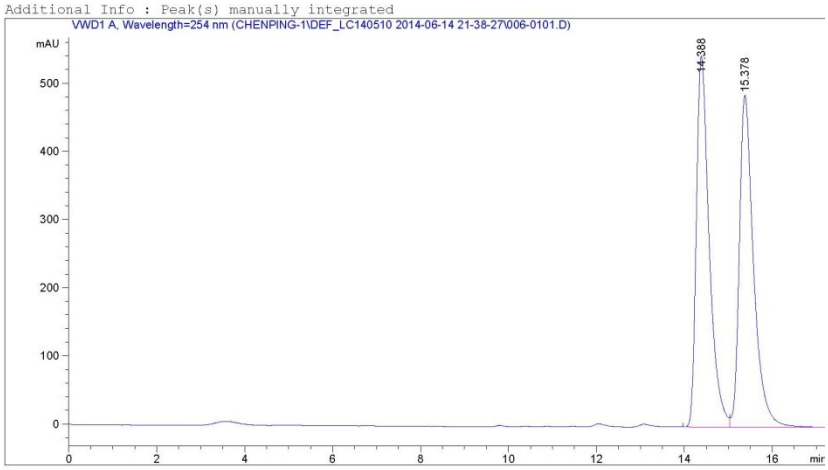
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

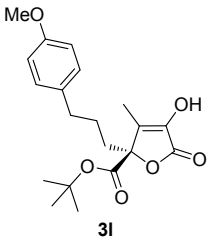
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.828	MM	0.1773	194.70197	18.30721	3.5867
2	6.379	MM	0.1988	5233.75586	438.75775	96.4133

Totals : 5428.45782 457.06496

Additional Info : Peak(s) manually integrated





3l

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=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  14.388 BV    0.3033 1.10201e4   544.12976  50.2522
   2  15.378 VB    0.3359 1.09095e4   486.69089  49.7478

Totals :                  2.19296e4  1030.82065
```
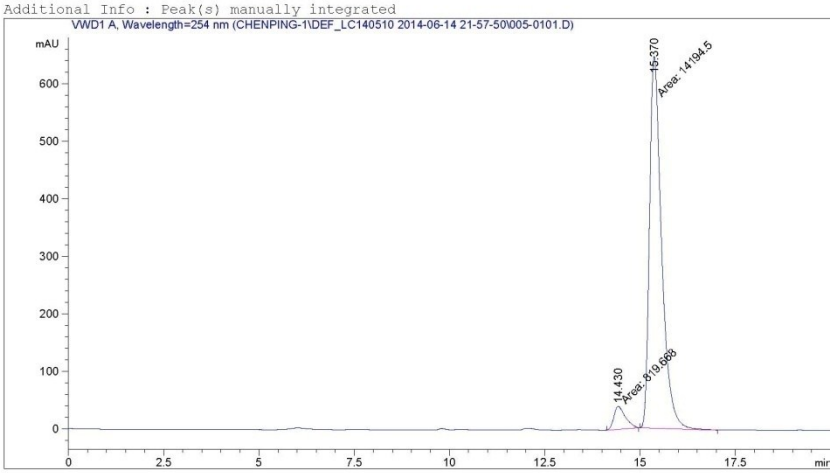
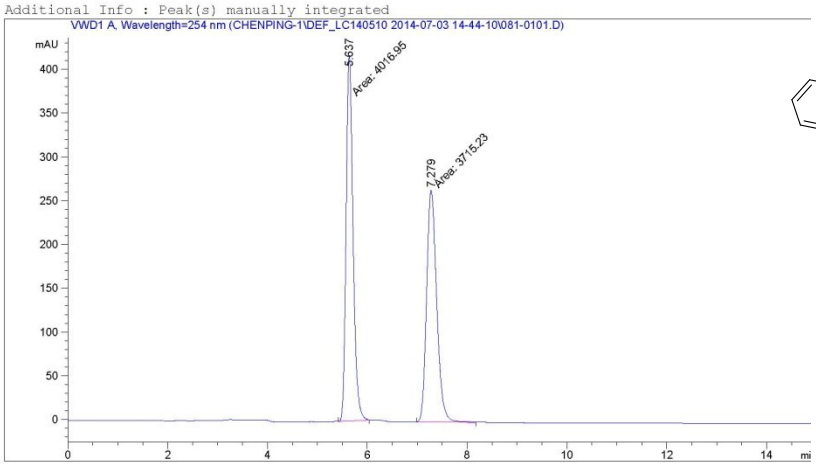
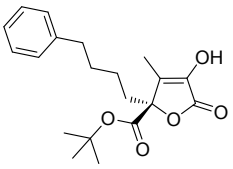

Additional Info : Peak(s) manually integrated




```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  14.430 MM    0.3441  819.66815   39.70047   5.4593
   2  15.370 MM    0.3660 1.41945e4   646.41071  94.5407

Totals :                  1.50141e4   686.11118
```

Additional Info : Peak(s) manually integrated

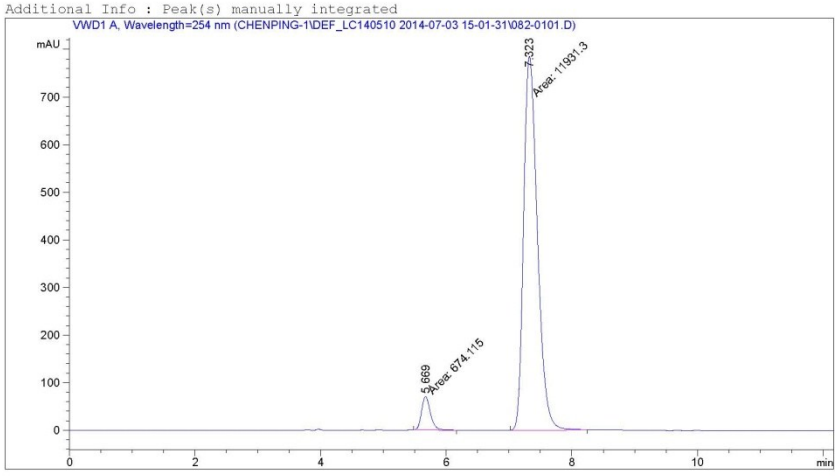




3m

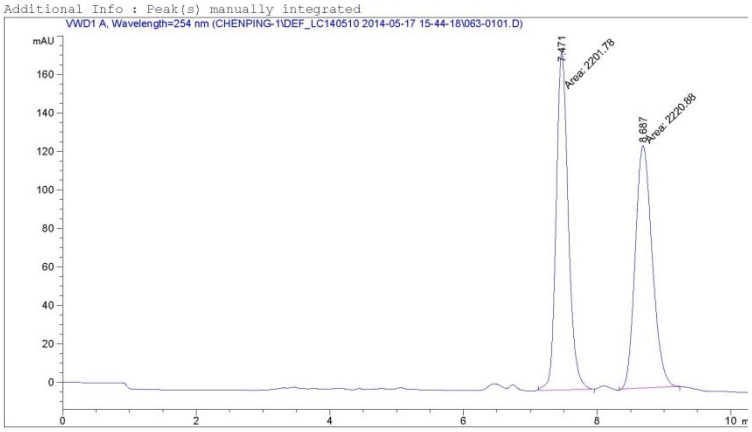
```
================================================================
                    Area Percent Report
================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.637 MM    0.1607 4016.94702  416.51282  51.9510
   2   7.279 MM    0.2339 3715.23242  264.78583  48.0490

Totals :                  7732.17944  681.29865
```

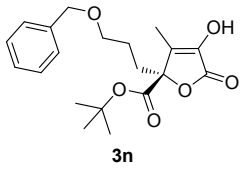
Additional Info : Peak(s) manually integrated




```
================================================================
                    Area Percent Report
================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.669 MM    0.1613  674.11542   69.66459   5.3478
   2   7.323 MM    0.2534 1.19313e4   784.84283  94.6522

Totals :                  1.26054e4   854.50742
```

Additional Info : Peak(s) manually integrated





3n

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======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs

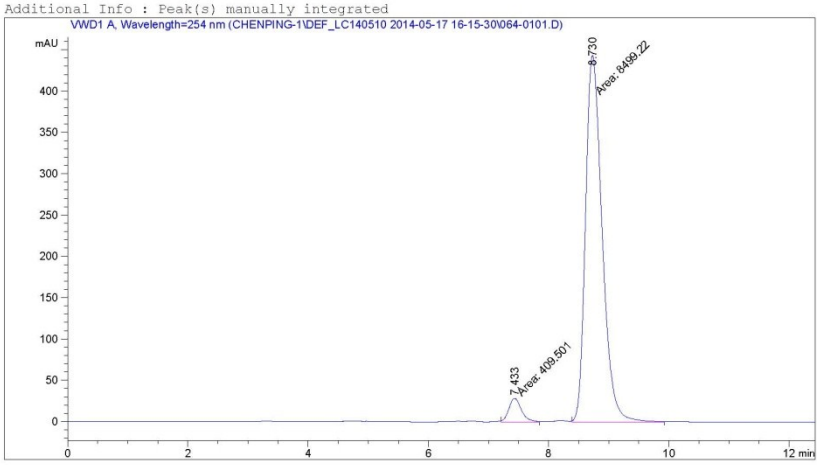

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.471 MM    0.2090 2201.77930  175.60349  49.7840
   2   8.687 MM    0.2940 2220.88306  125.89175  50.2160

Totals :                  4422.66235  301.49523

======================================================================
                        *** End of Report ***
```

Additional Info : Peak(s) manually integrated

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======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.433 MM    0.2393  409.50101   28.51761   4.5966
   2   8.730 MM    0.3193 8499.21875  443.61429  95.4034

Totals :                  8908.71976  472.13190
```
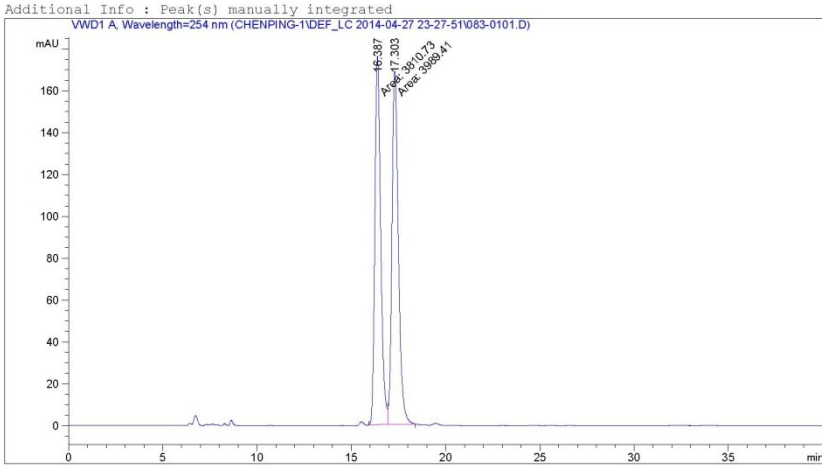
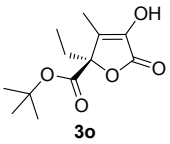

Additional Info : Peak(s) manually integrated

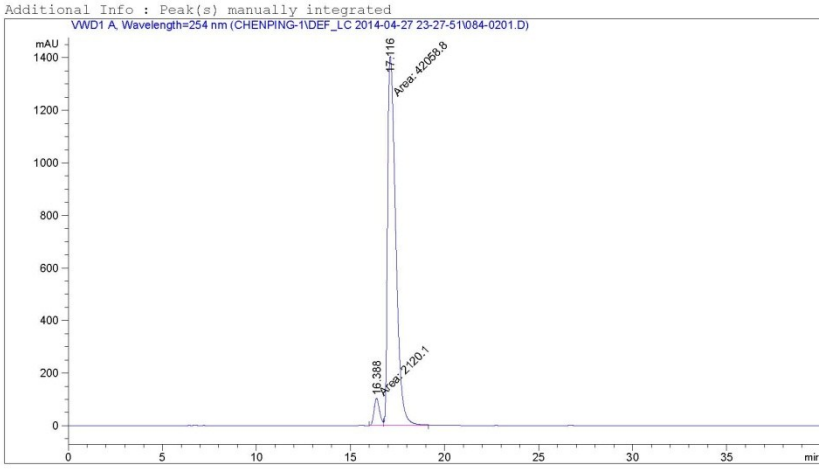




3o

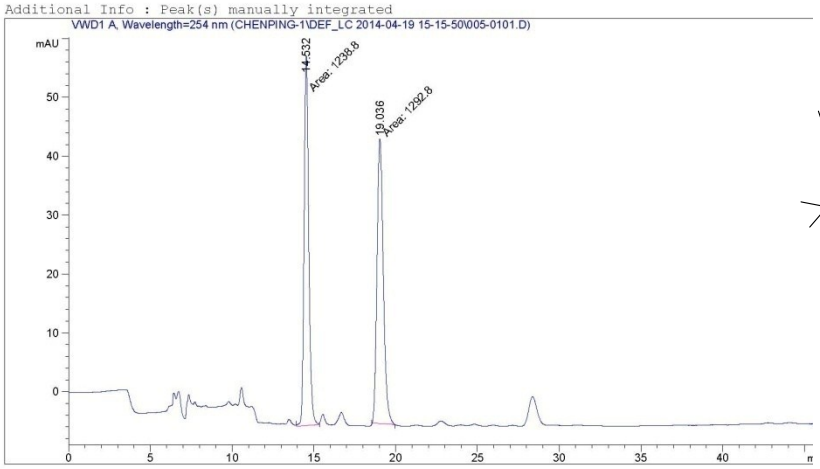
```
================================================================================
                          Area Percent Report
================================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  16.387 MF    0.3605 3810.73193  176.15533  48.8546
   2  17.303 FM    0.3938 3989.41040  168.85181  51.1454

Totals :                  7800.14233  345.00714
```

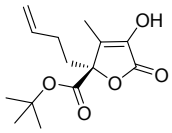
Additional Info : Peak(s) manually integrated




```
================================================================================
                          Area Percent Report
================================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  16.388 MF    0.3415 2120.09619  103.45605   4.7989
   2  17.116 FM    0.4990 4.20588e4  1404.63208  95.2011

Totals :                  4.41789e4  1508.08813
```

Additional Info : Peak(s) manually integrated





3p

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Area Percent Report

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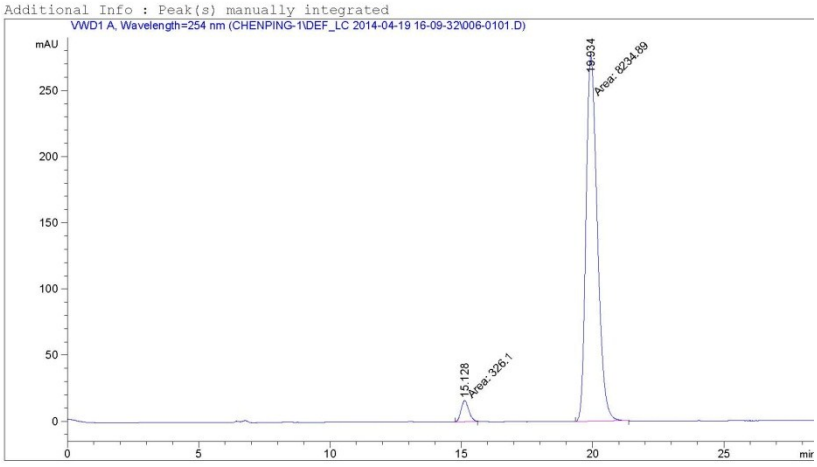
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.532	MM	0.3288	1238.80042	62.80086	48.9335
2	19.036	MM	0.4457	1292.79858	48.34789	51.0665

Totals : 2531.59900 111.14874

Additional Info : Peak(s) manually integrated



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Area Percent Report

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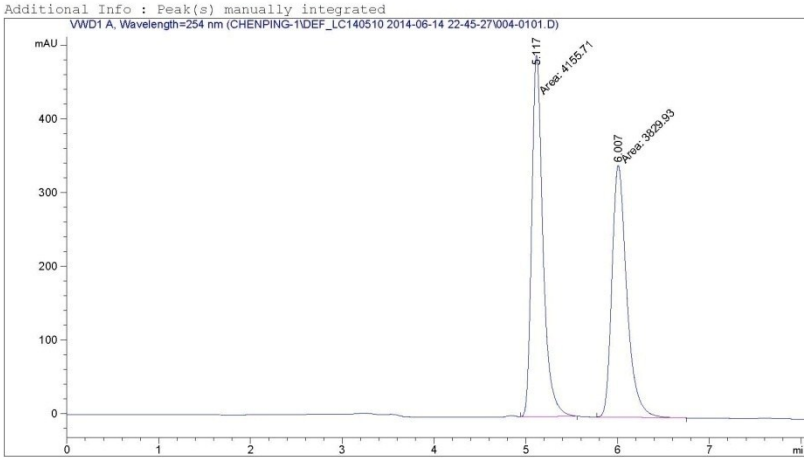
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

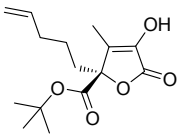
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.128	MM	0.3407	326.09976	15.95170	3.8091
2	19.934	MM	0.4977	8234.89453	275.76160	96.1909

Totals : 8560.99429 291.71329

Additional Info : Peak(s) manually integrated

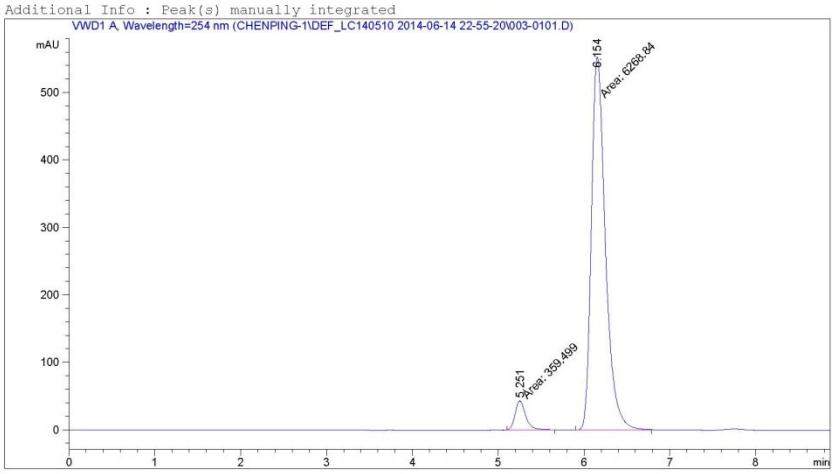




3q

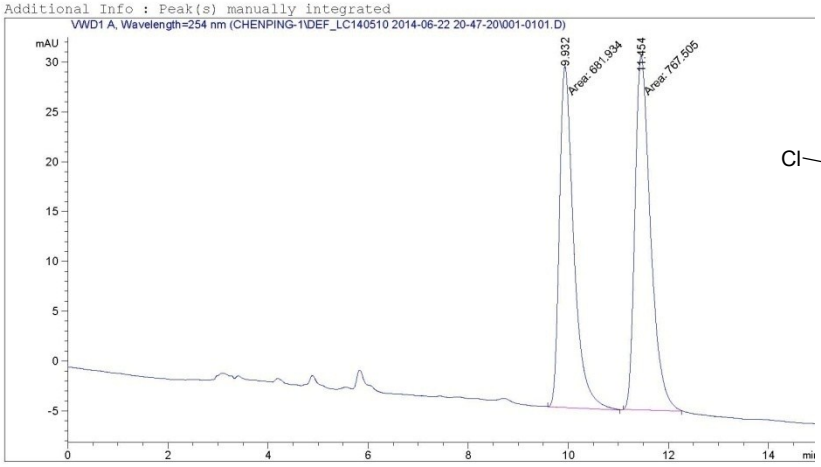
```
=====================================================================
                      Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.117 MM    0.1412 4155.70996  490.59387  52.0398
   2   6.007 MM    0.1867 3829.93433  341.88638  47.9602

Totals :                  7985.64429  832.48026
```

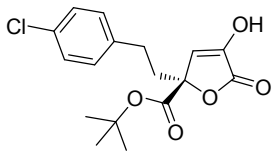
Additional Info : Peak(s) manually integrated




```
=====================================================================
                      Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.251 MM    0.1396  359.49936   42.91199   5.4237
   2   6.154 MM    0.1889 6268.83838  553.13757  94.5763

Totals :                  6628.33774  596.04957
```

Additional Info : Peak(s) manually integrated

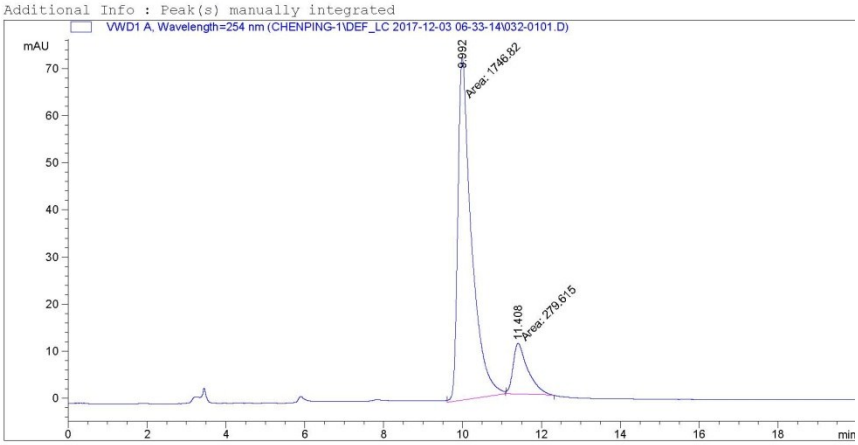




3r

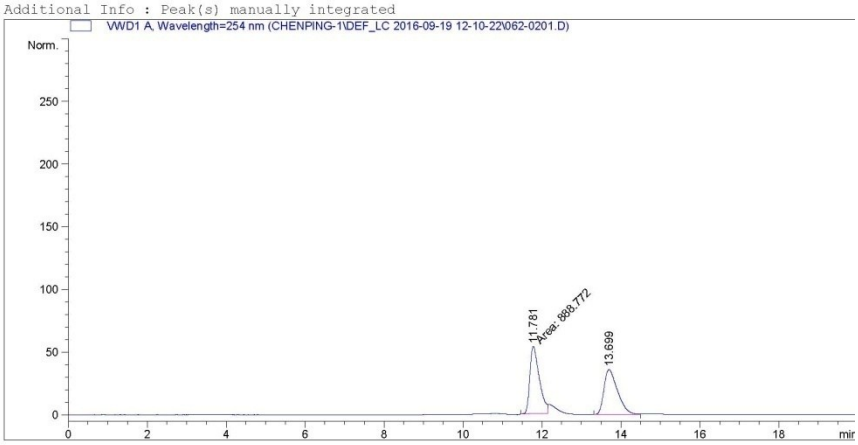
```
================================================================================
                              Area Percent Report
================================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.932 MM    0.3323  681.93384   34.20160  47.0481
   2  11.454 MM    0.3599  767.50464   35.54008  52.9519

Totals :                  1449.43848   69.74168
```

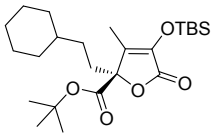
Additional Info : Peak(s) manually integrated




```
================================================================================
                              Area Percent Report
================================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1   9.992 MM    0.3991 1746.82422   72.95187  86.2017
   2  11.408 MM    0.4332  279.61481   10.75743  13.7983

Totals :                  2026.43903   83.70930
```

Additional Info : Peak(s) manually integrated





7

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Area Percent Report

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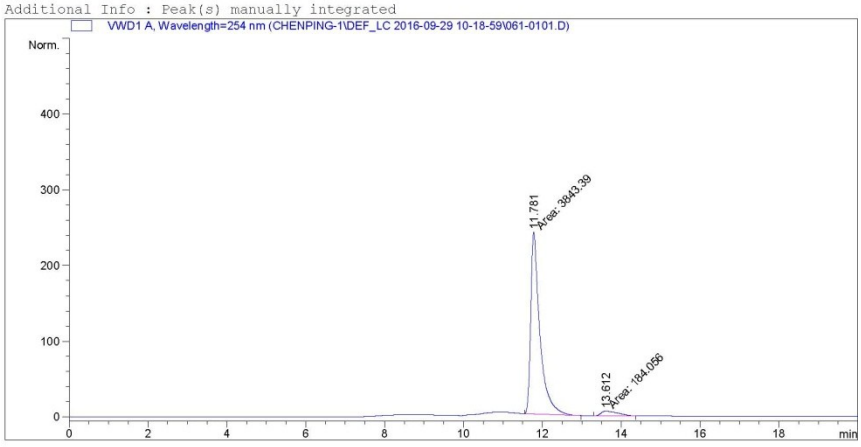
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	11.781	MM	0.2760	888.77216	53.67539	50.9727
2	13.699	BB	0.3575	854.85120	35.95080	49.0273
Totals :				1743.62335	89.62619	

Additional Info : Peak(s) manually integrated



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Area Percent Report

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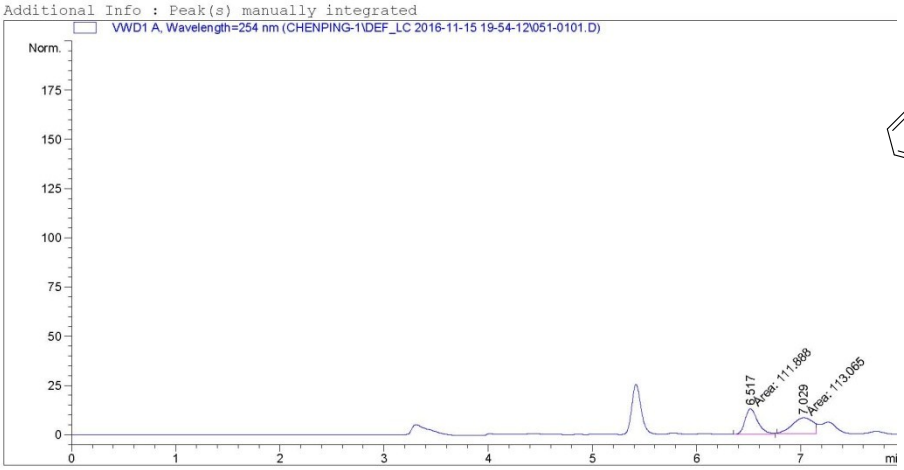
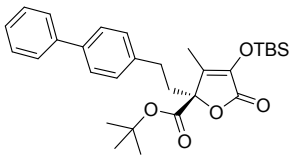
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	11.781	MM	0.2665	3843.38843	240.35664	95.4299
2	13.612	MM	0.4729	184.05629	6.48663	4.5701
Totals :				4027.44472	246.84328	

Additional Info : Peak(s) manually integrated





8

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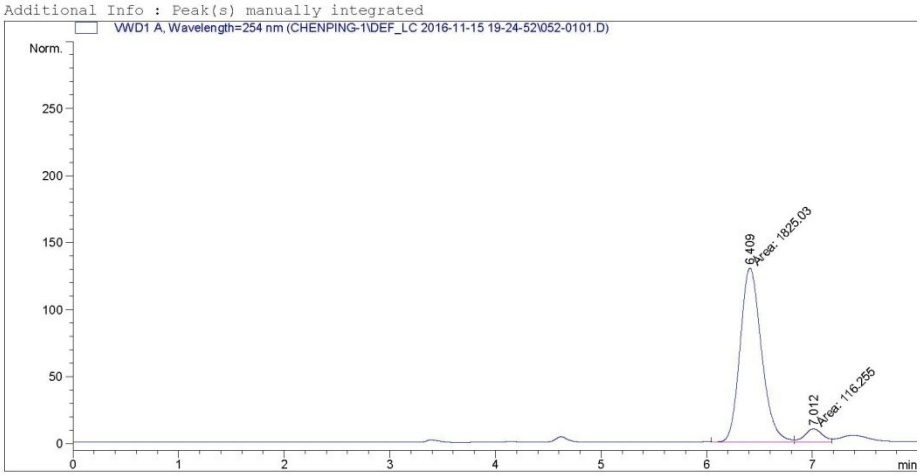
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1   6.517 MM    0.1422  111.88795   13.11751  49.7384
   2   7.029 MM    0.2327  113.06510    8.09761  50.2616
```

Additional Info : Peak(s) manually integrated



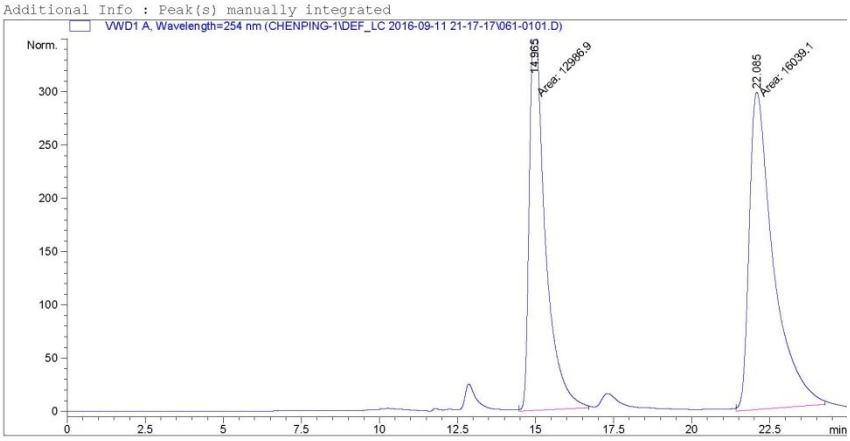

```
=====================================================================
                        Area Percent Report
=====================================================================

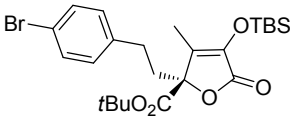
Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1   6.409 MF    0.2343 1825.02844  129.82613  94.0115
   2   7.012 FM    0.1962  116.25454    9.87466   5.9885
```

Additional Info : Peak(s) manually integrated





3f-TBS = **3'f**

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Area Percent Report

==========

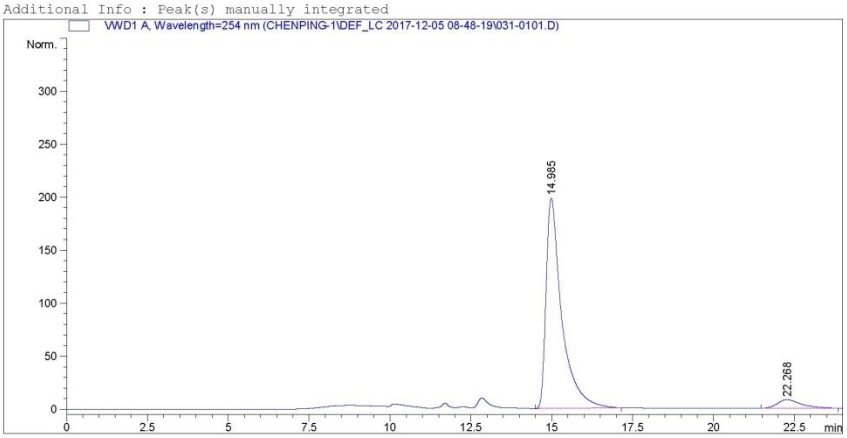
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	14.965	MM	0.5629	1.29869e4	384.49106	44.7422
2	22.085	MM	0.8961	1.60391e4	298.31088	55.2578

Totals : 2.90260e4 682.80194

Additional Info : Peak(s) manually integrated



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Area Percent Report

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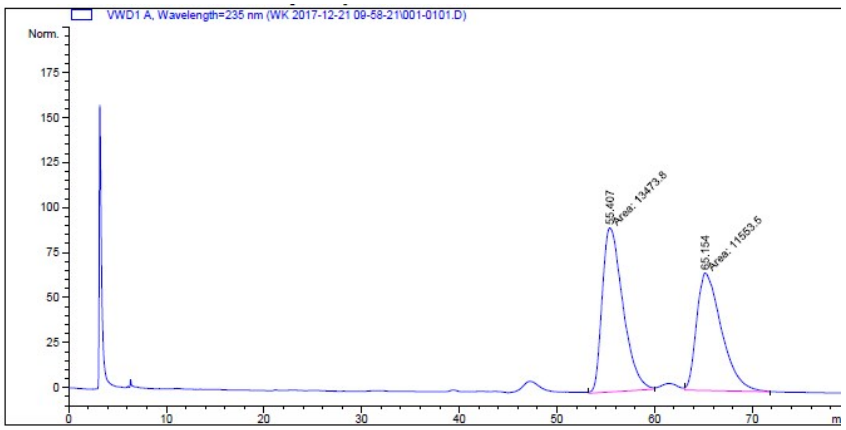
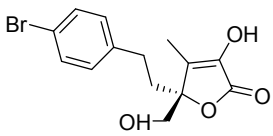
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	14.985	BB	0.4878	6659.89844	198.36076	93.9330
2	22.268	BB	0.7500	430.15573	8.20466	6.0670

Totals : 7090.05417 206.56543





9

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=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  55.407 MM    2.4649 1.34738e4    91.10563  53.8365
   2  65.154 MM    2.9555 1.15535e4    65.15263  46.1635
```

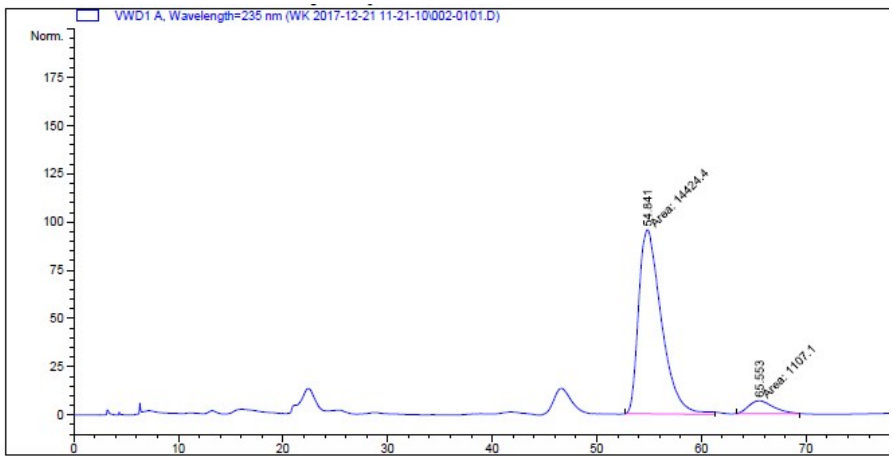


```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  54.841 MM    2.5221 1.44244e4    95.31974  92.8719
   2  65.553 MM    2.7517 1107.09656    6.70564   7.1281
```

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