Supporting Information

I_2-DMSO mediated multicomponent convergent synthesis of imidazo[2,1-*a*]isoquinoline derivatives *via* a triple *in situ* cross-trapping strategy

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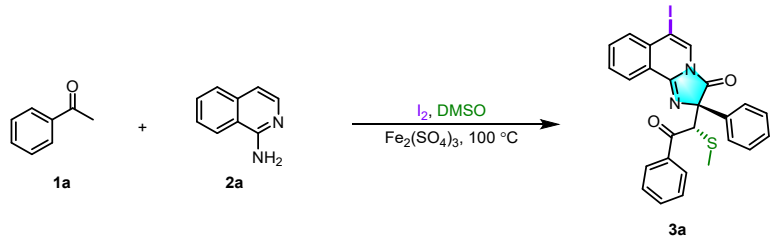
Contents

1. General

All of the substrates and reagents were commercially available and used without further purification. TLC analysis was performed using pre-coated glass plates. Flash column chromatography was performed on silica gel (200–300 mesh). ^{1}H NMR spectra were determined at 25 °C on a Varian Mercury 400 MHz spectrometer. Chemical shifts were provided in ppm relative to the internal standard of tetramethylsilane (TMS). ^{13}C spectra were recorded in $CDCl_3$ or DMSO-d_6 on 100 MHz NMR spectrometers and resonances (δ) in ppm. The data is being reported as s = singlet, d = doublet, t = triplet, m = multiplet or unresolved coupling constant(s) in Hz, integration. HRMS were obtained on Thermo Scientific Q Exactive equipped with an electron spray ionization source. Melting points were determined by using an electrothermal capillary melting point apparatus and not corrected. The X-ray crystal-structures were obtained on a Bruker APEX DUO CCD system.

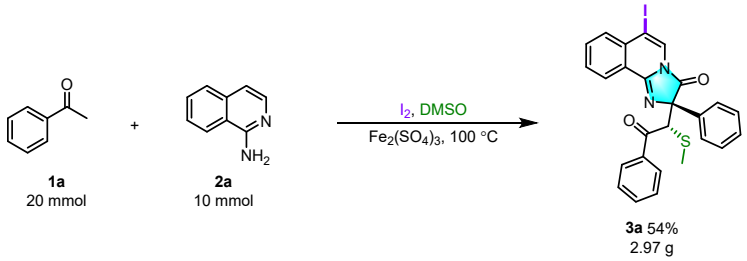
2. Experimental procedures

2.1 General procedure for the synthesis of 3 (3a as an example)



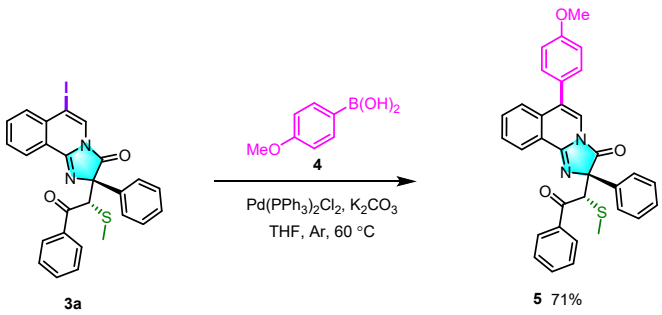
General procedure: A tube equipped with a magnetic stirring bar was charged with acetophenone (**1a**) (120.0 mg, 1.0 mmol), isoquinolin-1-amine (**2a**) (72.0 mg, 0.5 mmol), iodine (406.0 mg, 1.6 mmol) and $Fe_2(SO_4)_3$ (120.0 mg, 0.3 mmol) at room temperature, and DMSO (3 mL) was added. The resulting mixture was stirred at 100 °C for 1 h. After the reaction completed, the mixture was quenched with saturation $Na_2S_2O_3$ solution (50 mL), extracted with EtOAc (3 × 50 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 15:1) to yield the desired product **3a** (176.0 mg, yield 64%) as yellow solid (Rf = 0.3).

2.2 General procedure for the synthesis of 3a in a 10.0 mmol scale



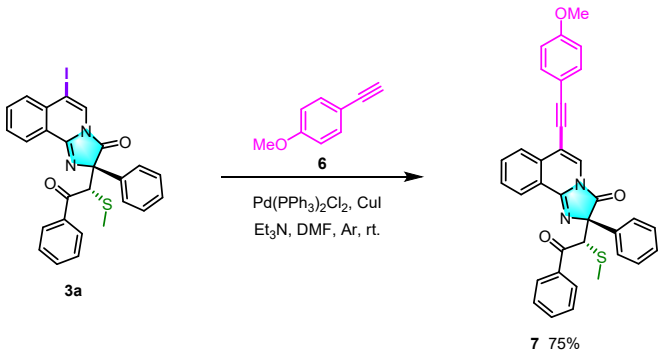
A 100 mL round-bottomed flask was charged with acetophenone (**1a**) (2.4 g, 20.0 mmol), isoquinolin-1-amine (**2a**) (1.44 g, 10.0 mmol), iodine (8.13 g, 32.0 mmol) and $Fe_2(SO_4)_3$ (2.40 g, 6.0 mmol) at room temperature, and DMSO (50 mL) was added. The resulting mixture was stirred at 100 °C for 1.5 h in oil bath. After the reaction completed, the mixture was quenched with saturation $Na_2S_2O_3$ solution (200 mL), extracted with EtOAc (3 × 200 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 15:1) to yield the desired product **3a** (2.97 g, yield 54%) as yellow solid (Rf = 0.3).

2.3 Procedure for the synthesis of 5 [1]



A 25 ml Schlenk tube equipped with a magnetic stirring bar was charged with a mixture of **3a** (110.0 mg, 0.2 mmol), **4** (30.4 mg, 0.2 mmol), $Pd(PPh_3)_2Cl_2$ (14.0 mg, 0.02 mmol), K_2CO_3 (82.8 mg, 0.6 mmol). Under reduced pressure, the tube was filled with argon for three times. After the addition of THF (2 mL), the reaction was stirred at 60 °C for 12 h. After the reaction completed, the mixture was quenched with saturation NaCl solution (50 mL), extracted with EtOAc (3 × 50 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 20:1) to yield the desired product **5** (75.3 mg, yield 71%) as yellow solid (Rf = 0.32).

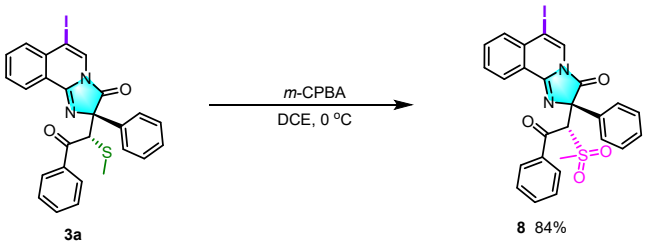
2.4 Procedure for the synthesis of 7 [1]



A 25 ml Schlenk tube equipped with a magnetic stirring bar was charged with a mixture of **3a** (110.0 mg, 0.2 mmol), **6** (31.7 mg, 0.24 mmol), $Pd(PPh_3)_2Cl_2$ (7.0 mg, 0.01 mmol), CuI (3.8 mg, 0.02 mmol). Under reduced pressure, the tube was filled with argon for three times. After the addition of DMF (1 mL) and Et_3N (2 mL), the reaction was stirred at room temperature for 12 h. After the reaction completed, the mixture was quenched with saturation NaCl solution (50 mL), extracted with EtOAc (3 × 50 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 30:1) to yield the desired product **7** (83.1

mg, yield 75%) as yellow solid (Rf = 0.28).

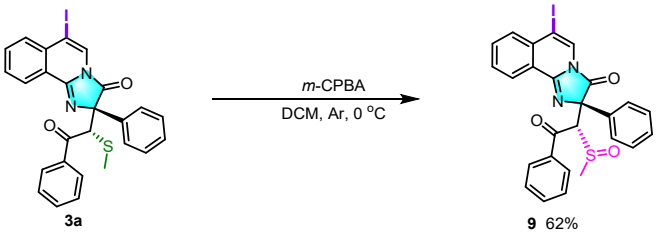
2.5 Procedure for the synthesis of 8 [2]



3a **8** 84%

A solution of **3a** (181.5 mg, 0.33 mmol) in 10 mL DCE was cooled to 0 °C. Then, *m*-CPBA (114.0 mg, 0.66 mmol) dissolved in 15 mL DCE was added drop wise to the stirred solution of **3a.** The reaction progress was monitored by TLC. After stirring for 3 h, water was added and the reaction mixture was extracted with CH_2Cl_2 (3 × 10 mL). The organic layer was dried over Na_2SO_4. Removal of the solvent followed by purification on silica gel (petroleum ether/EtOAc = 8:1) to yield the desired product **8** (161.3 mg, yield 84%) as a yellow solid (Rf = 0.32).

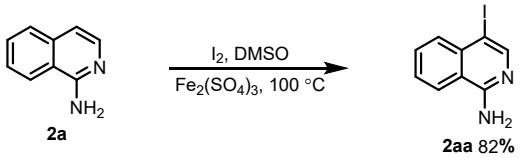
2.6 Procedure for the synthesis of 9 [3]



3a **9** 62%

A solution of **3a** (165.0 mg, 0.3 mmol) and *m*-CPBA (48.0 mg, 0.28 mmol) in dry CH_2Cl_2 (6 mL) was stirred under Ar at 0 ºC for 25 min. To the resulting suspension sat. $NaHCO_3$ (25 mL) was added at 0 ºC. The organic layer was diluted with EtOAc (50 mL), washed with sat. $NaHCO_3$ (3 × 100 mL), brine (3 × 100 mL), dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 5:1) to yield the desired product **9** (105.3 mg, yield 62%) as a yellow solid (Rf = 0.30).

2.7 Procedure for the synthesis of 2aa

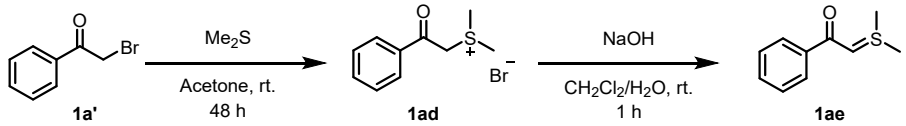


2a **2aa** 82%

A tube equipped with a magnetic stirring bar was charged with isoquinolin-1-amine (**2a**) (72.0 mg, 0.5 mmol), iodine (406.0 mg, 1.6 mmol) and $Fe_2(SO_4)_3$ (120.0 mg, 0.3 mmol) at room temperature, and DMSO (3 mL) was added. The resulting mixture was stirred at 100 °C for 1 h. After the reaction

completed, the mixture was quenched with saturation $Na_2S_2O_3$ solution (50 mL), extracted with EtOAc (3 × 50 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 8:1) to yield the product **2aa** (110.7 mg, yield 82%) as yellow solid (Rf = 0.3).

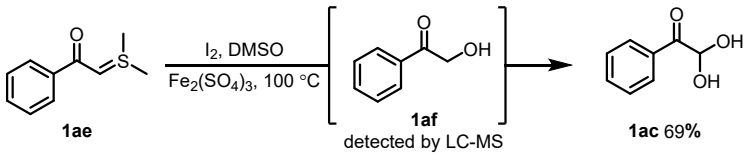
2.8 Procedure for the synthesis of 1ae [4]



Step-I: To a 0.5 M solution of bromoketone **1a'** (5 mmol, 1.0 equiv.) in acetone dimethyl sulfide (440 μL, 6.0 mmol, 1.2 equiv.) was added and the mixture was stirred for 48 h at room temperature. Then, the precipitate of sulfonium salt **1ad** was separated from the solution, washed with acetone and dried under reduced pressure to give pure sulfonium salt **1ad**, which was readily converted to the corresponding sulfonium ylide **1ae** (Step-II).

Step-II: To a suspension of sulfonium salt **1ad** (1.0 mmol, 1 equiv.) in 5 mL CH_2Cl_2 a solution of NaOH (5.0 mmol, 5 equiv.) in 5 mL H_2O was added and the mixture was intensively stirred for 1 h at room temperature. Then the reaction mixture was filtered through cotton wool. The organic layer was separated and the aqueous layer was washed with CH_2Cl_2 (5 × 15 mL). The combined organic layer was dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure. The residue was dried in a vacuum until constant weight to give sulfonium ylides **1ae**, which was immediately characterized and used in the next stage.

2.9 Procedure for the synthesis of 1ac from 1ae



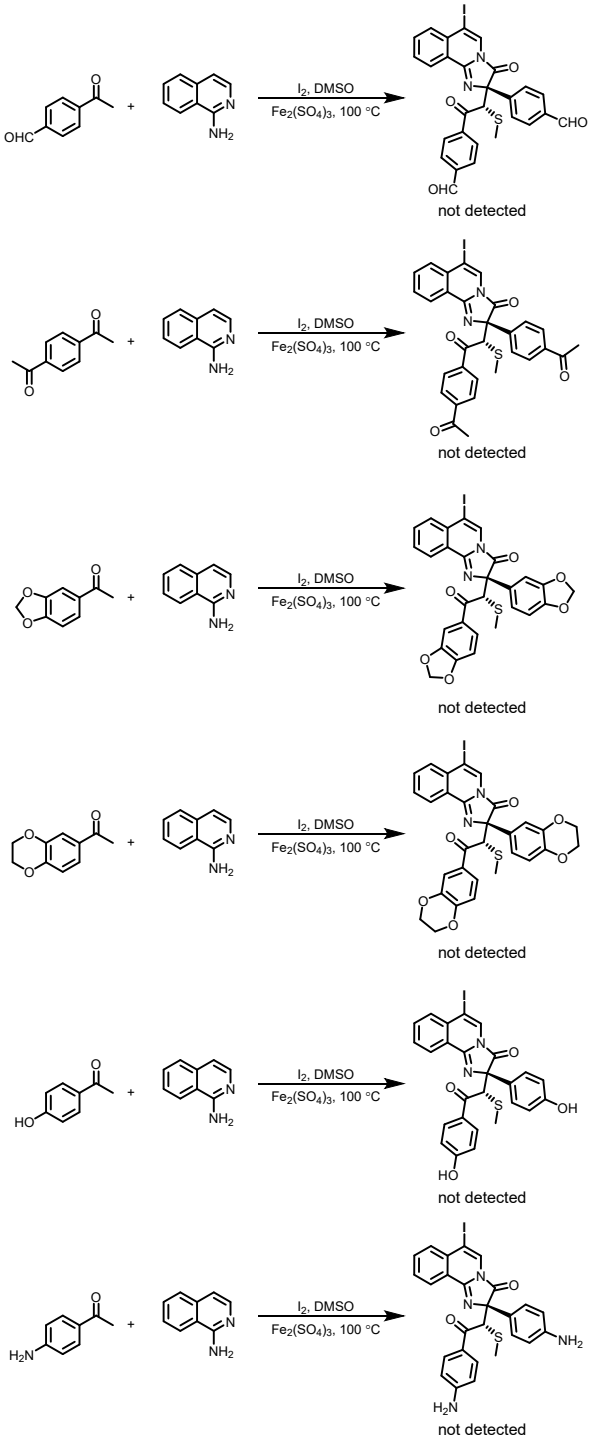
A tube equipped with a magnetic stirring bar was charged with sulfonium ylides (**1ae**) (90.0 mg, 0.5 mmol), iodine (203.0 mg, 1.6 mmol) and $Fe_2(SO_4)_3$ (60.0 mg, 0.3 mmol) at room temperature, and DMSO (3 mL) was added. The resulting mixture was stirred at 100 °C for 1 h. After the reaction completed, the mixture was quenched with saturation $Na_2S_2O_3$ solution (50 mL), extracted with EtOAc (3 × 50 mL). The combined organic layers were washed with brine, dried over anhydrous

Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1:1) to yield **1ac** (52.4 mg, yield 69%) as white solid (Rf = 0.2).

3. Substrate scope

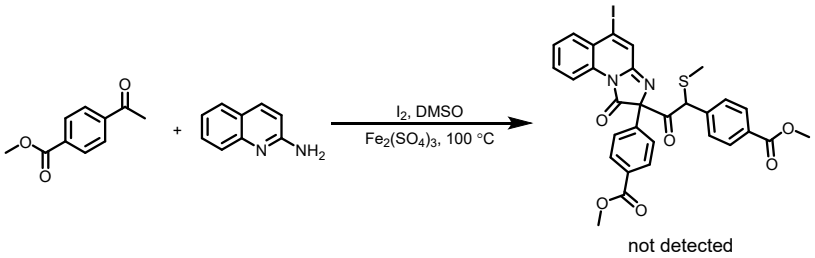
3.1 Substrate scope of methyl ketone

We have done several experiments using different acetophenone with other reactive functional groups, unfortunately, the desired product was not obtained by column chromatography. We speculate that the obstacle to this conversion is may be due to the fact that the substrate is too active, which increases the side reaction and complicates the reaction.

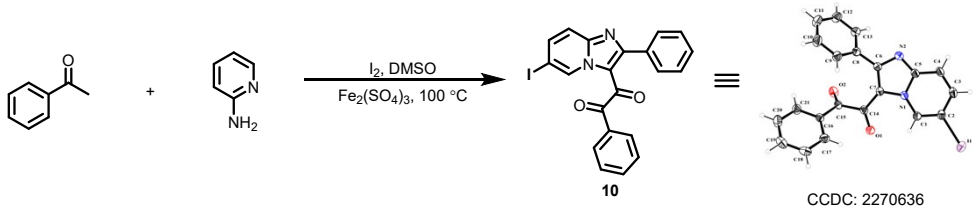


3.2 Substrate scope of amine

The 2-aminoquinoline was used to react under the standard conditions, unfortunately, the desired product was not isolated by column chromatography, and the desired product was also not detected by detection of the crude reaction extract by LC-MS analysis. When we used pyridin-2-amine to react under the standard conditions, this process was converted to other product.



not detected



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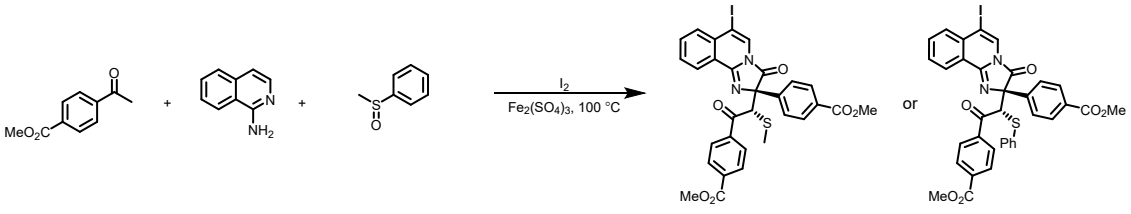
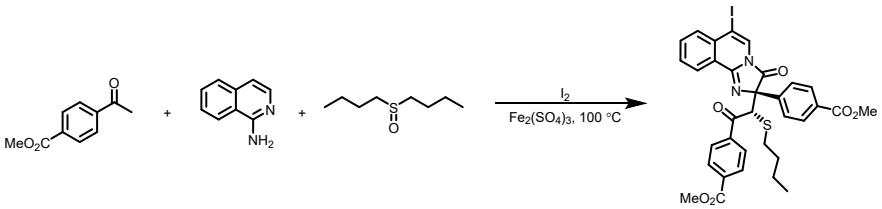
CCDC: 2270636

3.3 Substrate scope of sulfoxide

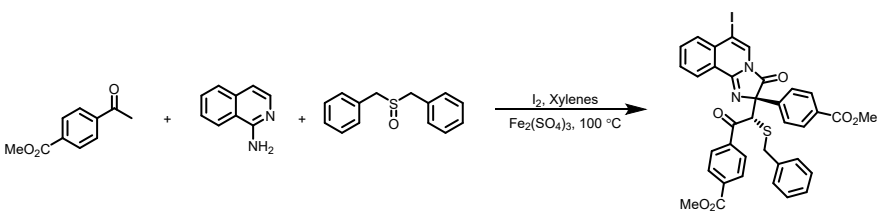
We have done several experiments using different solvents. Unfortunately, the desired product was not isolated by column chromatography, and the desired product was also not detected by detection of the crude reaction extract by LC-MS analysis when using other solvents.



not detected not detected



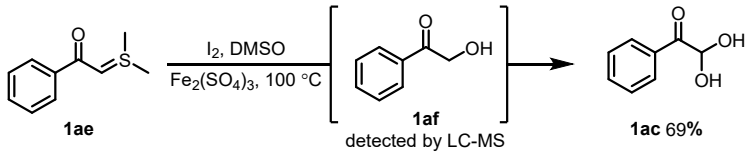
not detected



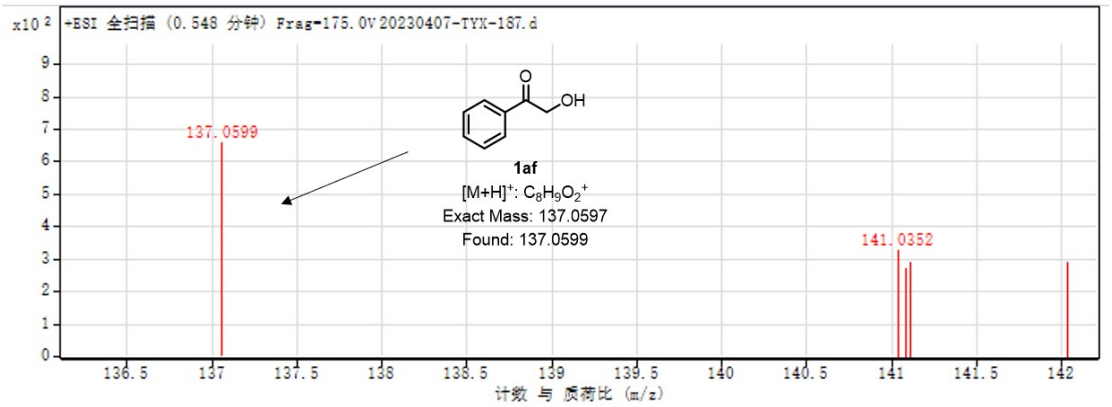
not detected

4. Mechanistic study

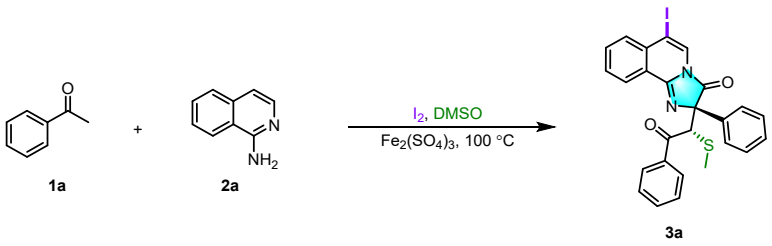
4.1 HPLC-MS of the intermediate 1af



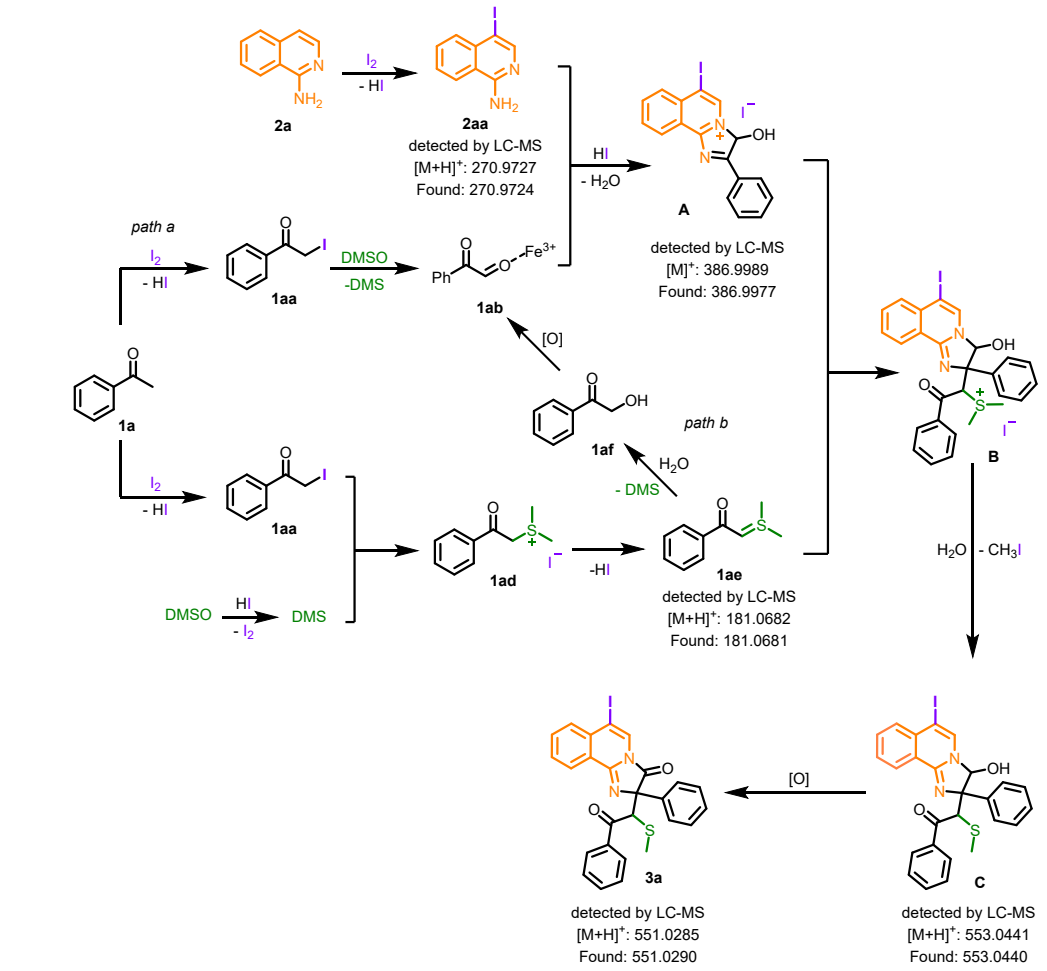
A tube equipped with a magnetic stirring bar was charged with sulfonium ylides (**1ae**) (90.0 mg, 0.5 mmol), iodine (203.0 mg, 1.6 mmol) and $Fe_2(SO_4)_3$ (60.0 mg, 0.3 mmol) at room temperature, and DMSO (3 mL) was added. The resulting mixture was stirred at 100 °C for 1 h. Then, the 1 mL of the reaction solution was quenched with 4 mL of saturation $Na_2S_2O_3$ solution, and then extracted with 3 mL of EtOAc. Then 0.5 mL of the extraction solution was added into the test bottle and diluted with 0.5 mL of MeOH. The samples were immediately monitored by HPLC-MS.

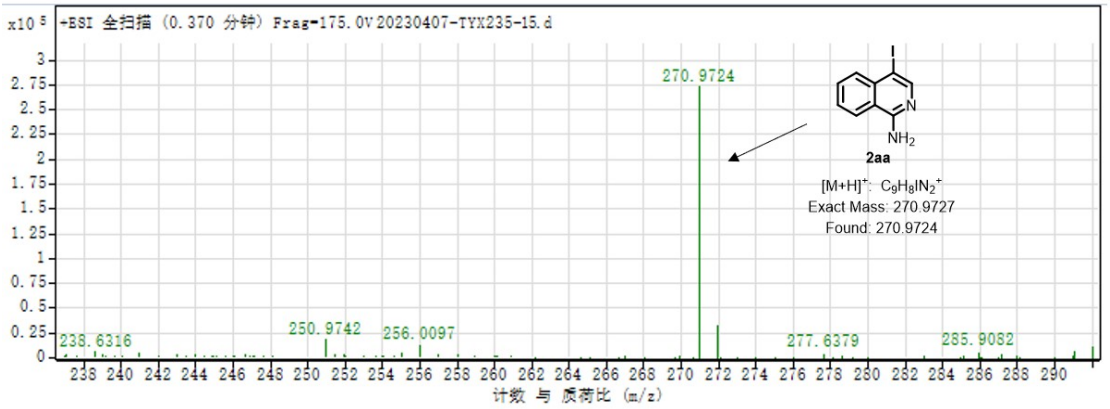


4.2 The mechanism of HPLC-MS



A tube equipped with a magnetic stirring bar was charged with acetophenone (**1a**) (120.0 mg, 1.0 mmol), isoquinolin-1-amine (**2a**) (72.0 mg, 0.5 mmol), iodine (406.0 mg, 1.6 mmol) and $Fe_2(SO_4)_3$ (120.0 mg, 0.3 mmol) at room temperature, and DMSO (3 mL) was added. The resulting mixture was stirred at 100 °C for 15 min. Then, the 0.5 mL of the reaction solution was diluted with 1.5 mL of EtOAc. The samples were immediately monitored by HPLC-MS.


2a
2aa
detected by LC-MS
[M+H]+: 270.9727
Found: 270.9724
A
detected by LC-MS
[M]+: 386.9989
Found: 386.9977
path a
1aa
1ab
1a
1af
path b
1ad
1ae
detected by LC-MS
[M+H]+: 181.0682
Found: 181.0681
B
C
3a
detected by LC-MS
[M+H]+: 551.0285
Found: 551.0290
detected by LC-MS
[M+H]+: 553.0441
Found: 553.0440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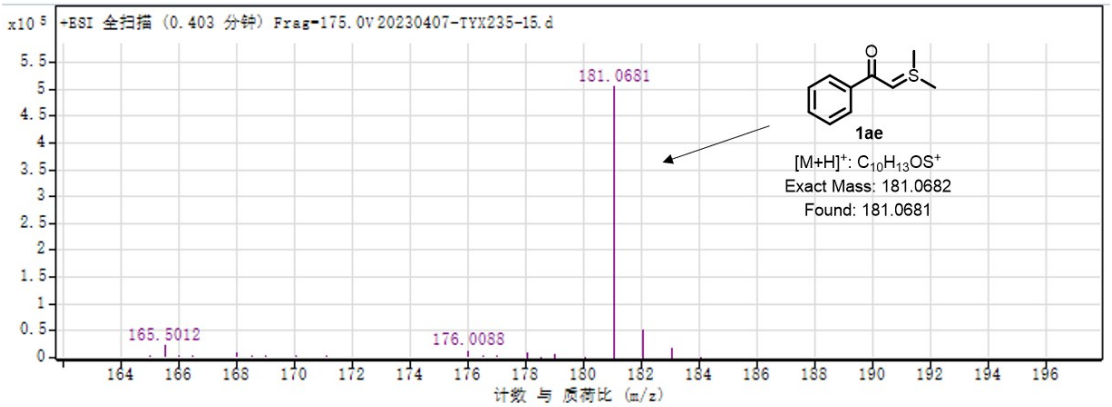
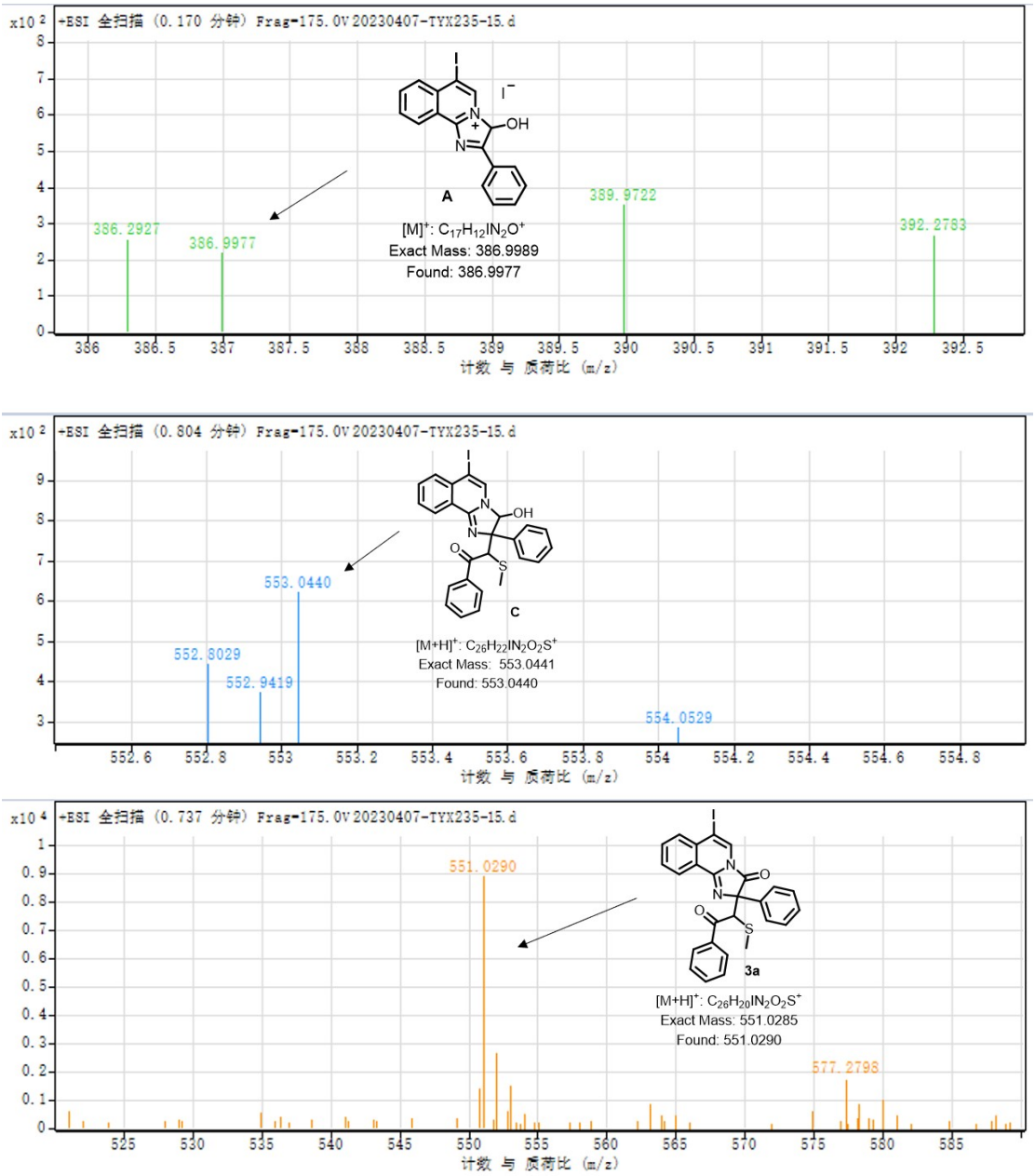
270.9724
2aa
[M+H]+: C9H8IN2+
Exact Mass: 270.9727
Found: 270.9724
238.6316
250.9742
256.0097
277.6379
285.9082
计数 与 质荷比 (m/z)

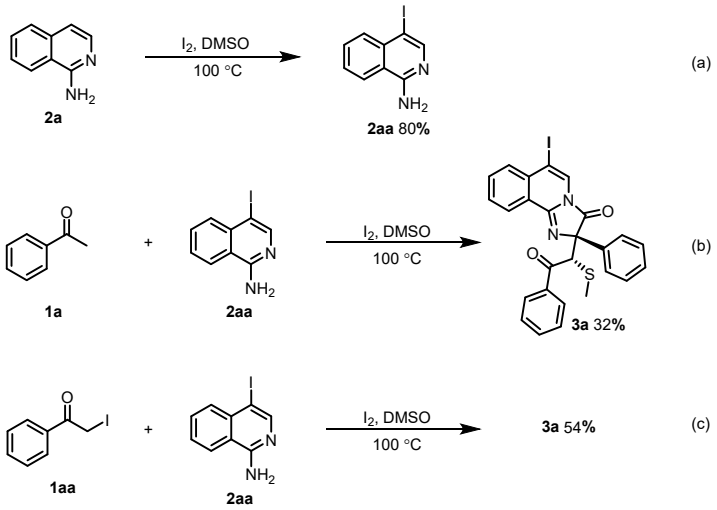

+ESI 全扫描 (0.403 分钟) Frag=175.0V 20230407-TYX235-15.d
181.0681
1ae
[M+H]+: C10H13OS+
Exact Mass: 181.0682
Found: 181.0681
165.5012
176.0088
计数 与 质荷比 (m/z)



4.3 Discuss the role of $Fe_2(SO4)_3$

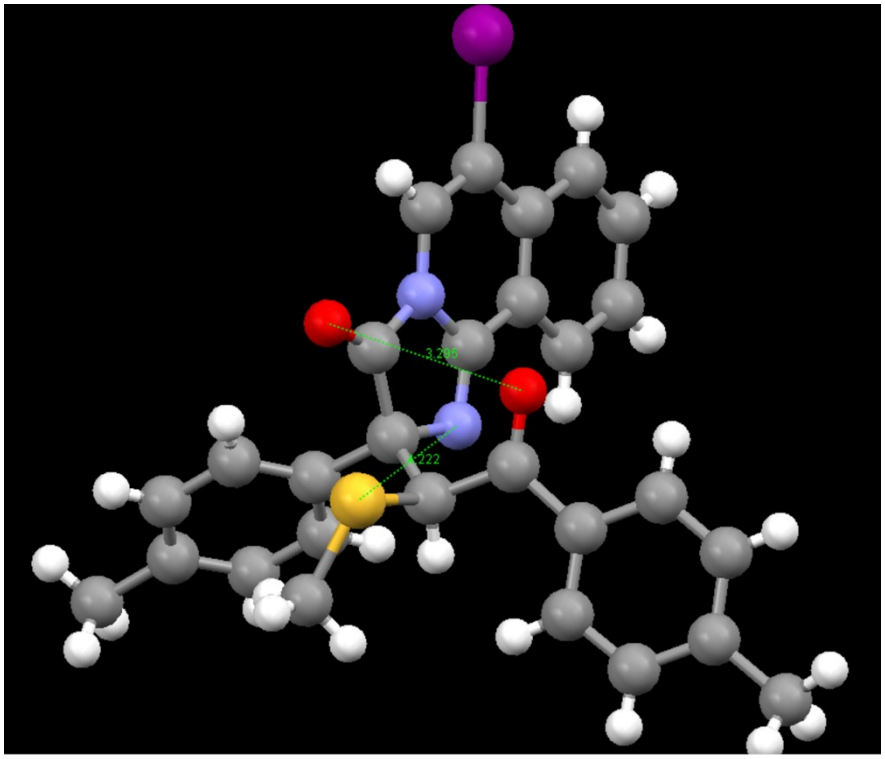
In order to further understand the role of $Fe_2(SO4)_3$, we conducted following control experiments. Isoquinolin-1-amine (**2a**) could be iodinated to 4-iodoisoquinolin-1-amine (**2aa**) in 80% yield without addition of $Fe_2(SO4)_3$ (a). In the absence of $Fe_2(SO4)_3$, iodoisoquinolin-1-amine (**2aa**) reacted with acetophenone (**1a**) providing the desired product 3a in 32% yield (b). Subsequently, replacing acetophenone (**1a**) with *α*-iodoacetophenone (**1aa**), the target product 3a was obtained in 54% yield. The above reactions effect were similar to that of with the additional of $Fe_2(SO4)_3$. Based on these supplementary experiments and literature review,[5] we speculate that

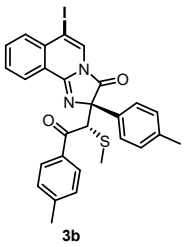
$Fe_2(SO_4)_3$ may act as a Lewis acid to active the carbonyl group of phenylglyoxal (**1ab**) and promote the cyclization process to form intermediate **A**.



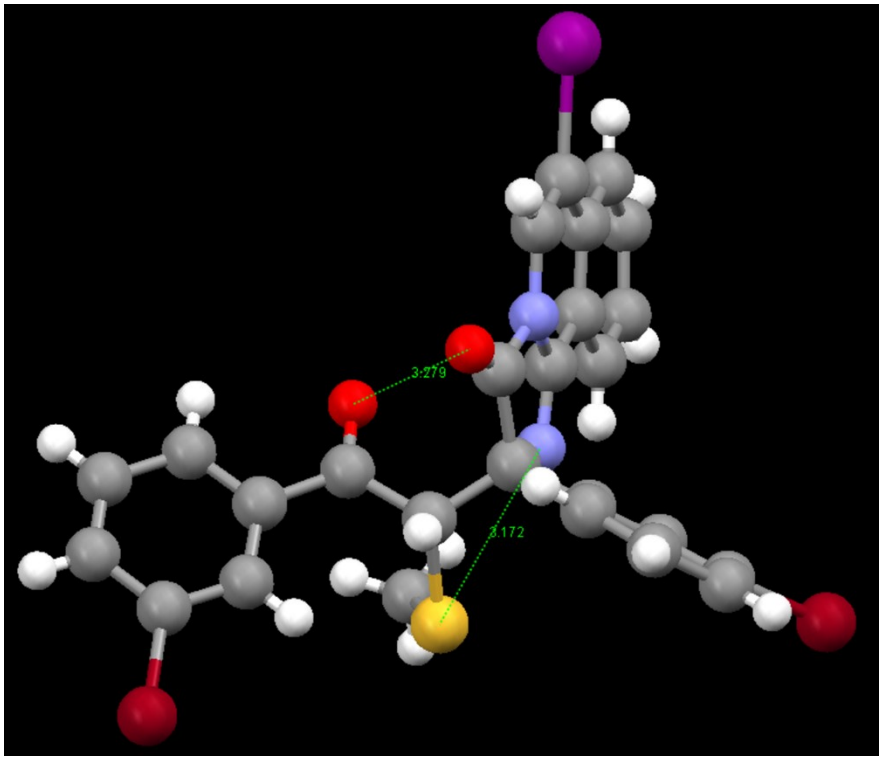
4.4 Discuss the stereoselectivity of the two chiral centers

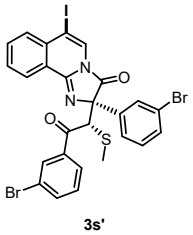
Through our unremitting efforts, we were fortunate to obtain the NMR spectra and confirm the molecular structure of the diastereoisomer **3s'** by X-ray crystallography. For other compounds, it's difficult to obtain their diastereoisomers. Through TLC analysis, we found that the diastereoisomers have lower polarity than the target product, and the separation between the two is good, the content ratio of the target product and its enantiomers is about 4:1. Unfortunately, our analytical technology is limited, we can only know from the experimental results that the energy of the target product is lower than its diastereoisomer, and it may has spatial advantages, which leads to the target product becoming the main product. By further analyzing the atomic distance between the single crystal structures of the two products, we found that the spatial distance between the two oxygen atoms in the target product (3.295 Å) was slightly larger than the diastereoisomer (3.279 Å), the spatial distance between the sulfur atom and the adjacent nitrogen atom in the target product (4.222 Å) was much larger than the diastereoisomer (3.172 Å). These were consistent with our experimental results, so this may be an important reason why the target product was the dominant structure.





3b





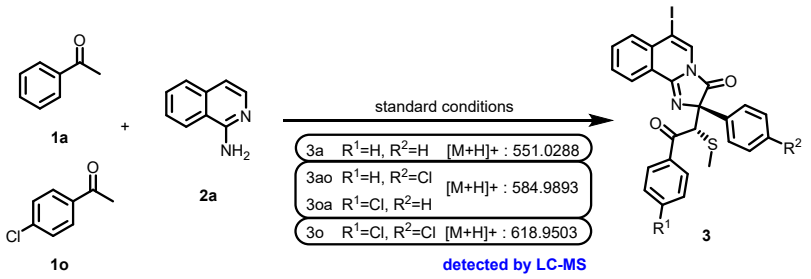
3s'

4.5 Studies of cross reaction

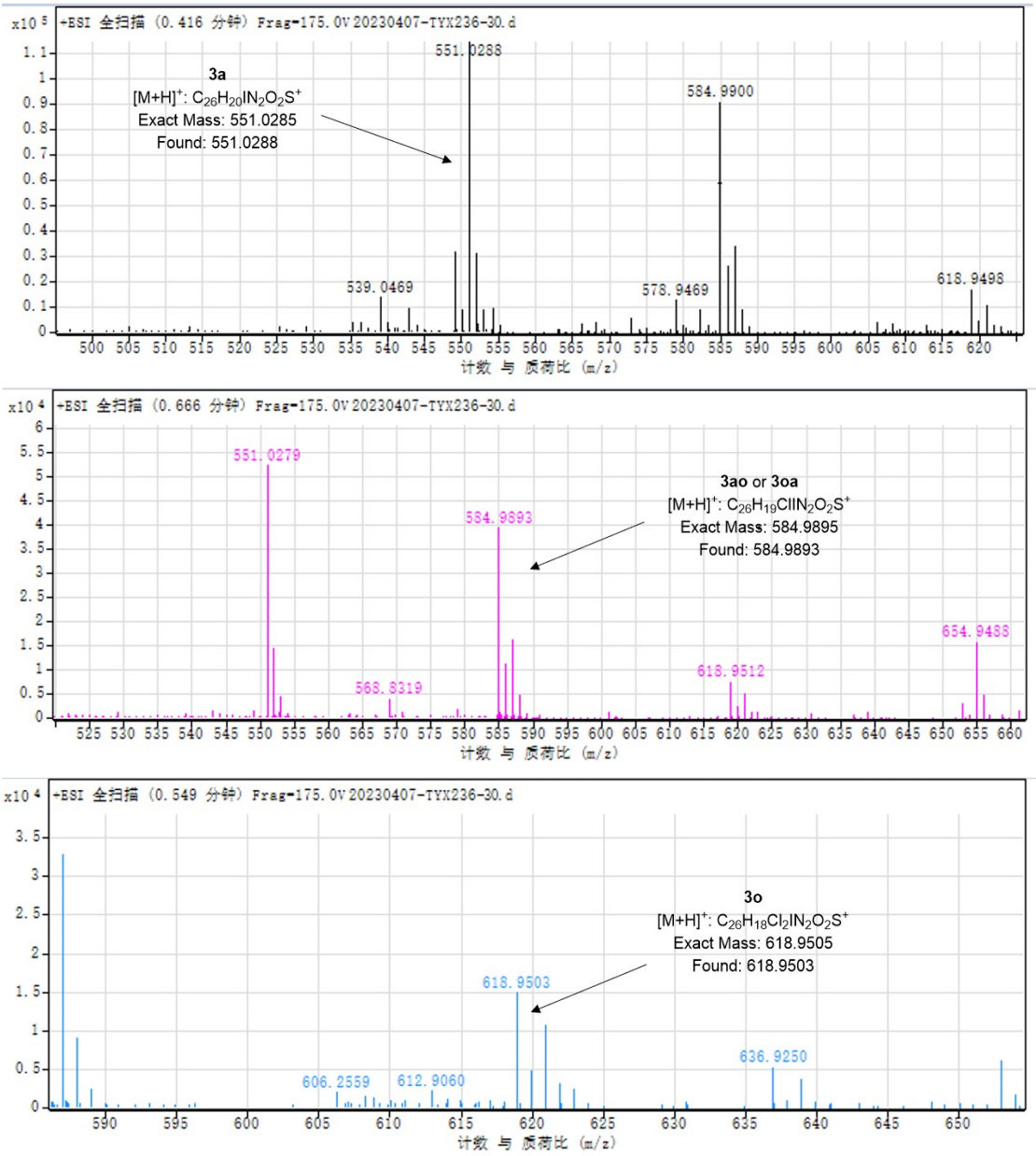
We conducted the following three sets of cross reactions. All the products were successfully identified by LC-MS analysis of the crude reaction extract, including the crossed products.

We first investigated the cross reaction using **1a** (0.5 mmol), **1o** (0.5 mmol) and **2a** (0.5 mmol)

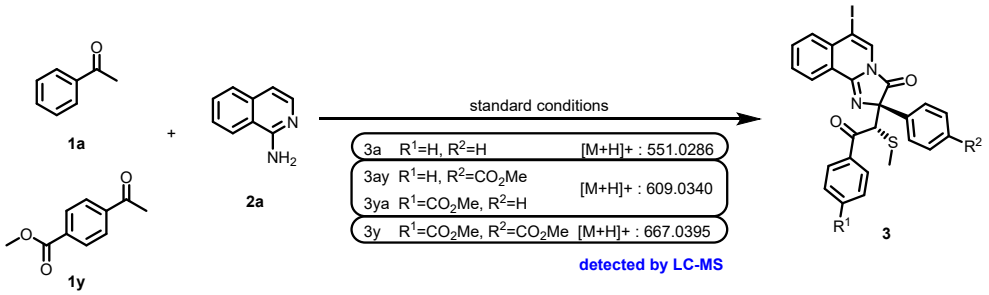
under the standard conditions.



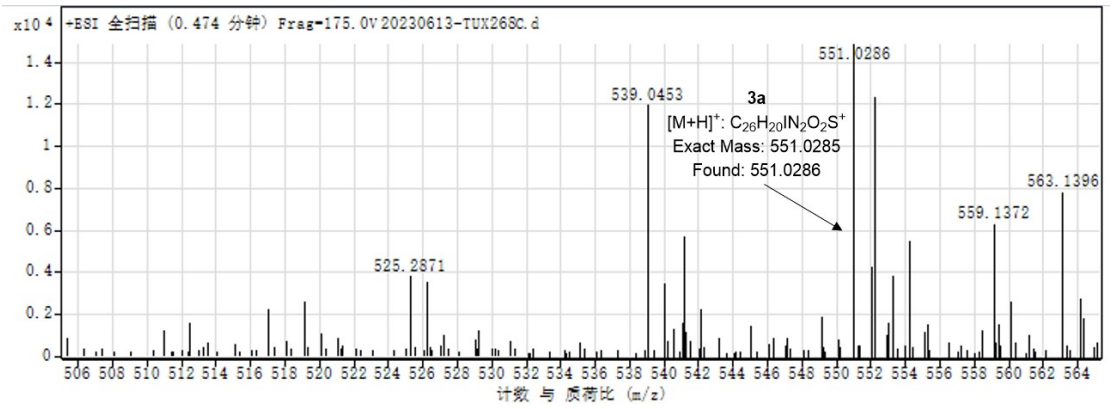
The LC-MS Spectra is listed below:

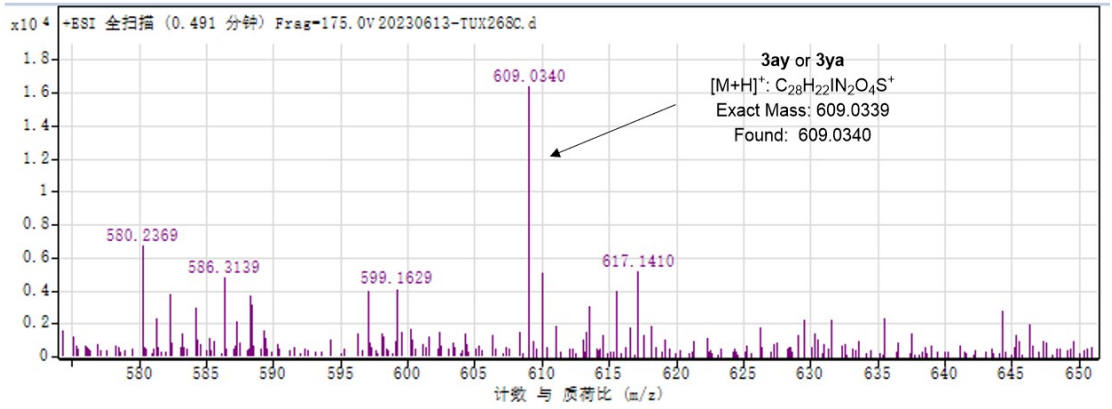


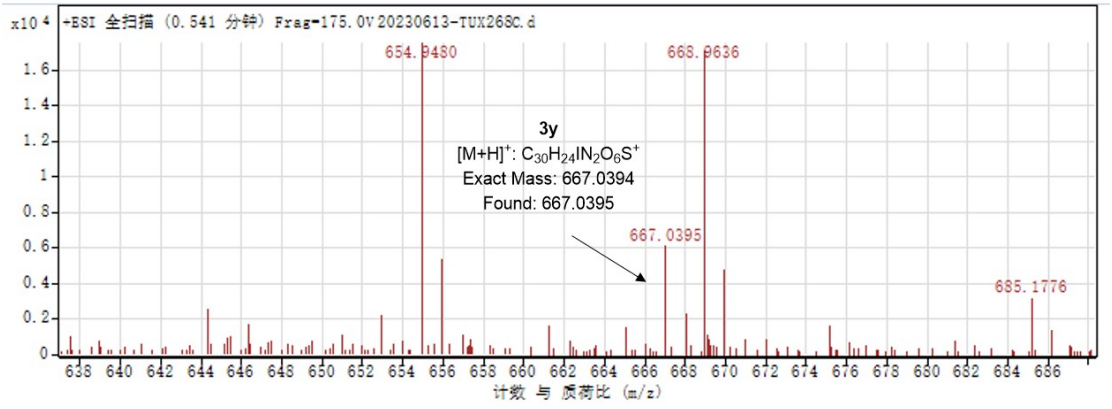
Then we investigated the cross reaction using **1a** (0.5 mmol), **1y** (0.5 mmol) and **2a** (0.5 mmol) under the standard conditions.



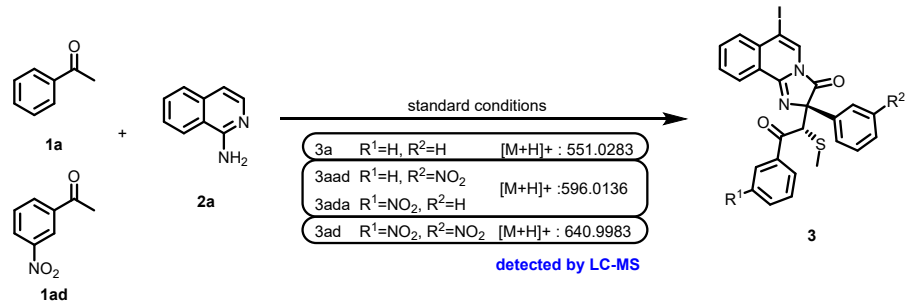
The LC-MS Spectra is listed below:



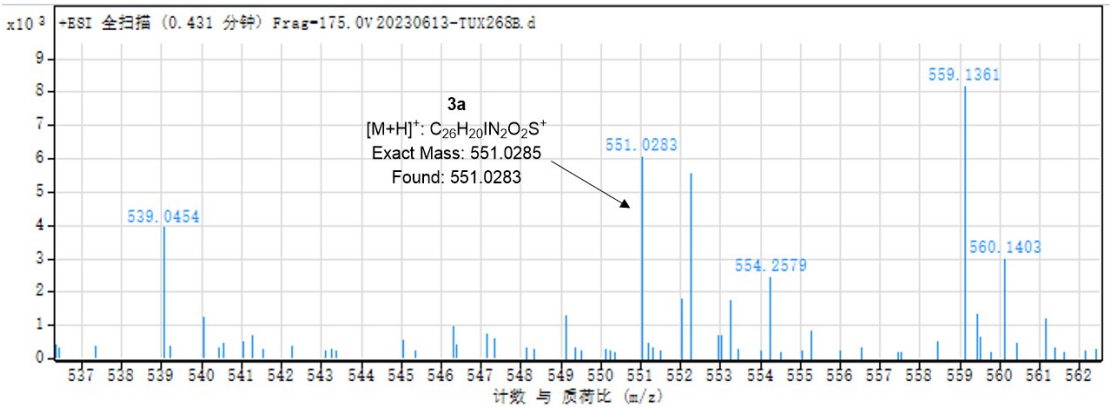


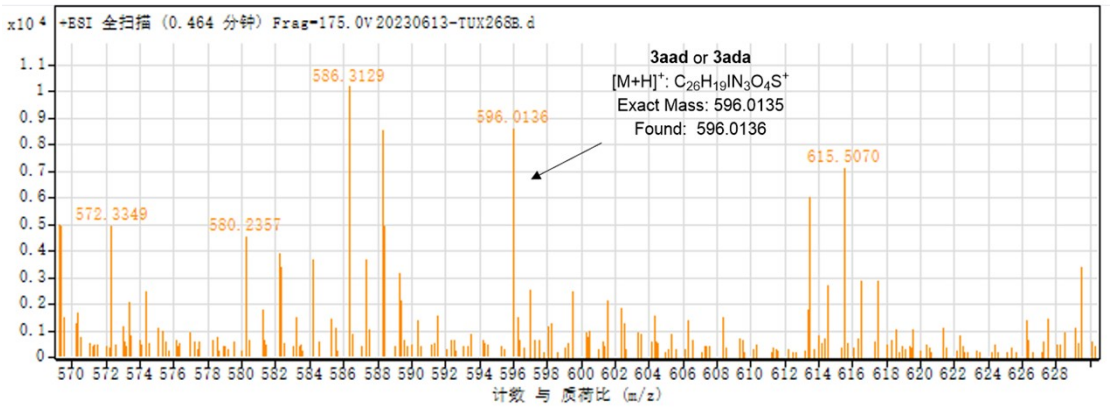


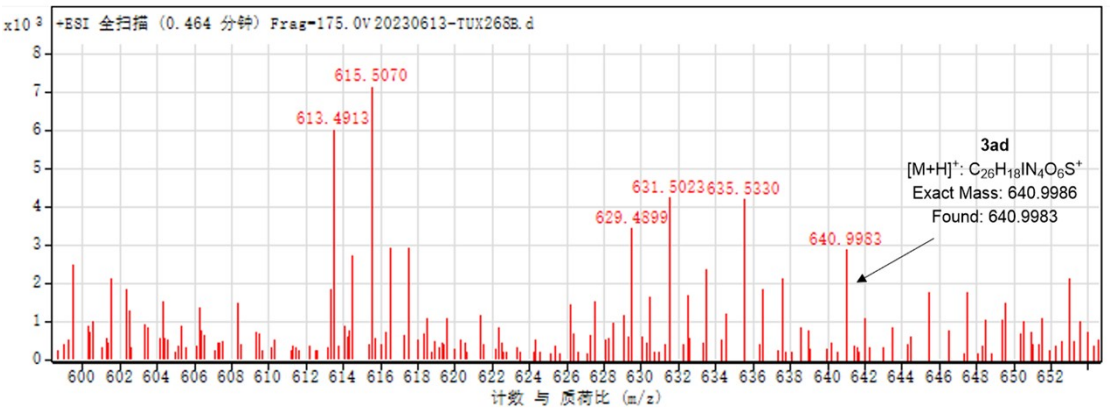
Next we investigated the cross reaction using **1a** (0.5 mmol), **1ad** (0.5 mmol) and **2a** (0.5 mmol) under the standard conditions.



The LC-MS Spectra is listed below:







References

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5. The crystallographic data

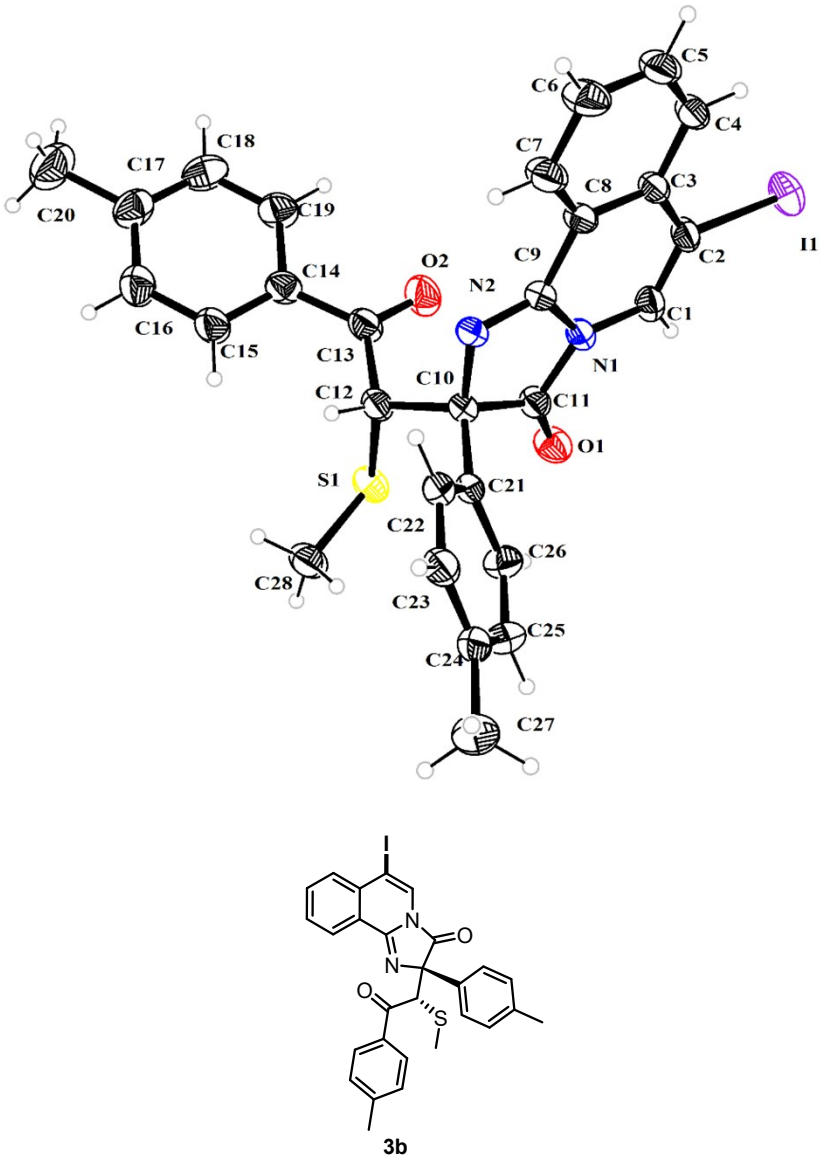


Figure S1. X-ray crystal structure of **3b** ORTEP (30%) drawing

Crystal Data for Compound **3b**: CCDC 2127420 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic.

Sample preparation: In a 10 mL glass bottle, 15 mg of pure **3b** was completely dissolved in the mixed solvent of 3 mL $CHCl_3$, and then 2 mL of n-hexane was added slowly. After a week of solvent evaporation, some yellow transparent crystals were obtained. The crystals were mounted on a glass fiber for diffraction experiments. Intensity data were collected on a Bruker SMART APEX CCD diffractometer with Mo Kα radiation (0.71073 Å) at room temperature.

Bond precision: C-C = 0.0048 A Wavelength=0.71073

Cell: a=13.900(5) b=11.046(4) c=17.684(7)
alpha=90 beta=109.022(6) gamma=90
Temperature: 296 K

	Calculated	Reported
Volume	2566.9(17)	2567.0(17)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C28 H23 I N2 O2 S	C28 H23 I N2 O2 S
Sum formula	C28 H23 I N2 O2 S	C28 H23 I N2 O2 S
Mr	578.44	578.44
Dx,g cm-3	1.497	1.497
Z	4	4
Mu (mm-1)	1.356	1.356
F000	1160.0	1160.0
F000'	1158.99	
h,k,lmax	19,15,24	19,15,24
Nref	7069	7004
Tmin,Tmax	0.729,0.873	0.561,0.746
Tmin'	0.659	

Correction method= # Reported T Limits: Tmin=0.561 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.991 Theta(max)= 29.380

R(reflections)= 0.0436(4808) wR2(reflections)= 0.1375(7004)

S = 1.035 Npar= 330

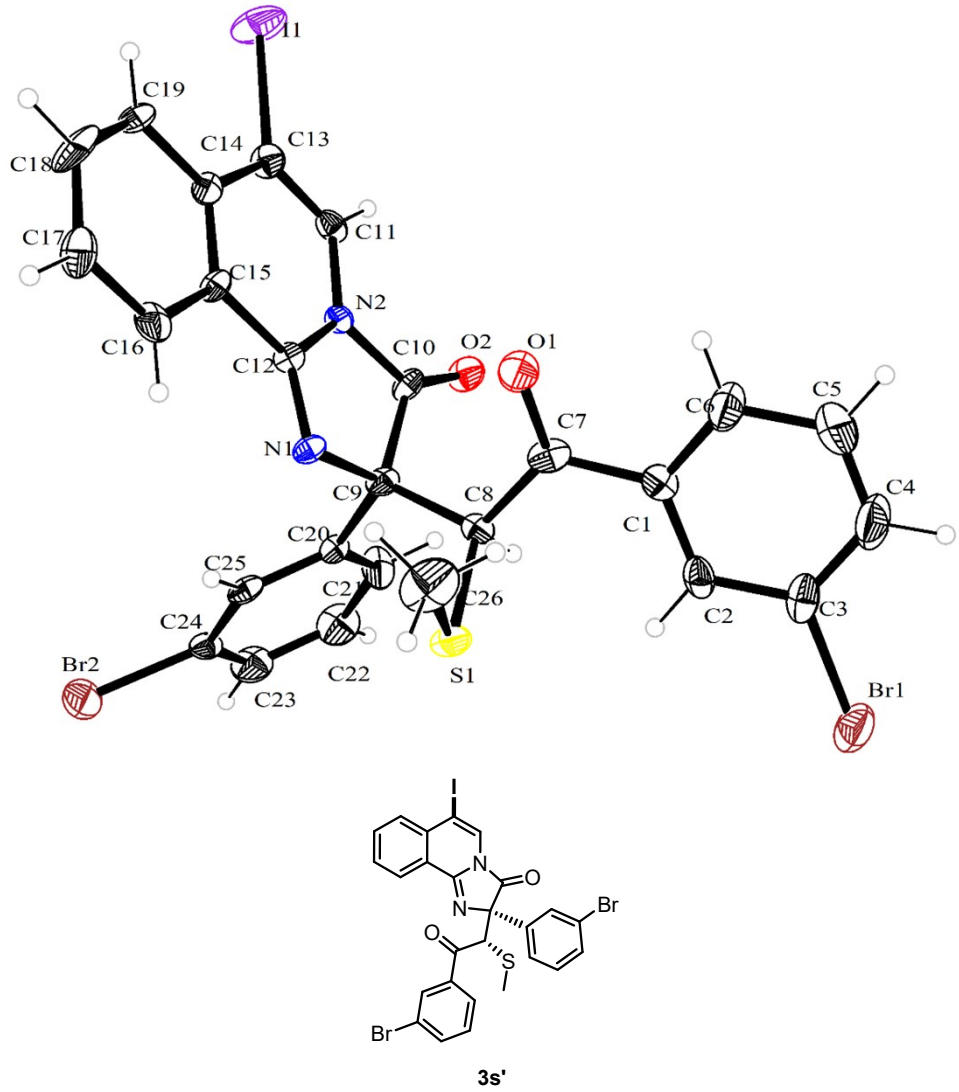


Figure S1. X-ray crystal structure of **3s'** ORTEP (30%) drawing

Crystal Data for Compound **3s'**: CCDC 2270637 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic.

Sample preparation: In a 10 mL glass bottle, 15 mg of pure **3s'** was completely dissolved in the mixed solvent of 3 mL $CHCl_3$, and then 2 mL of n-hexane was added slowly. After a week of solvent evaporation, some yellow transparent crystals were obtained. The crystals were mounted on a glass fiber for diffraction experiments. Intensity data were collected on a Bruker SMART APEX CCD diffractometer with Mo Kα radiation (0.71073 Å) at room temperature.

Bond precision: C-C = 0.0201 A Wavelength=0.71073

Cell: a=9.396(7) b=12.162(10) c=14.231(10)
alpha=110.606(11) beta=105.796(10) gamma=91.123(10)
Temperature: 296 K

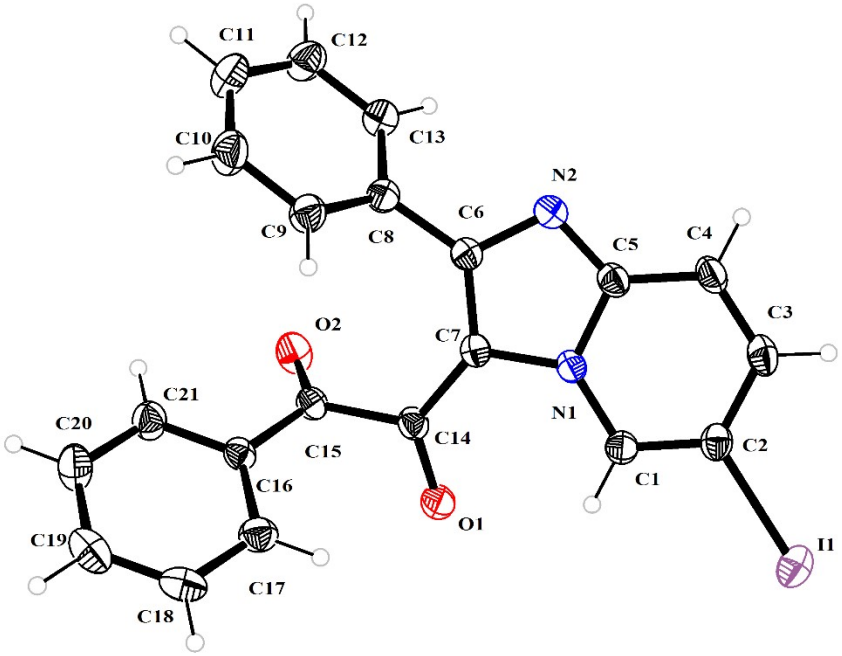
	Calculated	Reported
Volume	1452.6(19)	1452.5(19)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C26 H17 Br2 I N2 O2 S, C H Cl3	C26 H17 Br2 I N2 O2 S, C H Cl3
Sum formula	C27 H18 Br2 Cl3 I N2 O2 S	C27 H18 Br2 Cl3 I N2 O2 S
Mr	827.54	827.56
Dx,g cm-3	1.892	1.892
Z	2	2
Mu (mm-1)	4.230	4.230
F000	800.0	800.0
F000'	799.32	
h,k,lmax	11,14,16	11,14,16
Nref	5117	4967
Tmin,Tmax	0.608,0.655	0.229,0.746
Tmin'	0.596	

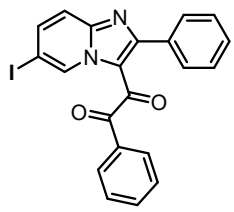
Correction method= # Reported T Limits: Tmin=0.229 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.971 Theta(max)= 25.000

R(reflections)= 0.0959(2566) wR2(reflections)= 0.2855(4967)

S = 0.967 Npar= 363





10

Figure S1. X-ray crystal structure of **10** ORTEP (30%) drawing

Crystal Data for Compound **10**: CCDC 2270636 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic.

Sample preparation: In a 10 mL glass bottle, 15 mg of pure **10** was completely dissolved in the mixed solvent of 3 mL $CHCl_3$, and then 2 mL of n-hexane was added slowly. After a week of solvent evaporation, some yellow transparent crystals were obtained. The crystals were mounted on a glass fiber for diffraction experiments. Intensity data were collected on a Bruker SMART APEX CCD diffractometer with Mo Kα radiation (0.71073 Å) at room temperature.

Bond precision: C-C = 0.0043 A Wavelength=0.71073

Cell: a=17.518(3) b=5.2658(9) c=20.162(3)
alpha=90 beta=107.568(2) gamma=90
Temperature: 296 K

	Calculated	Reported
Volume	1773.1(5)	1773.2(5)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C21 H13 I N2 O2	C21 H13 I N2 O2
Sum formula	C21 H13 I N2 O2	C21 H13 I N2 O2
Mr	452.23	452.23
Dx,g cm-3	1.694	1.694
Z	4	4
Mu (mm-1)	1.824	1.824
F000	888.0	888.0
F000'	886.43	
h,k,lmax	26,7,30	25,7,29
Nref	6127	5732
Tmin,Tmax	0.803,0.833	0.521,0.746
Tmin'	0.803	

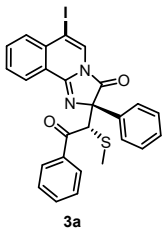
Correction method= # Reported T Limits: Tmin=0.521 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.936 Theta(max)= 31.969

R(reflections)= 0.0385(4474) wR2(reflections)= 0.1014(5732)

S = 1.034 Npar= 235

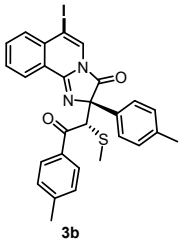
6. Spectroscopic data



3a

(*R*)-6-Iodo-2-((*S*)-1-(methylthio)-2-oxo-2-phenylethyl)-2-phenylimidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3a)

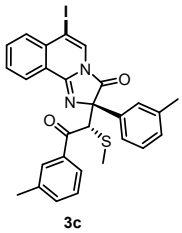
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (15:1 v/v) as eluent afforded **3a** (176.0 mg , yield 64%) as yellow solid (Rf = 0.3); m.p. 132-134 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, J = 7.6 Hz, 1H), 7.99–7.92 (m, 4H), 7.82 (s, 1H), 7.63 (d, J = 3.6 Hz, 2H), 7.55 (t, J = 7.2 Hz, 1H), 7.45–7.35 (m, 5H), 7.34–7.29 (m, 1H), 5.02 (s, 1H), 1.93 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.8, 177.5, 155.0, 135.9, 135.6, 134.6, 133.5, 133.4, 131.7, 129.0, 128.6, 128.5, 128.4, 128.3, 127.5, 127.2, 125.7, 123.4, 77.8, 76.1, 58.5, 16.1; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{20}IN_2O_2S^+$ 551.0285; Found 551.0287.



3b

(*R*)-6-Iodo-2-((*S*)-1-(methylthio)-2-oxo-2-(*p*-tolyl)ethyl)-2-(*p*-tolyl)imidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3b)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (15:1 v/v) as eluent afforded **3b** (176.3 mg yield 61%) as yellow solid (Rf = 0.28); m.p. 168-170 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, J = 7.6 Hz, 1H), 7.85 (d, J = 8.0 Hz, 4H), 7.80 (s, 1H), 7.59 (d, J = 3.6 Hz, 2H), 7.43–7.37 (m, 1H), 7.23–7.15 (m, 4H), 5.00 (s, 1H), 2.37 (s, 3H), 2.32 (s, 3H), 1.94 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.5, 177.6, 154.8, 144.3, 138.1, 134.5, 133.4, 132.94, 132.92, 131.6, 129.3, 128.9, 128.6, 127.3, 127.2, 125.6, 123.4, 77.7, 76.0, 58.3, 21.6, 21.1, 16.0; HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{28}H_{24}IN_2O_2S^+$ 579.0598; Found 579.0599.

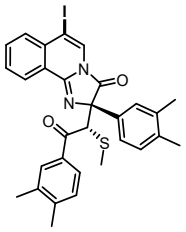


3c

(*R*)-6-Iodo-2-((*S*)-1-(methylthio)-2-oxo-2-(*m*-tolyl)ethyl)-2-(*m*-tolyl)imidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3c)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (30:1 v/v) as eluent afforded **3c** (167.6 mg, yield 58%) as yellow solid (Rf = 0.2); m.p. 163-165 °C; ^{1}H NMR

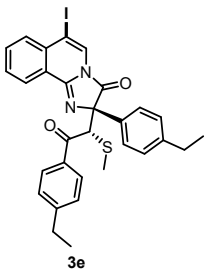
(400 MHz, $CDCl_3$) δ 8.30 (d, J = 7.6 Hz, 1H), 7.80 (s, 1H), 7.79–7.72 (m, 4H), 7.60 (d, J = 4.0 Hz, 2H), 7.45–7.39 (m, 1H), 7.36–7.24 (m, 3H), 7.12 (d, J = 7.6 Hz, 1H), 5.03 (s, 1H), 2.36 (s, 6H), 1.94 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.0, 177.5, 154.9, 138.4, 137.9, 135.8, 135.6, 134.6, 134.2, 133.4, 131.6, 129.1, 129.0, 128.9, 128.4, 128.1, 128.0, 127.2, 125.6, 124.5, 123.5, 77.8, 76.2, 58.3, 21.6, 21.3, 16.1; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{28}H_{24}IN_2O_2S^+$ 579.0598; Found 579.0600.



3d

(*R*)-2-(3,4-Dimethylphenyl)-2-((*S*)-2-(3,4-dimethylphenyl)-1-(methylthio)-2-oxoethyl)-6-iodoimidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3d)

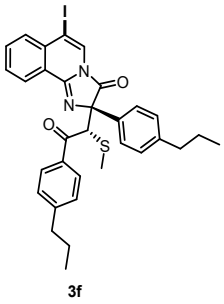
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (20:1 v/v) as eluent afforded **3d** (172.7 mg, yield 57%) as yellow solid (Rf = 0.3); m.p. 113-115 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, J = 7.6 Hz, 1H), 7.78 (s, 1H), 7.71 (s, 4H), 7.52 (s, 2H), 7.34 (s, 1H), 7.14 (d, J = 4.0 Hz, 2H), 5.05 (s, 1H), 2.27 (s, 3H), 2.23 (d, J = 2.8 Hz, 6H), 2.21 (s, 3H), 1.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.5, 177.5, 154.6, 142.9, 136.8, 136.6, 136.3, 134.3, 133.21, 133.18, 131.4, 129.7, 129.5, 129.4, 128.7, 128.4, 127.0, 126.1, 125.5, 124.8, 123.3, 77.6, 76.0, 58.0, 19.89, 19.86, 19.6, 19.3, 15.9; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{30}H_{28}IN_2O_2S^+$ 607.0911; Found 607.0912.



3e

(*R*)-2-(4-Ethylphenyl)-2-((*S*)-2-(4-ethylphenyl)-1-(methylthio)-2-oxoethyl)-6-iodoimidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3e)

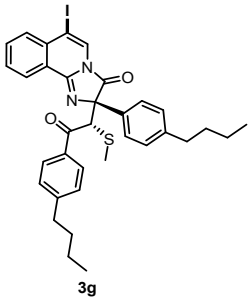
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (20:1 v/v) as eluent afforded **3e** (166.7 mg, yield 55%) as yellow solid (Rf = 0.28); m.p. 173-175 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, J = 6.8 Hz, 1H), 7.92–7.85 (m, 4H), 7.81 (s, 1H), 7.59 (d, J = 2.8 Hz, 2H), 7.44–7.38 (m, 1H), 7.25–7.18 (m, 4H), 5.01 (s, 1H), 2.71–2.58 (m, 4H), 1.94 (s, 3H), 1.25–1.17 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.5, 177.6, 154.8, 150.4, 144.4, 134.6, 133.4, 133.2, 131.6, 128.9, 128.7, 128.1, 127.7, 127.5, 127.2, 125.7, 123.5, 77.7, 76.0, 58.4, 28.9, 28.4, 16.0, 15.4, 15.1; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{30}H_{28}IN_2O_2S^+$ 607.0911; Found 607.0913.



3f

(*R*)-6-Iodo-2-((*S*)-1-(methylthio)-2-oxo-2-(4-propylphenyl)ethyl)-2-(4-propylphenyl)imidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3f)

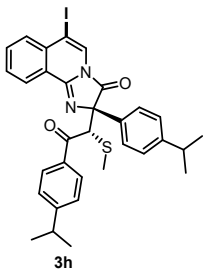
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (30:1 v/v) as eluent afforded **3f** (161.7 mg, yield 51%) as yellow solid (Rf = 0.29); m.p. 188-190 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, J = 6.8 Hz, 1H), 7.87 (t, J = 7.2 Hz, 4H), 7.81 (s, 1H), 7.60 (s, 2H), 7.41 (s, 1H), 7.24–7.15 (m, 4H), 5.00 (s, 1H), 2.63–2.53 (m, 4H), 1.93 (s, 3H), 1.68–1.55 (m, 4H), 0.95–0.87 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.6, 177.6, 154.8, 148.9, 142.9, 134.6, 133.4, 133.2, 131.6, 128.9, 128.7, 128.6, 128.3, 127.4, 127.2, 125.6, 123.5, 77.6, 76.0, 58.6, 38.0, 37.6, 24.4, 24.1, 16.1, 13.8; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{32}H_{32}IN_2O_2S^+$ 635.1224; Found 635.1223.



3g

(*R*)-2-(4-Butylphenyl)-2-((*S*)-2-(4-butylphenyl)-1-(methylthio)-2-oxoethyl)-6-iodoimidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3g)

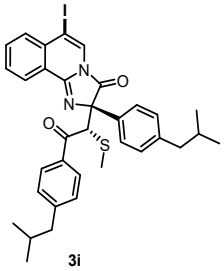
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (50:1 v/v) as eluent afforded **3g** (155.6 mg, yield 47%) as yellow solid (Rf = 0.2); m.p. 134-136 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, J = 7.6 Hz, 1H), 7.87 (t, J = 7.6 Hz, 4H), 7.80 (s, 1H), 7.58 (d, J = 3.2 Hz, 2H), 7.42–7.36 (m, 1H), 7.24–7.15 (m, 4H), 5.00 (s, 1H), 2.66–2.55 (m, 4H), 1.94 (s, 3H), 1.62–1.51 (m, 4H), 1.38–1.26 (m, 4H), 0.94–0.85 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.5, 177.6, 154.7, 149.2, 143.1, 134.5, 133.4, 133.1, 131.6, 128.9, 128.63, 128.60, 128.3, 127.4, 127.2, 125.6, 123.5, 77.6, 75.9, 58.5, 35.6, 35.2, 33.4, 33.1, 22.3, 22.2, 16.1, 13.89, 13.86; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{34}H_{36}IN_2O_2S^+$ 663.1537; Found 663.1537.



3h

(*R*)-6-Iodo-2-(4-isopropylphenyl)-2-((*S*)-2-(4-isopropylphenyl)-1-(methylthio)-2-oxoethyl)imidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3h)

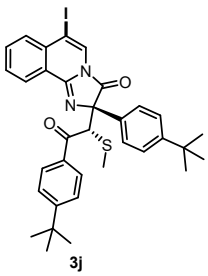
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (30:1 v/v) as eluent afforded **3h** (171.2 mg, yield 54%) as yellow solid (Rf = 0.32); m.p. 147-149 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, J = 8.0 Hz, 1H), 7.93 (d, J = 8.0 Hz, 2H), 7.89 (d, J = 8.0 Hz, 2H), 7.78 (s, 1H), 7.51 (d, J = 5.6 Hz, 2H), 7.36–7.31 (m, 1H), 7.27–7.22 (m, 4H), 5.03 (s, 1H), 2.94–2.83 (m, 2H), 1.95 (s, 3H), 1.22 (s, 6H), 1.20 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.3, 177.5, 154.8, 154.6, 148.9, 134.4, 133.3, 133.2, 133.1, 131.4, 128.8, 128.7, 127.5, 127.1, 126.6, 126.1, 125.5, 123.3, 77.5, 75.8, 58.3, 34.1, 33.6, 23.8, 23.49, 23.47, 15.9; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{32}H_{32}IN_2O_2S^+$ 635.1224; Found 635.1225.



3i

(*R*)-6-Iodo-2-(4-isobutylphenyl)-2-((*S*)-2-(4-isobutylphenyl)-1-(methylthio)-2-oxoethyl)imidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3i)

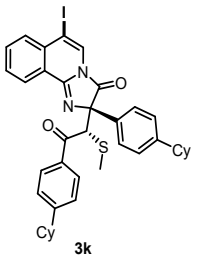
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (50:1 v/v) as eluent afforded **3i** (172.1 mg, yield 52%) as yellow solid (Rf = 0.3); m.p. 181-183 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, J = 7.6 Hz, 1H), 7.91–7.78 (m, 4H), 7.81 (s, 1H), 7.57 (d, J = 2.8 Hz, 2H), 7.44–7.36 (m, 1H), 7.20–7.10 (m, 4H), 4.99 (s, 1H), 2.49 (d, J = 7.2 Hz, 2H), 2.44 (d, J = 7.2 Hz, 2H), 1.93 (s, 3H), 1.90–1.79 (m, 2H), 0.91–0.83 (m, 12H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.7, 177.5, 154.8, 147.9, 141.9, 134.6, 133.4, 133.2, 133.1, 131.6, 129.3, 128.94, 128.89, 128.5, 127.3, 127.2, 125.6, 123.4, 77.7, 75.9, 58.7, 45.3, 45.0, 30.1, 30.0, 22.3, 16.2; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{34}H_{36}IN_2O_2S^+$ 663.1537; Found 663.1538.



3j

(*R*)-2-(4-(*tert*-Butyl)phenyl)-2-((*S*)-2-(4-(*tert*-butyl)phenyl)-1-(methylthio)-2-oxoethyl)-6-iodoimidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3j)

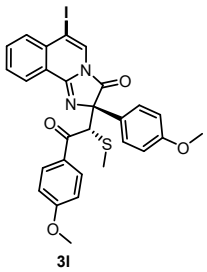
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (50:1 v/v) as eluent afforded **3j** (158.9 mg, yield 48%) as yellow solid (Rf = 0.30); m.p. 200-202 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, J = 6.8 Hz, 1H), 7.94–7.88 (m, 4H), 7.80 (s, 1H), 7.59 (d, J = 2.8 Hz, 2H), 7.45–7.37 (m, 5H), 5.03 (s, 1H), 1.95 (s, 3H), 1.30 (d, J = 6.8 Hz, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.4, 177.5, 157.1, 154.8, 151.3, 134.6, 133.4, 132.8, 131.6, 128.9, 128.5, 127.3, 127.2, 125.7, 125.5, 125.1, 123.4, 77.6, 75.9, 58.3, 35.1, 34.5, 31.2, 31.0, 16.0; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{34}H_{36}IN_2O_2S^+$ 663.1537; Found 663.1537.



3k

(*R*)-2-(4-Cyclohexylphenyl)-2-((*S*)-2-(4-cyclohexylphenyl)-1-(methylthio)-2-oxoethyl)-6-iodoimidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3k)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (30:1 v/v) as eluent afforded **3k** (224.9 mg, yield 63%) as yellow solid (Rf = 0.28); m.p. 183-185 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, J = 8.0 Hz, 1H), 7.92–7.84 (m, 4H), 7.78 (s, 1H), 7.56–7.50 (m, 2H), 7.38–7.32 (m, 1H), 7.25–7.18 (m, 4H), 5.01 (s, 1H), 2.56–2.42 (m, 2H), 1.93 (s, 3H), 1.81 (s, 8H), 1.75–1.68 (m, 2H), 1.42–1.29 (m, 8H), 1.27–1.18 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.4, 177.5, 154.6, 154.0, 148.1, 134.4, 133.3, 133.14, 133.12, 131.5, 128.8, 128.7, 127.5, 127.1, 127.0, 126.6, 125.5, 123.4, 77.5, 75.8, 58.4, 44.5, 44.0, 34.23, 34.21, 33.90, 33.88, 26.7, 26.6, 26.0, 25.9, 16.0; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{38}H_{40}IN_2O_2S^+$ 715.1850; Found 715.1847.

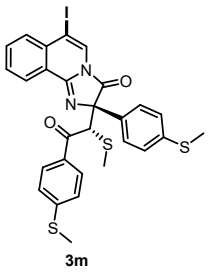


3l

(*R*)-6-Iodo-2-(4-methoxyphenyl)-2-((*S*)-2-(4-methoxyphenyl)-1-(methylthio)-2-oxoethyl)imidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3l)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded **3l** (137.3 mg, yield 45%) as yellow solid (Rf = 0.30); m.p. 144-146 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.08 (d, J = 7.6 Hz, 1H), 8.00 (d, J = 8.0 Hz, 2H), 7.84 (s, 3H), 7.70 (t, J = 7.2 Hz, 1H), 7.58 (d, J = 8.0 Hz, 1H), 7.48 (t, J = 7.2 Hz, 1H), 6.98 (t, J = 6.8 Hz, 4H), 5.21 (s, 1H), 3.81 (s, 3H), 3.74 (s, 3H), 1.83 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 192.0, 177.0, 163.6, 159.1, 153.9, 134.2, 134.1, 131.4, 131.2, 129.5, 129.0, 127.5, 127.4, 126.9, 125.0, 122.6, 114.0,

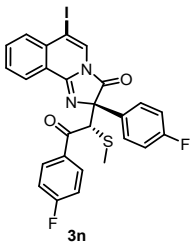
113.4, 78.1, 75.0, 58.1, 55.6, 55.1, 16.0; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{28}H_{24}IN_2O_4S^+$ 611.0496; Found 611.0494.



3m

(*R*)-6-Iodo-2-((*S*)-1-(methylthio)-2-(4-(methylthio)phenyl)-2-oxoethyl)-2-(4-(methylthio)phenyl)imidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3m)

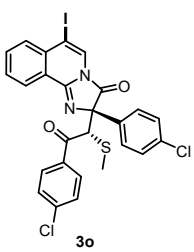
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (10:1 v/v) as eluent afforded **3m** (205.4 mg, yield 64%) as yellow solid (Rf = 0.28); m.p. 148-150 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, J = 8.0 Hz, 1H), 7.90 (d, J = 8.4 Hz, 2H), 7.85 (d, J = 8.4 Hz, 2H), 7.79 (s, 1H), 7.58 (d, J = 4.0 Hz, 2H), 7.44–7.37 (m, 1H), 7.25–7.16 (m, 4H), 4.95 (s, 1H), 2.45 (s, 3H), 2.44 (s, 3H), 1.95 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.7, 177.3, 154.9, 146.5, 139.0, 134.5, 133.5, 132.4, 131.6, 131.3, 129.0, 128.9, 127.9, 127.0, 125.8, 125.6, 124.7, 123.2, 77.9, 75.6, 58.2, 16.0, 15.4, 14.6; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{28}H_{24}IN_2O_2S_3^+$ 643.0039; Found 643.0040.



3n

(*R*)-2-(4-Fluorophenyl)-2-((*S*)-2-(4-fluorophenyl)-1-(methylthio)-2-oxoethyl)-6-iodoimidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3n)

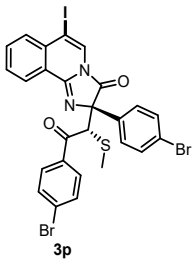
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (20:1 v/v) as eluent afforded **3n** (164.1 mg, yield 56%) as yellow solid (Rf = 0.3); m.p. 146-148 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, J = 8.0 Hz, 1H), 8.02–7.94 (m, 4H), 7.80 (s, 1H), 7.62 (d, J = 3.6 Hz, 2H), 7.48–7.41 (m, 1H), 7.12–7.02 (m, 4H), 4.89 (s, 1H), 1.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.3, 177.3, 167.1, 164.6, 163.9, 161.5, 155.2, 134.6, 133.7, 131.74, 131.70, 131.67, 131.6, 131.5, 131.3, 131.2, 129.44, 129.36, 129.1, 127.0, 125.6, 123.2, 115.8, 115.6, 115.2, 115.0, 78.0, 75.3, 58.6, 16.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -104.03, -113.19; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{18}F_2IN_2O_2S^+$ 587.0096; Found 587.0098.



3o

(*R*)-2-(4-Chlorophenyl)-2-((*S*)-2-(4-chlorophenyl)-1-(methylthio)-2-oxoethyl)-6-iodoimidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3o)

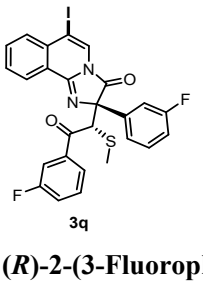
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (20:1 v/v) as eluent afforded **3o** (194.7 mg, yield 63%) as yellow solid (Rf = 0.3); m.p. 158-160 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, J = 8.0 Hz, 1H), 7.94–7.85 (m, 4H), 7.79 (s, 1H), 7.63 (d, J = 4.0 Hz, 2H), 7.49–7.42 (m, 1H), 7.39 (d, J = 8.4 Hz, 2H), 7.33 (d, J = 8.4 Hz, 2H), 4.88 (s, 1H), 1.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.4, 177.1, 155.4, 139.9, 134.63, 134.55, 134.3, 133.8, 133.7, 131.8, 130.0, 129.2, 128.95, 128.91, 128.4, 126.9, 125.6, 123.1, 78.2, 75.4, 58.5, 16.0; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{18}Cl_2IN_2O_2S^+$ 618.9505; Found 618.9507.



3p

(*R*)-2-(4-Bromophenyl)-2-((*S*)-2-(4-bromophenyl)-1-(methylthio)-2-oxoethyl)-6-iodoimidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3p)

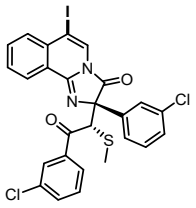
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (20:1 v/v) as eluent afforded **3p** (229.5 mg, yield 65%) as yellow solid (Rf = 0.3); m.p. 165-167 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, J = 7.6 Hz, 1H), 7.86 (d, J = 8.4 Hz, 2H), 7.80 (d, J = 8.8 Hz, 3H), 7.62 (s, 2H), 7.55 (d, J = 8.4 Hz, 2H), 7.51–7.42 (m, 3H), 4.87 (s, 1H), 1.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.6, 177.1, 155.4, 134.9, 134.6, 134.0, 133.8, 131.9, 131.8, 131.3, 130.0, 129.3, 129.2, 128.7, 126.9, 125.6, 123.1, 122.8, 78.2, 75.4, 58.4, 15.9; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{18}Br_2IN_2O_2S^+$ 706.8495; Found 706.8494.



3q

(*R*)-2-(3-Fluorophenyl)-2-((*S*)-2-(3-fluorophenyl)-1-(methylthio)-2-oxoethyl)-6-iodoimidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3q)

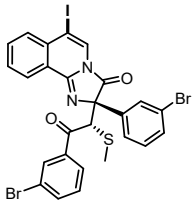
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (20:1 v/v) as eluent afforded **3q** (167.0 mg, yield 57%) as yellow solid (Rf = 0.3); m.p. 145-147 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, J = 7.6 Hz, 1H), 7.78 (d, J = 11.6 Hz, 2H), 7.75–7.68 (m, 2H), 7.62 (d, J = 8.8 Hz, 3H), 7.48–7.31 (m, 3H), 7.27–7.22 (m, 1H), 7.05–6.97 (m, 1H), 4.89 (s, 1H), 1.97 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.4, 191.3, 177.0, 163.9, 163.8, 161.4, 161.3, 155.5, 138.3, 138.2, 137.6, 137.5, 134.6, 133.8, 131.8, 130.3, 130.2, 129.7, 129.6, 129.2, 127.0, 125.7, 124.20, 124.17, 123.14, 123.11, 120.6, 120.4, 115.5, 115.34, 115.30, 115.0, 114.8, 78.2, 75.5, 58.6, 16.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -111.41, -111.98; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{18}F_2IN_2O_2S^+$ 587.0096; Found 587.0098.



3r

(*R*)-2-(3-Chlorophenyl)-2-((*S*)-2-(3-chlorophenyl)-1-(methylthio)-2-oxoethyl)-6-iodoimidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3r)

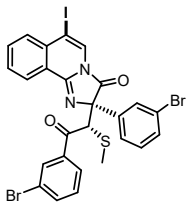
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (20:1 v/v) as eluent afforded **3r** (191.6 mg, yield 62%) as yellow solid (Rf = 0.3); m.p. 176-178 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, J = 6.4 Hz, 1H), 7.94 (d, J = 24.0 Hz, 3H), 7.78 (s, 2H), 7.60 (s, 2H), 7.46 (d, J = 19.6 Hz, 2H), 7.40–7.24 (m, 3H), 4.88 (s, 1H), 1.97 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.3, 176.9, 155.5, 137.7, 136.9, 134.8, 134.5, 134.3, 133.8, 133.3, 131.7, 129.9, 129.4, 129.2, 128.7, 128.6, 127.8, 126.8, 126.5, 125.7, 123.0, 78.2, 75.3, 58.6, 16.0; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{18}Cl_2IN_2O_2S^+$ 618.9505; Found 618.9504.



3s

(*R*)-2-(3-Bromophenyl)-2-((*S*)-2-(3-bromophenyl)-1-(methylthio)-2-oxoethyl)-6-iodoimidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3s)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (20:1 v/v) as eluent afforded **3s** (215.3 mg, yield 61%) as yellow solid (Rf = 0.3); m.p. 179-181 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, J = 7.6 Hz, 1H), 8.09 (d, J = 21.2 Hz, 2H), 7.96 (d, J = 8.0 Hz, 1H), 7.84 (d, J = 7.6 Hz, 1H), 7.77 (s, 1H), 7.67–7.57 (m, 3H), 7.47–7.39 (m, 2H), 7.32–7.21 (m, 2H), 4.86 (s, 1H), 1.97 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.2, 176.8, 155.5, 137.9, 137.1, 136.2, 134.5, 133.8, 131.7, 131.6, 131.5, 130.6, 130.1, 129.6, 129.1, 127.0, 126.8, 126.2, 125.7, 123.0, 122.8, 122.4, 78.2, 75.2, 58.7, 16.0; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{18}Br_2IN_2O_2S^+$ 706.8495; Found 706.8493.

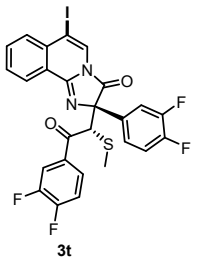


3s'

(*S*)-2-(3-Bromophenyl)-2-((*S*)-2-(3-bromophenyl)-1-(methylthio)-2-oxoethyl)-6-iodoimidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3s')

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (30:1 v/v) as eluent afforded **3s'** (63.5 mg, yield 18%) as yellow solid (Rf = 0.3); m.p. 168-170 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (d, J = 7.6 Hz, 1H), 8.08 (s, 2H), 7.89 (t, J = 6.8 Hz, 2H), 7.65–7.59 (m,

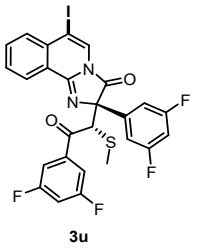
4H), 7.54–7.46 (m , 2H), 7.28–7.24 (m, 2H), 4.84 (s, 1H), 2.14 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.1, 178.6, 155.0, 139.7, 136.8, 136.3, 134.3, 133.6, 131.8, 131.7, 131.4, 130.2, 130.0, 129.8, 129.3, 127.0, 126.8, 125.6, 125.5, 123.6, 122.7, 122.5, 78.4, 58.3, 15.4; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{18}Br_2IN_2O_2S^+$ 706.8495; Found 706.8497.



3t

(*R*)-2-(3,4-Difluorophenyl)-2-((*S*)-2-(3,4-difluorophenyl)-1-(methylthio)-2-oxoethyl)-6-iodoimidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3t)

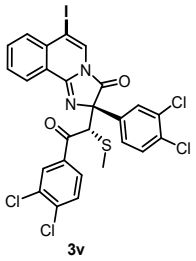
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (30:1 v/v) as eluent afforded **3t** (186.6 mg, yield 60%) as yellow solid (Rf = 0.28); m.p. 156-158 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (s, 1H), 7.97–7.59 (m, 7H), 7.48 (s, 1H), 7.29–7.09 (m, 2H), 4.80 (s, 1H), 2.00 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.1, 176.8, 155.7, 155.1, 155.0, 152.6, 152.4, 151.6, 151.5, 151.4, 151.2, 151.0, 149.2, 149.0, 148.9, 148.7, 148.6, 134.6, 134.0, 132.5, 132.2, 131.9, 129.3, 126.8, 125.7, 123.8, 122.9, 118.2, 118.0, 117.6, 117.4, 117.2, 117.0, 116.9, 116.8, 78.4, 74.7, 58.5, 15.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -128.34, -128.40, -135.45, -135.51, -136.48, -136.53, -137.33, -137.39; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{16}F_4IN_2O_2S^+$ 622.9908; Found 622.9907.



3u

(*R*)-2-(3,5-Difluorophenyl)-2-((*S*)-2-(3,5-difluorophenyl)-1-(methylthio)-2-oxoethyl)-6-iodoimidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3u)

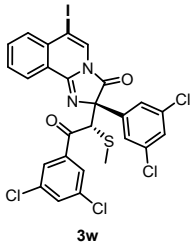
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (50:1 v/v) as eluent afforded **3u** (177.3 mg, yield 57%) as yellow solid (Rf = 0.2); m.p. 149-151 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, J = 8.0 Hz, 1H), 7.79 (s, 1H), 7.71–7.65 (m, 2H), 7.56–7.45 (m, 5H), 7.06–6.98 (m, 1H), 6.82–6.74 (m, 1H), 4.76 (s, 1H), 2.01 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.9, 176.5, 164.2, 164.1, 163.9, 163.8, 161.7, 161.6, 161.5, 161.3, 156.0, 139.4, 138.3, 138.2, 138.1, 134.7, 134.1, 131.9, 129.4, 126.8, 125.8, 122.9, 111.8, 111.7, 111.6, 111.5, 111.0, 110.9, 110.8, 110.7, 109.1, 108.9, 108.6, 104.4, 104.1, 103.9, 78.5, 75.0, 58.6, 15.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ -107.56, -108.62; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{16}F_4IN_2O_2S^+$ 622.9908; Found 622.9907.



3v

(*R*)-2-(3,4-Dichlorophenyl)-2-((*S*)-2-(3,4-dichlorophenyl)-1-(methylthio)-2-oxoethyl)-6-iodoimidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3v)

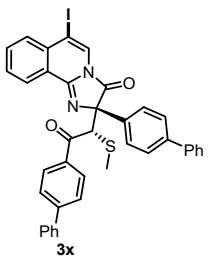
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (30:1 v/v) as eluent afforded **3v** (181.8 mg, yield 53%) as yellow solid (Rf = 0.3); m.p. 185-187 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, J = 7.6 Hz, 1H), 8.05 (s, 2H), 7.86 (d, J = 8.4 Hz, 1H), 7.77 (d, J = 10.0 Hz, 2H), 7.69–7.63 (m, 2H), 7.52–7.42 (m, 3H), 4.80 (s, 1H), 2.00 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.2, 176.7, 155.8, 138.1, 135.8, 134.62, 134.57, 133.9, 133.2, 132.8, 132.4, 131.8, 130.63, 130.61, 130.0, 129.6, 129.3, 127.6, 126.9, 126.7, 125.7, 122.8, 78.5, 74.7, 58.4, 15.8; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{16}Cl_4IN_2O_2S^+$ 686.8726; Found 686.8725.



3w

(*R*)-2-(3,5-Dichlorophenyl)-2-((*S*)-2-(3,5-dichlorophenyl)-1-(methylthio)-2-oxoethyl)-6-iodoimidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3w)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (50:1 v/v) as eluent afforded **3w** (185.2 mg, yield 54%) as yellow solid (Rf = 0.2); m.p. 180-182 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, J = 7.6 Hz, 1H), 7.88 (s, 2H), 7.80 (s, 3H), 7.71–7.64 (m, 2H), 7.56–7.47 (m, 2H), 7.33 (s, 1H), 4.73 (s, 1H), 2.02 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.9, 176.4, 156.0, 138.9, 137.6, 135.6, 134.9, 134.7, 134.1, 133.2, 131.9, 129.4, 128.8, 127.0, 126.7, 126.2, 125.9, 122.8, 78.6, 74.7, 58.7, 15.9; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{16}Cl_4IN_2O_2S^+$ 686.8726; Found 686.8726.

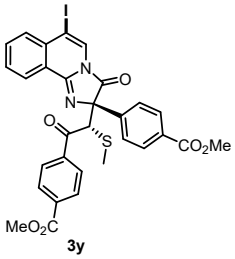


3x

(*R*)-2-([1,1'-Biphenyl]-4-yl)-2-((*S*)-2-([1,1'-biphenyl]-4-yl)-1-(methylthio)-2-oxoethyl)-6-iodoimidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3x)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (20:1 v/v) as eluent afforded **3x** (231.7 mg, yield 66%) as yellow solid (Rf = 0.3); m.p. 198-200 °C; ^{1}H NMR

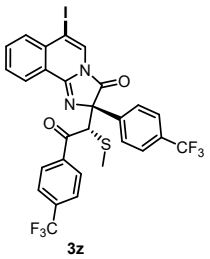
(400 MHz, $CDCl_3$) δ 8.31 (d, J = 7.6 Hz, 1H), 8.11 (d, J = 7.6 Hz, 2H), 8.03 (d, J = 7.6 Hz, 2H), 7.80 (s, 1H), 7.64–7.51 (m, 10H), 7.40–7.27 (m, 7H), 5.13 (s, 1H), 2.01 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.2, 177.4, 155.0, 145.9, 141.0, 140.2, 139.4, 134.9, 134.4, 134.0, 133.4, 131.5, 129.1, 128.9, 128.8, 128.6, 128.2, 128.0, 127.3, 127.10, 127.06, 126.9, 126.8, 125.5, 123.2, 77.9, 75.9, 58.4, 16.0; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{38}H_{28}IN_2O_2S^+$ 703.0911; Found 703.0910.



3y

Methyl 4-((*R*)-6-iodo-2-((*S*)-2-(4-(methoxycarbonyl)phenyl)-1-(methylthio)-2-oxoethyl)-3-oxo-2,3-dihydroimidazo[2,1-*a*]isoquinolin-2-yl)benzoate (3y)

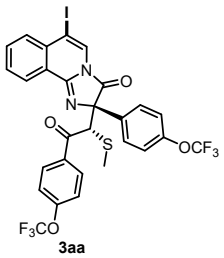
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (8:1 v/v) as eluent afforded **3y** (209.8 mg, yield 63%) as yellow solid (Rf = 0.3); m.p. 169-171 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, J = 8.0 Hz, 1H), 8.10–8.02 (m, 6H), 7.99 (d, J = 8.4 Hz, 2H), 7.80 (s, 1H), 7.66–7.60 (m, 2H), 7.49–7.42 (m, 1H), 5.00 (s, 1H), 3.92 (s, 3H), 3.90 (s, 3H), 1.95 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.9, 176.8, 166.5, 165.9, 155.5, 140.7, 138.8, 134.5, 134.0, 133.8, 131.7, 130.0, 129.7, 129.4, 129.2, 128.4, 127.5, 126.8, 125.6, 123.0, 78.3, 75.8, 58.7, 52.4, 52.1, 16.1; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{30}H_{24}IN_2O_6S^+$ 667.0394; Found 667.0396.



3z

(*R*)-6-Iodo-2-((*S*)-1-(methylthio)-2-oxo-2-(4-(trifluoromethyl)phenyl)ethyl)-2-(4-(trifluoromethyl)phenyl)imidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3z)

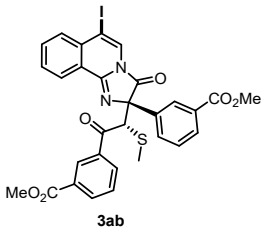
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (8:1 v/v) as eluent afforded **3z** (205.8 mg, yield 60%) as yellow solid (Rf = 0.3); m.p. 150-152 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, J = 6.8 Hz, 1H), 8.14 (d, J = 7.6 Hz, 2H), 8.06 (d, J = 7.6 Hz, 2H), 7.81 (s, 1H), 7.72–7.61 (m, 6H), 7.49 (s, 1H), 4.98 (s, 1H), 1.99 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.4, 176.9, 155.8, 139.7, 138.2, 134.9, 134.7, 134.5, 134.0, 131.9, 130.8, 130.5, 129.3, 128.9, 128.0, 126.8, 125.70, 125.67, 125.2, 125.14, 125.11, 124.8, 123.0, 122.5, 122.0, 78.5, 75.6, 58.6, 15.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.63, -63.17; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{28}H_{18}F_6IN_2O_2S^+$ 687.0032; Found 687.0029.



3aa

(*R*)-6-Iodo-2-((*S*)-1-(methylthio)-2-oxo-2-(4-(trifluoromethoxy)phenyl)ethyl)-2-(4-(trifluoromethoxy)phenyl)imidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3aa)

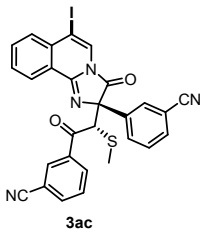
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (50:1 v/v) as eluent afforded **3aa** (211.8 mg, yield 59%) as yellow solid (Rf = 0.3); m.p. 139-141 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, J = 7.6 Hz, 1H), 8.08–7.97 (m, 4H), 7.80 (s, 1H), 7.65 (d, J = 3.2 Hz, 2H), 7.50–7.43 (m, 1H), 7.28–7.19 (m, 4H), 4.90 (s, 1H), 1.98 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.2, 177.2, 155.5, 152.8, 149.3, 134.7, 134.4, 133.8, 133.5, 131.8, 130.7, 129.2, 127.0, 125.6, 124.2, 124.1, 123.1, 121.6, 121.5, 120.5, 120.3, 119.1, 118.9, 116.5, 116.3, 78.2, 75.3, 58.6, 15.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.57, -57.79; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{28}H_{18}F_6IN_2O_4S^+$ 718.9931; Found 718.9932.



3ab

Methyl 3-((*R*)-6-iodo-2-((*S*)-2-(3-(methoxycarbonyl)phenyl)-1-(methylthio)-2-oxoethyl)-3-oxo-2,3-dihydroimidazo[2,1-*a*]isoquinolin-2-yl)benzoate (3ab)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded **3ab** (186.5 mg, yield 56%) as yellow solid (Rf = 0.3); m.p.133-135 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 (d, J = 10.8 Hz, 2H), 8.40–7.98 (m, 5H), 7.83 (s, 1H), 7.64 (s, 2H), 7.57–7.40 (m, 3H), 5.01 (s, 1H), 3.93 (s, 6H), 1.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.9, 177.1, 166.8, 166.0, 155.5, 136.3, 135.5, 134.7, 134.2, 133.8, 132.8, 132.1, 131.8, 130.6, 130.3, 129.7, 129.6, 129.2, 128.9, 128.8, 128.3, 127.0, 125.9, 123.1, 78.2, 75.5, 58.9, 52.4, 52.2, 16.1; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{30}H_{24}IN_2O_6S^+$ 667.0394; Found 667.0395.

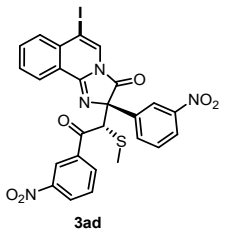


3ac

3-((*R*)-2-((*S*)-2-(3-Cyanophenyl)-1-(methylthio)-2-oxoethyl)-6-iodo-3-oxo-2,3-dihydroimidazo[2,1-*a*]isoquinolin-2-yl)benzonitrile (3ac)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (8:1 v/v) as eluent afforded **3ac** (192.0 mg, yield 64%) as yellow solid (Rf = 0.3); m.p. 175-177 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (s, 4H), 8.16 (d, J = 6.4 Hz, 1H), 7.88–7.76 (m, 2H), 7.73–7.57 (m, 4H),

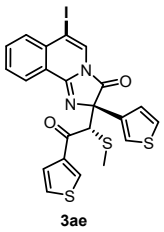
7.51 (s, 2H), 4.86 (s, 1H), 2.01 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.5, 176.5, 156.1, 137.2, 136.3, 135.9, 134.6, 134.1, 132.5, 132.4, 132.1, 132.0, 131.9, 131.5, 129.6, 129.4, 128.9, 126.6, 125.7, 122.7, 118.5, 117.6, 113.1, 112.4, 78.6, 74.8, 58.8, 15.8; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{28}H_{18}IN_4O_2S^+$ 601.0190; Found 601.0190.



3ad

(*R*)-6-Iodo-2-((*S*)-1-(methylthio)-2-(3-nitrophenyl)-2-oxoethyl)-2-(3-nitrophenyl)imidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3ad)

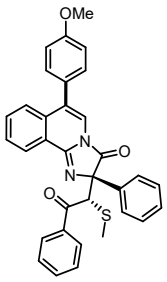
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded **3ad** (185.6 mg, yield 58%) as yellow solid (Rf = 0.28); m.p. 201-203 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.89 (s, 1H), 8.83 (s, 1H), 8.45–8.35 (m, 3H), 8.28–8.18 (m, 2H), 7.82 (s, 1H), 7.73–7.62 (m, 3H), 7.62–7.50 (m, 2H), 4.92 (s, 1H), 2.04 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.4, 176.6, 156.3, 148.3, 148.1, 137.8, 136.3, 134.7, 134.3, 133.7, 132.0, 129.9, 129.5, 129.1, 127.8, 126.7, 125.9, 123.8, 123.6, 123.0, 122.8, 78.8, 74.8, 59.1, 15.8; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{18}IN_4O_6S^+$ 640.9986; Found 640.9984.



3ae

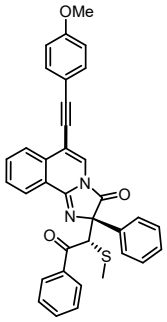
(*R*)-6-Iodo-2-((*S*)-1-(methylthio)-2-oxo-2-(thiophen-3-yl)ethyl)-2-(thiophen-3-yl)imidazo[2,1-*a*]isoquinolin-3(2*H*)-one (3ae)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (10:1 v/v) as eluent afforded **3ae** (140.5 mg, yield 50%) as yellow solid (Rf = 0.32); m.p. 167-169 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, J = 8.0 Hz, 1H), 8.19 (d, J = 1.6 Hz, 1H), 7.79 (s, 1H), 7.69 (d, J = 2.0 Hz, 1H), 7.61 (d, J = 4.0 Hz, 2H), 7.56 (d, J = 4.8 Hz, 1H), 7.49 (d, J = 5.2 Hz, 1H), 7.46–7.39 (m, 1H), 7.33–7.24 (m, 2H), 4.74 (s, 1H), 2.01 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.2, 177.1, 155.3, 139.8, 135.8, 134.6, 133.6, 133.3, 131.7, 129.0, 127.4, 127.1, 126.9, 126.2, 125.6, 125.5, 123.9, 123.3, 77.9, 74.7, 60.1, 16.2; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{22}H_{16}IN_2O_2S_3^+$ 562.9413; Found 562.9415.



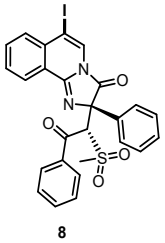
5

(*R*)-6-(4-Methoxyphenyl)-2-((*S*)-1-(methylthio)-2-oxo-2-phenylethyl)-2-phenylimidazo[2,1-*a*]isoquinolin-3(2*H*)-one (5): Yellow solid; 75.3 mg (yield 71%); m.p. 155-157 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (s, 1H), 8.07–7.92 (m, 4H), 7.57–7.48 (m, 2H), 7.46–7.35 (m, 7H), 7.34–7.30 (m, 2H), 7.29–7.23 (m, 1H), 6.99 (d, J = 8.4 Hz, 2H), 5.09 (s, 1H), 3.86 (s, 3H), 1.97 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.9, 179.3, 159.4, 155.9, 136.4, 135.8, 135.5, 135.2, 133.2, 132.7, 130.8, 130.2, 128.53, 128.50, 128.2, 128.0, 127.7, 127.5, 126.0, 123.5, 122.3, 118.5, 114.0, 76.3, 58.2, 55.3, 16.1; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{33}H_{27}N_2O_3S^+$ 531.1737; Found 531.1736.



7

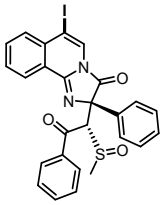
(*R*)-6-((4-Methoxyphenyl)ethynyl)-2-((*S*)-1-(methylthio)-2-oxo-2-phenylethyl)-2-phenylimidazo[2,1-*a*]isoquinolin-3(2*H*)-one (7): Yellow solid; 83.1 mg (yield 75%); m.p. 151-153 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (d, J = 7.2 Hz, 1H), 7.97 (t, J = 8.8 Hz, 5H), 7.71 (t, J = 6.8 Hz, 1H), 7.55 (s, 2H), 7.49 (d, J = 8.0 Hz, 3H), 7.44–7.35 (m, 5H), 6.89 (d, J = 6.8 Hz, 2H), 5.02 (s, 1H), 3.82 (s, 3H), 2.15 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.7, 180.0, 159.8, 154.6, 138.0, 135.4, 133.8, 133.4, 133.1, 132.9, 128.7, 128.5, 128.44, 128.40, 127.1, 126.2, 125.4, 123.6, 123.5, 114.8, 114.1, 105.3, 93.8, 81.9, 77.6, 58.5, 55.3, 15.5; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{35}H_{27}N_2O_3S^+$ 555.1737; Found 555.1731.



8

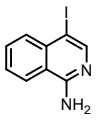
(*R*)-6-Iodo-2-((*S*)-1-(methylsulfonyl)-2-oxo-2-phenylethyl)-2-phenylimidazo[2,1-*a*]isoquinolin-3(2*H*)-one (8): Yellow solid; 161.3 mg (yield 84%); m.p. 225-227 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 (d, J = 7.6 Hz, 1H), 7.79–7.69 (m, 5H), 7.66–7.58 (m, 3H), 7.53 (t, J = 7.6 Hz, 1H), 7.37 (t, J = 7.6 Hz, 2H), 7.12–7.06 (m, 3H), 6.06 (s, 1H), 3.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.3, 177.4, 157.1, 137.6, 134.9, 134.3, 134.1, 133.9, 132.2, 129.6, 128.9, 128.6, 127.0,

126.7, 125.5, 123.0, 78.7, 74.0, 73.8, 41.8; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{20}IN_2O_4S^+$ 583.0183; Found 583.0179.



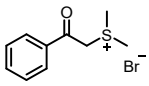
9

(*R*)-6-Iodo-2-((*S*)-1-((*S*)-methylsulfinyl)-2-oxo-2-phenylethyl)-2-phenylimidazo[2,1-*a*]isoquinolin-3(2*H*)-one (9): Yellow solid; 105.3 mg (yield 62%); m.p. 221-223 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, J = 6.8 Hz, 1H), 8.00 (d, J = 7.2 Hz, 2H), 7.82 (d, J = 8.0 Hz, 3H), 7.63–7.55 (m, 3H), 7.45 (s, 3H), 7.37–7.27 (m, 3H), 5.51 (s, 1H), 2.55 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.5, 177.5, 155.7, 136.7, 134.4, 134.3, 133.8, 131.8, 129.7, 129.2, 128.9, 128.7, 127.5, 126.8, 125.8, 123.0, 78.7, 77.5, 74.3, 38.0; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{20}IN_2O_3S^+$ 567.0234; Found 567.0231.



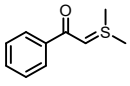
2aa

4-Iodoisoquinolin-1-amine (2aa): Yellow solid; 110.7 mg (yield 82%); m.p. 133-135 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (s, 1H), 7.91 (d, J = 8.4 Hz, 1H), 7.74–7.66 (m, 2H), 7.53 (t, J = 7.6 Hz, 1H), 5.44 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.4, 148.5, 137.4, 131.6, 131.3, 127.2, 123.0, 119.2, 82.7; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_9H_8IN_2^+$ 270.9727; Found 270.9723.



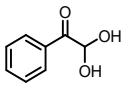
1ad

Dimethyl(2-oxo-2-phenylethyl)sulfoniumbromide (1ad): Colorless solid; 962.0 mg (yield 74%);^{1}H NMR (400 MHz, DMSO-d_6) δ 8.05 (d, J = 7.6 Hz, 2H), 7.79 (t, J = 7.6 Hz, 1H), 7.64 (t, J = 7.6 Hz, 2H), 5.70 (s, 2H), 3.06 (s, 6H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 191.4, 135.1, 133.9, 129.2, 128.7, 52.8, 24.5; The ^{1}H NMR and ^{13}C NMR spectra data are consistent with the reported literature.



1ae

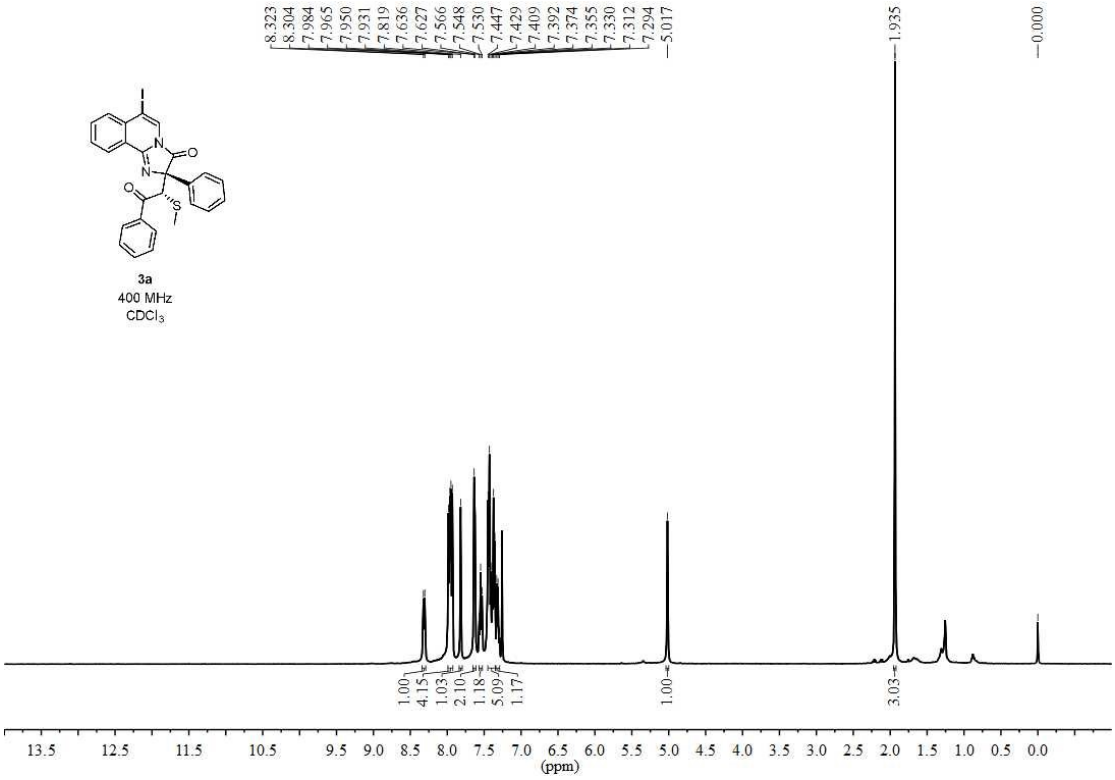
2-(Dimethyl-λ^4-sulfaneylidene)-1-phenylethan-1-one (1ae): Yellow solid; 120.6 mg (yield 67%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78–7.74 (m, 2H), 7.35–7.30 (m, 3H), 4.31 (s, 1H), 2.84 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 182.0, 140.5, 129.0, 127.4, 125.9, 52.3, 28.1; The ^{1}H NMR and ^{13}C NMR spectra data are consistent with the reported literature.

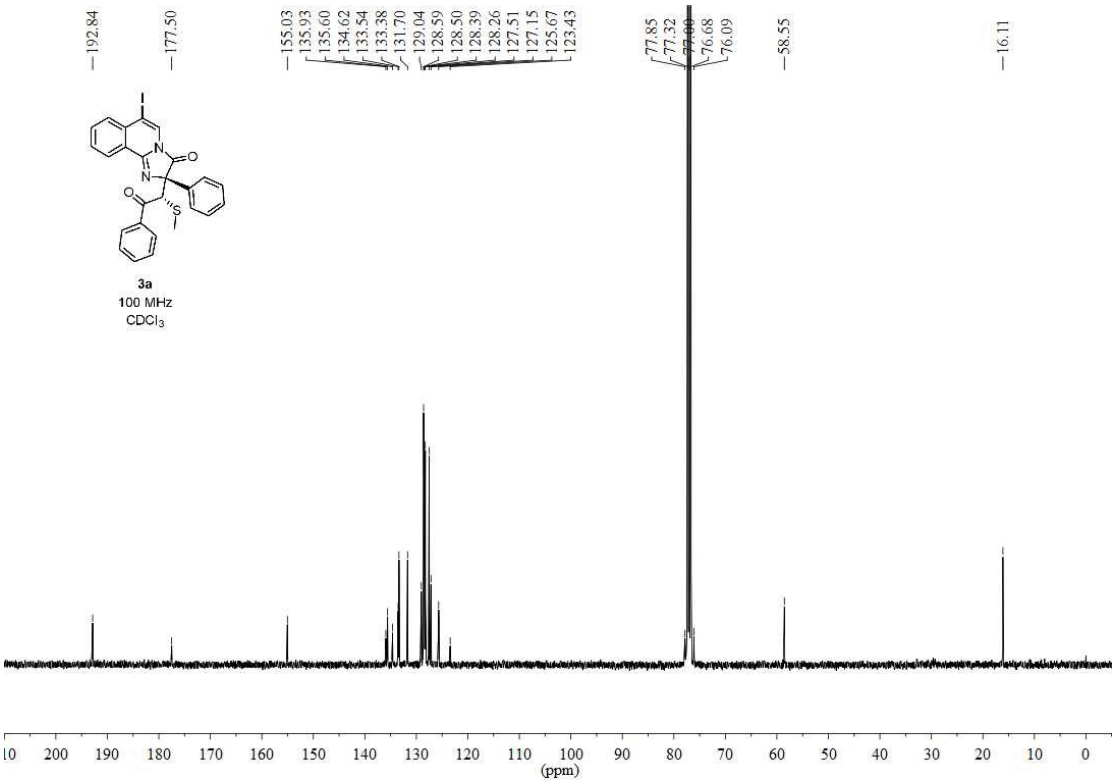


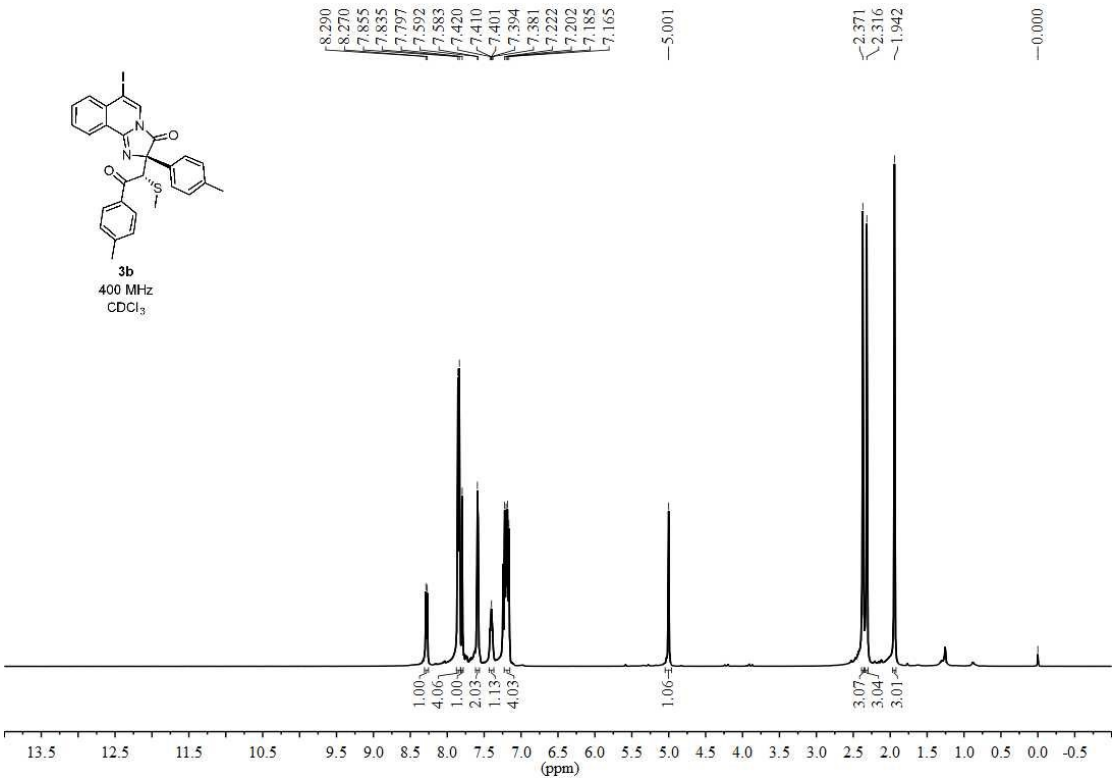
1ac

2,2-Dihydroxy-1-phenylethan-1-one (1ac): White solid; 52.4 mg (yield 69%); ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.12 (d, J = 7.6 Hz, 2H), 7.68–7.61 (m, 1H), 7.58–7.50 (m, 2H), 6.82 (d, J = 7.2 Hz, 2H), 5.76 (t, J = 7.2 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 196.3, 133.8, 133.4, 129.5, 128.6, 89.2; The ^{1}H NMR and ^{13}C NMR spectra data are consistent with the reported literature.

7. Copies of ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra



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7.401
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7.202
7.185
7.165
5.001
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2.316
1.942
0.000
3b
400 MHz
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1.00
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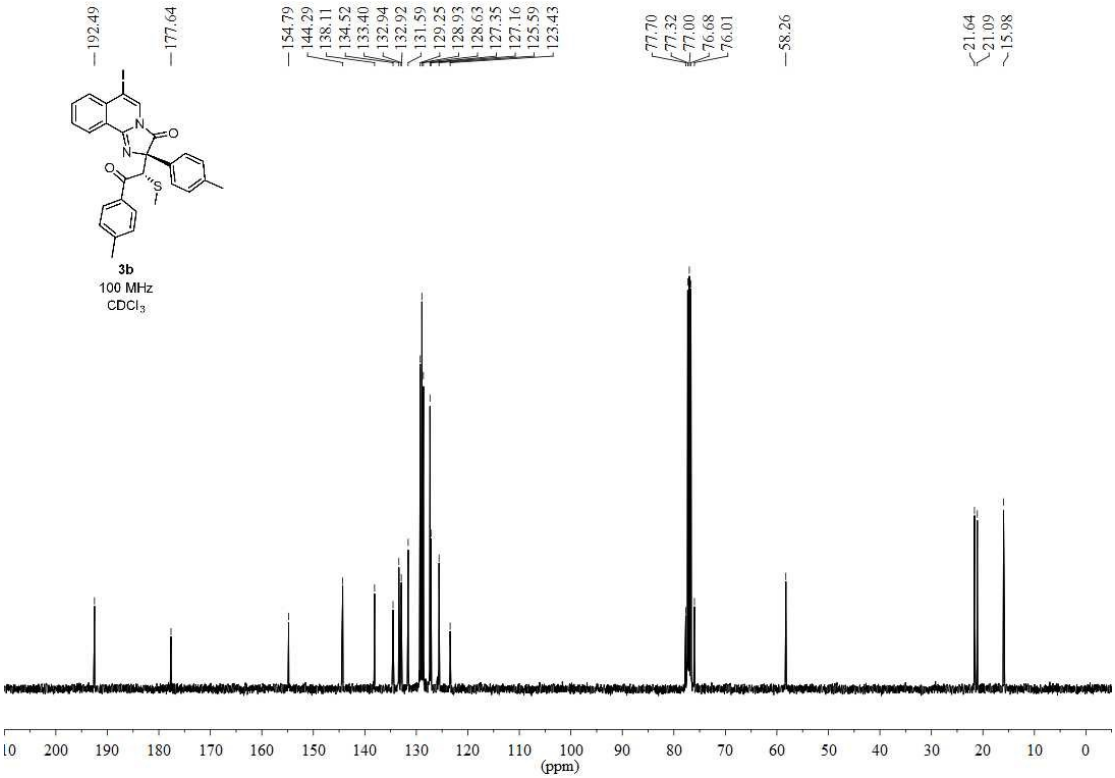
1.13
4.03
1.06
3.07
3.04
3.01
(ppm)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128.63
127.35
127.16
125.59
123.43
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76.01
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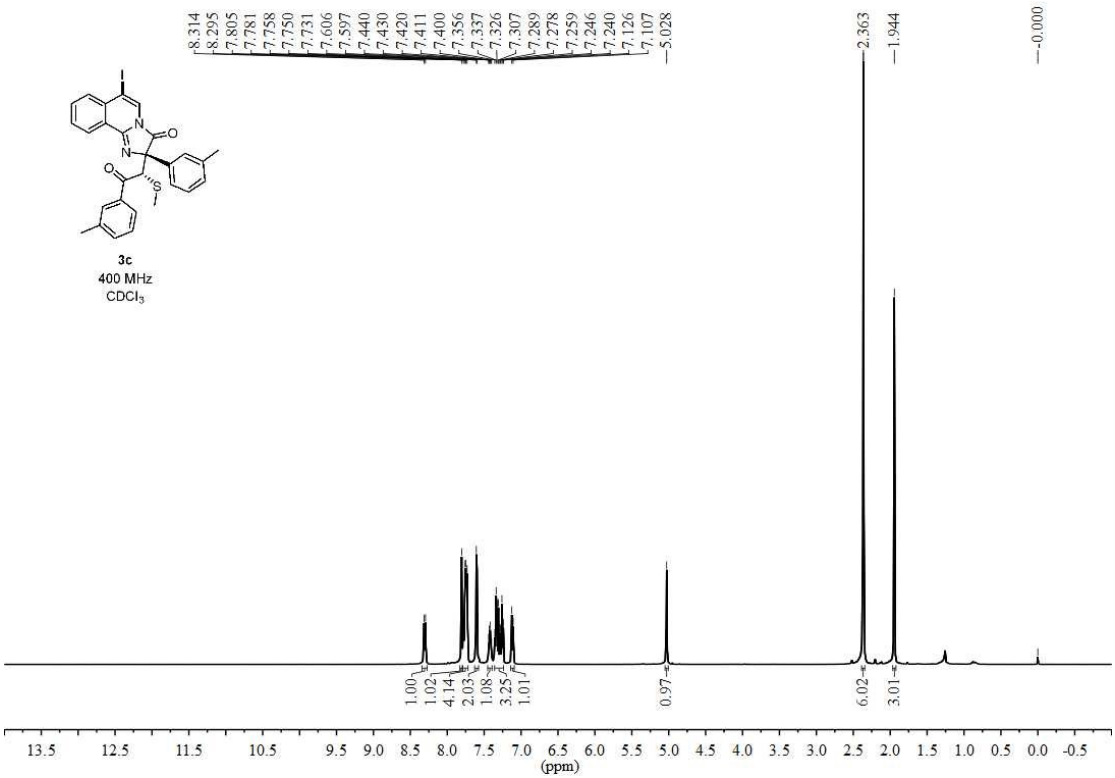
21.09
15.98
3b
100 MHz
CDCl3
(ppm)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7.400
7.356
7.337
7.326
7.307
7.289
7.278
7.259
7.246
7.240
7.126
7.107
5.028
2.363
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1.00
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4.14
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1.08
3.25
1.01
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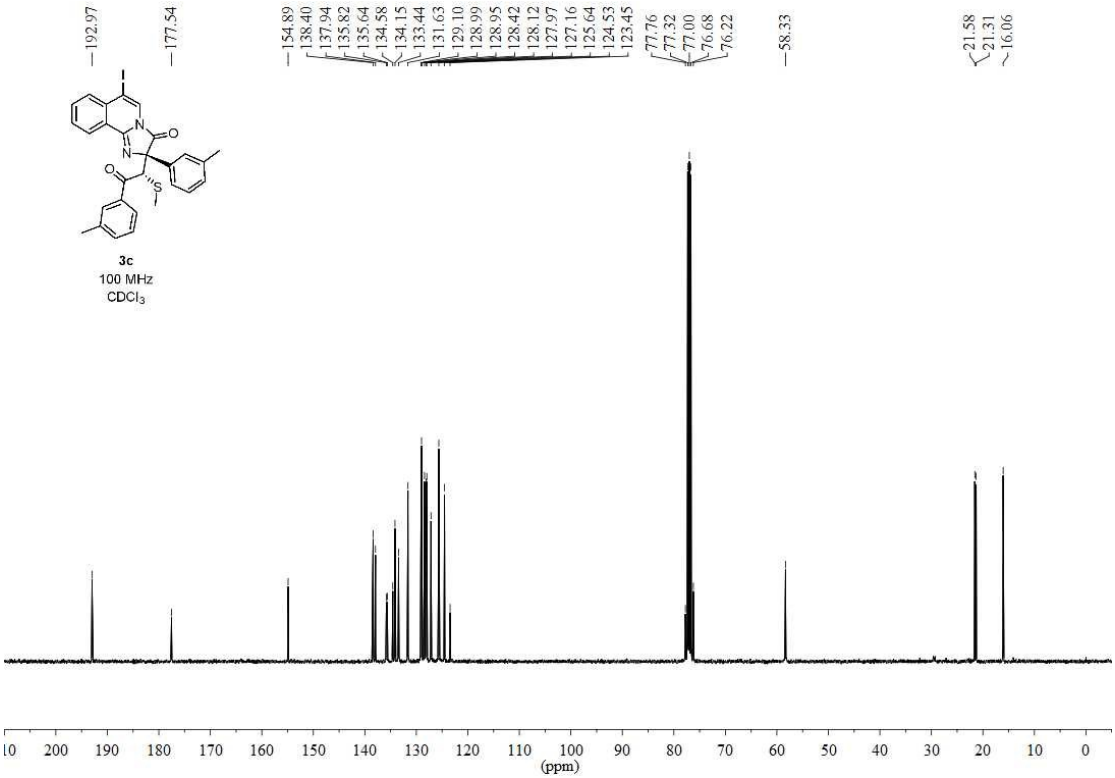
6.02
3.01
3c
400 MHz
CDCl3
(ppm)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131.63
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127.16
125.64
124.53
123.45
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76.22
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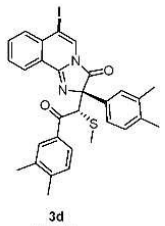
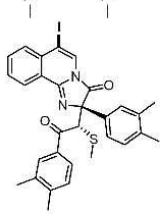
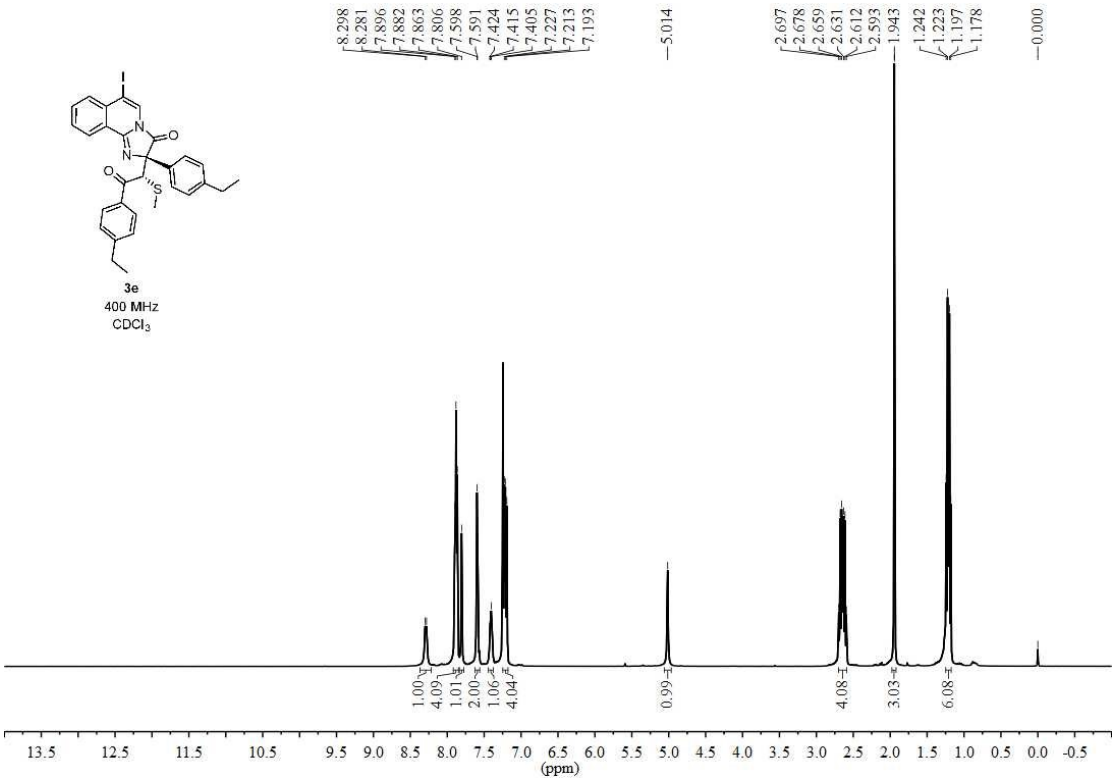
16.06
3c
100 MHz
CDCl3
(ppm)



3d
400 MHz
$CDCl_3$



3d
100 MHz
$CDCl_3$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7.193
5.014
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2.678
2.659
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2.612
2.593
1.943
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1.223
1.197
1.178
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1.06
4.04
0.99
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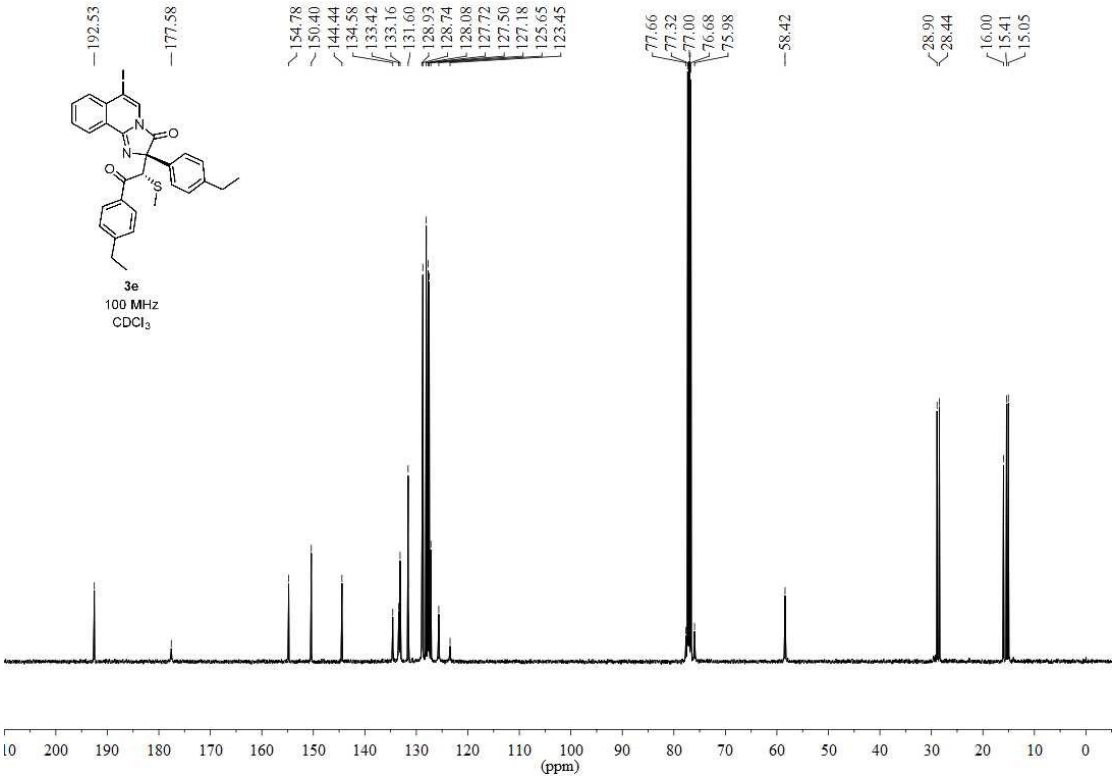
6.08
(ppm)
3e
400 MHz
CDCl3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127.50
127.18
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123.45
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77.32
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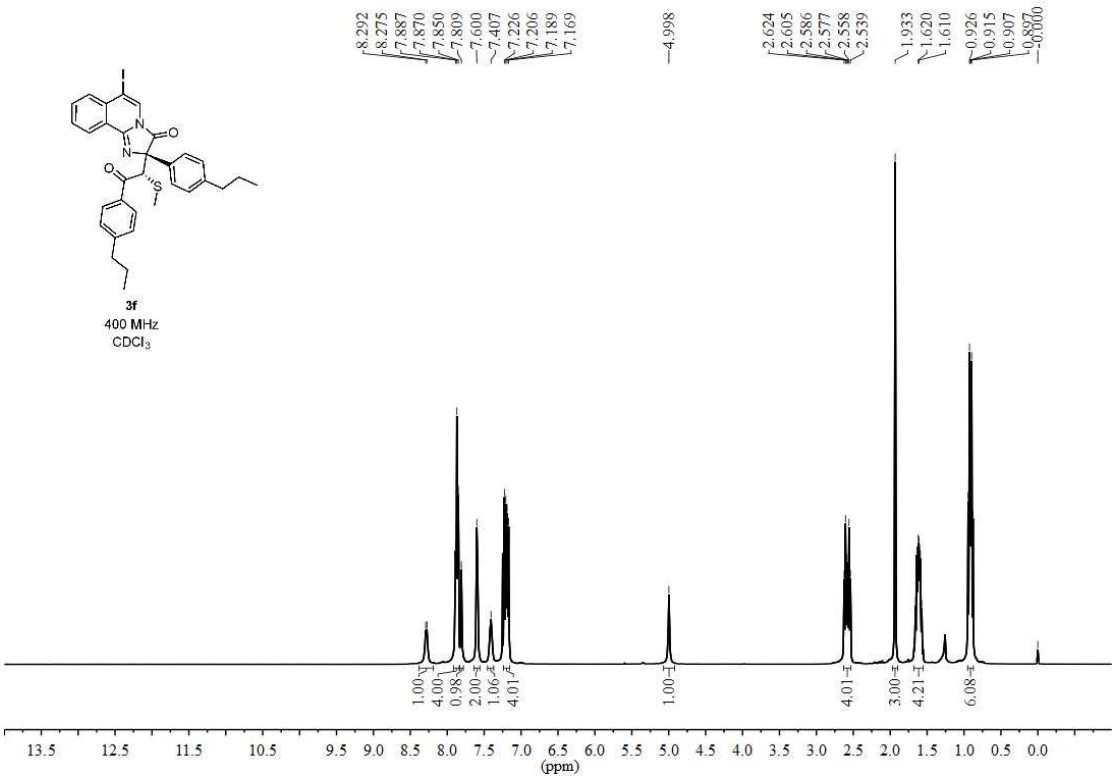
15.05
(ppm)
3e
100 MHz
CDCl3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7.206
7.189
7.169
4.998
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2.605
2.586
2.577
2.558
2.539
1.933
1.620
1.610
0.926
0.915
0.907
0.897
0.000
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4.01
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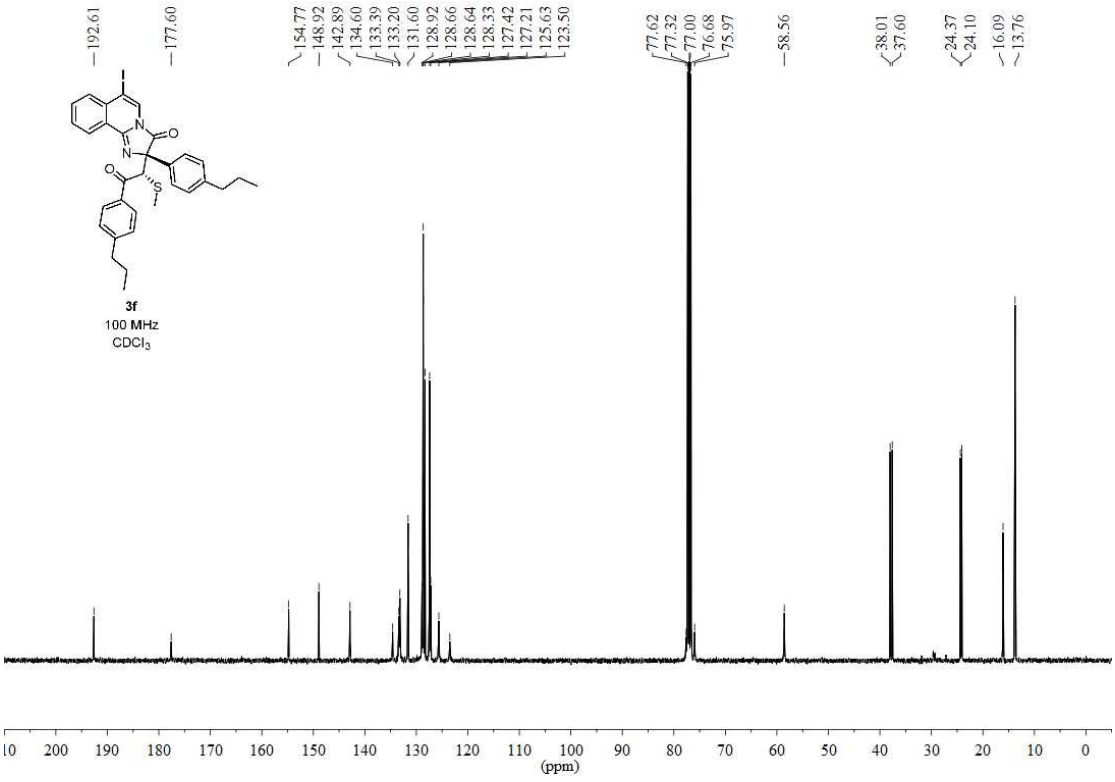
(ppm)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123.50
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16.09
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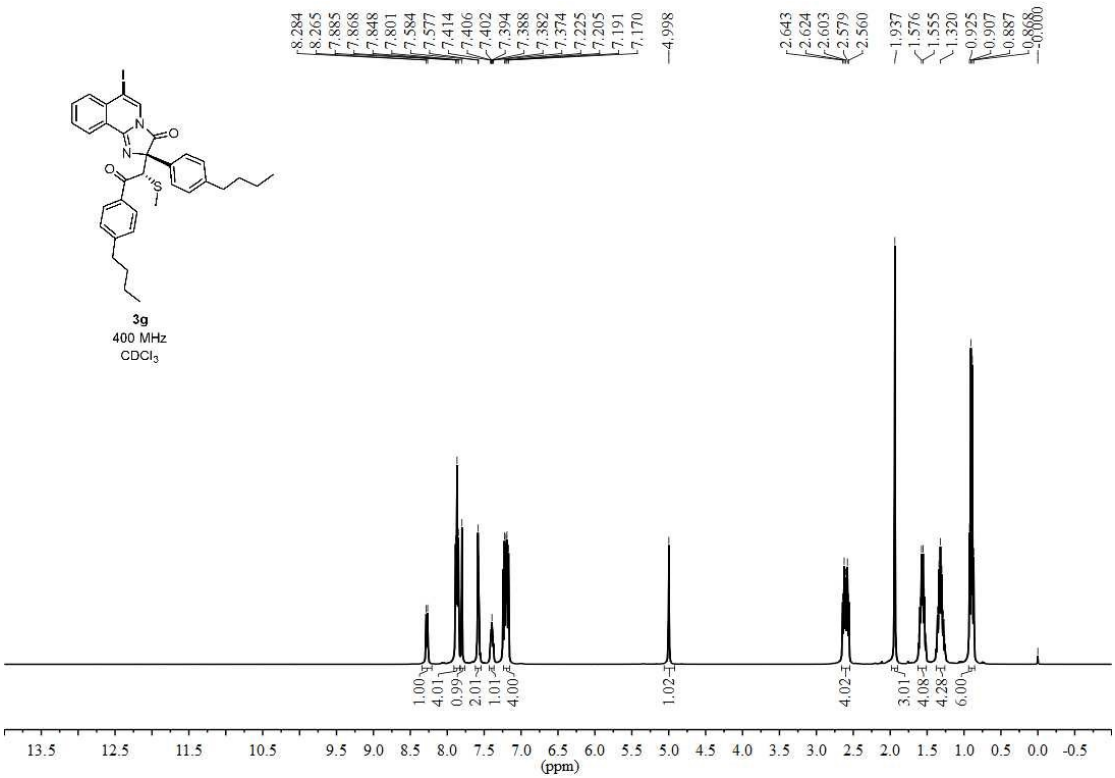
(ppm)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1.02
4.02
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4.28
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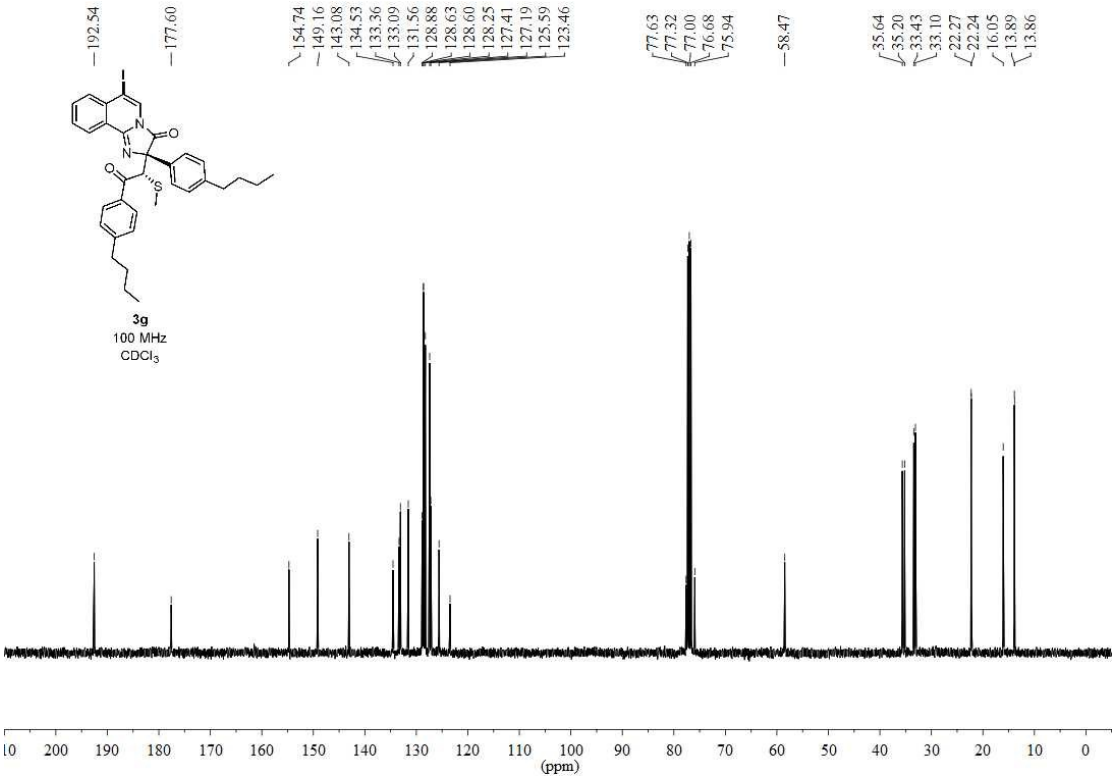
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33.10
22.27
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100 MHz
CDCl3
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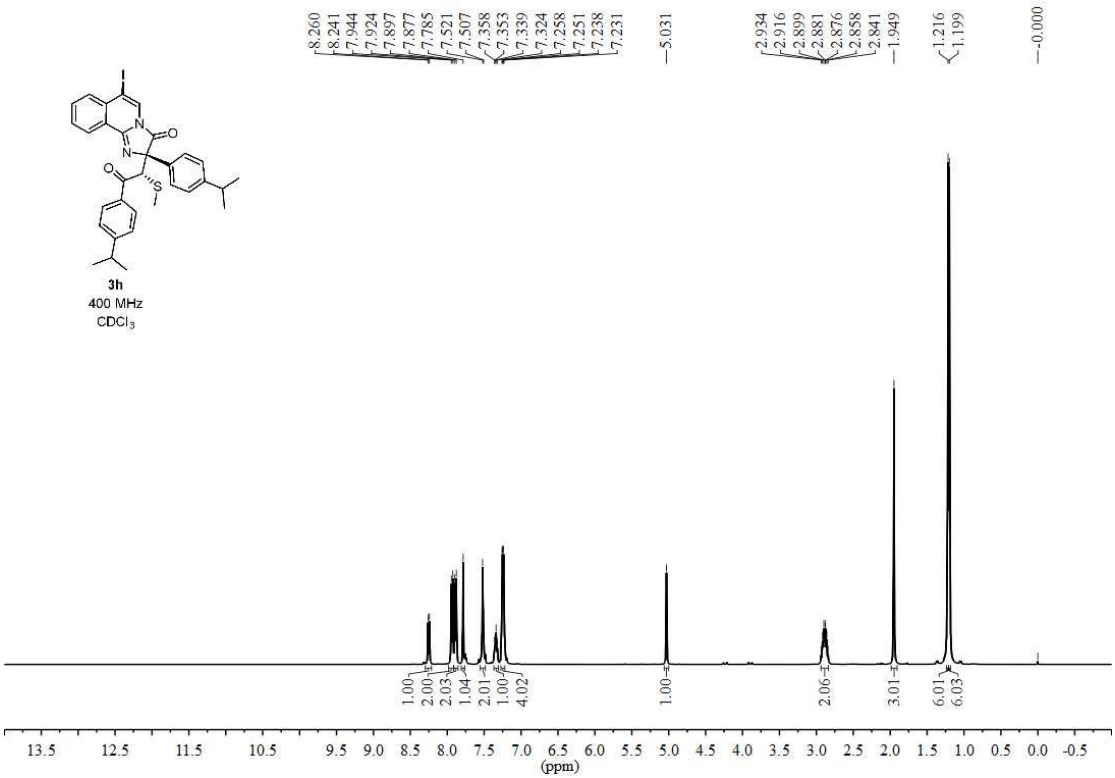
(ppm)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CDCl3
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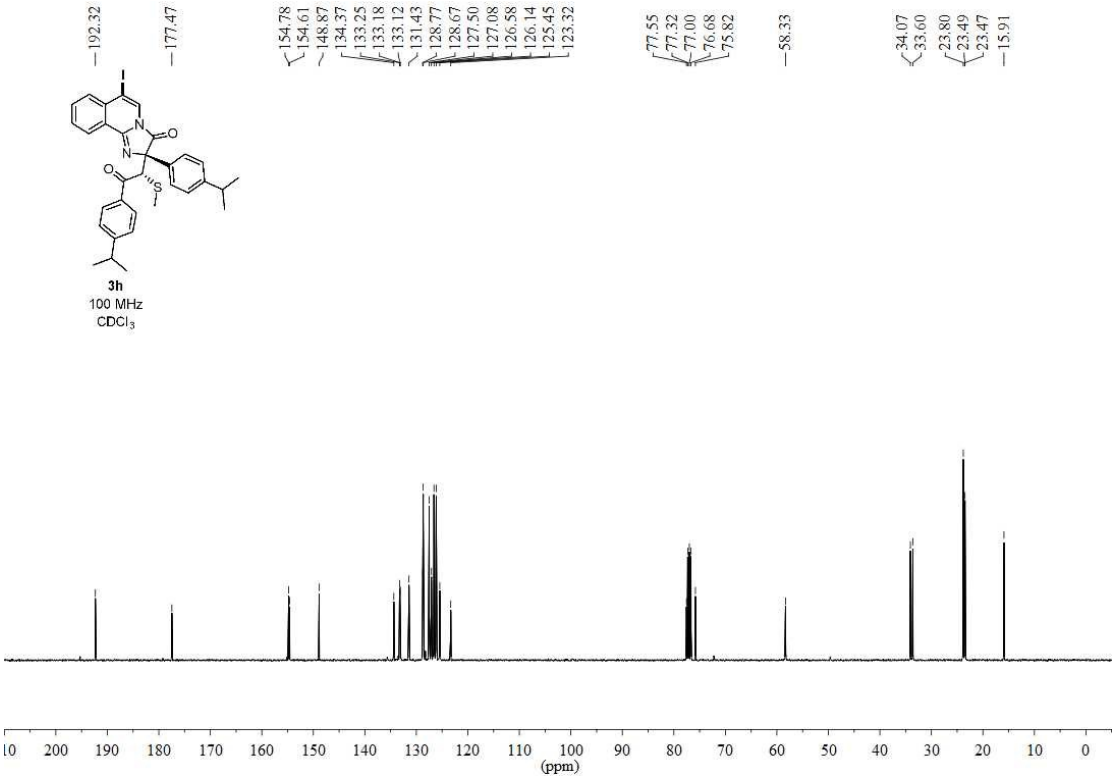
(ppm)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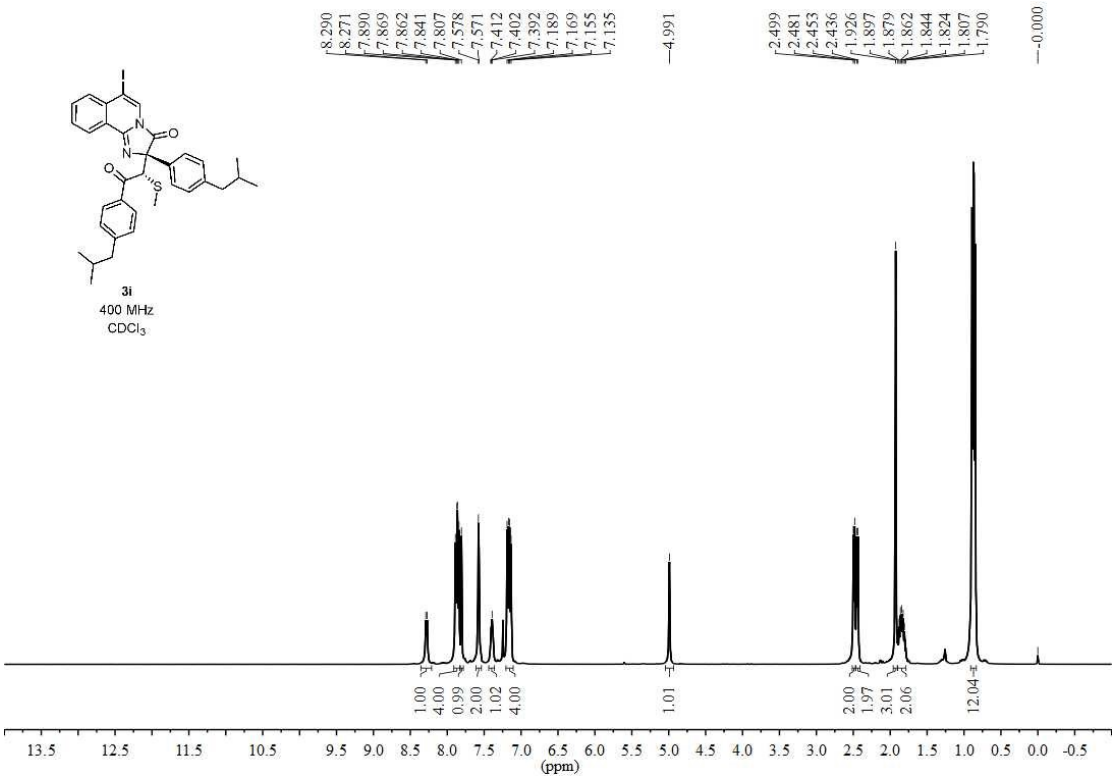
(ppm)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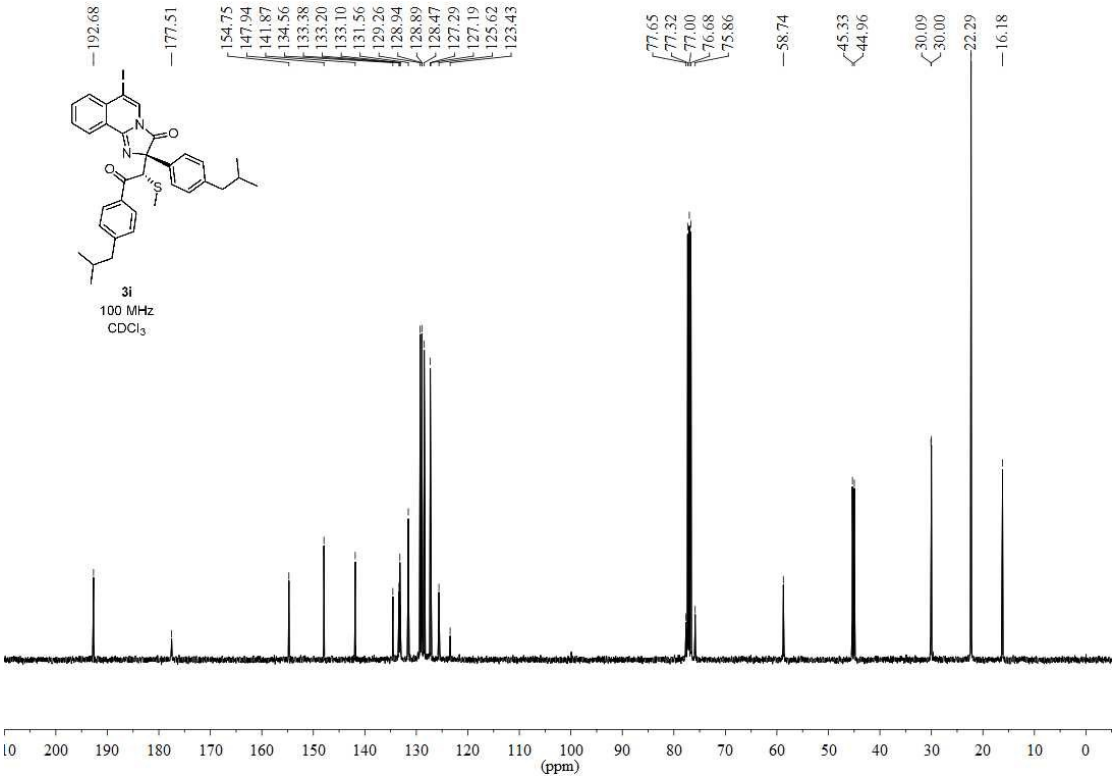
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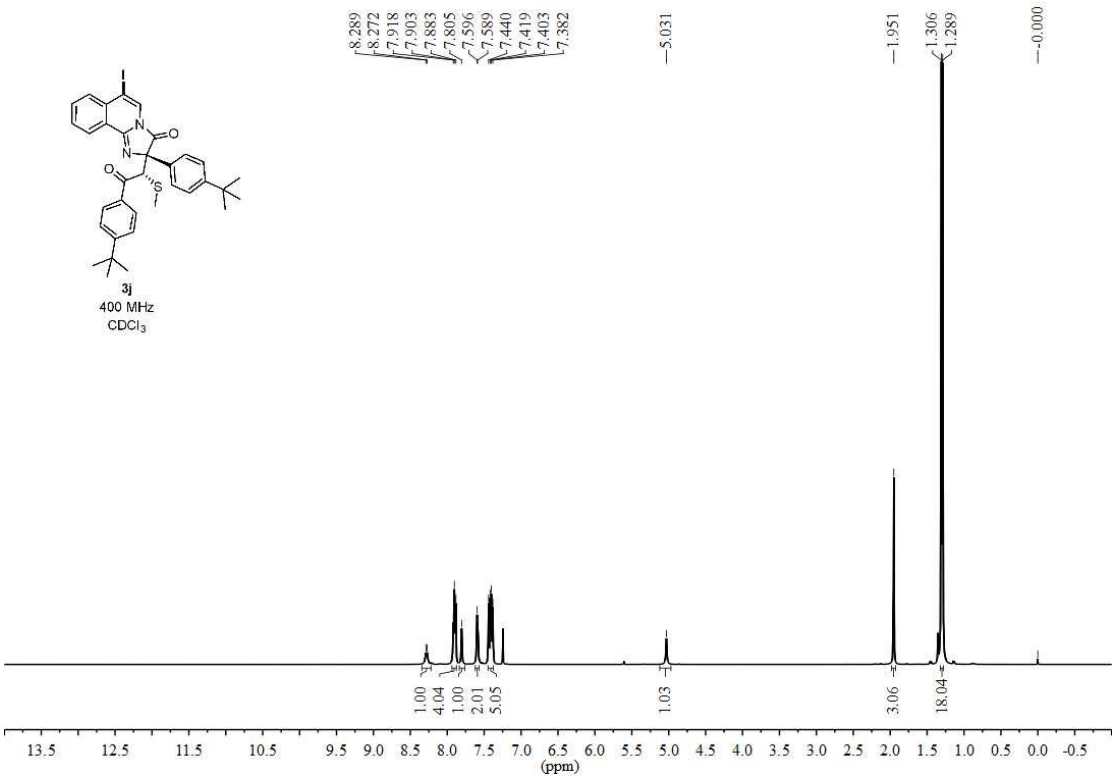
(ppm)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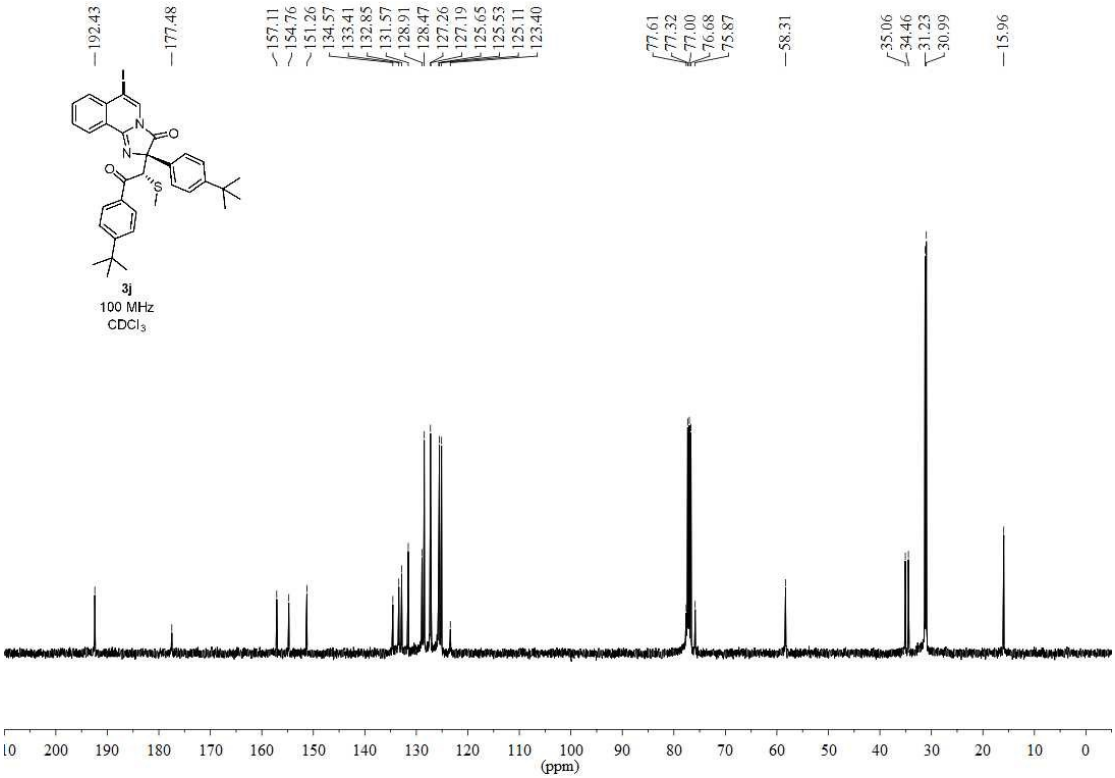
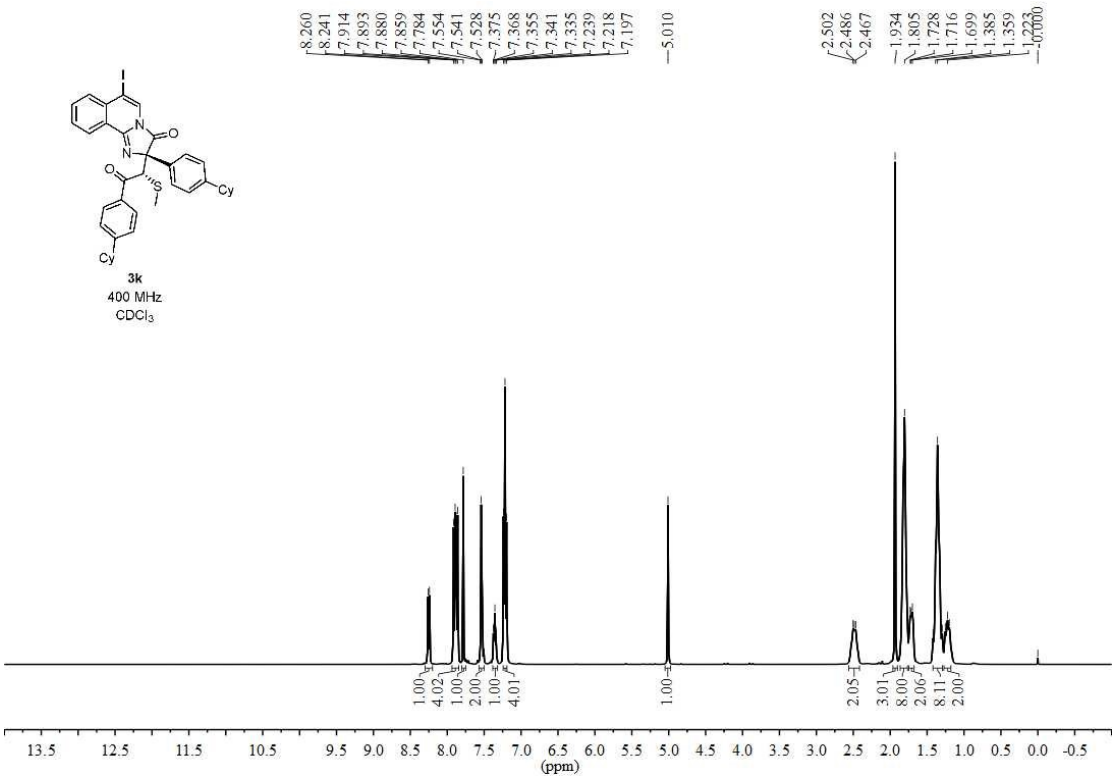
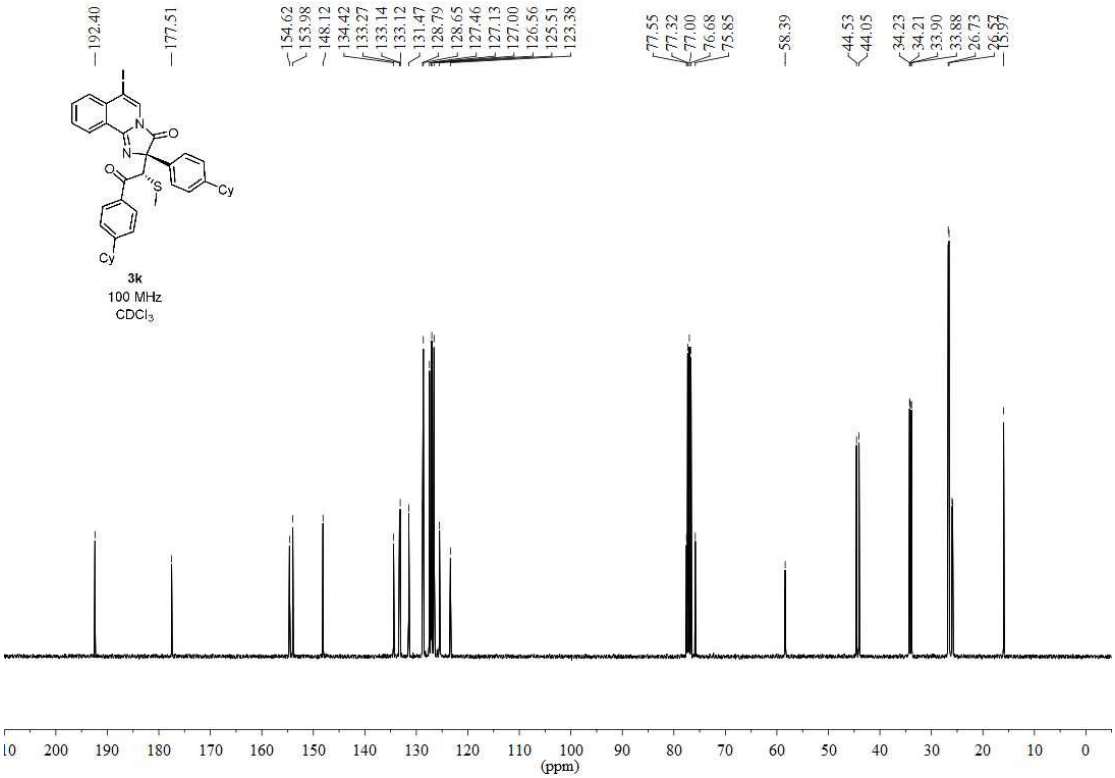
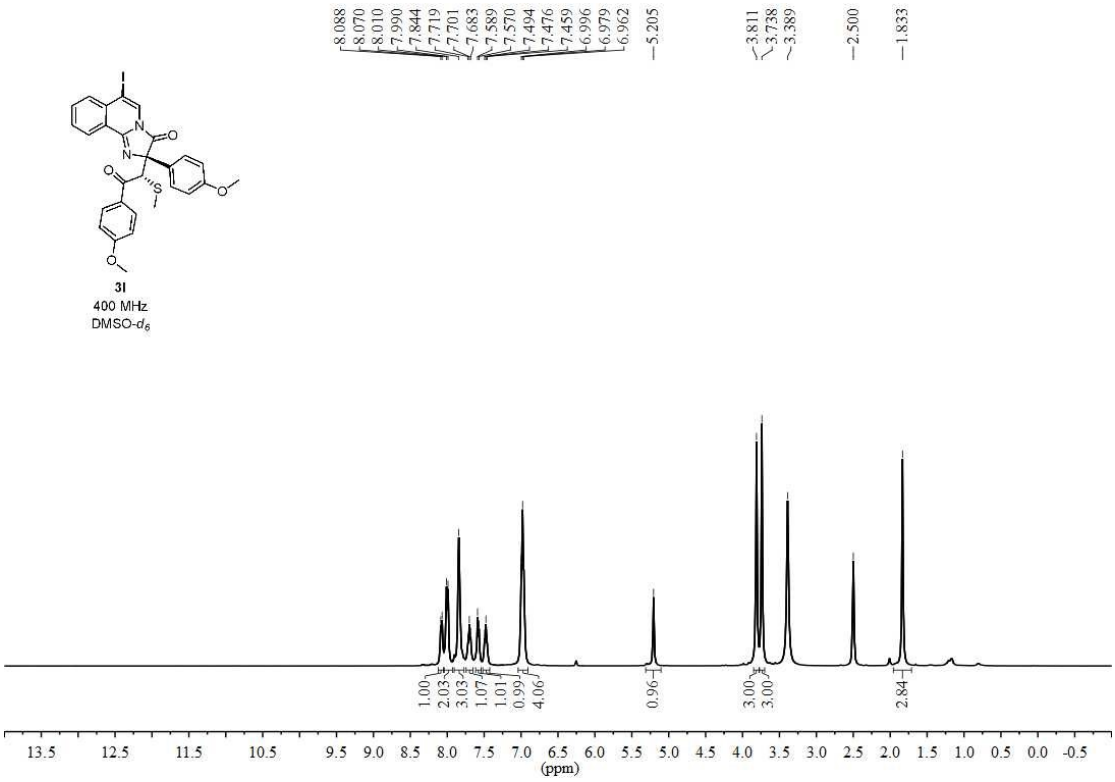
7.440
7.419
7.403
7.382
5.031
1.951
1.306
1.289
0.000
3j
400 MHz
CDCl3
1.00
4.04
1.00
2.01
5.05
1.03
3.06
18.04
(ppm)

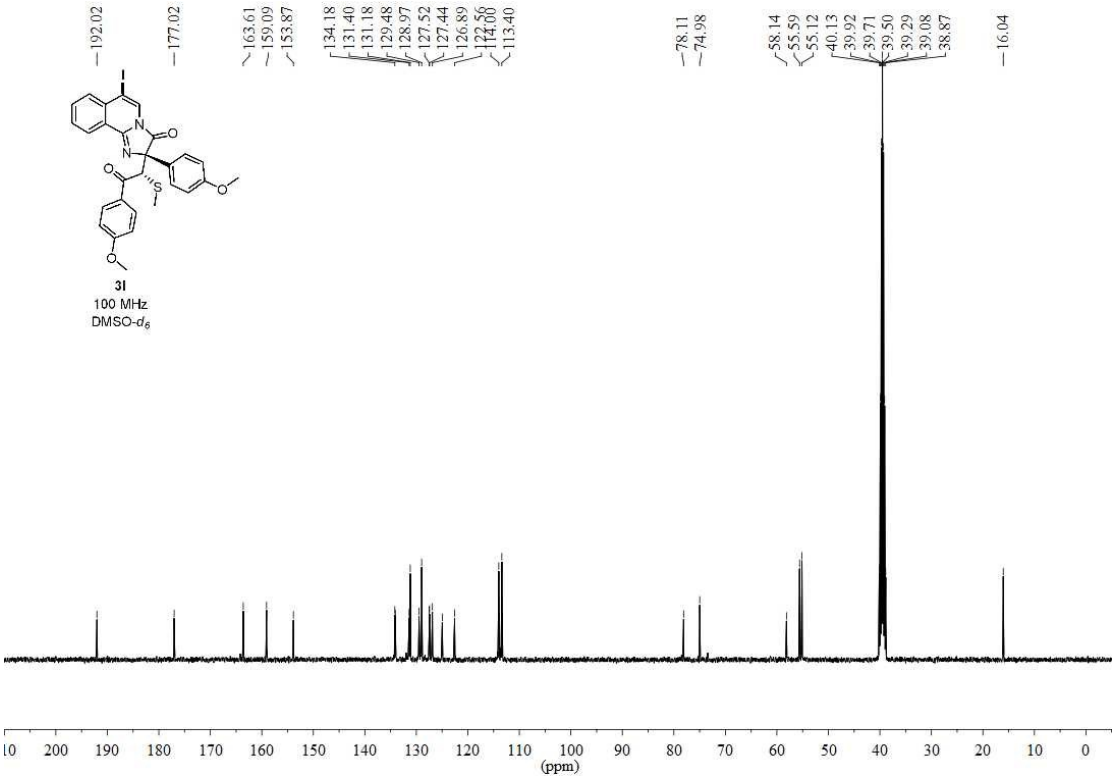

192.43
177.48
157.11
154.76
151.26
134.57
133.41
132.85
131.57
128.91
128.47
127.26
127.19
125.65
125.53
125.11
123.40
77.61
77.32
77.00
76.68
75.87
58.31
35.06
34.46
31.23
30.99
15.96
3j
100 MHz
CDCl3
(ppm)


3k
400 MHz
CDCl3
(ppm)

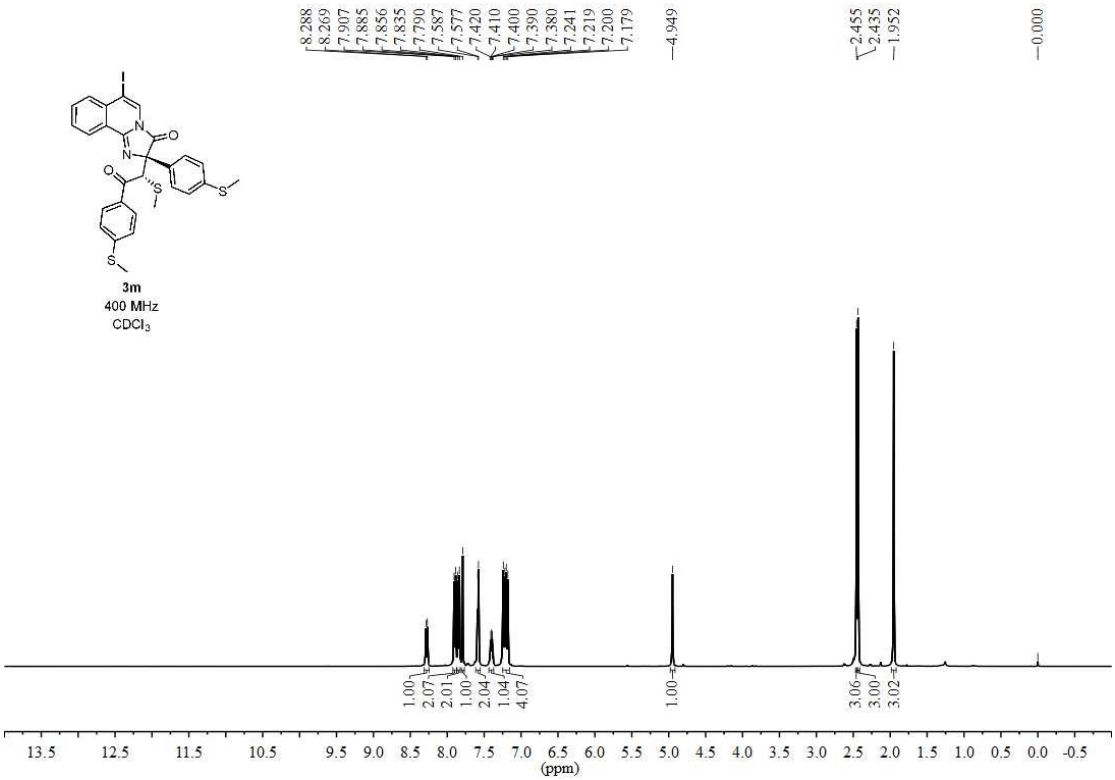

3k
100 MHz
CDCl3
(ppm)



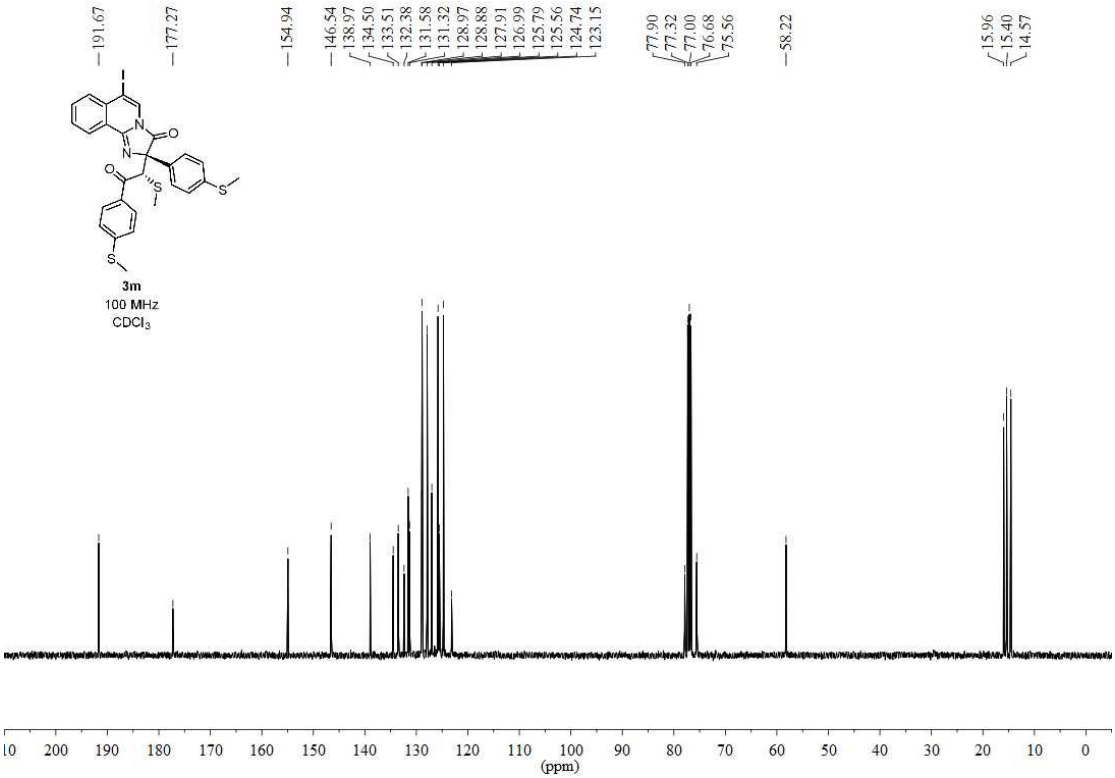
3l
400 MHz
DMSO-d_6



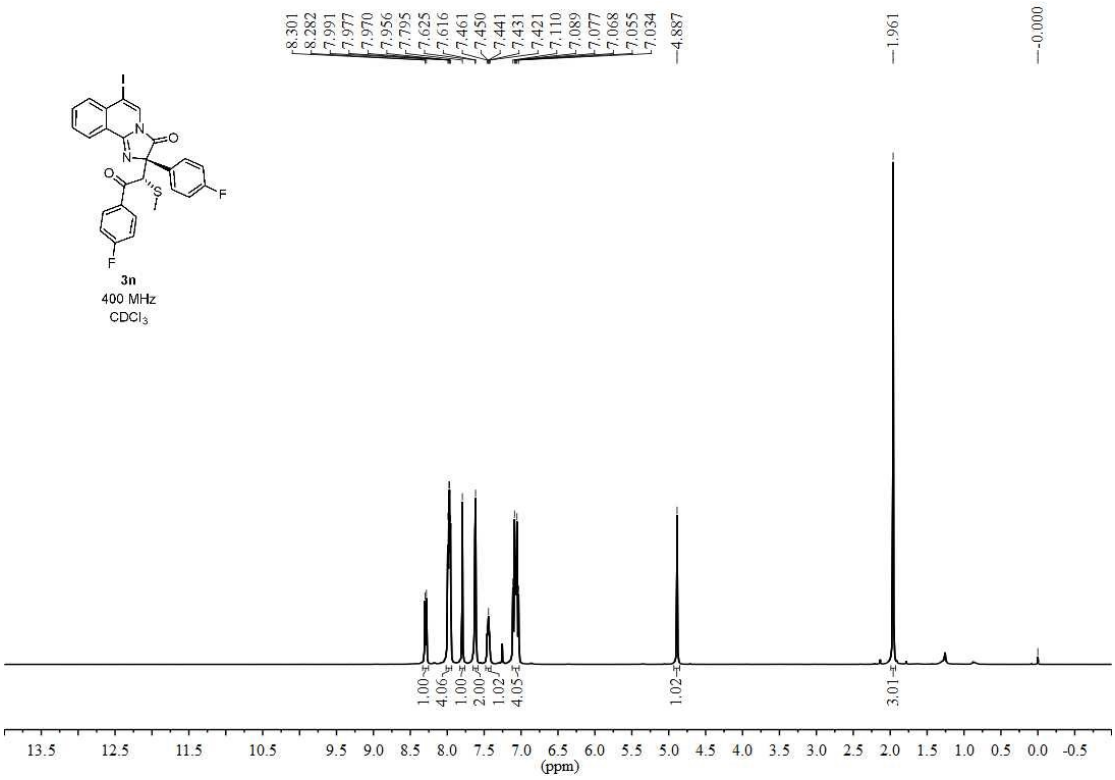
3l
100 MHz
DMSO-d_6

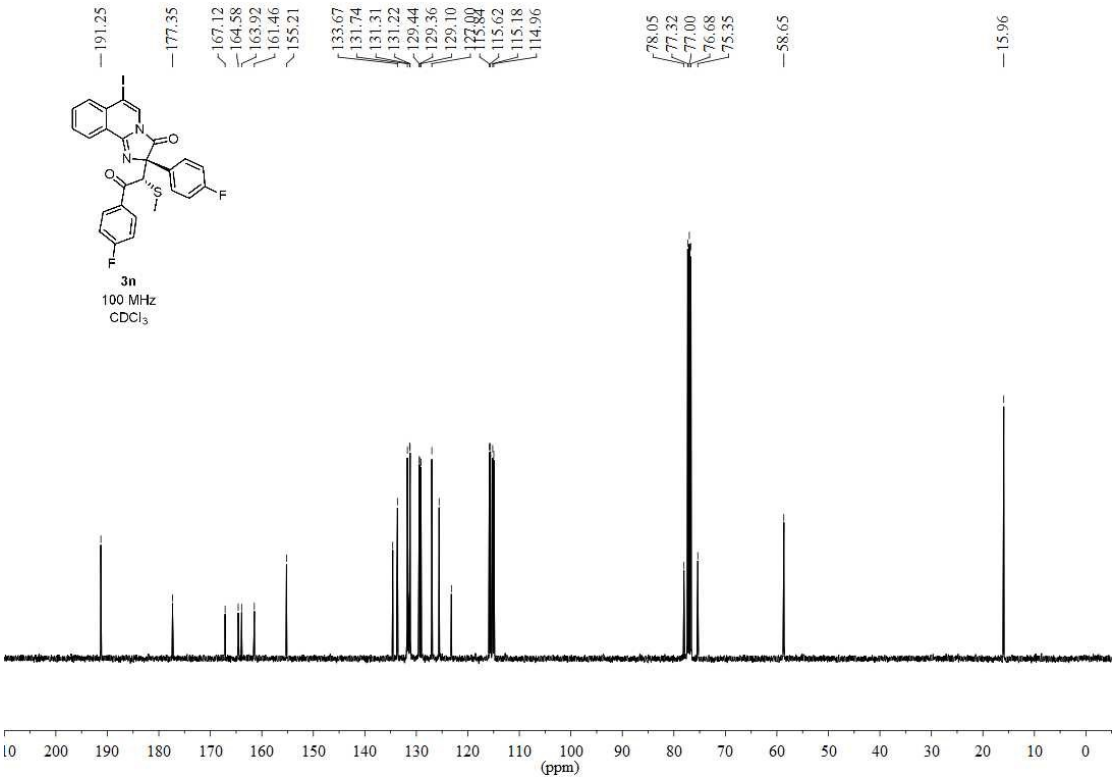


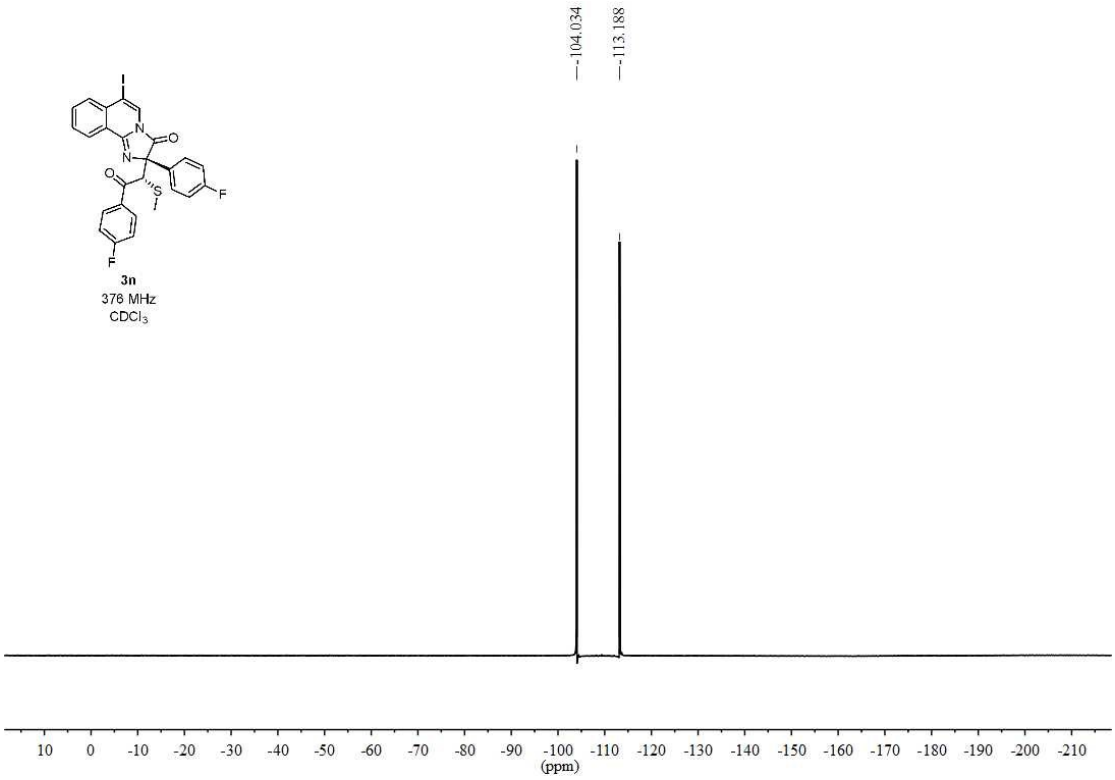
3m
400 MHz
$CDCl_3$

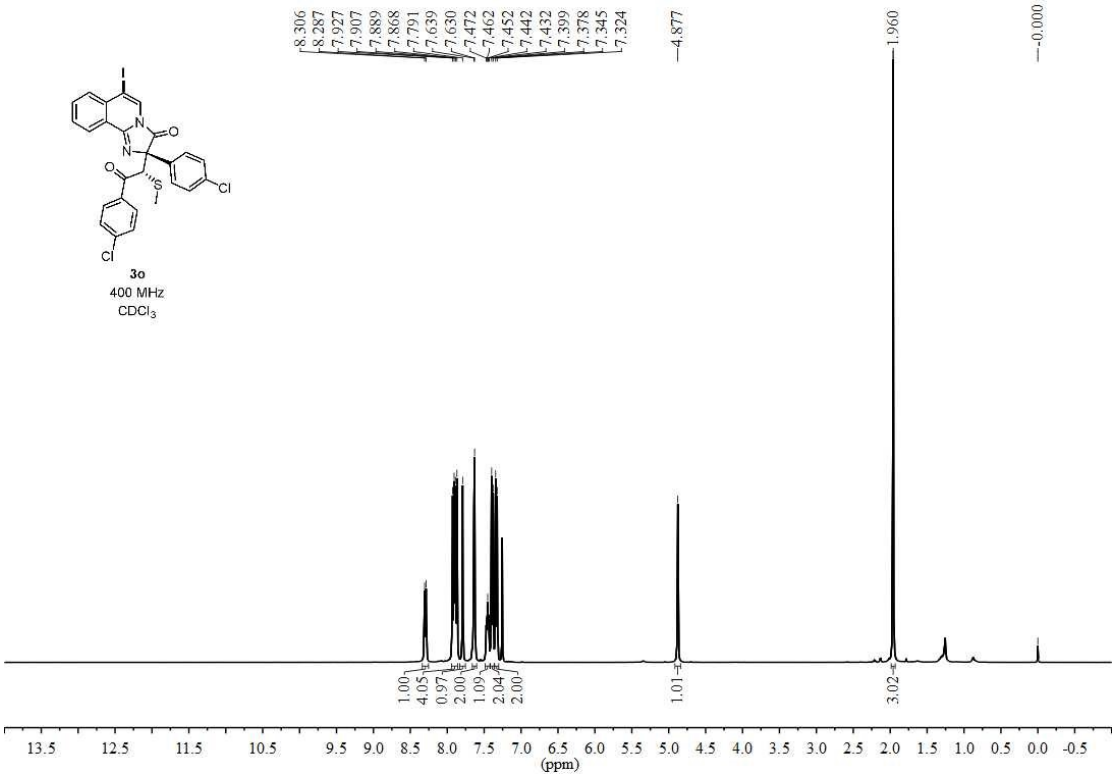


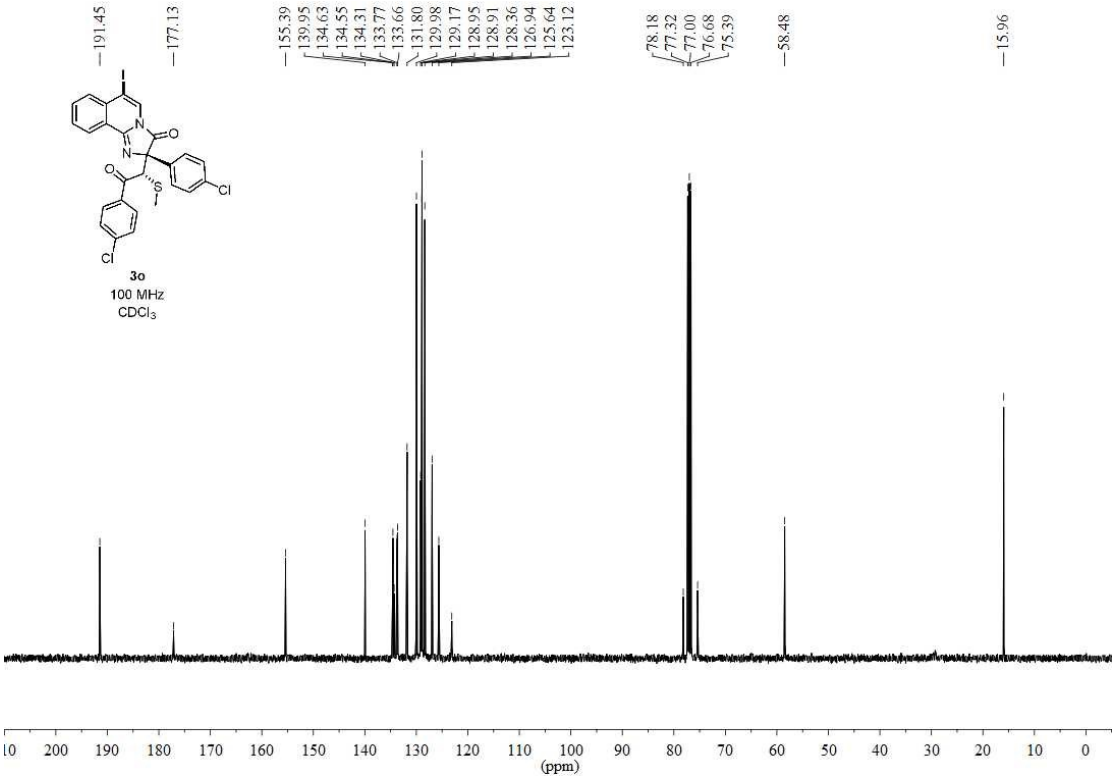
3m
100 MHz
$CDCl_3$

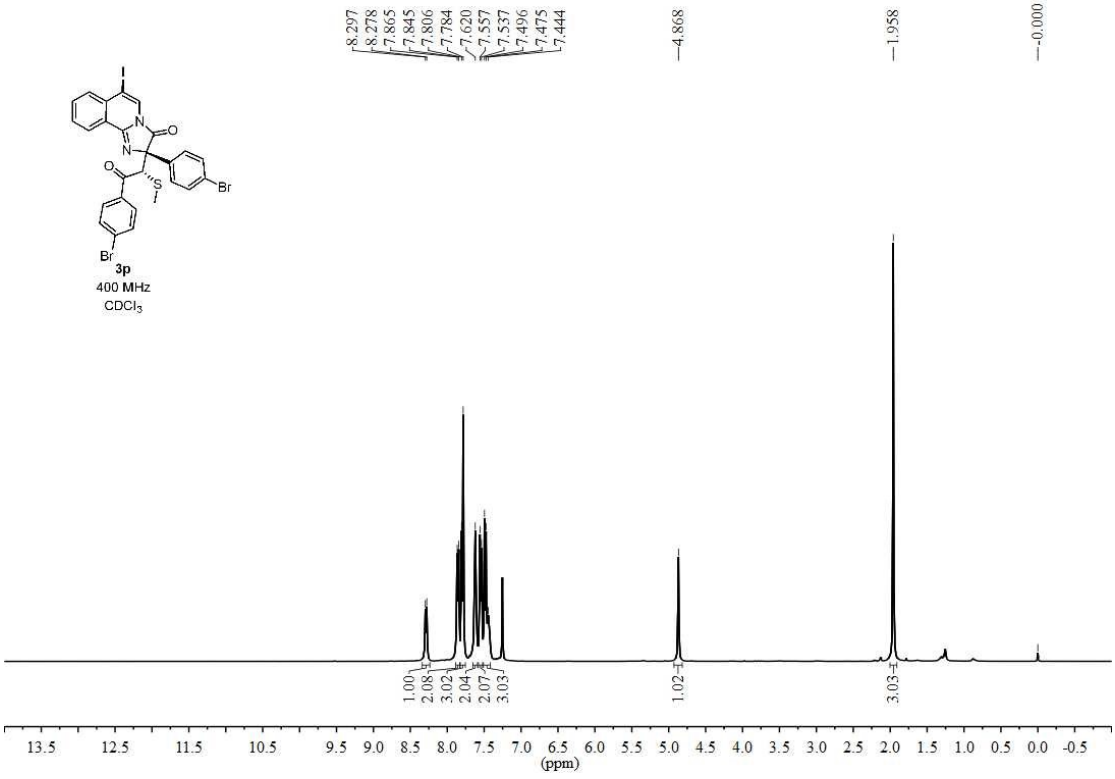

8.301
8.282
7.991
7.977
7.970
7.956
7.795
7.625
7.616
7.461
7.450
7.441
7.431
7.421
7.110
7.089
7.077
7.068
7.055
7.034
4.887
1.961
0.000
3n
400 MHz
CDCl3
1.00
4.06
1.00
2.00
1.02
4.05
1.02
3.01
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
(ppm)

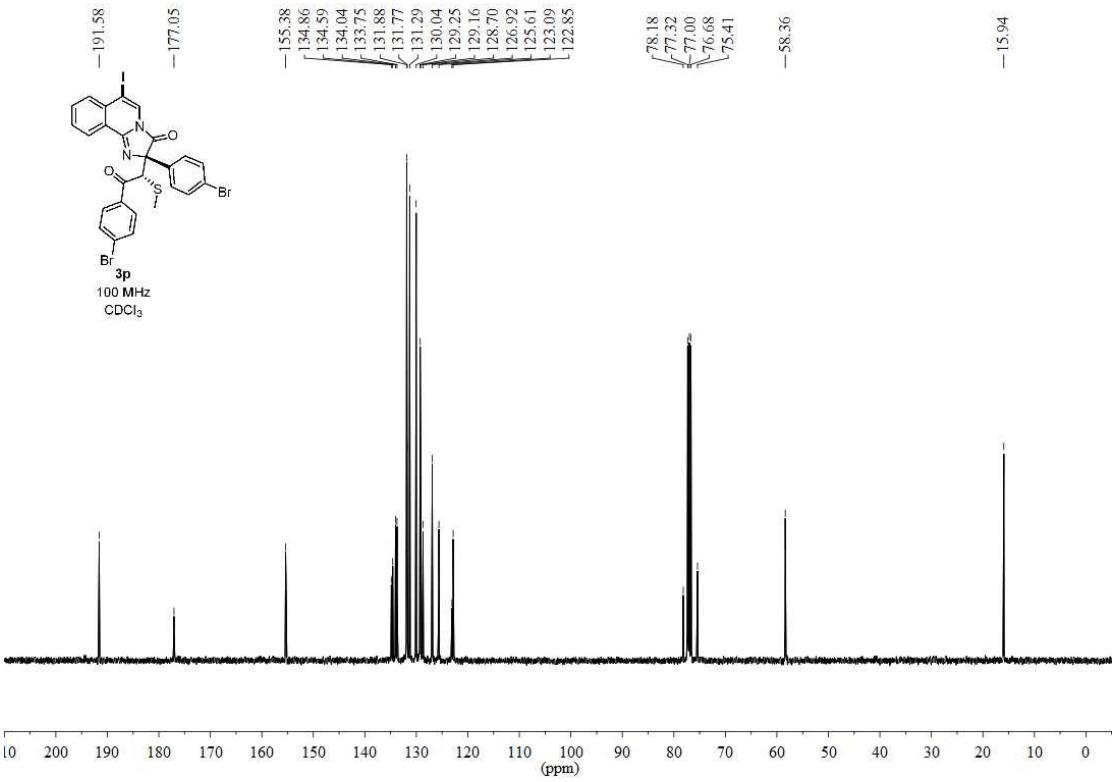

191.25
177.35
167.12
164.58
163.92
161.46
155.21
133.67
131.74
131.31
131.22
129.44
129.36
129.10
127.00
115.84
115.62
115.18
114.96
78.05
77.32
77.00
76.68
75.35
58.65
15.96
3n
100 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

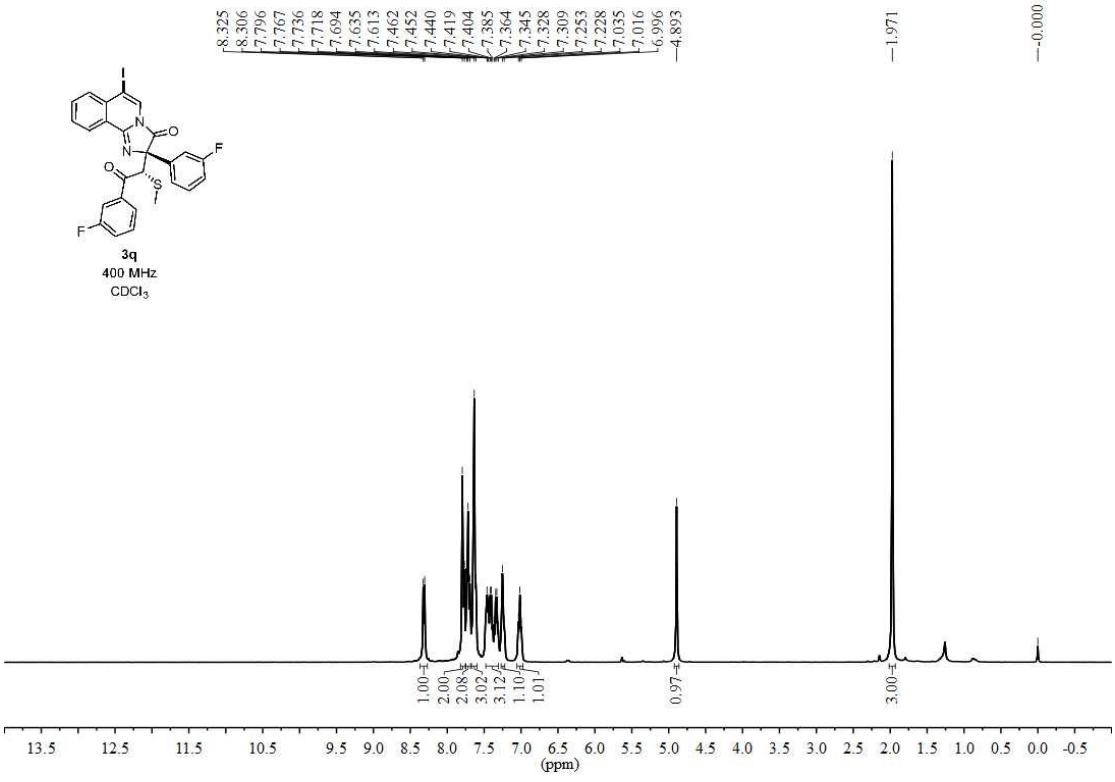

-104.034
-113.188
3n
376 MHz
CDCl3
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
(ppm)

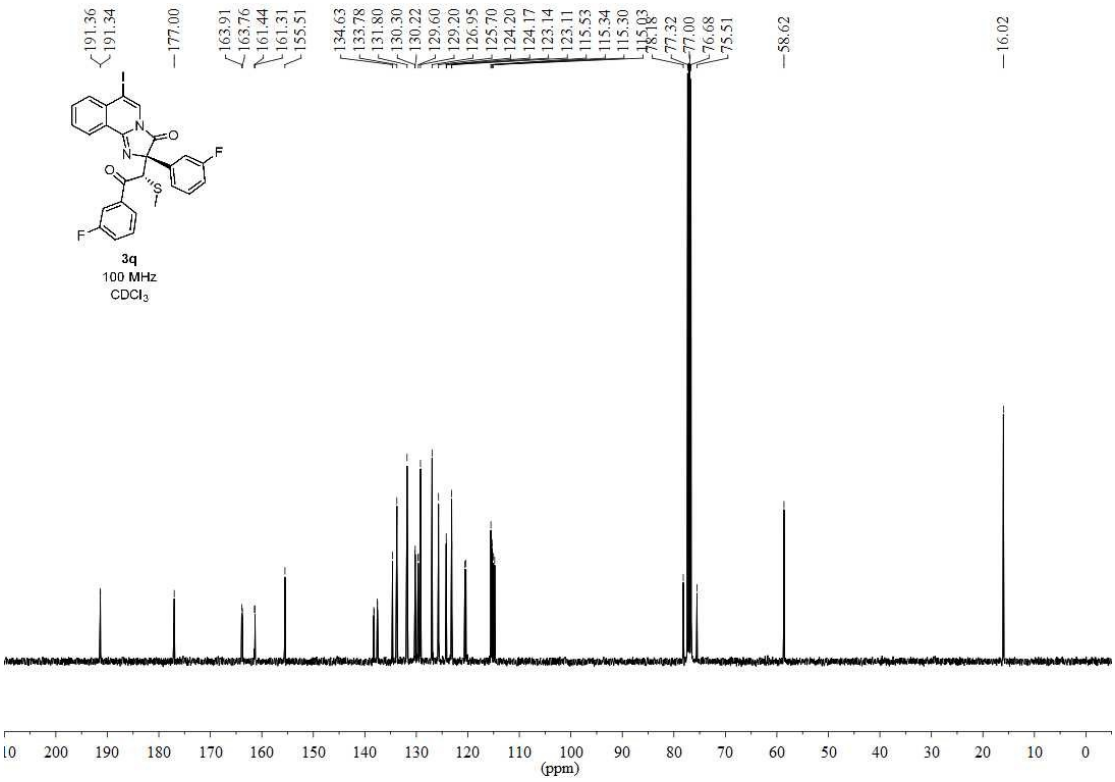

8.306
8.287
7.927
7.907
7.889
7.868
7.791
7.639
7.630
7.472
7.462
7.452
7.442
7.432
7.399
7.378
7.345
7.324
4.877
1.960
0.000
3o
400 MHz
CDCl3
1.00
4.05
0.97
2.00
1.09
2.04
2.00
1.01
3.02
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
(ppm)

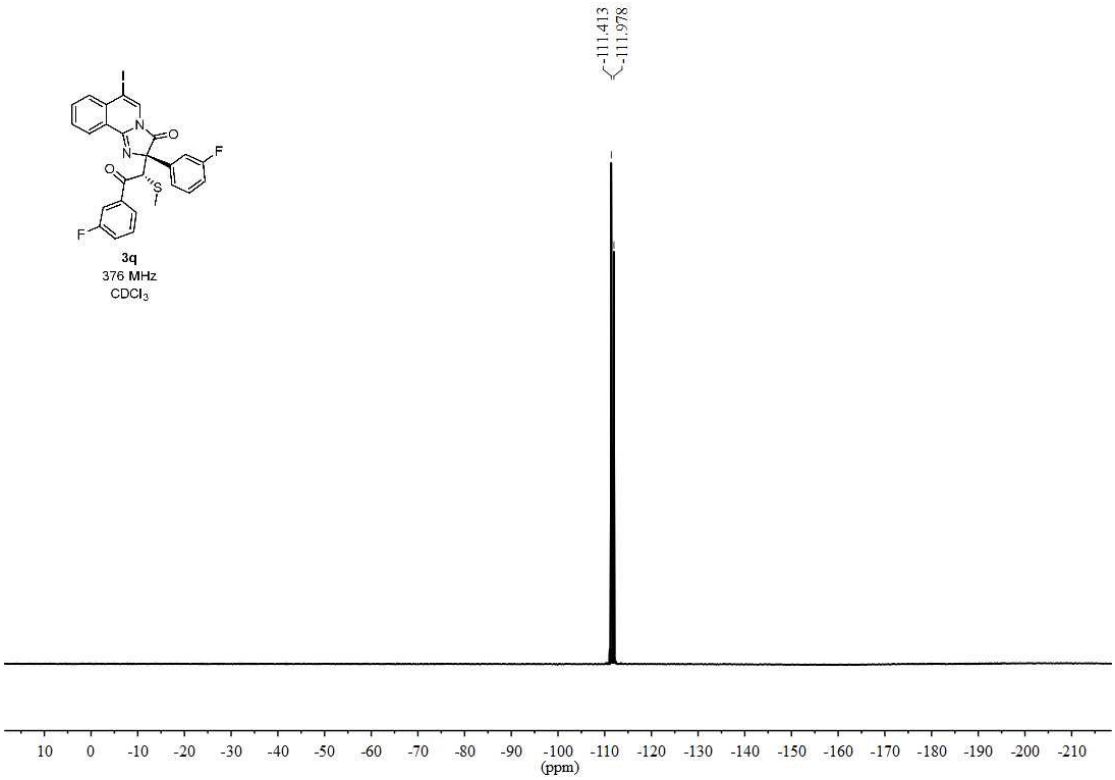

191.45
177.13
155.39
139.95
134.63
134.55
134.31
133.77
133.66
131.80
129.98
129.17
128.95
128.91
128.36
126.94
125.64
123.12
78.18
77.32
77.00
76.68
75.39
58.48
15.96
3o
100 MHz
CDCl3
(ppm)

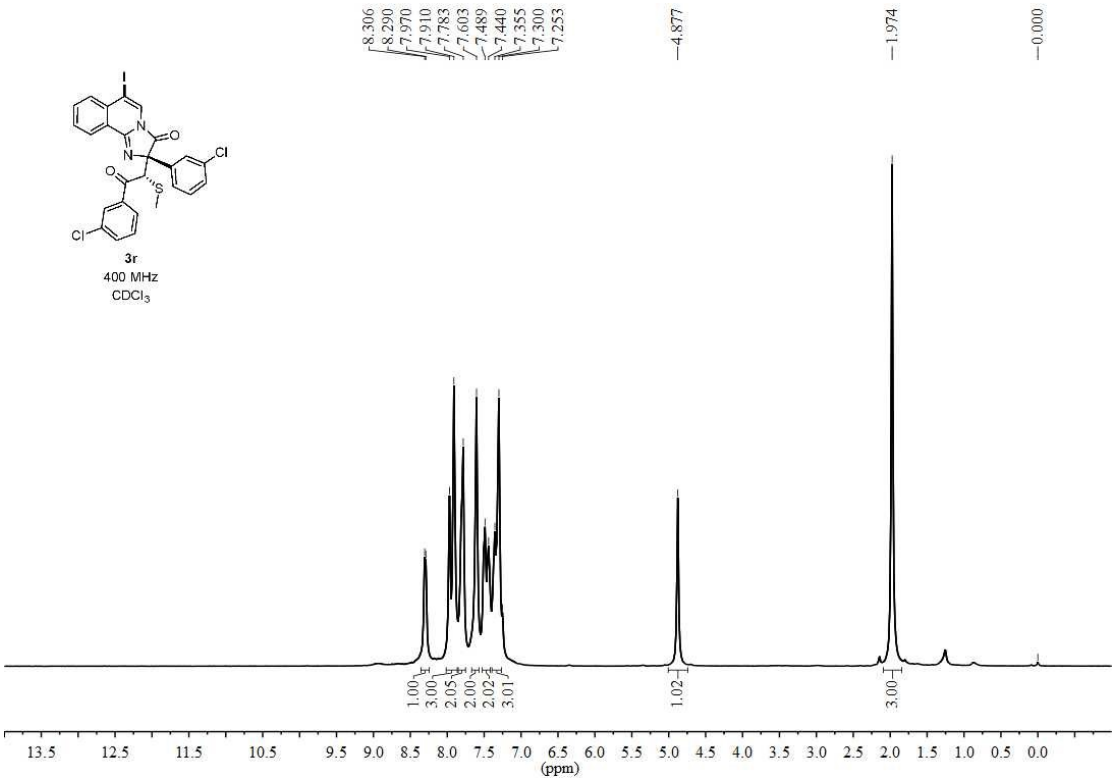

8.297
8.278
7.865
7.845
7.806
7.784
7.620
7.557
7.537
7.496
7.475
7.444
4.868
1.958
0.000
1.00
2.08
3.02
2.04
2.07
3.03
1.02
3.03
3p
400 MHz
CDCl3
(ppm)

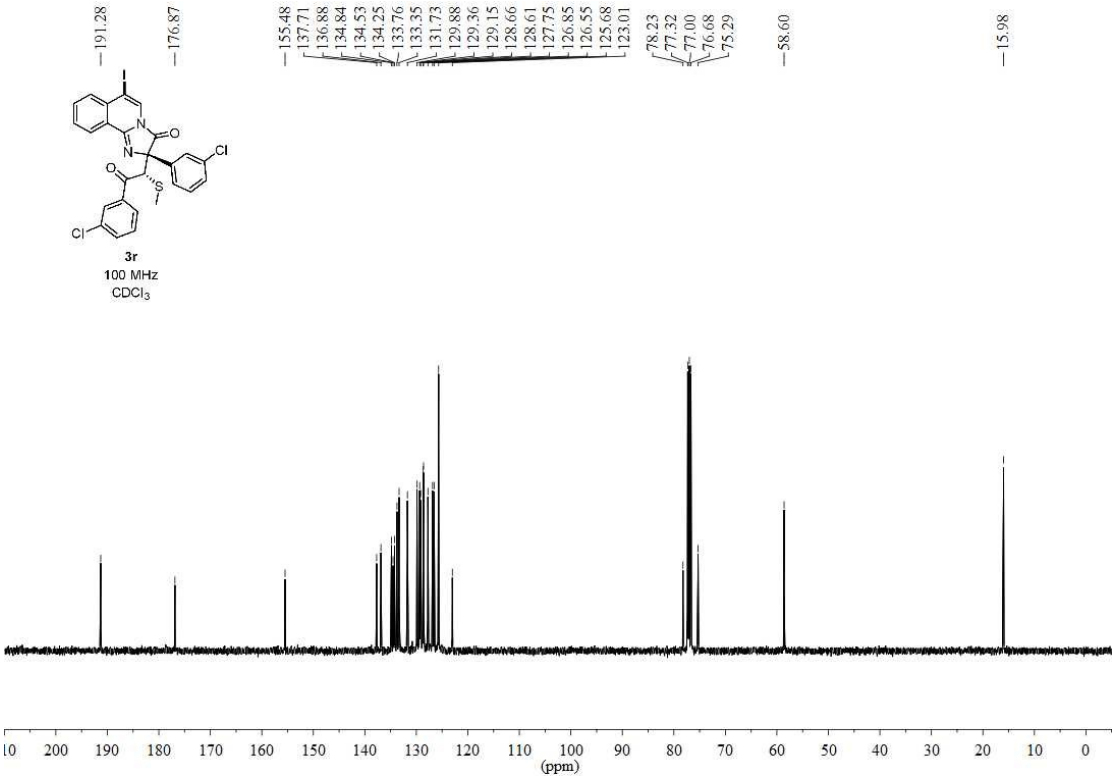

191.58
177.05
155.38
134.86
134.59
134.04
133.75
131.88
131.77
131.29
130.04
129.25
129.16
128.70
126.92
125.61
123.09
122.85
78.18
77.32
77.00
76.68
75.41
58.36
15.94
3p
100 MHz
CDCl3
(ppm)

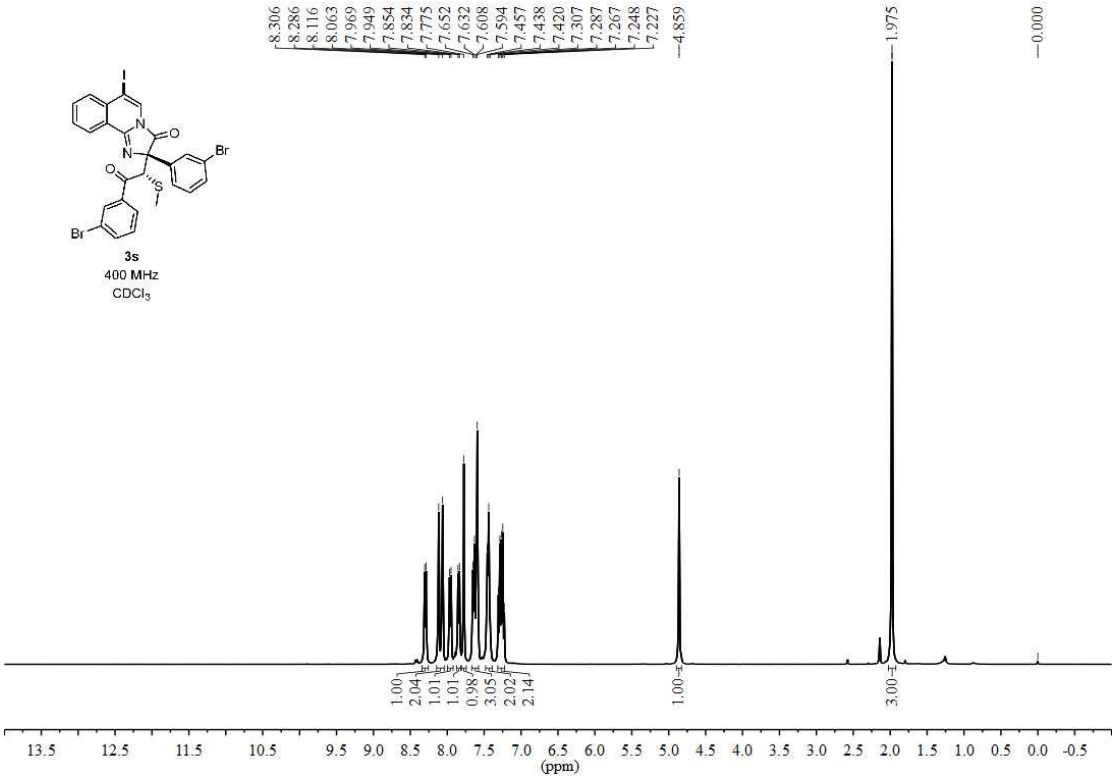

8.325
8.306
7.796
7.767
7.736
7.718
7.694
7.635
7.613
7.462
7.452
7.440
7.419
7.404
7.385
7.364
7.345
7.328
7.309
7.253
7.228
7.035
7.016
6.996
4.893
1.971
-0.000
1.00
2.00
2.08
3.02
3.12
1.10
1.01
0.97
3.00
3q
400 MHz
CDCl3
(ppm)

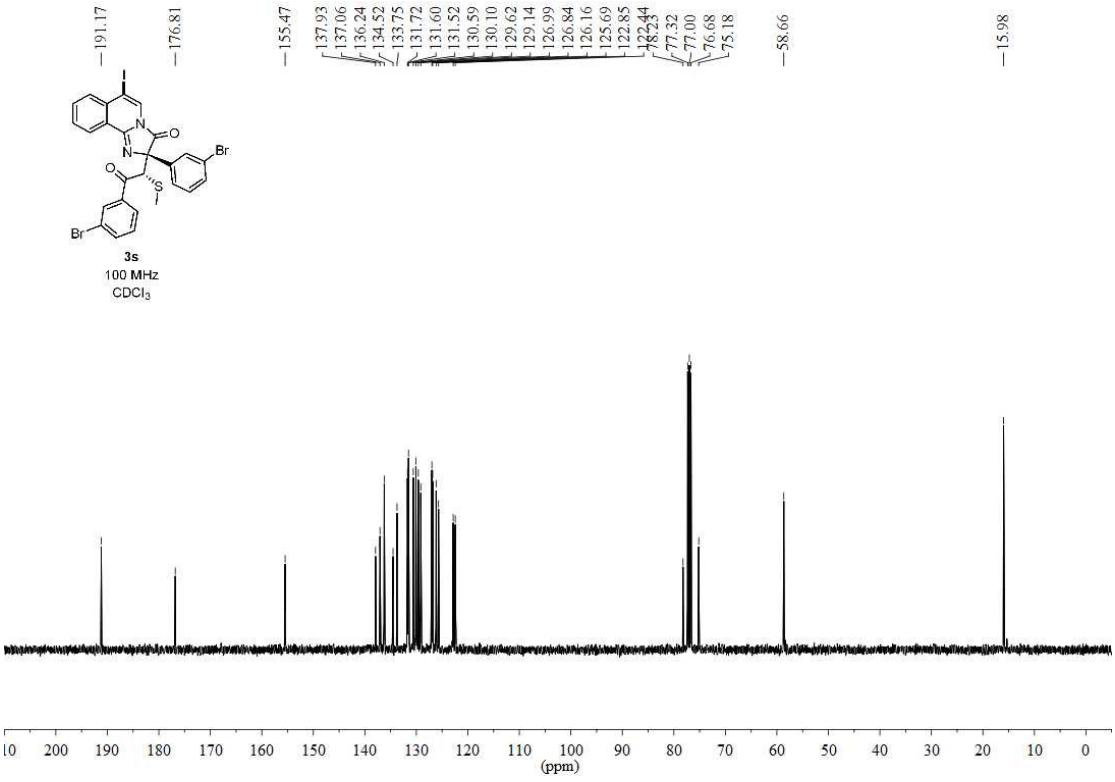

191.36
191.34
177.00
163.91
163.76
161.44
161.31
155.51
134.63
133.78
131.80
130.30
130.22
129.60
129.20
126.95
125.70
124.20
124.17
123.14
123.11
115.53
115.34
115.30
115.03
78.18
77.32
77.00
76.68
75.51
58.62
16.02
3q
100 MHz
CDCl3
(ppm)

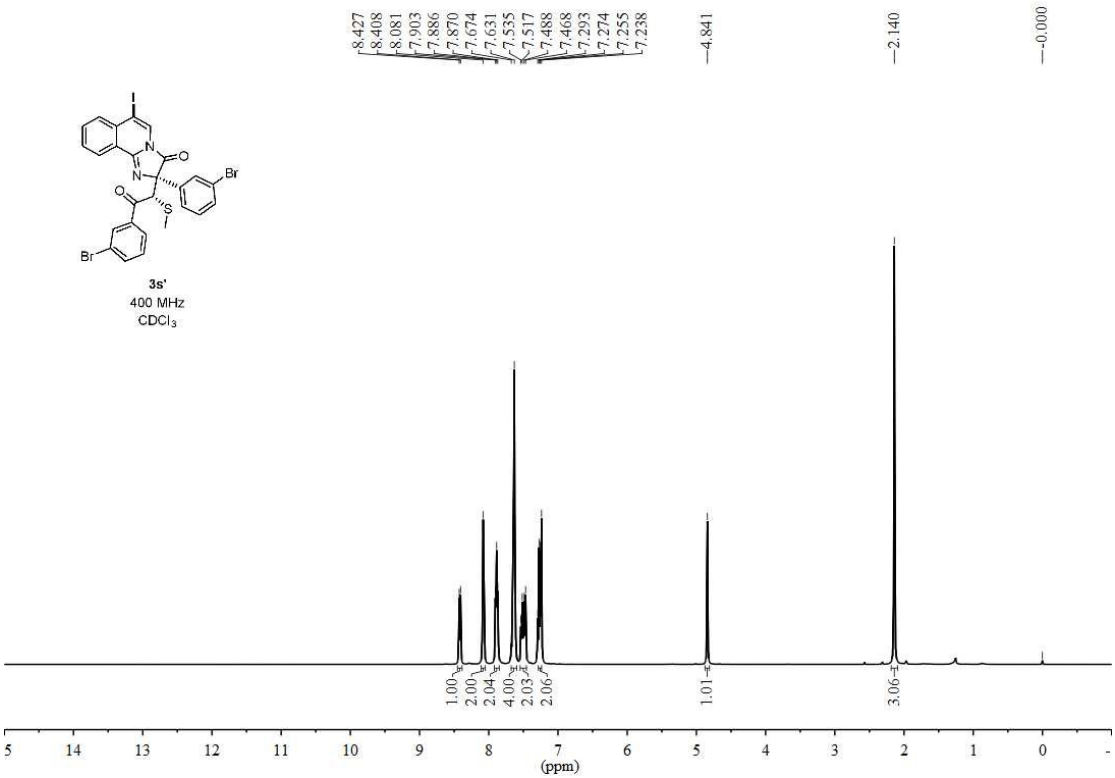

-111.413
-111.978
3q
376 MHz
CDCl3
(ppm)

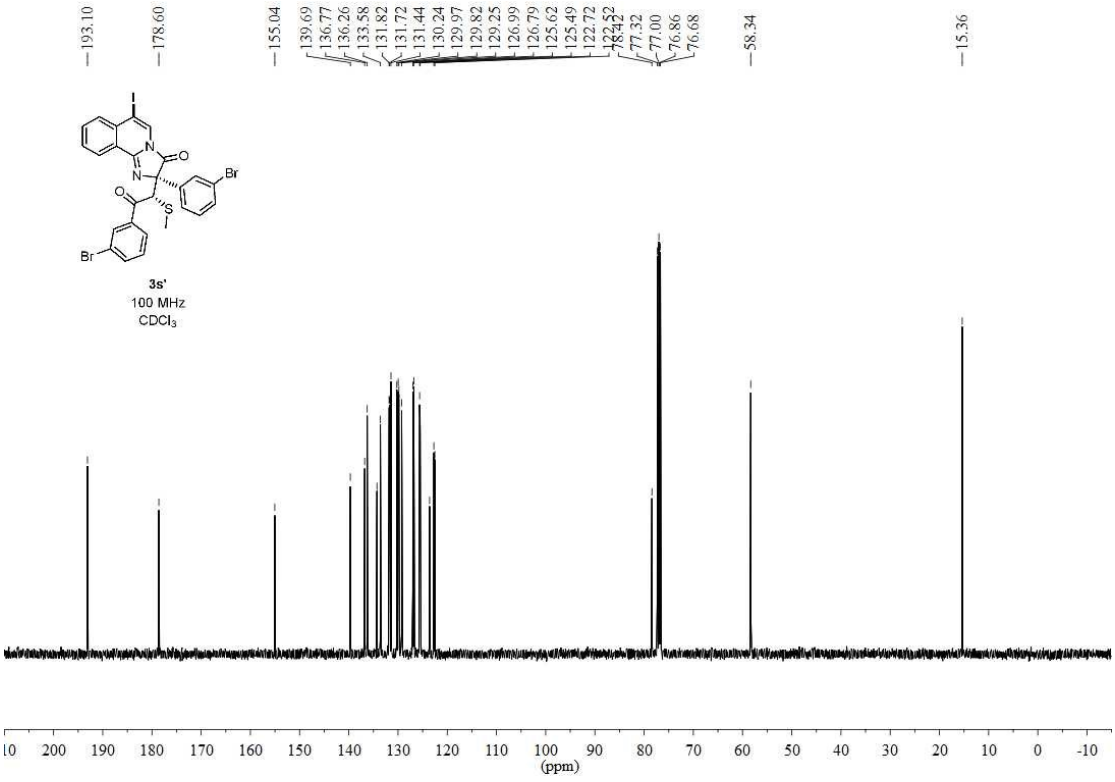

8.306
8.290
7.970
7.910
7.783
7.603
7.489
7.440
7.355
7.300
7.253
4.877
1.974
0.000
3r
400 MHz
CDCl3
1.00
3.00
2.05
2.00
2.02
3.01
1.02
3.00
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)

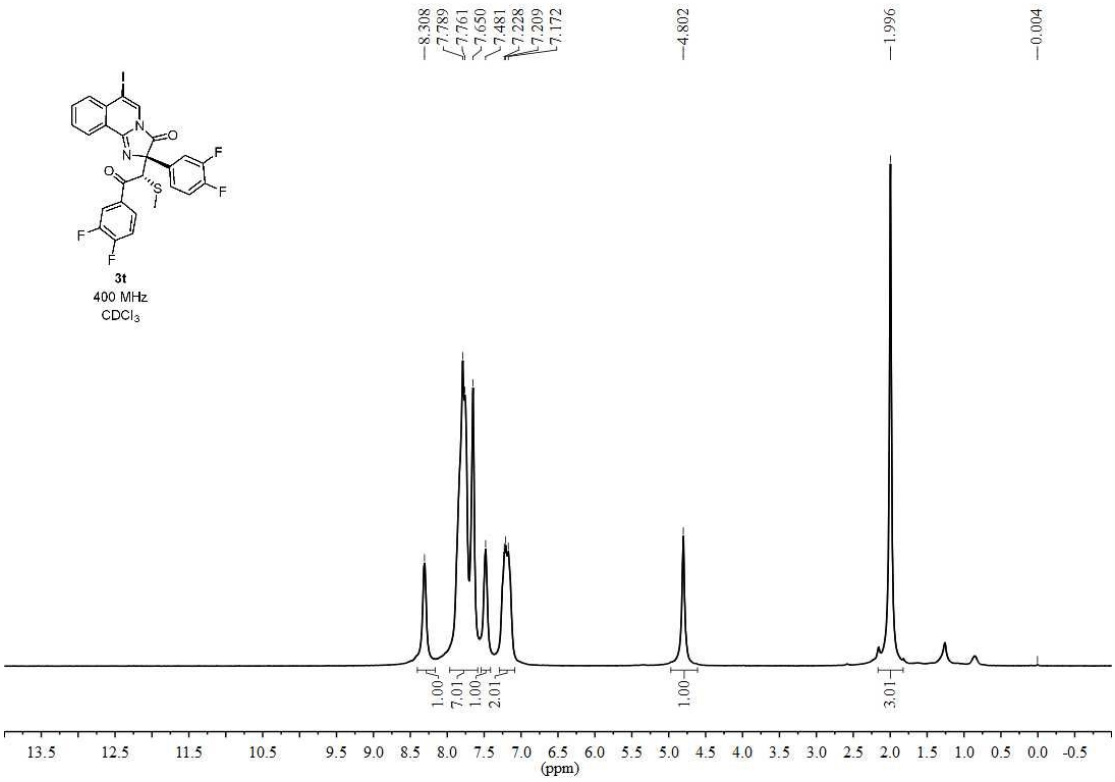

191.28
176.87
155.48
137.71
136.88
134.84
134.53
134.25
133.76
133.35
131.73
129.88
129.36
129.15
128.66
128.61
127.75
126.85
126.55
125.68
123.01
78.23
77.32
77.00
76.68
75.29
58.60
15.98
3r
100 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

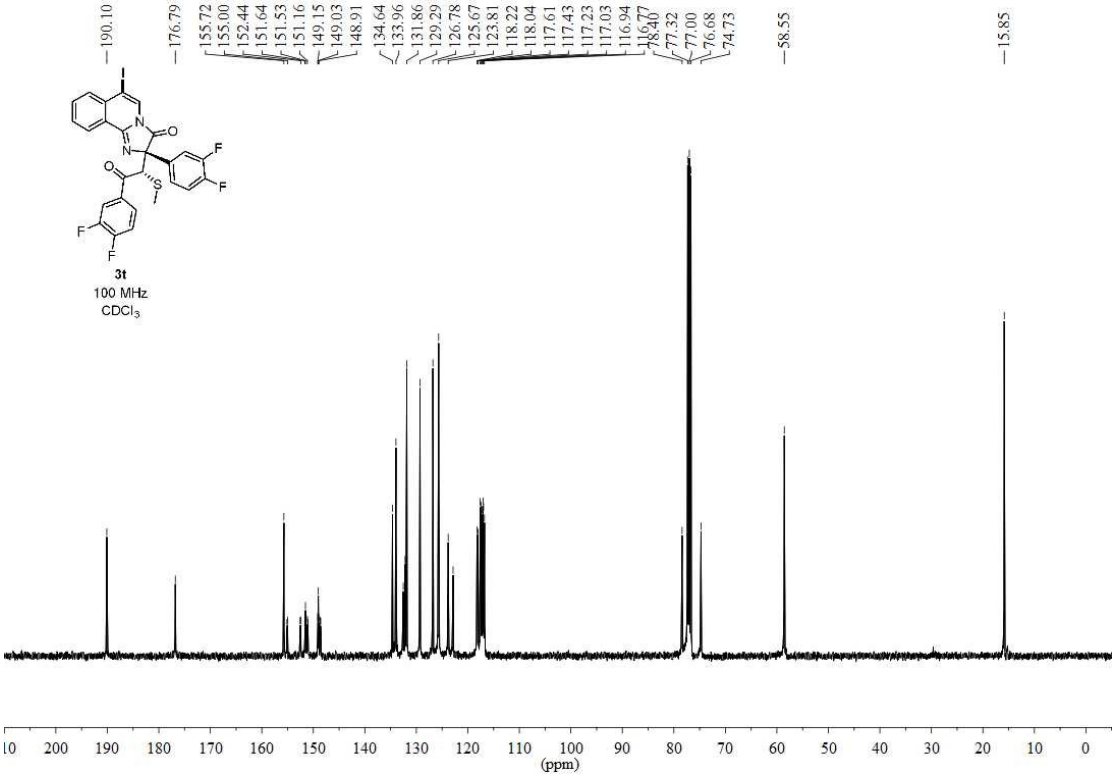

3s
400 MHz
CDCl3
8.306
8.286
8.116
8.063
7.969
7.949
7.854
7.834
7.775
7.652
7.632
7.608
7.594
7.457
7.438
7.420
7.307
7.287
7.267
7.248
7.227
4.859
1.975
0.000
1.00
2.04
1.01
1.01
0.98
3.05
2.02
2.14
1.00
3.00
(ppm)

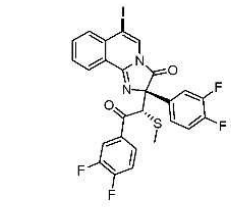

3s
100 MHz
CDCl3
191.17
176.81
155.47
137.93
137.06
136.24
134.52
133.75
131.72
131.60
131.52
130.59
130.10
129.62
129.14
126.99
126.84
126.16
125.69
122.85
122.44
78.23
77.32
77.00
76.68
75.18
58.66
15.98
(ppm)


8.427
8.408
8.081
7.903
7.886
7.870
7.674
7.631
7.535
7.517
7.488
7.468
7.293
7.274
7.255
7.238
4.841
2.140
0.000
3s'
400 MHz
CDCl3
1.00
2.00
2.04
4.00
2.03
2.06
1.01
3.06
(ppm)

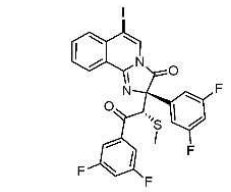

193.10
178.60
155.04
139.69
136.77
136.26
133.58
131.82
131.72
131.44
130.24
129.97
129.82
129.25
126.99
126.79
125.62
125.49
122.72
77.32
77.00
76.86
76.68
58.34
15.36
3s'
100 MHz
CDCl3
(ppm)


8.308
7.789
7.761
7.650
7.481
7.228
7.209
7.172
4.802
1.996
0.004
3t
400 MHz
CDCl3
1.00
7.01
1.00
2.01
1.00
3.01
(ppm)

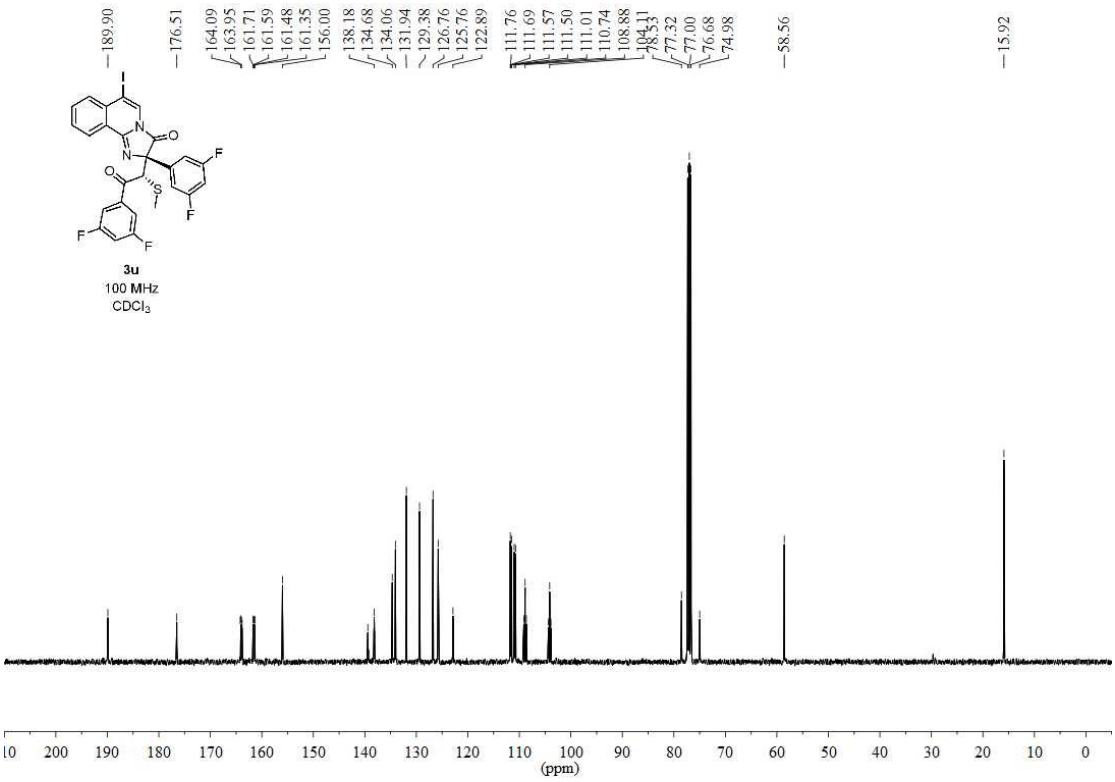

190.10
176.79
155.72
155.00
152.44
151.64
151.53
151.16
149.15
149.03
148.91
134.64
133.96
131.86
129.29
126.78
125.67
123.81
118.22
118.04
117.61
117.43
117.23
117.03
116.94
116.77
78.40
77.32
77.00
76.68
74.73
58.55
15.85
3t
100 MHz
CDCl3
(ppm)

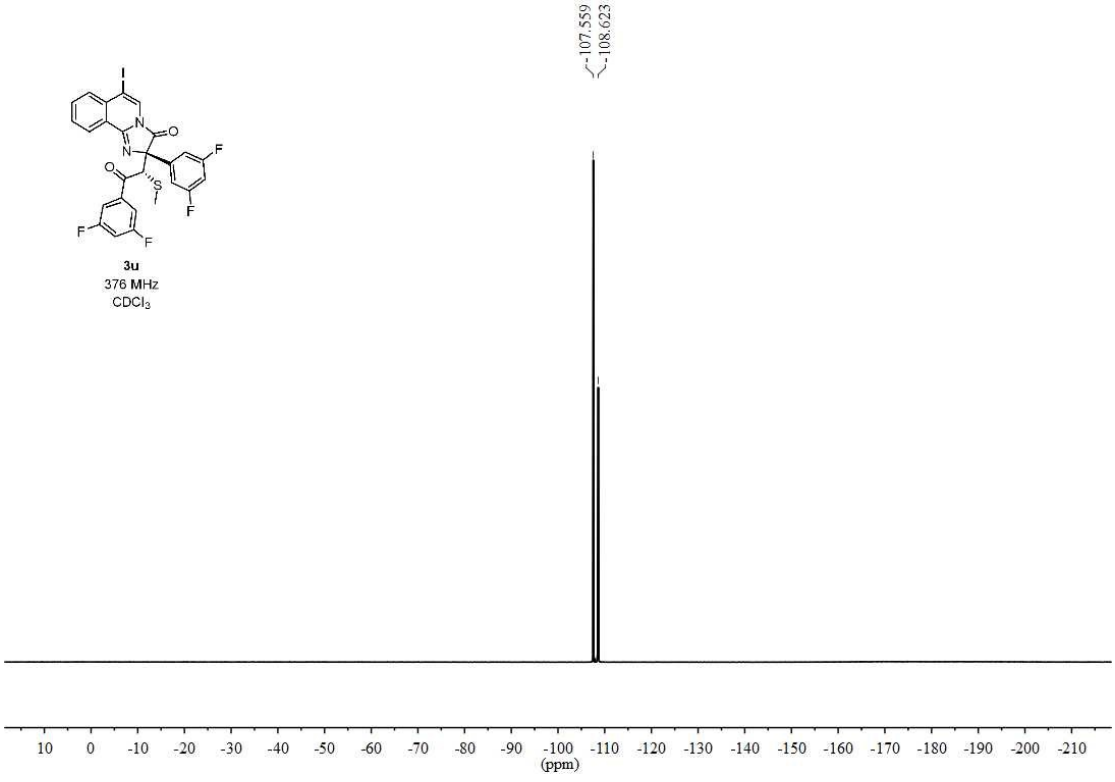


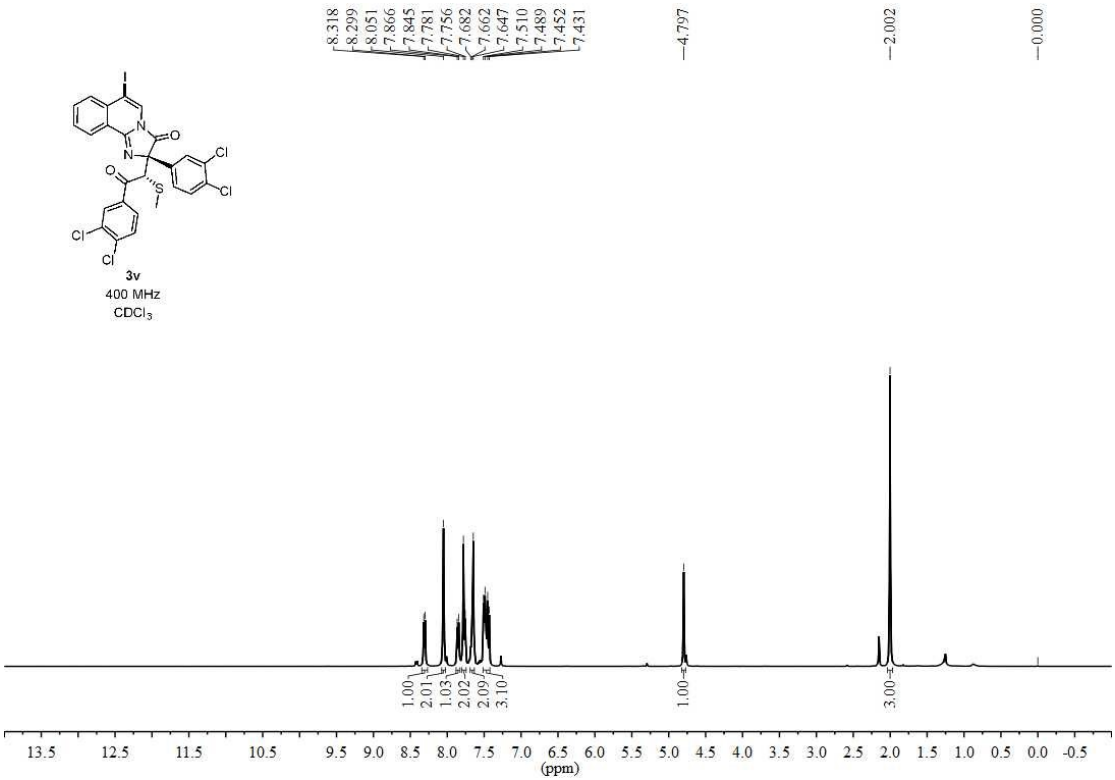
3t
376 MHz
$CDCl_3$

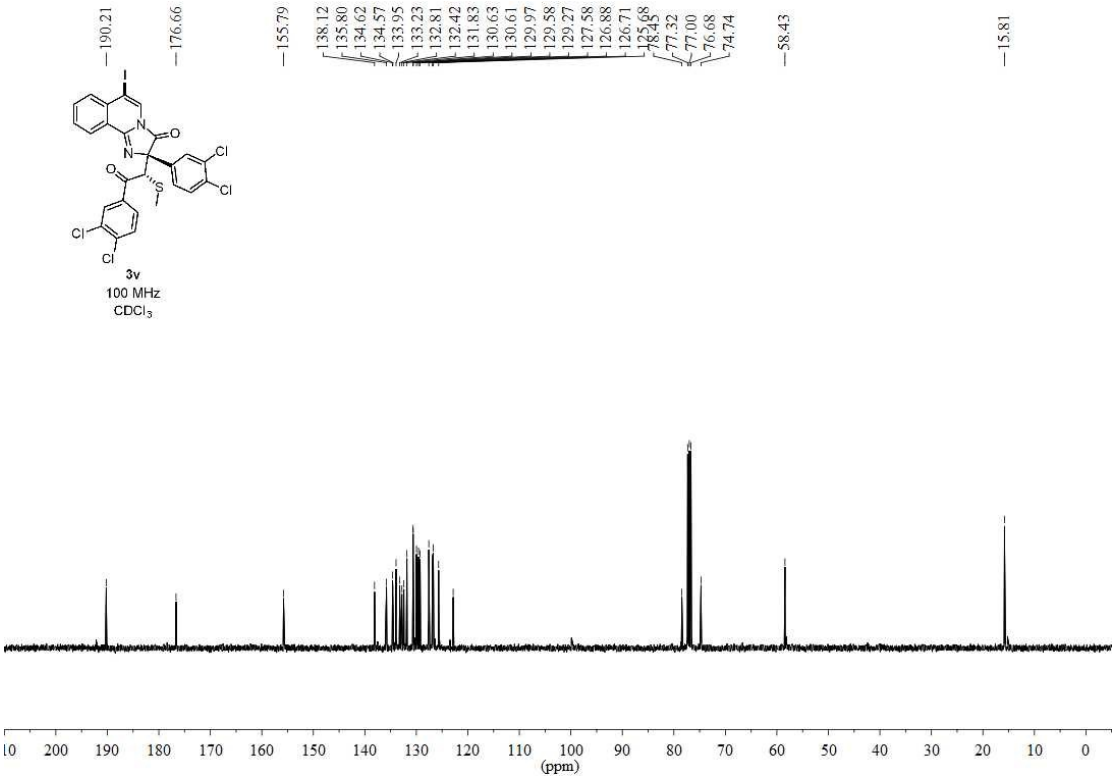


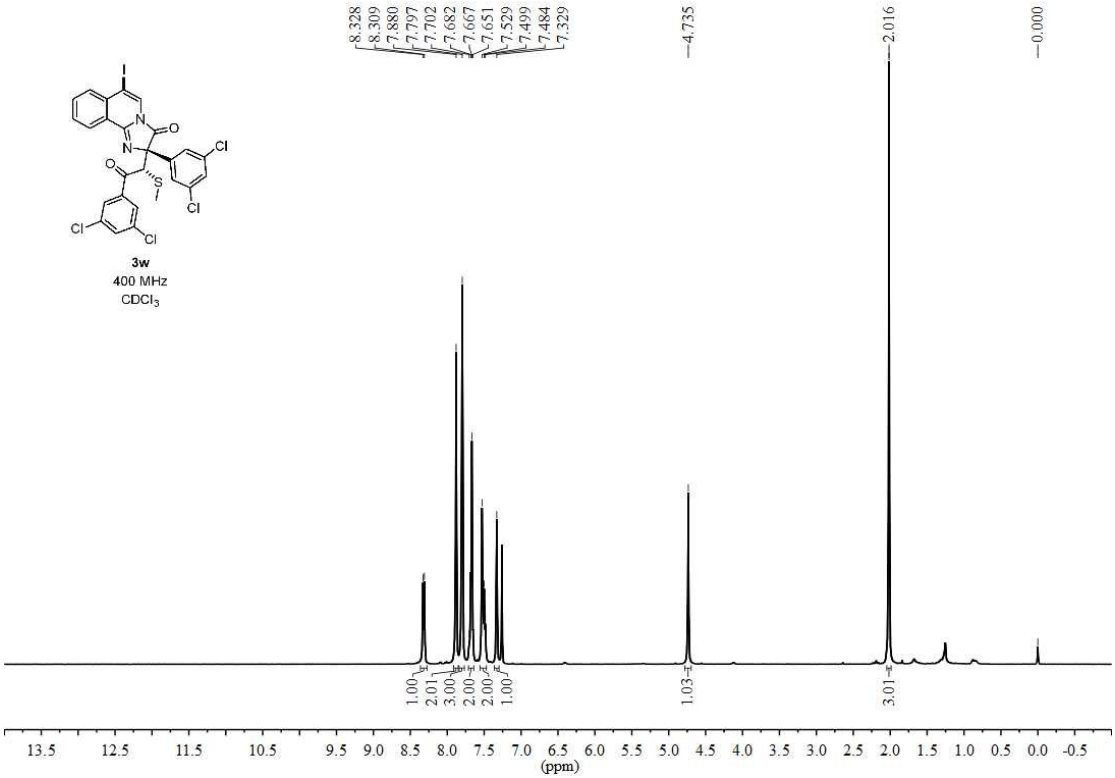
3u
400 MHz
$CDCl_3$

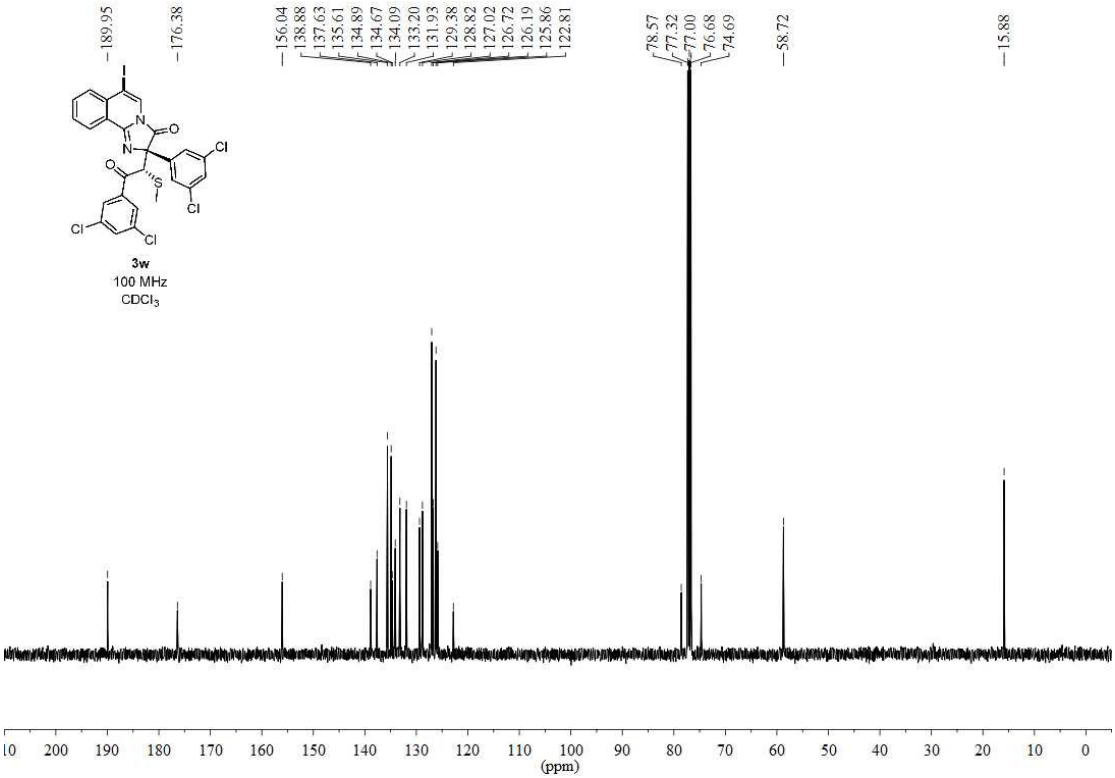

189.90
176.51
164.09
163.95
161.71
161.59
161.48
161.35
156.00
138.18
134.68
134.06
131.94
129.38
126.76
125.76
122.89
111.76
111.69
111.57
111.50
111.01
110.74
108.88
104.11
78.53
77.32
77.00
76.68
74.98
58.56
15.92
3u
100 MHz
CDCl3
(ppm)

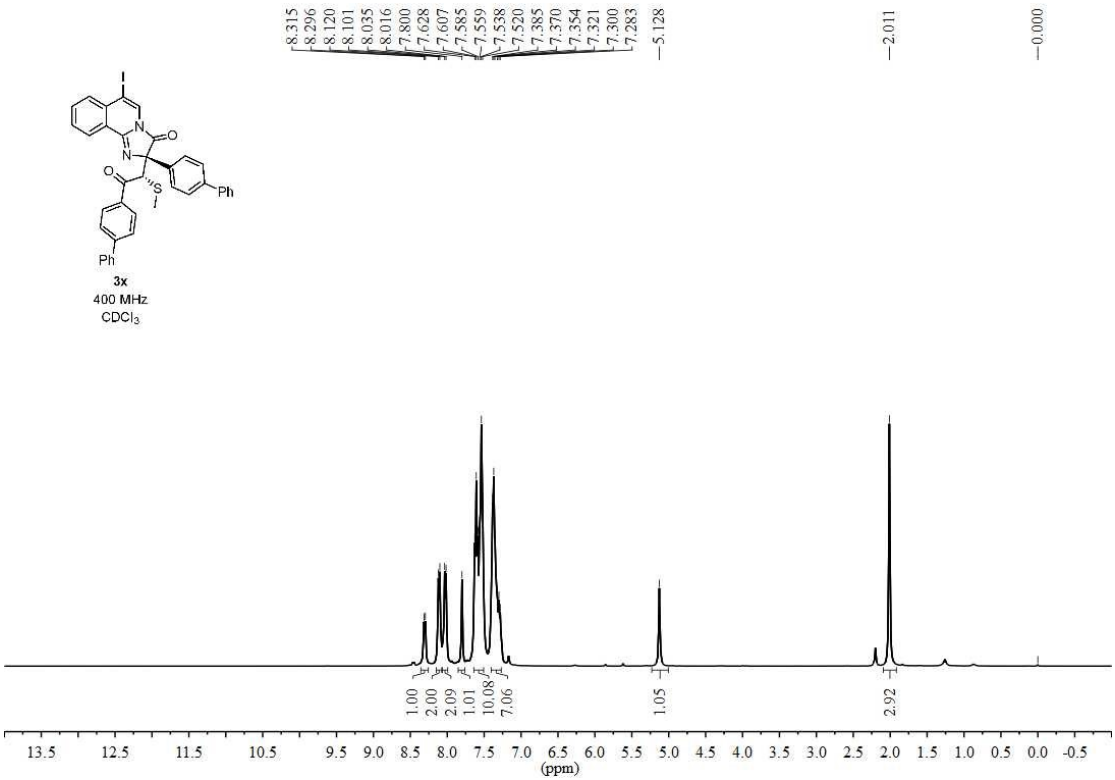

107.559
108.623
3u
376 MHz
CDCl3
(ppm)

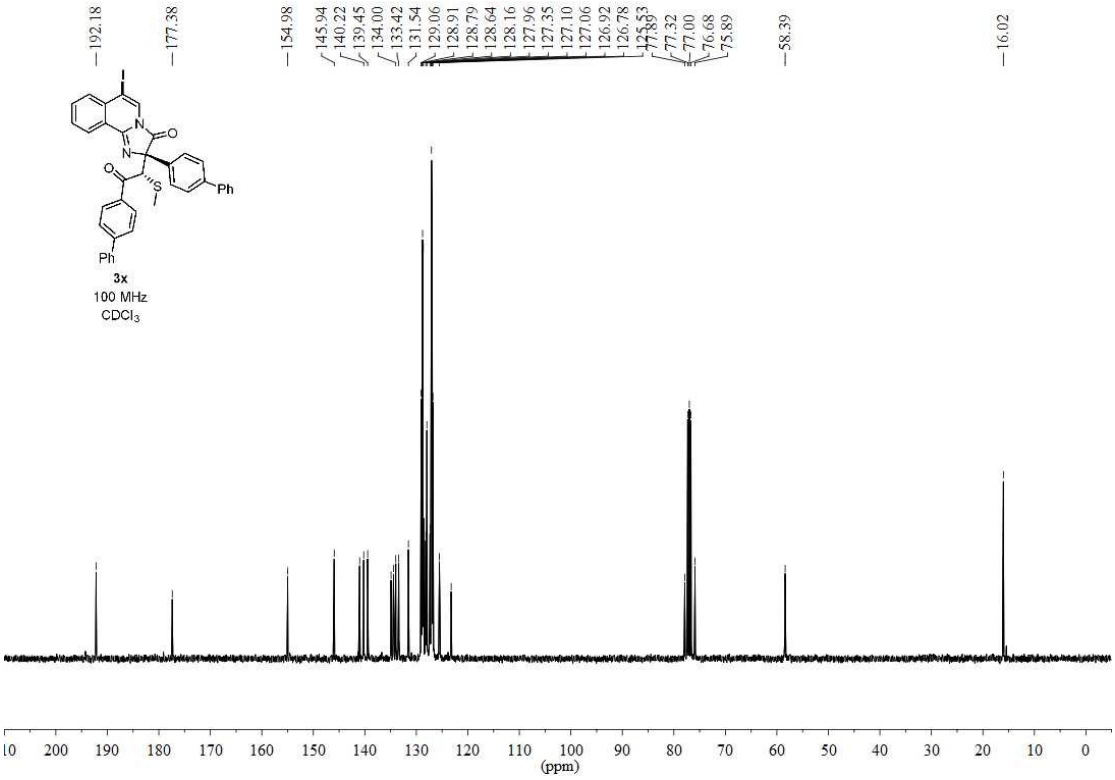

8.318
8.299
8.051
7.866
7.845
7.781
7.756
7.682
7.662
7.647
7.510
7.489
7.452
7.431
4.797
2.002
0.000
3v
400 MHz
CDCl3
1.00
2.01
1.03
2.02
2.09
3.10
1.00
3.00
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
(ppm)

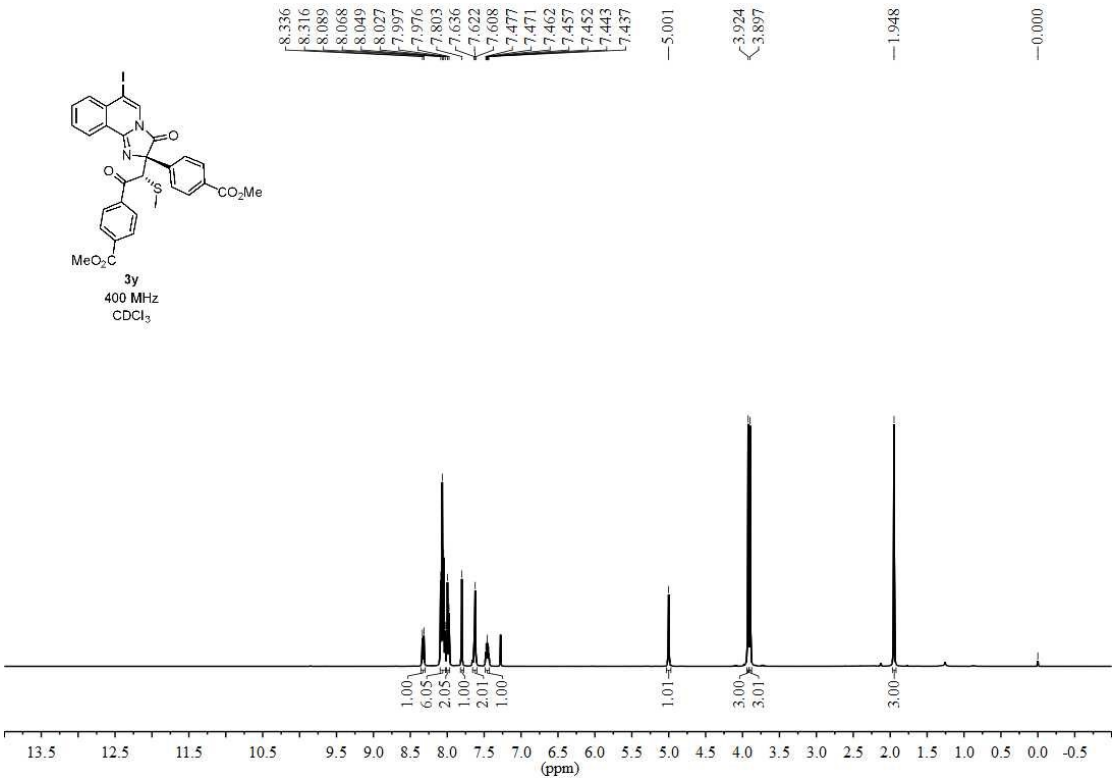

190.21
176.66
155.79
138.12
135.80
134.62
134.57
133.95
133.23
132.81
132.42
131.83
130.63
130.61
129.97
129.58
129.27
127.58
126.88
126.71
125.68
78.45
77.32
77.00
76.68
74.74
58.43
15.81
3v
100 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

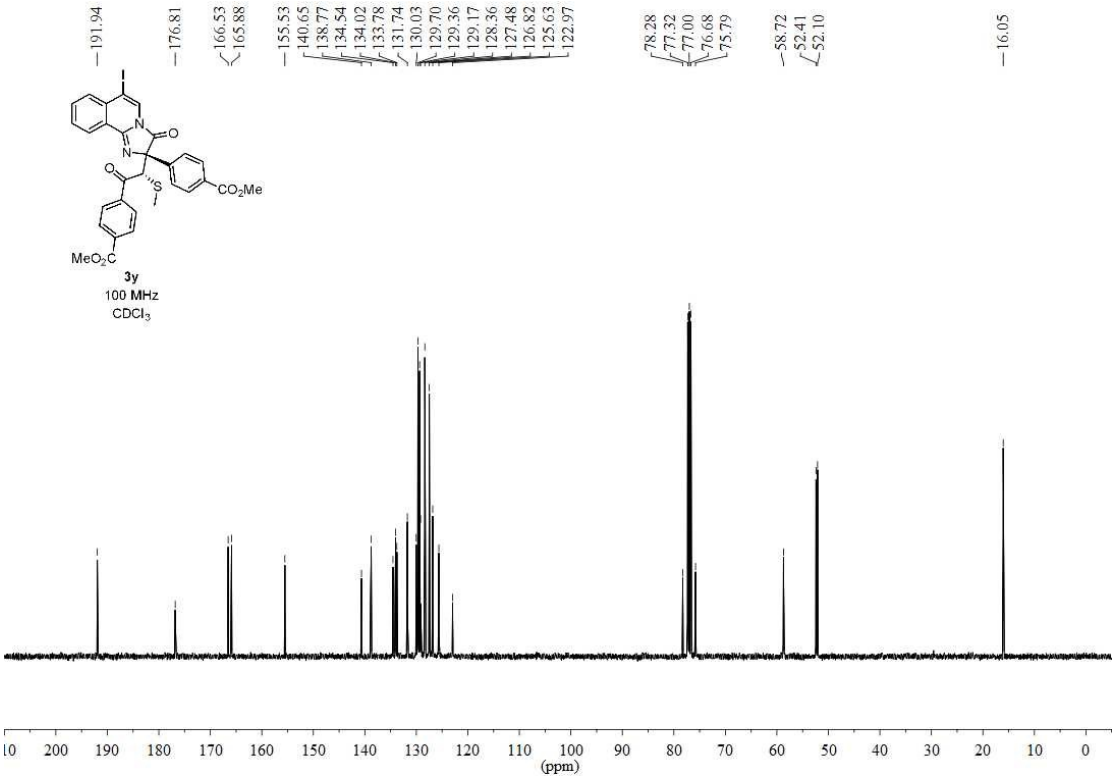

8.328
8.309
7.880
7.797
7.702
7.682
7.667
7.651
7.529
7.499
7.484
7.329
4.735
2.016
0.000
3w
400 MHz
CDCl3
1.00
2.01
3.00
2.00
2.00
1.00
1.03
3.01
(ppm)

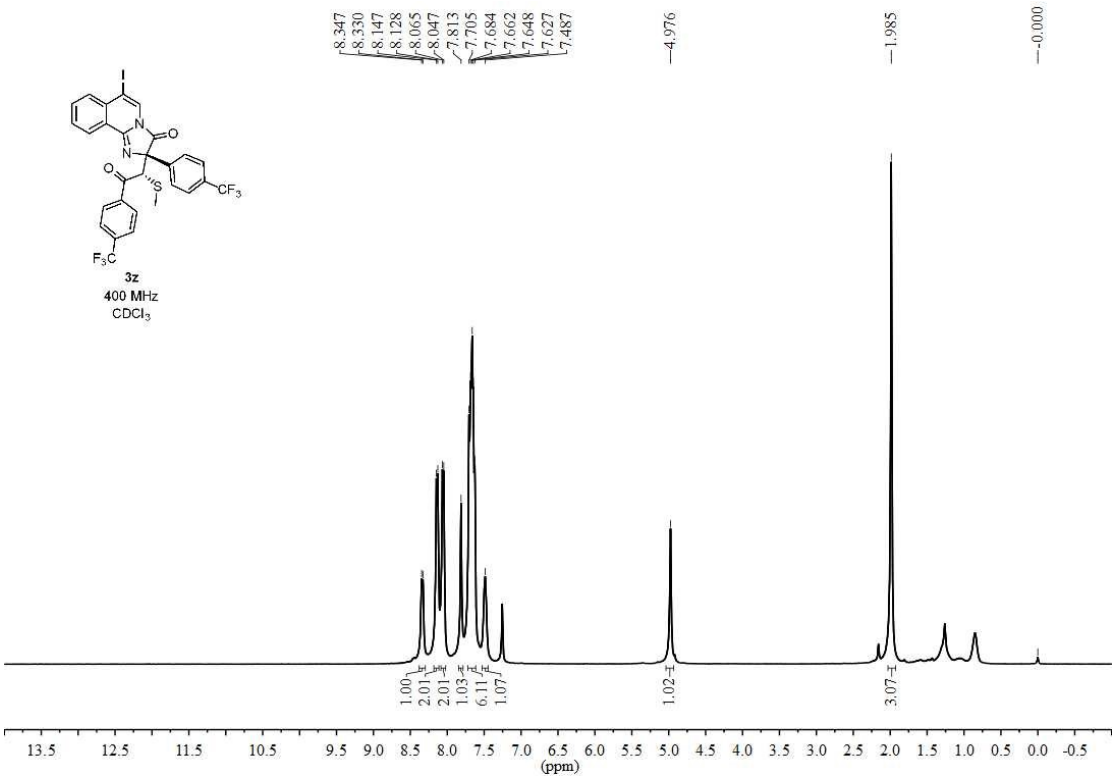

189.95
176.38
156.04
138.88
137.63
135.61
134.89
134.67
134.09
133.20
131.93
129.38
128.82
127.02
126.72
126.19
125.86
122.81
78.57
77.32
77.00
76.68
74.69
58.72
15.88
3w
100 MHz
CDCl3
(ppm)

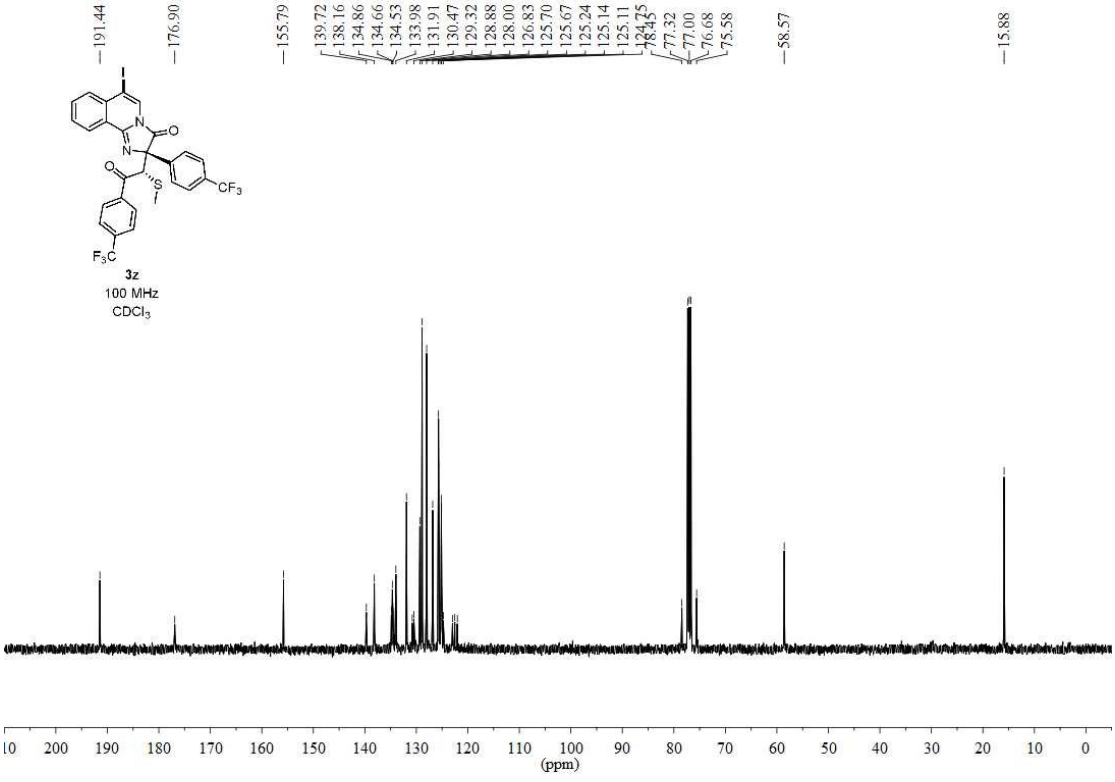

8.315
8.296
8.120
8.101
8.035
8.016
7.800
7.628
7.607
7.585
7.559
7.538
7.520
7.385
7.370
7.354
7.321
7.300
7.283
5.128
2.011
0.000
3x
400 MHz
CDCl3
1.00
2.00
2.09
1.01
10.08
7.06
1.05
2.92
(ppm)

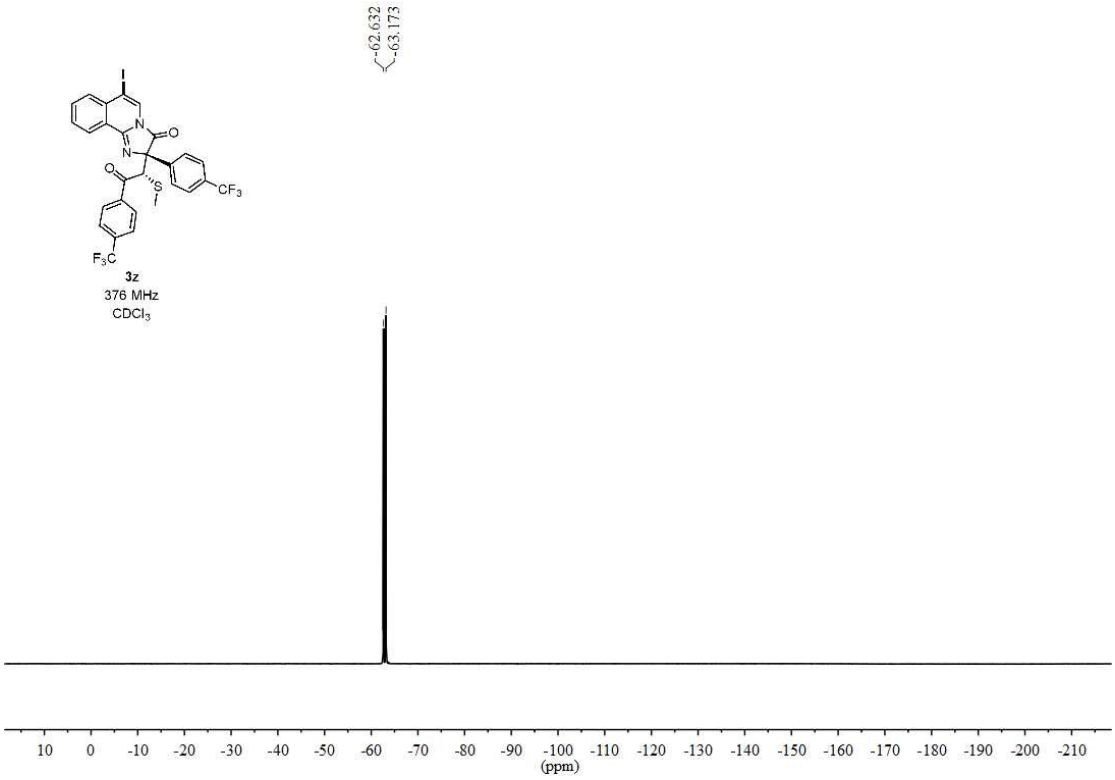

192.18
177.38
154.98
145.94
140.22
139.45
134.00
133.42
131.54
129.06
128.91
128.79
128.64
128.16
127.96
127.35
127.10
127.06
126.92
126.78
125.53
77.32
77.00
76.68
75.89
58.39
16.02
3x
100 MHz
CDCl3
(ppm)

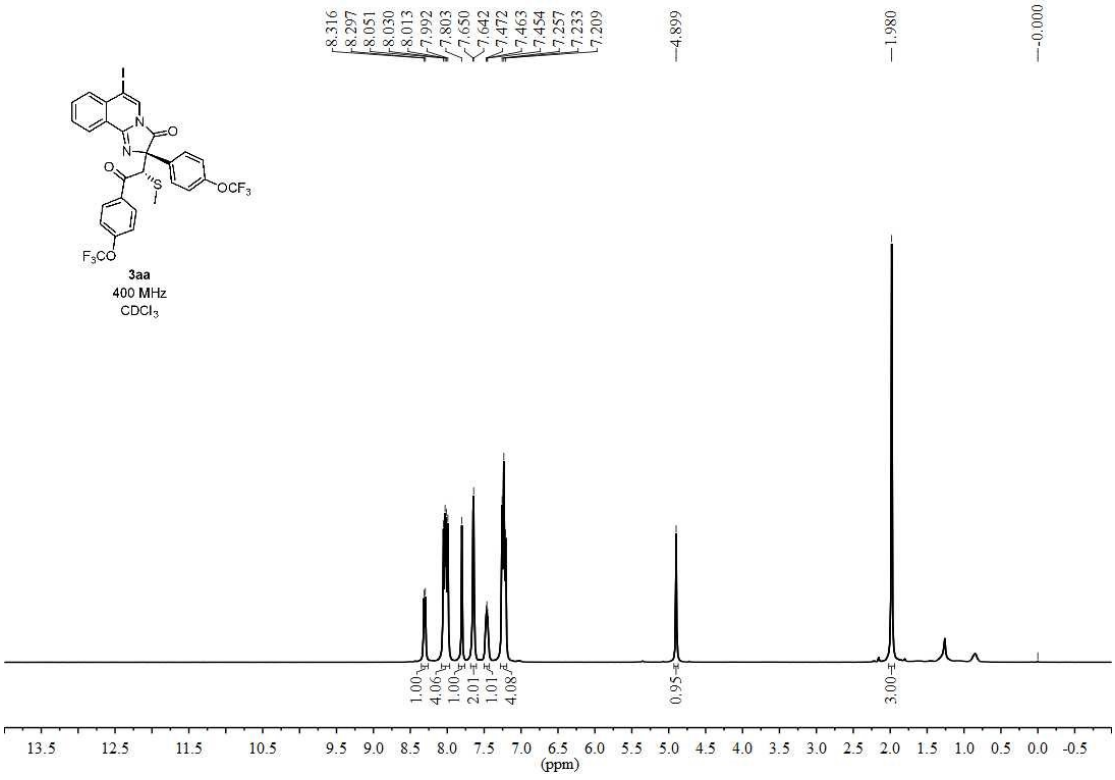

8.336
8.316
8.089
8.068
8.049
8.027
7.997
7.976
7.803
7.636
7.622
7.608
7.477
7.471
7.462
7.457
7.452
7.443
7.437
5.001
3.924
3.897
1.948
0.000
3y
400 MHz
CDCl3
1.00
6.05
2.05
1.00
2.01
1.00
1.01
3.00
3.01
3.00
(ppm)

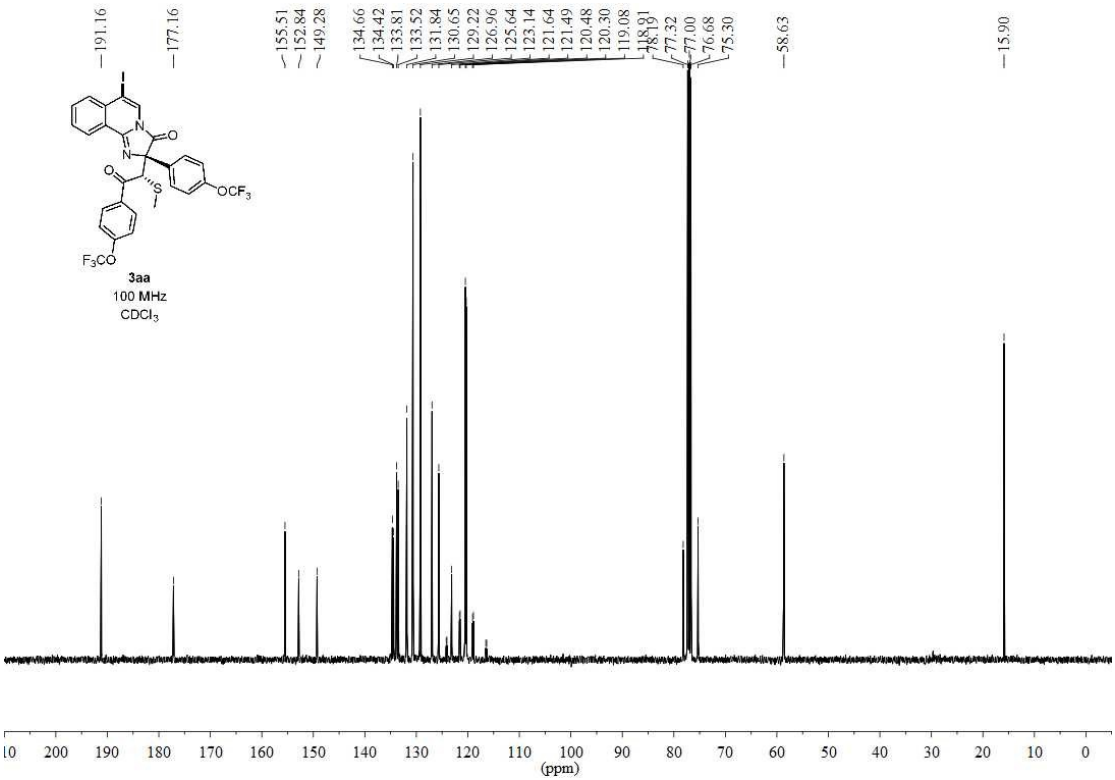

191.94
176.81
166.53
165.88
155.53
140.65
138.77
134.54
134.02
133.78
131.74
130.03
129.70
129.36
129.17
128.36
127.48
126.82
125.63
122.97
78.28
77.32
77.00
76.68
75.79
58.72
52.41
52.10
16.05
3y
100 MHz
CDCl3
(ppm)

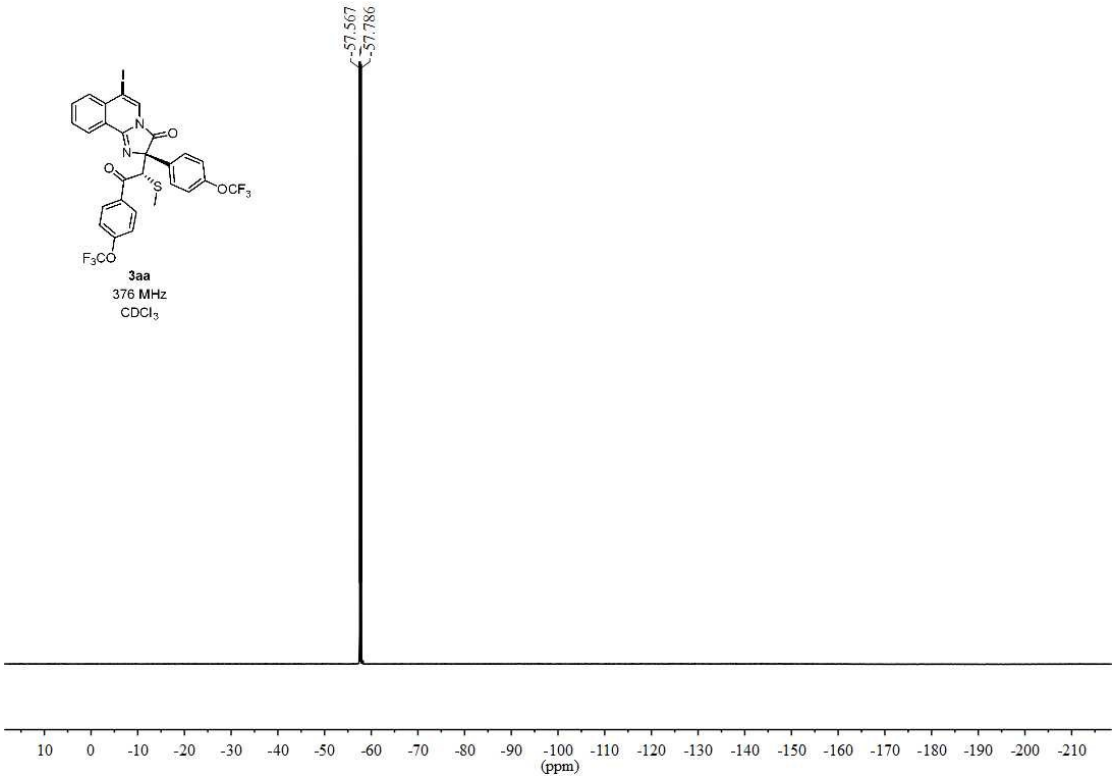

8.347
8.330
8.147
8.128
8.065
8.047
7.813
7.705
7.684
7.662
7.648
7.627
7.487
4.976
1.985
0.000
3z
400 MHz
CDCl3
1.00
2.01
2.01
1.03
6.11
1.07
1.02
3.07
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
(ppm)

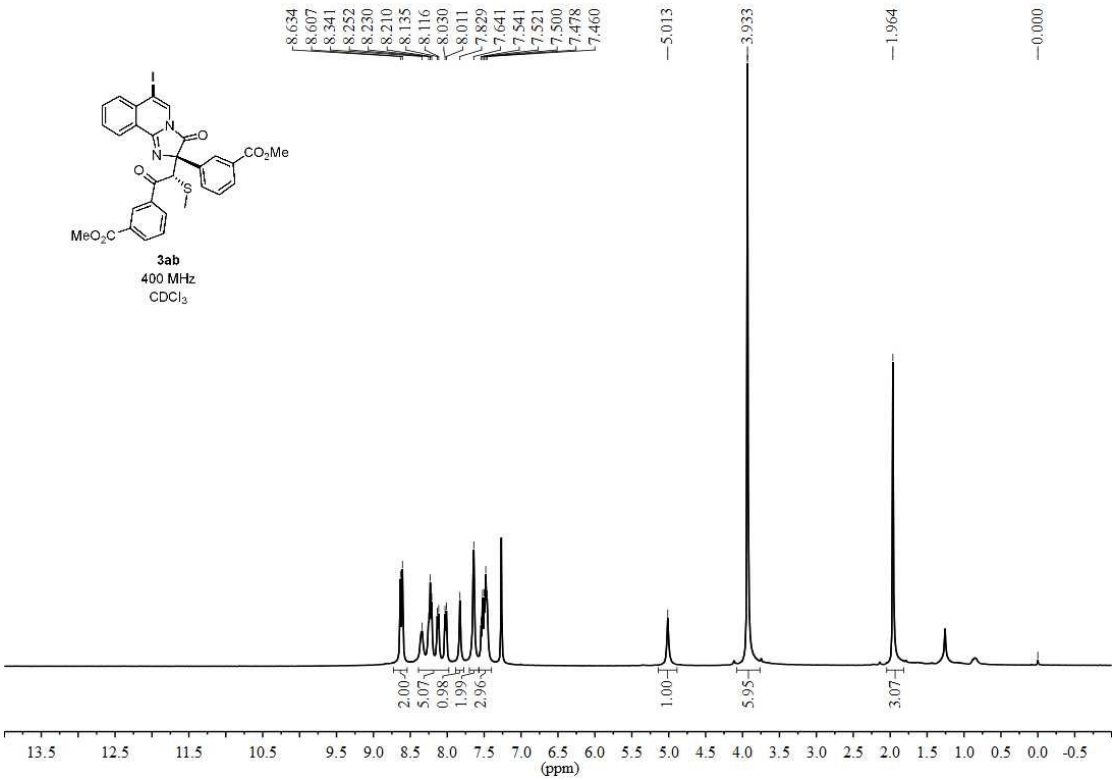

191.44
176.90
155.79
139.72
138.16
134.86
134.66
134.53
133.98
131.91
130.47
129.32
128.88
128.00
126.83
125.70
125.67
125.24
125.14
125.11
124.75
78.45
77.32
77.00
76.68
75.58
58.57
15.88
3z
100 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

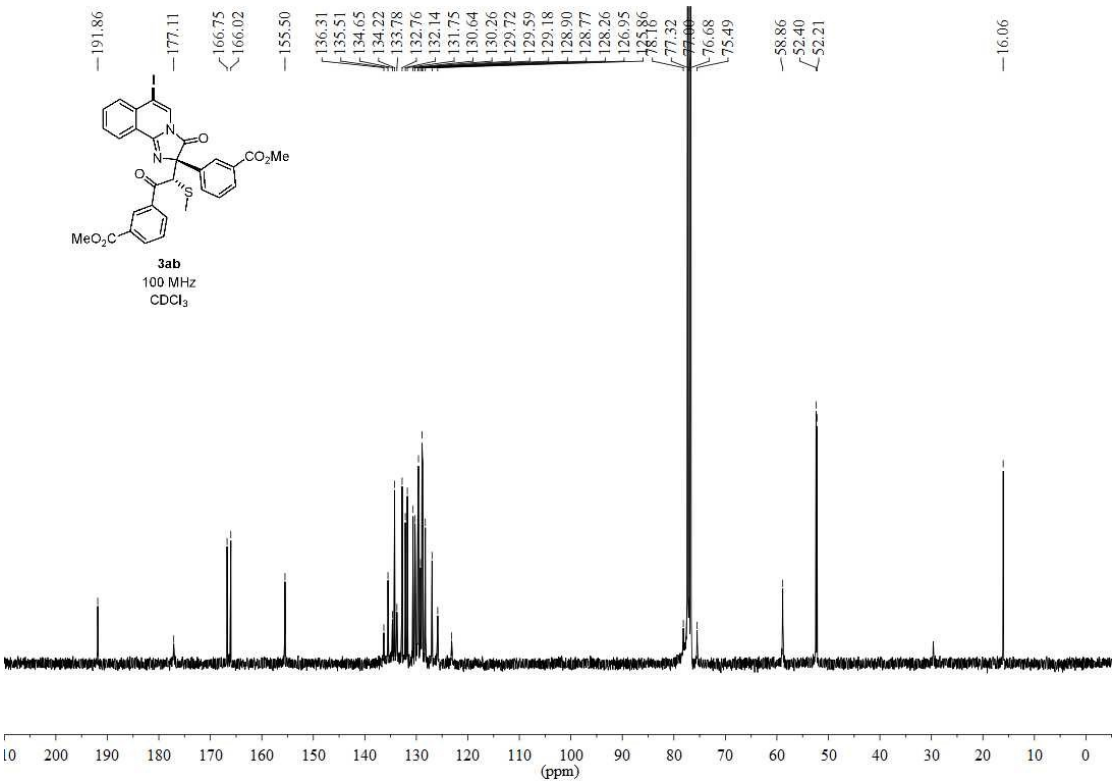

-62.632
-63.173
3z
376 MHz
CDCl3
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
(ppm)

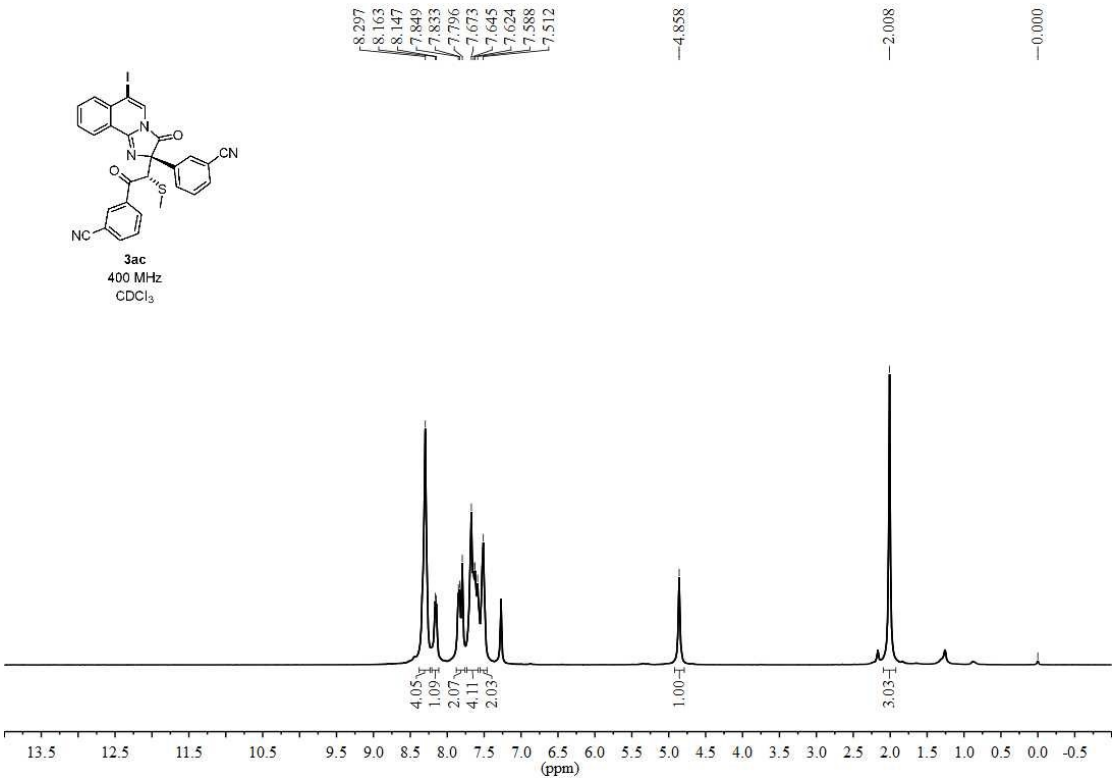

8.316
8.297
8.051
8.030
8.013
7.992
7.803
7.650
7.642
7.472
7.463
7.454
7.257
7.233
7.209
4.899
1.980
0.000
3aa
400 MHz
CDCl3
1.00
4.06
1.00
2.01
1.01
4.08
0.95
3.00
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
(ppm)

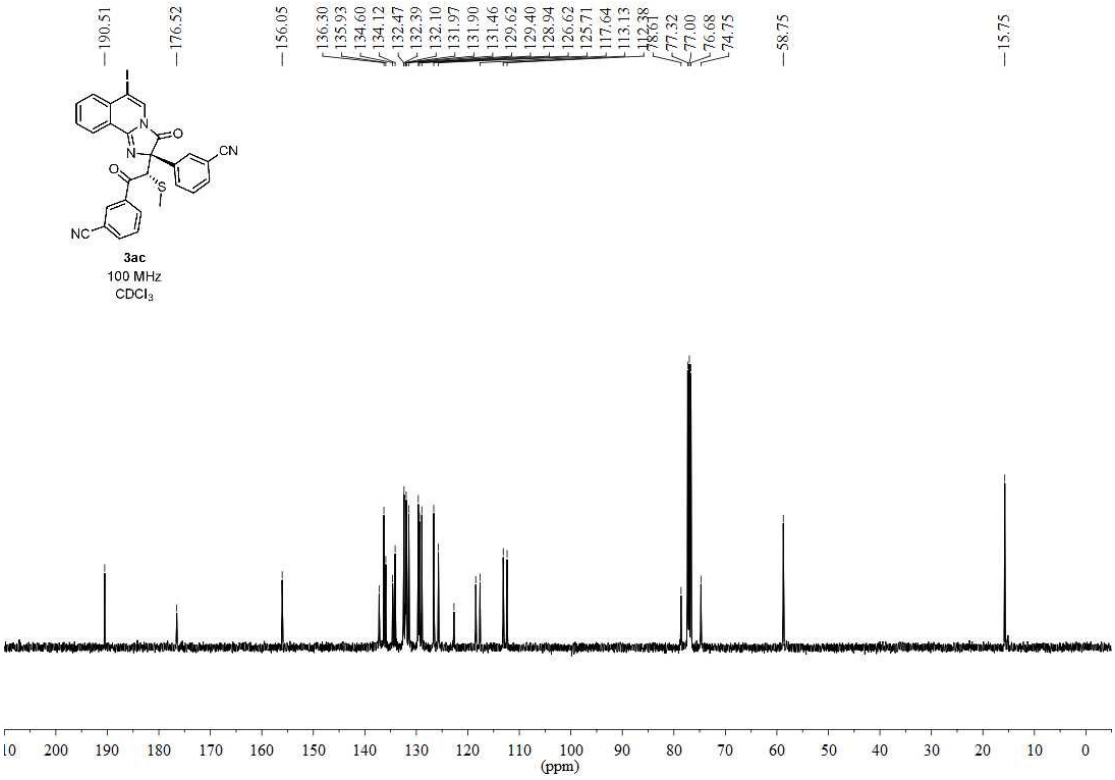

191.16
177.16
155.51
152.84
149.28
134.66
134.42
133.81
133.52
131.84
130.65
129.22
126.96
125.64
123.14
121.64
121.49
120.48
120.30
119.08
118.91
78.19
77.32
77.00
76.68
75.30
58.63
15.90
OCF3
F3CO
3aa
100 MHz
CDCl3
(ppm)

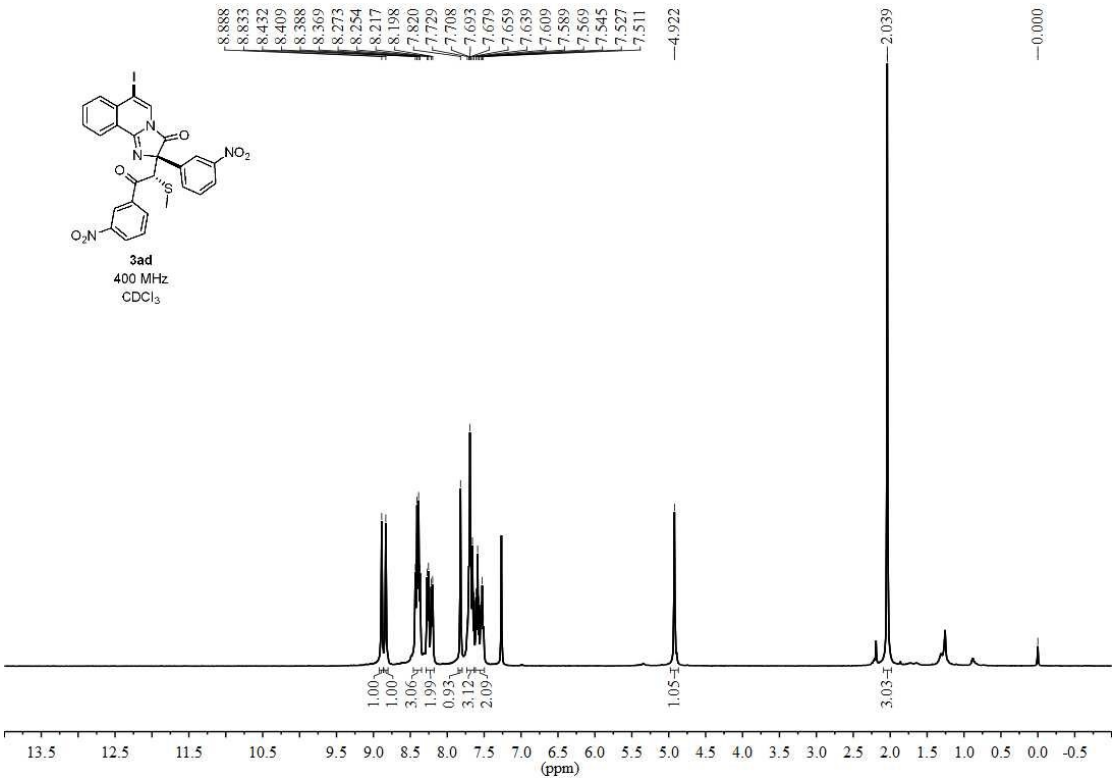

57.567
57.786
OCF3
F3CO
3aa
376 MHz
CDCl3
(ppm)

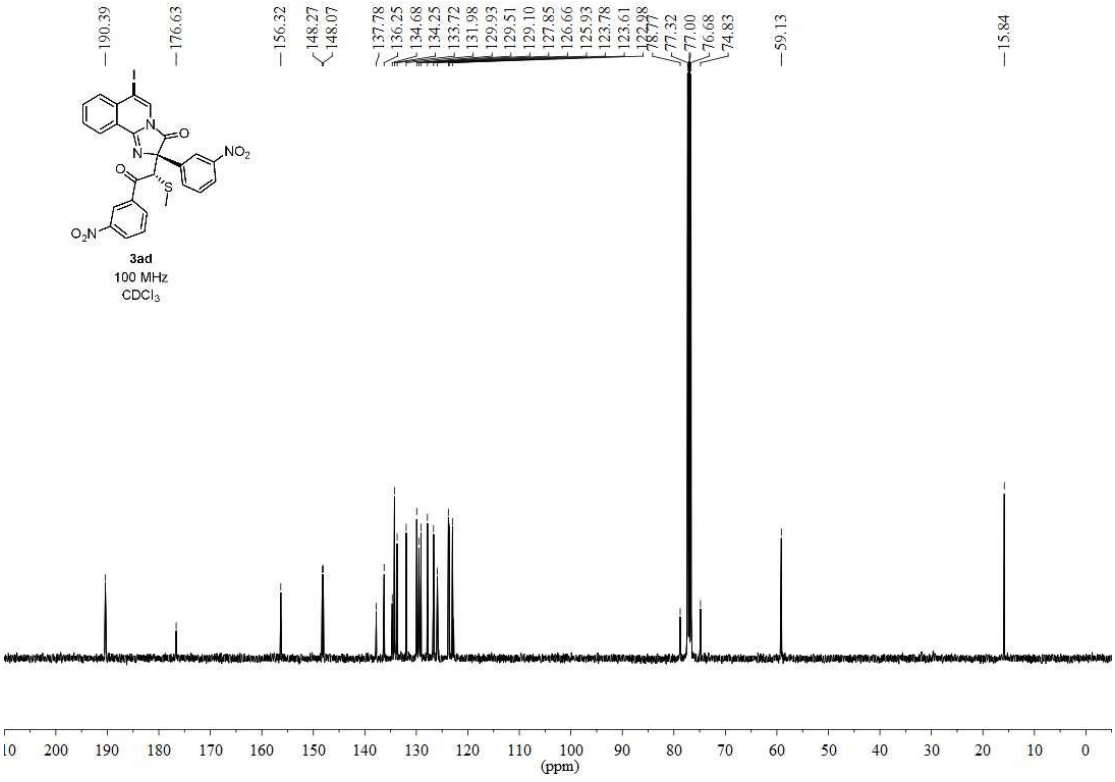

8.634
8.607
8.341
8.252
8.230
8.210
8.135
8.116
8.030
8.011
7.829
7.641
7.541
7.521
7.500
7.478
7.460
5.013
3.933
1.964
0.000
2.00
5.07
0.98
1.99
2.96
1.00
5.95
3.07
(ppm)
3ab
400 MHz
CDCl3


191.86
177.11
166.75
166.02
155.50
136.31
135.51
134.65
134.22
133.78
132.76
132.14
131.75
130.64
130.26
129.72
129.59
129.18
128.90
128.77
128.26
126.95
125.86
78.16
77.32
76.68
75.49
58.86
52.40
52.21
16.06
(ppm)
3ab
100 MHz
CDCl3


8.297
8.163
8.147
7.849
7.833
7.796
7.673
7.645
7.624
7.588
7.512
4.858
2.008
0.000
3ac
400 MHz
CDCl3
4.05
1.09
2.07
4.11
2.03
1.00
3.03
(ppm)


190.51
176.52
156.05
136.30
135.93
134.60
134.12
132.47
132.39
132.10
131.97
131.90
131.46
129.62
129.40
128.94
126.62
125.71
117.64
113.13
112.38
78.61
77.32
77.00
76.68
74.75
58.75
15.75
3ac
100 MHz
CDCl3
(ppm)


8.888
8.833
8.432
8.409
8.388
8.369
8.273
8.254
8.217
8.198
7.820
7.729
7.708
7.693
7.679
7.659
7.639
7.609
7.589
7.569
7.545
7.527
7.511
4.922
2.039
0.000
3ad
400 MHz
CDCl3
1.00
1.00
3.06
1.99
0.93
3.12
2.09
1.05
3.03
(ppm)


190.39
176.63
156.32
148.27
148.07
137.78
136.25
134.68
134.25
133.72
131.98
129.93
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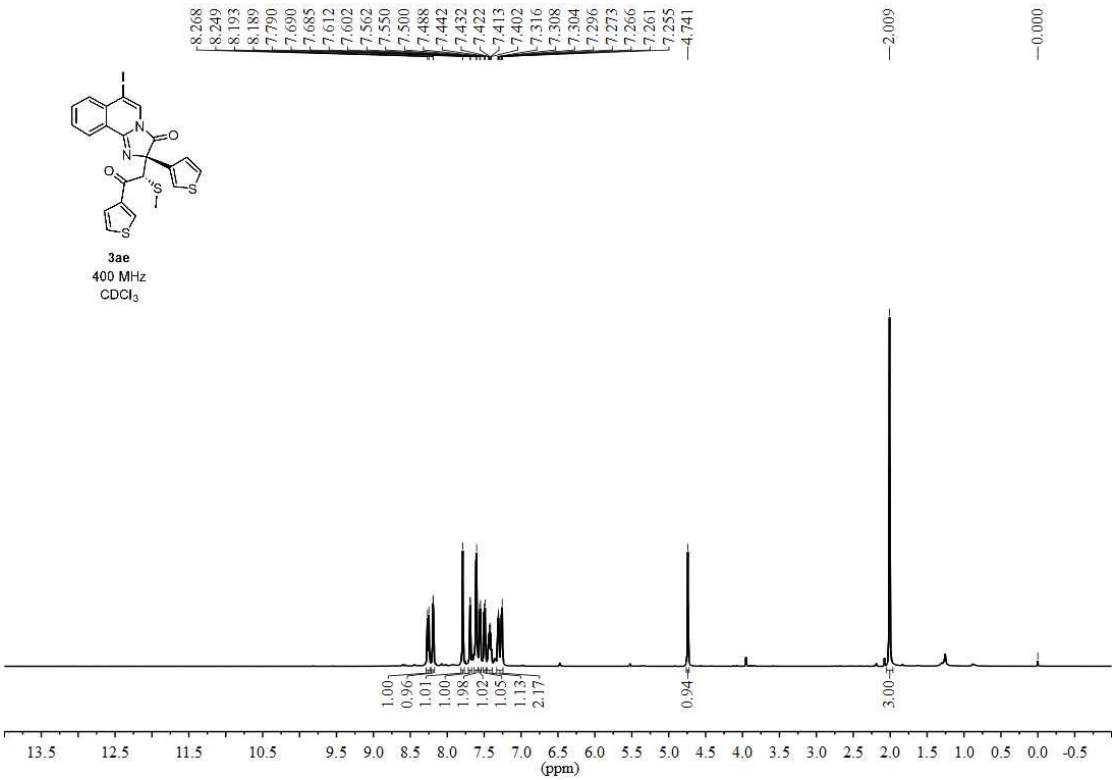
129.10
127.85
126.66
125.93
123.78
123.61
122.98
78.77
77.32
77.00
76.68
74.83
59.13
15.84
3ad
100 MHz
CDCl3
(ppm)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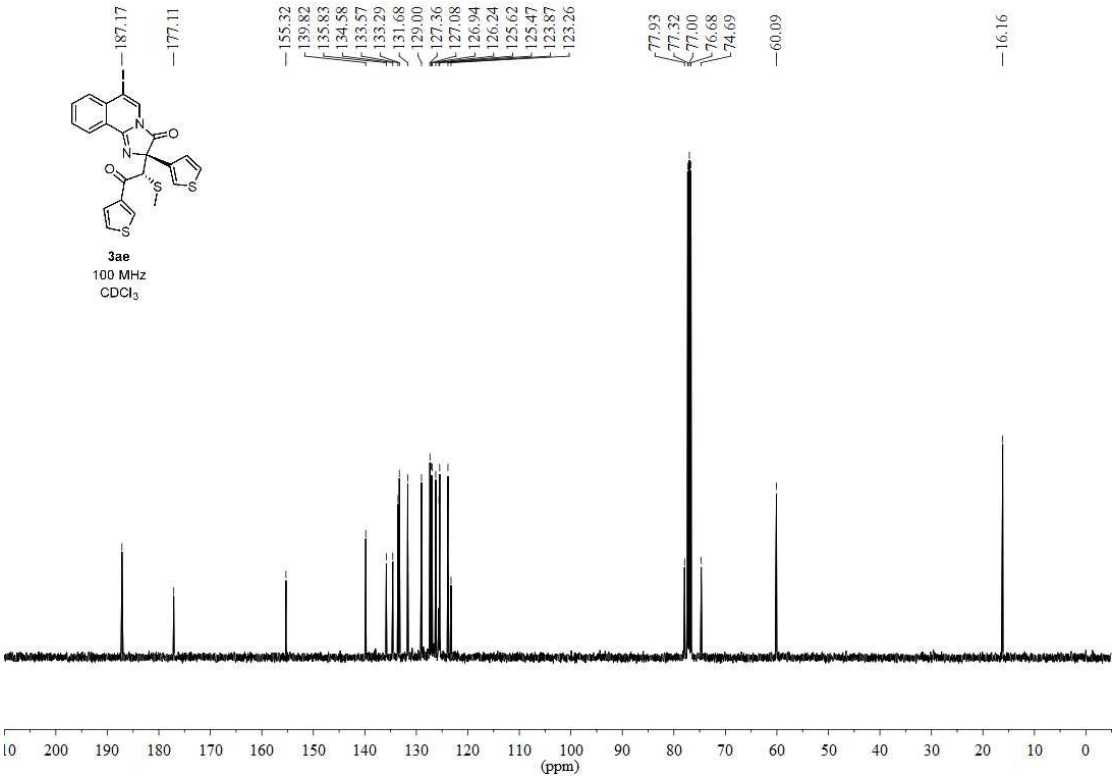
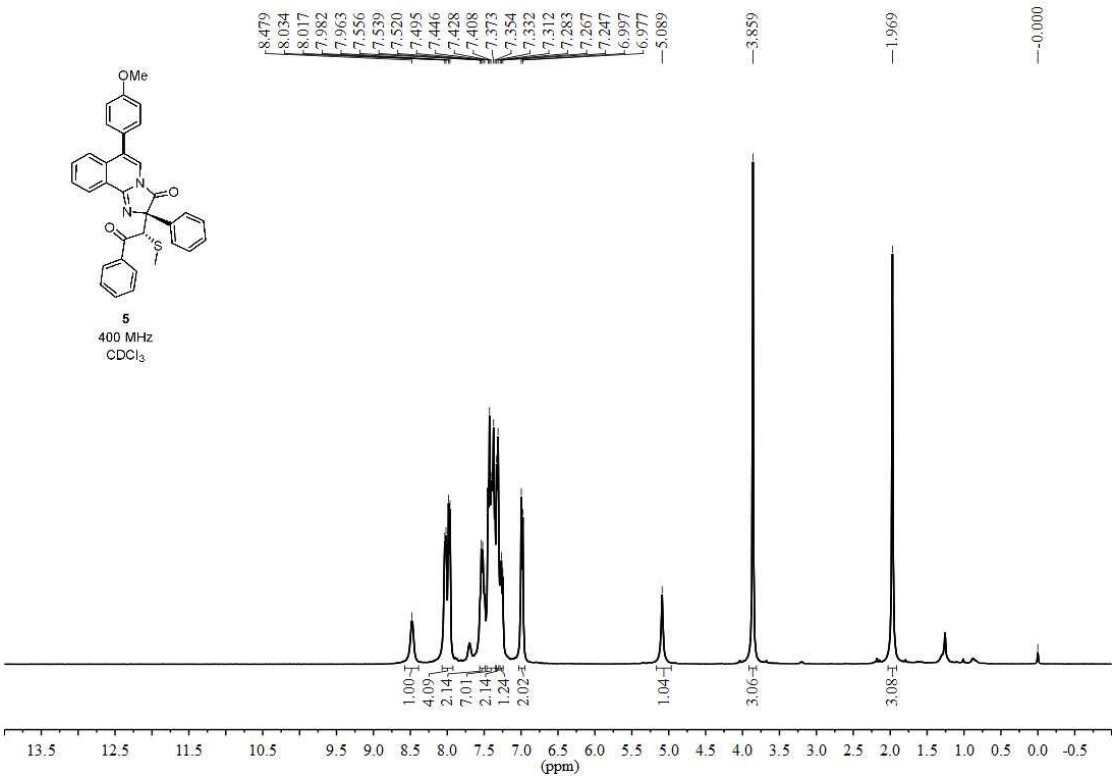
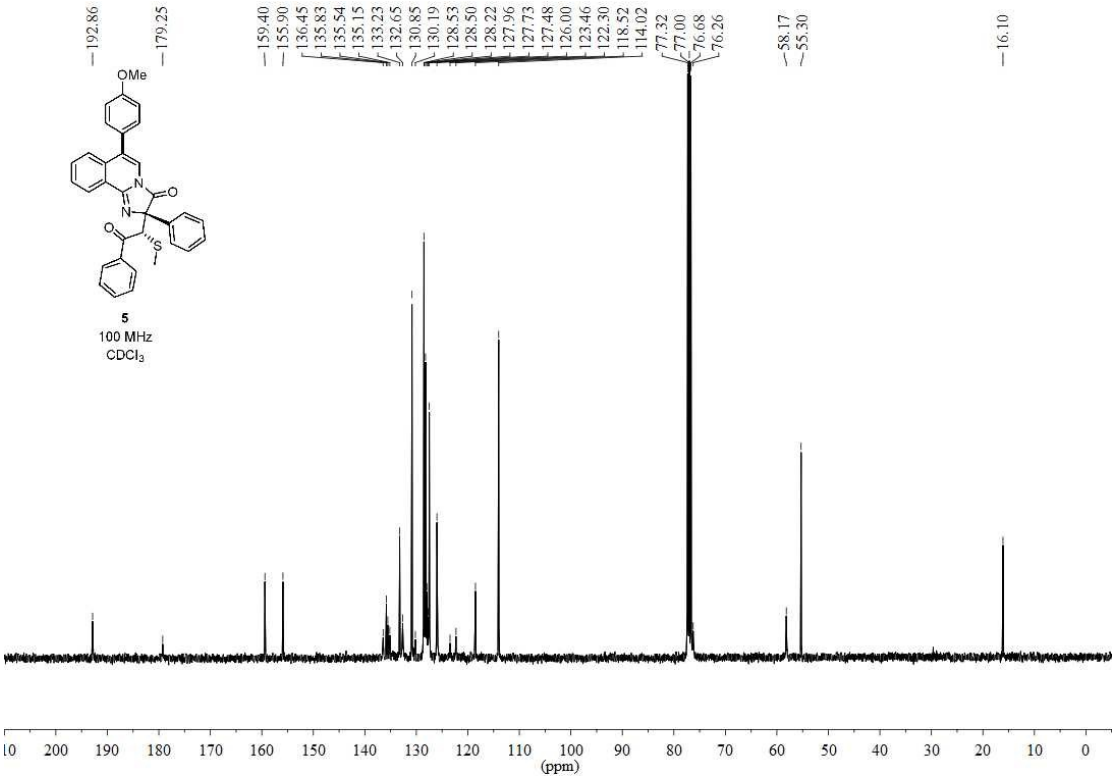
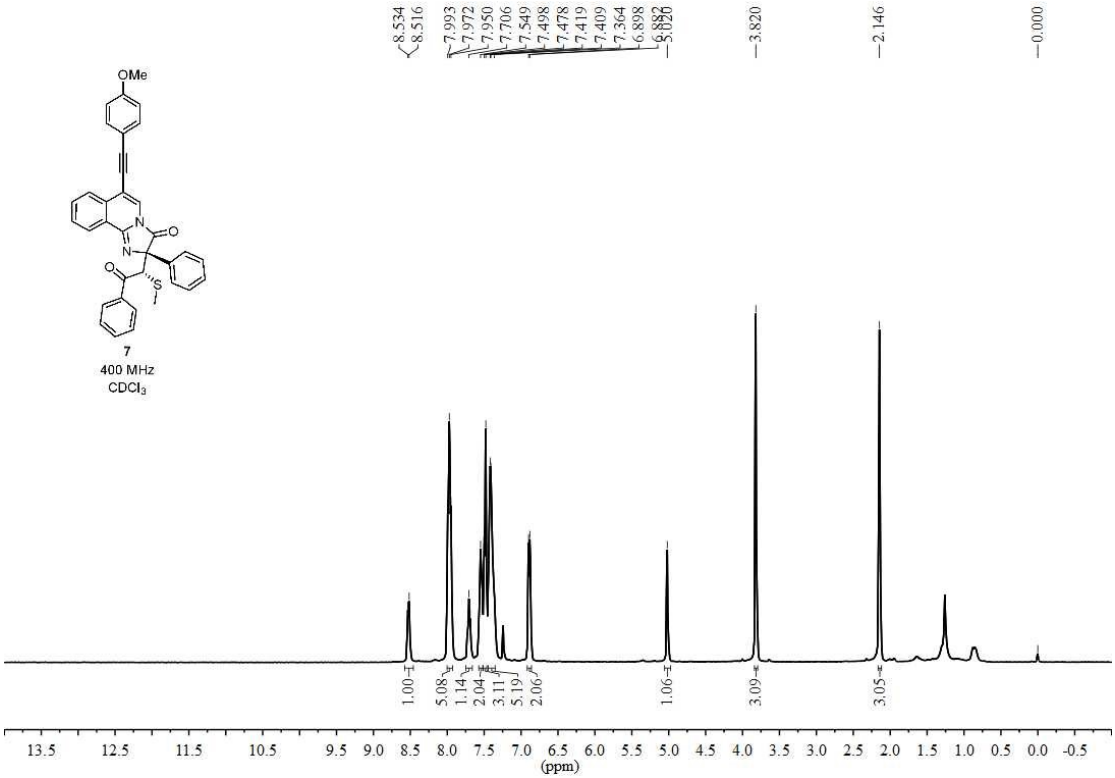
8.189
7.790
7.690
7.685
7.612
7.602
7.562
7.550
7.500
7.488
7.442
7.432
7.422
7.413
7.402
7.316
7.308
7.304
7.296
7.273
7.266
7.261
7.255
4.741
2.009
0.000
3ae
400 MHz
CDCl3
1.00
0.96
1.01
1.00
1.98
1.02
1.05
1.13
2.17
0.94
3.00
(ppm)


187.17
177.11
155.32
139.82
135.83
134.58
133.57
133.29
131.68
129.00
127.36
127.08
126.94
126.24
125.62
125.47
123.87
123.26
77.93
77.32
77.00
76.68
74.69
60.09
16.16
3ae
100 MHz
CDCl3
(ppm)


8.479
8.034
8.017
7.982
7.963
7.556
7.539
7.520
7.495
7.446
7.428
7.408
7.373
7.354
7.332
7.312
7.283
7.267
7.247
6.997
6.977
5.089
3.859
1.969
0.000
OMe
5
400 MHz
CDCl3
1.00
4.09
2.14
7.01
2.14
1.24
2.02
1.04
3.06
3.08
(ppm)


192.86
179.25
159.40
155.90
136.45
135.83
135.54
135.15
133.23
132.65
130.85
130.19
128.53
128.50
128.22
127.96
127.73
127.48
126.00
123.46
122.30
118.52
114.02
77.32
77.00
76.68
76.26
58.17
55.30
16.10
OMe
5
100 MHz
CDCl3
(ppm)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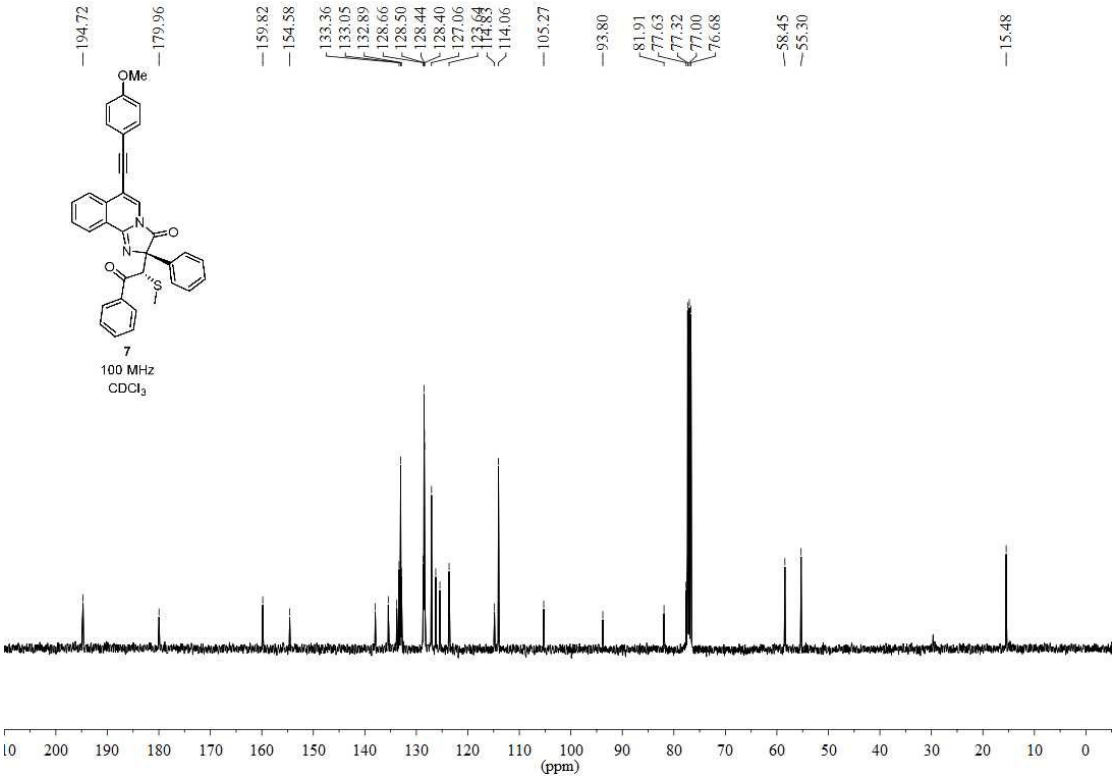
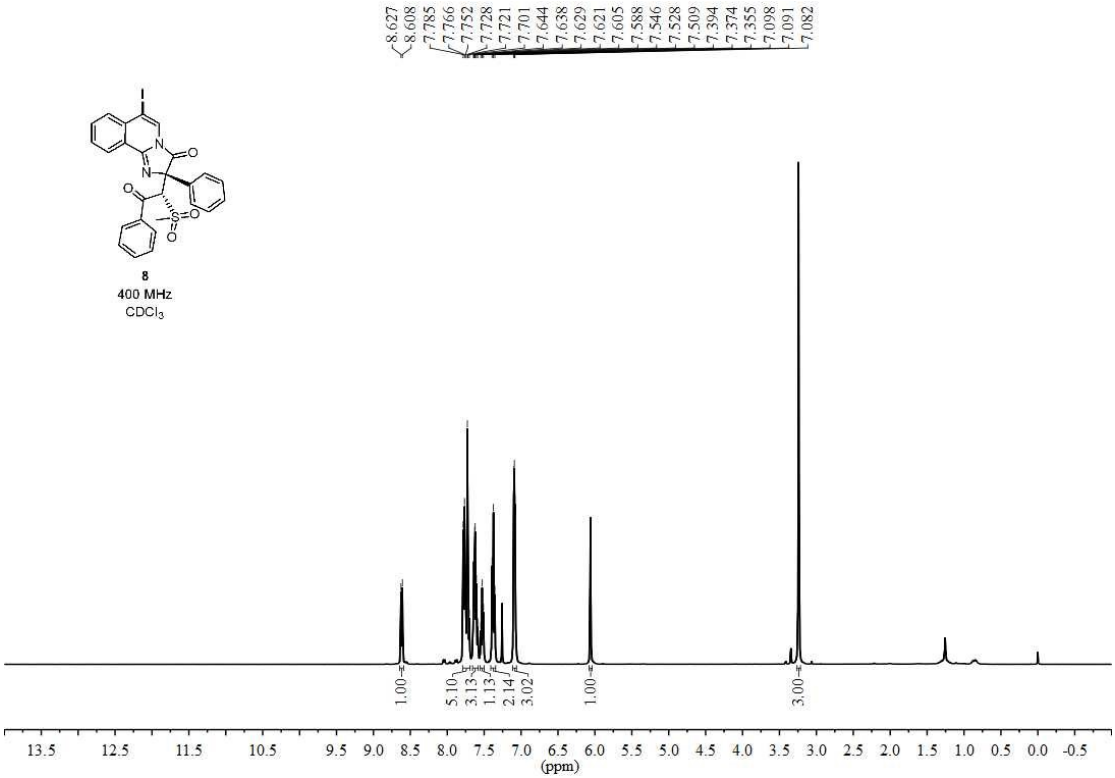
8.516
7.993
7.972
7.950
7.706
7.549
7.498
7.478
7.419
7.409
7.364
6.898
3.820
2.146
0.000
OMe
7
400 MHz
CDCl3
1.00
5.08
1.14
2.04
3.11
5.19
2.06
1.06
3.09
3.05
(ppm)


194.72
179.96
159.82
154.58
133.36
133.05
132.89
128.66
128.50
128.44
128.40
127.06
123.64
114.85
114.06
105.27
93.80
81.91
77.63
77.32
77.00
76.68
58.45
55.30
15.48
OMe
7
100 MHz
CDCl3
(ppm)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8.608
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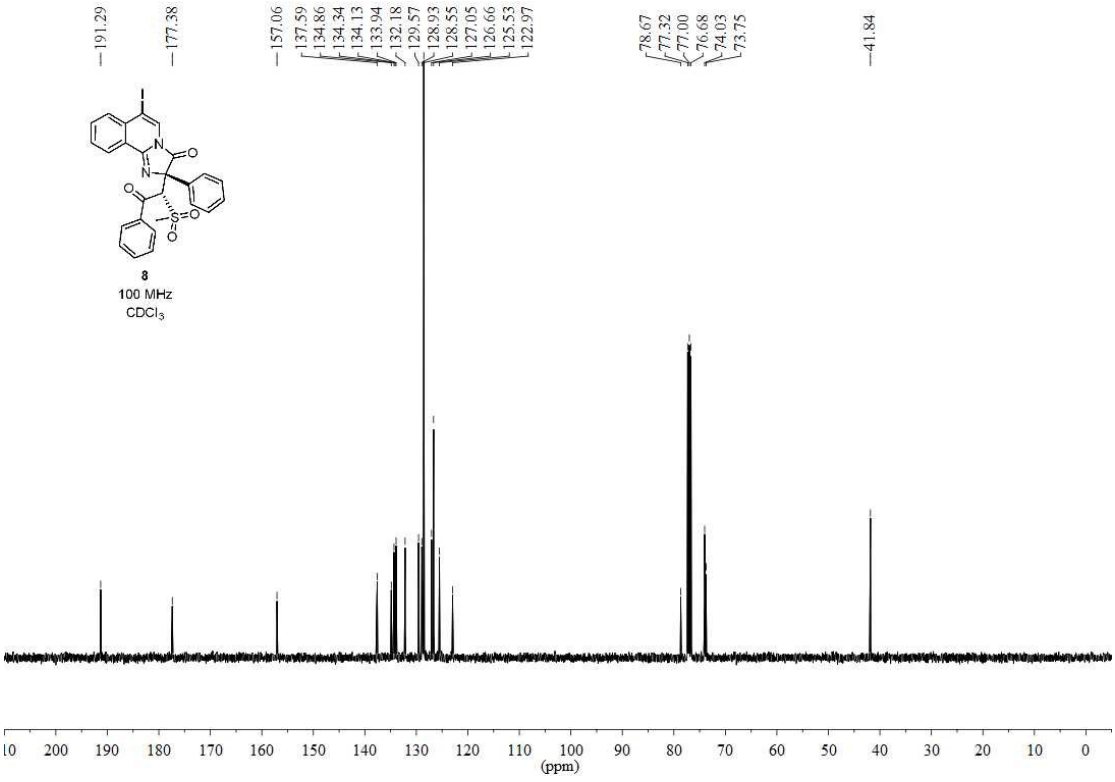
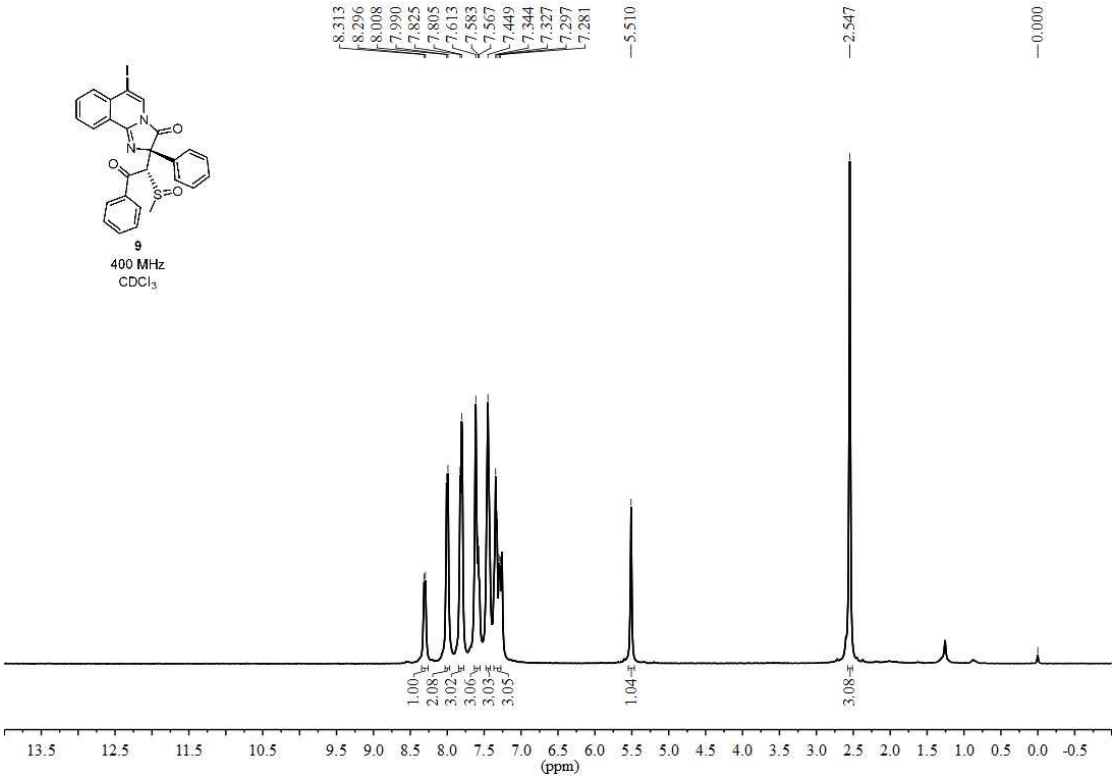
7.766
7.752
7.728
7.721
7.701
7.644
7.638
7.629
7.621
7.605
7.588
7.546
7.528
7.509
7.394
7.374
7.355
7.098
7.091
7.082
8
400 MHz
CDCl3
1.00
5.10
3.13
1.13
2.14
3.02
1.00
3.00
(ppm)


191.29
177.38
157.06
137.59
134.86
134.34
134.13
133.94
132.18
129.57
128.93
128.55
127.05
126.66
125.53
122.97
78.67
77.32
77.00
76.68
74.03
73.75
41.84
8
100 MHz
CDCl3
(ppm)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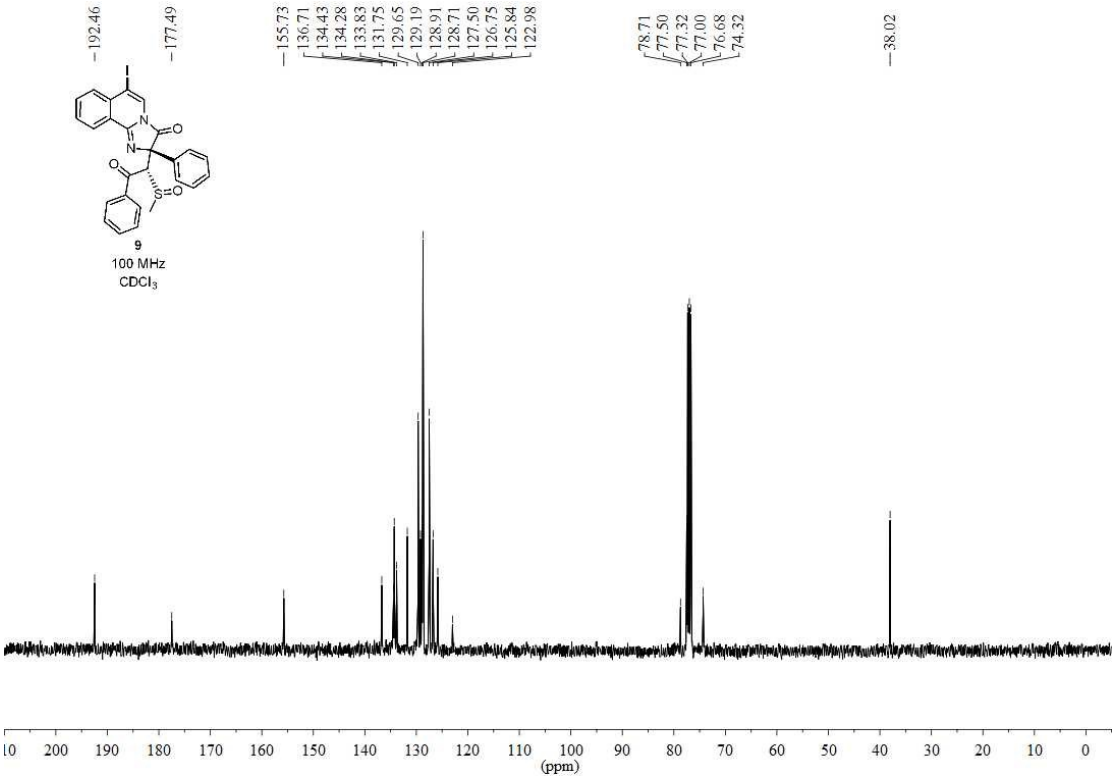
8.008
7.990
7.825
7.805
7.613
7.583
7.567
7.449
7.344
7.327
7.297
7.281
5.510
2.547
0.000
9
400 MHz
CDCl3
1.00
2.08
3.02
3.06
3.03
3.05
1.04
3.08
(ppm)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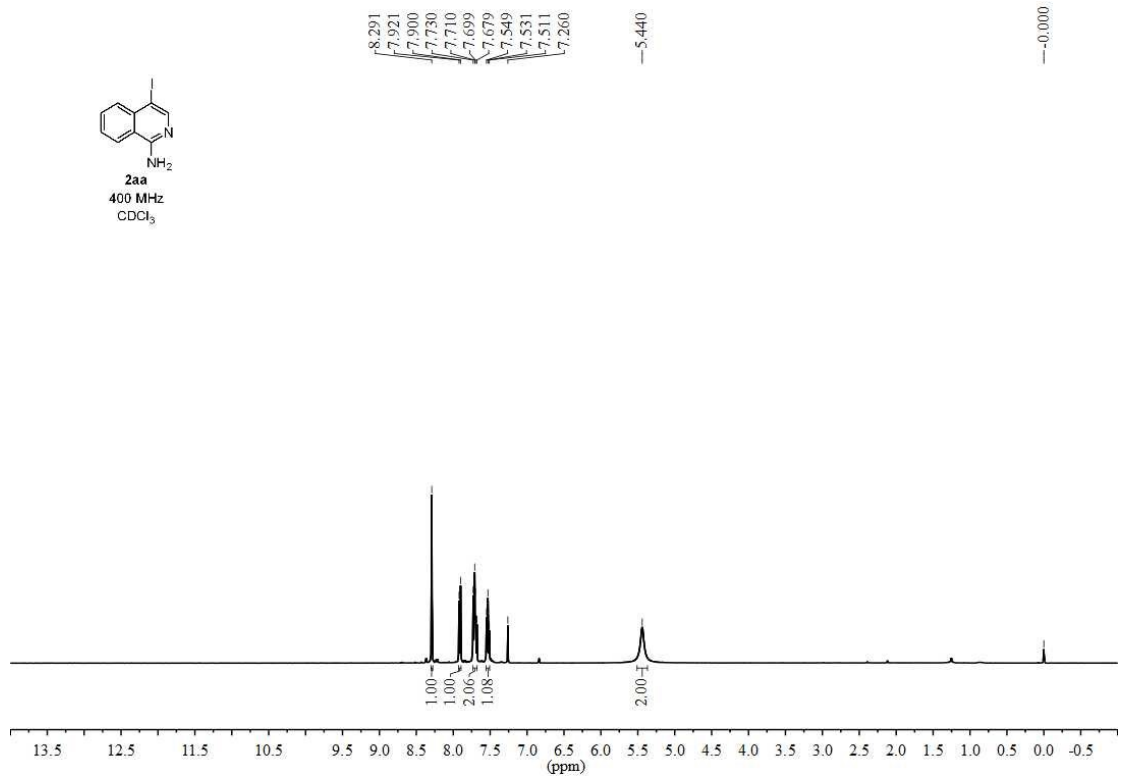
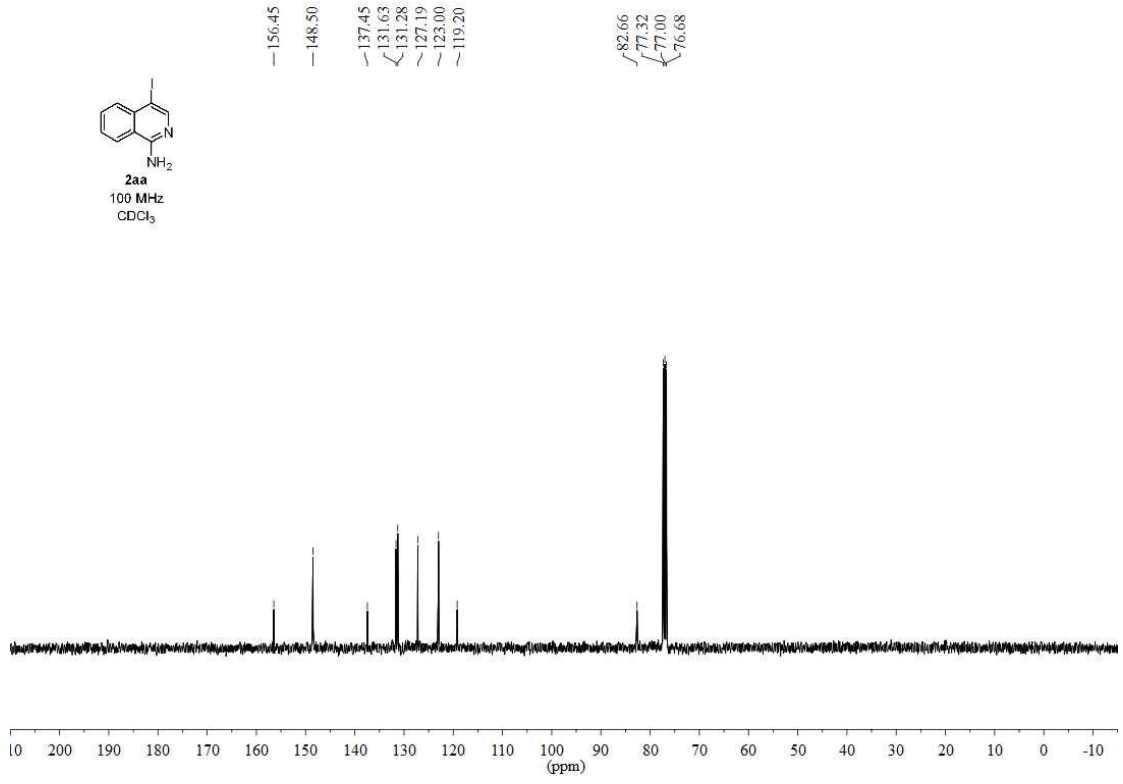
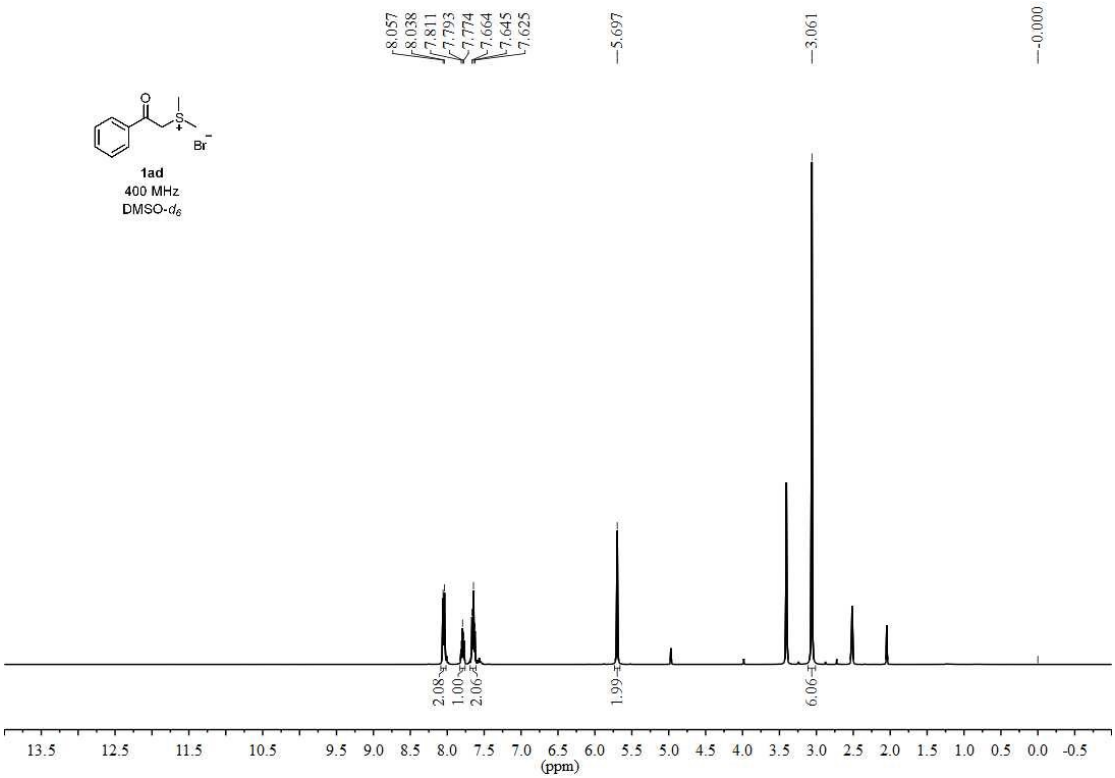
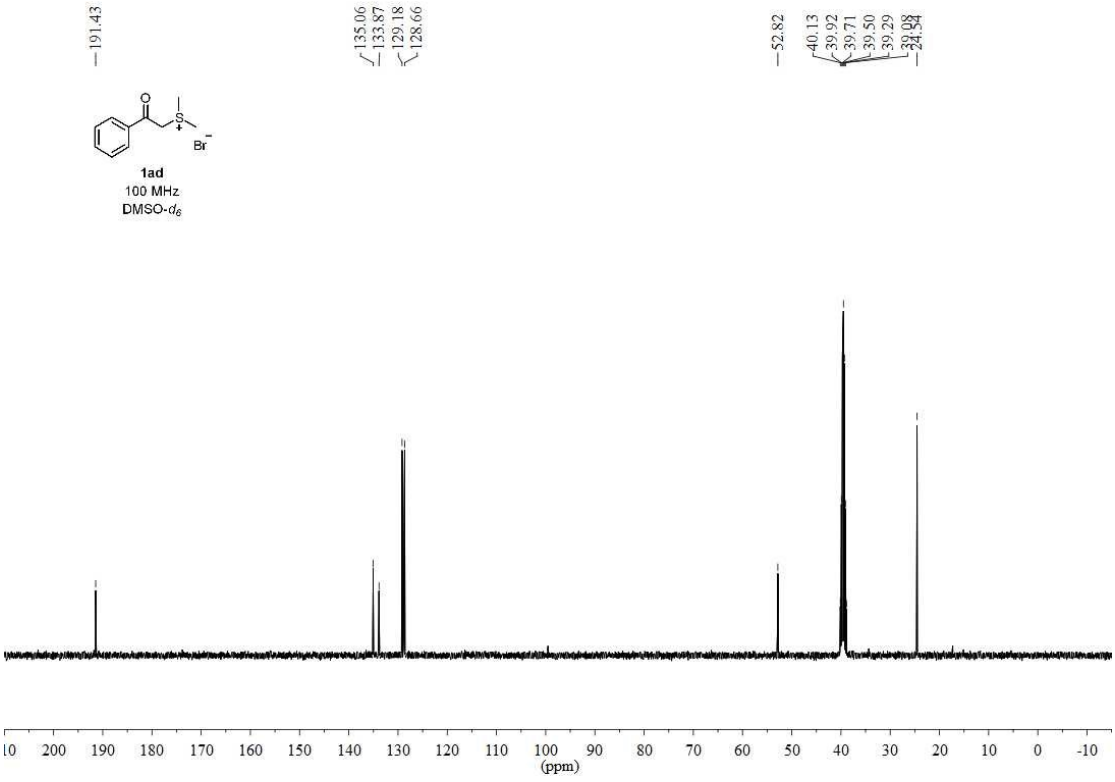
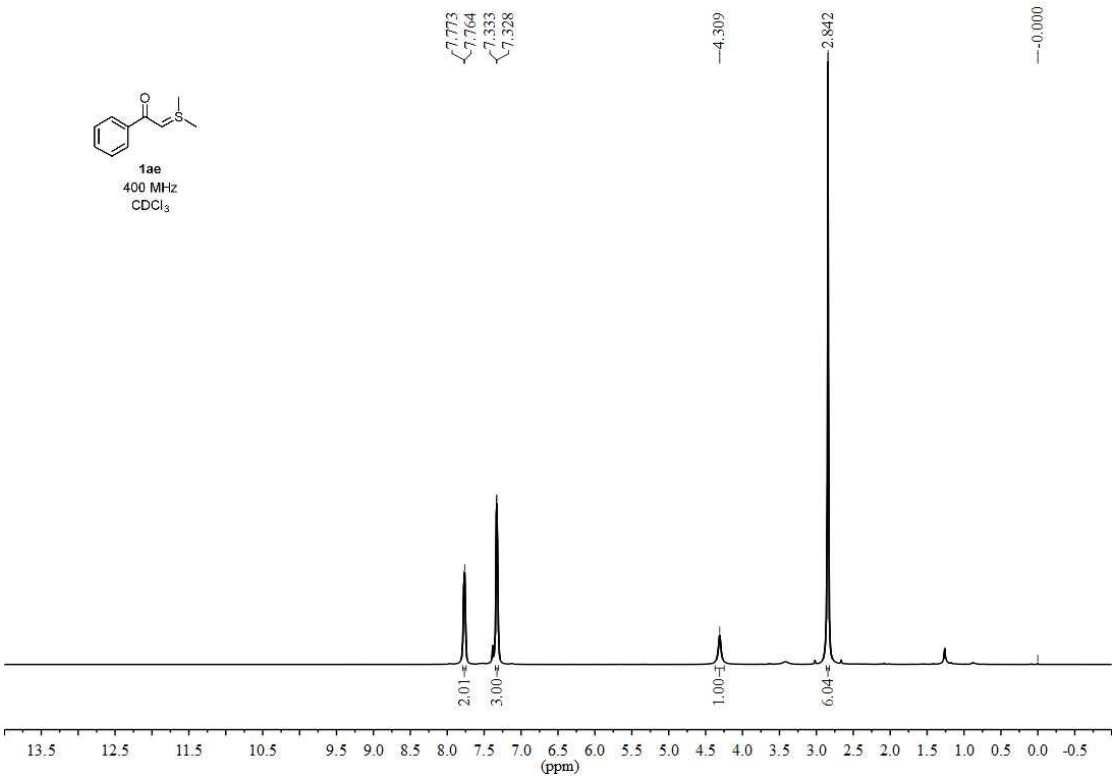
177.49
155.73
136.71
134.43
134.28
133.83
131.75
129.65
129.19
128.91
128.71
127.50
126.75
125.84
122.98
78.71
77.50
77.32
77.00
76.68
74.32
38.02
9
100 MHz
CDCl3
(ppm)

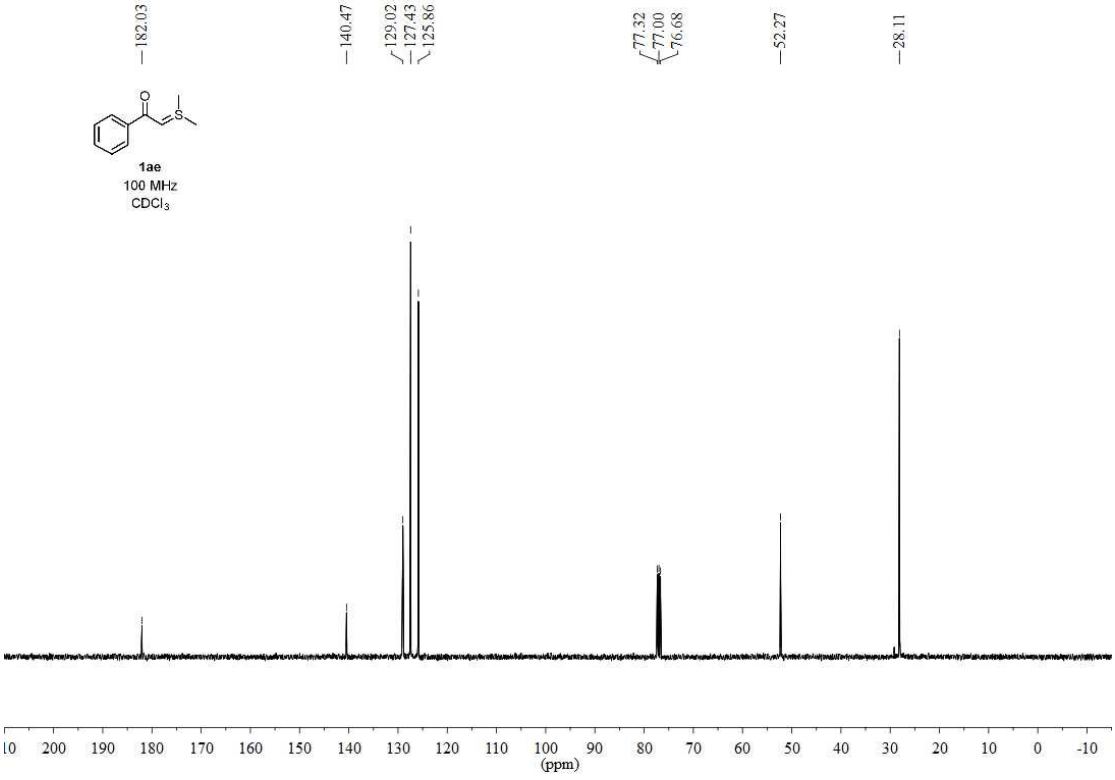

8.291
7.921
7.900
7.730
7.710
7.699
7.679
7.549
7.531
7.511
7.260
5.440
0.000
I
N
NH2
2aa
400 MHz
CDCl3
1.00
1.00
2.06
1.08
2.00
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
(ppm)

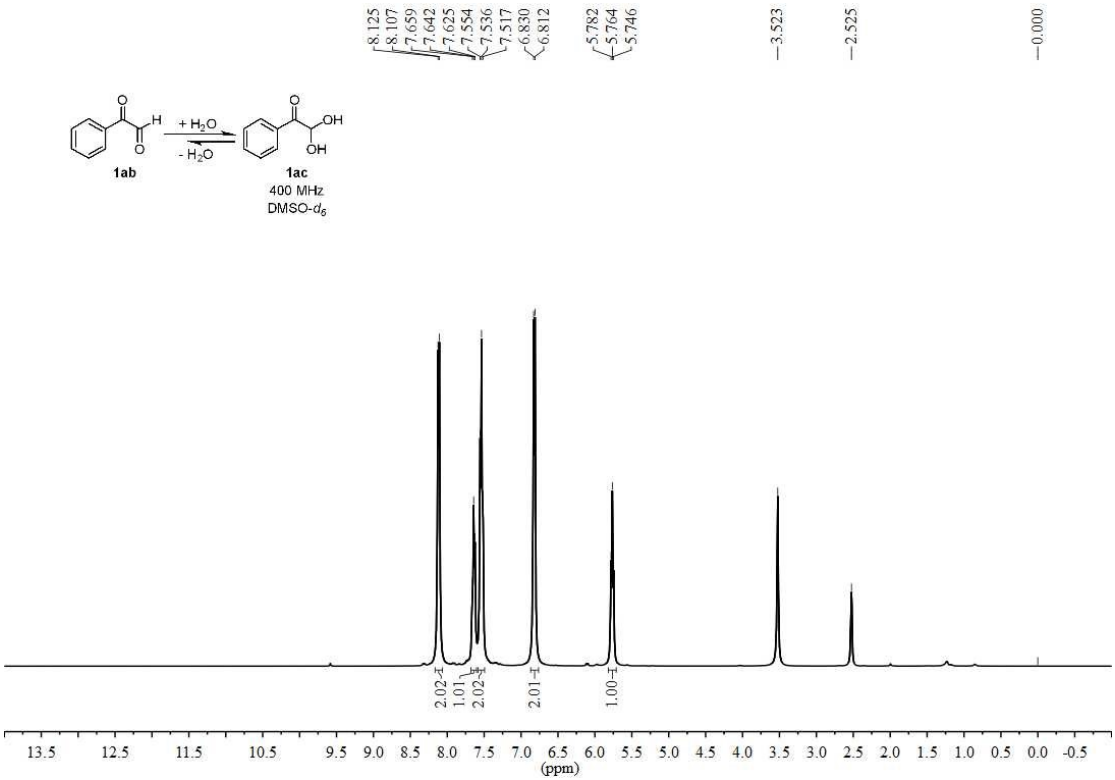

156.45
148.50
137.45
131.63
131.28
127.19
123.00
119.20
82.66
77.32
77.00
76.68
I
N
NH2
2aa
100 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
(ppm)

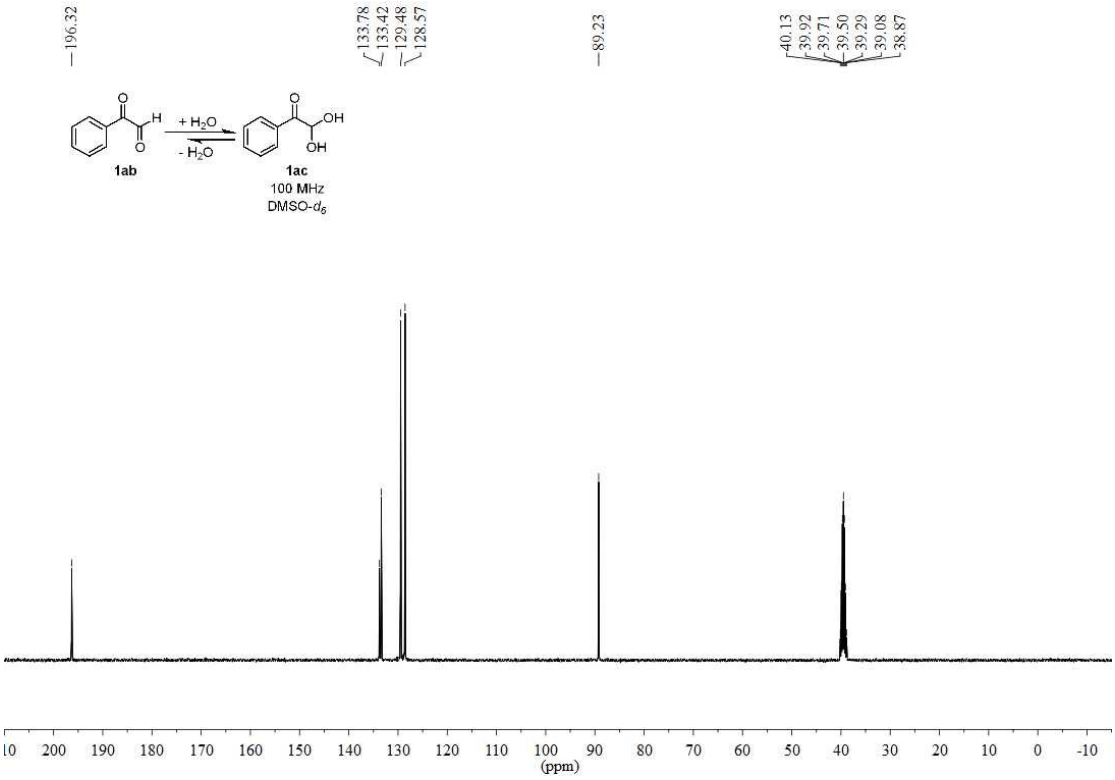

8.057
8.038
7.811
7.793
7.774
7.664
7.645
7.625
5.697
3.061
0.000
1ad
400 MHz
DMSO-d_6
2.08
1.00
2.06
1.99
6.06
(ppm)


191.43
135.06
133.87
129.18
128.66
52.82
40.13
39.92
39.71
39.50
39.29
39.08
24.54
1ad
100 MHz
DMSO-d_6
(ppm)


7.773
7.764
7.333
7.328
4.309
2.842
0.000
1ae
400 MHz
CDCl3
2.01
3.00
1.00
6.04
(ppm)


182.03
140.47
129.02
127.43
125.86
77.32
77.00
76.68
52.27
28.11
1ae
100 MHz
CDCl3
(ppm)


8.125
8.107
7.659
7.642
7.625
7.554
7.536
7.517
6.830
6.812
5.782
5.764
5.746
3.523
2.525
0.000
+ H2O
- H2O
1ab
1ac
400 MHz
DMSO-d6
2.02
1.01
2.02
2.01
1.00
(ppm)


196.32
133.78
133.42
129.48
128.57
89.23
40.13
39.92
39.71
39.50
39.29
39.08
38.87
+ H2O
- H2O
1ab
1ac
100 MHz
DMSO-d6
(ppm)