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Supporting Information

An Efficient Synthsis of gem-Diiodoolefins and (*E*)-iodoalkenes from Propargylic Amides with Cu(I)/Cu(III) Cycle

Shuo Zhang,[a] Ying Chen,[a] Jianwu Wang,*[a] Yue Pan,[a] Zhenghu Xu*[a,b] and Chen-Ho Tung[a]

[a] Key Lab for Colloid and Interface Chemistry of Education Ministry School of chemistry and Chemical Engineering, Shandong University Jinan 250100, PR China.
E-mail: xuzh@sdu.edu.cn; jwwang@sdu.edu.cn

[b]State Key Laboratory of Organometallic Chemistry Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences Shanghai 200032, PR China

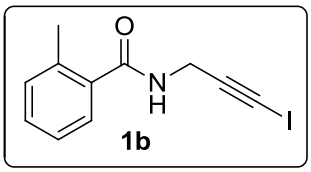
[c] Key Laboratory of Photochemical Conversion and Optoelectronic Materials, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing 100190, PR China.

†

General information

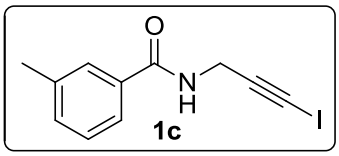
Unless otherwise noted, all the reagents were obtained commercially and used without further purification and reactions were monitored by TLC. All NMR spectra were recorded on Bruker-400 MHz spectrometer or Bruker-300 MHz. HRMS were measured on the Q-TOF6510 instruments.

Synthesis of the starting materials



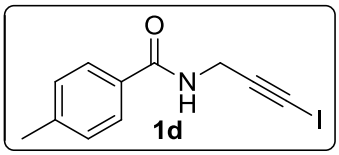
1b

Yield: (2.10g, 70%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.31 (m, 2H), 7.22-7.17 (m, 2H), 5.98 (s, 1H), 4.36 (d, *J* = 5.3 Hz,2H), 2.43 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.46, 136.43, 135.36, 131.15, 130.24, 126.77, 125.78, 89.54, 31.43, 19.82, 0.03. HRMS (ESI, m/z) calcd for $C_{11}H_{10}INO$ $[M+H]^+$ 299.9880, found 299.9882.



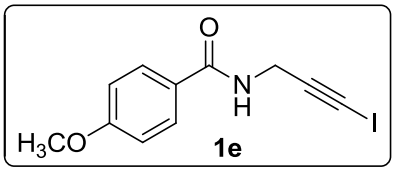
1c

Yield: (2.15g, 72%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.85 (s, 1H), 7.65-7.61 (m, 2H), 7.32 (d, *J* = 4.1 Hz, 2H), 4.14 (d, *J* = 5.4 Hz, 2H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.41, 138.09, 134.18, 132.48, 128.70, 128.31, 124.86, 90.67, 30.84, 21.39, 8.04. HRMS (ESI, m/z) calcd for $C_{11}H_{10}INO$ $[M+H]^+$ 299.9880, found 299.9886.



1d

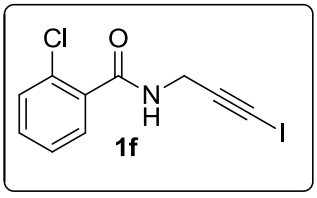
Yield: (2.0g, 67%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.82 (s, 1H), 7.73 (d, *J* = 7.5 Hz, 2H), 7.24 (d, *J* = 6.8 Hz, 2H), 4.14 (d, *J* = 5.3 Hz, 2H), 2.32 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.19, 141.85, 131.38, 129.35, 127.76, 90.75, 30.81, 21.44, 8.07. HRMS (ESI, m/z) calcd for $C_{11}H_{10}INO$ $[M+H]^+$ 299.9880, found 299.9885.



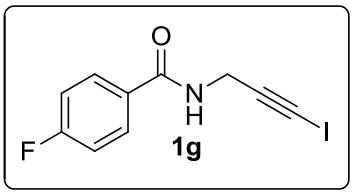
1e

Yield: (1.73g, 1.55%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8.7 Hz, 2H), 6.92 (d,

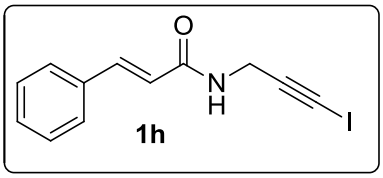
J = 8.8Hz, 2H), 6.25 (s, 1H), 4.40 (d, *J* = 5.2 Hz,2H), 3.85 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.35, 161.69, 129.11, 125.85, 113.49, 90.36, 55.29, 30.32, 7.47. HRMS (ESI, m/z) calcd for $C_{11}H_{10}INO_2$ $[M+H]^+$ 315.9829, found 315.9836.



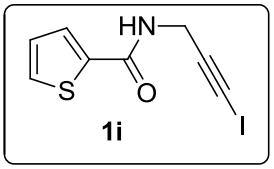
Yield: (1.44g, 45%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.86 (s, 1H), 7.48-7.34 (m, 4H), 4.13 (d, *J* = 5.5 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 165.94, 136.11, 130.94, 129.91, 129.63, 128.84, 127.06, 89.49, 30.21, 8.12. HRMS (ESI, m/z) calcd for $C_{10}H_7ClINO$ $[M+H]^+$ 319.9334, found 319.9334.



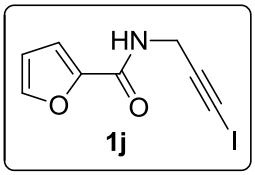
Yield: (1.88g, 62%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (t, *J* = 6.8 Hz, 2H), 7.11 (d, *J* = 8.1Hz, 2H), 6.35 (s, 1H), 4.39 (d, *J* = 4.6 Hz,2H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 165.80, 164.97,162.51, 130.29, 130.25, 130.17, 130.05, 115.57, 115.28, 90.18, 30.62, 8.03. HRMS (ESI, m/z) calcd for $C_{10}H_7FINO$ $[M+H]^+$ 303.9629, found 303.9628.



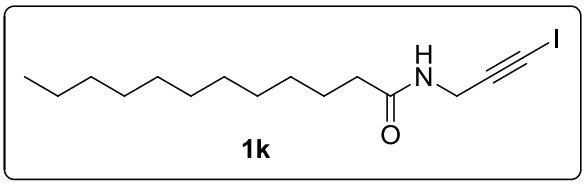
Yield: (1.77g, 57%). ^{1}H NMR (400 MHz,DMSO-d_6) δ 8.54 (s, 1H), 7.53 (d, *J* = 6.7 Hz, 2H), 7.41-7.35 (m, 4H), 6.59 (d, *J* = 15.8 Hz, 1H), 4.10 (d, *J* = 5.1 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.10, 139.91, 135.19, 130.08, 129.41, 128.06, 121.86, 90.36, 30.42, 8.59. HRMS (ESI, m/z) calcd for $C_{12}H_{10}INO$ $[M+H]^+$ 311.9880, found 311.9881.



Yield: (1.89g, 65%). ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.97 (t, *J* = 5.4 Hz, 1H), 7.79-7.77 (m, 2H), 7.17-7.14 (m, 1H), 4.17 (d, *J* = 5.7 Hz, 2H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 160.77, 139.11, 131.17, 128.45, 127.97, 89.90, 30.21, 8.10. HRMS (ESI, m/z) calcd for C_8H_6INOS $[M+H]^+$ 291.9288, found 291.9289.

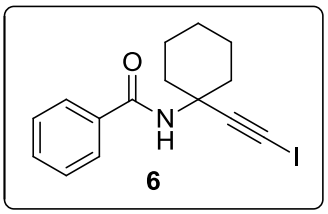


Yield: (1.93g, 70%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (s, 1H), 7.12 (d, *J* = 3.4Hz, 1H), 6.63 (s, 1H), 6.49 (dd, J_1 = 3.2 Hz, J_2 = 1.5 Hz, 1H), 4.36 (d, *J* = 5.6 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.84, 147.37, 144.22, 112.24, 89.33, 33.98, 30.68, 0.19. HRMS (ESI, m/z) calcd for $C_8H_6INO_2$ $[M+H]^+$ 275.9516, found 275.9518.



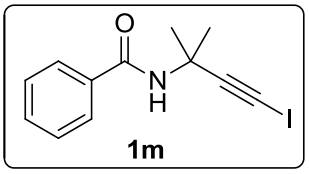
1k

Yield: (2.36g, 65%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.71 (s, 1H), 4.20 (d, *J* = 5.3 Hz, 2H), 2.18 (t, *J* = 7.5 Hz, 2H), 1.62 (t, *J* = 6.8 Hz, 2H), 1.28-1.25 (m, 16H), 0.87 (t, *J* = 6.4 Hz). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.67, 100.06, 89.85, 36.48, 32.76, 31.90, 30.99, 29.60, 29.47, 29.33, 29.26, 25.55, 22.68, 14.11. HRMS (ESI, m/z) calcd for $C_{15}H_{26}INO$ $[M+H]^+$ 364.1132, found 364.1141.



6

Yield: (2.47g, 70%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.2 Hz, 2H), 7.49-7.40 (m, 3H), 6.09 (s, 1H), 3.09-3.05 (m, 2H), 2.23-1.93 (m, 2H), 1.71-1.60 (m, 5H), 1.42-1.35 (m, 1H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 165.82, 134.96, 131.06, 128.04, 127.50, 95.62, 52.65, 36.41, 24.91, 22.01, 6.95. HRMS (ESI, m/z) calcd for $C_{15}H_{16}INO$ $[M+H]^+$ 354.0349, found 354.0345.



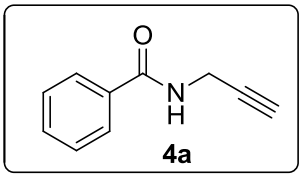
1m

Yield: (2.13g, 68%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 7.2 Hz, 2H), 7.48 (d, *J* = 7.2 Hz, 1H), 7.41 (t, *J* = 7.7 Hz, 2H), 6.21 (s, 1H), 1.76 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.35, 134.88, 131.50, 128.54, 126.89, 97.38, 50.17, 29.03, -2.05. HRMS (ESI, m/z) calcd for $C_{12}H_{12}INO$ $[M+H]^+$ 314.0036, found 314.0026.

General procedure for the synthesis of alkynyl amides **4a-4n**.

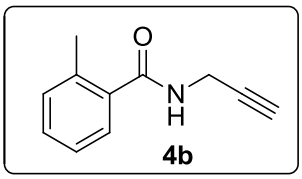
The corresponding Propynylamine (10 mmol) was dissolved in DCM, (30 mL). The solution was added triethylamine (24 mmol), chloride (12 mmol) and 4-dimethylaminopyridine (0.8 mmol) , the resulting solution

was allowed to reach room temperature. The reaction was stired at room temperature for 3h. And then was successively diluted with water. The aqueous layer was extracted with CH_2Cl_2, and the combined organic layers were washed with satd. $NaHCO_3$ followed by water and brine, dried over Na_2SO_4 and concentrated under reduced pressure to obtain the crude alkynyl amides. Silica gel chromatography gave the desired alkynyl amides **4a-4n**.



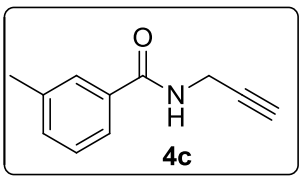
4a

Known compound. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, J = 7.4 Hz, 2H), 7.50-7.40 (m, 3H), 6.39 (s, 1H), 4.24 (dd, J_1 = 5.1 Hz, J_2 = 2.5 Hz, 2H), 2.27 (t, J = 2.4 Hz, 1H).



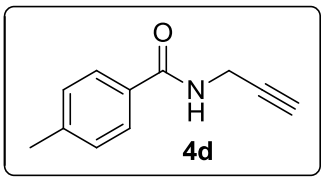
4b

Known compound. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.30 (m, 2H), 7.23-7.18 (m, 2H), 5.97 (s, 1H), 4.23 (dd, J_1 = 5.1 Hz, J_2 = 2.4 Hz, 2H), 2.45 (s, 3H), 2.27 (t, J = 2.4 Hz, 1H).



4c

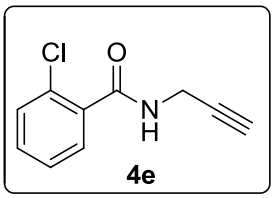
Known compound. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61-7.55 (m, 2H), 7.32-7.31 (m, 2H), 6.28 (s, 1H), 4.25 (dd, J_1 = 5.2Hz, J_2 = 2.5 Hz, 2H), 2.40(s, 3H), 2.28 (t, J = 2.4 Hz, 1H).



4d

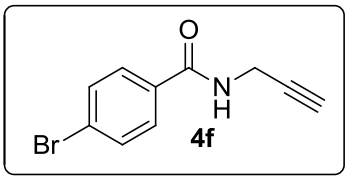
Known compound. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, J = 8.1 Hz, 2H), 7.23 (d. J = 8.1 Hz, 2H), 6.36 (s, 1H), 4.24 (dd, J_1 = 5.2 Hz, J_2= 2.5 Hz, 2H), 2.39 (s, 3H), 2.27

(t, *J* = 2.4 Hz, 1H).



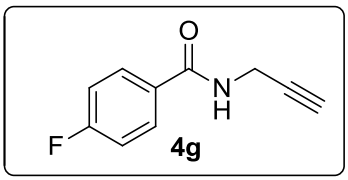
4e

Known compound. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 1.4 Hz, 1H), 7.68-7.30 (m, 3H), 6.46 (s, 1H), 4.27 (dd, J_1 = 5.2 Hz, J_2 = 2.5 Hz, 2H), 2.29 (t, *J* = 2.6 Hz, 1H).



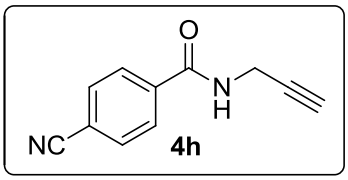
4f

Known compound. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.5 Hz, 2H), 7.57 (d, *J* = 8.5 Hz, 2H), 6.38 (s, 1H), 4.24 (dd, J_1= 5.1 Hz, J_2 = 2.5 Hz, 2H), 2.28 (t, *J* =2.5 Hz, 1 H)



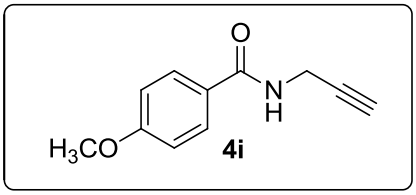
4g

Known compound. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82-7.79 (m, 2H), 7.09 (t, *J* = 8.6 Hz, 2H), 6.62 (s, 1H) 4.22 (dd, J_1 = 5.2 Hz, J_2 = 2.5 Hz, 2H), 2.27 (d, *J* = 2.6 Hz, 1H).



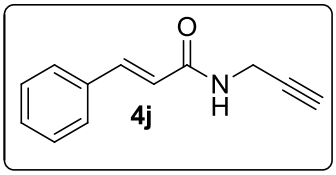
4h

Known compound. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, J = 8.3 Hz, 2H), 7.75 (d, *J* = 8.4 Hz, 2H), 6.45 (s, 1H), 4.26 (dd, J_1 = 5.2 Hz, J_2 = 2.6 Hz, 2H), 2.30 (t, *J* = 2.5 Hz, 1H).



4i

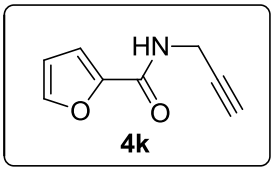
Known compound. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8.7 Hz, 2H), 6.91 (d, *J* =8.8 Hz, 2H), 6.30 (s, 1H), 4.23 (dd, J_1 = 5.1 Hz, J_2 = 2.4 Hz, 2H), 3.84 (s, 3H).



4j

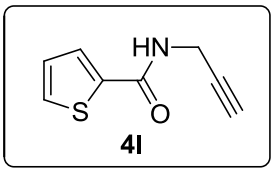
Known compound. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 15.9 Hz, 1H),

7.51-7.46 (m, 2H), 7.37-7.31 (m, 3H), 6.45 (d, J = 15.9 Hz, 1H), 6.18 (s, 1H), 4.20 (dd, J_1 = 5.2 Hz, J_2 = 2.5 Hz, 2H), 2.26 (t, J = 2.5 Hz, 1H)



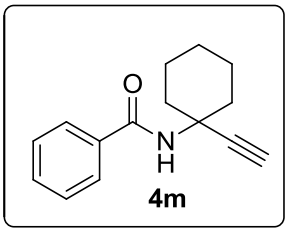
4k

Known compound. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, J = 0.8 Hz, 1H), 7.14 (d, J = 3.4 Hz, 1H), 6.50 (dd, J_1 = 3.4 Hz, J_2 = 1.7 Hz, 2H), 4.23 (dd, J_1 = 5.4 Hz, J_2 = 2.6 Hz, 2H), 2.27 (t, J = 2.5 Hz, 1H),



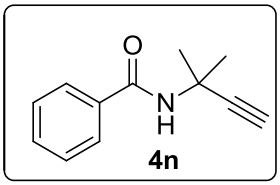
4l

Known compound. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, J = 3.7 Hz, 1H), 7.49 (d, 5.0 Hz, 1H), 7.08 (t, J = 4.1 Hz, 1H), 6.22 (s, 1H), 4.22 (dd, J_1 = 5.1 Hz, J_2 = 2.4 Hz, 2H), 2.28 (t, J = 2.4 Hz, 1H).



4m

Known compound. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76-7.74 (m, 2H), 7.48-7.38 (m, 3H), 6.14 (s, 1H), 2.44 (s, 1H), 2.24-2.20 (m, 2H), 1.98-1.91 (m, 2H), 1.76-1.63 (m, 5H), 1.60-1.58 (m, 1H)

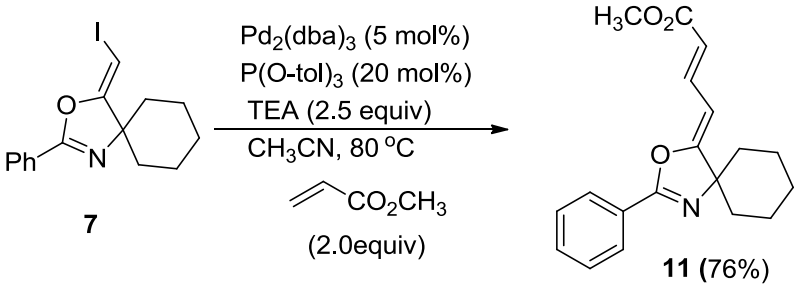


4n

Known compound. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75-7.73 (m, 2H), 7.50-7.39 (m, 3H), 6.20 (s, 1H), 2.38 (s, 1H), 1.76 (s, 6H).

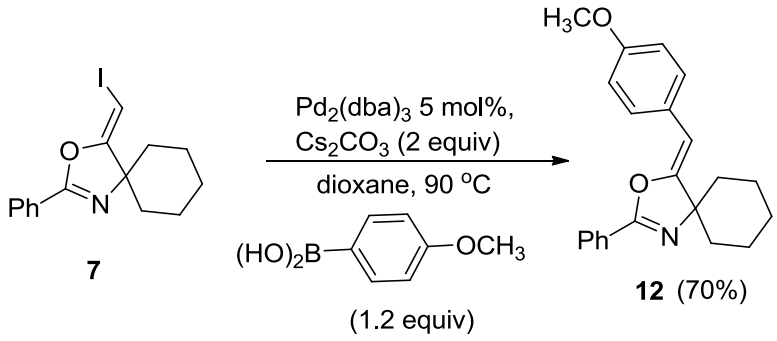
Synthetic applications:

Procedure for Synthesis of compound **11**



To a mixture of $Pd_2(dba)_3$ (0.01 mmol), P(O-tol) $_3$ (0.04 mmol), compound **10** (0.2 mmol) in CH_3CN (2 ml) under N_2 atmosphere, methyl acrylate (0.4 mmol) and Et_3N (0.5 mmol) was added. The system was stirred at 80℃ overnight. The resulting mixture was washed with water and extracted with DCM. The organic layer was filtered on celite and evaporated under reduced pressure. Purification by flash column chromatography afforded the desired product **11** (47.27 mg, 76%).

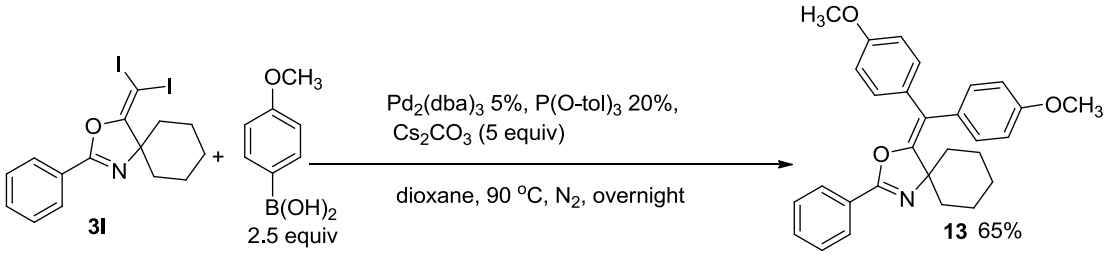
Procedure for Synthesis of compound **12**



To a mixture of Pd_2dba_3 (0.01 mmol), Cs_2CO_3 (0.5 mmol), 4-Methoxyphenylboronic acid (0.24 mmol), compound **10** (0.2 mmol)

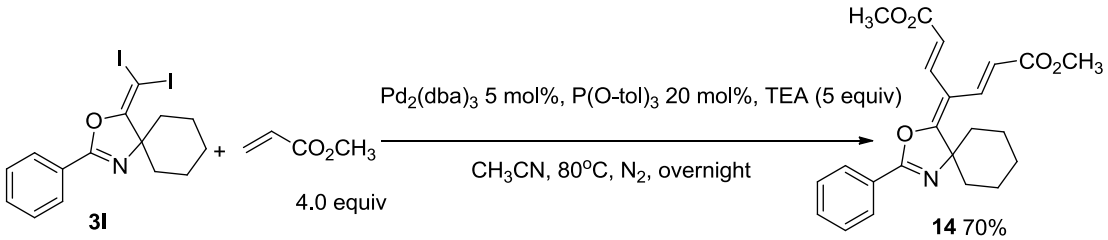
in dioxane (2 ml) under N_2 atmosphere was stirred at 90℃ overnight. The resulting mixture was washed with water and extracted with DCM. The organic layer was filtered on celite and evaporated under reduced pressure. Purification by flash column chromatography afforded the desired product **12** (46.62 mg, 70%).

Procedure for Synthesis of compound **13**



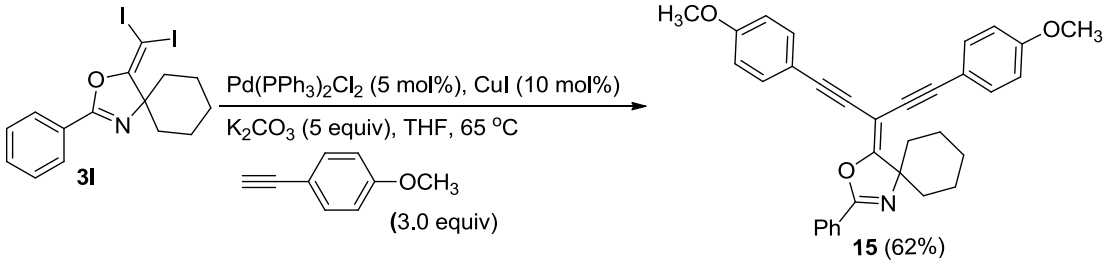
To a mixture of Pd_2dba_3 (0.02 mmol), Cs_2CO_3 (1 mmol), 4-Methoxyphenylboronic acid (0.5 mmol), compound **3l** (0.2 mmol) in dioxane (2 ml) under N_2 atmosphere was stirred at 90℃ overnight. The resulting mixture was washed with water and extracted with DCM. The organic layer was filtered on celite and evaporated under reduced pressure. Purification by flash column chromatography afforded the desired product **13** (57.07 mg, 65%).

Procedure for Synthesis of compound **14**



To a mixture of $Pd_2(dba)_3$ (0.02 mmol), P(O-tol) $_3$ (0.08 mmol), compound **2l** (0.2 mmol) in CH_3CN (2 ml) under N_2 atmosphere, compound **6** (0.24 mmol) and Et_3N (1 mmol) was added. The system was stirred at 80℃ overnight. The resulting mixture was washed with water and extracted with DCM. The organic layer was filtered on celite and evaporated under reduced pressure. Purification by flash column chromatography afforded the desired product **14** (55.3 mg, 70%).

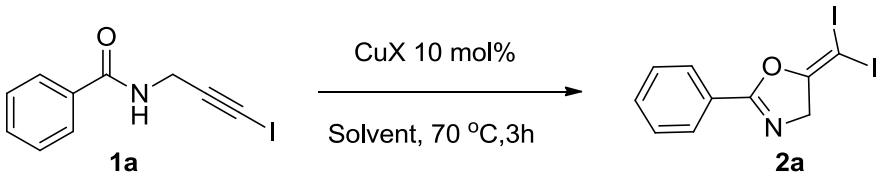
Procedure for Synthesis of compound **15**



To a mixture of $Pd(PPh_3)_2Cl_2$ (0.02 mmol), CuI (0.04 mmol), K_2CO_3 (1 mmol), compound **3l** (0.2 mmol) in THF (2 ml) under N_2 atmosphere, 4-Methoxyphenylacetylene (0.6 mmol) was added. The system was stirred at 65℃ overnight. The resulting mixture was washed with water and extracted with DCM. The organic layer was filtered on celite and evaporated under reduced pressure. Purification by flash column chromatography afforded the desired product **15** (58.44 mg, 62%).

Optimization of reaction conditions:

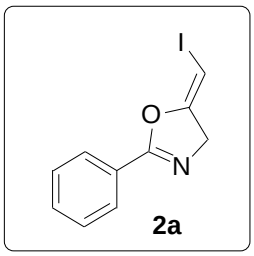
Table 1. Optimization of Reaction Conditions



Entry	Catalyst	Solvent	Yield(%)[a]
1	CuI	DCE	90
2	CuCl	DCE	86
3	CuBr	DCE	72
4	$Cu(acac)_2$	DCE	75
5	$CuSO_4$	DCE	95
6	1,10-Phen-CuI	DCE	83
7	IPRCuI	DCE	69
8	$CuCl_2$	DCE	79
9	$Cu(OAc)_2$	DCE	75
10	$Cu(PF_4)$ $(CH_3CN)_4$	DCE	50
11	$Cu(PF_4)_2$	DCE	46
12	$Cu(NO_3)_2$	DCE	40
13	$Cu(ClO_4)_2$	DCE	43
14	$CuSO_4$	CH_3CN	26
15	$CuSO_4$	Dioxane	76
16	$CuSO_4$	THF	84
17	$CuSO_4$	Toluene	75

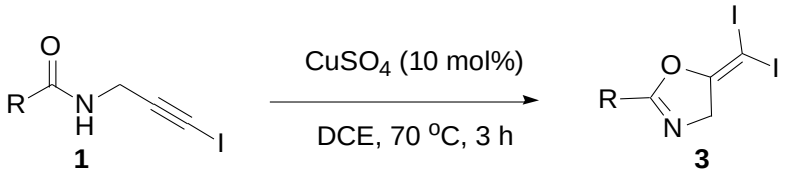
a: Isolated yields were reported. Reaction conditions: **1a** (0.1 mmol) , CuX (0.01 mmol) in solvent (1 mL) was stirred at 70℃ for 3 h.

Characterization Data



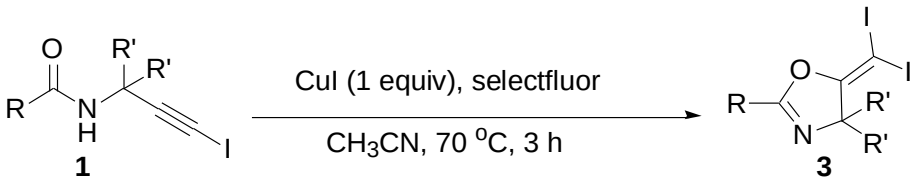
^{1}H NMR (300 MHz, DMSO-d_6) δ 7.89-7.86 (m, 2H), 7.62-7.57 (m, 1H), 7.54-7.49 (m, 2H), 5.44 (t, *J*= 2.4 Hz, 1H), 4.67 (d, *J* = 2.4 Hz, 2H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 161.14, 159.58, 132.77, 129.41, 128.05, 126.24, 58.45, 43.72. HRMS (ESI, m/z) calcd for $C_{10}H_8INO$ $[M+H]^+$ 285.9723, found 285.9719.

Condition A:

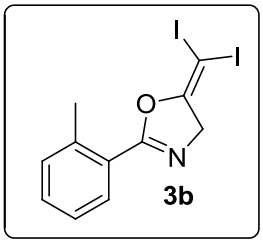


[a] Reaction conditions: **1** (0.2 mmol), $CuSO_4$ (0.02 mmol) in DCE (2 mL) was stirred at 70℃ for 3 h. Isolated yields were reported.

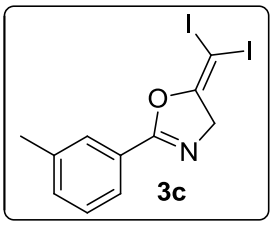
Condition B:



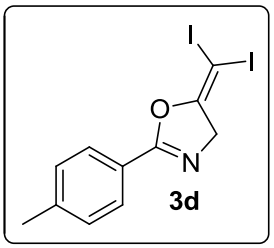
[a] Reaction conditions: **1a** (0.2 mmol), CuI (0.2 mmol), selectfluor (0.24 mmol), in CH_3CN (2 mL) was stirred at 70℃ for 3 h. Isolated yields were reported.



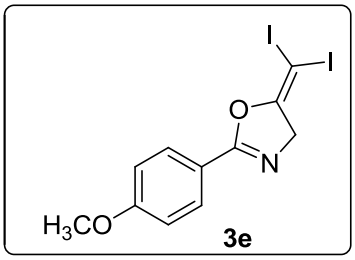
Yield: condition A (41.13 mg,97%), condition B (75.47 mg, 89%) ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.79-7.76 (m, 1H), 7.52-7.46 (m, 1H), 7.36, (t, *J* = 7.2 Hz, 2H), 4.64 (s, 2H), 2.57 (s, 3H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 161.13, 158.50, 138.60, 131.64, 131.61, 129.21, 126.11, 125.03, 61.41, 21.50, -16.01. HRMS (ESI, m/z) calcd for $C_{11}H_9I_2NO$ $[M+H]^+$ 425.8846, found 425.8845.



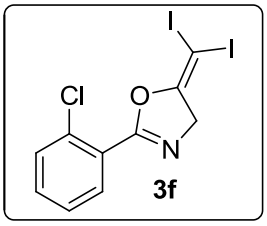
Yield: condition A (40.28 mg, 95%), condition B(77.17 mg, 91%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78-7.75 (m, 2H), 7.35 (d, *J* = 5.3 Hz, 2H), 4.61 (s, 2H), 2.41 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 160.99, 158.71, 138.38, 133.09, 128.91, 127.72, 125.86, 124.66, 61.11, 20.86, -15.53. HRMS (ESI, m/z) calcd for $C_{11}H_9I_2NO$ $[M+H]^+$ 425.8846, found 425.8845.



Yield: condition A (41.13 mg, 97%), condition B (74.63 mg, 88%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.0 Hz, 2H), 7.26 (d, *J* = 7.7 Hz, 2H), 4.61 (s, 2H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 160.91, 158.76, 142.62, 129.58, 127.40, 123.15, 61.07, 21.14, -15.72. HRMS (ESI, m/z) calcd for $C_{11}H_9I_2NO$ $[M+H]^+$ 425.8846, found 425.8850.

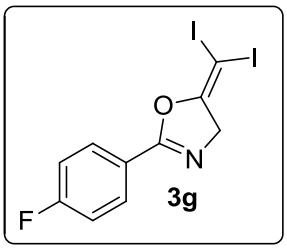


Yield: condition A (38.28 mg, 87%), condition B (79.21 mg, 91%) ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.78 (d, *J* = 8.7 Hz, 2H), 7.07 (d, *J* = 8.7 Hz, 2H), 4.54, (s, 2H), 3.80 (s, 3H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 162.39, 160.66, 158.83, 129.30, 118.09, 114.44, 61.01, 55.46, -15.92. HRMS (ESI, m/z) calcd for $C_{11}H_9I_2NO_2$ $[M+H]^+$ 441.8795, found 441.8793.

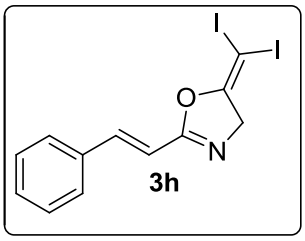


Yield: condition A (32.49 mg, 73%), condition B (71.11 mg, 80%)^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87-7.85 (m, 1H), 7.49-7.43, (m, 2H), 7.39-7.34 (m, 1H), 4.68 (s, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 159.83, 158.91, 133.64, 132.69, 131.79,

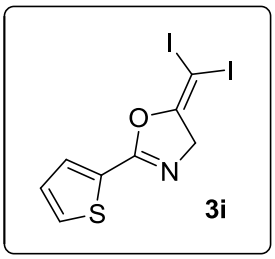
131.44, 128.03, 125.89, 61.91, -14.62. HRMS (ESI, m/z) calcd for $C_{10}H_6ClI_2NO$ $[M+H]^+$ 445.8300, found 445.8300.



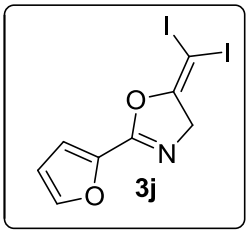
Yield: condition A (30.89 mg, 72%), condition B (64.35 mg, 75%) ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.92-7.88 (m, 2H), 7.41-7.35, (m, 2H), 4.58, (s, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 166.15, 163.66, 160.54, 159.08, 130.63, 130.54, 122.99, 122.97, 116.83, 116.61, 61.67, -14.87. HRMS (ESI, m/z) calcd for $C_{10}H_6FI_2NO$ $[M+H]^+$ 429.8596, found 429.8578.



Yield: condition A (38.02 mg, 87%), condition B (71.67 mg, 82%) ^{1}H NMR (400 MHz,DMSO-d_6) δ 7.68-7.67 (m, 2H), 7.40-7.38 (m, 4H), 6.79 (d, *J* = 16.3 Hz, 1H), 4.50 (s, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.50, 158.97, 141.11, 134.78, 130.59, 129.41, 128.46, 114.46, 61.73, -15.77. HRMS (ESI, m/z) calcd for $C_{12}H_9I_2NO$ $[M+H]^+$ 437.8846, found 437.8843.

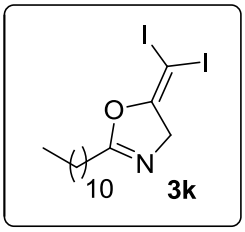


Yield: condition A (39.20 mg, 94%), condition B (75.06 mg, 90%) ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.91 (s, *J* = 3.8Hz, 1H), 7.64 (d, *J* = 3.9 Hz, 1H), 7.23 (t, *J* =3.9 Hz, 1H), 4.57, (s, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.89, 157.31, 132.80, 131.65, 128.87, 128.45, 61.57, -14.70. HRMS (ESI, m/z) calcd for $C_8H_5I_2NOS$ $[M+H]^+$ 417.8254, found 417.8254.



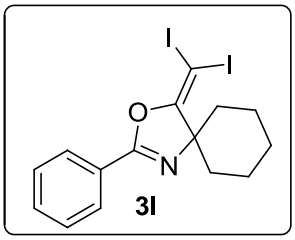
Yield: condition A (39.28 mg, 98%), condition B (73.78 mg, 92%) ^{1}H NMR (400

MHz, DMSO-d_6) δ 7.97 (s, 1H), 7.12 (d, *J* = 3.3 Hz, 1H), 6.69 (q, *J* = 1.5 Hz, 1H), 4.55 (s, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.53, 153.81, 147.69, 141.28, 116.34, 112.77, 61.47, -14.74. HRMS (ESI, m/z) calcd for $C_8H_5I_2NO$ $[M+H]^+$ 401.8482, found 401.8485.



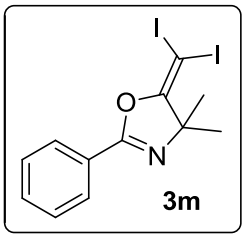
3k

Yield: condition A (27.38 mg, 56%), condition B (76.28 mg, 78%) ^{1}H NMR (400 MHz, DMSO-d_6) δ 4.31 (s, 2H), 2.30 (t, *J* = 6.9 Hz, 2H), 1.53 (t, *J* = 6.6 Hz, 2H), 1.28-1.21 (m, 16H), 0.83 (t, J= 5.8 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 61.14, 31.78, 29.47, 29.33, 29.21, 29.08, 28.76, 27.93, 25.23, 22.59, 14.44, -16.48. HRMS (ESI, m/z) calcd for $C_{15}H_{25}I_2NO$ $[M+H]^+$ 490.0098, found 490.0099.



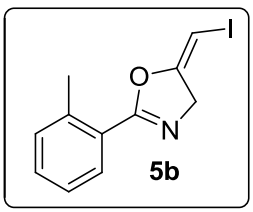
3l

Yield: condition B (84.30 mg, 88%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00-7.97 (m, 2H), 7.51-7.42, (m, 3H), 2.59-2.52, (m, 2H), 1.94- 1.58 (m, 7H), 1.41-1.35 (m, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.77, 155.69, 131.89, 128.53, 128.34, 126.20, 77.43, 77.11, 76.79, 75.53, 33.95, 25.48, 22.34, -24.04. HRMS (ESI, m/z) calcd for $C_{15}H_{15}I_2NO$ $[M+H]^+$ 479.9316, found 479.9327.



3m

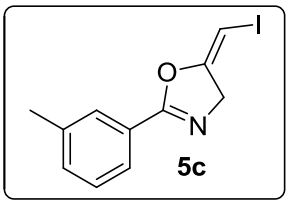
Yield: condition B (72.87 mg, 83%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95-7.93 (m, 2H), 7.54-7.42, (m, 3H), 1.69 (s, 6H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.32, 155.92, 132.88, 129.47, 128.08, 125.81, 71.83, 26.10, -14.55. HRMS (ESI, m/z) calcd for $C_{12}H_{11}I_2NO$ $[M+H]^+$ 439.9003, found 439.8956.



5b

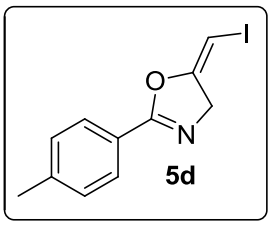
Yield: (55.02 mg, 92%) ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.72-7.69 (m, 2H),

7.43-7.41(m, 2H), 6.05 (t, *J* = 4.0 Hz, 1H), 4.61(d, *J* = 4.0 Hz, 2H), 2.37(s, 3H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 162.45, 157.46, 138.34, 132.90, 128.84, 127.86, 126.03, 124.68, 60.44， 49.20, 20.78. HRMS (ESI, m/z) calcd for $C_{11}H_{10}INO$ $[M+H]^+$ 299.9880, found 299.9879.



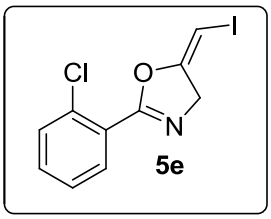
5c

Yield: (49.64 mg, 83%) ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.72-7.69 (m, 2H), 7.43-7.41, (m, 2H), 6.05 (t, *J* = 3.1 Hz, 1H), 4.61(d, *J* =3.3 Hz, 2H), 2.37 (s, 3H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 162.45, 157.46, 138.34, 132.90, 128.84, 127.86, 126.03, 124.68, 60.43, 20.77. HRMS (ESI, m/z) calcd for $C_{11}H_{10}INO$ $[M+H]^+$ 299.9880, found 299.9885.



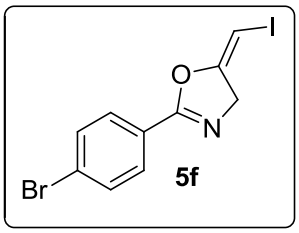
5d

Yield: (53.22 mg, 89%) ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.79 (d, *J* = 8.4 Hz, 2H), 7.34 (d, *J* = 8.1 Hz, 2H), 6.04 (t, *J* = 3.0 Hz, 1H), 4.59 (d, *J* = 3.3Hz, 2H), 2.38 (s, 3H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 162.39, 157.49, 142.40, 129.49, 127.46, 123.33, 60.40, 49.08, 21.10. HRMS (ESI, m/z) calcd for $C_{11}H_{10}INO$ $[M+H]^+$ 299.9880, found 299.9879o.



5e

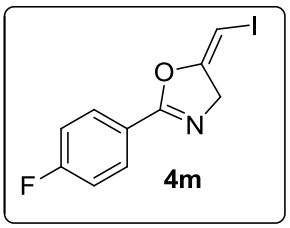
Yield: (46.08 mg, 72%) ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.77 (d, *J* = 7.6 Hz, 1H), 7.58 (t, *J* = 6.7 Hz, 2H), 7.45(t, *J* = 7.4 Hz, 1H), 6.02 (t, *J* = 2.9 Hz, 1H). 4.62(d, *J* = 3.0 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.24, 157.51, 133.49, 132.58, 131.79, 131.30, 127.98, 126.24, 61.33, 50.10. HRMS (ESI, m/z) calcd for $C_{10}H_7ClINO$ $[M+H]^+$ 319.9334, found 319.9334.



5f

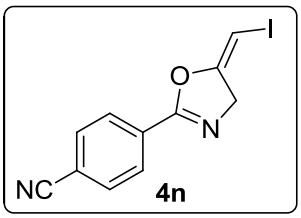
Yield: (53.14 mg, 73%) ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.79 (d, *J* = 8.4 Hz, 2H),

7.72 (d, *J* = 8.4 Hz, 2H), 6.05 (t, *J* = 3.0 Hz, 1H), 4.58 (d, *J*= 3.0 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.21, 157.74, 132.55, 129.91, 126.53, 125.76, 61.02, 50.13. HRMS (ESI, m/z) calcd for $C_{10}H_7BrINO$ $[M+H]^+$ 363.8828, found 363.8828.



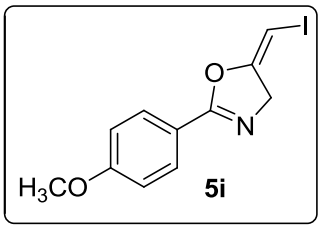
4m

Yield: (41.21 mg, 68%) ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.99-7.92 (m, 2H), 7.42-7.34 (m, 2H), 6.07 (t, *J* = 3.3 Hz, 1H), 4.61 (d, *J*= 3.3 Hz, 2H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 165.99, 162.67, 161.52, 157.38, 130.24, 130.12, 122.71, 122.67, 116.30, 116.00, 60.45, 49.45. HRMS (ESI, m/z) calcd for $C_{10}H_7FINO$ $[M+H]^+$ 303.9629, found 303.9627.



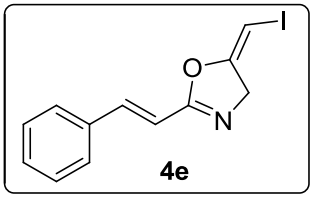
4n

Yield: (45.88 mg, 74%) ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.21-8.01 (m, 4H), 6.11 (s, 1H), 4.65(s, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.81, 157.51, 133.39, 130.62, 128.69, 118.53, 114.96, 61.14, 50.51. HRMS (ESI, m/z) calcd for $C_{11}H_7IN_2O$ $[M+H]^+$ 310.9676, found 310.9686.



5i

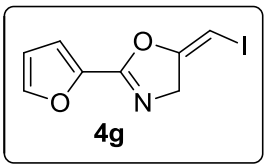
Yield: (51.66 mg, 82%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.8 Hz, 2H), 6.94 (d, *J* = 8.8 Hz, 2H), 5.74 (t, *J* = 3.0 Hz, 1H), 4.60 (d, *J* = 3.0 Hz, 2H), 3.86(s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.27, 162.18, 157.56, 129.36, 118.28, 114.33, 60.32, 55.43, 48.91. HRMS (ESI, m/z) calcd for $C_{11}H_{10}INO_2$ $[M+H]^+$ 315.9829, found 315.9828.



4e

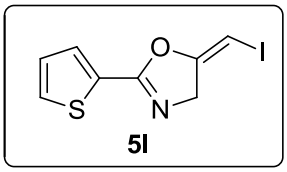
Yield: (57.85 mg, 93%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 1.4 Hz, 2H), 7.37 (m, 4H), 6.77 (d, *J* = 16.4 Hz, 1H), 5.92, (t, *J* = 3.0 Hz, 1H), 4.49, (d, *J* = 2.7 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 167.68, 162.39, 145.81, 139.66, 135.23, 134.11, 133.15, 119.17, 65.78, 53.88. HRMS (ESI, m/z) calcd for $C_{12}H_{10}INO$ $[M+H]^+$

311.9880, found 311.9888.



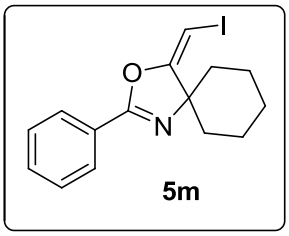
4g

Yield: (50.6 mg, 92%) ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.95 (s, 1H), 7.14 (d, *J* = 3.2 Hz, 1H), 6.68 (t, *J* = 1.6 Hz, 1H), 6.02 (t, *J* = 2.9 Hz, 1H), 4.55 (d, *J* = 2.9 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 157.21, 155.17, 147.59, 141.44, 116.16, 112.71, 60.69, 50.07. HRMS (ESI, m/z) calcd for $C_8H_6INO_2$ $[M+H]^+$ 275.9516, found 275.9515.



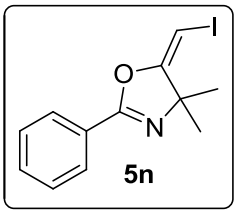
5l

Yield: (52.38 mg, 90%) ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.88 (d, *J* = 5.0 Hz, 1H), 7.65 (d, *J* = 3.6 Hz, 1H), 7.20 (t, *J* = 4.0 Hz, 1H), 6.04 (t, *J* = 2.8 Hz, 1H), 4.56 (d, *J*= 3.0 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.50, 162.38, 137.31, 136.29, 133.56, 133.46, 65.62, 54.74. HRMS (ESI, m/z) calcd for C_8H_6INOS $[M+H]^+$ 291.9288, found 291.9307



5m

Yield: (52.25 mg, 74%) ^{1}H NMR (400 MHz,$CDCl_3$) δ 8.04 (d, *J* = 8.0 Hz, 2H), 7.52-7.43 (m, 3H), 5.06, (s, 1H), 1.88-1.59, (m, 10H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 167.49, 156.87, 132.15, 128.85, 127.68, 125.97, 73.48, 44.44, 24.85, 21.76. HRMS (ESI, m/z) calcd for $C_{15}H_{16}INO$ $[M+H]^+$ 354.0349, found 354.0346.



5n

Yield: (56.34 mg, 90%) ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.85-7.83 (m, 2H), 7.56-7.45 (m, 3H), 5.98, (s, 1H), 1.56, (s, 6H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.79, 157.96, 132.57, 129.28, 128.11, 126.08, 71.21, 48.37, 26.09. HRMS (ESI, m/z) calcd for $C_{12}H_{12}INO$ $[M+H]^+$ 314.0036, found 314.0029.

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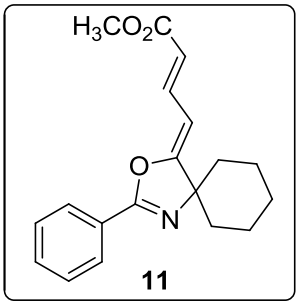
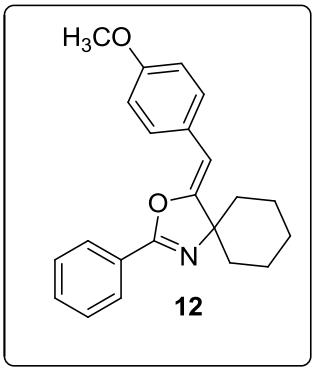
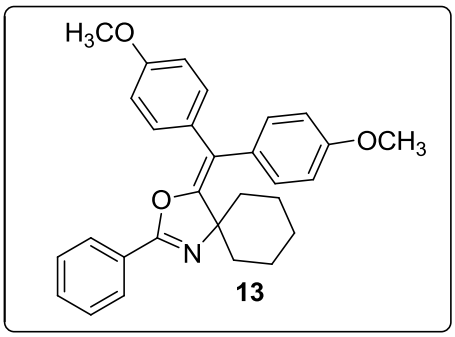


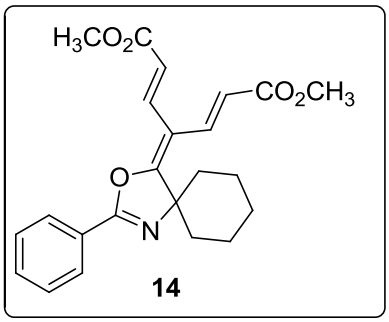
Yield: (47.27 mg, 76%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 7.2Hz, 2H), 7.81-7.75, (m, 1H), 7.53-7.45 (m, 3H), 5.83 (d, *J*= 15.4 Hz, 1H), 5.44 (d, J = 11.4 Hz, 1H), 3.77 (s, 3H), 1.92-1.38 (m, 10H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.01, 167.82, 158.52, 138.82, 131.84, 128.52, 128.33, 126.68, 116.85, 97.88, 73.64, 51.43, 38.57, 25.53, 22.06. HRMS (ESI, m/z) calcd for $C_{19}H_{21}NO_3$ $[M+H]^+$ 312.1594, found 312.1590.



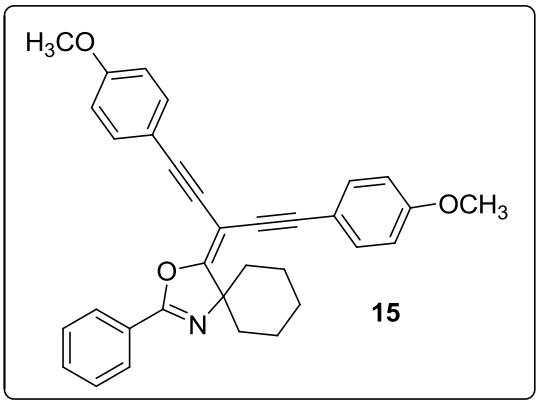
Yield: (46.62 mg, 70%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 6.9 Hz, 2H), 7.61-7.47, (m, 5H), 6.95 (d, *J* = 8.7 Hz, 2H), 5.47 (s, 1H), 3.84 (s, 1H), 1.97-1.41 (m, 10H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.79, 159.11, 157.83, 131.50, 129.11, 128.48, 128.27, 128.14, 127.49, 113.99, 98.94, 73.65, 55.31, 39.45, 25.80, 22.42. HRMS (ESI, m/z) calcd for $C_{22}H_{23}NO_2$ $[M+H]^+$ 334.1802, found 334.1803.



Yield: (57.18 mg, 65%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04-8.02 (m, 2H), 7.50-7.43, (m, 5H), 7.40-7.38 (m, 2H), 7.21 (d, *J*= 8.6 Hz, 1H), 6.94-6.85 (m, 4H), 3.87 (s, 3H), 3.81 (s, 3H)1.90-1.84 (m, 2H), 1.86-1.83 (m, 3H), 1.67-1.44 (s, 5H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.78, 158.02, 157.82, 156.76, 133.16, 132.96, 131.27, 130.00, 128.39, 128.16, 127.71, 114.84, 113.25, 113.12, 74.38, 55.24, 37.68, 29.71, 25.78, 22.39. HRMS (ESI, m/z) calcd for $C_{29}H_{29}NO_3$ $[M+H]^+$ 440.2220, found 440.2227.

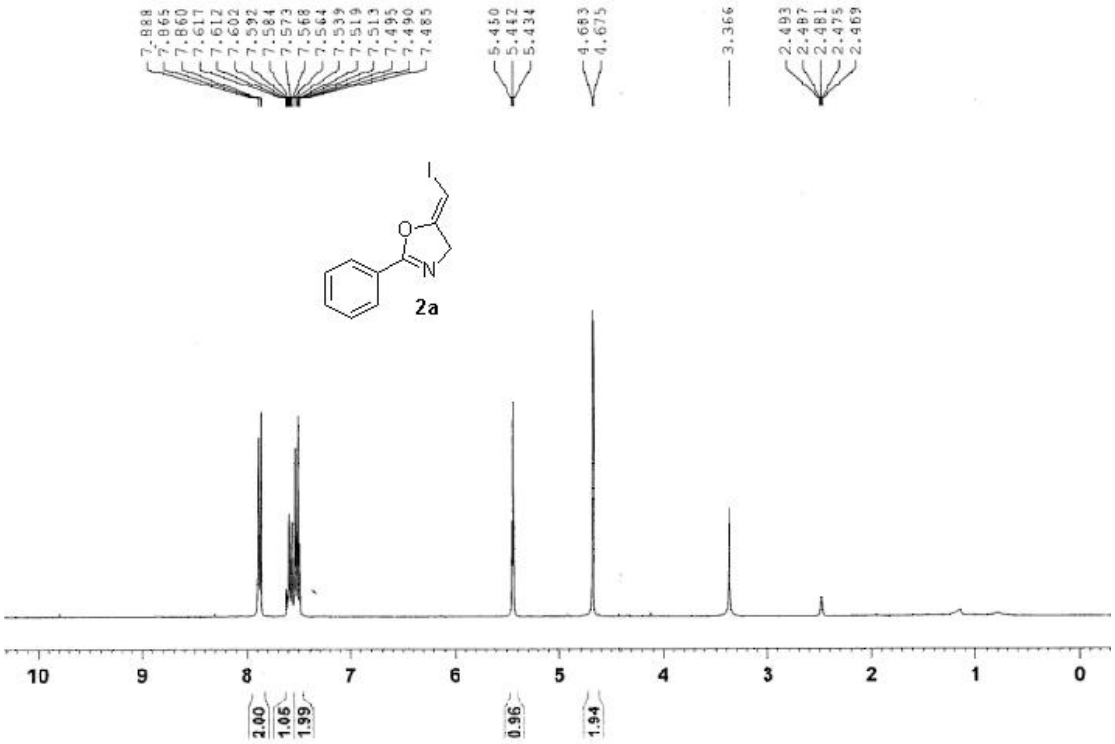


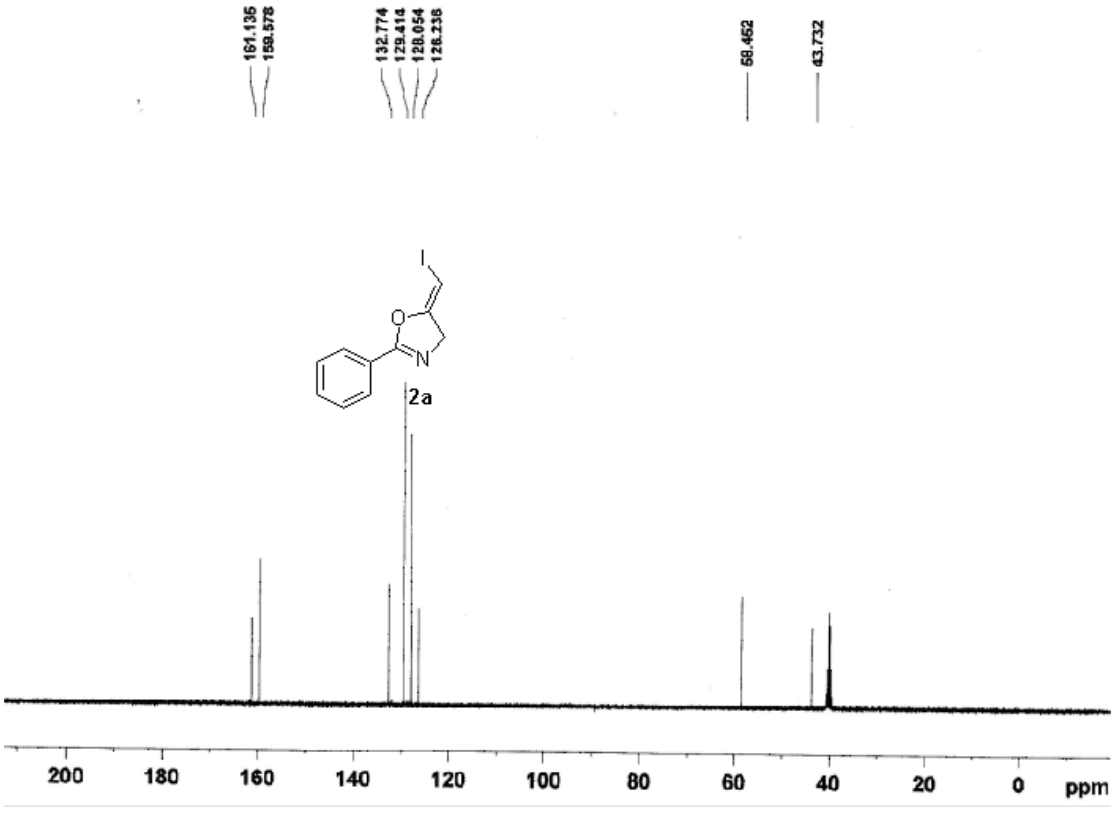
Yield: (55.44 mg, 70%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.3 Hz, 2H), 7.90 (d, *J* = 15.8 Hz, 1H), 7.68 (d, *J* = 16.2 Hz, 1H), 7.54-7.46 (m, 3H), 6.34 (d, *J*= 16.2 Hz, 1H), 6.13(d, *J* = 15.7 Hz, 1H), 3.82-3.81 (m, 6H), 2.13-1.96 (m, 6H), 1.92-1.73 (m, 4H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.91, 167.68, 167.49, 157.44, 138.37, 137.75, 132.07, 128.65, 128.31, 126.15, 121.07, 118.24, 107.74, 76.29, 51.67, 36.75, 29.69, 25.52, 22.28. HRMS (ESI, m/z) calcd for $C_{23}H_{25}NO_5$ $[M+H]^+$ 396.1805, found 396.1807.

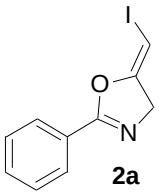


Yield: (60.51 mg, 62%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 7.5 Hz, 2H), 7.53-7.46, (m, 7H), 6.91-6.89 (m, 4H), 3.84 (s, 6H), 2.62-2.56 (m, 2H), 1.95-1.87 (m, 3H), 1.73-1.37 (m, 5H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 173.52, 158.54, 156.96, 131.96, 131.36, 130.78, 127.46, 127.33, 125.53, 114.59, 114.52, 113.07, 112.92, 91.54, 91.50, 79.38, 74.95, 54.30, 54.28, 33.35, 24.86, 21.29. HRMS (ESI, m/z) calcd for $C_{33}H_{29}NO_3$ $[M+H]^+$ 488.2220, found 488.2219.

NMR spectra for the products

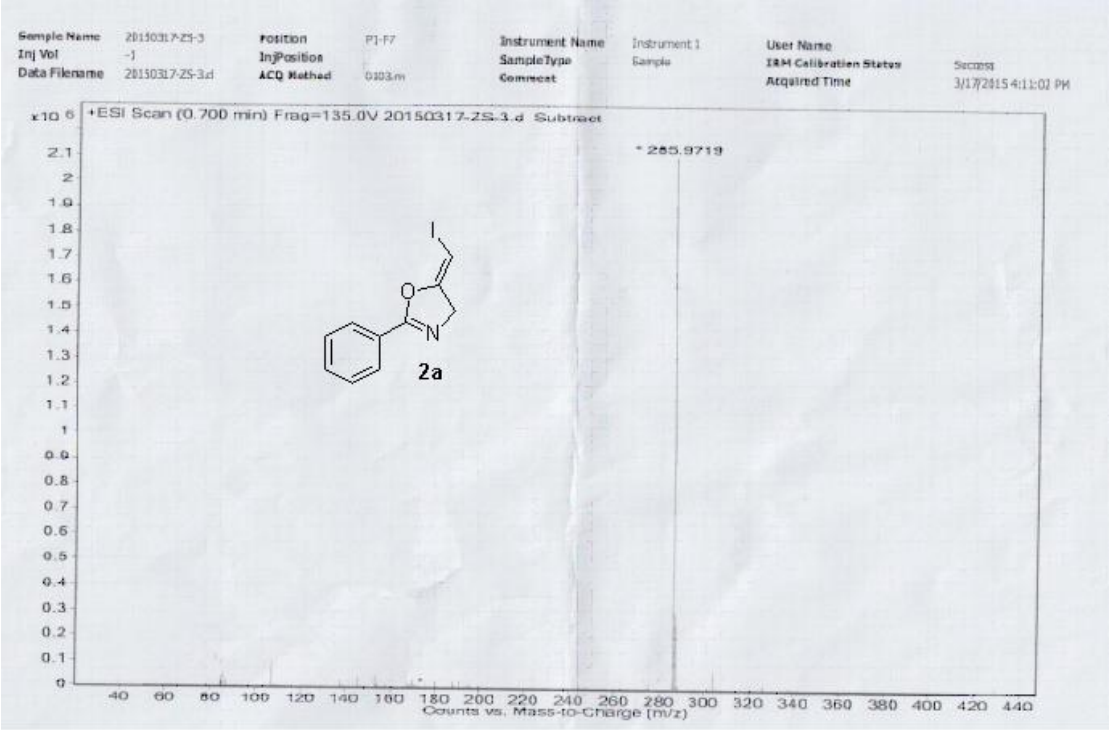




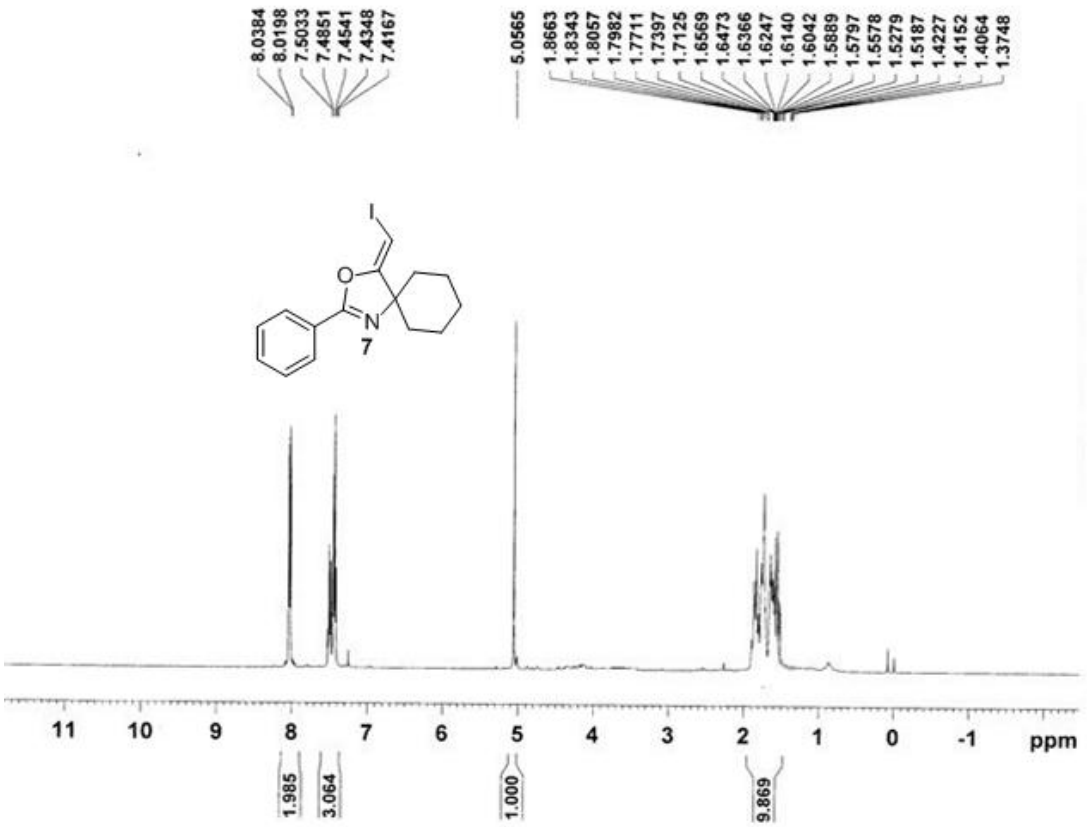


2a

Chemical Formula: $C_{10}H_8INO$
Exact Mass: 284.9651
Molecular Weight: 285.0811
m/z: 353.0277 : 284.9651 (100.0%), 285.9684 (11.1%)
Elemental Analysis: C, 42.13; H, 2.83; I, 44.52; N, 4.91; O, 5.61



HRMS (ESI, m/z) calcd for $C_{10}H_8INO\,[M+H]^+$ **285.9723**, found **285.9719.**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7.5033
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7.4541
7.4348
7.4167
5.0565
1.8663
1.8343
1.8057
1.7982
1.7711
1.7397
1.7125
1.6569
1.6473
1.6366
1.6247
1.6140
1.6042
1.5889
1.5797
1.5578
1.5279
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1.4152
1.4064
1.3748
I
O
N
7
11
10
9
8
7
6
5
4
3
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ppm
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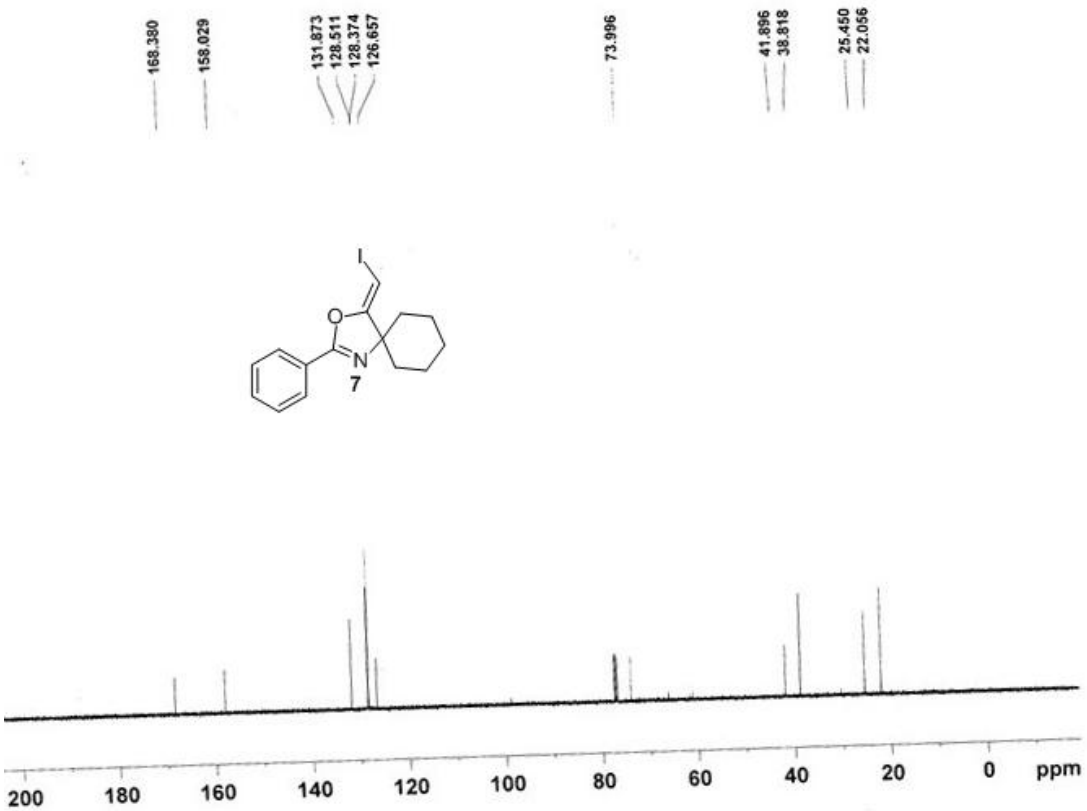
1.000
9.869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128.374
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41.896
38.818
25.450
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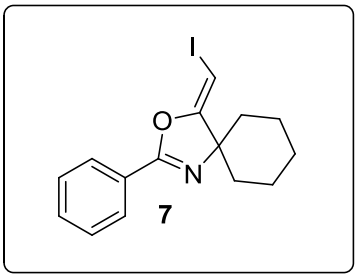
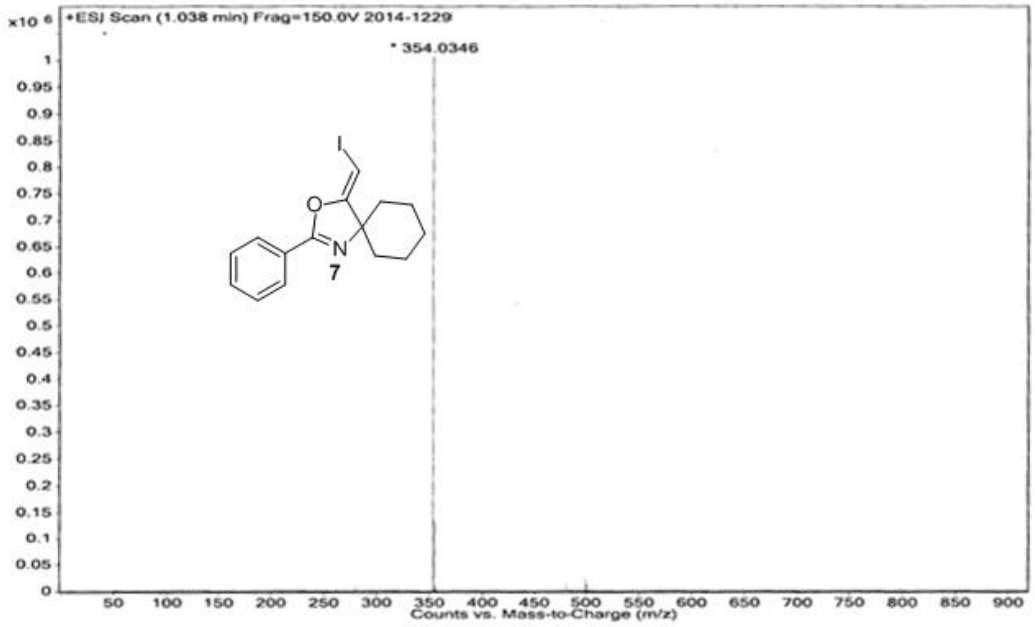
O
N
7
200
180
160
140
120
100
80
60
40
20
0
ppm

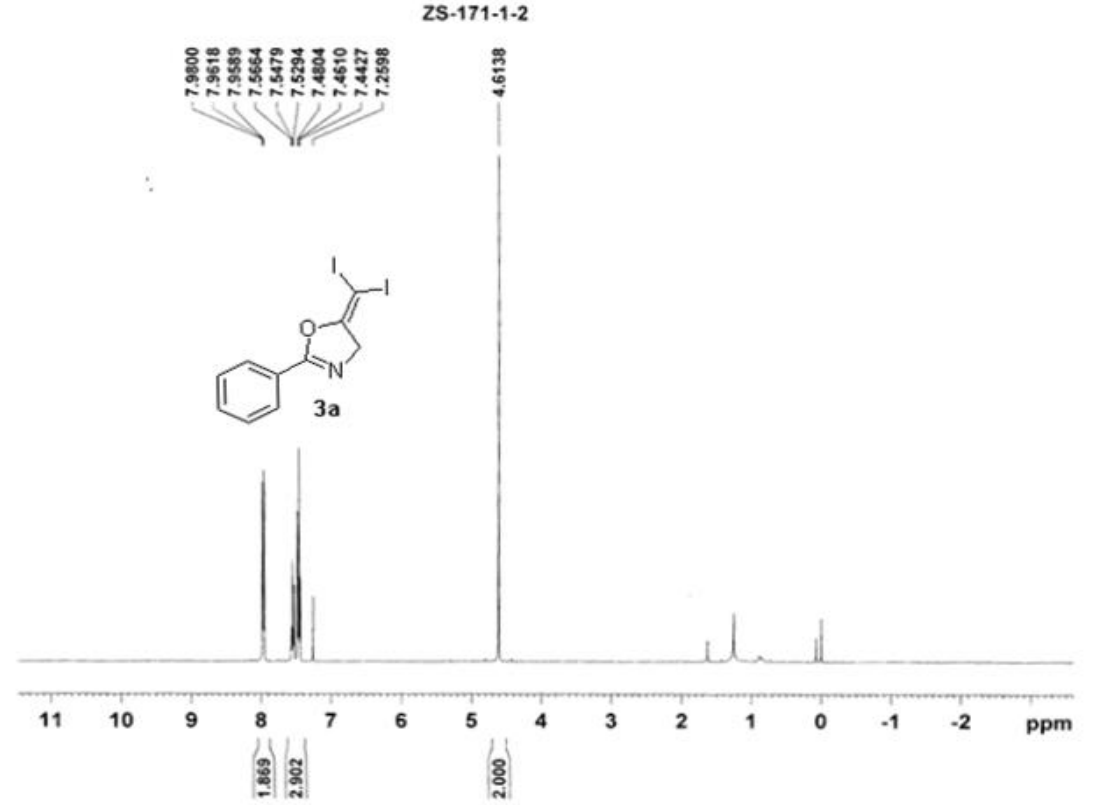


Chemical Formula: $C_{15}H_{16}INO$
Exact Mass: 353.0277
Molecular Weight: 353.1981
m/z: 353.0277 (100.0%), 354.0310 (16.2%), 355.0344 (1.2%)
Elemental Analysis: C, 51.01; H, 4.57; I, 35.93; N, 3.97; O, 4.53

Sample Name	2014-1229	**Position**	P1-C9	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	2014-1229	**ACQ Method**	0103.m	**Comment**		**Acquired Time**	12/29/2014 10:28:35 AM



HRMS (ESI, m/z) calcd for $C_{15}H_{16}INO$ $[M+H]^+$ **354.0349**, found **354.0346.**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7.4427
7.2598
4.6138
I
I
O
N
3a
11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
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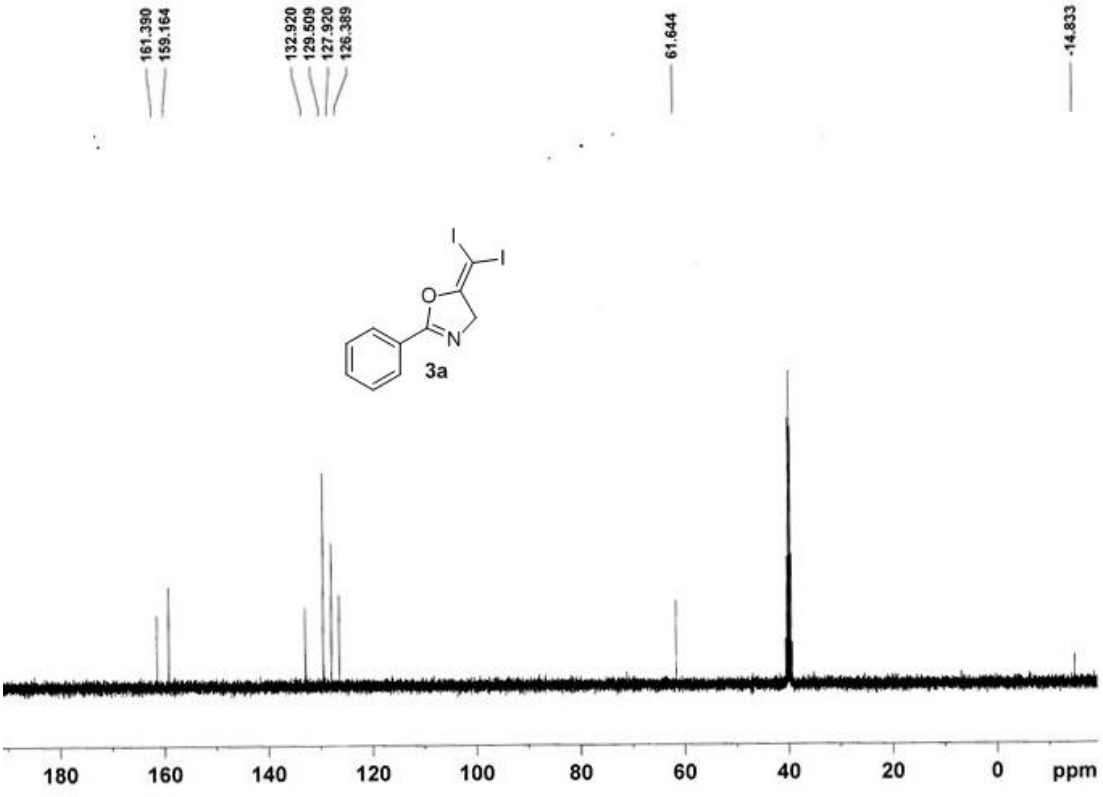
2.000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I
I
O
N
3a
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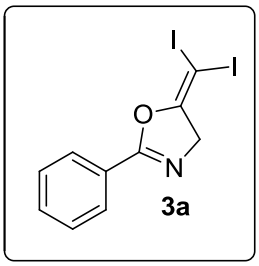
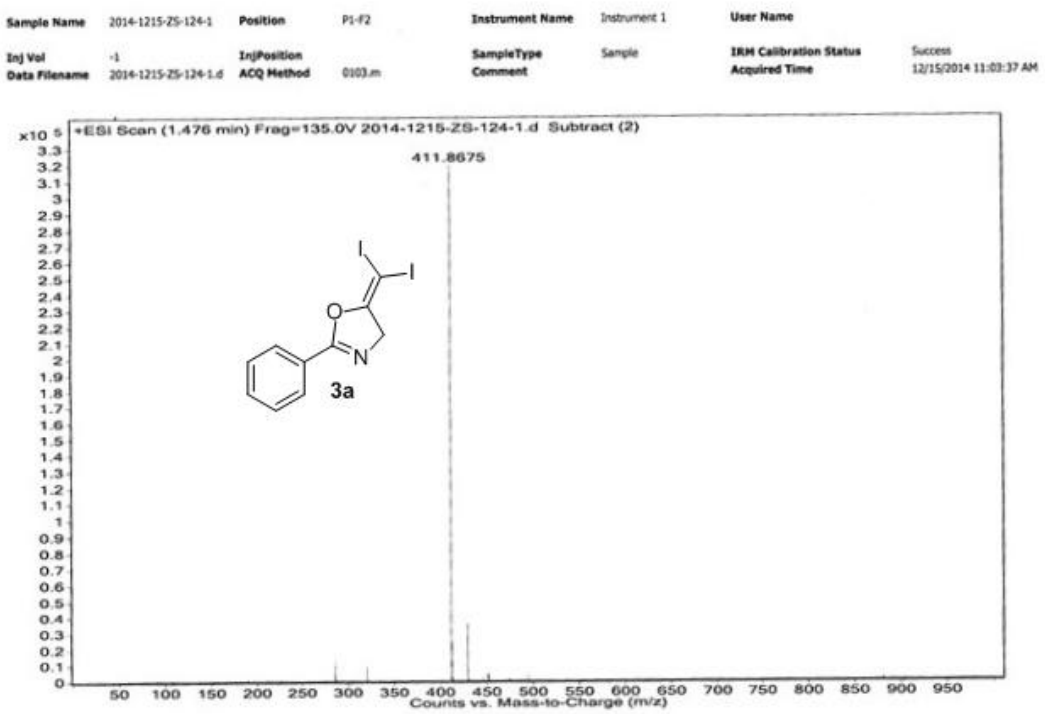
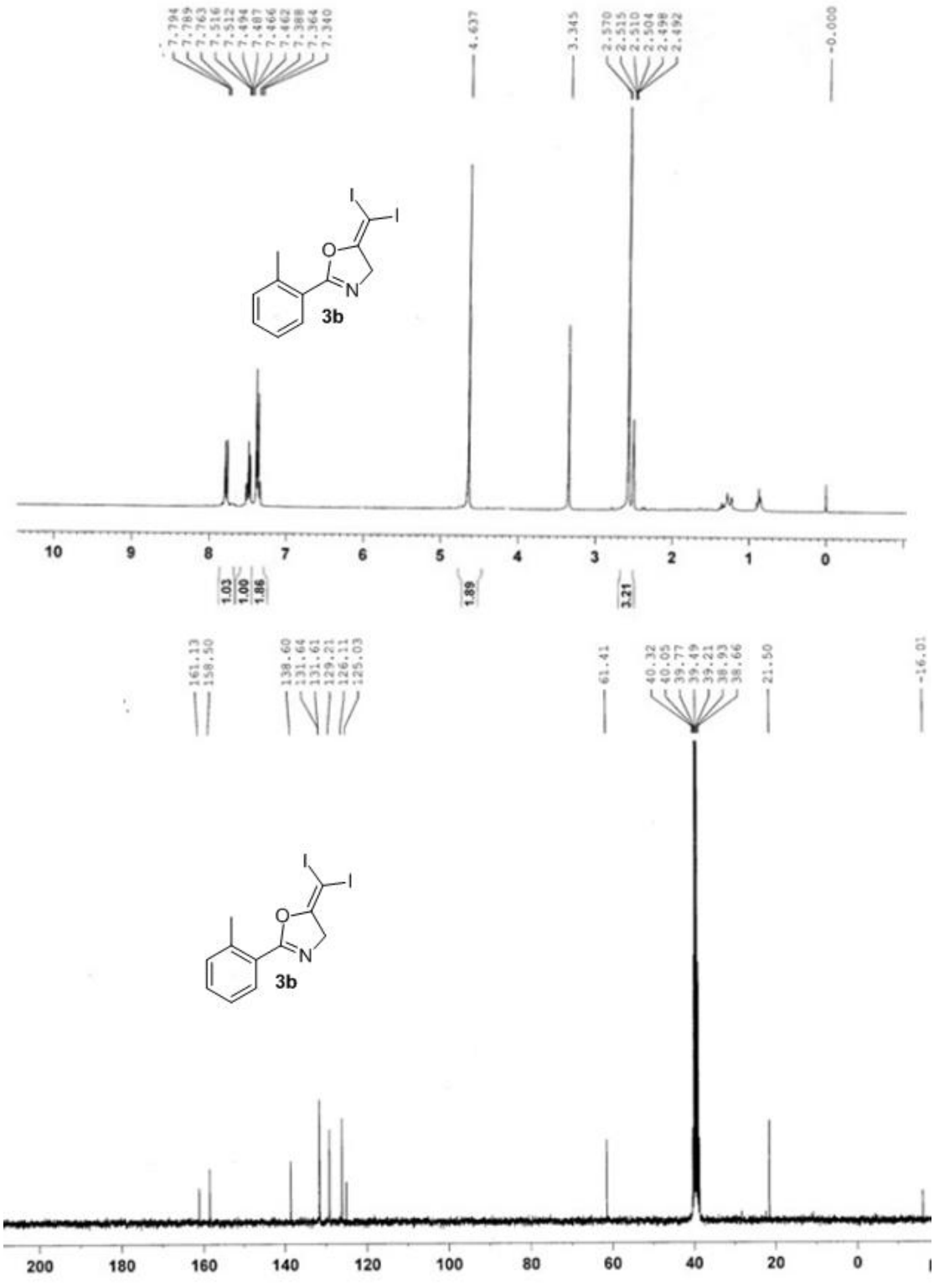


Chemical Formula: $C_{10}H_7I_2NO$
Exact Mass: 410.86
Molecular Weight: 410.98
m/z: 410.86 (100.0%), 411.87 (10.9%)
Elemental Analysis: C, 29.22; H, 1.72; I, 61.76; N, 3.41; O, 3.89



HRMS (ESI, m/z) calcd for $C_{10}H_7I_2NO$ $[M+H]^+$ **411.8690,** found **411.8675.**


7.794
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7.512
7.494
7.487
7.466
7.462
7.388
7.364
7.340
4.637
3.345
2.570
2.515
2.510
2.504
2.498
2.492
0.000
I
I
O
N
3b
10
9
8
7
6
5
4
3
2
1
0
1.03
1.00
1.86
1.89
3.21
161.13
158.50
138.60
131.64
131.61
129.21
126.11
125.03
61.41
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40.05
39.77
39.49
39.21
38.93
38.66
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140
120
100
80
60
40
20
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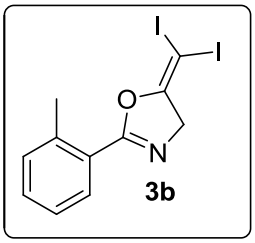
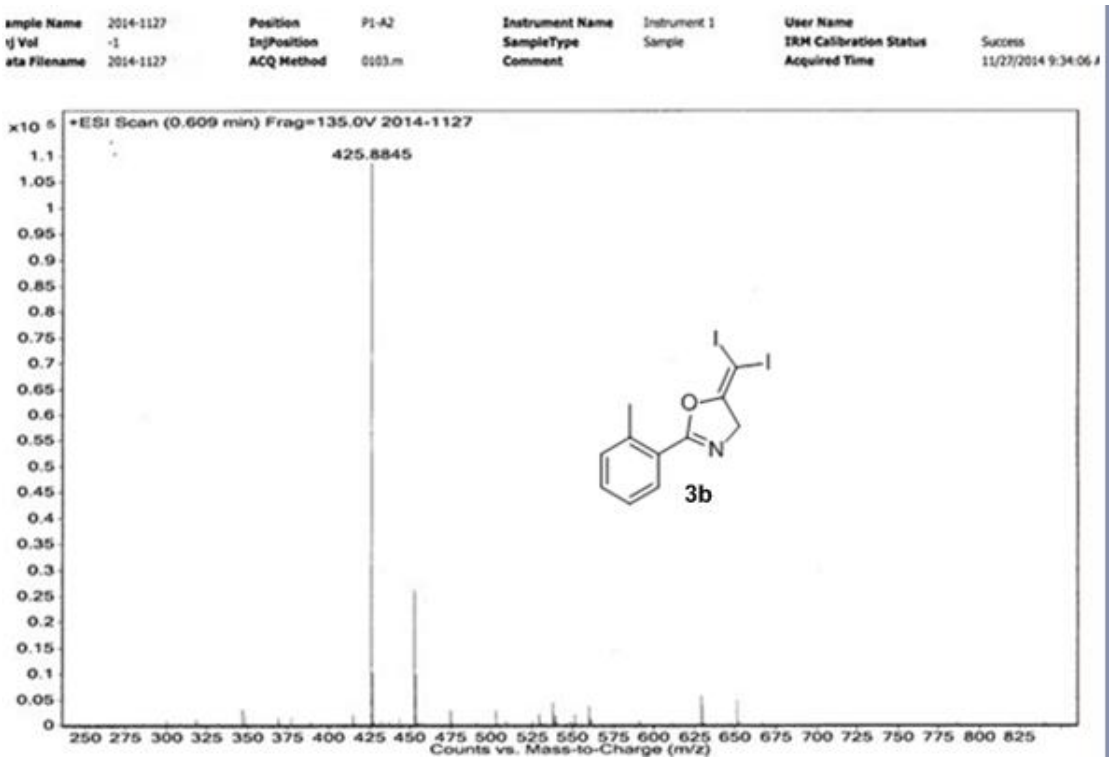
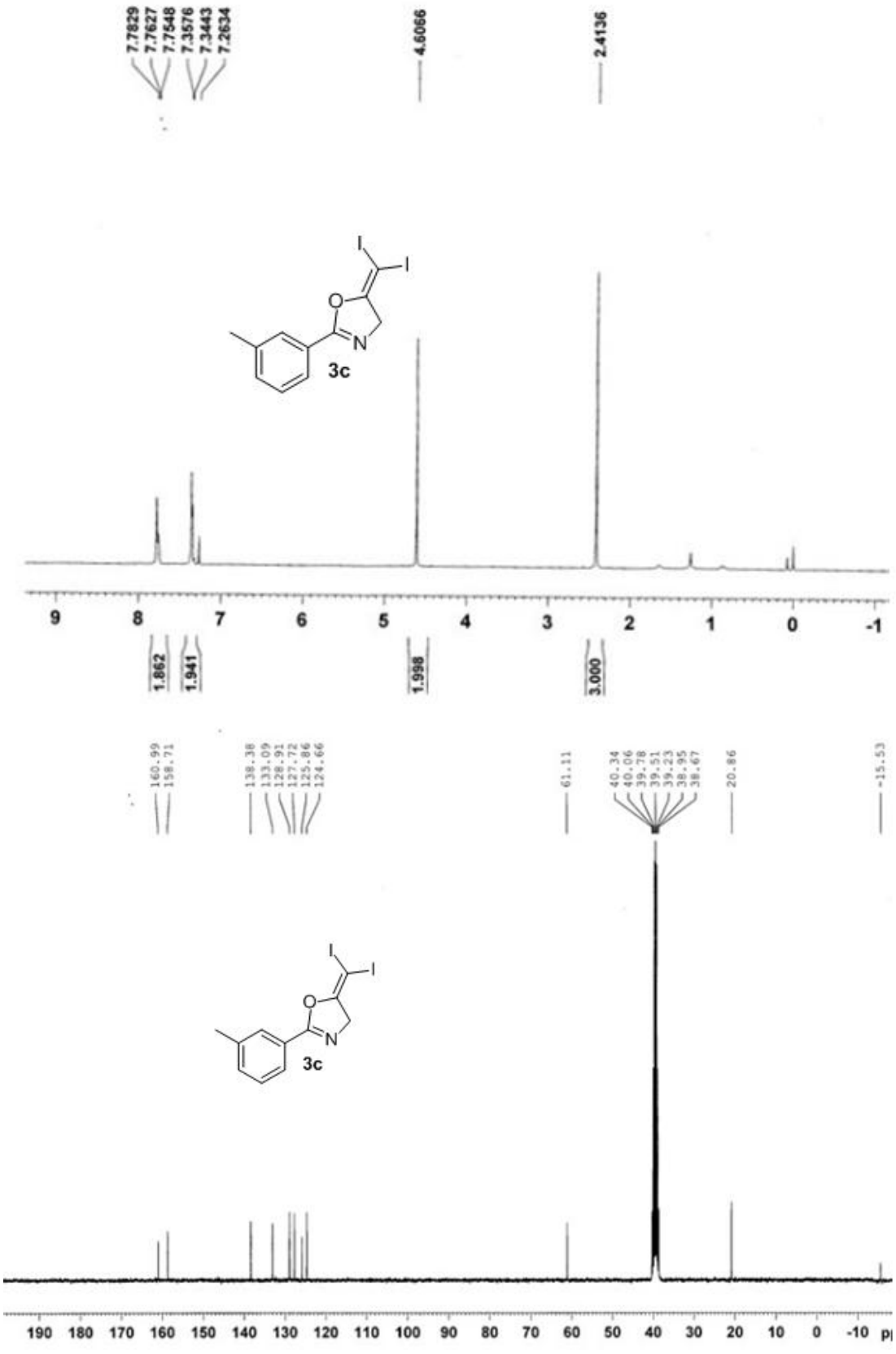


Chemical Formula: $C_{11}H_9I_2NO$
Exact Mass: 424.88
Molecular Weight: 425.00
m/z: 424.88 (100.0%), 425.88 (12.0%)
Elemental Analysis: C, 31.09; H, 2.13; I, 59.72; N, 3.30; O, 3.76



HRMS (ESI, m/z) calcd for $C_{11}H_9I_2NO$ $[M+H]^+$ **425.8846**, found **425.8845.**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7.2634
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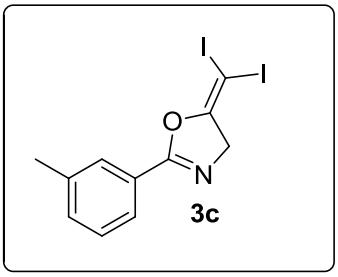
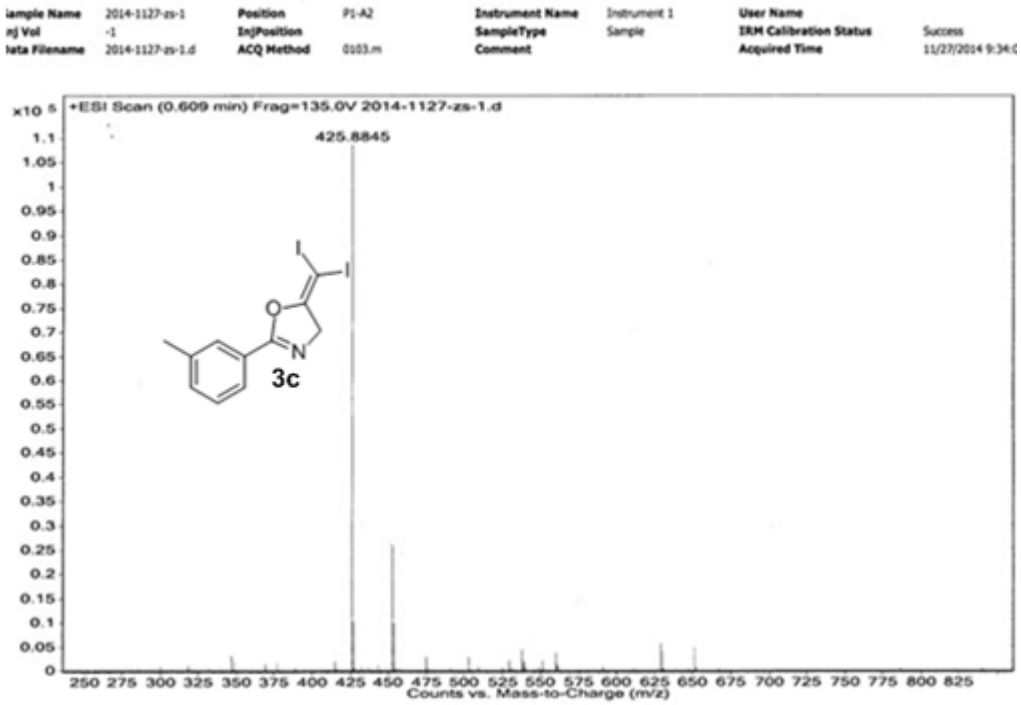
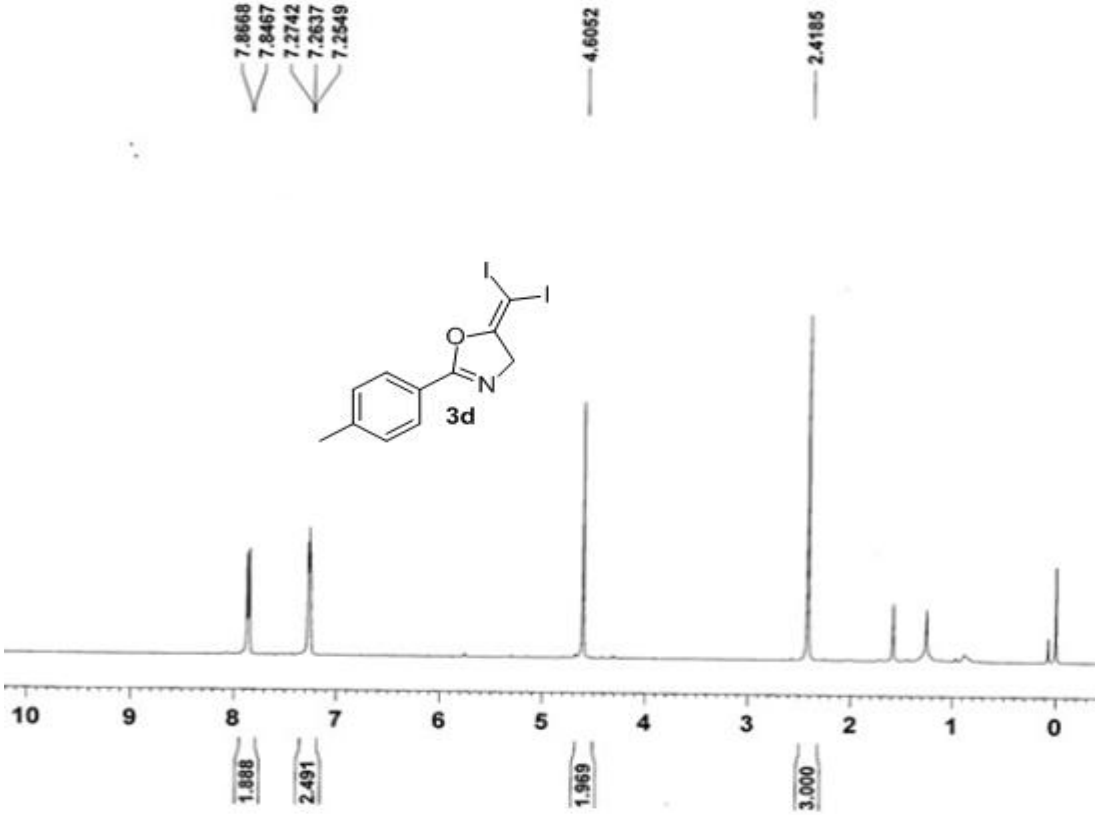
I
I
O
N
3c
9
8
7
6
5
4
3
2
1
0
-1
1.862
1.941
1.998
3.000
160.99
158.71
138.38
133.09
128.91
127.72
125.86
124.66
61.11
40.34
40.06
39.78
39.51
39.23
38.95
38.67
20.86
-15.53
I
I
O
N
3c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

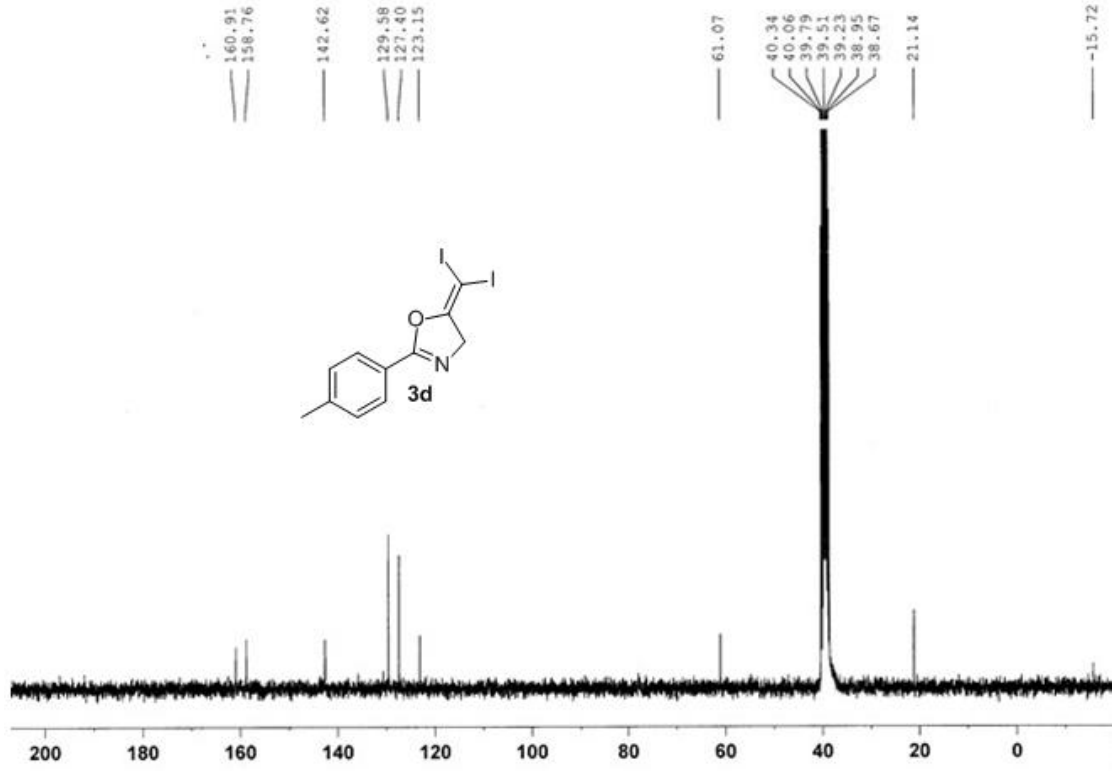


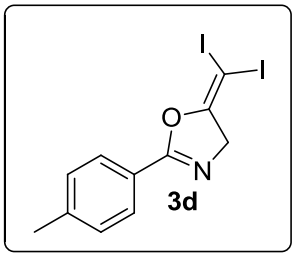
Chemical Formula: $C_{11}H_9I_2NO$
Exact Mass: 424.88
Molecular Weight: 425.00
m/z: 424.88 (100.0%), 425.88 (12.0%)
Elemental Analysis: C, 31.09; H, 2.13; I, 59.72; N, 3.30; O, 3.76



HRMS (ESI, m/z) calcd for $C_{11}H_9I_2NO$ $[M+H]^+$ **425.8846**, found **425.8845.**

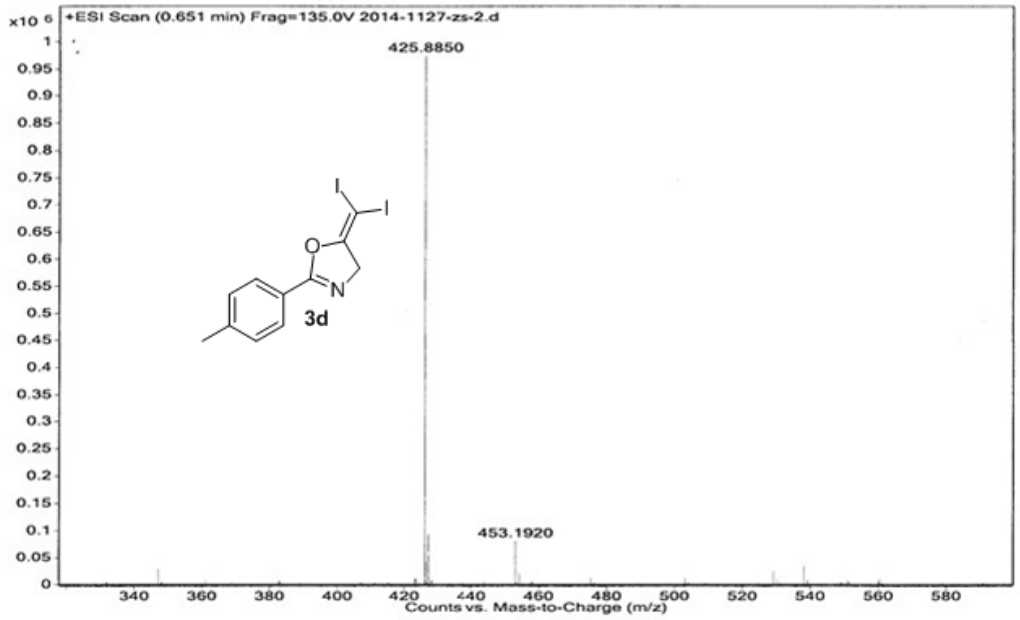

7.8668
7.8467
7.2742
7.2637
7.2549
4.6052
2.4185
I
I
O
N
3d
10
9
8
7
6
5
4
3
2
1
0
1.888
2.491
1.969
3.000


160.91
158.76
142.62
129.58
127.40
123.15
61.07
40.34
40.06
39.79
39.51
39.23
38.95
38.67
21.14
-15.72
I
I
O
N
3d
200
180
160
140
120
100
80
60
40
20
0

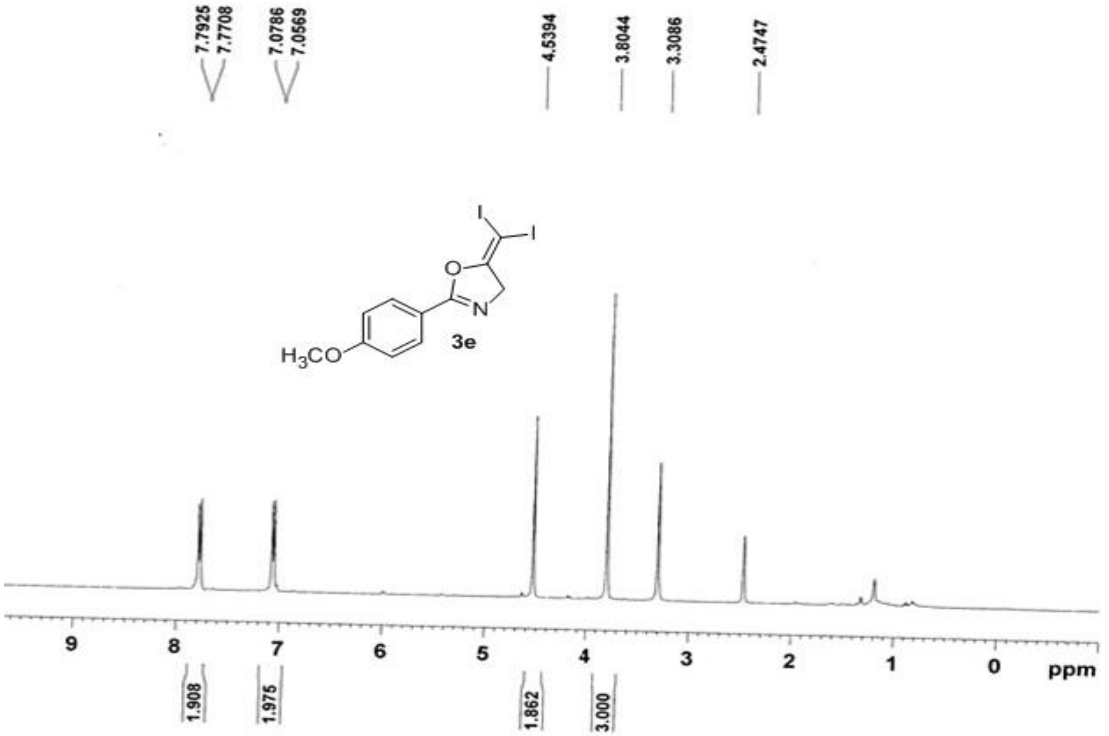


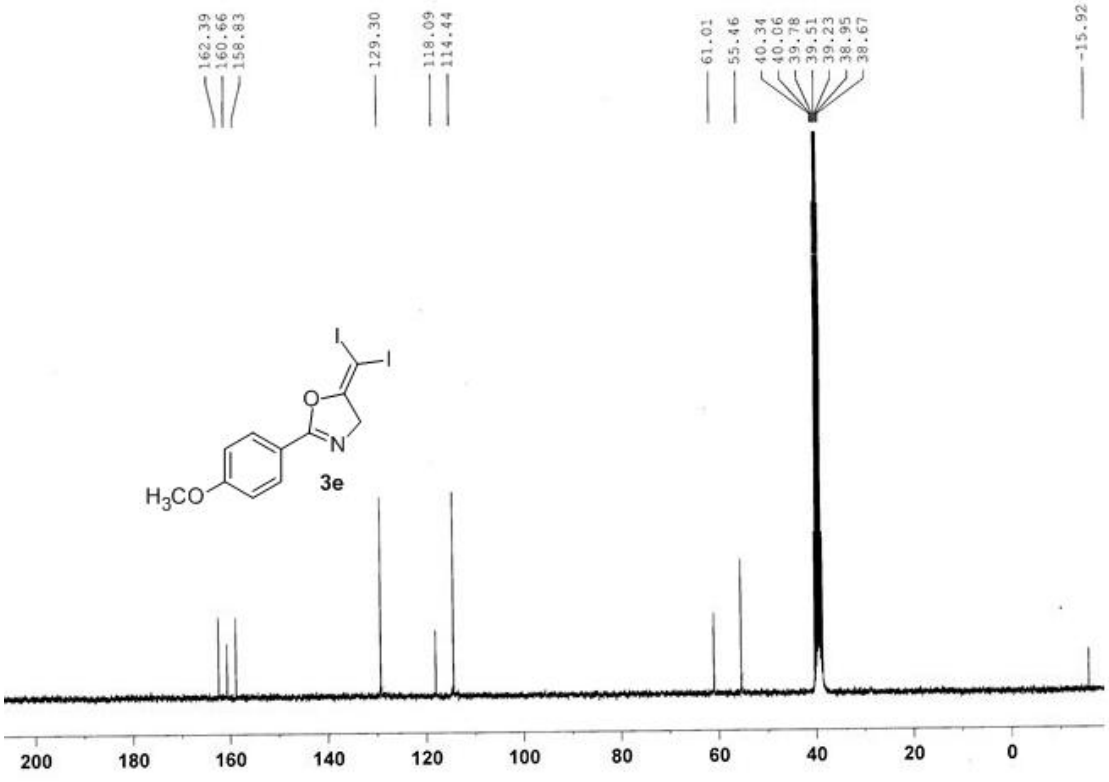
Chemical Formula: $C_{11}H_9I_2NO$
Exact Mass: 424.88
Molecular Weight: 425.00
m/z: 424.88 (100.0%), 425.88 (12.0%)
Elemental Analysis: C, 31.09; H, 2.13; I, 59.72; N, 3.30; O, 3.76

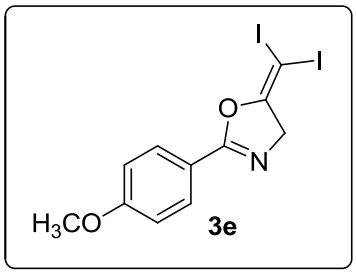
Sample Name	2014-1127-zs-2	**Position**	P1-B2	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	2014-1127-zs-2.d	**ACQ Method**	0103.m	**Comment**		**Acquired Time**	11/27/2014 9:36:23 AM



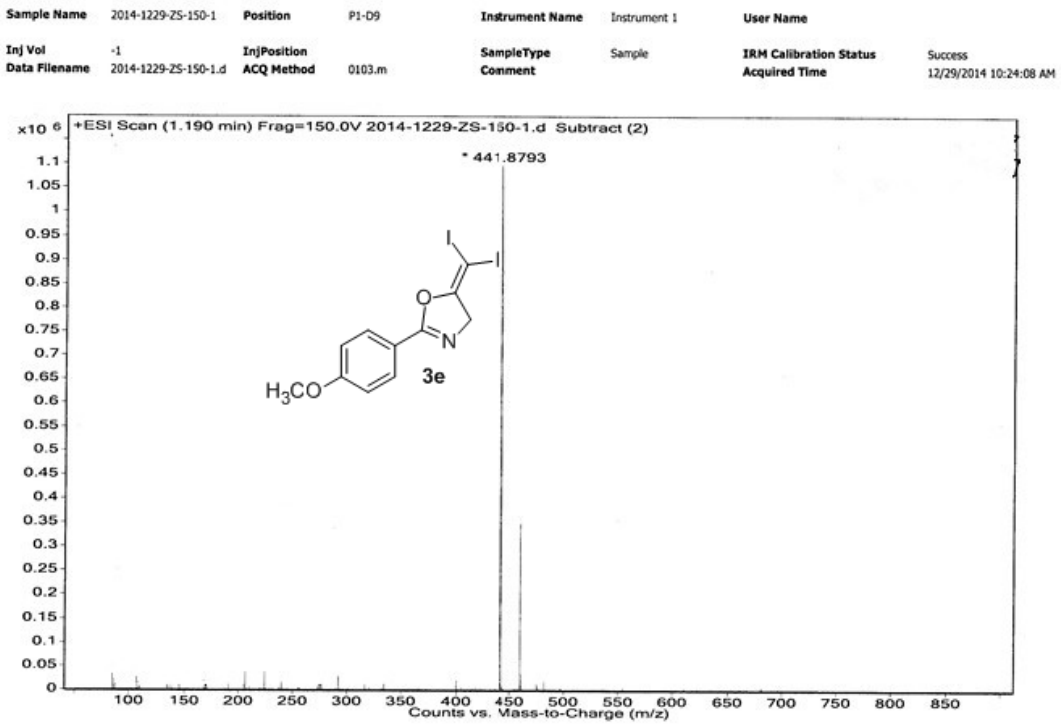
HRMS (ESI, m/z) calcd for $C_{11}H_9I_2NO$ $[M+H]^+$ **425.8846**, found **425.8850.**


7.7925
7.7708
7.0786
7.0569
4.5394
3.8044
3.3086
2.4747
I
I
O
N
H3CO
3e
9
8
7
6
5
4
3
2
1
0
ppm
1.908
1.975
1.862
3.000

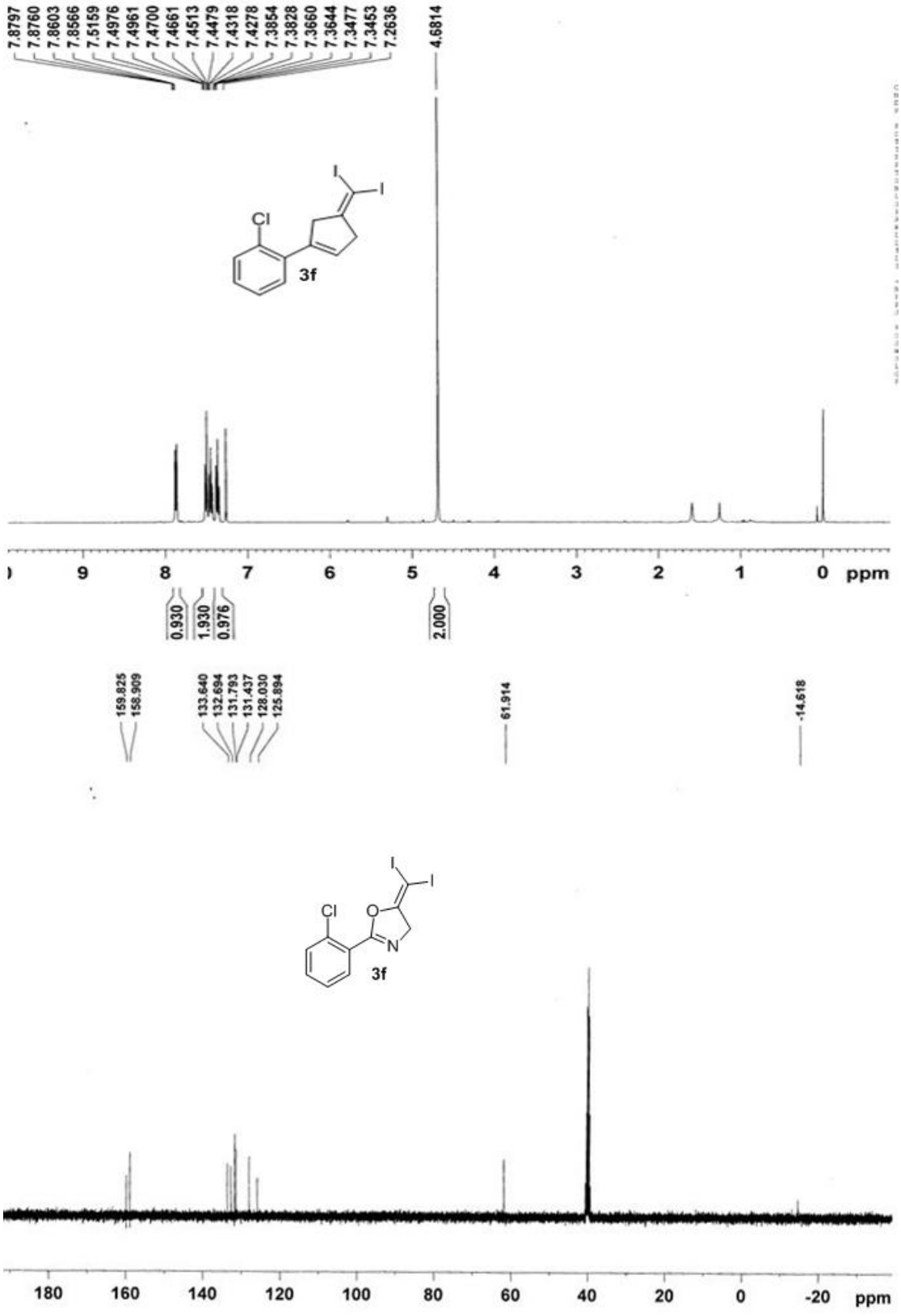

162.39
160.66
158.83
129.30
118.09
114.44
61.01
55.46
40.34
40.06
39.78
39.51
39.23
38.95
38.67
-15.92
I
I
O
N
H3CO
3e
200
180
160
140
120
100
80
60
40
20
0

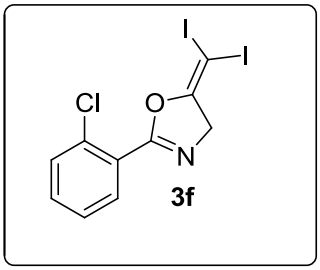


Chemical Formula: $C_{11}H_9I_2NO_2$
Exact Mass: 440.87
Molecular Weight: 441.00
m/z: 440.87 (100.0%), 441.88 (12.1%), 442.88 (1.1%)
Elemental Analysis: C, 29.96; H, 2.06; I, 57.55; N, 3.18; O, 7.26

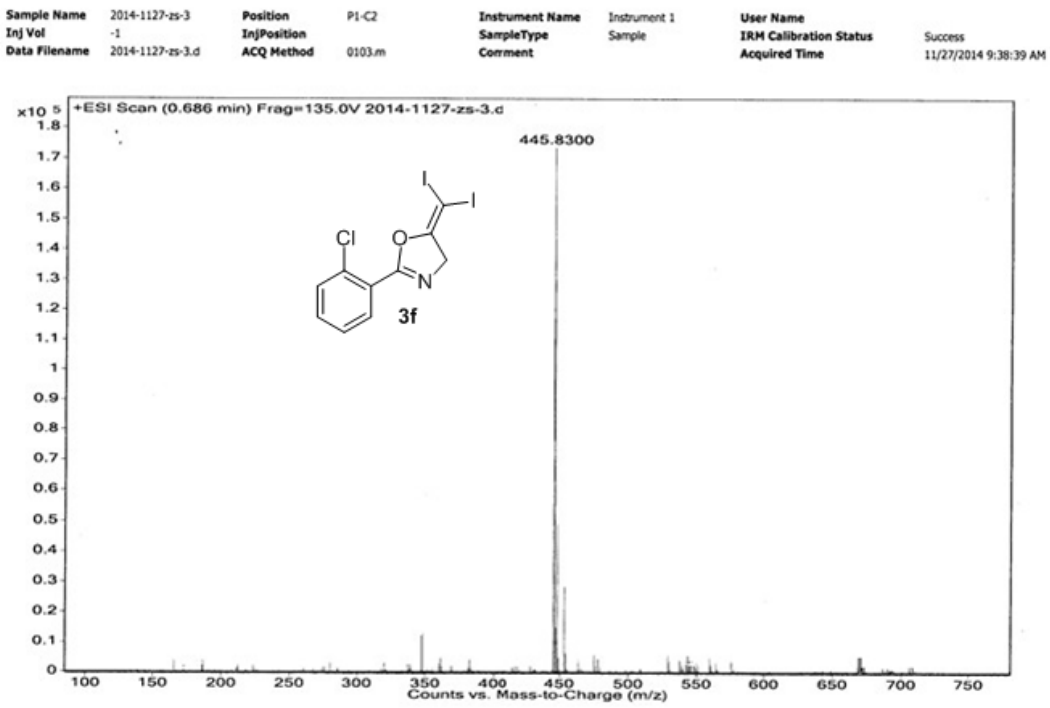


HRMS (ESI, m/z) calcd for $C_{11}H_9I_2NO_2$ $[M+H]^+$ **441.8795,** found **441.8793.**

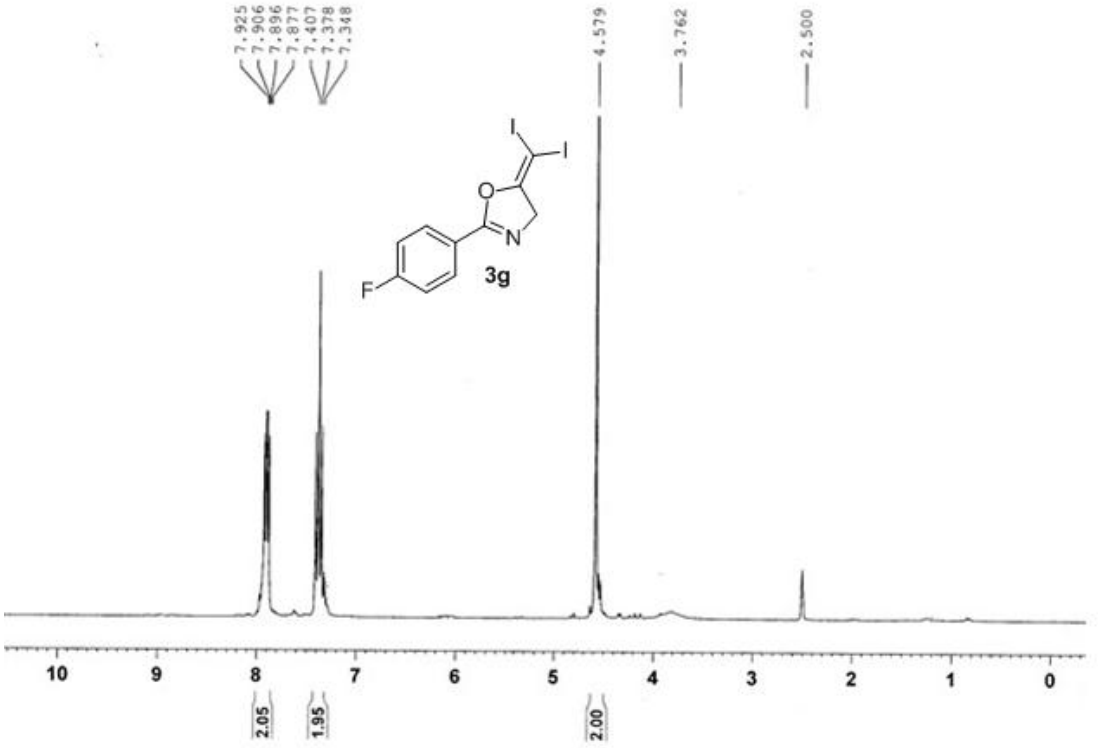

7.8797
7.8760
7.8603
7.8566
7.5159
7.4976
7.4961
7.4700
7.4661
7.4513
7.4479
7.4318
7.4278
7.3854
7.3828
7.3660
7.3644
7.3477
7.3453
7.2636
4.6814
I
I
Cl
3f
9
8
7
6
5
4
3
2
1
0
ppm
0.930
1.930
0.976
2.000
159.825
158.909
133.640
132.694
131.793
131.437
128.030
125.894
61.914
-14.618
I
I
Cl
O
N
3f
180
160
140
120
100
80
60
40
20
0
-20
ppm

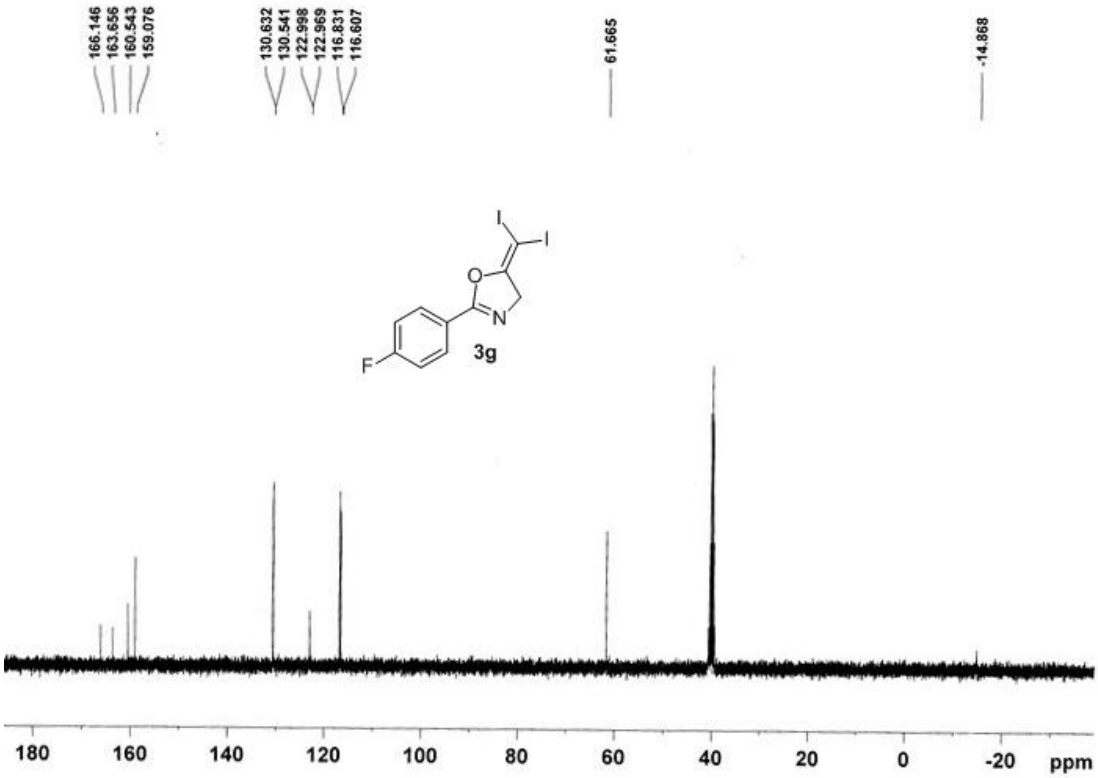


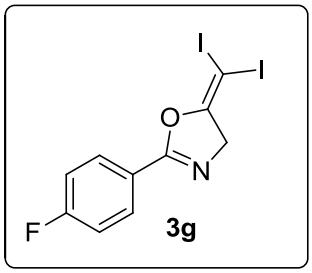
Chemical Formula: $C_{10}H_6ClI_2NO$
Exact Mass: 444.82
Molecular Weight: 445.42
m/z: 444.82 (100.0%), 446.82 (32.0%), 445.83 (10.9%), 447.82 (3.6%)
Elemental Analysis: C, 26.96; H, 1.36; Cl, 7.96; I, 56.98; N, 3.14; O, 3.59



HRMS (ESI, m/z) calcd for $C_{10}H_6ClI_2NO$ $[M+H]^+$ **445.8300,** found **445.8300.**

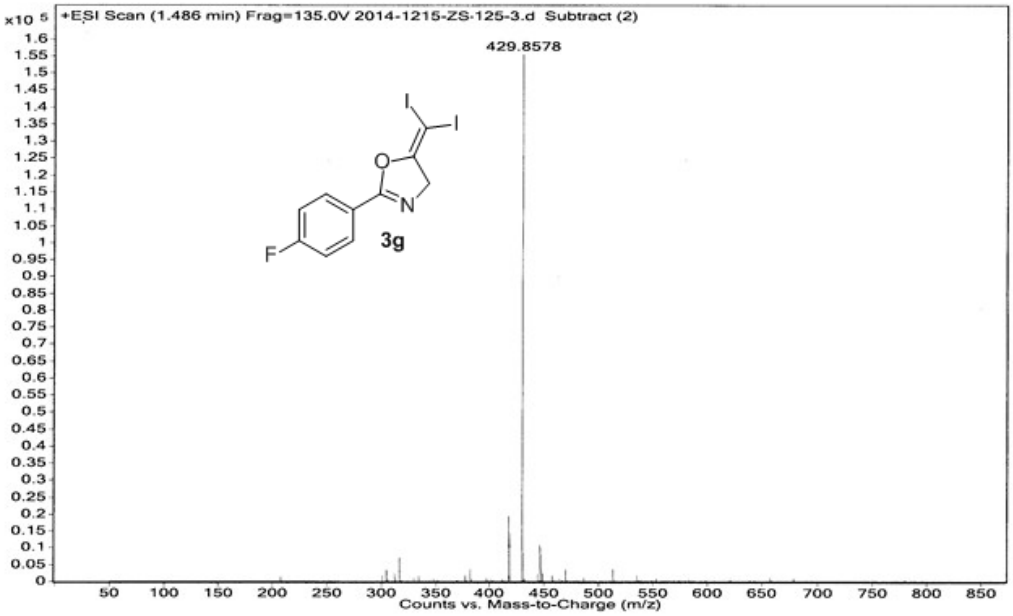

7.925
7.906
7.896
7.877
7.407
7.378
7.348
4.579
3.762
2.500
I
I
O
N
F
3g
10
9
8
7
6
5
4
3
2
1
0
2.05
1.95
2.00


166.146
163.656
160.543
159.076
130.632
130.541
122.998
122.969
116.831
116.607
61.665
-14.868
I
I
O
N
F
3g
180
160
140
120
100
80
60
40
20
0
-20
ppm

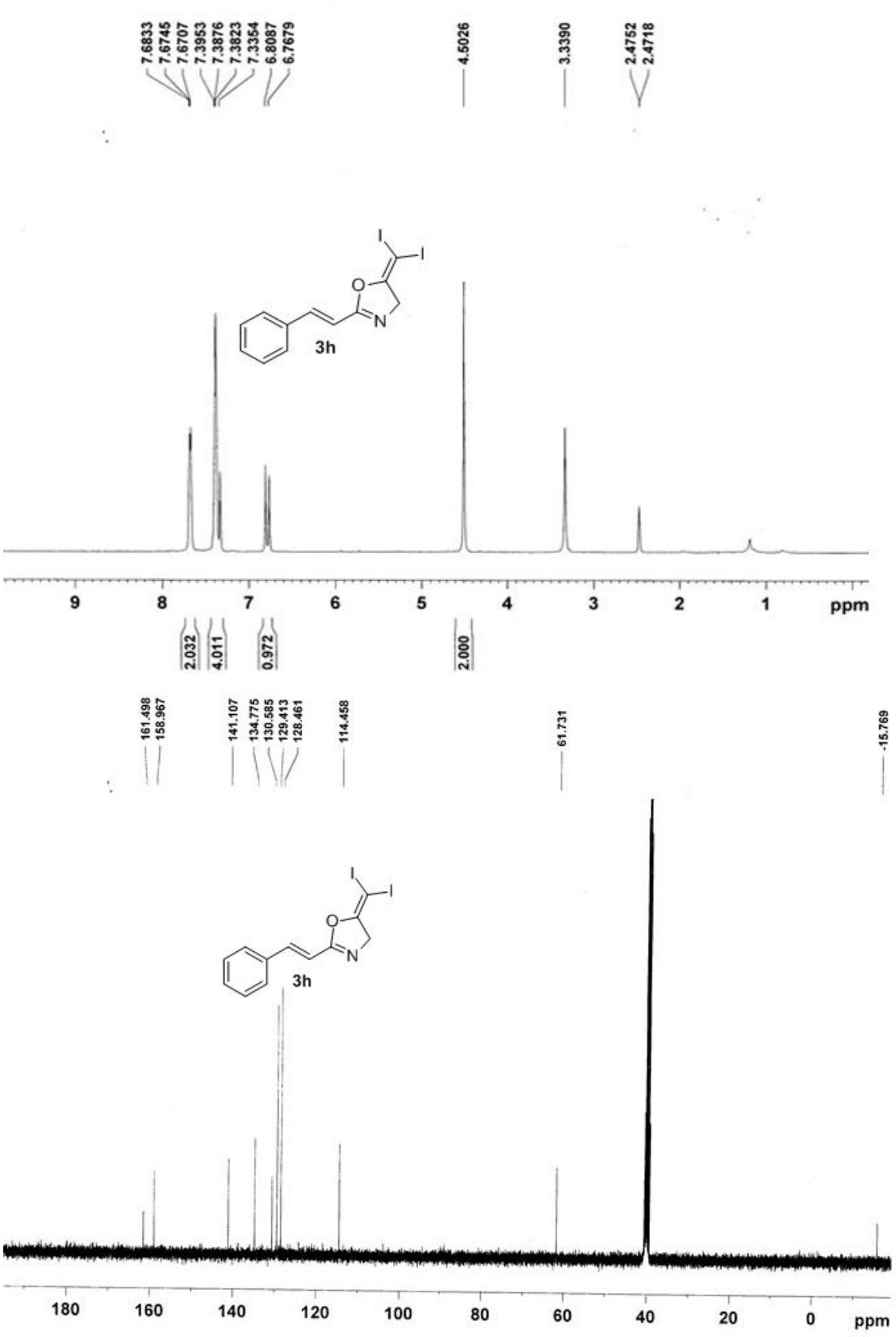


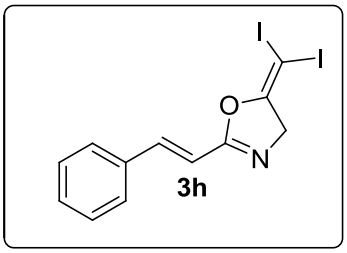
Chemical Formula: $C_{10}H_6FI_2NO$
Exact Mass: 428.85
Molecular Weight: 428.97
m/z: 428.85 (100.0%), 429.86 (10.9%)
Elemental Analysis: C, 28.00; H, 1.41; F, 4.43; I, 59.17; N, 3.27; O, 3.73

Sample Name	2014-1215-ZS-125-3	**Position**	P1-C2	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	2014-1215-ZS-125-3.d	**ACQ Method**	0103.m	**Comment**		**Acquired Time**	12/15/2014 11:12:44 AM

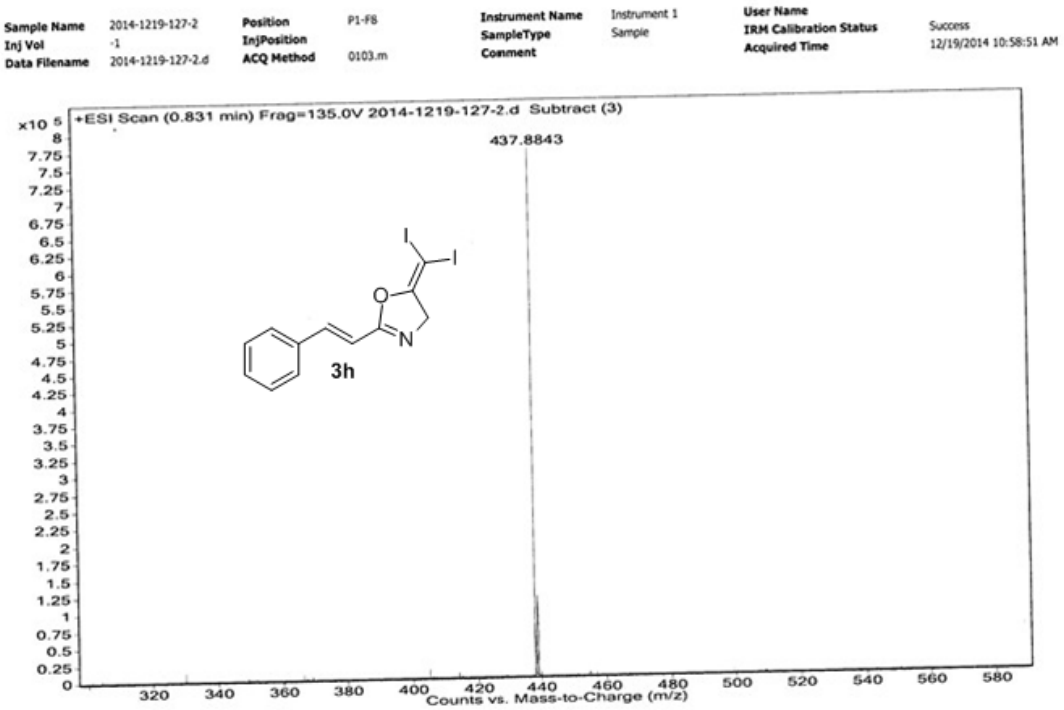


HRMS (ESI, m/z) calcd for $C_{10}H_6FI_2NO$ $[M+H]^+$ **429.8596,** found **429.8578.**

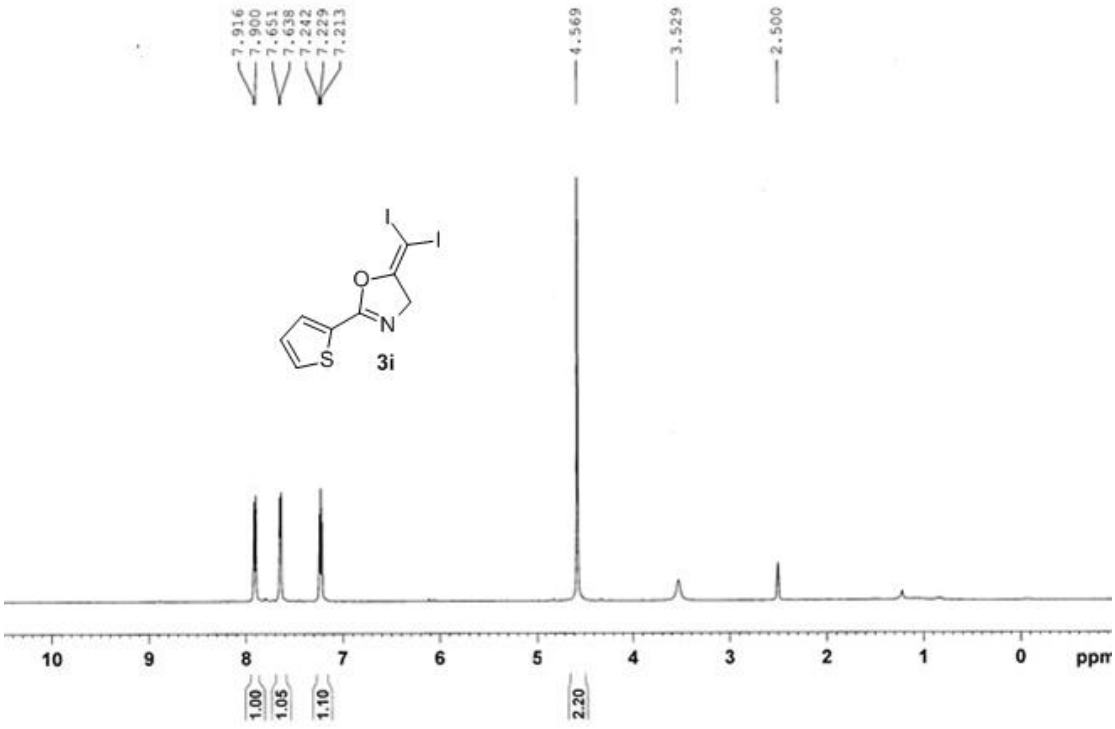

7.6833
7.6745
7.6707
7.3953
7.3876
7.3823
7.3354
6.8087
6.7679
4.5026
3.3390
2.4752
2.4718
I
I
O
N
3h
9
8
7
6
5
4
3
2
1
ppm
2.032
4.011
0.972
2.000
161.498
158.967
141.107
134.775
130.585
129.413
128.461
114.458
61.731
-15.769
I
I
O
N
3h
180
160
140
120
100
80
60
40
20
0
ppm

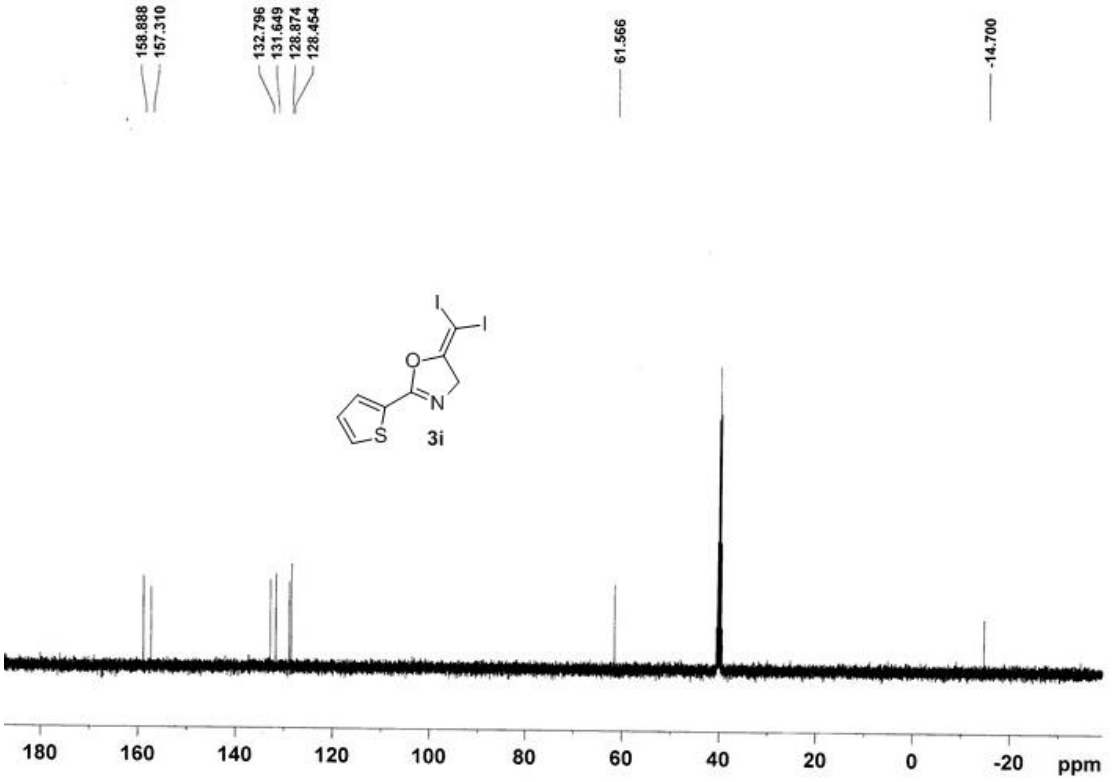


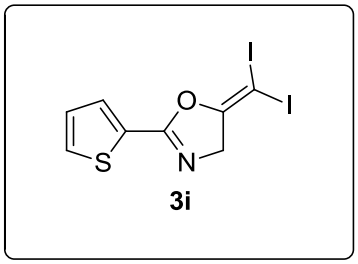
Chemical Formula: $C_{12}H_9I_2NO$
Exact Mass: 436.88
Molecular Weight: 437.01
m/z: 436.88 (100.0%), 437.88 (13.1%), 438.88 (1.0%)
Elemental Analysis: C, 32.98; H, 2.08; I, 58.08; N, 3.21; O, 3.66



HRMS (ESI, m/z) calcd for $C_{12}H_9I_2NO$ $[M+H]^+$ **437.8846,** found **437.8843.**


7.916
7.900
7.651
7.638
7.242
7.229
7.213
4.569
3.529
2.500
I
I
O
N
S
3i
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.05
1.10
2.20

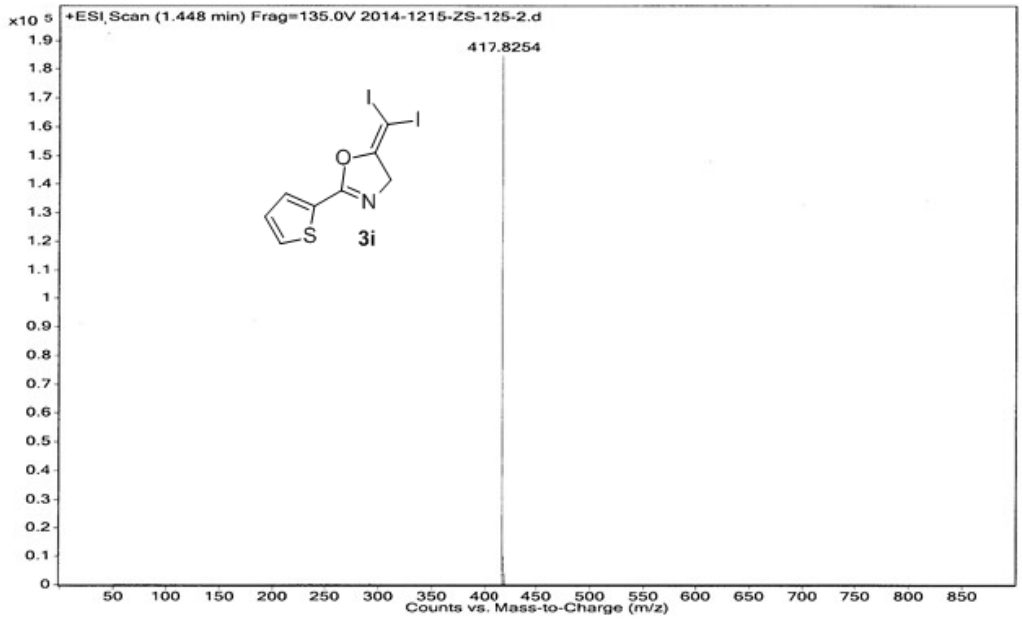

158.888
157.310
132.796
131.649
128.874
128.454
61.566
-14.700
I
I
O
N
S
3i
180
160
140
120
100
80
60
40
20
0
-20
ppm



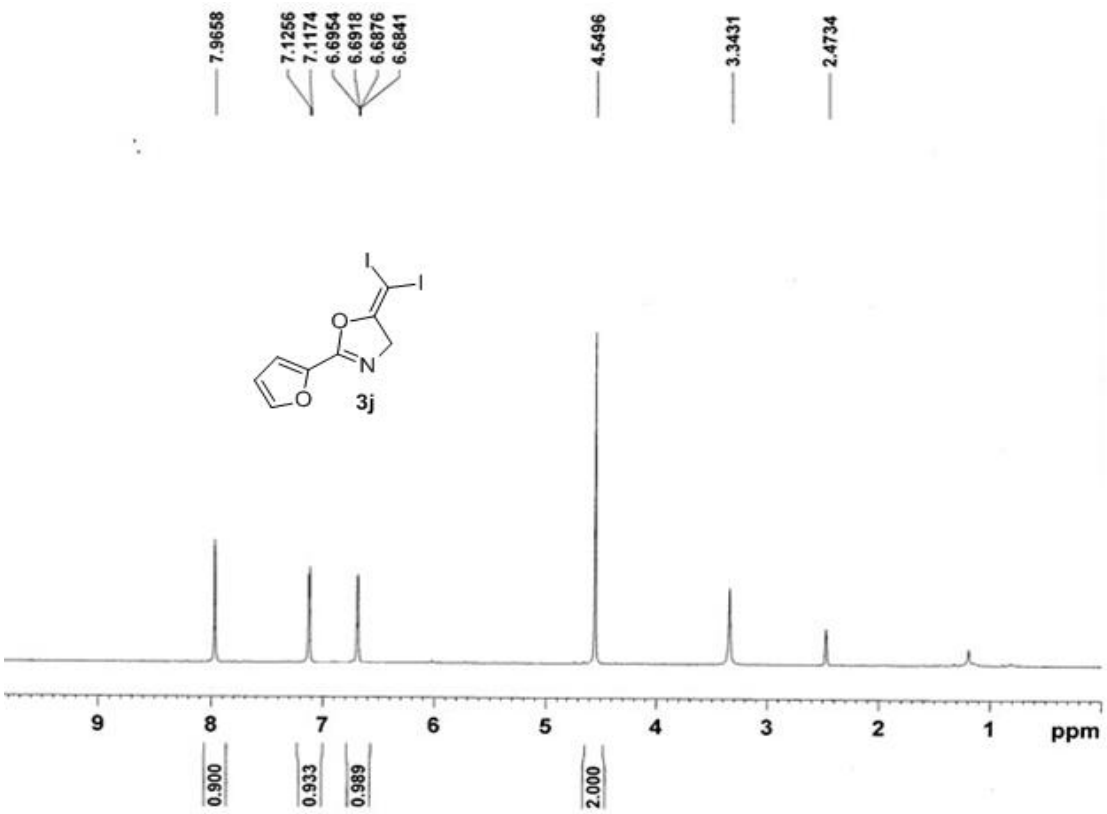
3i

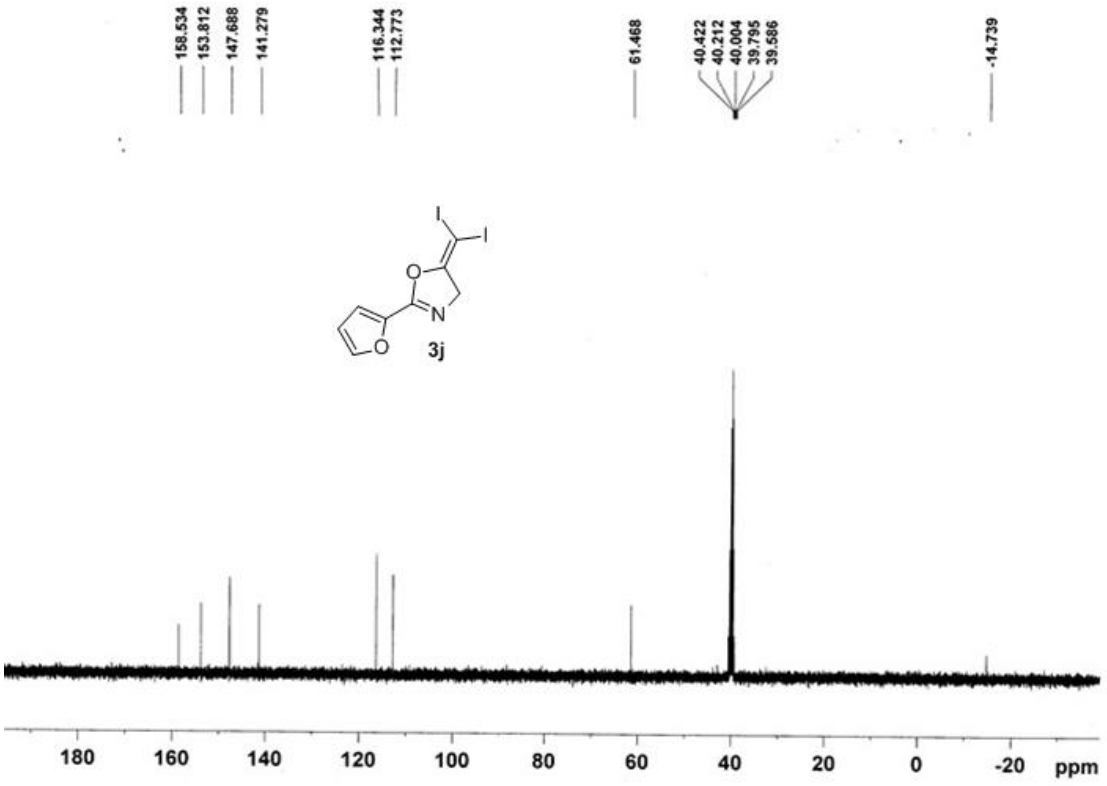
Chemical Formula: $C_8H_5I_2NOS$
Exact Mass: 416.8181
Molecular Weight: 417.0053
m/z: 416.8181 (100.0%), 417.8215 (8.7%), 418.8139 (4.5%)
Elemental Analysis: C, 23.04; H, 1.21; I, 60.86; N, 3.36; O, 3.84; S, 7.69

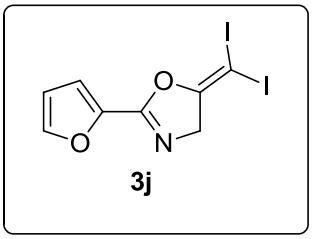
Sample Name	2014-1215-ZS-125-2	**Position**	P1-D2	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	2014-1215-ZS-125-2.d	**ACQ Method**	0103.m	**Comment**		**Acquired Time**	12/15/2014 11:10:27 AM



HRMS (ESI, m/z) calcd for $C_8H_5I_2NOS$ $[M+H]^+$ **417.8254,** found **417.8254.**


7.9658
7.1256
7.1174
6.6954
6.6918
6.6876
6.6841
4.5496
3.3431
2.4734
I
I
O
N
O
3j
9
8
7
6
5
4
3
2
1
ppm
0.900
0.933
0.989
2.000

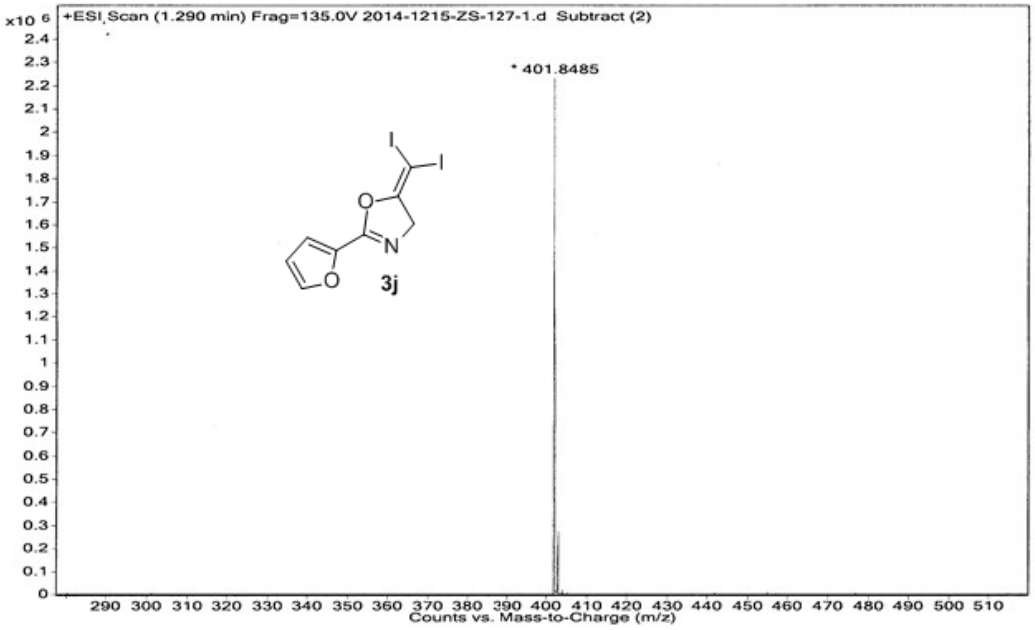

158.534
153.812
147.688
141.279
116.344
112.773
61.468
40.422
40.212
40.004
39.795
39.586
-14.739
I
I
O
N
O
3j
180
160
140
120
100
80
60
40
20
0
-20
ppm



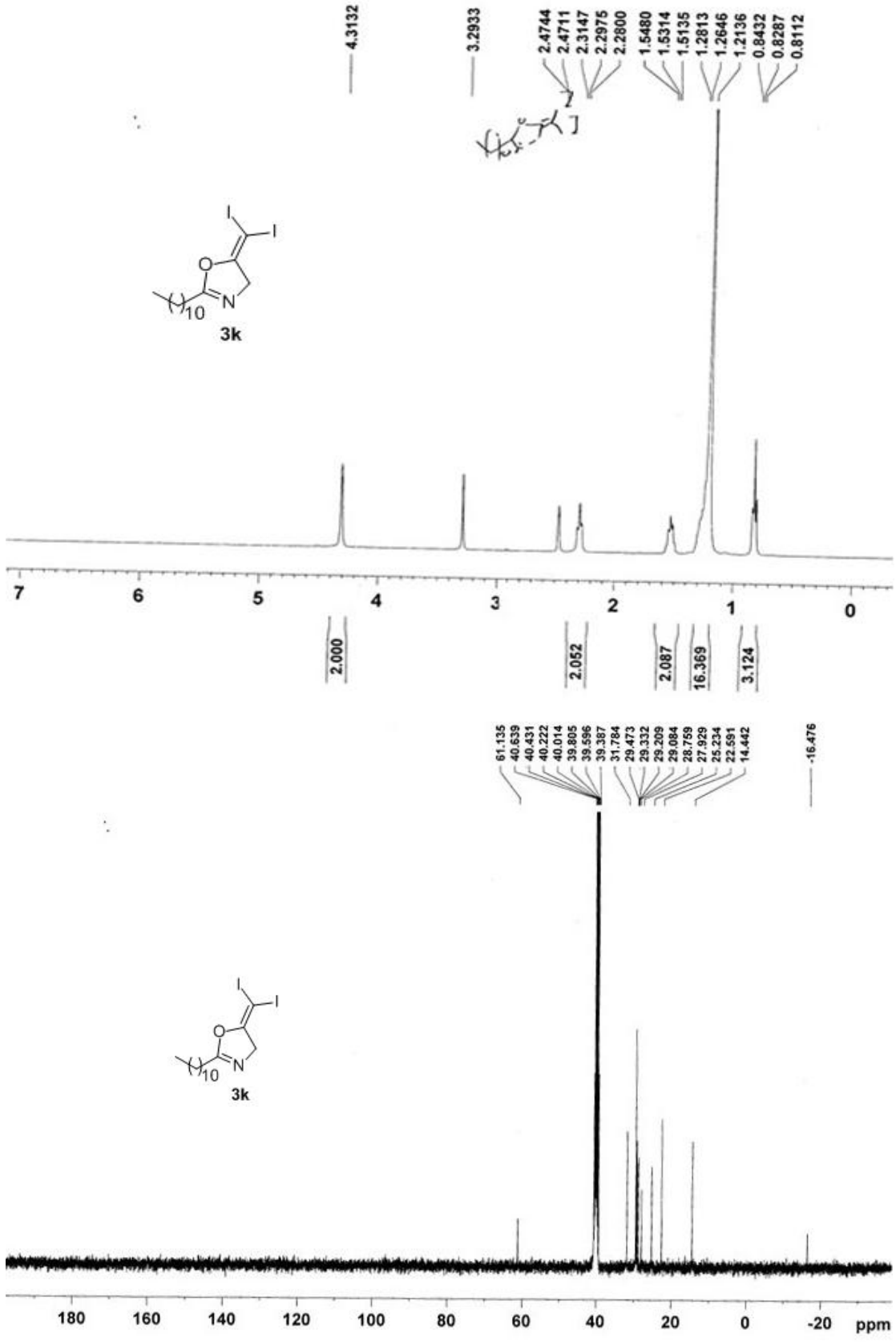
3j

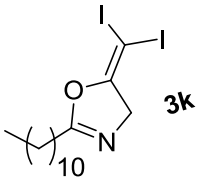
Chemical Formula: $C_8H_5I_2NO_2$
Exact Mass: 400.84
Molecular Weight: 400.94
m/z: 400.84 (100.0%), 401.84 (9.0%)
Elemental Analysis: C, 23.97; H, 1.26; I, 63.30; N, 3.49; O, 7.98

Sample Name	2014-1215-ZS-127-1	**Position**	P1-E2	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	2014-1215-ZS-127-1.d	**ACQ Method**	0103.m	**Comment**		**Acquired Time**	12/15/2014 11:08:10 AM

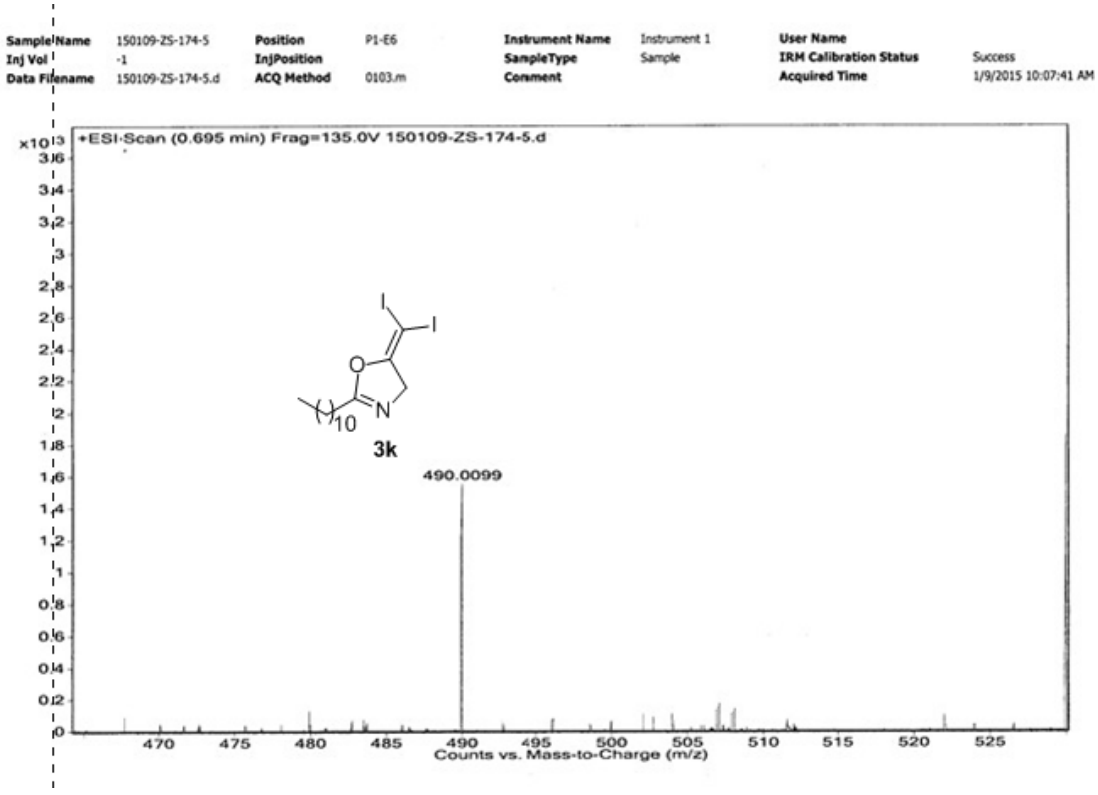


HRMS (ESI, m/z) calcd for $C_8H_5I_2NO$ $[M+H]^+$ **401.8482**, found **401.8485.**

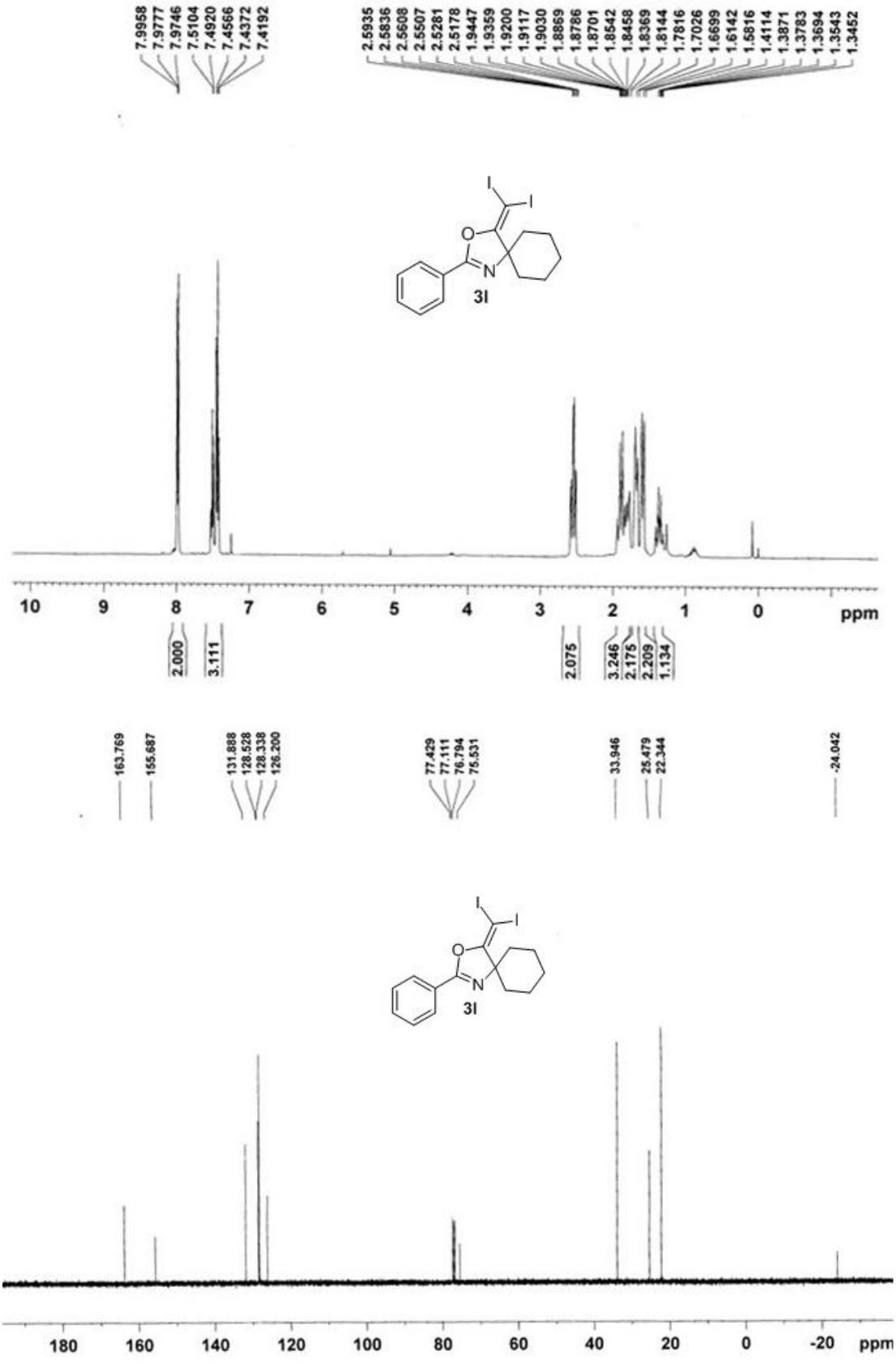

4.3132
3.2933
2.4744
2.4711
2.3147
2.2975
2.2800
1.5480
1.5314
1.5135
1.2813
1.2646
1.2136
0.8432
0.8287
0.8112
3k
7
6
5
4
3
2
1
0
2.000
2.052
2.087
16.369
3.124
61.135
40.639
40.431
40.222
40.014
39.805
39.596
39.387
31.784
29.473
29.332
29.209
29.084
28.759
27.929
25.234
22.591
14.442
-16.476
3k
180
160
140
120
100
80
60
40
20
0
-20
ppm

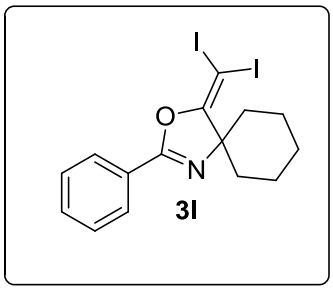


Chemical Formula: $C_{15}H_{25}I_2NO$
Exact Mass: 489.0026
Molecular Weight: 489.1740
m/z: 489.0026 (100.0%), 490.0059 (16.2%), 491.0093 (1.2%)
Elemental Analysis: C, 36.83; H, 5.15; I, 51.89; N, 2.86; O, 3.27



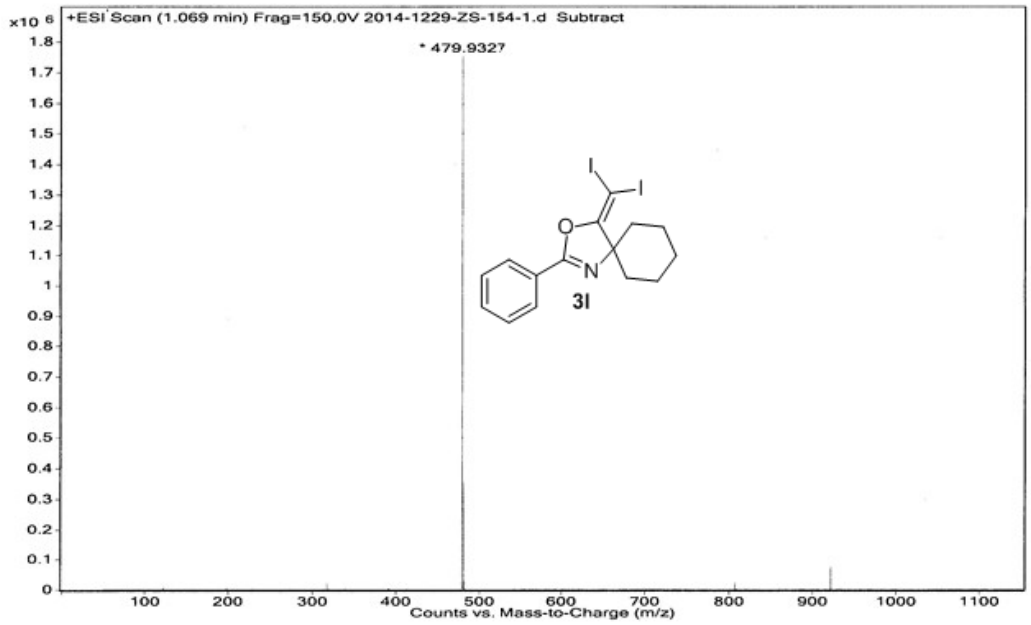
HRMS (ESI, m/z) calcd for $C_{15}H_{25}I_2NO$ $[M+H]^+$ **490.0098**, found **490.0099.**


7.9958
7.9777
7.9746
7.5104
7.4920
7.4566
7.4372
7.4192
2.5935
2.5836
2.5608
2.5507
2.5281
2.5178
1.9447
1.9359
1.9200
1.9117
1.9030
1.8869
1.8786
1.8701
1.8542
1.8458
1.8369
1.8144
1.7816
1.7026
1.6699
1.6142
1.5816
1.4114
1.3871
1.3783
1.3694
1.3543
1.3452
I
I
O
N
3l
10
9
8
7
6
5
4
3
2
1
0
ppm
2.000
3.111
2.075
3.246
2.175
2.209
1.134
163.769
155.687
131.888
128.528
128.338
126.200
77.429
77.111
76.794
75.531
33.946
25.479
22.344
-24.042
I
I
O
N
3l
180
160
140
120
100
80
60
40
20
0
-20
ppm

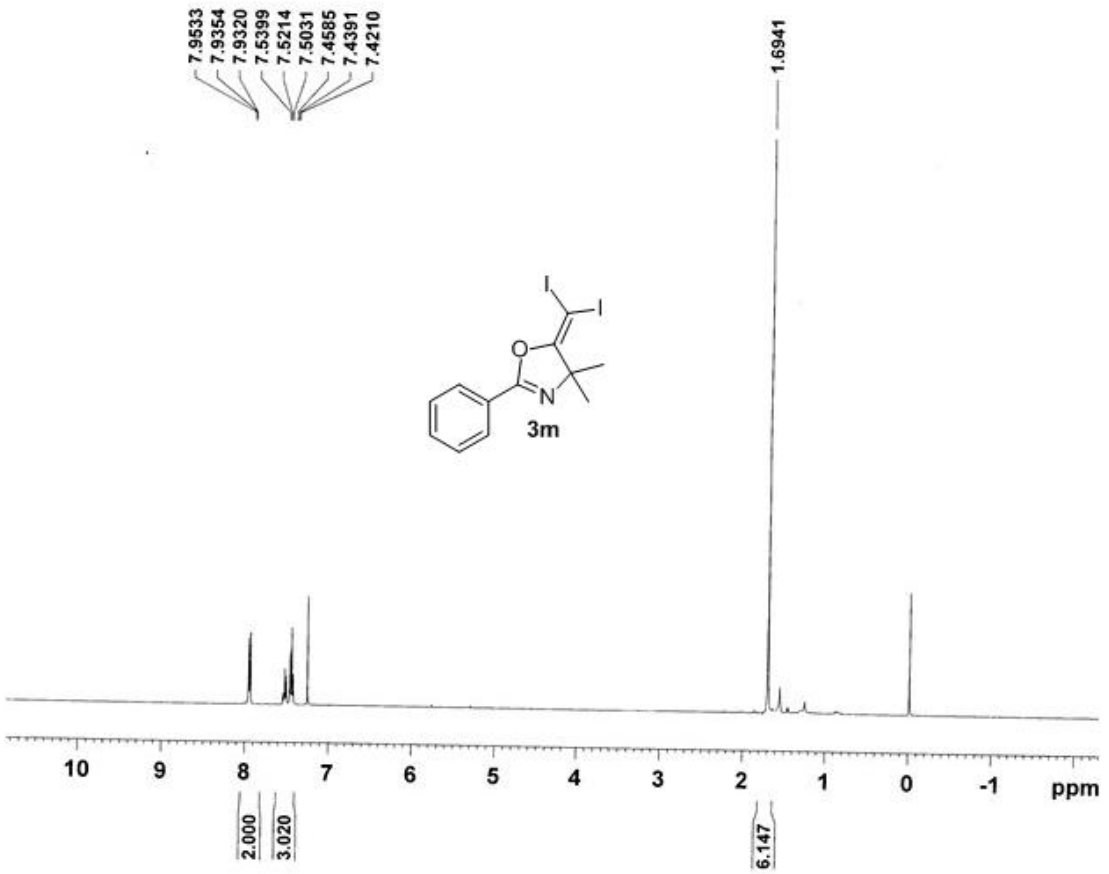


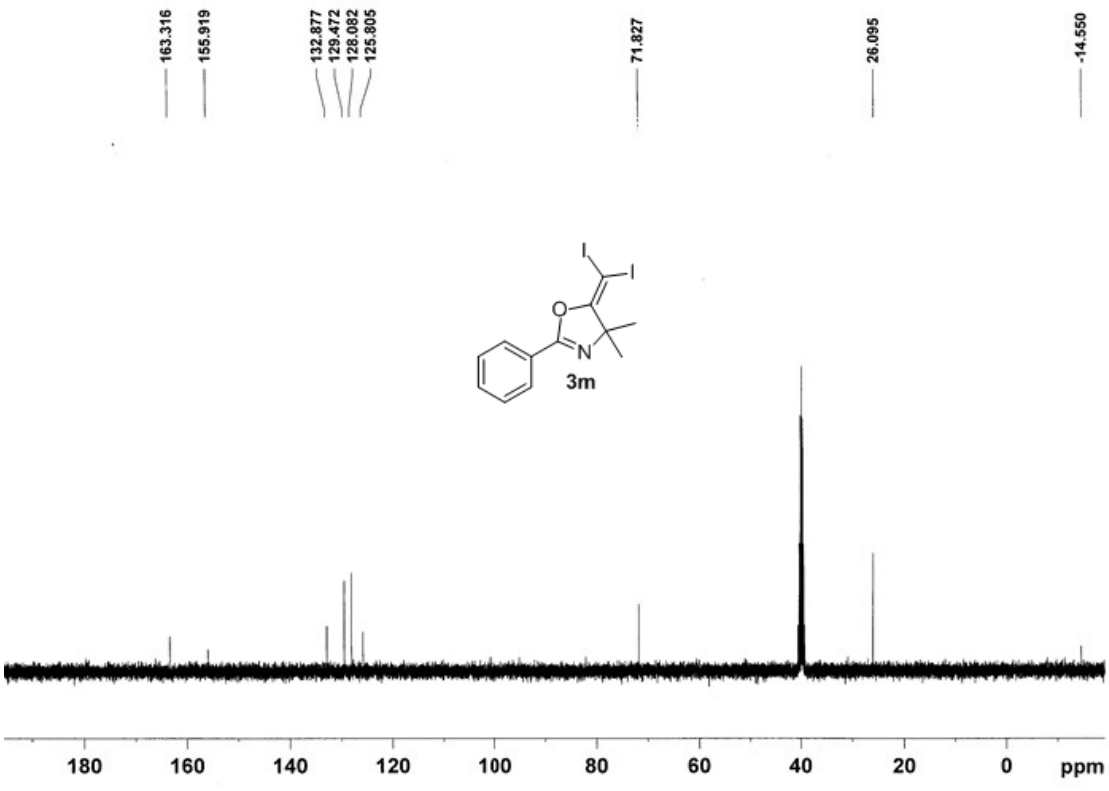
Chemical Formula: $C_{15}H_{15}I_2NO$
Exact Mass: 478.92
Molecular Weight: 479.09
m/z: 478.92 (100.0%), 479.93 (16.4%), 480.93 (1.5%)
Elemental Analysis: C, 37.60; H, 3.16; I, 52.98; N, 2.92; O, 3.34

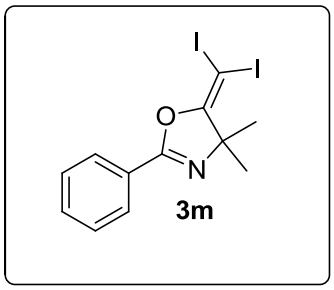
Sample Name	2014-1229-ZS-154-1	**Position**	P1-B9	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	2014-1229-ZS-154-1.d	**ACQ Method**	0103.m	**Comment**		**Acquired Time**	12/29/2014 10:30:49 AM



HRMS (ESI, m/z) calcd for $C_{15}H_{15}I_2NO$ $[M+H]^+$ **479.9316**, found **479.9327.**

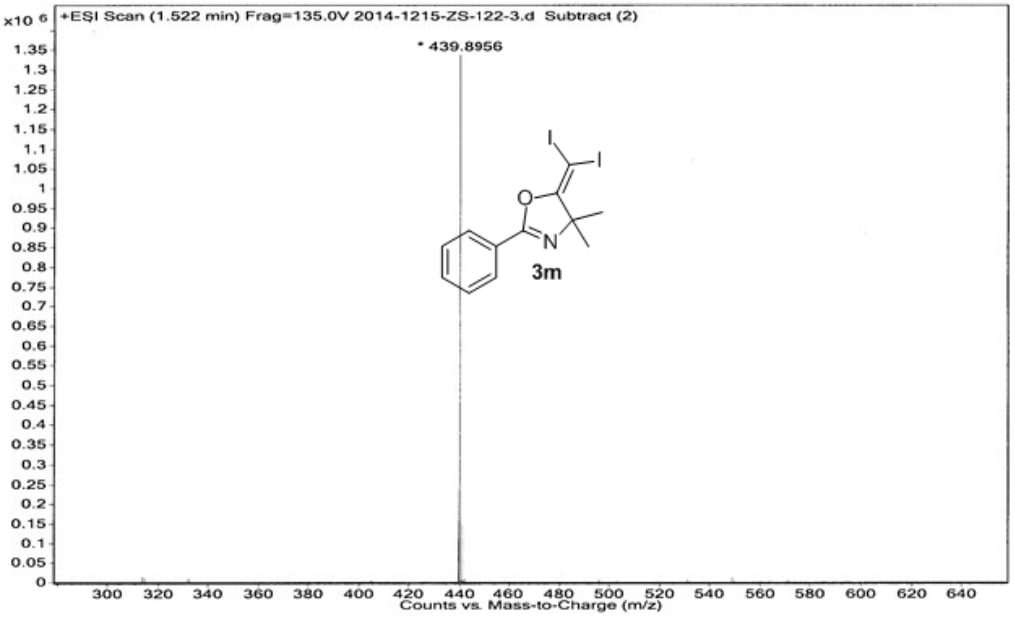

7.9533
7.9354
7.9320
7.5399
7.5214
7.5031
7.4585
7.4391
7.4210
1.6941
I
I
O
N
3m
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
2.000
3.020
6.147


163.316
155.919
132.877
129.472
128.082
125.805
71.827
26.095
-14.550
I
I
O
N
3m
180
160
140
120
100
80
60
40
20
0
ppm

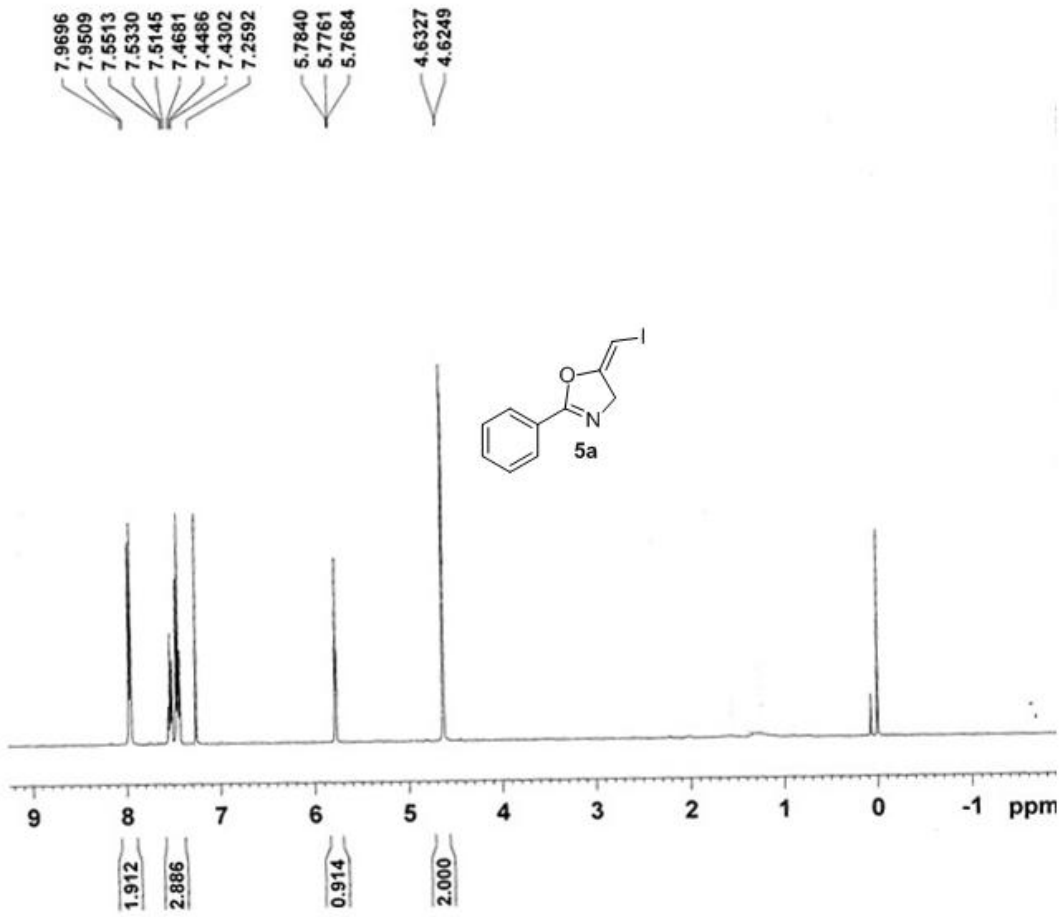


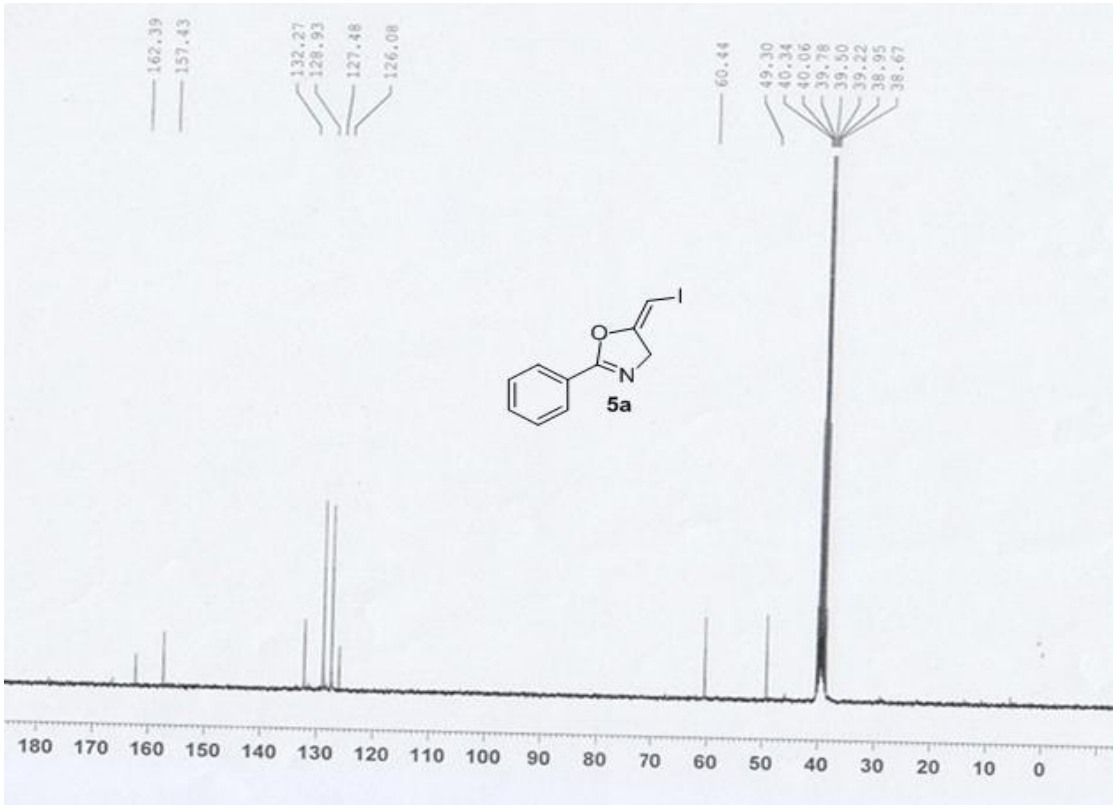
Chemical Formula: $C_{12}H_{11}I_2NO$
Exact Mass: 438.89
Molecular Weight: 439.03
m/z: 438.89 (100.0%), 439.90 (13.1%)
Elemental Analysis: C, 32.83; H, 2.53; I, 57.81; N, 3.19; O, 3.64

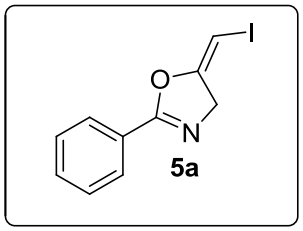
Sample Name	2014-1215-ZS-122-3	**Position**	P1-C1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	2014-1215-ZS-122-3.d	**ACQ Method**	0103.m	**Comment**		**Acquired Time**	12/15/2014 10:46:31 AM



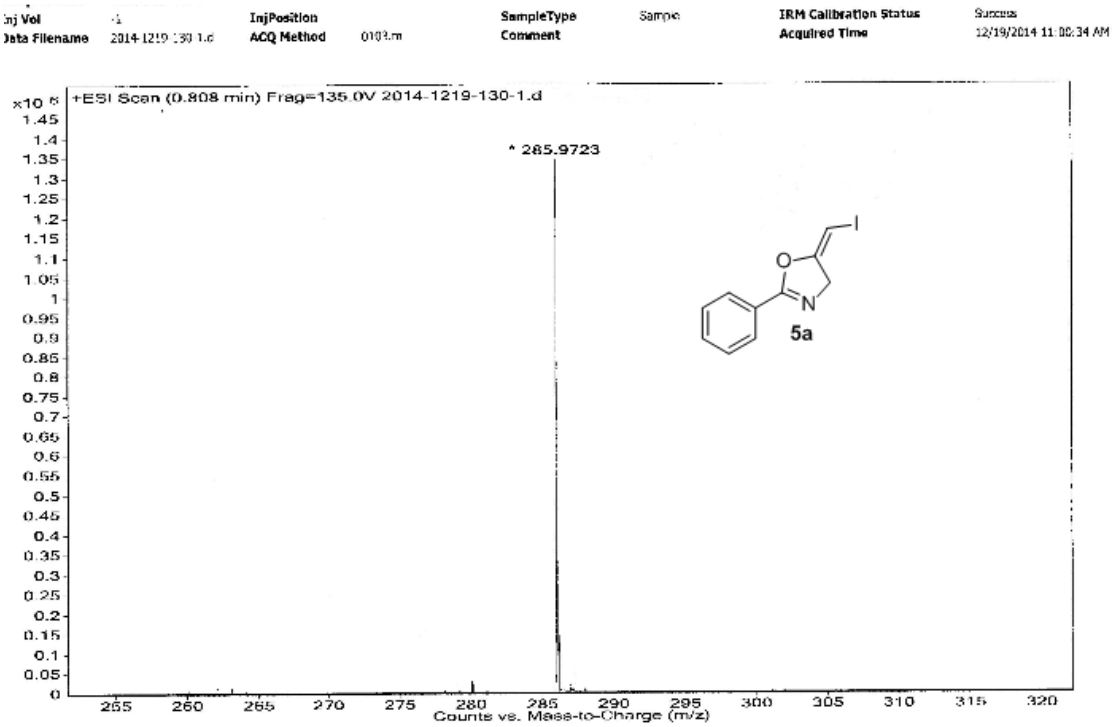
HRMS (ESI, m/z) calcd for $C_{12}H_{11}I_2NO$ $[M+H]^+$ **439.9003**, found **439.8956.**


7.9696
7.9509
7.5513
7.5330
7.5145
7.4681
7.4486
7.4302
7.2592
5.7840
5.7761
5.7684
4.6327
4.6249
I
O
N
5a
9
8
7
6
5
4
3
2
1
0
-1
ppm
1.912
2.886
0.914
2.000

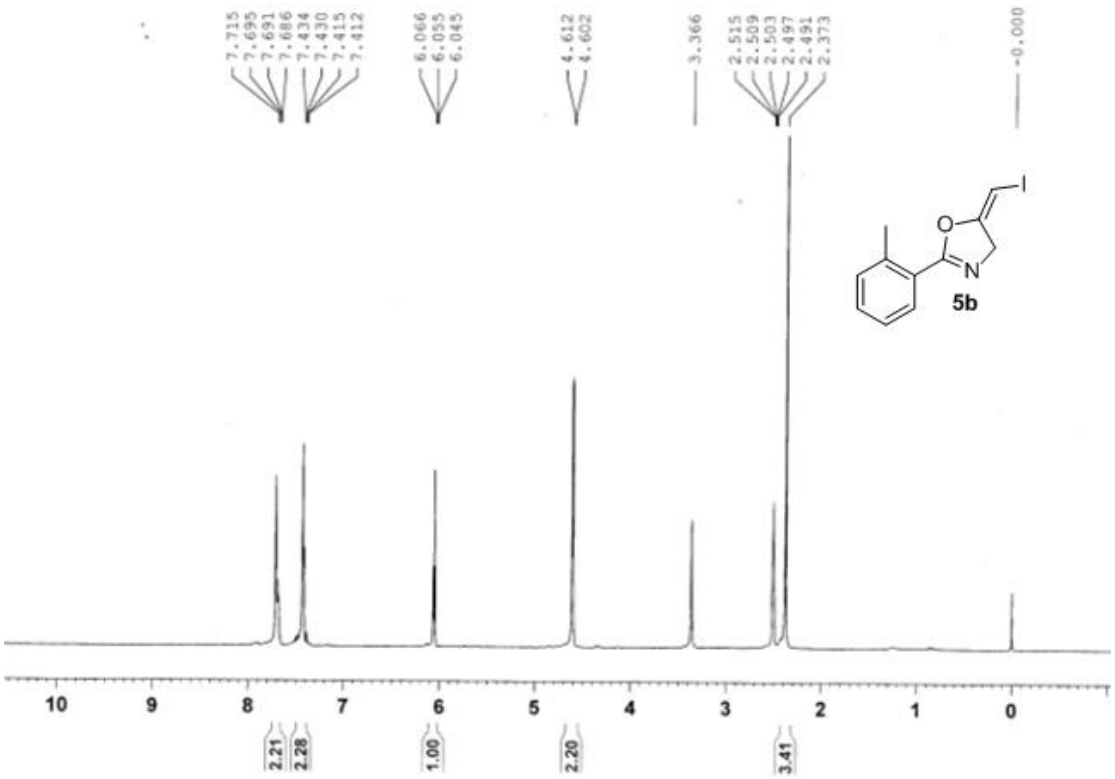

162.39
157.43
132.27
128.93
127.48
126.08
60.44
49.30
40.34
40.06
39.78
39.50
39.22
38.95
38.67
I
O
N
5a
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

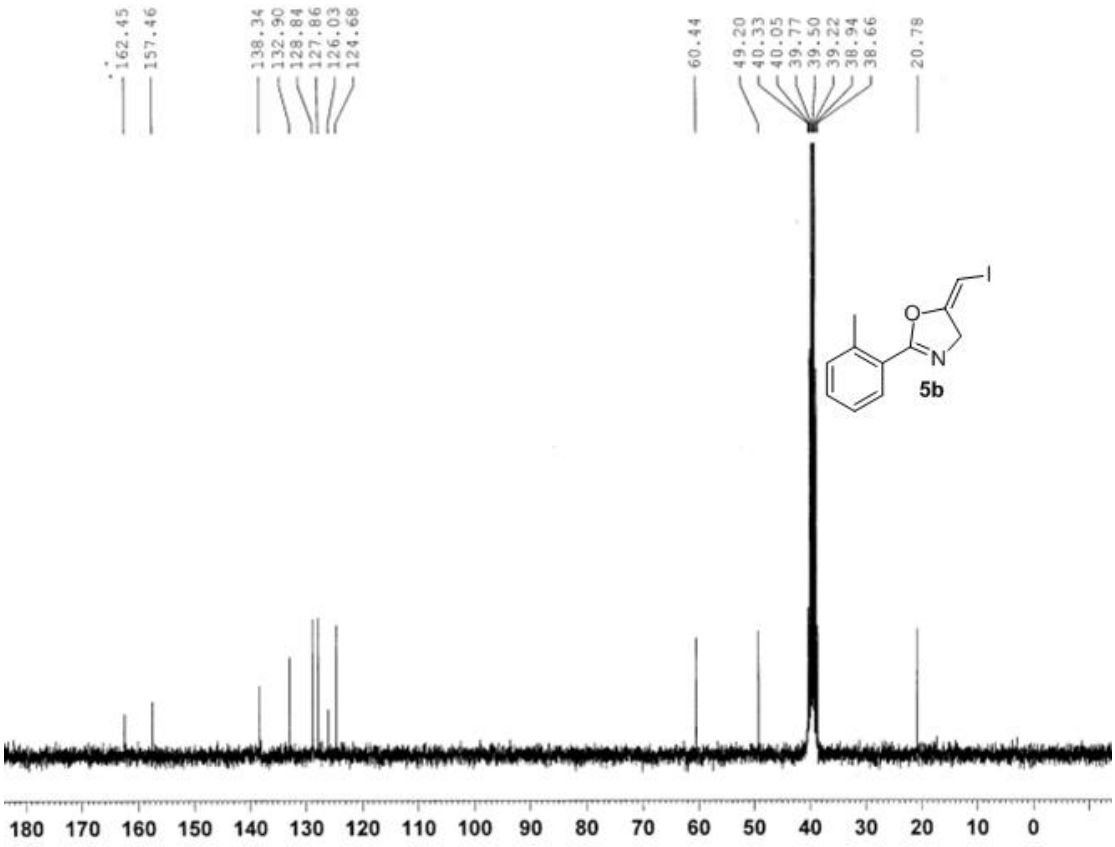


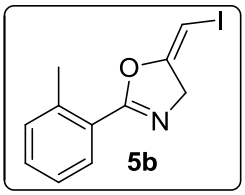
Chemical Formula: $C_{10}H_8INO$
Exact Mass: 284.97
Molecular Weight: 285.08
m/z: 284.97 (100.0%), 285.97 (10.9%)
Elemental Analysis: C, 42.13; H, 2.83; I, 44.52; N, 4.91; O, 5.61



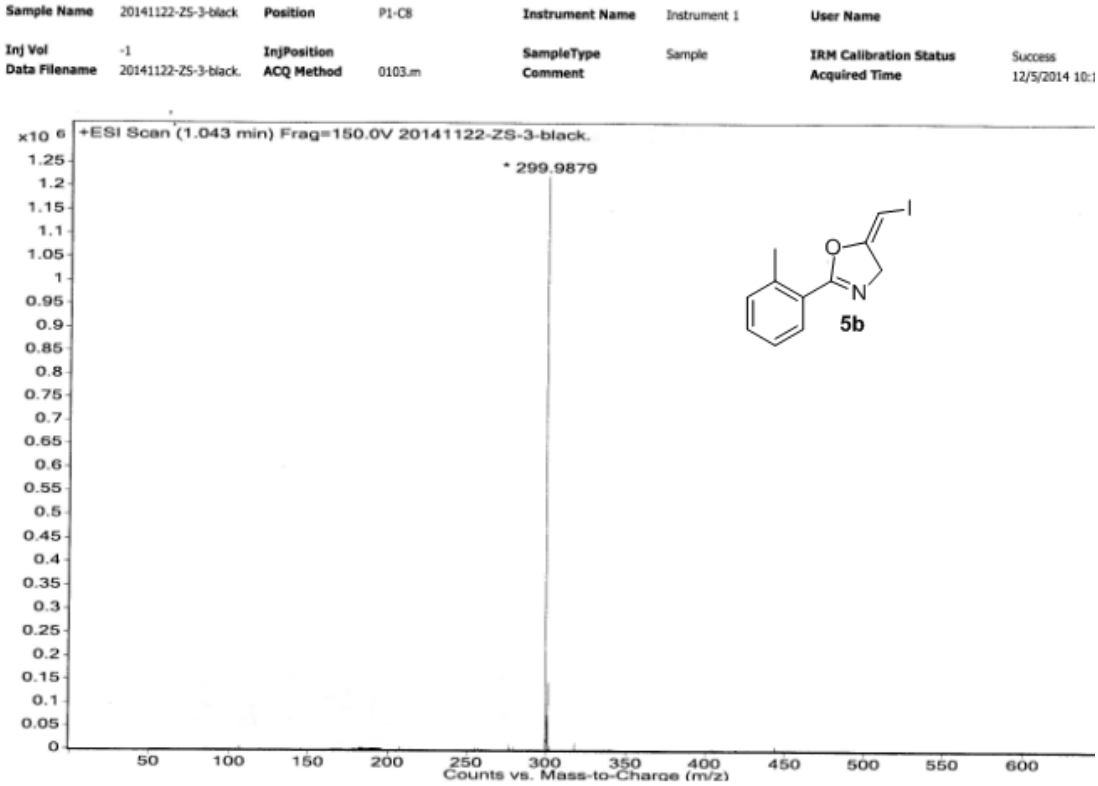
HRMS (ESI, m/z) calcd for $C_{10}H_8INO$ $[M+H]^+$ **285.9723**, found **285.9723**.


7.715
7.695
7.691
7.686
7.434
7.430
7.415
7.412
6.066
6.055
6.045
4.612
4.602
3.366
2.515
2.509
2.503
2.497
2.491
2.373
-0.000
I
O
N
5b
10
9
8
7
6
5
4
3
2
1
0
2.21
2.28
1.00
2.20
3.41

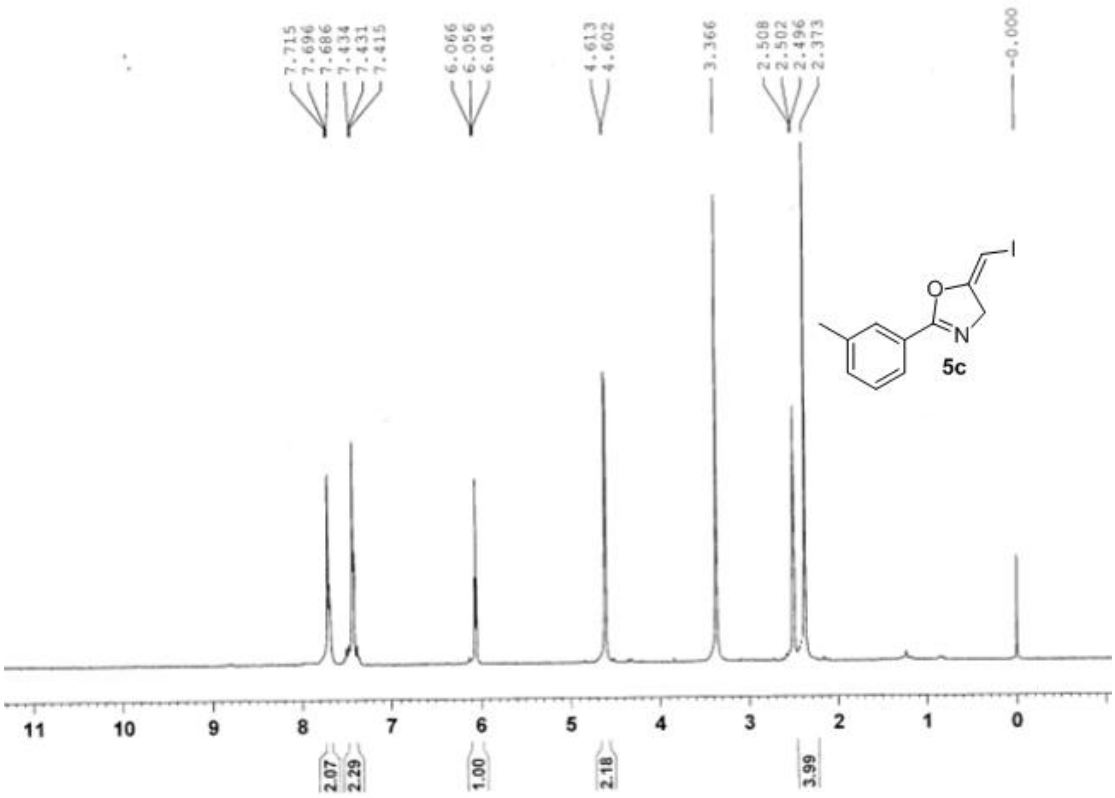

162.45
157.46
138.34
132.90
128.84
127.86
126.03
124.68
60.44
49.20
40.33
40.05
39.77
39.50
39.22
38.94
38.66
20.78
I
O
N
5b
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

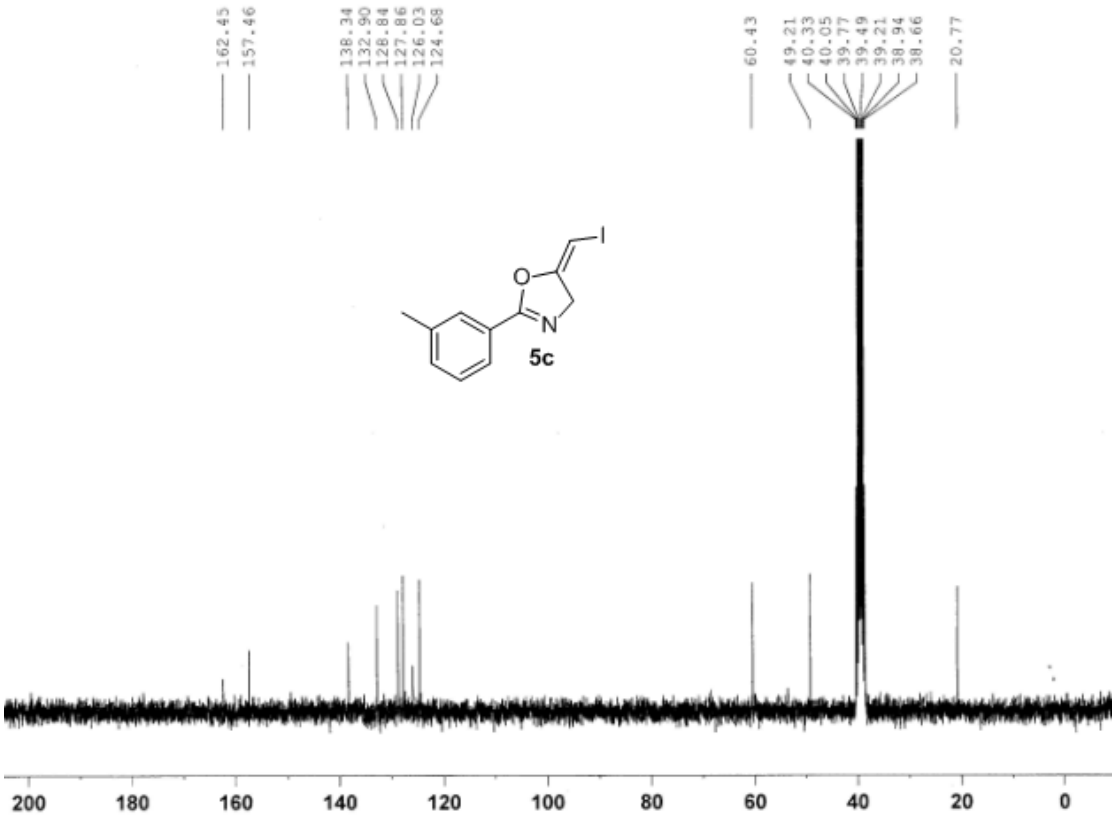


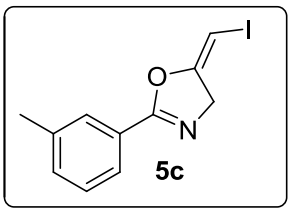
Chemical Formula: $C_{11}H_{10}INO$
Exact Mass: 298.98
Molecular Weight: 299.11
m/z: 298.98 (100.0%), 299.98 (12.3%)
Elemental Analysis: C, 44.17; H, 3.37; I, 42.43; N, 4.68; O, 5.35



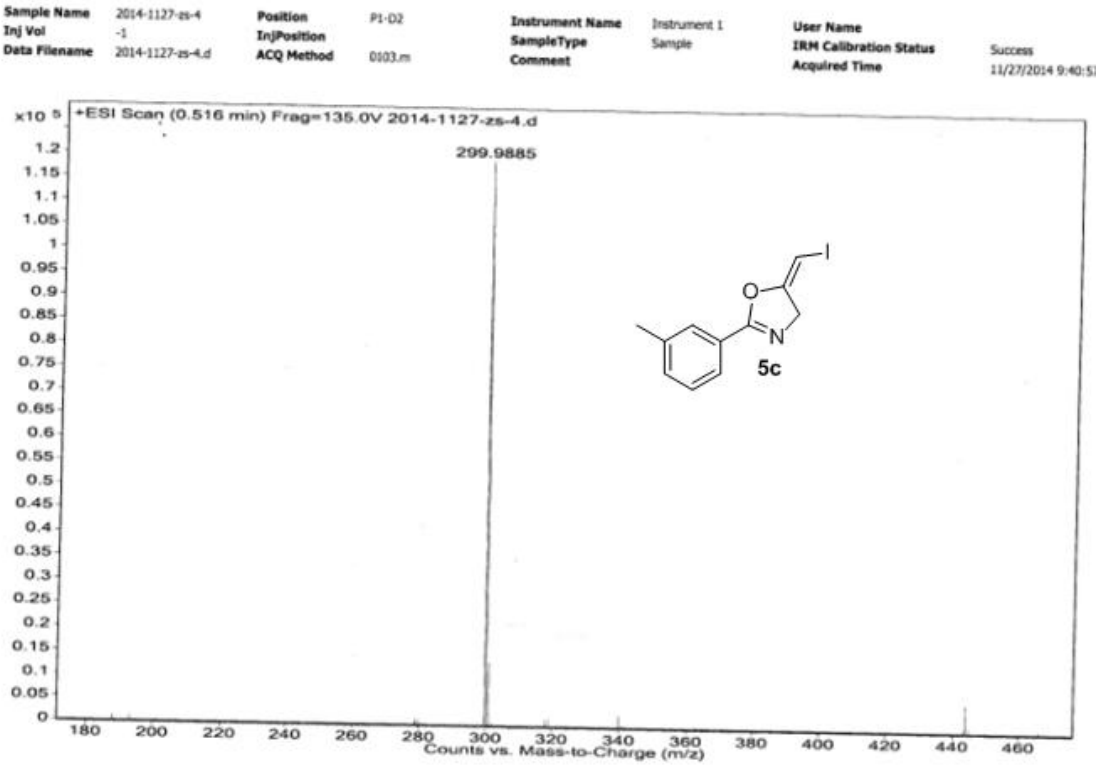
HRMS (ESI, m/z) calcd for $C_{11}H_{10}INO$ $[M+H]^+$ **299.9880**, found **299.9879.**


7.715
7.696
7.686
7.434
7.431
7.415
6.066
6.056
6.045
4.613
4.602
3.366
2.508
2.502
2.496
2.373
-0.000
I
O
N
5c
11
10
9
8
7
6
5
4
3
2
1
0
2.07
2.29
1.00
2.18
3.99

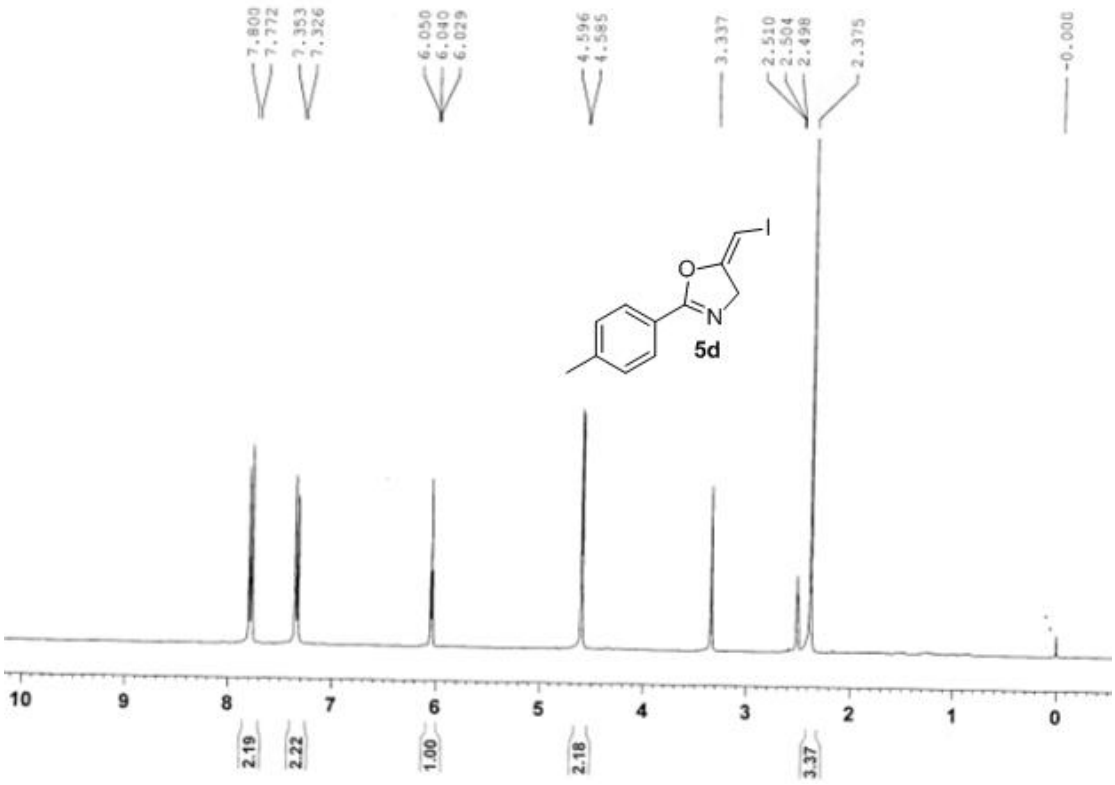

162.45
157.46
138.34
132.90
126.84
127.86
126.03
124.68
60.43
49.21
40.33
40.05
39.77
39.49
39.21
38.94
38.66
20.77
I
O
N
5c
200
180
160
140
120
100
80
60
40
20
0

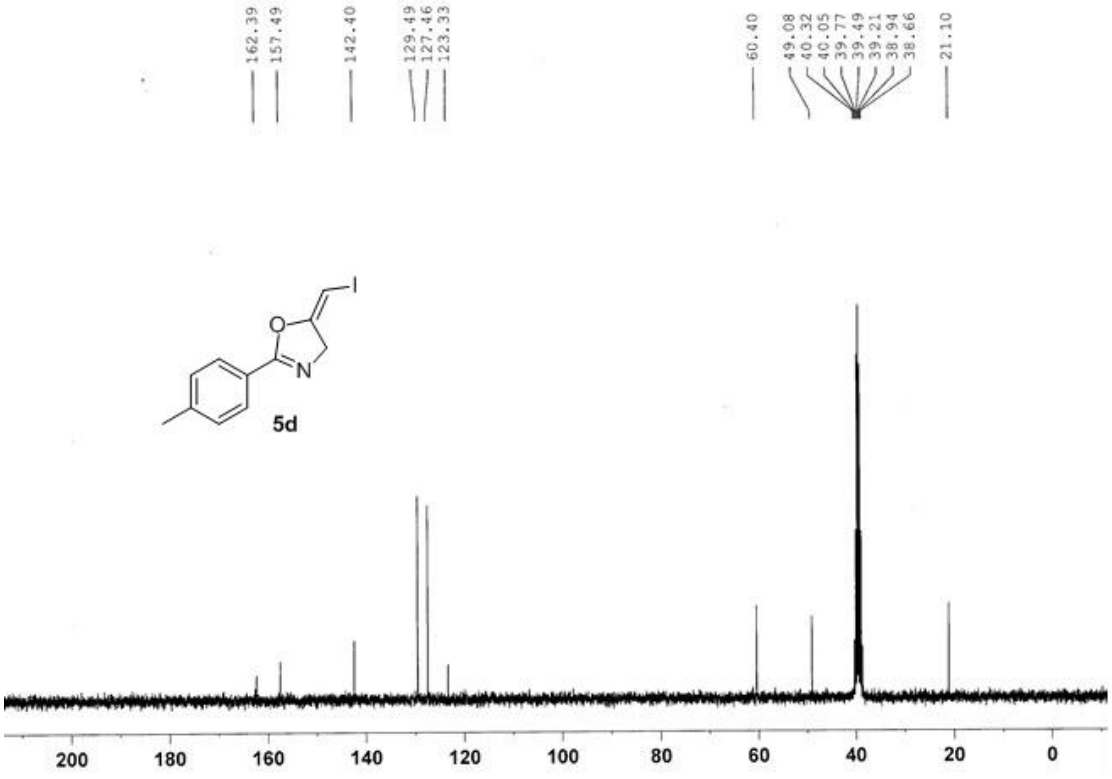


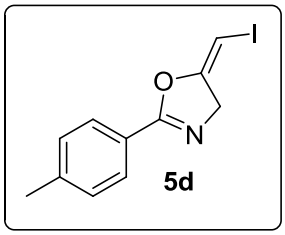
Chemical Formula: $C_{11}H_{10}INO$
Exact Mass: 298.98
Molecular Weight: 299.11
m/z: 298.98 (100.0%), 299.98 (12.3%)
Elemental Analysis: C, 44.17; H, 3.37; I, 42.43; N, 4.68; O, 5.35



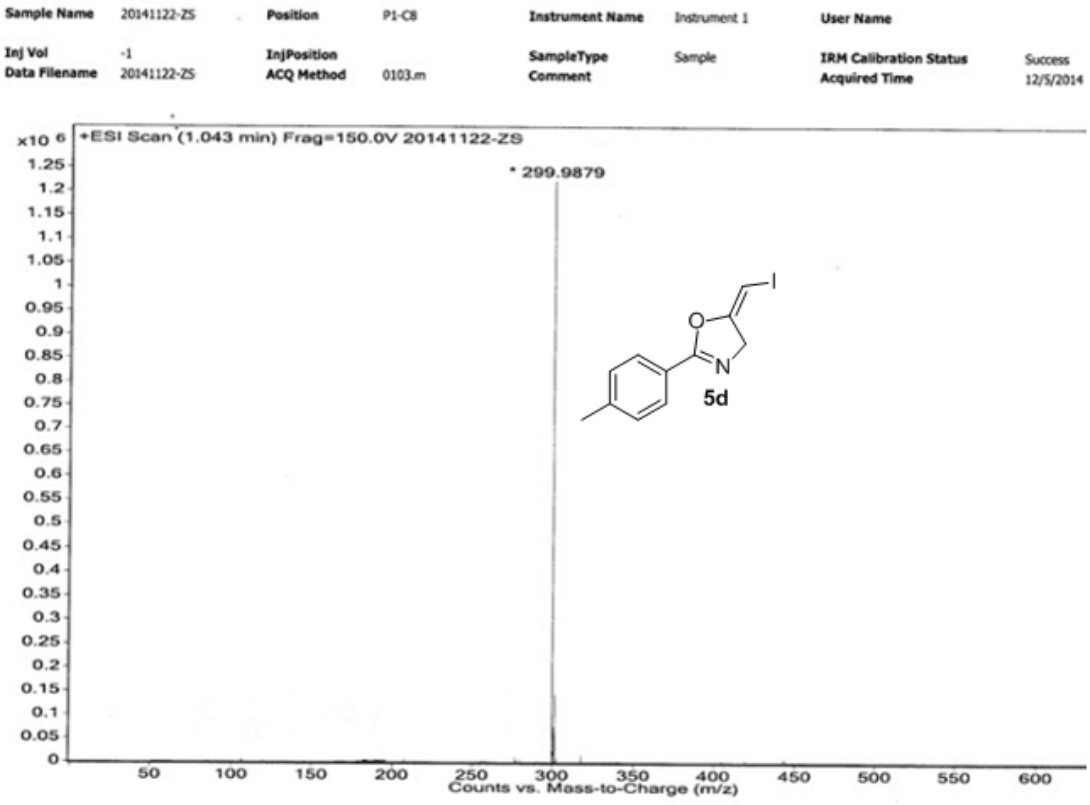
HRMS (ESI, m/z) calcd for $C_{11}H_{10}INO$ $[M+H]^+$ **299.9880**, found **299.9885.**


7.800
7.772
7.353
7.326
6.050
6.040
6.029
4.596
4.585
3.337
2.510
2.504
2.498
2.375
-0.000
I
O
N
5d
10
9
8
7
6
5
4
3
2
1
0
2.19
2.22
1.00
2.18
3.37

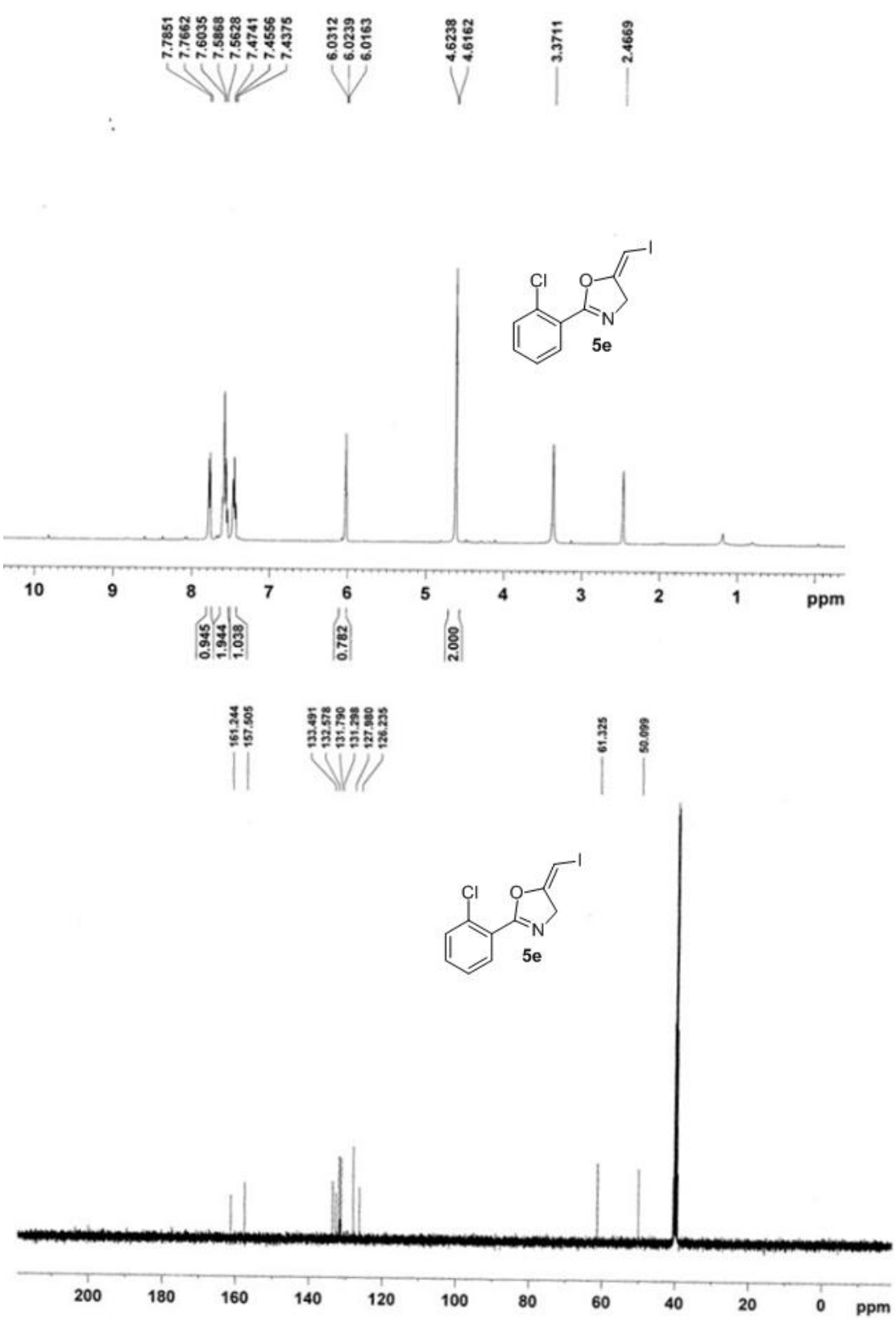

162.39
157.49
142.40
129.49
127.46
123.33
60.40
49.08
40.32
40.05
39.77
39.49
39.21
38.94
38.66
21.10
I
O
N
5d
200
180
160
140
120
100
80
60
40
20
0

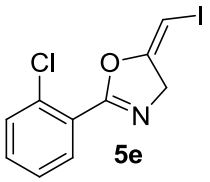


Chemical Formula: $C_{11}H_{10}INO$
Exact Mass: 298.98
Molecular Weight: 299.11
m/z: 298.98 (100.0%), 299.98 (12.3%)
Elemental Analysis: C, 44.17; H, 3.37; I, 42.43; N, 4.68; O, 5.35

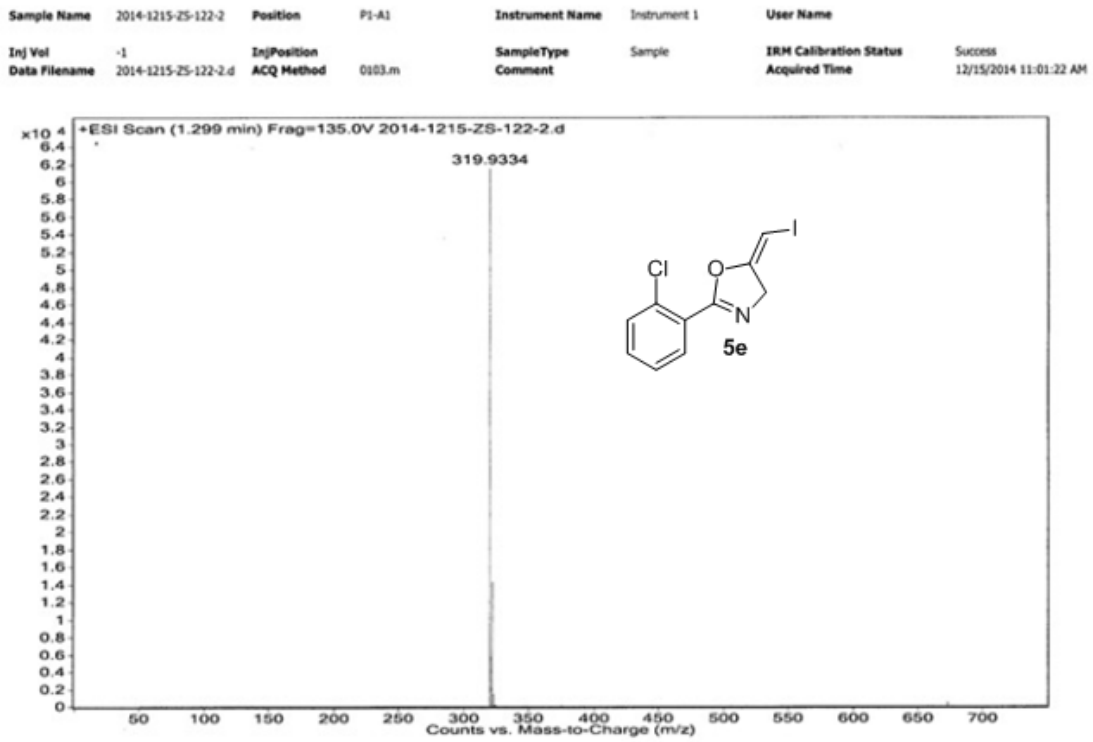


HRMS (ESI, m/z) calcd for $C_{11}H_{10}INO$ $[M+H]^+$ **299.9880**, found **299.9879.**

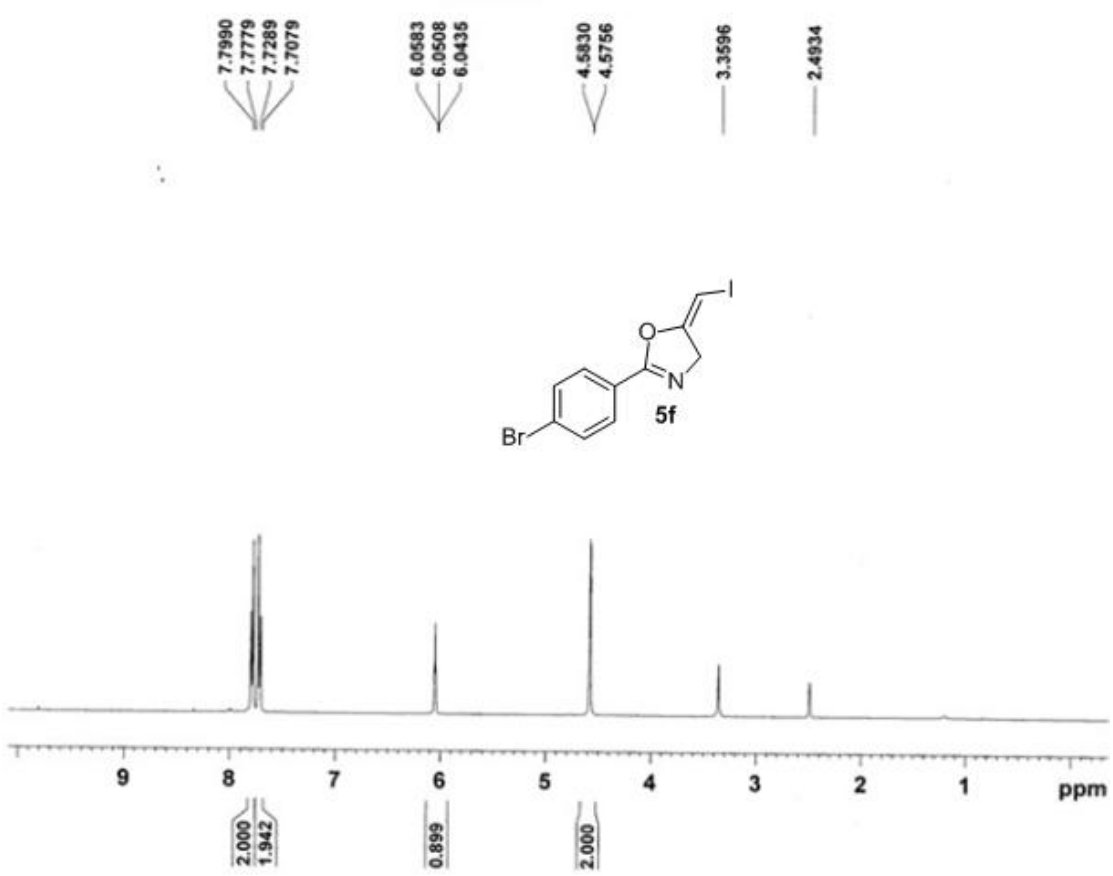

7.7851
7.7662
7.6035
7.5868
7.5628
7.4741
7.4556
7.4375
6.0312
6.0239
6.0163
4.6238
4.6162
3.3711
2.4669
Cl
O
N
I
5e
10
9
8
7
6
5
4
3
2
1
ppm
0.945
1.944
1.038
0.782
2.000
161.244
157.505
133.491
132.578
131.790
131.298
127.980
126.235
61.325
50.099
Cl
O
N
I
5e
200
180
160
140
120
100
80
60
40
20
0
ppm

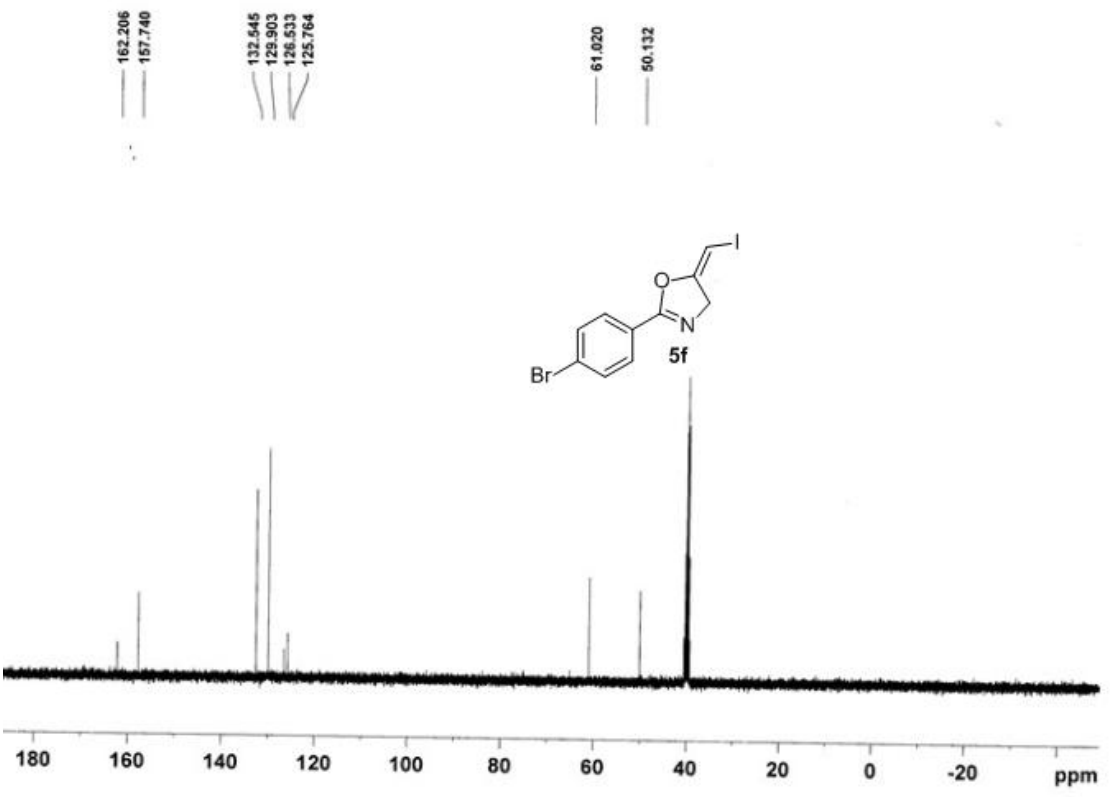


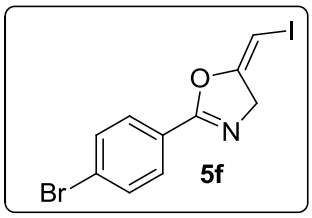
Chemical Formula: $C_{10}H_7ClINO$
Exact Mass: 318.9261
Molecular Weight: 319.5261
m/z: 318.9261 (100.0%), 320.9231 (32.0%), 319.9294 (10.8%), 321.9265 (3.5%)
Elemental Analysis: C, 37.59; H, 2.21; Cl, 11.10; I, 39.72; N, 4.38; O, 5.01



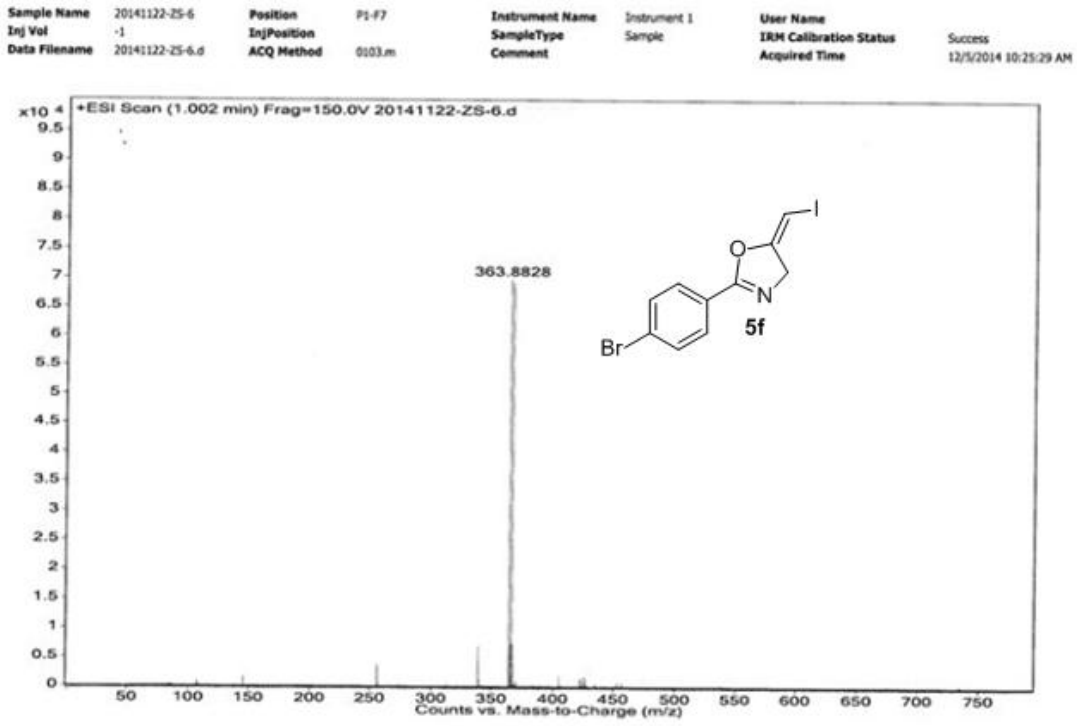
HRMS (ESI, m/z) calcd for $C_{10}H_7ClINO$ $[M+H]^+$ **319.9334**, found **319.9334.**


7.7990
7.7779
7.7289
7.7079
6.0583
6.0508
6.0435
4.5830
4.5756
3.3596
2.4934
I
O
N
Br
5f
9
8
7
6
5
4
3
2
1
ppm
2.000
1.942
0.899
2.000

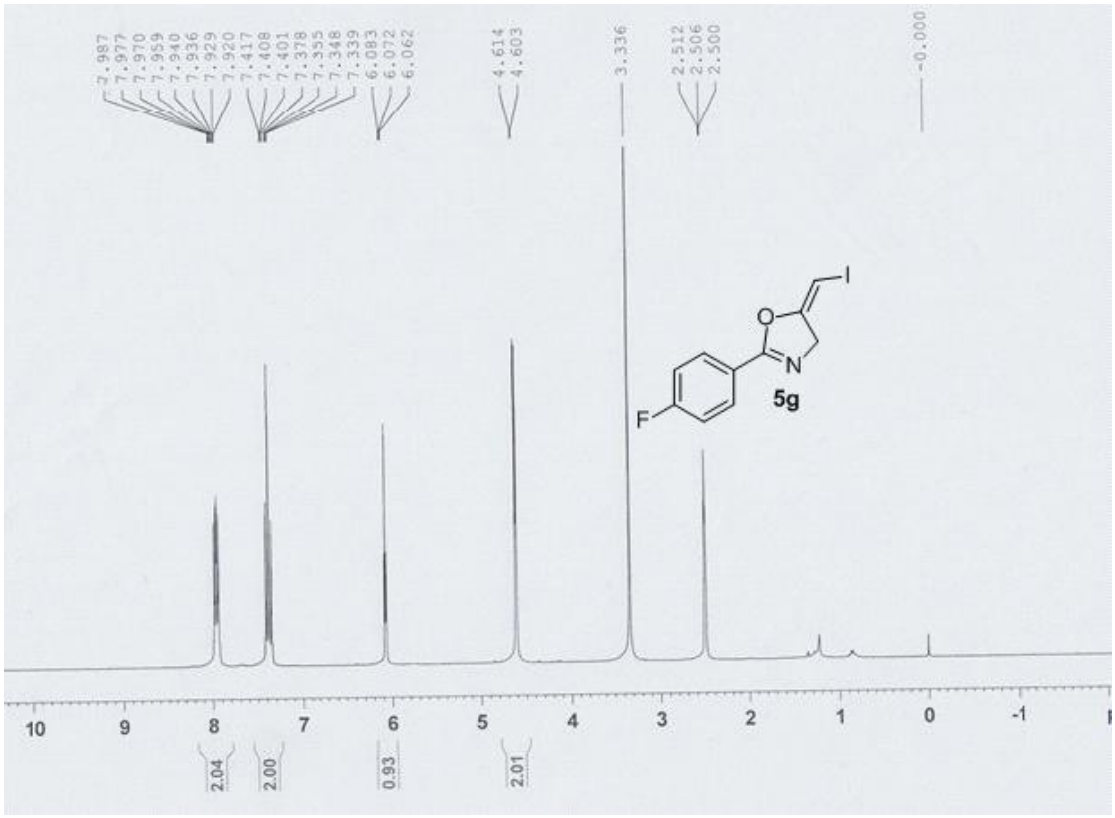

162.206
157.740
132.545
129.903
126.533
125.764
61.020
50.132
I
O
N
Br
5f
180
160
140
120
100
80
60
40
20
0
-20
ppm

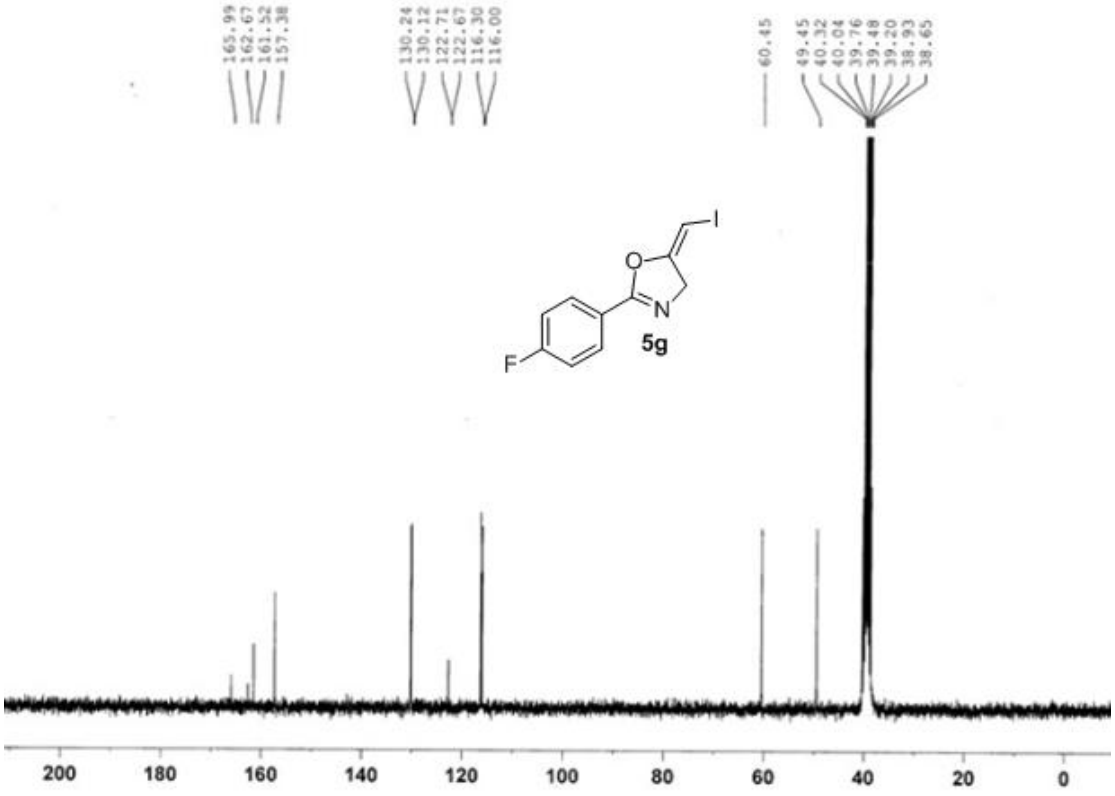


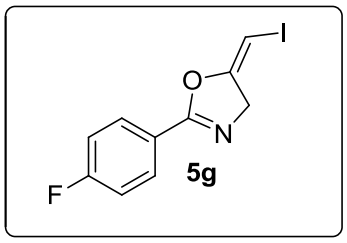
Chemical Formula: $C_{10}H_7BrINO$
Exact Mass: 362.88
Molecular Weight: 363.98
m/z: 362.88 (100.0%), 364.87 (97.3%), 363.88 (10.9%), 365.88 (10.7%)
Elemental Analysis: C, 33.00; H, 1.94; Br, 21.95; I, 34.87; N, 3.85; O, 4.40



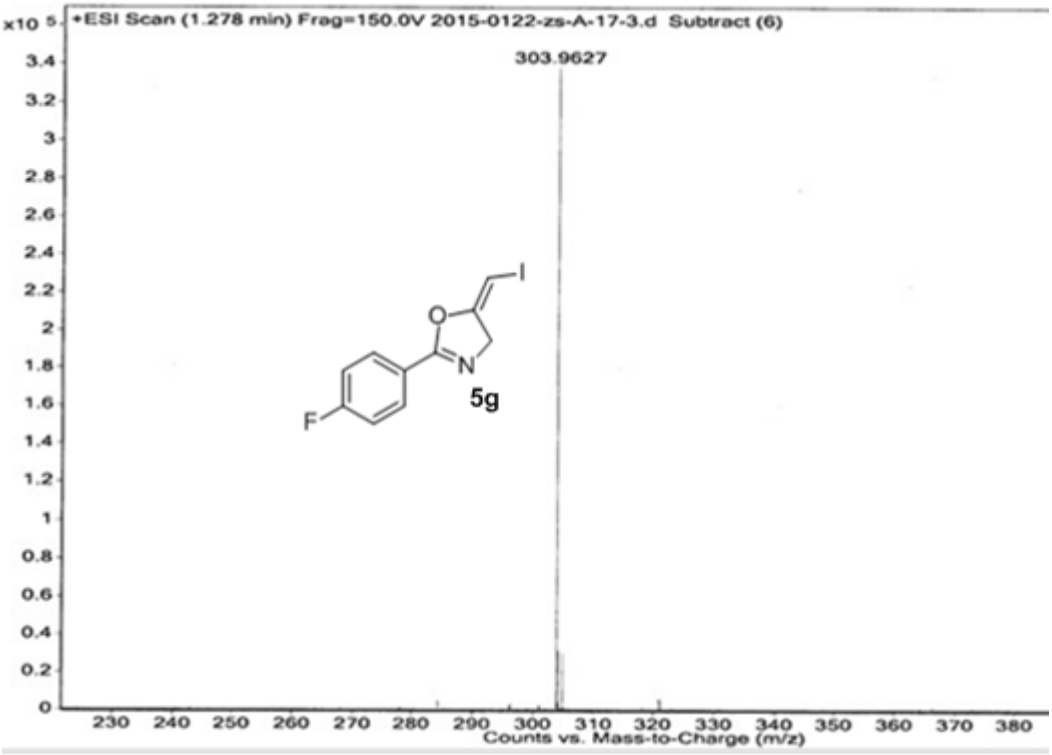
HRMS (ESI, m/z) calcd for $C_{10}H_7BrINO\,[M+H]^+$ **363.8828,** found **363.8828.**


7.987
7.977
7.970
7.959
7.940
7.936
7.929
7.920
7.417
7.408
7.401
7.378
7.355
7.348
7.339
6.083
6.072
6.062
4.614
4.603
3.336
2.512
2.506
2.500
-0.000
O
N
I
F
5g
10
9
8
7
6
5
4
3
2
1
0
-1
2.04
2.00
0.93
2.01

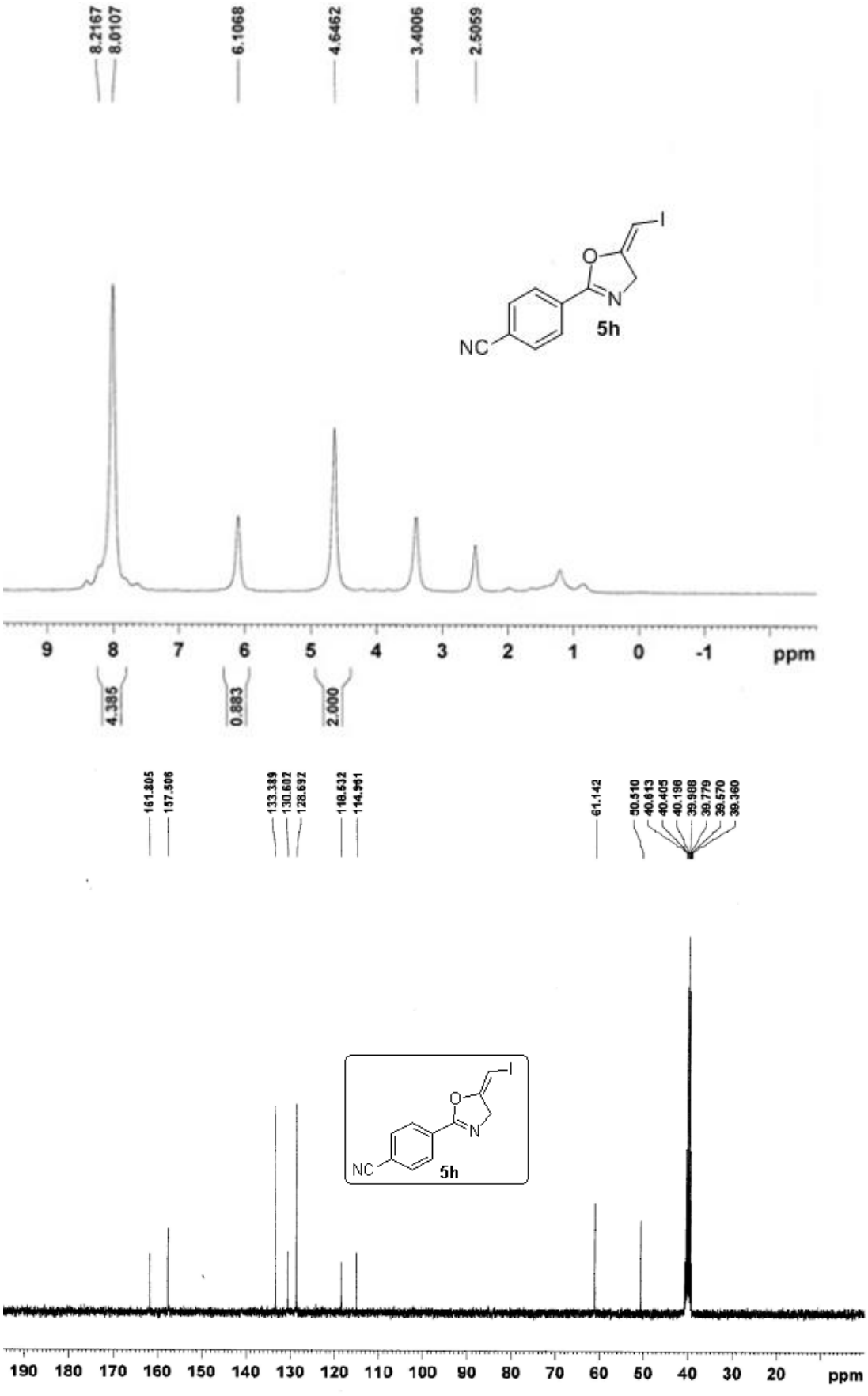

165.99
162.67
161.52
157.38
130.24
130.12
122.71
122.67
116.30
116.00
60.45
49.45
40.32
40.04
39.76
39.48
39.20
38.93
38.65
O
N
I
F
5g
200
180
160
140
120
100
80
60
40
20
0

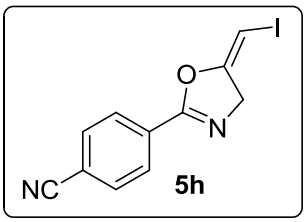


Chemical Formula: $C_{10}H_7FINO$
Exact Mass: 302.96
Molecular Weight: 303.07
m/z: 302.96 (100.0%), 303.96 (10.9%)
Elemental Analysis: C, 39.63; H, 2.33; F, 6.27; I, 41.87; N, 4.62; O, 5.28

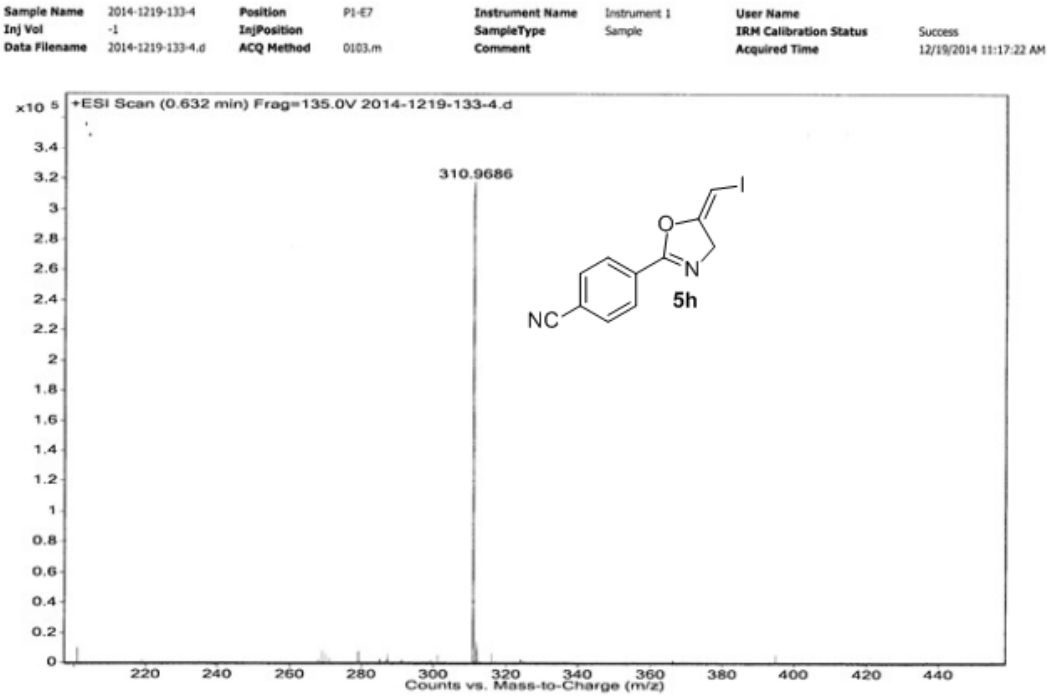


HRMS (ESI, m/z) calcd for $C_{10}H_7FINO\,[M+H]^+$ **303.9629**, found **303.9627.**

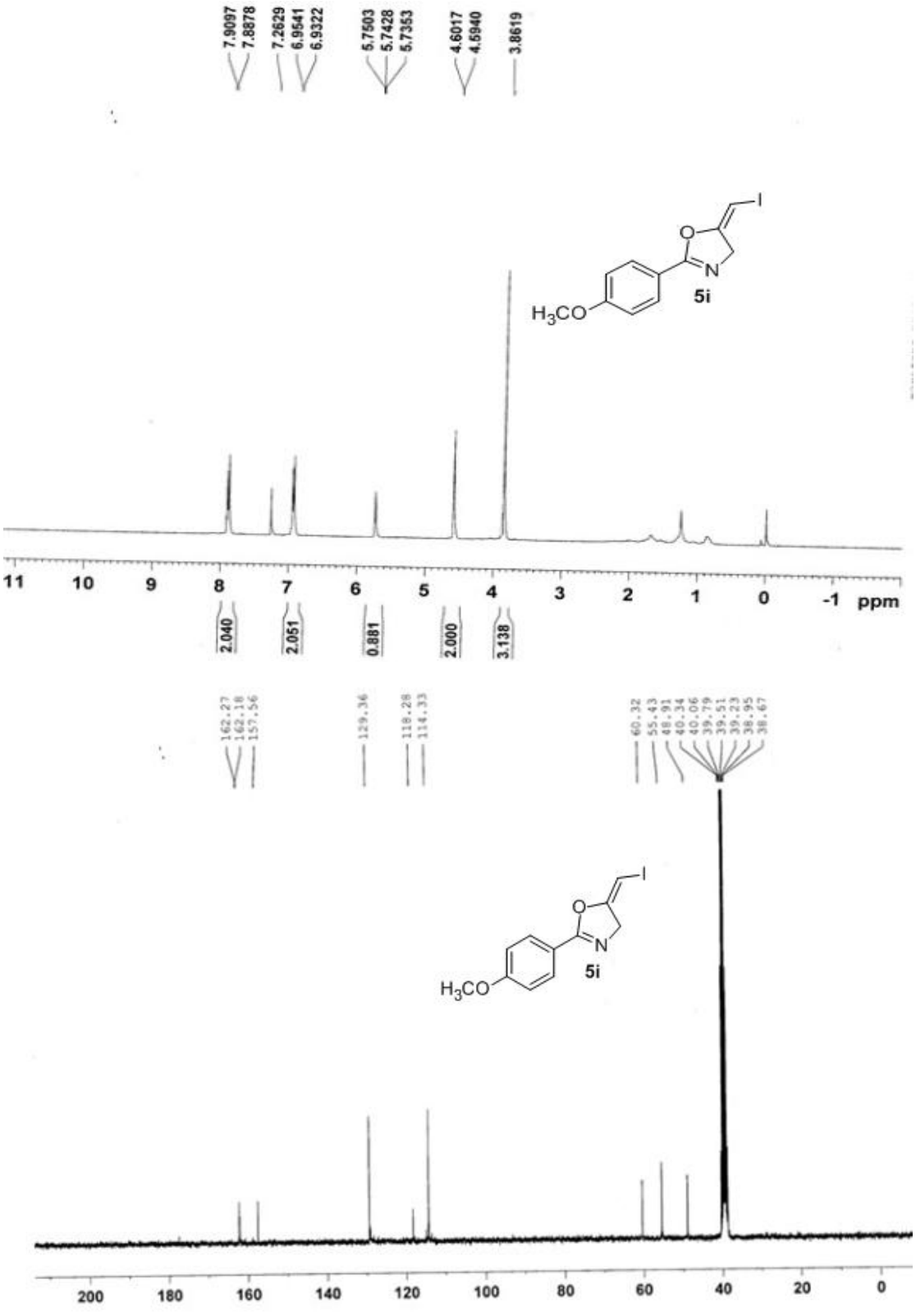

8.2167
8.0107
6.1068
4.6462
3.4006
2.5059
I
O
N
NC
5h
9
8
7
6
5
4
3
2
1
0
-1
ppm
4.385
0.883
2.000
161.805
157.506
133.389
130.602
128.692
118.532
114.961
61.142
50.510
40.613
40.405
40.196
39.988
39.779
39.570
39.360
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

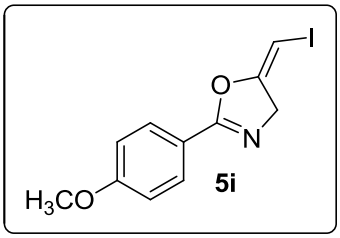


Chemical Formula: $C_{11}H_7IN_2O$
Exact Mass: 309.96
Molecular Weight: 310.09
m/z: 309.96 (100.0%), 310.96 (12.7%)
Elemental Analysis: C, 42.61; H, 2.28; I, 40.92; N, 9.03; O, 5.16

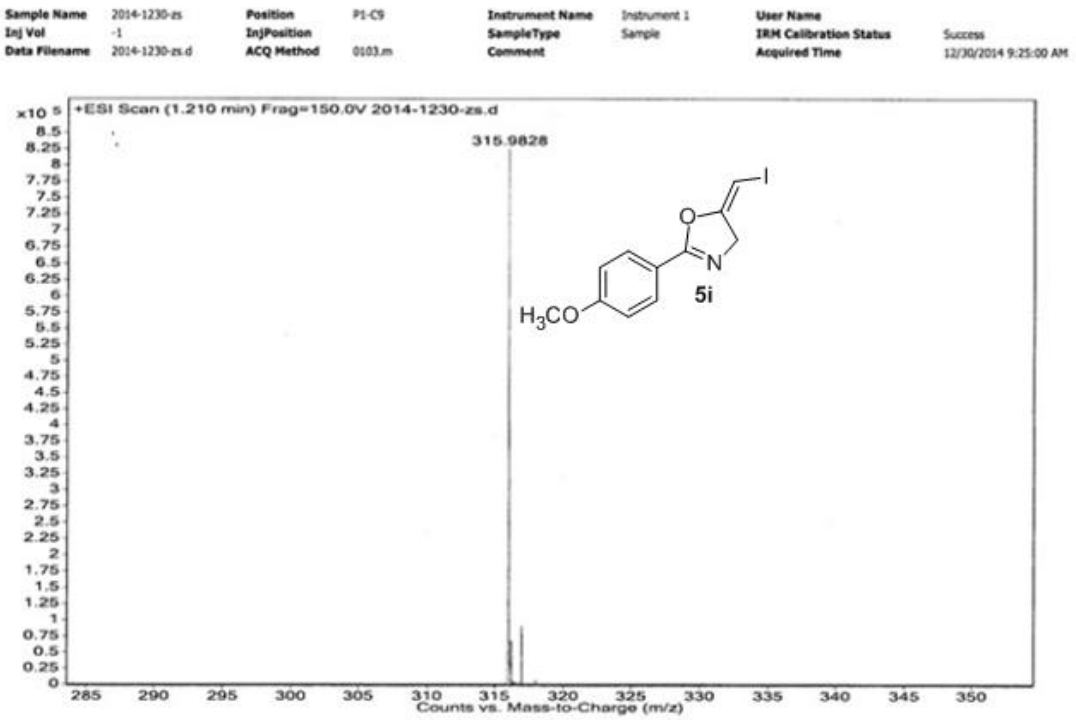


HRMS (ESI, m/z) calcd for $C_{11}H_7IN_2O$ $[M+H]^+$ **310.9676**, found **310.9686.**

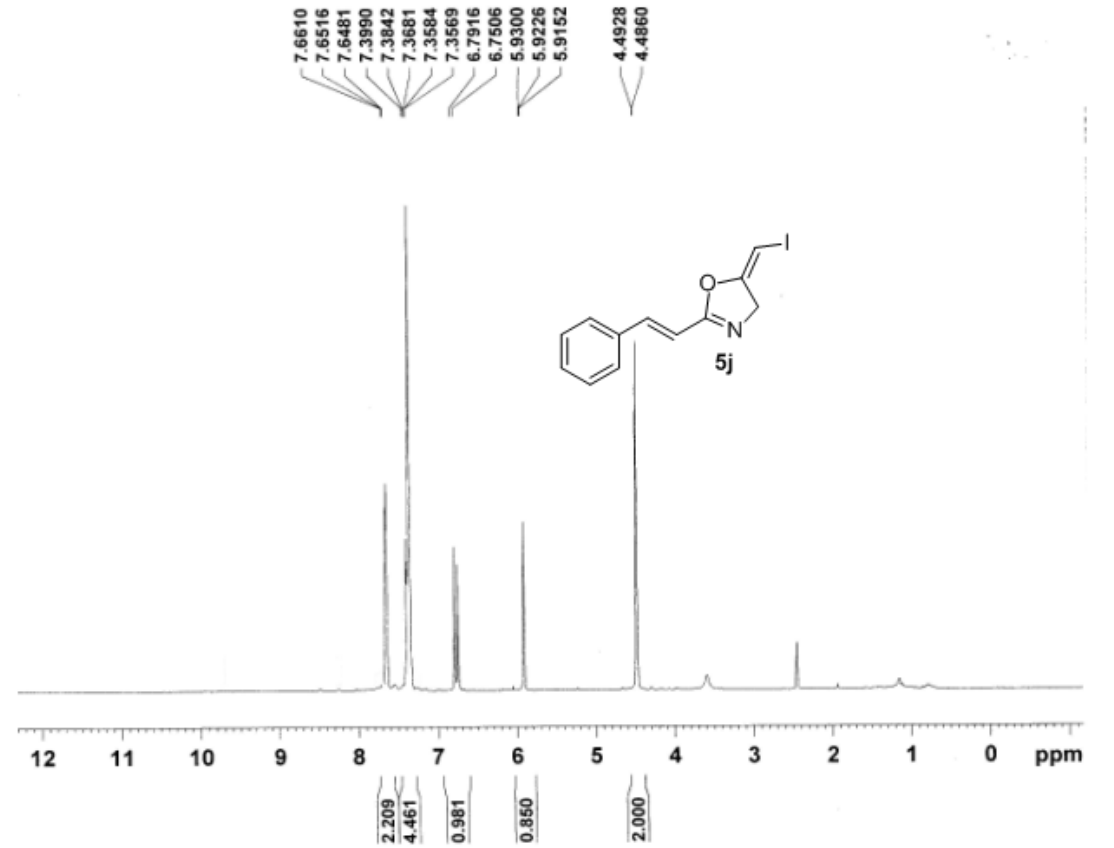

7.9097
7.8878
7.2629
6.9541
6.9322
5.7503
5.7428
5.7353
4.6017
4.6940
3.8619
I
O
N
H3CO
5i
11
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
2.040
2.051
0.881
2.000
3.138
162.27
162.18
157.56
129.36
118.28
114.33
60.32
55.43
48.91
40.34
40.06
39.79
39.51
39.23
38.95
38.67
I
O
N
H3CO
5i
200
180
160
140
120
100
80
60
40
20
0

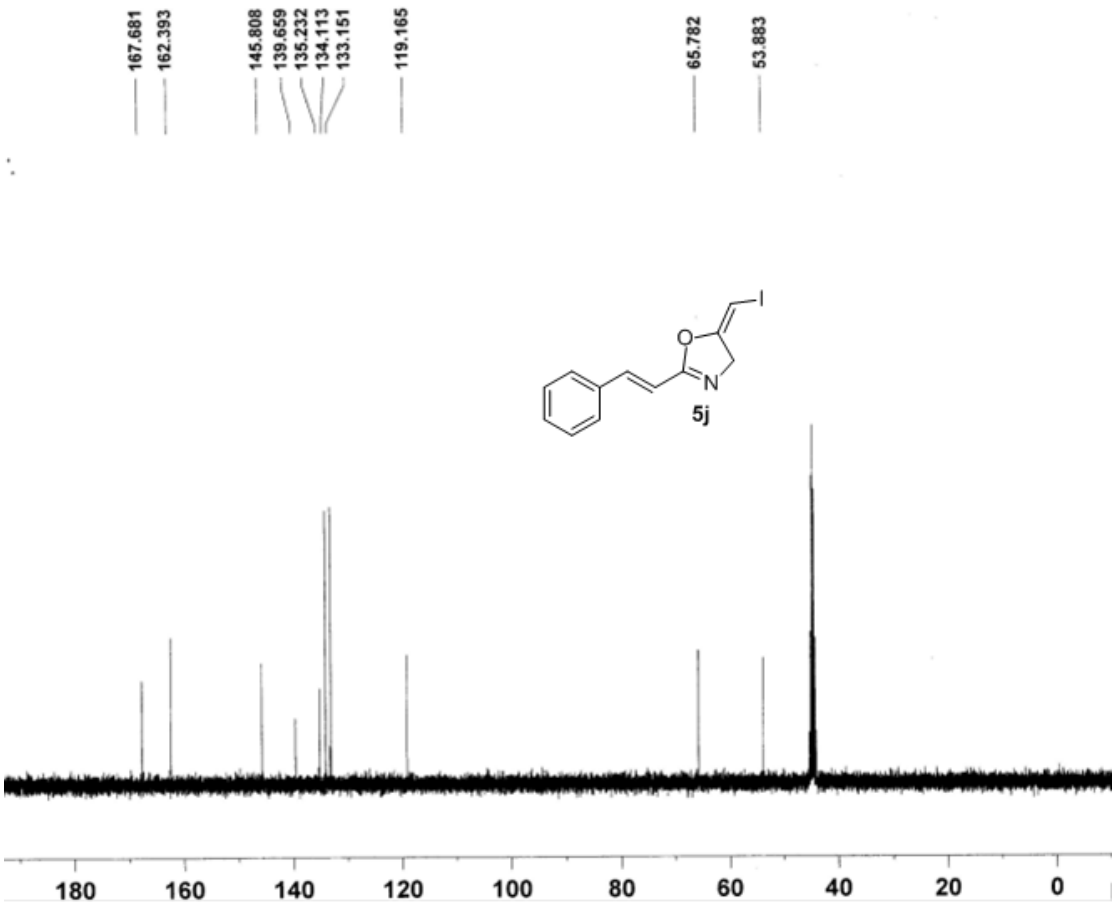


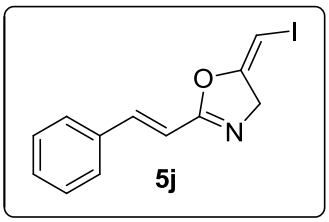
Chemical Formula: $C_{11}H_{10}INO_2$
Exact Mass: 314.98
Molecular Weight: 315.11
m/z: 314.98 (100.0%), 315.98 (12.1%), 316.98 (1.1%)
Elemental Analysis: C, 41.93; H, 3.20; I, 40.27; N, 4.45; O, 10.15



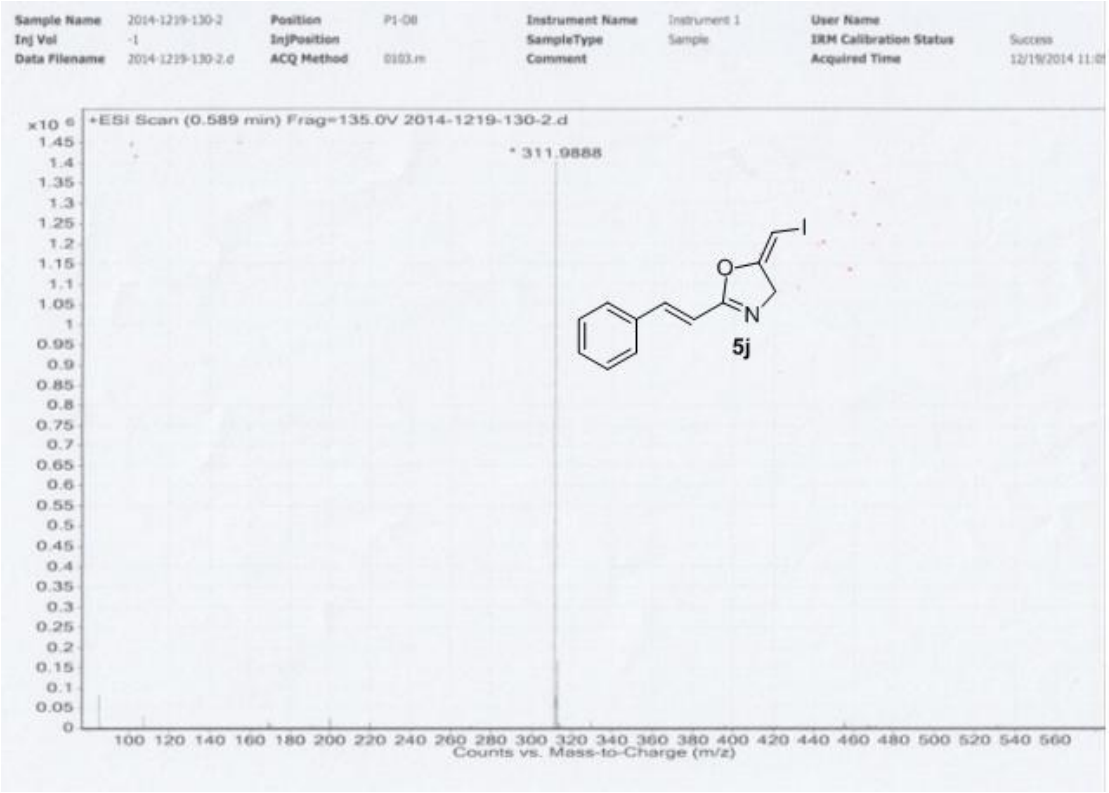
HRMS (ESI, m/z) calcd for $C_{11}H_{10}INO_2$ $[M+H]^+$ **315.9829**, found **315.9828.**


7.6610
7.6516
7.6481
7.3990
7.3842
7.3681
7.3584
7.3569
6.7916
6.7506
5.9300
5.9226
5.9152
4.4928
4.4860
I
O
N
5j
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.209
4.461
0.981
0.850
2.000

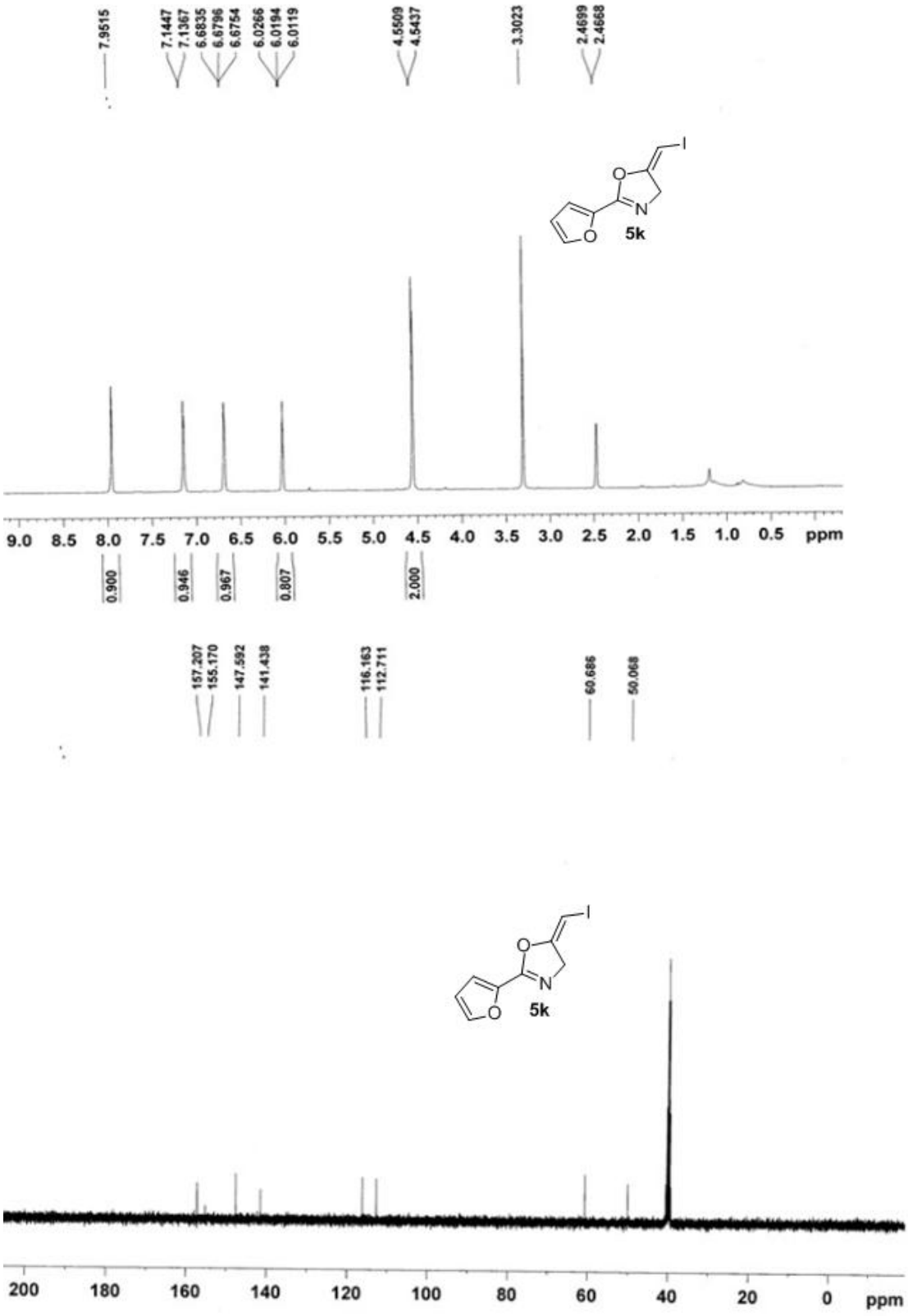

167.681
162.393
145.808
139.659
135.232
134.113
133.151
119.165
65.782
53.883
I
O
N
5j
180
160
140
120
100
80
60
40
20
0

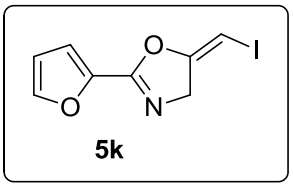


Chemical Formula: $C_{12}H_{10}INO$
Exact Mass: 310.98
Molecular Weight: 311.12
m/z: 310.98 (100.0%), 311.98 (13.4%)
Elemental Analysis: C, 46.33; H, 3.24; I, 40.79; N, 4.50; O, 5.14

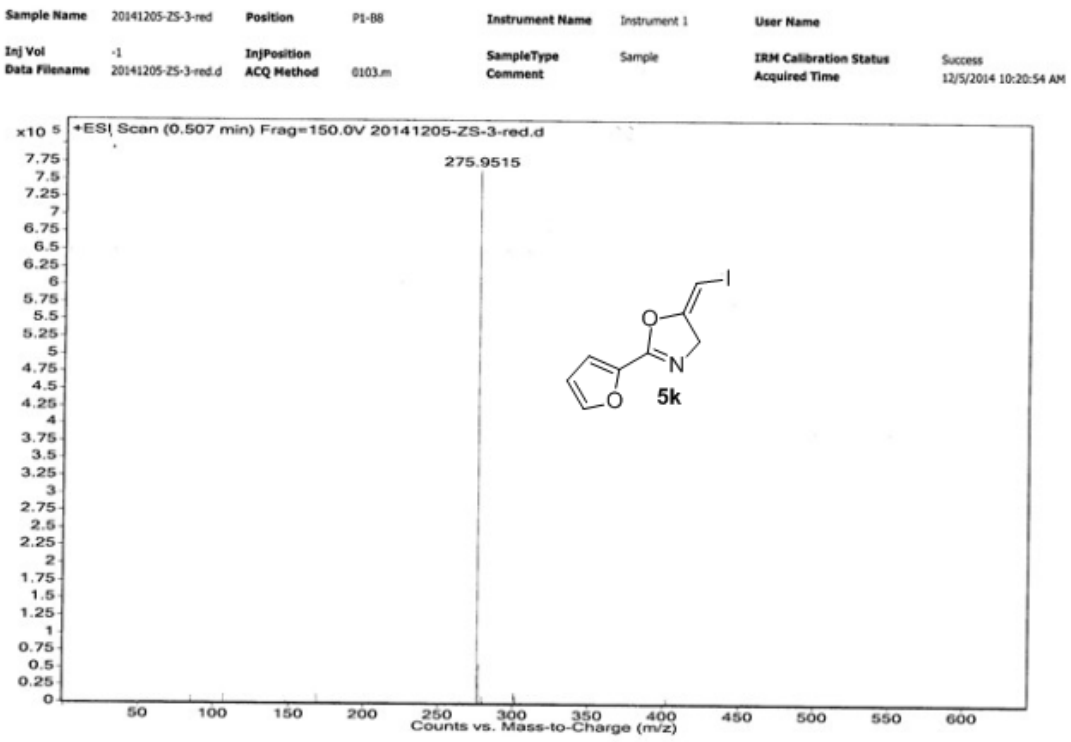


HRMS (ESI, m/z) calcd for $C_{12}H_{10}INO$ $[M+H]^+$ **311.9880**, found **311.9888.**

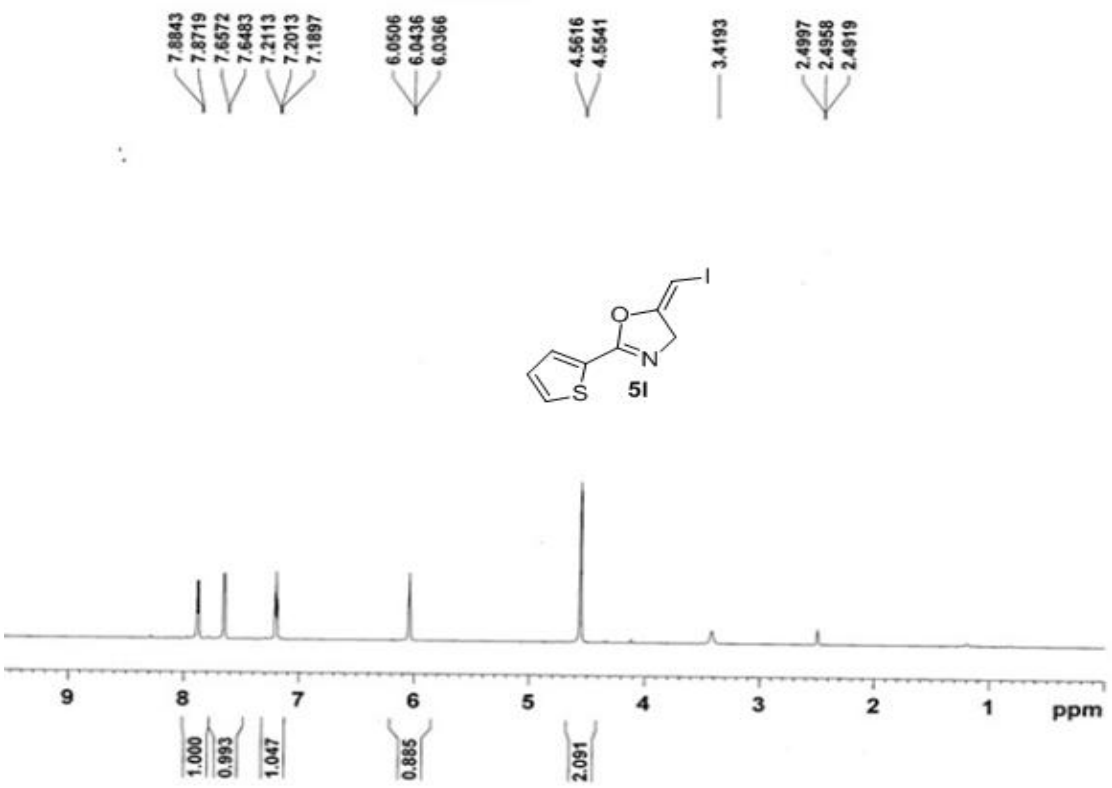

7.9515
7.1447
7.1367
6.6835
6.6796
6.6754
6.0266
6.0194
6.0119
4.5509
4.5437
3.3023
2.4699
2.4668
I
O
N
O
5k
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.900
0.946
0.967
0.807
2.000
157.207
155.170
147.592
141.438
116.163
112.711
60.686
50.068
I
O
N
O
5k
200 180 160 140 120 100 80 60 40 20 0 ppm

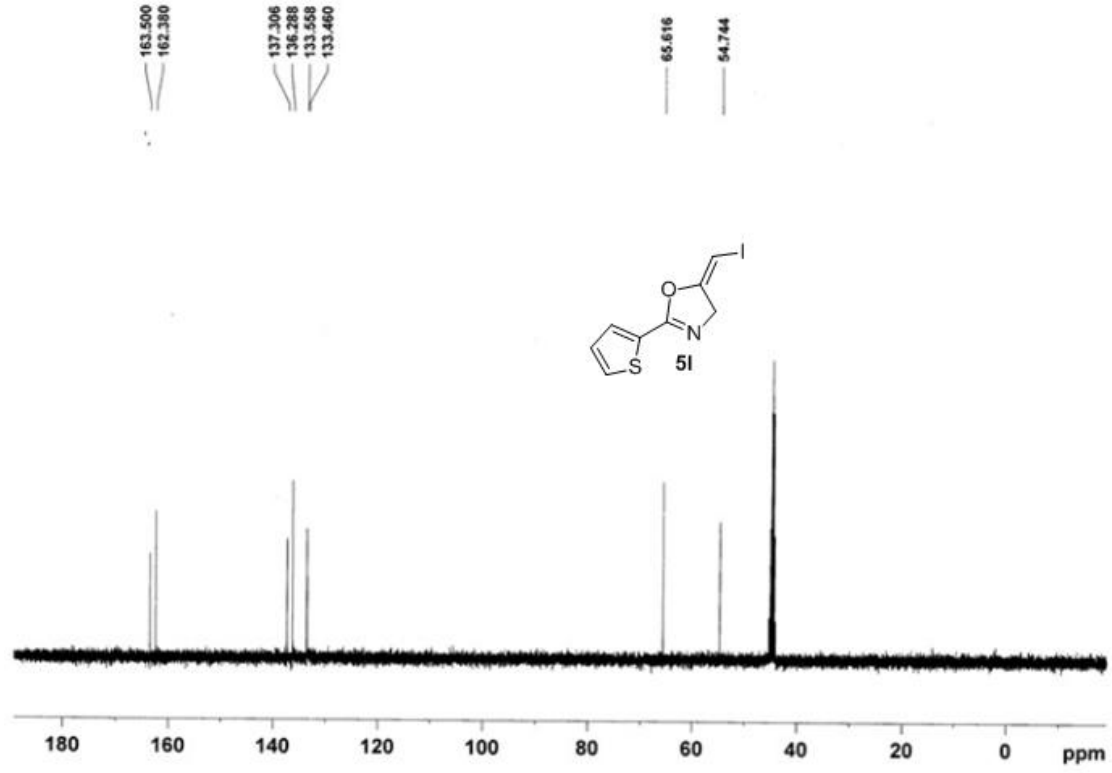


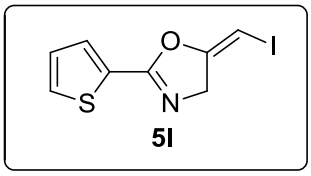
Chemical Formula: $C_8H_6INO_2$
Exact Mass: 274.9443
Molecular Weight: 275.0432
m/z: 274.9443 (100.0%), 275.9477 (8.7%)
Elemental Analysis: C, 34.93; H, 2.20; I, 46.14; N, 5.09; O, 11.63



HRMS (ESI, m/z) calcd for $C_8H_6INO_2$ $[M+H]^+$ **275.9516**, found **275.9515.**

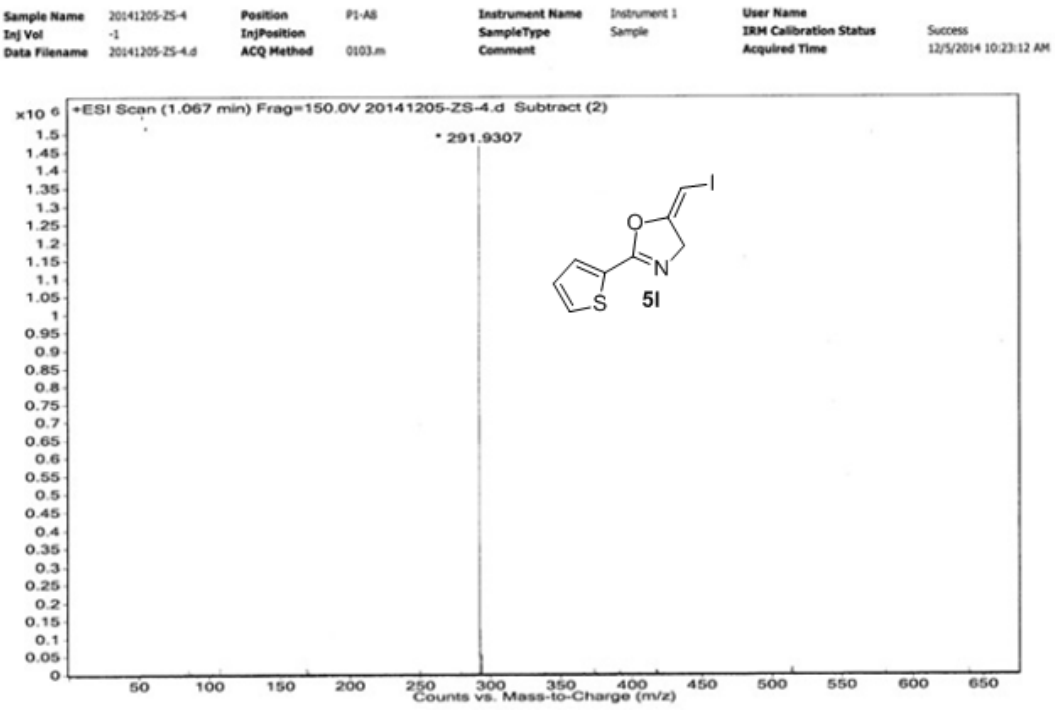

7.8843
7.8719
7.6572
7.6483
7.2113
7.2013
7.1897
6.0506
6.0436
6.0366
4.5616
4.5541
3.4193
2.4997
2.4958
2.4919
I
O
N
S
5l
9
8
7
6
5
4
3
2
1
ppm
1.000
0.993
1.047
0.885
2.091


163.500
162.380
137.306
136.288
133.558
133.460
65.616
54.744
I
O
N
S
5l
180
160
140
120
100
80
60
40
20
0
ppm

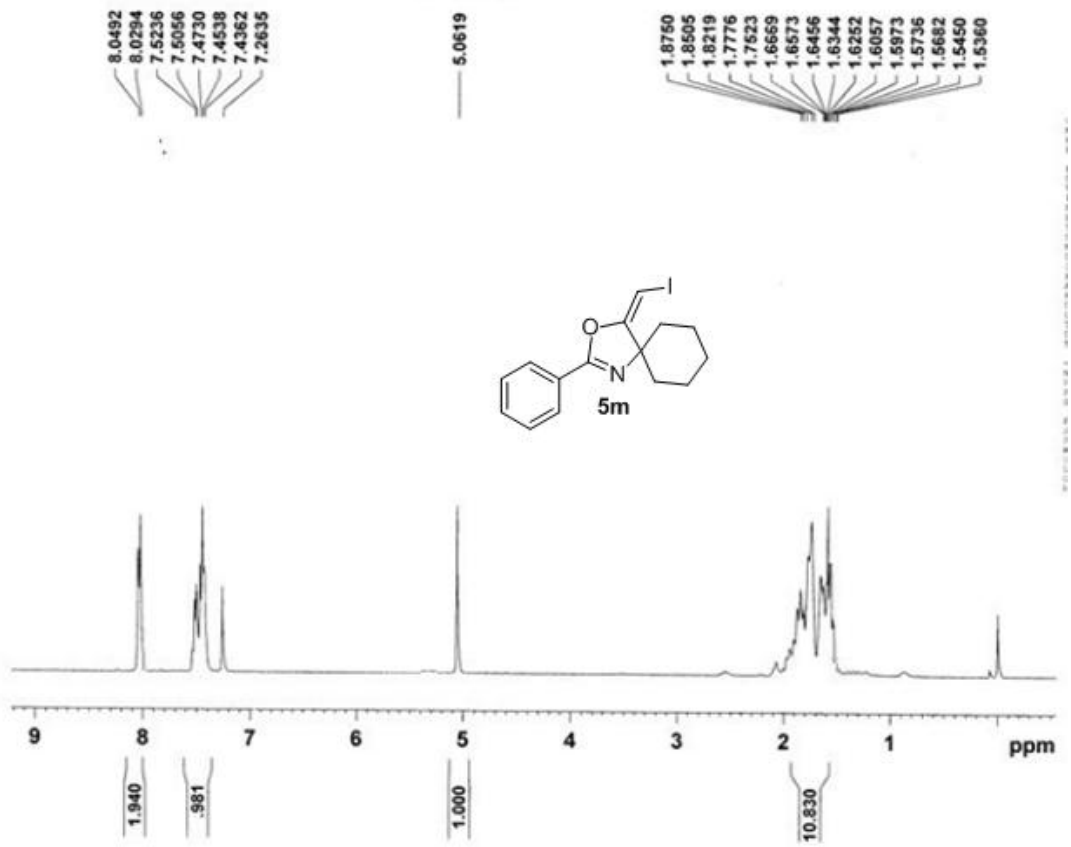


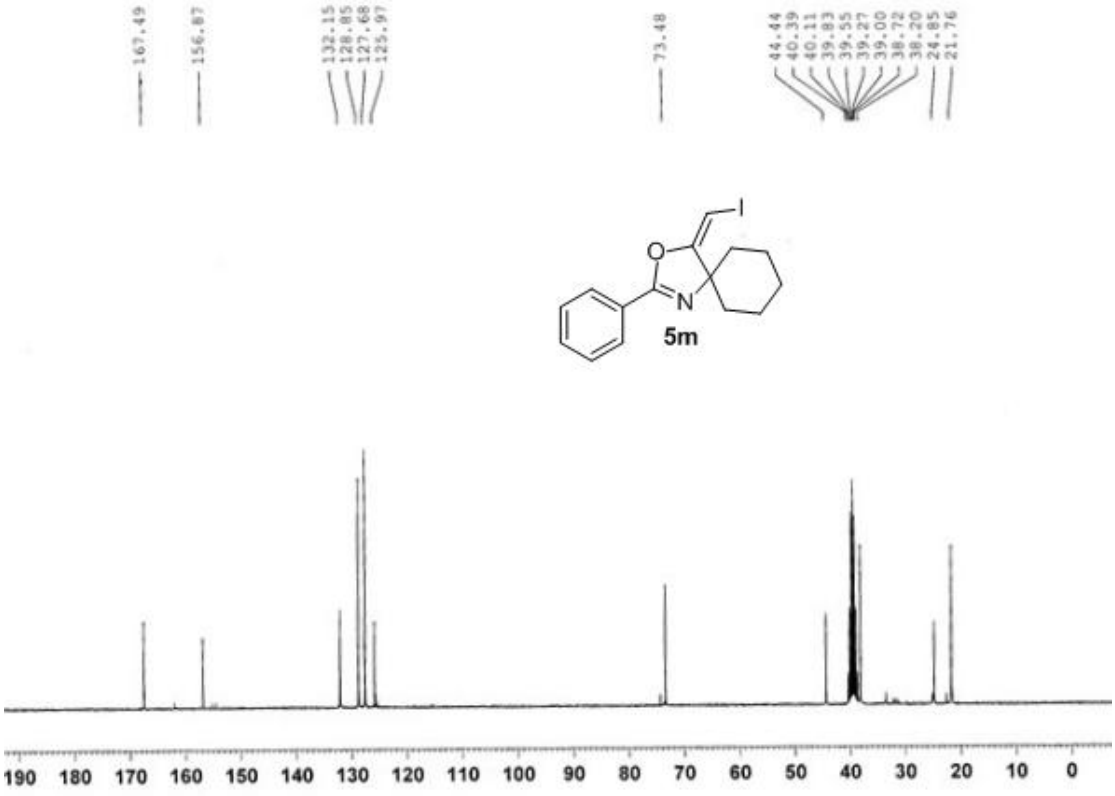
5l

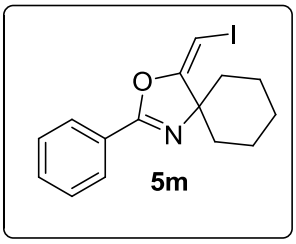
Chemical Formula: C_8H_6INOS
Exact Mass: 290.92
Molecular Weight: 291.11
m/z: 290.92 (100.0%), 291.92 (9.8%), 292.92 (4.6%)
Elemental Analysis: C, 33.01; H, 2.08; I, 43.59; N, 4.81; O, 5.50; S, 11.01



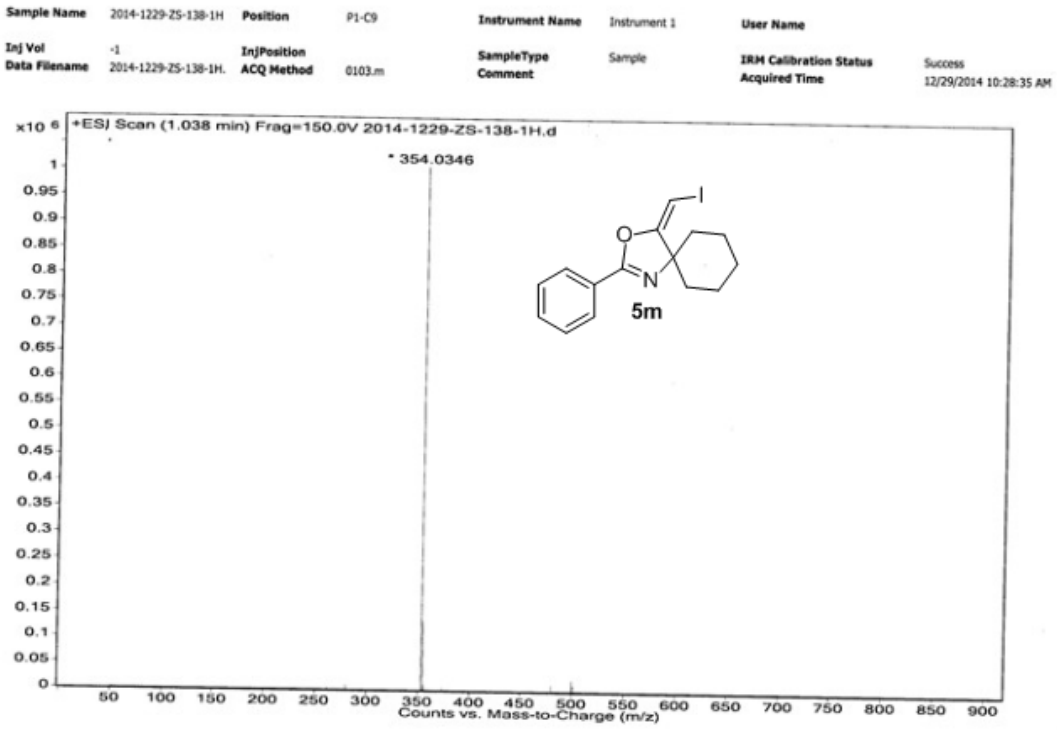
HRMS (ESI, m/z) calcd for C_8H_6INOS $[M+H]^+$ **291.9288**, found **291.9307.**


8.0492
8.0294
7.5236
7.5056
7.4730
7.4538
7.4362
7.2635
5.0619
1.8750
1.8505
1.8219
1.7776
1.7523
1.6669
1.6573
1.6456
1.6344
1.6252
1.6057
1.5973
1.5736
1.5682
1.5450
1.5360
I
O
N
5m
9
8
7
6
5
4
3
2
1
ppm
1.940
.981
1.000
10.830

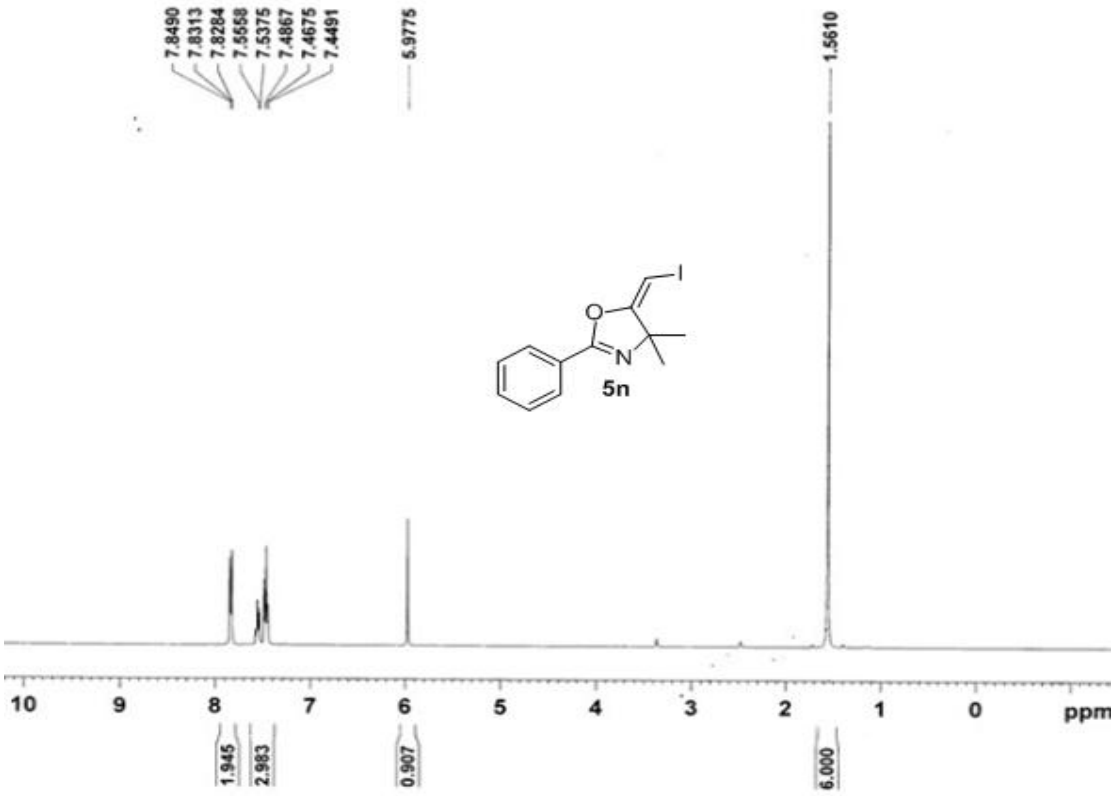

167.49
156.87
132.15
128.85
127.68
125.97
73.48
44.44
40.39
40.11
39.83
39.55
39.27
39.00
38.72
38.20
24.85
21.76
I
O
N
5m
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

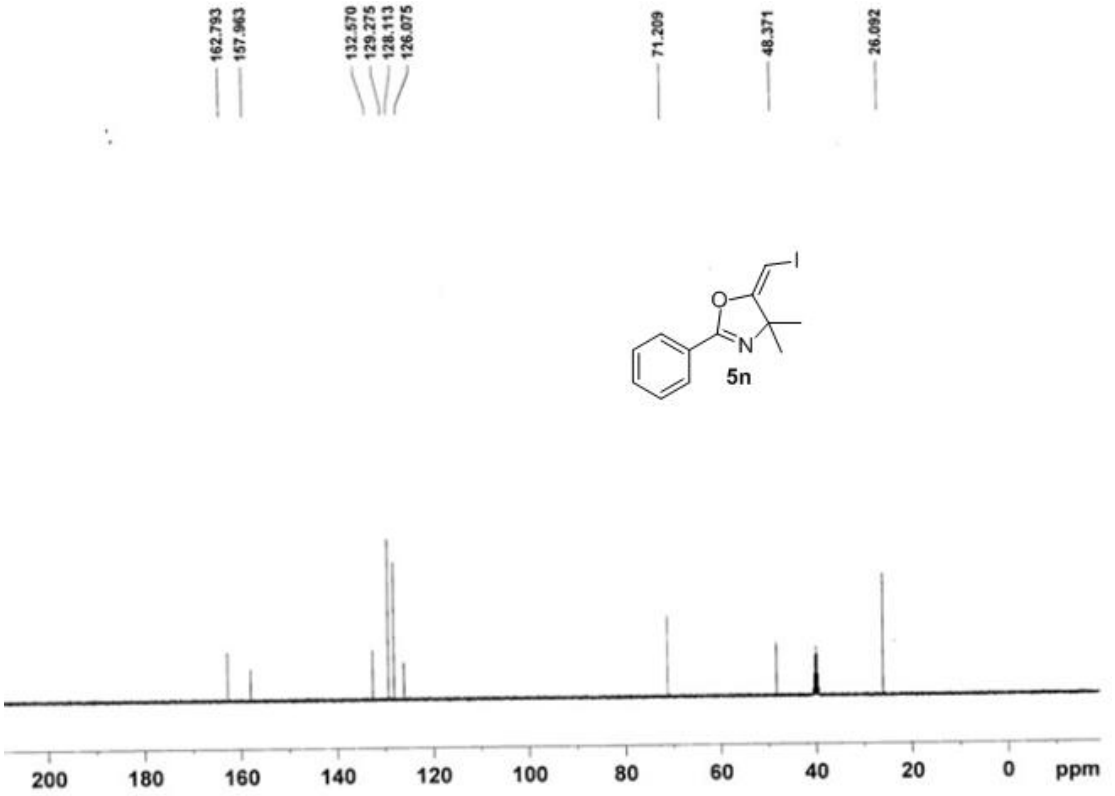


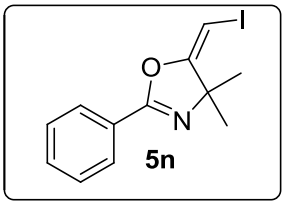
Chemical Formula: $C_{15}H_{16}INO$
Exact Mass: 353.03
Molecular Weight: 353.20
m/z: 353.03 (100.0%), 354.03 (16.4%), 355.03 (1.5%)
Elemental Analysis: C, 51.01; H, 4.57; I, 35.93; N, 3.97; O, 4.53



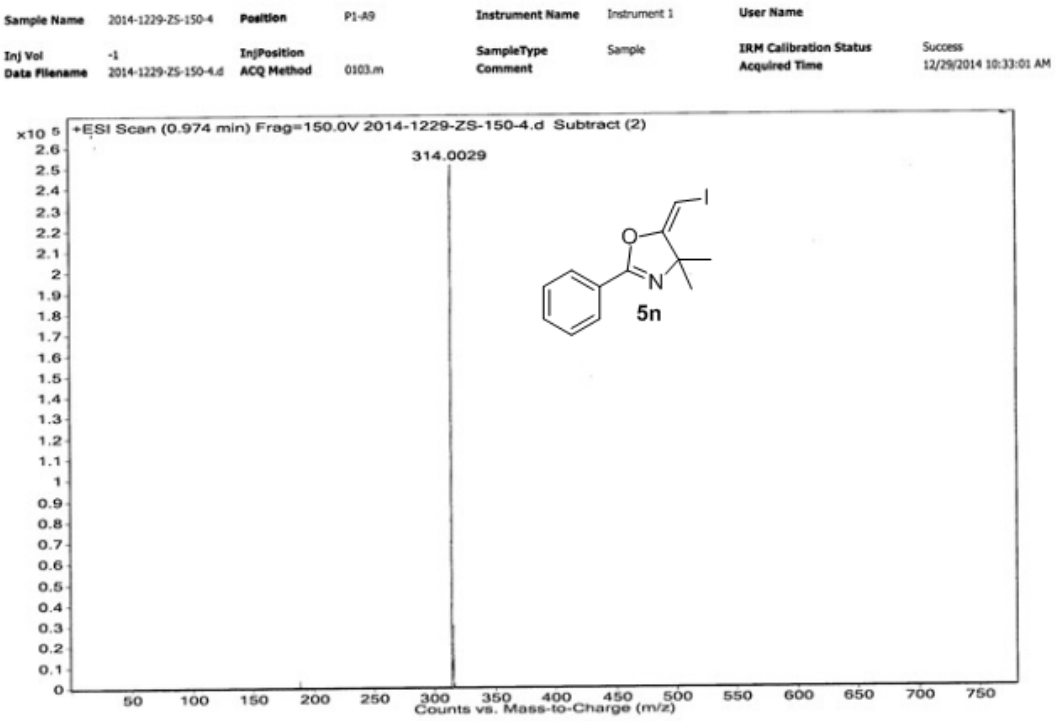
HRMS (ESI, m/z) calcd for $C_{15}H_{16}INO$ $[M+H]^+$ **354.0349,** found **354.0346.**


7.8490
7.8313
7.8284
7.5558
7.5375
7.4867
7.4675
7.4491
5.9775
1.5610
I
O
N
5n
10
9
8
7
6
5
4
3
2
1
0
ppm
1.945
2.983
0.907
6.000

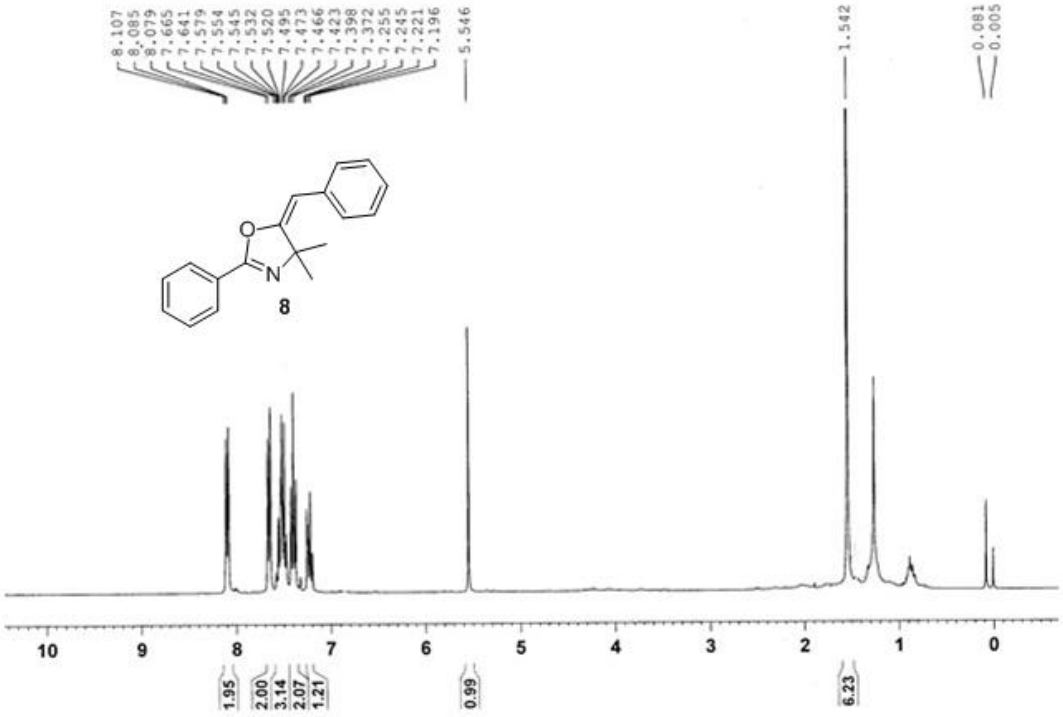

162.793
157.963
132.570
129.275
128.113
126.075
71.209
48.371
26.092
I
O
N
5n
200
180
160
140
120
100
80
60
40
20
0
ppm

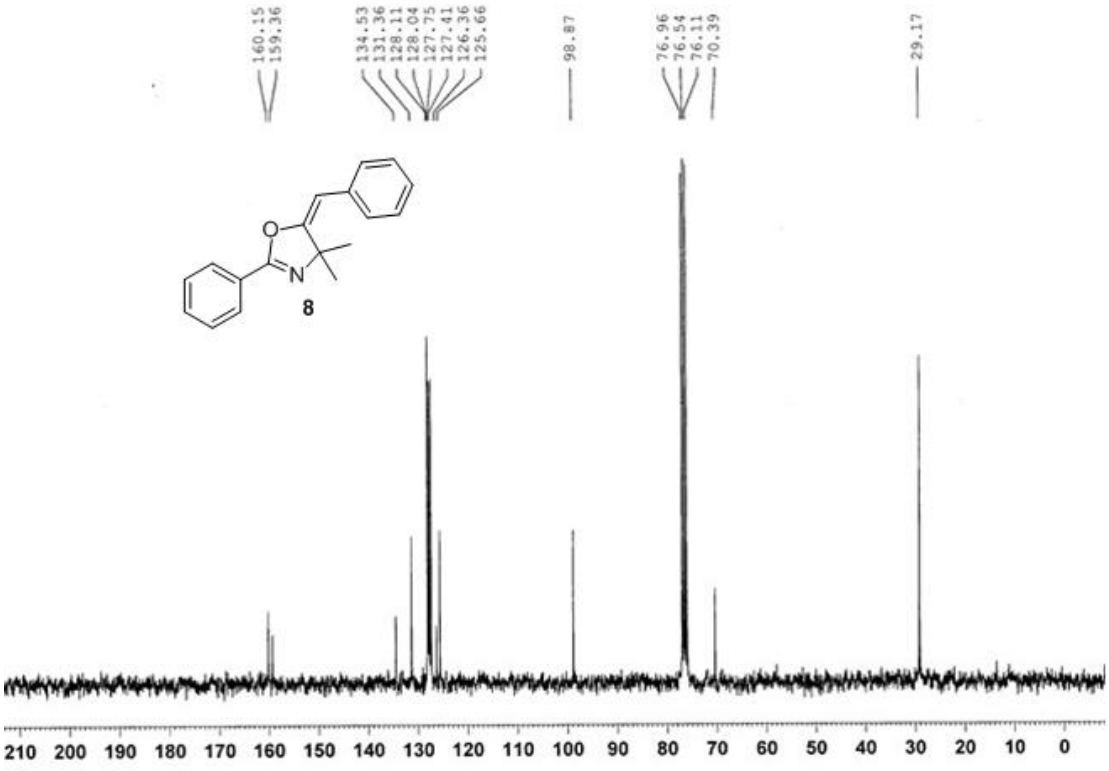


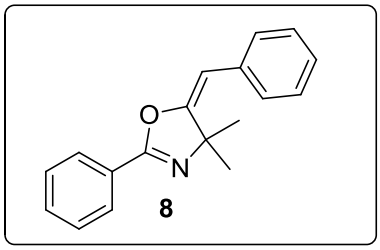
Chemical Formula: $C_{12}H_{12}INO$
Exact Mass: 313.00
Molecular Weight: 313.13
m/z: 313.00 (100.0%), 314.00 (13.2%), 315.00 (1.0%)
Elemental Analysis: C, 46.03; H, 3.86; I, 40.53; N, 4.47; O, 5.11



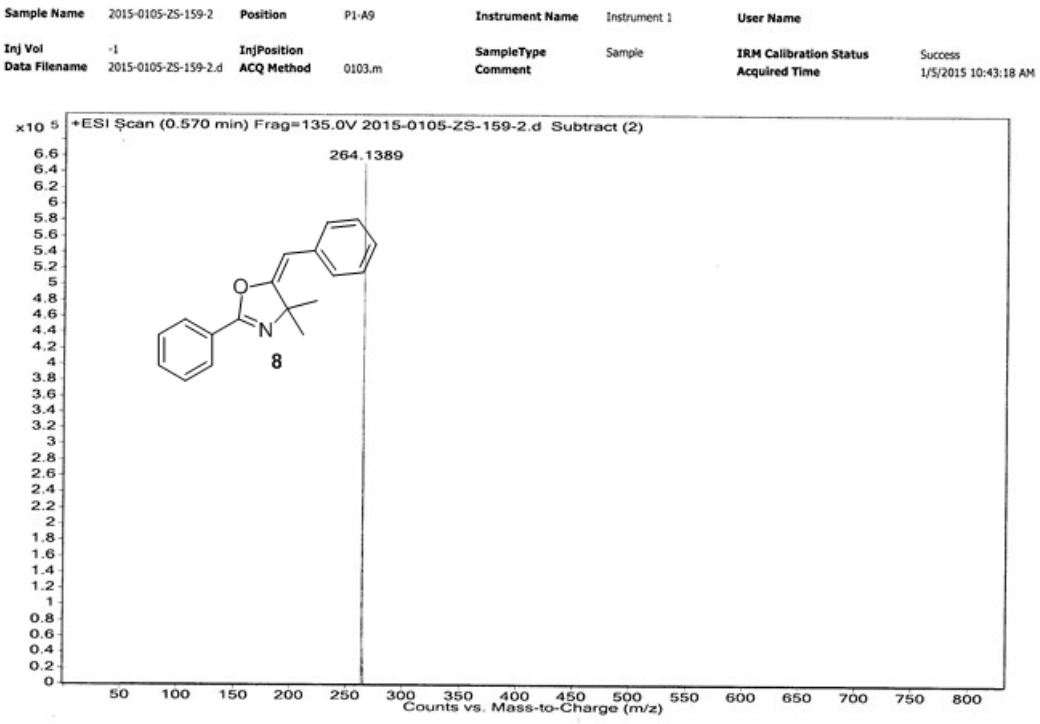
HRMS (ESI, m/z) calcd for $C_{12}H_{12}INO$ $[M+H]^+$ **314.0036**, found **314.0029.**


8.107
8.085
8.079
7.665
7.641
7.579
7.554
7.545
7.532
7.520
7.495
7.473
7.466
7.423
7.398
7.372
7.255
7.245
7.221
7.196
5.546
1.542
0.081
0.005
8
10
9
8
7
6
5
4
3
2
1
0
1.95
2.00
3.14
2.07
1.21
0.99
6.23

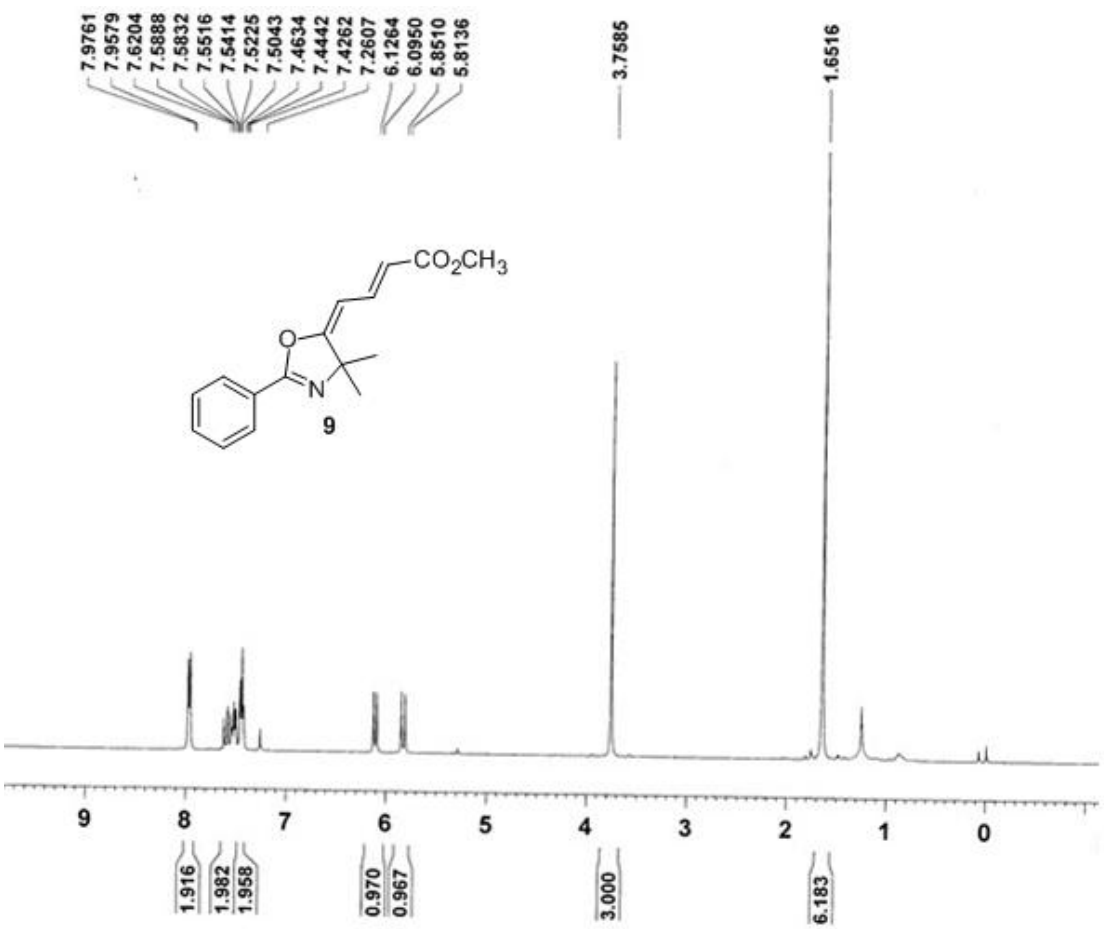

160.15
159.36
134.53
131.36
128.11
128.04
127.75
127.41
126.36
125.66
98.87
76.96
76.54
76.11
70.39
29.17
8
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

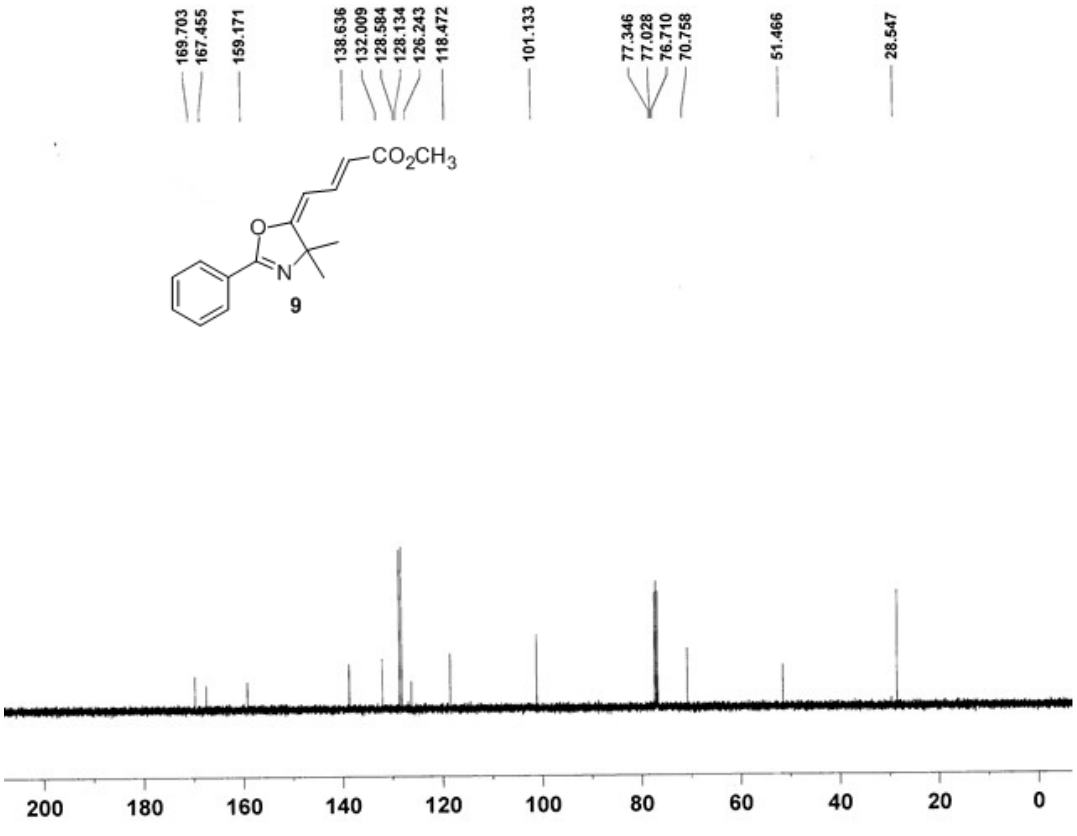


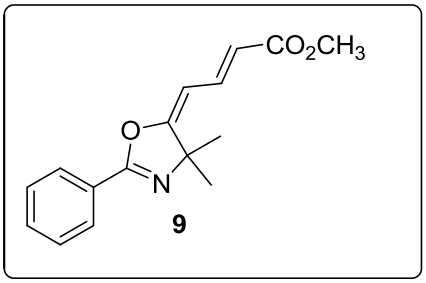
Chemical Formula: $C_{18}H_{17}NO$
Exact Mass: 263.1310
Molecular Weight: 263.3337
m/z: 263.1310 (100.0%), 264.1344 (19.5%), 265.1377 (1.8%)
Elemental Analysis: C, 82.10; H, 6.51; N, 5.32; O, 6.08



HRMS (ESI, m/z) calcd for $C_{18}H_{17}NO\,[M+H]^+$ **264.1383**, found **264.1389.**

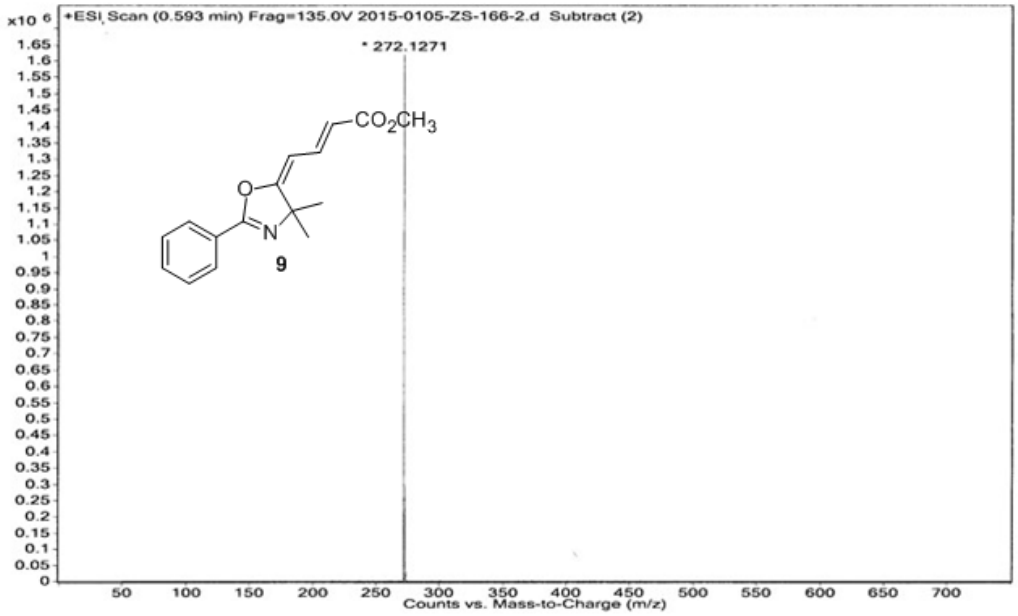

7.9761
7.9579
7.6204
7.5888
7.5832
7.5516
7.5414
7.5225
7.5043
7.4634
7.4442
7.4262
7.2607
6.1264
6.0950
5.8510
5.8136
3.7585
1.6516
CO2CH3
O
N
9
9 8 7 6 5 4 3 2 1 0
1.916
1.982
1.958
0.970
0.967
3.000
6.183


169.703
167.455
159.171
138.636
132.009
128.584
128.134
126.243
118.472
101.133
77.346
77.028
76.710
70.758
51.466
28.547
CO2CH3
O
N
9
200 180 160 140 120 100 80 60 40 20 0

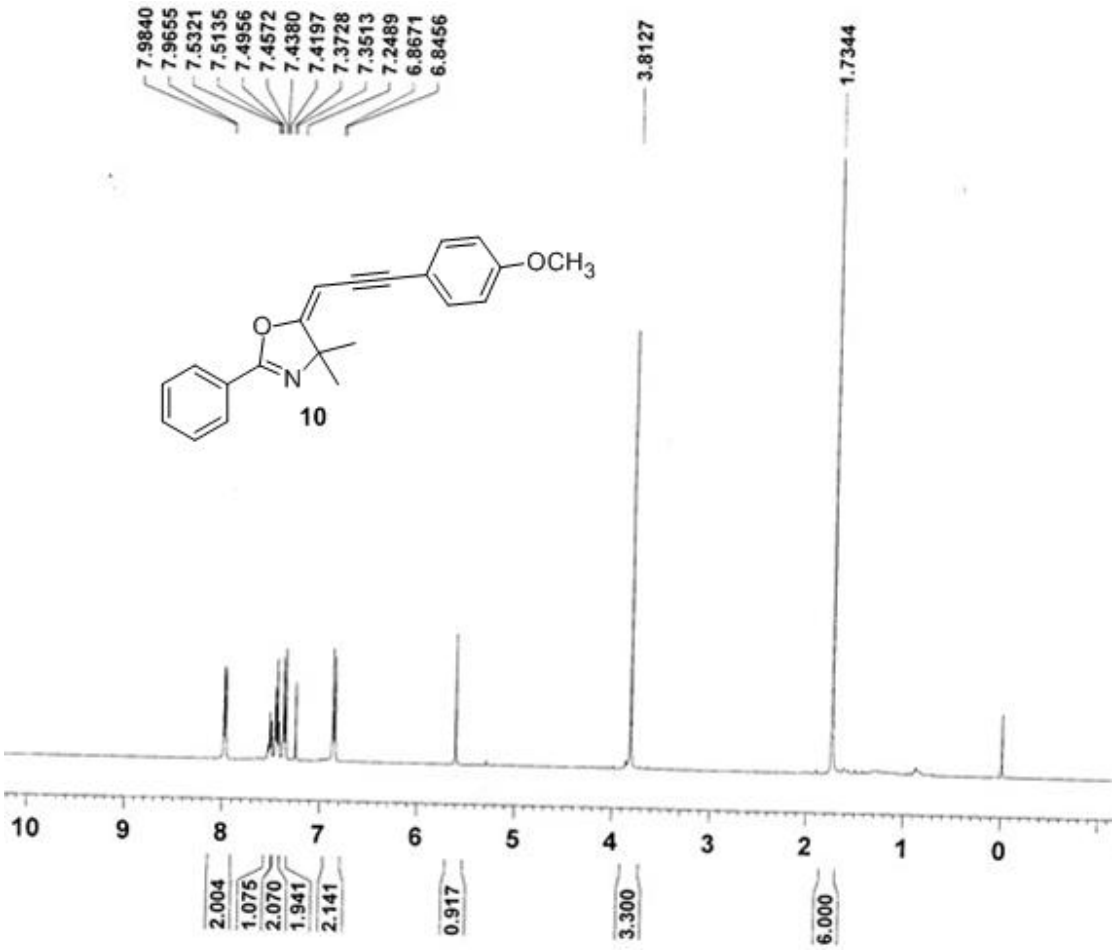


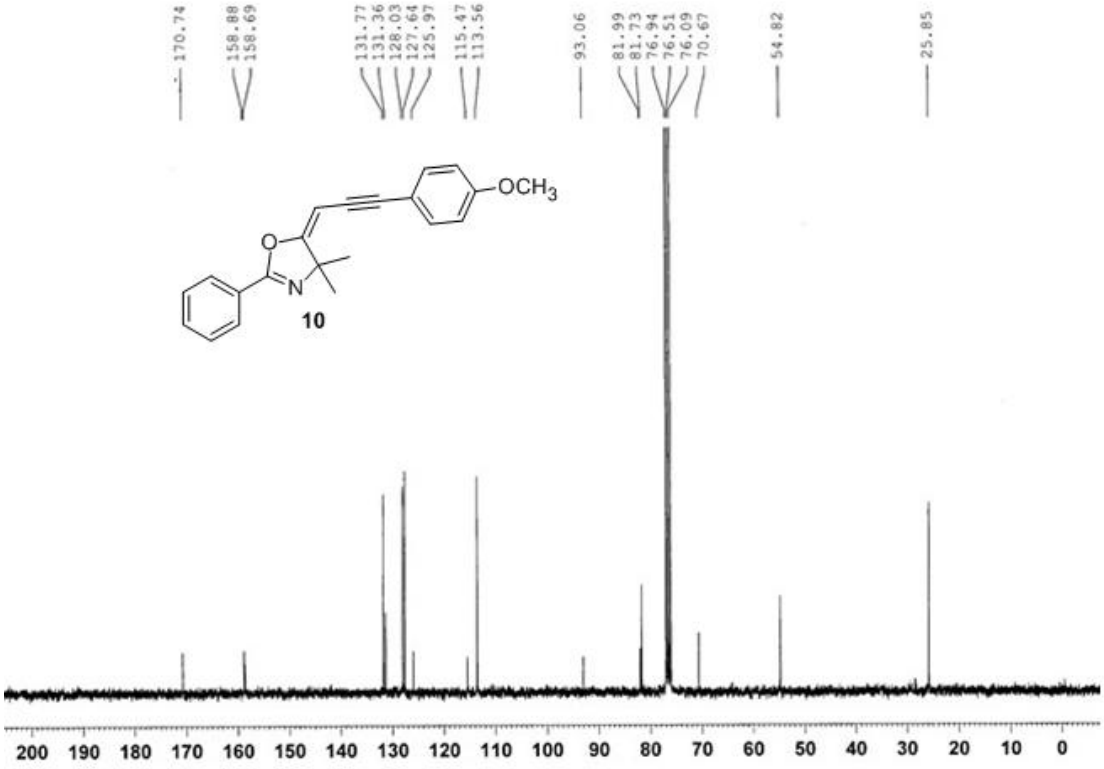
Chemical Formula: $C_{16}H_{17}NO_3$
Exact Mass: 271.1208
Molecular Weight: 271.3111
m/z: 271.1208 (100.0%), 272.1242 (17.3%), 273.1276 (1.4%)
Elemental Analysis: C, 70.83; H, 6.32; N, 5.16; O, 17.69

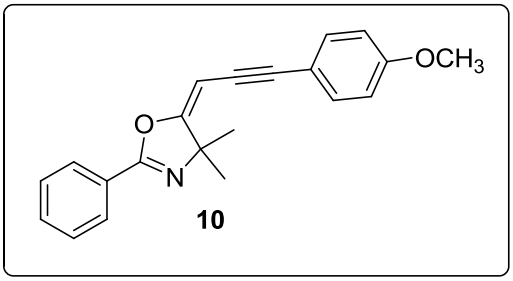
Sample Name	2015-0105-ZS-166-2	**Position**	P1-C9	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	2015-0105-ZS-166-2.d	**ACQ Method**	0103.m	**Comment**		**Acquired Time**	1/5/2015 10:38:48 AM



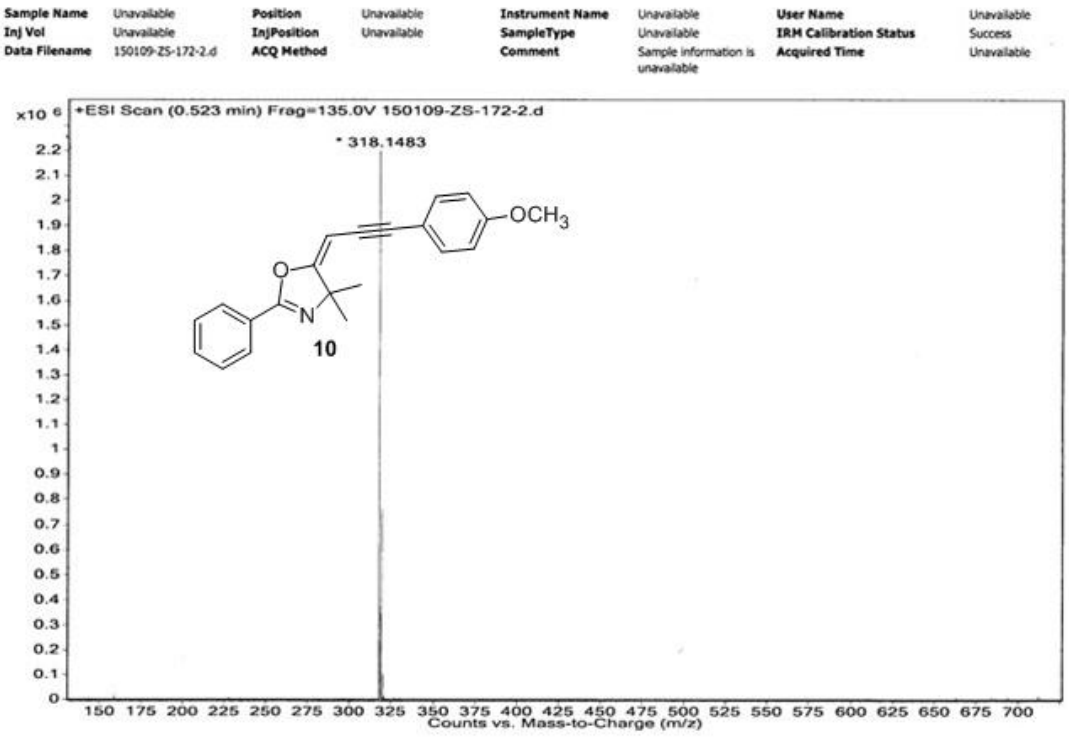
HRMS (ESI, m/z) calcd for $C_{16}H_{17}NO_3$ $[M+H]^+$ **272.1281**, found **264.1271.**


7.9840
7.9655
7.5321
7.5135
7.4956
7.4572
7.4380
7.4197
7.3728
7.3513
7.2489
6.8671
6.8456
3.8127
1.7344
OCH3
O
N
10
10 9 8 7 6 5 4 3 2 1 0
2.004
1.075
2.070
1.941
2.141
0.917
3.300
6.000

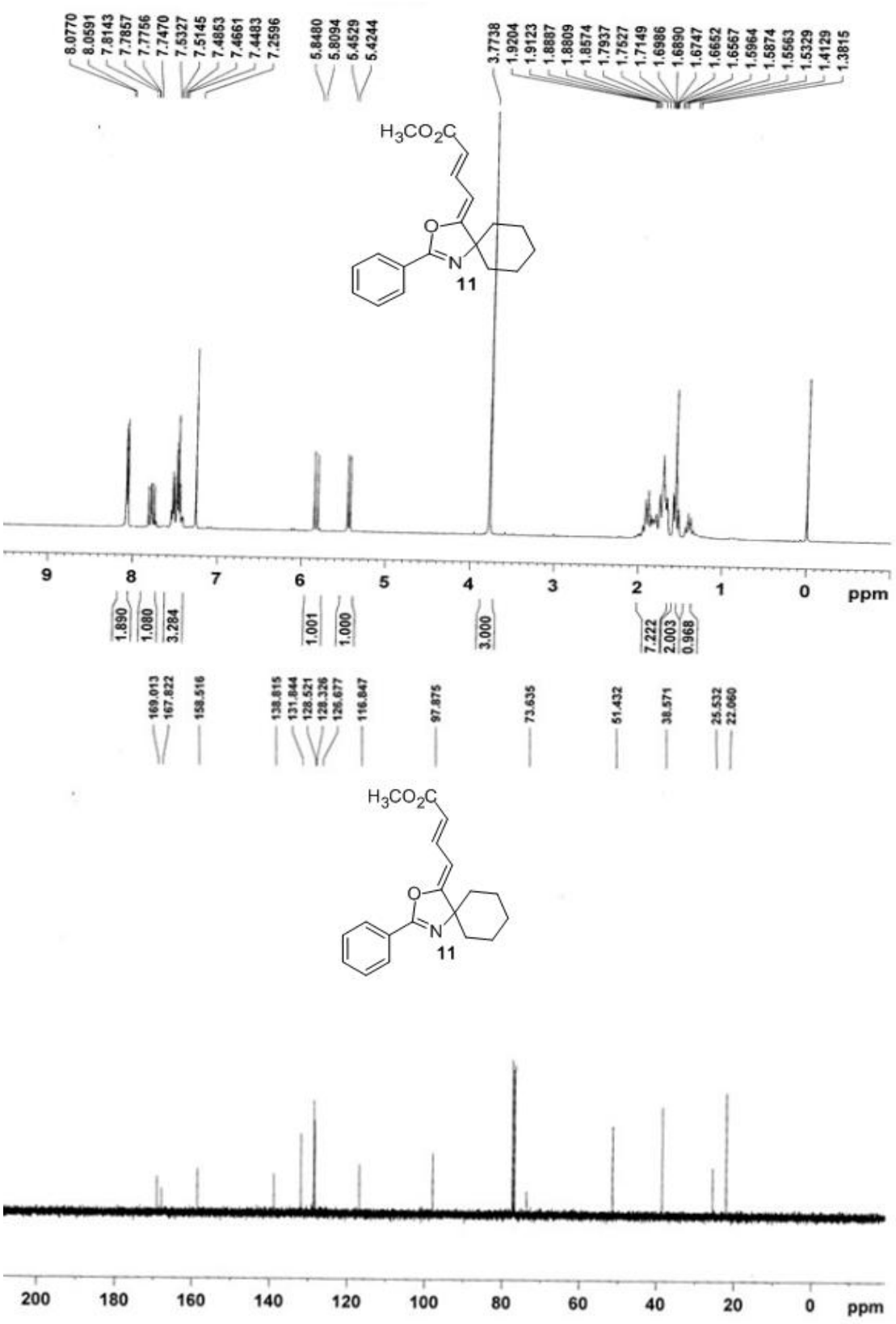

170.74
158.88
158.69
131.77
131.36
128.03
127.64
125.97
115.47
113.56
93.06
81.99
81.73
76.94
76.51
76.09
70.67
54.82
25.85
OCH3
O
N
10
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

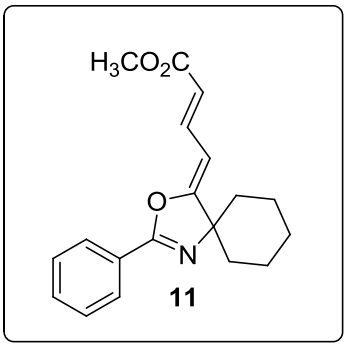


Chemical Formula: $C_{21}H_{19}NO_2$
Exact Mass: 317.1416
Molecular Weight: 317.3811
m/z: 317.1416 (100.0%), 318.1449 (22.7%), 319.1483 (2.5%)
Elemental Analysis: C, 79.47; H, 6.03; N, 4.41; O, 10.08



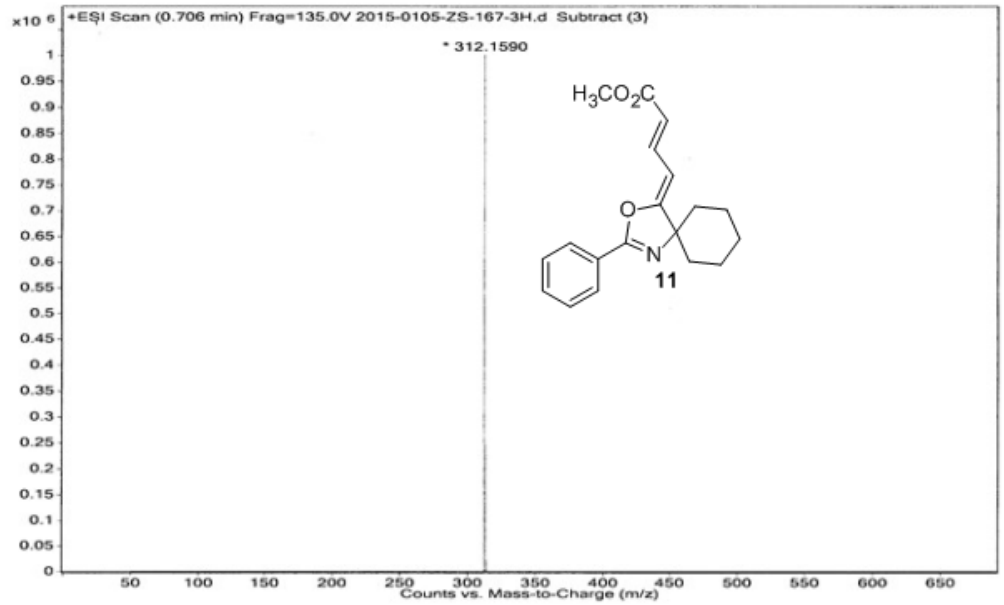
HRMS (ESI, m/z) calcd for $C_{21}H_{19}NO_2$ $[M+H]^+$**318.1489,** found **318.1483.**


8.0770
8.0591
7.8143
7.7857
7.7756
7.7470
7.5327
7.5145
7.4853
7.4661
7.4483
7.2596
5.8480
5.8094
5.4529
5.4244
3.7738
1.9204
1.9123
1.8887
1.8809
1.8574
1.7937
1.7527
1.7149
1.6986
1.6890
1.6747
1.6652
1.6567
1.5964
1.5874
1.5563
1.5329
1.4129
1.3815
H3CO2C
O
N
11
9
8
7
6
5
4
3
2
1
0
ppm
1.890
1.080
3.284
1.001
1.000
3.000
7.222
2.003
0.968
169.013
167.822
158.516
138.815
131.844
128.521
128.326
126.677
116.847
97.875
73.635
51.432
38.571
25.532
22.060
H3CO2C
O
N
11
200
180
160
140
120
100
80
60
40
20
0
ppm

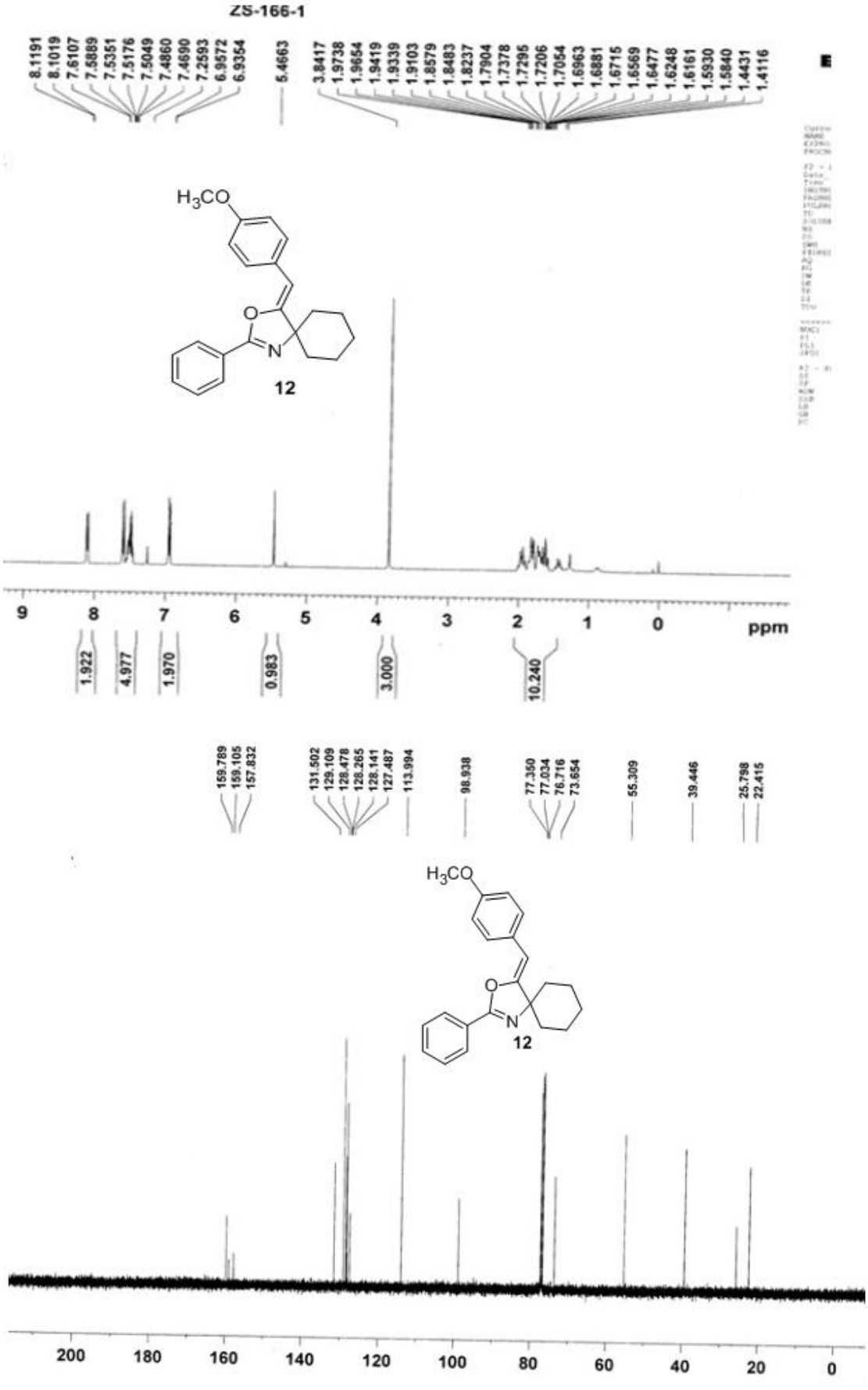


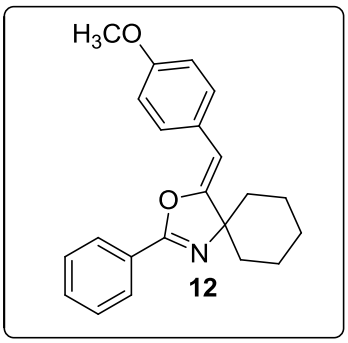
Chemical Formula: $C_{19}H_{21}NO_3$
Exact Mass: 311.1521
Molecular Weight: 311.3749
m/z: 311.1521 (100.0%), 312.1555 (20.5%), 313.1589 (2.0%)
Elemental Analysis: C, 73.29; H, 6.80; N, 4.50; O, 15.41

Sample Name	2015-0105-ZS-167-3H	**Position**	P1-B8	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	2015-0105-ZS-167-3H.	**ACQ Method**	0103.m	**Comment**		**Acquired Time**	1/5/2015 11:01:43 AM

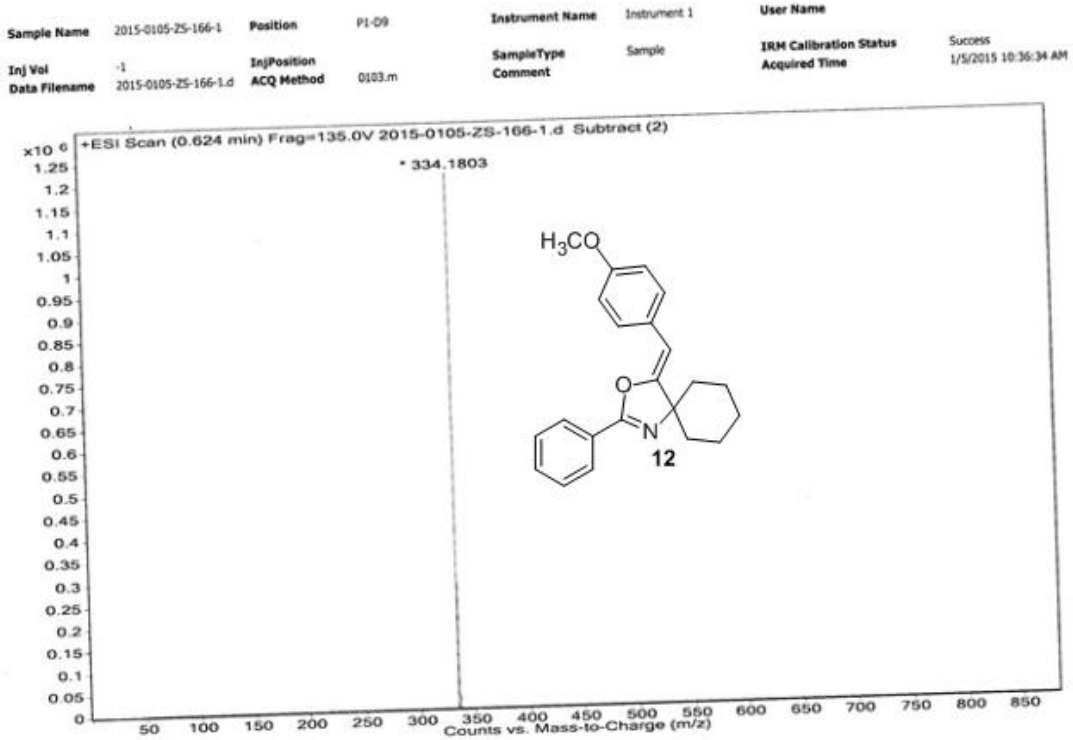


HRMS (ESI, m/z) calcd for $C_{19}H_{21}NO_3$ $[M+H]^+$ **312.1594,** found **312.1590.**

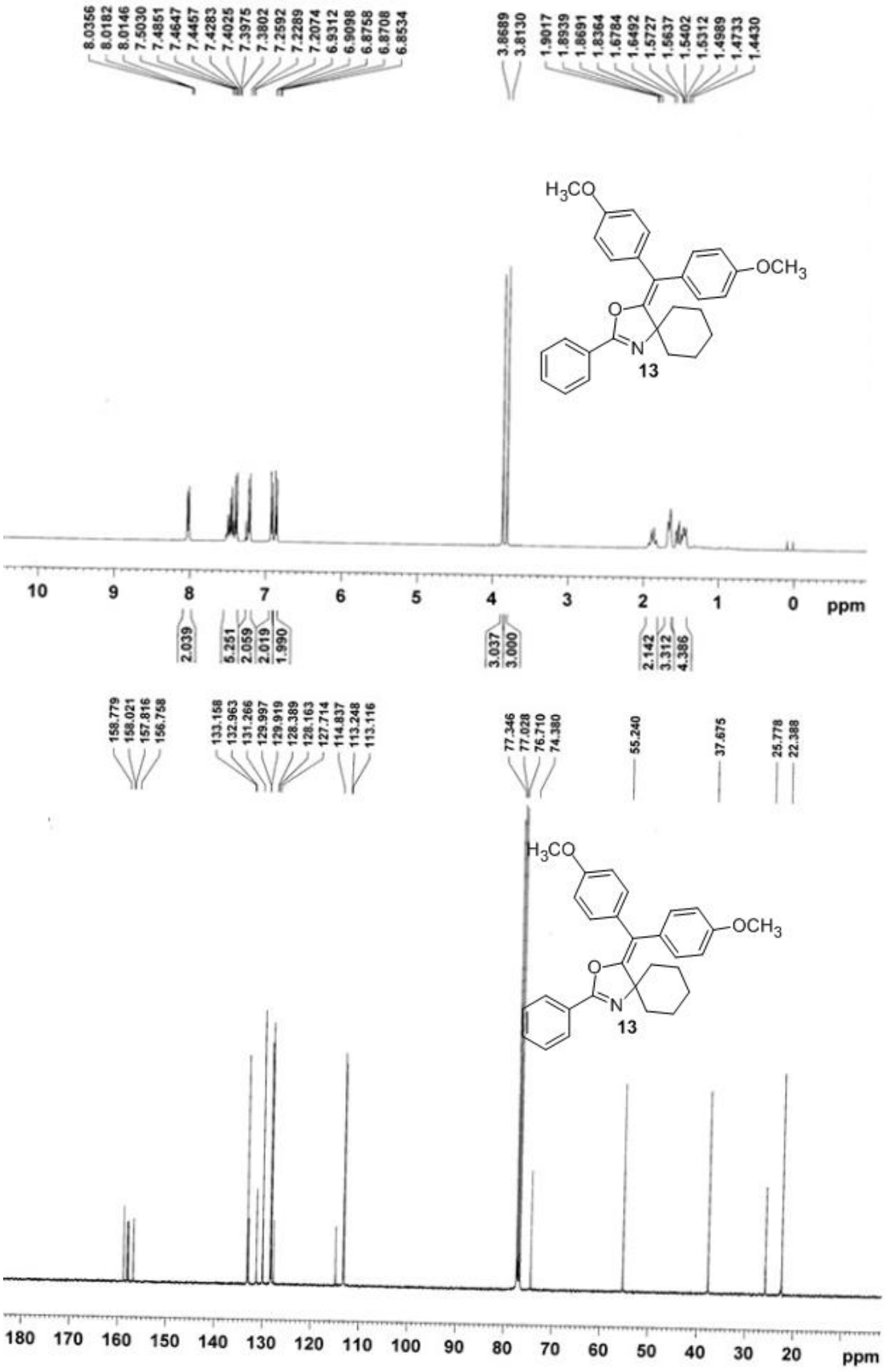

ZS-166-1
8.1191
8.1019
7.6107
7.5889
7.5351
7.5176
7.5049
7.4860
7.4690
7.2593
6.9572
6.9354
5.4663
3.8417
1.9738
1.9654
1.9419
1.9339
1.9103
1.8579
1.8483
1.8237
1.7904
1.7378
1.7295
1.7206
1.7054
1.6963
1.6881
1.6715
1.6569
1.6477
1.6248
1.6161
1.5930
1.5840
1.4431
1.4116
H3CO
O
N
12
9
8
7
6
5
4
3
2
1
0
ppm
1.922
4.977
1.970
0.983
3.000
10.240
159.789
159.105
157.832
131.502
129.109
128.478
128.265
128.141
127.487
113.994
98.938
77.350
77.034
76.716
73.654
55.309
39.446
25.798
22.415
H3CO
O
N
12
200
180
160
140
120
100
80
60
40
20
0

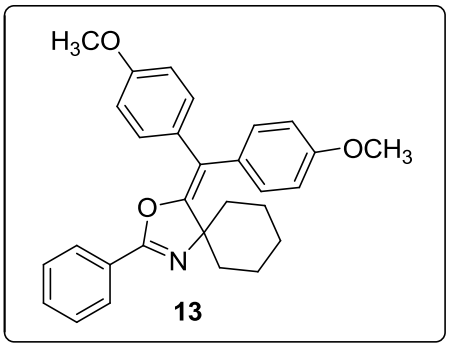


Chemical Formula: $C_{22}H_{23}NO_2$
Exact Mass: 333.1729
Molecular Weight: 333.4235
m/z: 333.1729 (100.0%), 334.1762 (23.8%), 335.1796 (2.7%)
Elemental Analysis: C, 79.25; H, 6.95; N, 4.20; O, 9.60

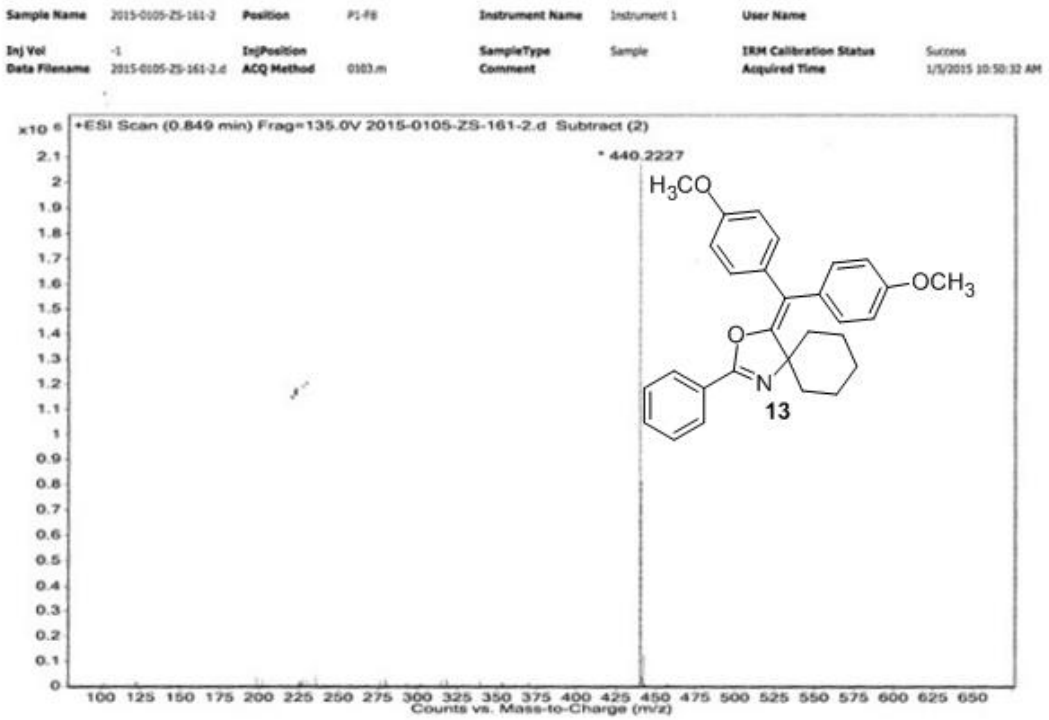


HRMS (ESI, m/z) calcd for $C_{22}H_{23}NO_2$ $[M+H]^+$ **334.1802**, found **334.1803.**

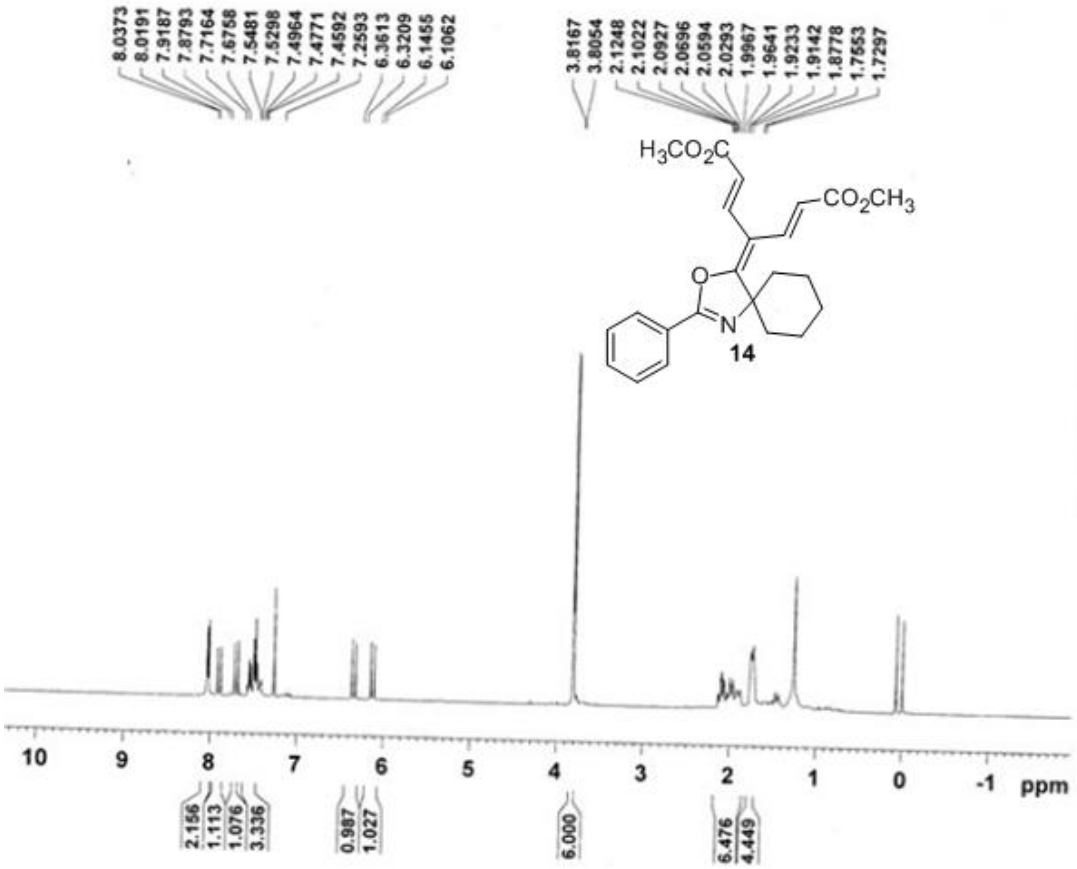

8.0356
8.0182
8.0146
7.5030
7.4851
7.4647
7.4457
7.4283
7.4025
7.3975
7.3802
7.2592
7.2289
7.2074
6.9312
6.9098
6.8758
6.8708
6.8534
3.8689
3.8130
1.9017
1.8939
1.8691
1.8364
1.6784
1.6492
1.5727
1.5637
1.5402
1.5312
1.4989
1.4733
1.4430
H3CO
OCH3
O
N
13
10 9 8 7 6 5 4 3 2 1 0 ppm
2.039
5.251
2.059
2.019
1.990
3.037
3.000
2.142
3.312
4.386
158.779
158.021
157.816
156.758
133.158
132.963
131.266
129.997
129.919
128.389
128.163
127.714
114.837
113.248
113.116
77.346
77.028
76.710
74.380
55.240
37.675
25.778
22.388
H3CO
OCH3
O
N
13
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

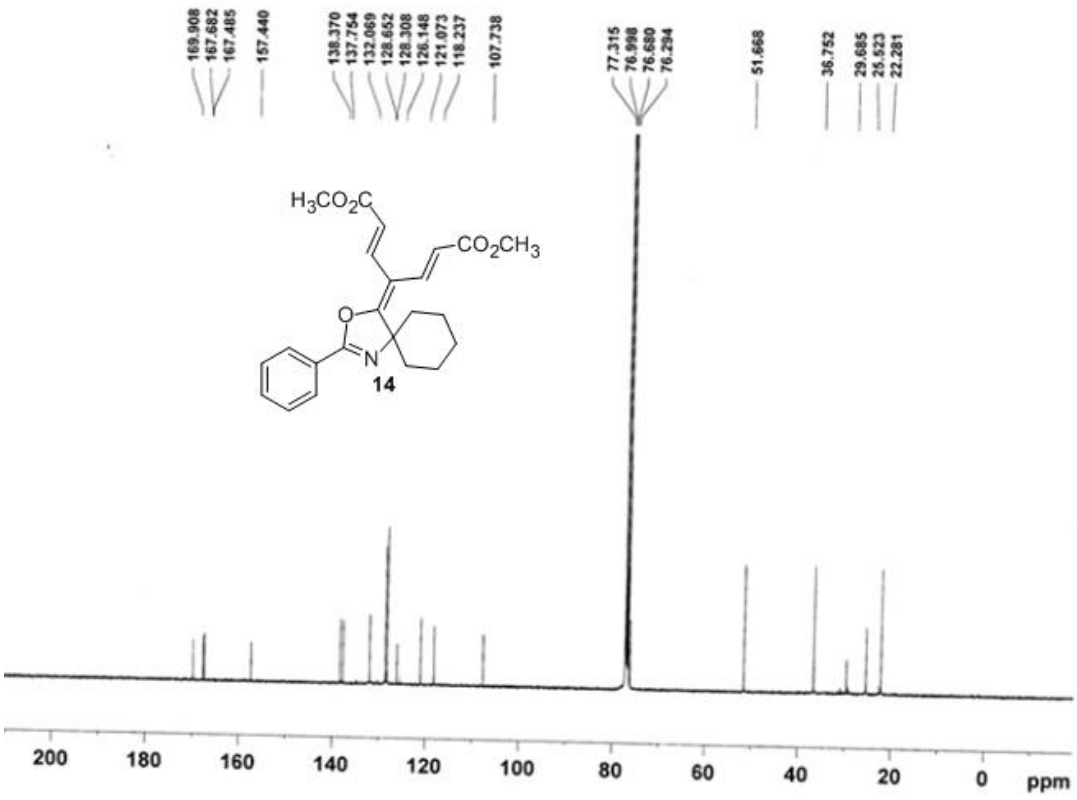


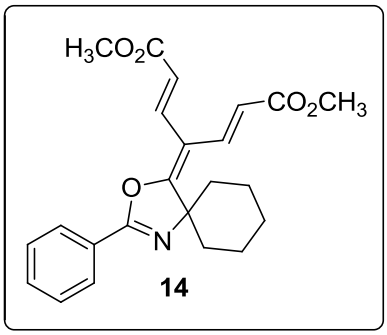
Chemical Formula: $C_{28}H_{26}NO_2$
Exact Mass: 408.1964
Molecular Weight: 408.5115
m/z: 408.1964 (100.0%), 409.1997 (30.3%), 410.2031 (4.4%)
Elemental Analysis: C, 82.32; H, 6.42; N, 3.43; O, 7.83



HRMS (ESI, m/z) calcd for $C_{29}H_{29}NO_3$ $[M+H]^+$ **440.2220,** found 440.**2227.**

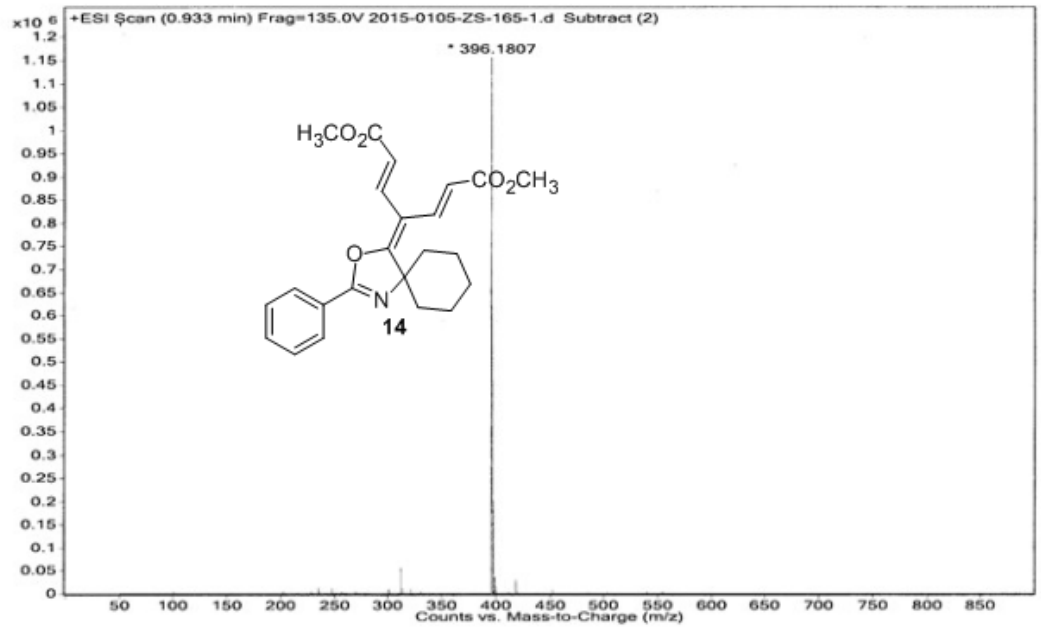

8.0373
8.0191
7.9187
7.8793
7.7164
7.6758
7.5481
7.5298
7.4964
7.4771
7.4592
7.2593
6.3613
6.3209
6.1455
6.1062
3.8167
3.8054
2.1248
2.1022
2.0927
2.0696
2.0594
2.0293
1.9967
1.9641
1.9233
1.9142
1.8778
1.7553
1.7297
H3CO2C
CO2CH3
O
N
14
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
2.156
1.113
1.076
3.336
0.987
1.027
6.000
6.476
4.449


169.908
167.682
167.485
157.440
138.370
137.754
132.069
128.652
128.308
126.148
121.073
118.237
107.738
77.315
76.998
76.680
76.294
51.668
36.752
29.685
25.523
22.281
H3CO2C
CO2CH3
O
N
14
200
180
160
140
120
100
80
60
40
20
0
ppm

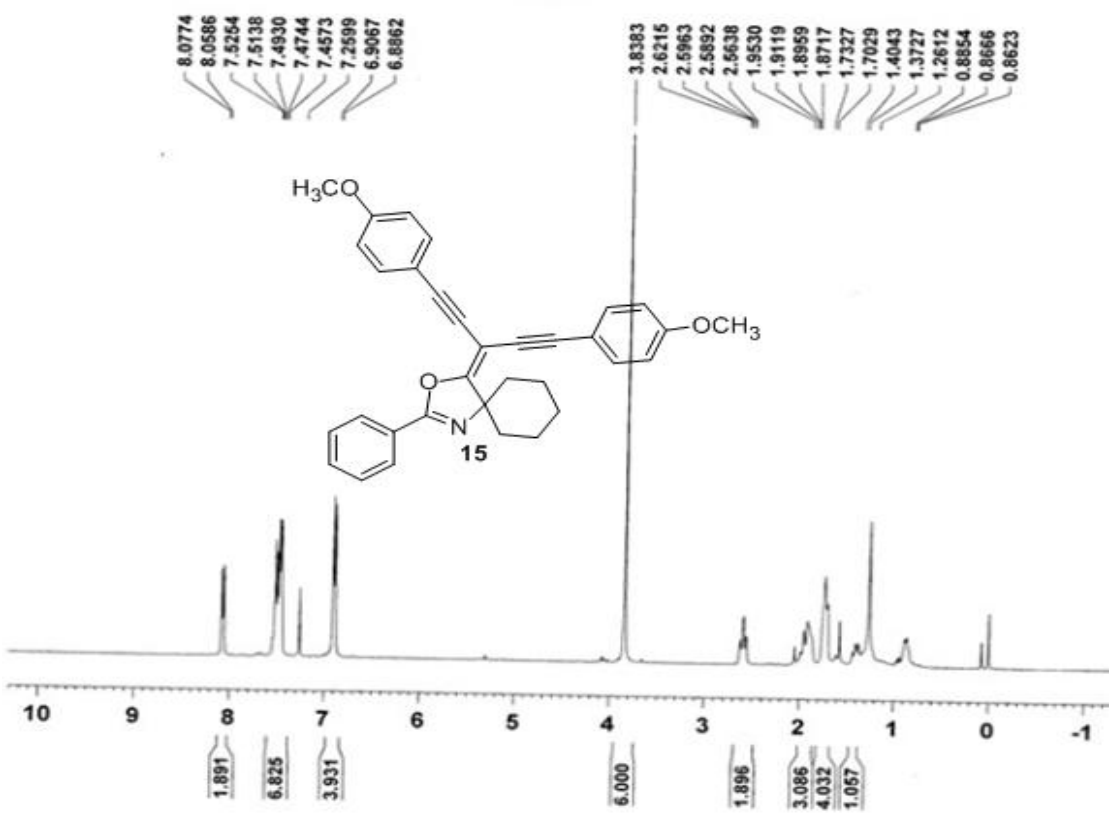


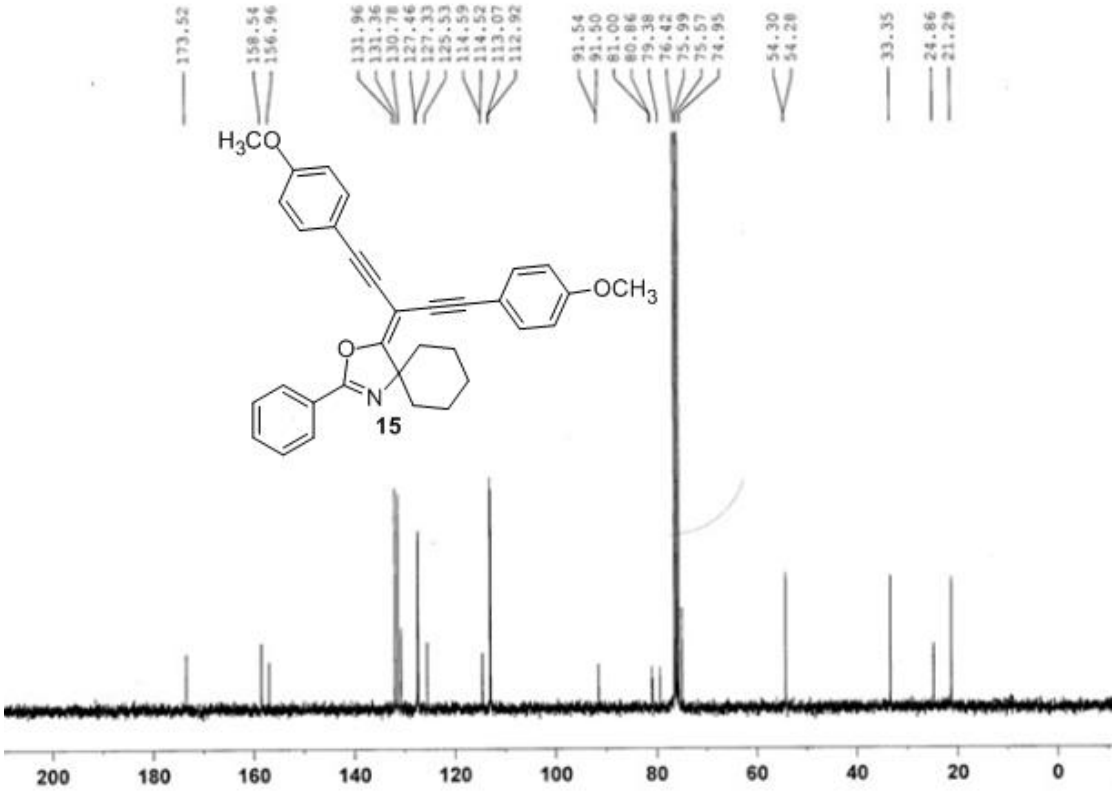
Chemical Formula: $C_{23}H_{25}NO_5$
Exact Mass: 395.1733
Molecular Weight: 395.4483
m/z: 395.1733 (100.0%), 396.1766 (24.9%), 397.1800 (3.0%), 397.1775 (1.0%)
Elemental Analysis: C, 69.86; H, 6.37; N, 3.54; O, 20.23

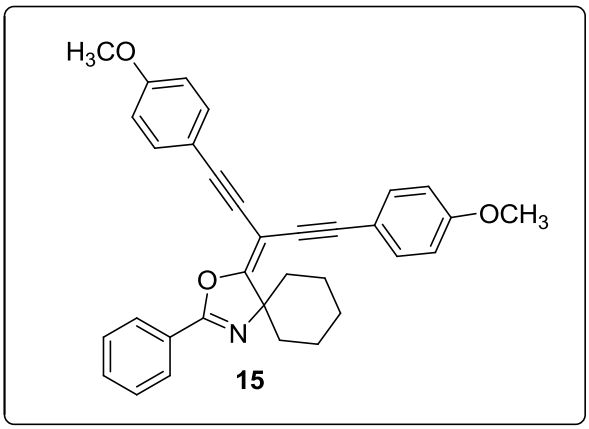
Sample Name	2015-0105-ZS-165-1	**Position**	P1-B9	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	2015-0105-ZS-165-1.d	**ACQ Method**	0103.m	**Comment**		**Acquired Time**	1/5/2015 10:41:01 AM



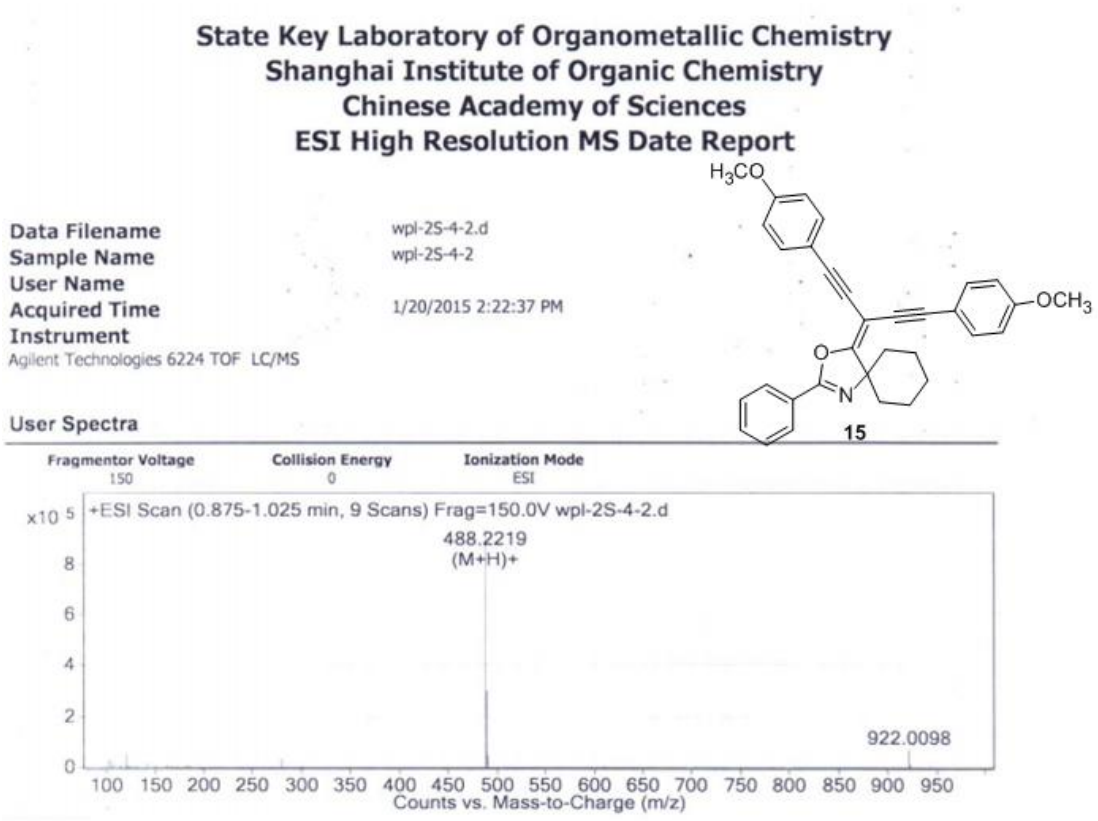
HRMS (ESI, m/z) calcd for $C_{23}H_{25}NO_5$ $[M+H]^+$ **396.1805**, found **396.1807.**


8.0774
8.0586
7.5264
7.5138
7.4930
7.4744
7.4573
7.2599
6.9067
6.8862
3.8383
2.6215
2.5963
2.5892
2.5638
1.9530
1.9119
1.8959
1.8717
1.7327
1.7029
1.4043
1.3727
1.2612
0.8854
0.8666
0.8623
H3CO
OCH3
O
N
15
10
9
8
7
6
5
4
3
2
1
0
-1
1.891
6.825
3.931
6.000
1.896
3.086
4.032
1.057


173.52
158.54
156.96
131.96
131.36
130.78
127.46
127.33
125.53
114.59
114.52
113.07
112.92
91.54
91.50
81.00
80.86
79.38
76.42
75.99
75.57
74.95
54.30
54.28
33.35
24.86
21.29
H3CO
OCH3
O
N
15
200
180
160
140
120
100
80
60
40
20
0



Chemical Formula: $C_{33}H_{29}NO_3$
Exact Mass: 487.2147
Molecular Weight: 487.5883
m/z: 487.2147 (100.0%), 488.2181 (35.7%), 489.2215 (6.2%)
Elemental Analysis: C, 81.29; H, 5.99; N, 2.87; O, 9.84



HRMS (ESI, m/z) calcd for $C_{33}H_{29}NO_3$ $[M+H]^+$ **488.2220**, found **488.2219.**