Electronic Supplementary Material (ESI) for Green Chemistry.

Supporting Information

Sunlight-promoted cyclization versus decarboxylation in reaction of alkynoates with *N*-iodosuccinimide: an easy access to 3-iodocoumarins

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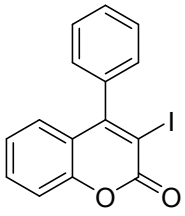
Table of Contends

1. General information

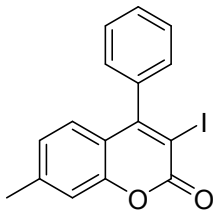
All manipulations were carried out under air atmosphere. Commercially available reagents were used as received without purification. Column chromatography was carried out on silica gel (300–400 mesh). Analytical thin–layer chromatography was performed on glass plates of Silica Gel GF–254 with detection by UV. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AVANCE 400M spectrometer with TMS as reference. High resolution mass spectra (HRMS) were measured with a LTQ-Orbitrap XL (Thermofisher, U. S. A.). Melting point determination was taken on a Melt–Temp apparatus (X-4) from Beijing Fukai Electro–optic Instrument Plant and was uncorrected.

2. General procedure for sunlight-promoted cyclization of alkynoates using NIS

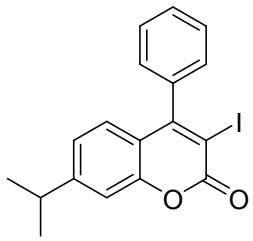
A sealable reaction tube equipped with a magnetic stirrer bar was charged with phenyl 3-phenylpropiolate **1a** (44.4 mg, 0.2 mmol), NIS **2** (*N*-iodosuccinimide, 0.3 mmol, 67.5 mg) and acetonitrile (2.5 mL). The rubber septum was then replaced by a Teflon–coated screw cap, and the reaction tube was exposed to sun light at room temperature for 6 h. After completion of the reaction, it was diluted with ethyl acetate, washed with water, dried over $MgSO_4$. After the solvent was removed under reduced pressure, the residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1 to 20:1) to afford the corresponding product **3a** in 98% yield (68.2 mg).



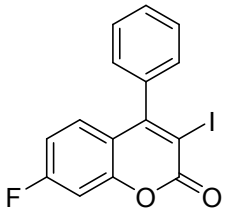
***3-iodo-4-phenyl-2H-chromen-2-one (3a)*:** White solid. mp 126−128 °C. Yield: 68.2 mg (98%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62−7.51 (m, 4H), 7.40 (d, *J* = 8.3 Hz, 1H), 7.25 (d, *J* = 7.3 Hz, 2H), 7.16 (t, *J* = 7.6 Hz, 1H), 7.05 (d, *J* = 8.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.8, 158.1, 153.2, 139.0, 132.4, 129.4, 129.0, 127.9, 127.8, 124.7, 120.1, 116.7, 92.4. HRMS (ESI-TOF) calcd for $C_{15}H_{10}IO_2$ $[M+H]^+$ 348.9725, found 348.9733. IR (cm^{-1}): 1745, 1704, 1591, 1545, 1445, 1273, 978, 752, 699.



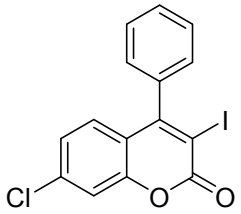
***3-iodo-7-methyl-4-phenyl-2H-chromen-2-one (3b)*:** White solid. mp 157−159 °C. Yield: 68.8 mg (95%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55−7.39 (m, 3H), 7.21−7.06 (m, 3H), 6.94−6.78 (m, 2H), 2.34 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.7, 158.2, 153.3, 143.8, 139.2, 129.3, 128.9, 127.8, 127.6, 125.8, 117.8, 116.8, 90.7, 21.8. HRMS (ESI-TOF) calcd for $C_{16}H_{11}IO_2Na$ $[M+Na]^+$ 384.9702, found 384.9705. IR (cm^{-1}): 1718, 1615, 1585, 1533, 1490, 1440, 1345, 1253, 1132, 960, 729, 697.



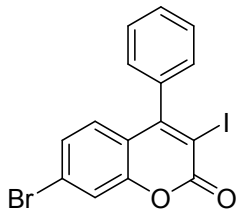
***3-iodo-7-isopropyl-4-phenyl-2H-chromen-2-one (3c)*:** White solid. mp 92−94 °C. Yield: 66.5 mg (85%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54−7.41 (m, 3H), 7.22−7.09 (m, 3H), 6.98−6.83 (m, 2H), 2.97−2.83 (m, 1H), 1.18 (d, *J* = 6.9 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.7, 157.3, 153.6, 152.4, 138.1, 128.2, 127.8, 126.8, 126.7, 122.3, 117.1, 113.2, 89.7, 76.4, 76.4, 76.1, 33.2, 22.5. HRMS (ESI-TOF) calcd for $C_{18}H_{15}IO_2Na$ $[M+Na]^+$ 413.0015, found 413.0020. IR (cm^{-1}): 1752, 1720, 1617, 1586, 1413, 995.



***7-fluoro-3-iodo-4-phenyl-2H-chromen-2-one (3d)*:** Light yellow solid. mp 187−189 °C. Yield: 59.0 mg (81%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55−7.45 (m, 3H), 7.21−7.12 (m, 2H), 7.05 (dd, *J* = 8.7, 2.5 Hz, 1H), 7.01−6.94 (m, 1H), 6.81 (td, *J* = 8.4, 2.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.9, 163.4, 160.2, 157.8, 154.3, 154.2, 138.9, 129.8, 129.7, 129.5, 129.1, 127.7, 117.0, 117.0, 112.9, 112.7, 104.4, 104.1, 90.7, 90.7. HRMS (ESI-TOF) calcd for $C_{15}H_8FIO_2Na$ $[M+Na]^+$ 388.9451, found 388.9434. IR (cm^{-1}): 1721, 1604, 1267, 1142, 1000, 857, 778, 758, 698, 533.

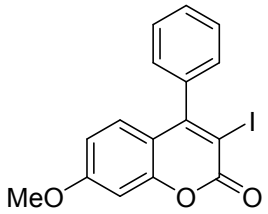


***7-chloro-3-iodo-4-phenyl-2H-chromen-2-one (3e)*:** Yellow solid. mp 168−170 °C. Yield: 57.4 mg (75%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61−7.52 (m, 3H), 7.41 (d, *J* = 2.0 Hz, 1H), 7.26−7.20 (m, 2H), 7.12 (dd, *J* = 8.6, 2.0 Hz, 1H), 6.99 (d, *J* = 8.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.1, 157.5, 153.3, 138.6, 138.3, 129.6, 129.1, 128.8, 127.7, 125.3, 118.7, 116.9, 92.2. HRMS (ESI-TOF) calcd for $C_{15}H_8{}^{35}ClIO_2Na$ $[M+Na]^+$ 404.9156, found 404.9161. IR (cm^{-1}): 1749, 1585, 1398, 986, 864, 758, 698.

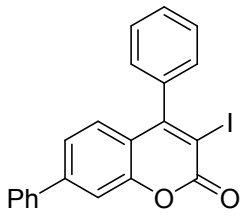


***7-bromo-3-iodo-4-phenyl-2H-chromen-2-one (3f)*:** Light yellow solid. mp 170−172 °C. Yield: 61.1 mg (72%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64−7.51 (m, 4H), 7.33−7.18 (m, 3H), 6.97−6.87 (m,

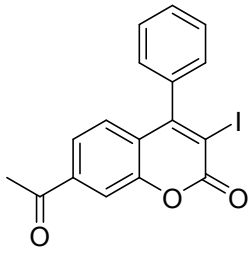
1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.2, 157.4, 153.3, 138.6, 129.6, 129.1, 128.9, 128.1, 127.8, 126.3, 119.9, 119.1, 92.4. HRMS (ESI-TOF) calcd for $C_{15}H_8{}^{80}BrIO_2Na$ $[M+Na]^+$ 448.8650, found 448.8645. IR (cm^{-1}): 1748, 1585, 1394, 983, 755, 695.



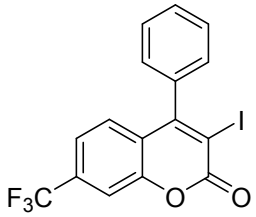
***3-iodo-7-methoxy-4-phenyl-2H-chromen-2-one (3g)*:** White solid. mp 161−163 °C. Yield: 49.9 mg (66%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59−7.50 (m, 3H), 7.25−7.19 (m, 2H), 6.94 (d, J = 8.9 Hz, 1H), 6.90−6.84 (m, 1H), 6.70 (dd, J = 8.9, 2.5 Hz, 1H), 3.87 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.2, 160.7, 158.4, 155.0, 139.2, 129.2, 129.0, 128.9, 127.8, 114.0, 112.8, 100.4, 87.6, 55.9. HRMS (ESI-TOF) calcd for $C_{16}H_{11}IO_3Na$ $[M+Na]^+$ 400.9651, found 400.9661. IR (cm^{-1}): 1717, 1619, 1585, 1534, 1292, 1155, 1134.



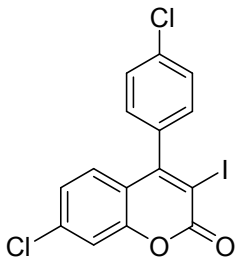
***3-iodo-4,7-diphenyl-2H-chromen-2-one (3h)*:** Light yellow solid. mp 122−124 °C. Yield: 62.0 mg (73%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66−7.53 (m, 6H), 7.52−7.35 (m, 4H), 7.30−7.23 (m, 2H), 7.10 (d, J = 8.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.5, 158.2, 153.6, 145.5, 139.0, 138.9, 129.4, 129.2, 129.0, 128.8, 128.3, 127.9, 127.2, 123.5, 119.0, 114.7, 91.8. HRMS (ESI-TOF) calcd for $C_{21}H_{13}IO_2Na$ $[M+Na]^+$ 446.9858, found 446.9856. IR (cm^{-1}): 1710, 1616, 1588, 1576, 1401, 984, 748.



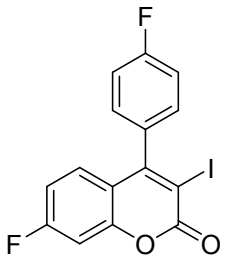
***7-acetyl-3-iodo-4-phenyl-2H-chromen-2-one (3i)*:** Yellow solid. mp 185−187 °C. Yield: 56.6 mg (73%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 1.7 Hz, 1H), 7.71 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.64−7.53 (m, 3H), 7.30−7.21 (m, 2H), 7.15 (d, *J* = 8.3 Hz, 1H), 2.64 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.3, 159.9, 157. 6, 153.0, 139.6, 138.6, 129.6, 129.2, 128.2, 127.7, 123.9, 123.1, 116.6, 95.5, 26.9. HRMS (ESI-TOF) calcd for $C_{17}H_{11}IO_3Na$ $[M+Na]^+$ 412.9651, found 412.9638. IR (cm^{-1}): 1735, 1585, 1409, 1276, 1211, 964, 707.



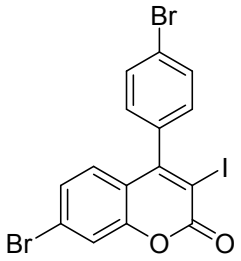
***3-iodo-4-phenyl-7-(trifluoromethyl)-2H-chromen-2-one (3j)*:** Light yellow solid. mp 149−152 °C. Yield: 66.6 mg (80%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67−7.54 (m, 4H), 7.39 (dd, *J* = 8.4, 1.7 Hz, 1H), 7.30−7.23 (m, 2H), 7.20 (d, *J* = 8.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.7, 157.2, 152.8, 138.4, 134.3 (q, *J* = 34.3 Hz), 129.7, 129.2, 128.8, 127.7, 127.1 (q, *J* = 273.7 Hz), 122.4, 121.2, 114.2, 95.3. HRMS (ESI-TOF) calcd for $C_{16}H_8F_3IO_2Na$ $[M+Na]^+$ 438.9419, found 438.9409. IR (cm^{-1}): 1732, 1414, 1347, 1333, 1318, 1178, 1133, 986.



***7-chloro-4-(4-chlorophenyl)-3-iodo-2H-chromen-2-one (3k)*:** Yellow solid. mp 173−175 °C. Yield: 61.5 mg (74%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60−7.54 (m, 2H), 7.40 (d, *J* = 2.0 Hz, 1H), 7.23−7.18 (m, 2H), 7.15 (dd, *J* = 8.6, 2.1 Hz, 1H), 6.98 (d, *J* = 8.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.9, 157.2, 153.3, 138.5, 136.9, 135.8, 129.6, 129.3, 128.5, 125.4, 118.5, 117.0, 92.5. HRMS (ESI-TOF) calcd for $C_{15}H_7{}^{35}Cl_2IO_2Na$ $[M+Na]^+$ 438.8766, found 438.8756. IR (cm^{-1}): 1723, 1599, 1585, 1488, 1397, 1337, 1077, 988, 803, 803.

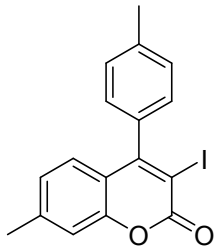


***7-fluoro-4-(4-fluorophenyl)-3-iodo-2H-chromen-2-one (3l)*:** Light yellow solid. mp 145−147 °C. Yield: 59.0 mg (77%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34−7.20 (m, 4H), 7.16−7.10 (m, 1H), 7.06 (dd, *J* = 8.9, 6.0 Hz, 1H), 6.97−6.87 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.0, 164.4 (d, *J* = 101.0 Hz), 161.9, 159.3 (d, *J* = 161.6 Hz), 154.1, 134.7, 129.9, 129.5 (d, *J* = 10.1 Hz), 116.9, 116.3 (d, *J* = 22.2 Hz), 112.8 (d, *J* = 22.2 Hz), 104.4 (d, *J* = 25.2 Hz), 91.4 (d, *J* = 4.0 Hz). HRMS (ESI-TOF) calcd for $C_{15}H_7F_2IO_2Na$ $[M+Na]^+$ 406.9357, found 406.9345. IR (cm^{-1}): 1721, 1600, 1505, 1343, 1271, 1231, 1158, 1105, 999, 841, 812, 536.

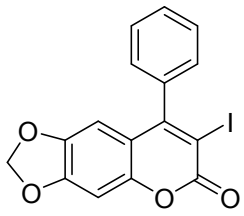


***7-bromo-4-(4-bromophenyl)-3-iodo-2H-chromen-2-one (3m)*:** Light yellow solid. mp 200−202 °C. Yield: 70.3 mg (70%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76−7.68 (m, 2H), 7.57 (d, *J* = 1.9 Hz, 1H), 7.29 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.16−7.08 (m, 2H), 6.90 (d, *J* = 8.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.0, 157.1, 153.3, 137.3, 132.5, 129.5, 128.5, 128.2, 126.5, 124.0, 120.0, 118.7, 92.7.

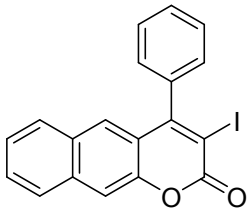
HRMS (ESI-TOF) calcd for $C_{15}H_7{}^{80}Br_2IO_2Na$ $[M+Na]^+$ 526.7755, found 526.7759. IR (cm^{-1}): 1752, 1483, 1392, 983, 800.



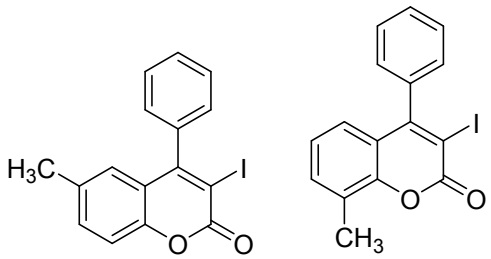
***3-iodo-7-methyl-4-(p-tolyl)-2H-chromen-2-one (3n)*:** Yellow solid. mp 157−159 °C. Yield: 68.4 mg (91%). ^1H NMR (400 MHz, $CDCl_3$) δ 7.27 (d, J = 7.8 Hz, 2H), 7.10 (s, 1H), 7.08−7.00 (m, 2H), 6.87 (d, J = 1.0 Hz, 2H), 2.39 (s, 3H), 2.33 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.9, 158.3, 153.2, 143.8, 139.3, 136.2, 129.5, 127.8, 127.7, 125.8, 117.9, 116.7, 90.7, 21.8, 21.5. HRMS (ESI-TOF) calcd for $C_{17}H_{13}IO_2Na$ $[M+Na]^+$ 398.9858, found 398.9848. IR (cm^{-1}): 1618, 1536, 1506, 1341, 1257, 1131, 1032, 987, 806, 732.



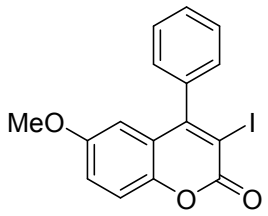
***7-iodo-8-phenyl-6H-[1,3]dioxolo[4,5-g]chromen-6-one (3o)*:** White solid. mp 236−238 °C. Yield: 67.5 mg (86%). ^1H NMR (400 MHz, $CDCl_3$) δ 7.56−7.41 (m, 3H), 7.17−7.07 (m, 2H), 6.79 (s, 1H), 6.30 (s, 1H), 5.96 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.6, 158.5, 151.6, 150.4, 145.1, 139.5, 129.3, 129.0, 127.7, 114.1, 105.3, 102.6, 97.9, 88.3. HRMS (ESI-TOF) calcd for $C_{16}H_9IO_4Na$ $[M+Na]^+$ 414.9444, found 414.9441. IR (cm^{-1}): 1706, 1542, 1478, 1441, 1265, 1206, 1030, 991, 931, 867, 580.



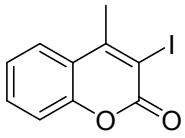
***3-iodo-4-phenyl-2H-benzo[g]chromen-2-one (3p)*:** Light yellow solid. mp 123−125 °C. Yield: 65.3 mg (82%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.72−8.58 (m, 1H), 7.92−7.78 (m, 1H), 7.73−7.47 (m, 6H), 7.36−7.21 (m, 2H), 7.03 (d, *J* = 8.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.5, 158.2, 150.6, 139.5, 134.9, 129.3, 129.2, 129.0, 127.8, 127.8, 127.5, 124.5, 123.3, 122.7, 122.6, 115.4, 91.4. HRMS (ESI-TOF) calcd for $C_{19}H_{11}IO_2Na$ $[M+Na]^+$ 420.9702, found 420.9708. IR (cm^{-1}): 1723, 1394, 1051, 756, 669.



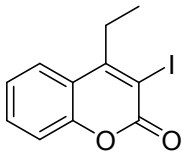
***3-iodo-6-methyl-4-phenyl-2H-chromen-2-one (3q1)*, *3-iodo-8-methyl-4-phenyl-2H-chromen-2-one (3q2)*:** Light yellow solid. mp 136−138 °C. Yield: 65.9 mg (91%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55−7.41 (m, 3H), 7.38−7.27 (m, 1H), 7.25−6.93 (m, 3H), 6.82−6.69 (m, 1H), 2.44 (s, 1H), 2.20 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.0, 159.7, 157.2, 157.0, 150.5, 150.3, 138.4, 138.1, 133.4, 132.6, 132.4, 128.2, 128.2, 127.9, 127.9, 127.8, 126.8, 126.7, 126.5, 125.1, 124.7, 123.1, 118.9, 118.7, 115.4, 91.3, 91.0, 19.8, 14.6. HRMS (ESI-TOF) calcd for $C_{16}H_{11}IO_2Na$ $[M+Na]^+$ 384.9699, found 384.9706. IR (cm^{-1}):1720, 1545, 1274, 1247, 990, 955, 813, 752, 698.



***3-iodo-6-methoxy-4-phenyl-2H-chromen-2-one (3r)*:** Light yellow solid. mp 150−152 °C. Yield: 68.1 mg (90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62−7.50 (m, 3H), 7.32 (d, *J* = 9.0 Hz, 1H), 7.27−7.21 (m, 2H), 7.13 (dd, *J* = 9.0, 2.9 Hz, 1H), 6.46 (d, *J* = 2.9 Hz, 1H), 3.66 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.4, 158.2, 156.1, 147.7, 139.1, 129.4, 129.0, 127.8, 120.5, 119.4, 117.6, 110.8, 93.1, 55.8. HRMS (ESI-TOF) calcd for $C_{16}H_{11}IO_3Na$ $[M+Na]^+$ 400.9651, found 400.9641. IR (cm^{-1}): 1723, 1709, 1549, 1478, 1423, 1266, 1228, 1140, 1034, 990, 731, 700.



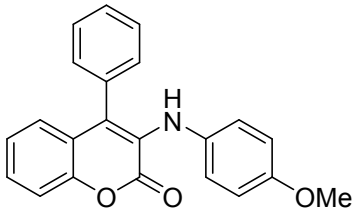
***3-iodo-4-methyl-2H-chromen-2-one (3t)*:** Light yellow solid. mp 100−102 °C. Yield: 47.5 mg (83%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.63−7.54 (m, 1H), 7.39−7.24 (m, 2H), 2.72 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.7, 156.5, 152.5, 132.3, 125.2, 124.8, 119.2, 116.9, 93.1, 25.5. HRMS (ESI-TOF) calcd for $C_{10}H_7IO_2Na$ $[M+Na]^+$ 308.9389, found 308.9388. IR (cm^{-1}): 1724, 1597, 1547, 1444, 1178, 1074, 962, 747, 730.



***4-ethyl-3-iodo-2H-chromen-2-one (3u)*:** Yellow solid. mp 89−91 °C. Yield: 53.4 mg (89%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.0 Hz, 1H), 7.58 (t, *J* = 7.8 Hz, 1H), 7.39−7.26 (m, 2H), 3.10 (q, *J* = 7.5 Hz, 2H), 1.28 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.2, 157.8, 153.0, 132.2, 124.9, 124.8, 118.1, 117.1, 91.9, 31.7, 12.2. HRMS (ESI-TOF) calcd for $C_{11}H_9IO_2Na$ $[M+Na]^+$ 322.9545, found 322.9541. IR (cm^{-1}): 1594, 1544, 1443, 977, 753.

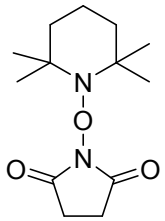
3. Pd-catalyzed Buchwald-Hartwig amination of compound 3a with *p*-anisidine

A mixture of compound **3a** (0.15 mmol), *p*-anisidine (1.2 equiv), $Pd_2(dba)_3$ (2.5 mol %), Xantphos (5 mol %), and K_2CO_3 (2.0 equiv) in toluene (1.0 mL) was stirred at 80 °C for 16 h. After completion of the reaction as indicated by TLC, the mixture was cooled to room temperature and purified directly by flash column chromatography on silica gel to afford the corresponding product **4a** in 72% yield.



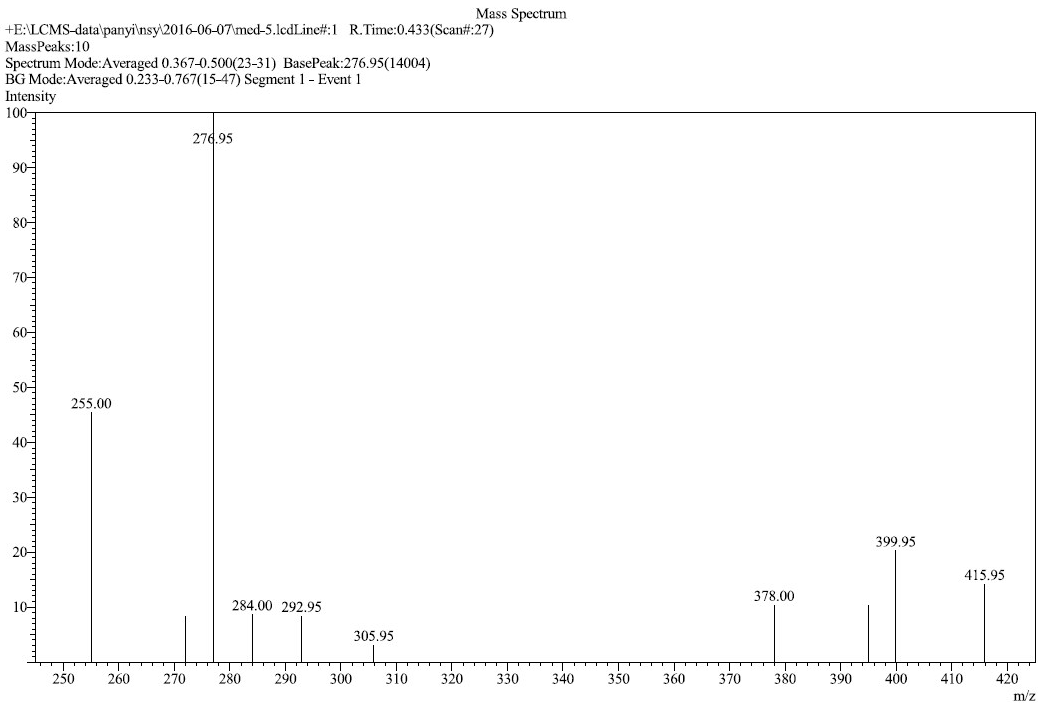
***3-((4-methoxyphenyl)amino)-4-phenyl-2H-chromen-2-one (4a)*:** Yellow oil. Yield: 71.0 mg (72%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43−7.30 (m, 2H), 7.29−7.08 (m, 7H), 6.65−6.57 (m, 2H), 6.55−6.47 (m, 2H), 6.20 (s, 1H), 3.68 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.4, 155.6, 149.3, 134.2, 133.3, 129.6, 128.5, 128.1, 127.9, 127.7, 127.3, 125.0, 124.4, 123.3, 121.8, 116.4, 113.6, 55.5. HRMS (ESI-TOF) calcd for $C_{22}H_{17}NO_3Na$ $[M+Na]^+$ 366.1106, found 366. 1106. IR (cm^{-1}): 1734, 1709, 1701, 1510, 1240, 1124, 1112, 756.

4. Mass spectrum of TEMPO-trapped adduct

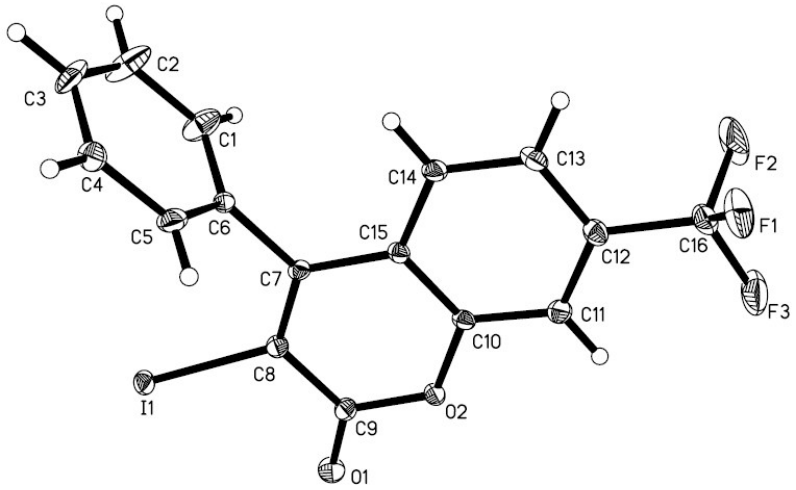


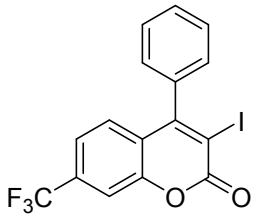
ESI-MS ([M+H]$^+$) m/z calcd for $[C_{13}H_{23}N_2O_3]^+$ 255.1, found 255.0.

ESI-MS ([M+Na]$^+$) m/z calcd for $[C_{13}H_{22}N_2O_3Na]^+$ 277.1, found 276.9.



5. X-ray analysis of 3j





CCDC 1451801

Bond distance:
C1 C2 1.379(6)
C1 C6 1.382(5)
C1 H1 0.9300
C2 C3 1.374(6)
C2 H2 0.9300
C3 C4 1.363(6)
C3 H3 0.9300
C4 C5 1.375(5)
C4 H4 0.9300
C5 C6 1.378(5)
C5 H5 0.9300
C6 C7 1.498(4)

C7 C8 1.347(5)
C7 C15 1.452(5)
C8 C9 1.469(5)
C8 I1 2.072(4)
C9 O1 1.198(4)
C9 O2 1.369(4)
C10 C11 1.375(6)
C10 O2 1.378(4)
C10 C15 1.401(5)
C11 C12 1.380(5)
C11 H11 0.9300
C12 C13 1.391(5)
C12 C16 1.504(5)
C13 C14 1.375(5)
C13 H13 0.9300
C14 C15 1.405(5)
C14 H14 0.9300
C16 F2 1.307(5)
C16 F3 1.328(5)
C16 F1 1.333(5)

Bond angle
C2 C1 C6 119.4(4)
C2 C1 H1 120.3
C6 C1 H1 120.3
C3 C2 C1 120.5(4)
C3 C2 H2 119.7
C1 C2 H2 119.7
C4 C3 C2 119.9(4)
C4 C3 H3 120.0
C2 C3 H3 120.0
C3 C4 C5 120.4(4)
C3 C4 H4 119.8
C5 C4 H4 119.8
C4 C5 C6 120.0(3)
C4 C5 H5 120.0
C6 C5 H5 120.0
C5 C6 C1 119.8(3)
C5 C6 C7 119.1(3)
C1 C6 C7 121.1(3)
C8 C7 C15 118.4(3)
C8 C7 C6 122.0(3)

C15 C7 C6 119.5(3)
C7 C8 C9 122.8(4)
C7 C8 I1 122.8(3)
C9 C8 I1 114.3(2)
O1 C9 O2 117.1(3)
O1 C9 C8 126.6(3)
O2 C9 C8 116.2(3)
C11 C10 O2 116.8(3)
C11 C10 C15 122.4(3)
O2 C10 C15 120.8(3)
C10 C11 C12 118.3(3)
C10 C11 H11 120.9
C12 C11 H11 120.9
C11 C12 C13 121.5(3)
C11 C12 C16 120.2(3)
C13 C12 C16 118.2(3)
C14 C13 C12 119.4(3)
C14 C13 H13 120.3
C12 C13 H13 120.3
C13 C14 C15 120.9(3)
C13 C14 H14 119.5
C15 C14 H14 119.5
C10 C15 C14 117.5(3)
C10 C15 C7 118.8(3)
C14 C15 C7 123.7(3)
F2 C16 F3 107.9(4)
F2 C16 F1 106.5(3)
F3 C16 F1 104.7(3)
F2 C16 C12 112.3(3)
F3 C16 C12 113.4(3)
F1 C16 C12 111.5(3)
C9 O2 C10 122.7(3)

6. Computational details

The structures of the reactants, transition states, intermediates and products in acetonitrile solution are optimized by using the UB3LYP method.[1] The DGDZVP basis set is employed for the iodine atom, and the 6-311G(d,p) basis set is used for all the other atoms. The self-consistent reaction field method (SCRF) with polarizable continuum model (PCM) is applied to take the effect of the solvent into consideration (the acetonitrile solvent is considered).[2] The nature of the minima and the transition states are checked by the vibrational frequencies analysis. Intrinsic reaction coordinate calculations are performed to confirm that each transition state connects with the desired reactants and products. All calculations are carried out using the Gaussian 09 program.[3]

Reference:

1) A. D. Becke, J. Chem. Phys. 1993, 98, 5648.
2) J. Tomasi, M. Persico, Chem. Rev. 1994, 94, 2027.
3) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

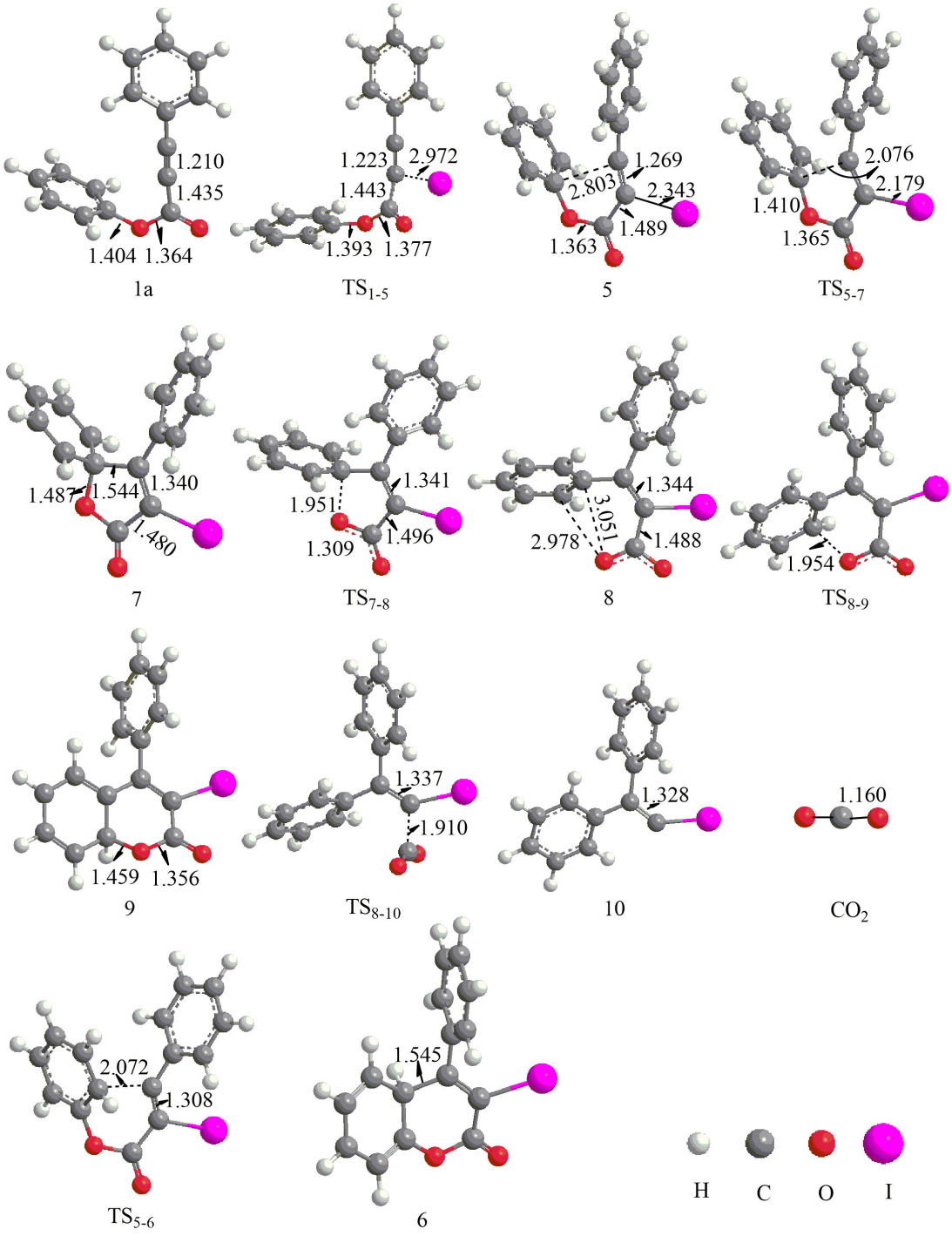


Figure S1 Optimized structures of reactants, intermediates, transition states and products for the title reaction calculated at 298.15 K and 1.0 atm in acetonitrile solvent. All bond lengths are in Å.

Table S1 Computed energies and cartesian coordinates of all species

1a

B3LYP free energy in acetonitrile solution: -728.037699 a.u.

Symbol	X	Y	Z
C	2.66103400	-1.90483800	1.20801700
C	2.69721200	-2.60135700	0.00012800
C	2.66193900	-1.90482000	-1.20777800
C	2.58507300	-0.51301600	-1.21397500
C	2.54132400	0.16166100	0.00009000
C	2.58416400	-0.51303400	1.21417900
C	0.14633800	1.50026800	-0.00045900
C	-0.93159500	0.95016300	-0.00024600
C	-2.18702100	0.28430700	-0.00011700
C	-2.24271800	-1.12201300	-0.00062800
C	-3.47280200	-1.76775200	-0.00052400
C	-4.65462800	-1.02535700	0.00009200
C	-4.60725200	0.36940900	0.00060100
C	-3.38295200	1.02616000	0.00048900
H	2.69416800	-2.44245000	2.14827500
H	2.75895800	-3.68314600	0.00014400
H	2.69577800	-2.44241900	-2.14801800
H	2.56351500	0.04593800	-2.14142600
H	2.56191900	0.04590300	2.14162300
H	-1.32169800	-1.69158400	-0.00110200
H	-3.51117800	-2.85053700	-0.00091700
H	-5.61189400	-1.53343600	0.00017500
H	-5.52543000	0.94458500	0.00108100
H	-3.33875900	2.10821900	0.00086700
C	1.36244000	2.26312700	-0.00012200
O	1.39857800	3.46935800	0.00000800
O	2.53533200	1.56582700	0.00009200

TS_{1-5}

B3LYP free energy in acetonitrile solution: -7647.879113 a.u.

Symbol	X	Y	Z
C	-4.24000000	2.16516800	0.52078800
C	-5.03513600	1.96821800	-0.60519700
C	-4.83247800	0.84006000	-1.40176300
C	-3.84058500	-0.08120000	-1.08110400
C	-3.05498000	0.13216400	0.04940700
C	-3.24525800	1.24731300	0.86137400
C	0.08698600	-0.08543600	0.76975300
C	0.96859000	0.72166500	0.50737400
C	2.00176700	1.61945000	0.18803900
C	2.00693300	2.28035300	-1.06046300
C	3.02704500	3.16807000	-1.36375500
C	4.04597300	3.40641800	-0.43731800
C	4.04773600	2.75818700	0.80078300
C	3.03396800	1.86868100	1.11967000
H	-4.38984900	3.03556700	1.14879500
H	-5.80688600	2.68446600	-0.85987500
H	-5.44597500	0.67534200	-2.27986700
H	-3.66516300	-0.95950100	-1.68966200
H	-2.64542400	1.40080100	1.74949000
H	1.21201500	2.08591600	-1.76904800
H	3.03367000	3.67549800	-2.32044100
H	4.84171900	4.10033400	-0.68103000
H	4.84093200	2.94979300	1.51274600
H	3.02289300	1.35991300	2.07511000
C	-1.14109000	-0.64321300	1.28531000
O	-1.31869000	-0.95973600	2.42769000
O	-2.08971200	-0.83915400	0.30586400
I	1.30740500	-2.54363000	-0.37117100

5

B3LYP free energy in acetonitrile solution: -7647.885447 a.u.

Symbol	X	Y	Z
C	3.50380900	-1.53488600	-1.03579000
C	4.04001800	-1.39260700	0.24406500
C	3.25756600	-1.67302600	1.36483800
C	1.93731000	-2.08920100	1.21320500
C	1.41443600	-2.20635700	-0.07158800
C	2.18459000	-1.94972300	-1.20192300
C	-0.90275200	-0.53491400	-0.09148700
C	0.08577000	0.26188300	-0.09283400
C	0.90260300	1.38846600	-0.07450800
C	1.42493900	1.88057900	1.14936400
C	2.23448500	3.00416700	1.15151600
C	2.54673900	3.65370300	-0.04686400
C	2.04252500	3.17322100	-1.25980400
C	1.23064900	2.05204400	-1.28537400
H	4.11281800	-1.32789400	-1.90763300
H	5.06761900	-1.07247400	0.36800500
H	3.67573700	-1.57463500	2.35952200
H	1.31878200	-2.32532500	2.07036100
H	1.75181800	-2.07780700	-2.18632200
H	1.18115000	1.37248600	2.07338100
H	2.62683600	3.37933800	2.08907900
H	3.18221100	4.53108800	-0.03587700
H	2.28604500	3.67907200	-2.18636200
H	0.83673900	1.67522800	-2.22062700
I	-3.01569800	0.45884400	0.11029300
C	-1.02585500	-2.01258900	-0.23000000
O	-2.06369000	-2.60280600	-0.34418800
O	0.13009900	-2.73498700	-0.23905800

$TS_{5\text{-}7}$

B3LYP free energy in acetonitrile solution: -7647.871680 a.u.

Symbol	X	Y	Z
C	-3.30961100	-1.43880900	1.21696200
C	-3.97413400	-1.21476700	0.00080700
C	-3.31008900	-1.43894300	-1.21558400
C	-1.98901000	-1.83743900	-1.23002700
C	-1.26823000	-1.91310400	0.00031300
C	-1.98852700	-1.83730300	1.23092800
C	0.97208300	-0.62943900	-0.00012900
C	-0.22659600	-0.11652500	0.00002800
C	-0.91205900	1.13901900	0.00003400
C	-1.26091300	1.76034400	-1.21540800
C	-1.92379700	2.98183800	-1.20824100
C	-2.25704600	3.59587600	0.00001700
C	-1.92362500	2.98194800	1.20828400
C	-1.26074100	1.76045300	1.21546900
H	-3.84534700	-1.32887400	2.15235700
H	-5.01355800	-0.91091600	0.00099300
H	-3.84619100	-1.32910900	-2.15078000
H	-1.46617400	-2.05207400	-2.15375100
H	-1.46532800	-2.05183600	2.15447000
H	-1.00106200	1.28434500	-2.15281600
H	-2.18078800	3.45649400	-2.14801800
H	-2.77474200	4.54790600	0.00001100
H	-2.18048200	3.45669100	2.14805300
H	-1.00075700	1.28454200	2.15288400
I	2.82705900	0.51521300	-0.00043000
C	1.11099600	-2.10515000	-0.00009000
O	2.11815400	-2.75571600	-0.00023100
O	-0.10964600	-2.71821100	0.00013300

7

B3LYP free energy in acetonitrile solution: -7647.892338 a.u.

Symbol	X	Y	Z
C	-3.61061400	-1.06669400	1.30076300
C	-4.33570600	-1.13535800	0.08639400
C	-3.64280200	-1.27682900	-1.13931000
C	-2.28092600	-1.32379500	-1.18344700
C	-1.44364900	-1.24010100	0.05867700
C	-2.24933300	-1.11828200	1.31817600
C	0.84618300	-0.77812600	0.00803700
C	-0.34213500	-0.15911900	-0.01166400
C	-0.65175900	1.28120900	-0.01550500
C	-1.51345500	1.84478600	-0.96802300
C	-1.78747200	3.20957700	-0.94853600
C	-1.22273300	4.02651900	0.02937000
C	-0.37486500	3.47311700	0.98784400
C	-0.08516300	2.11249900	0.96338700
H	-4.15059000	-0.98001200	2.23698100
H	-5.41738900	-1.09817900	0.09730800
H	-4.20671700	-1.35691600	-2.06189500
H	-1.74718100	-1.45076300	-2.11801500
H	-1.69190100	-1.07817900	2.24656900
H	-1.95548100	1.22141900	-1.73387300
H	-2.44459600	3.63341000	-1.69892100
H	-1.44327900	5.08754300	0.04571800
H	0.06217400	4.10003000	1.75627100
H	0.56688900	1.68728200	1.71605400
I	2.78915400	0.02943300	-0.11565200
C	0.67187200	-2.24592900	0.09627400
O	1.50194700	-3.11638600	0.13142600
O	-0.65966800	-2.50191800	0.13716700

$TS_{7\text{-}8}$

B3LYP free energy in acetonitrile solution: -7647.882934 a.u.

Symbol	X	Y	Z
C	3.81111600	-1.07519900	-1.18841500
C	4.53938000	-1.02899500	0.01200000
C	3.89143000	-0.74975200	1.22922800
C	2.53456300	-0.53294100	1.25967300
C	1.74888000	-0.65471200	0.05914900
C	2.45109300	-0.86802400	-1.18262300
C	-0.63610800	-0.86470100	0.04029400
C	0.38856600	0.00130100	0.02640000
C	0.35276200	1.48196300	0.01505600
C	-0.45363700	2.17935800	0.92744100
C	-0.46498600	3.57072100	0.94062500
C	0.32026000	4.28799600	0.03915400
C	1.13019500	3.60514400	-0.86683900
C	1.15747700	2.21372800	-0.87180200
H	4.32365900	-1.26766500	-2.12298100
H	5.60973400	-1.19466600	-0.00141200
H	4.46918300	-0.68876600	2.14345100
H	2.02817300	-0.29690900	2.18719900
H	1.87734400	-0.90372300	-2.10032800
H	-1.05468500	1.63114500	1.64124000
H	-1.08552700	4.09385700	1.65882100
H	0.30647600	5.37166300	0.04739200
H	1.74597400	4.15493500	-1.56894400
H	1.79585700	1.69789200	-1.57843200
I	-2.69904300	-0.42544800	-0.14703700
C	-0.25857700	-2.30675000	0.17549800
O	-1.04405200	-3.23843400	0.22035500
O	1.03887500	-2.46204600	0.25438700

8

B3LYP free energy in acetonitrile solution: -7647.887419 a.u.

Symbol	X	Y	Z
C	0.55799200	0.05258100	-0.05776400
C	-0.38208900	-0.90884200	-0.08437700
C	2.01158100	-0.28685800	-0.03746800
C	2.54468400	-1.13950100	0.93810500
C	2.87296400	0.30905000	-0.96990500
C	3.91217800	-1.39642600	0.97407700
H	1.89129900	-1.58507000	1.67727000
C	4.23577300	0.02976500	-0.94579100
H	2.47229200	0.98134700	-1.71930100
C	4.75928500	-0.82034200	0.02858900
H	4.31514300	-2.04736600	1.74123700
H	4.88968300	0.48260300	-1.68195500
H	5.82308600	-1.02636700	0.05482200
C	0.22959800	1.50367200	-0.02108100
C	0.76095900	2.31029600	0.99564100
C	-0.57191000	2.09131100	-1.01070400
C	0.46310900	3.66815500	1.04232200
H	1.39582200	1.86852600	1.75442400
C	-0.84713000	3.45632000	-0.97348000
H	-0.95443100	1.48628300	-1.82347900
C	-0.33951500	4.24482500	0.05696100
H	0.86345300	4.27829000	1.84349400
H	-1.45522300	3.90166800	-1.75208200
H	-0.56014600	5.30543400	0.08871100
I	-2.49929100	-0.56743200	0.15047600
C	-0.29532300	-2.38029400	-0.28960700
O	-1.44261400	-2.97779500	-0.25927900
O	0.73118000	-3.01891900	-0.49465700

TS_{8-9}

B3LYP free energy in acetonitrile solution: -7647.880698 a.u.

Symbol	X	Y	Z
C	-4.71097800	-0.06126600	0.00009900
C	-4.07814500	0.96831000	0.73175200
C	-2.69354000	1.12027000	0.69758300
C	-1.91240200	0.24038200	-0.04855500
C	-2.54821900	-0.80141100	-0.80695900
C	-3.96919600	-0.92259400	-0.77154200
C	0.18677500	-0.94934600	0.02991700
C	-0.44216700	0.25288400	-0.01370000
C	0.22767400	1.58099600	0.00025800
C	-0.01050800	2.48862900	-1.04097800
C	0.59804700	3.74081600	-1.03600700
C	1.42586300	4.11209300	0.02280900
C	1.64653800	3.22433700	1.07523300
C	1.05714300	1.96316400	1.06242300
H	-5.79066600	-0.14658300	0.02641500
H	-4.67572500	1.64127800	1.33443100
H	-2.21964900	1.90121500	1.27869100
H	-4.44606400	-1.68456600	-1.37483100
H	-0.66155100	2.20730500	-1.86065100
H	0.42045100	4.42761100	-1.85538000
H	1.89164100	5.09074600	0.03088700
H	2.27794900	3.51278700	1.90756500
H	1.22815400	1.27807700	1.88366200
I	2.30296100	-1.15261200	-0.16690000
C	-0.51321500	-2.25058100	0.34134000
O	0.10533100	-3.21436400	0.77115300
O	-1.80908300	-2.31105200	0.19071900
H	-2.03346700	-1.17618200	-1.68208300

9

B3LYP free energy in acetonitrile solution: -7647.896804 a.u.

Symbol	X	Y	Z
C	4.72294500	0.24260000	-0.04592300
C	4.01792400	1.47505700	-0.21644400
C	2.62709900	1.51228300	-0.17967000
C	1.88264500	0.36206200	0.07110700
C	2.58764900	-0.90503400	0.46422800
C	4.06120200	-0.90642000	0.22782100
C	-0.11817000	-0.96342400	0.00250700
C	0.45196900	0.28765700	0.02222400
C	-0.34229600	1.54935000	-0.02365200
C	-0.41437800	2.37472100	1.10426400
C	-1.14715900	3.55891800	1.06167900
C	-1.79647100	3.93857800	-0.11206500
C	-1.71500900	3.12745600	-1.24335300
C	-0.99636400	1.93533500	-1.19922300
H	5.80087200	0.23356900	-0.15789800
H	4.57218600	2.37973000	-0.43249600
H	2.11219300	2.44103000	-0.39094900
H	2.58814627	-1.36760105	1.46726117
H	4.57414100	-1.85343000	0.34390400
H	0.09520200	2.08486800	2.01604500
H	-1.20647900	4.18573500	1.94394600
H	-2.36062100	4.86348800	-0.14615600
H	-2.21161700	3.42134300	-2.16086900
H	-0.93595800	1.30506400	-2.07878200
I	-2.21628900	-1.27796100	0.14267400
C	0.66680700	-2.19118700	-0.25147900
O	0.19322400	-3.25991300	-0.56313600
O	2.01742200	-2.07099500	-0.20337900

$TS_{8\text{-}10}$

B3LYP free energy in acetonitrile solution: -7647.875757 a.u.

Symbol	X	Y	Z
C	0.48433700	0.15898900	-0.03218200
C	-0.44625400	-0.80189400	-0.01504500
C	1.94218300	-0.16809700	-0.07600500
C	2.52964400	-1.01915400	0.86919000
C	2.75055700	0.42720200	-1.05532400
C	3.89796100	-1.28144700	0.82432100
H	1.92188800	-1.45776300	1.65042800
C	4.11241900	0.15045200	-1.10499100
H	2.30762700	1.09809400	-1.78198100
C	4.69057400	-0.70413300	-0.16452400
H	4.34199800	-1.93408800	1.56701800
H	4.72462500	0.60525600	-1.87512600
H	5.75375100	-0.91155500	-0.20014600
C	0.13122300	1.60701400	0.06651600
C	0.65925700	2.37701000	1.11324700
C	-0.68306000	2.22172000	-0.89369000
C	0.36248700	3.73281500	1.20548400
H	1.29622500	1.90931500	1.85477100
C	-0.96062100	3.58333000	-0.80878600
H	-1.07973000	1.64024100	-1.71660500
C	-0.44680500	4.33955800	0.24411400
H	0.76594000	4.31678100	2.02444700
H	-1.57726000	4.05298800	-1.56623700
H	-0.67194900	5.39746400	0.31324800
I	-2.53694300	-0.74466900	-0.02855800
C	0.05607300	-2.64432300	0.03431100
O	0.40413200	-2.77280800	-1.10986400
O	-0.12975700	-3.11763200	1.11035900

10

B3LYP free energy in acetonitrile solution: -7459.267578 a.u.

Symbol	X	Y	Z
C	0.50743400	-0.14849600	-0.03331100
C	-0.43355900	-1.08526000	-0.06365400
C	1.94043400	-0.56983100	-0.05095100
C	2.33365400	-1.80707600	0.48409500
C	2.91937600	0.25363700	-0.62611700
C	3.66313000	-2.21257700	0.43390000
H	1.58989500	-2.44189500	0.95186100
C	4.25061200	-0.15445700	-0.67391600
H	2.63723500	1.21256300	-1.04341800
C	4.62812100	-1.38795400	-0.14600600
H	3.94886800	-3.16895900	0.85718600
H	4.99301800	0.49370800	-1.12578300
H	5.66516100	-1.70165500	-0.17934600
C	0.18102400	1.31331900	0.02498400
C	0.64545900	2.08964800	1.09563600
C	-0.58597000	1.92316900	-0.97411600
C	0.33792400	3.44559100	1.16844400
H	1.24358200	1.62823200	1.87309100
C	-0.88504800	3.28269700	-0.90386000
H	-0.93831100	1.33445100	-1.81282900
C	-0.42769300	4.04627900	0.16860700
H	0.69662500	4.03324800	2.00589600
H	-1.47346000	3.74403000	-1.68884600
H	-0.66308200	5.10291100	0.22447000
I	-2.49337600	-1.21073100	0.00972300

$TS_{5\text{-}6}$

B3LYP free energy in acetonitrile solution: -7647.862952 a.u.

Symbol	X	Y	Z
C	-3.26971500	0.05909500	0.68902200
C	-4.12050200	-0.30036500	-0.33837800
C	-3.90026600	-1.47698600	-1.07237400
C	-2.80694700	-2.29980400	-0.77521600
C	-1.96250600	-1.93907800	0.25183100
C	-2.11880500	-0.73226800	0.98835500
C	0.56645500	-0.79844700	0.25188400
C	-0.34905800	0.13239200	0.34264000
C	-0.41614200	1.56361700	0.21270700
C	-1.13394700	2.15641400	-0.84187300
C	-1.19781700	3.54098100	-0.94942900
C	-0.57312600	4.35148400	-0.00042700
C	0.12539700	3.77025800	1.05859800
C	0.20781500	2.38691700	1.16896400
H	-3.46494300	0.94383500	1.28161100
H	-4.98320800	0.31590700	-0.56241100
H	-4.57680200	-1.75377700	-1.87131600
H	-2.61231800	-3.20695700	-1.33334800
H	-1.71608900	-0.68974700	1.99523400
H	-1.62397000	1.52866400	-1.57570300
H	-1.73991400	3.98913600	-1.77396500
H	-0.63198700	5.43028700	-0.08471800
H	0.61069200	4.39580900	1.79876800
H	0.75230500	1.93554800	1.98929700
I	2.63907200	-0.30149000	-0.38138100
C	0.40594200	-2.24145200	0.57140400
O	1.29811400	-3.00085400	0.82961400
O	-0.87627200	-2.74243500	0.54582700

6

B3LYP free energy in acetonitrile solution: -7647.883615 a.u.

Symbol	X	Y	Z
C	4.50623500	-0.08069200	-0.73068200
C	3.97828000	1.18966000	-0.38851600
C	2.77350300	1.32527600	0.23287200
C	1.95522600	0.13470800	0.66480400
C	2.54139300	-1.14117600	0.15615200
C	3.74774900	-1.24152100	-0.46631700
C	-0.19943000	-0.96677100	0.16361200
C	0.45560400	0.19697900	0.29477300
C	-0.17699400	1.53619500	0.18293300
C	-0.45790900	2.27584900	1.33771400
C	-1.02923600	3.54238700	1.23482700
C	-1.30959700	4.08556100	-0.01797800
C	-1.01945300	3.35651400	-1.17029800
C	-0.45614400	2.08632800	-1.07331200
H	5.46445200	-0.16258900	-1.22614400
H	4.54622700	2.07989300	-0.63580700
H	2.39284600	2.30457700	0.49077300
H	1.95686900	0.10605900	1.77517700
H	4.09820400	-2.22058600	-0.77119900
H	-0.24222200	1.85802400	2.31443300
H	-1.25382600	4.10338400	2.13456000
H	-1.75068000	5.07248500	-0.09591500
H	-1.23248600	3.77463700	-2.14730200
H	-0.23176100	1.52083800	-1.96994400
I	-2.29801900	-1.08590900	-0.23102300
C	0.44684200	-2.28403900	0.38390300
O	-0.12774500	-3.32604600	0.55948600
O	1.81661800	-2.29584400	0.38409800

CO_2

B3LYP free energy in acetonitrile solution: -188.652742 a.u.

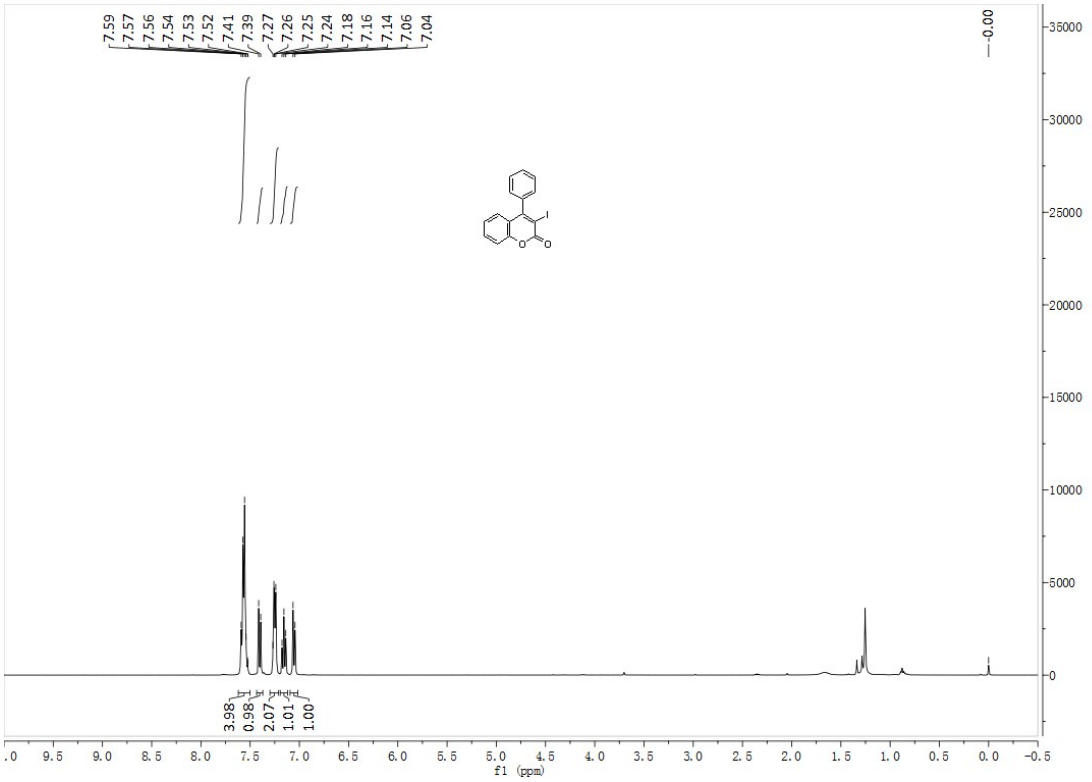
Symbol	X	Y	Z
C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16027800
O	0.00000000	0.00000000	-1.16027800

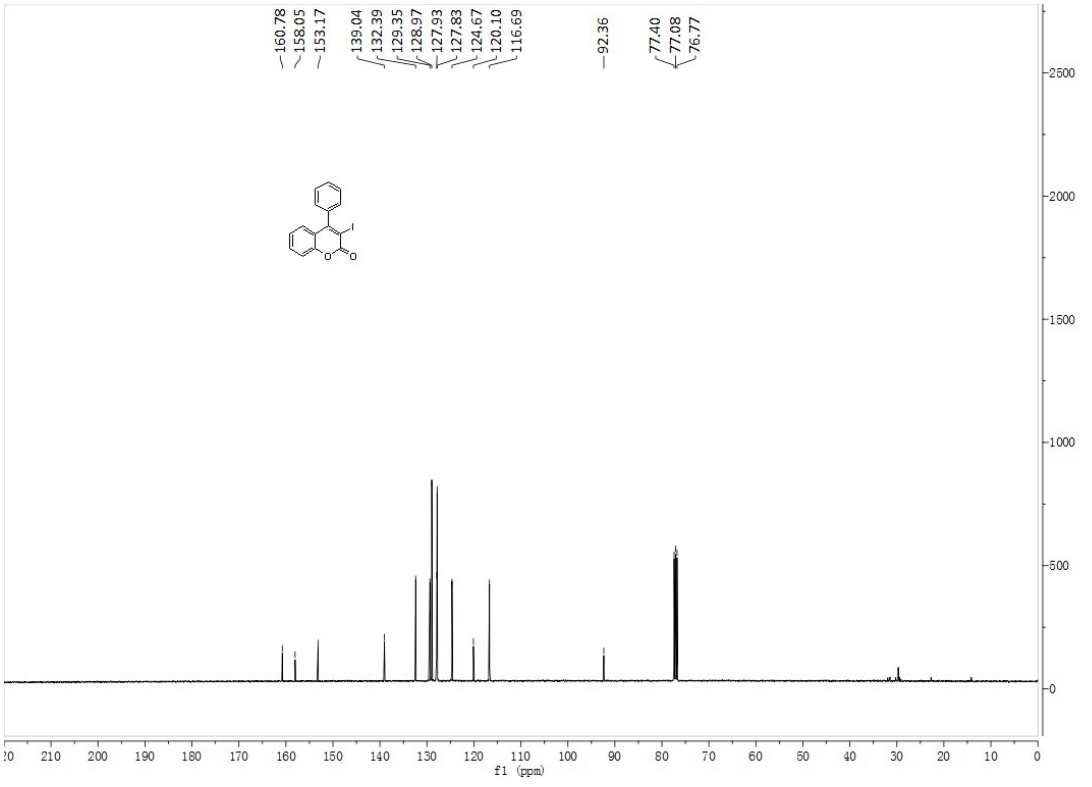
I radical

B3LYP free energy in acetonitrile solution: -6919.857070 a.u.

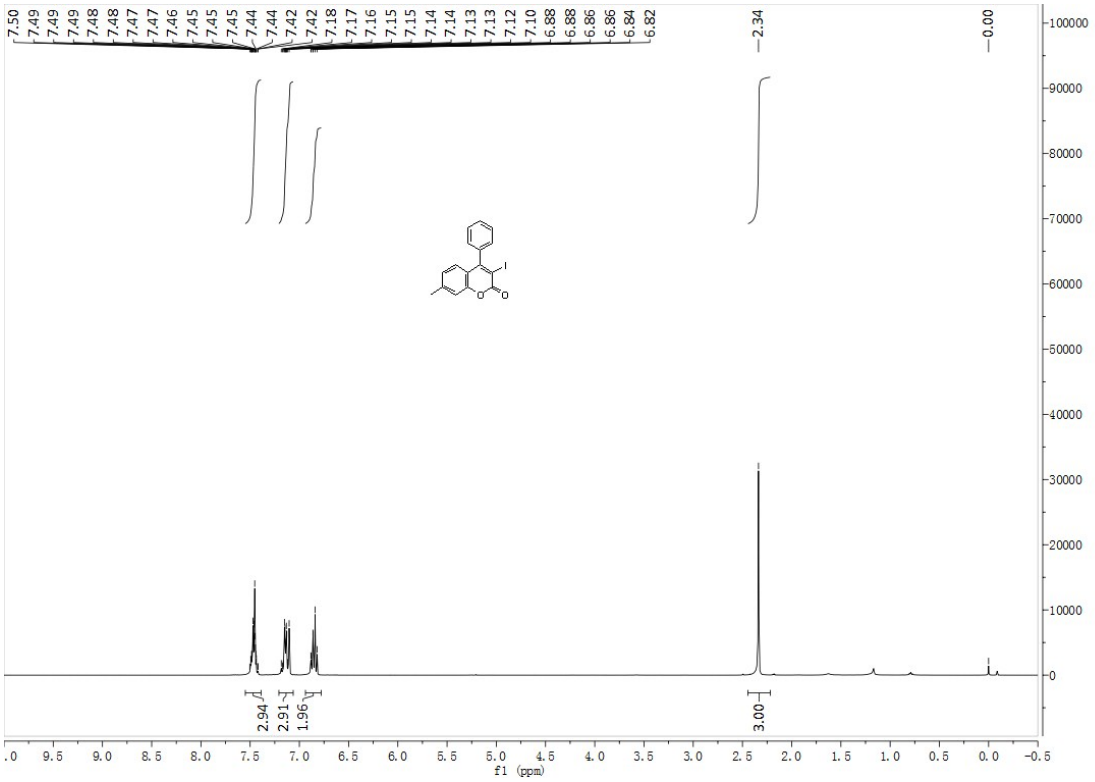
7. ^{1}H and ^{13}C NMR spectra of 3 and 4a

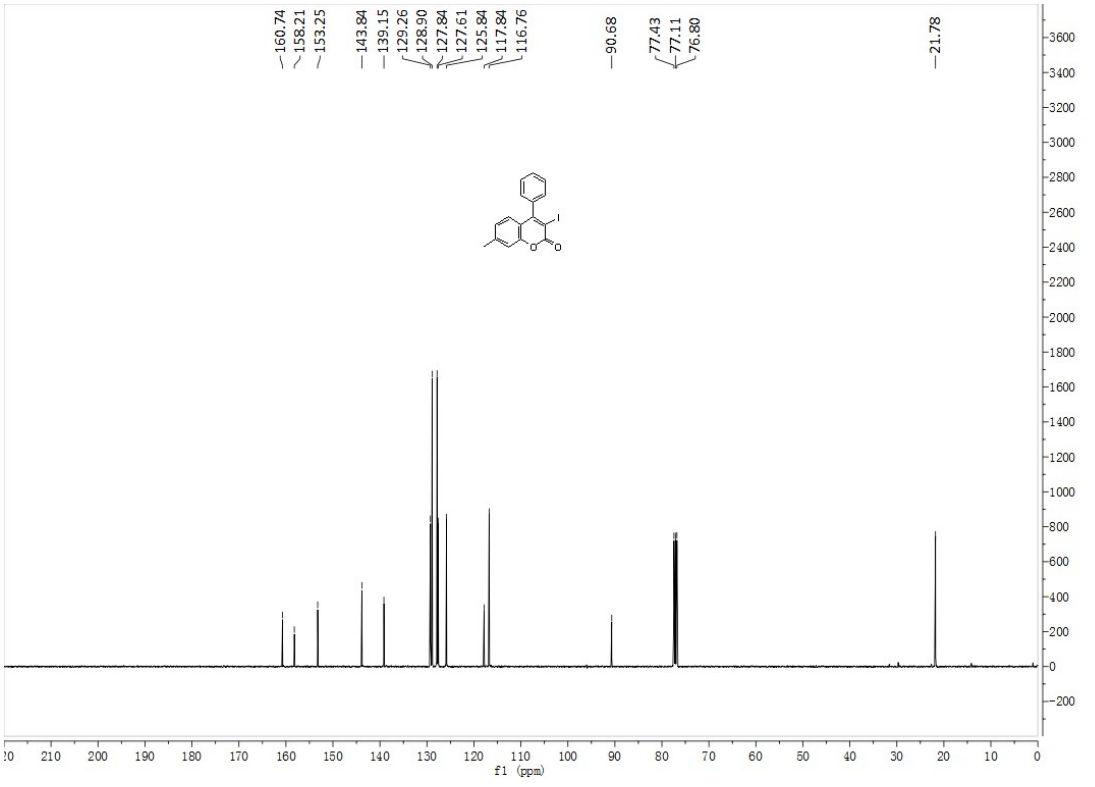
^{1}H and ^{13}C NMR spectra of **3a**



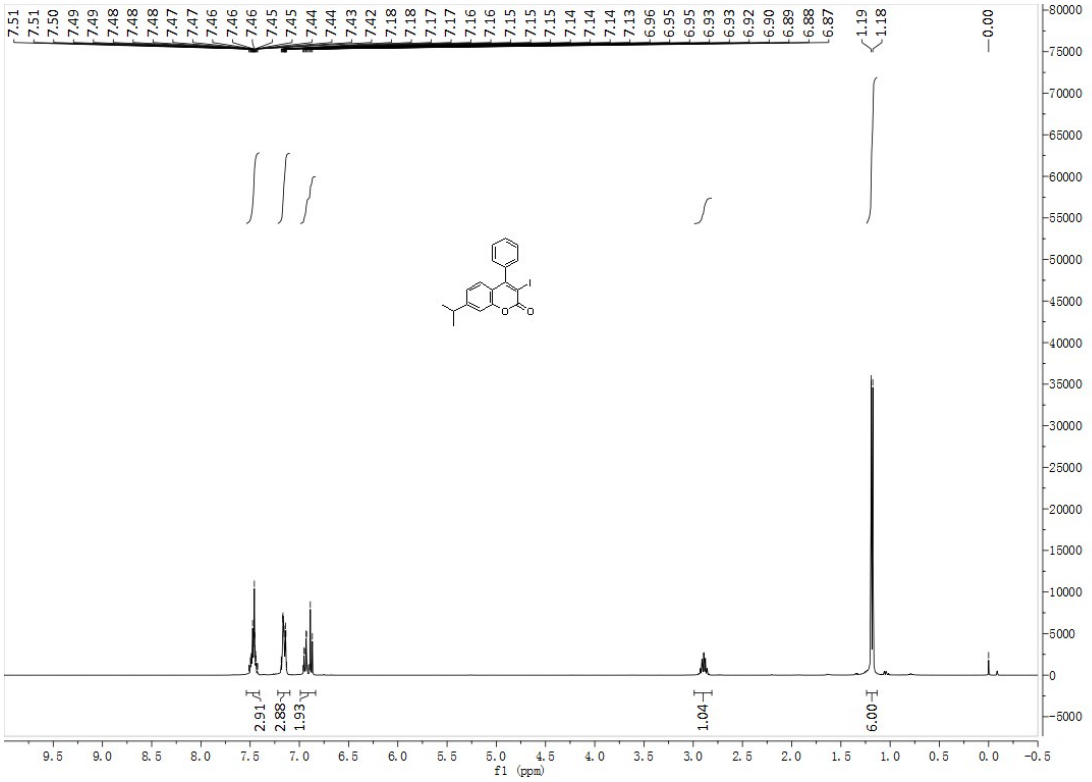


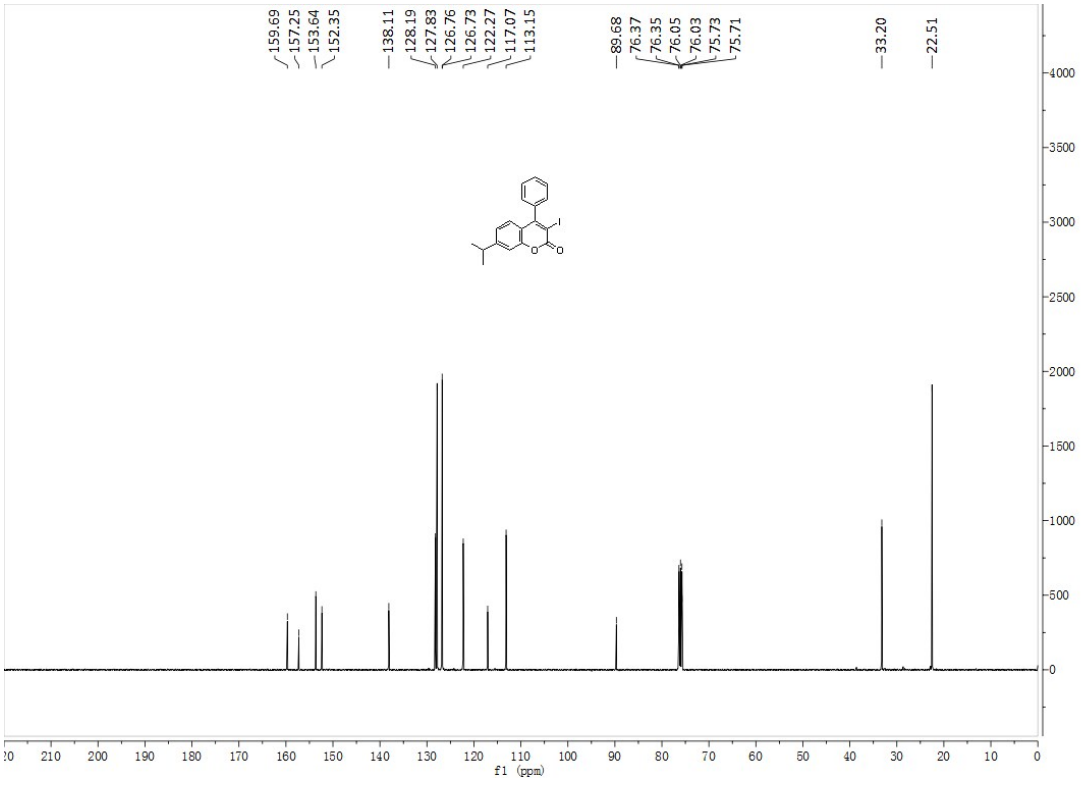
^{1}H and ^{13}C NMR spectra of **3b**



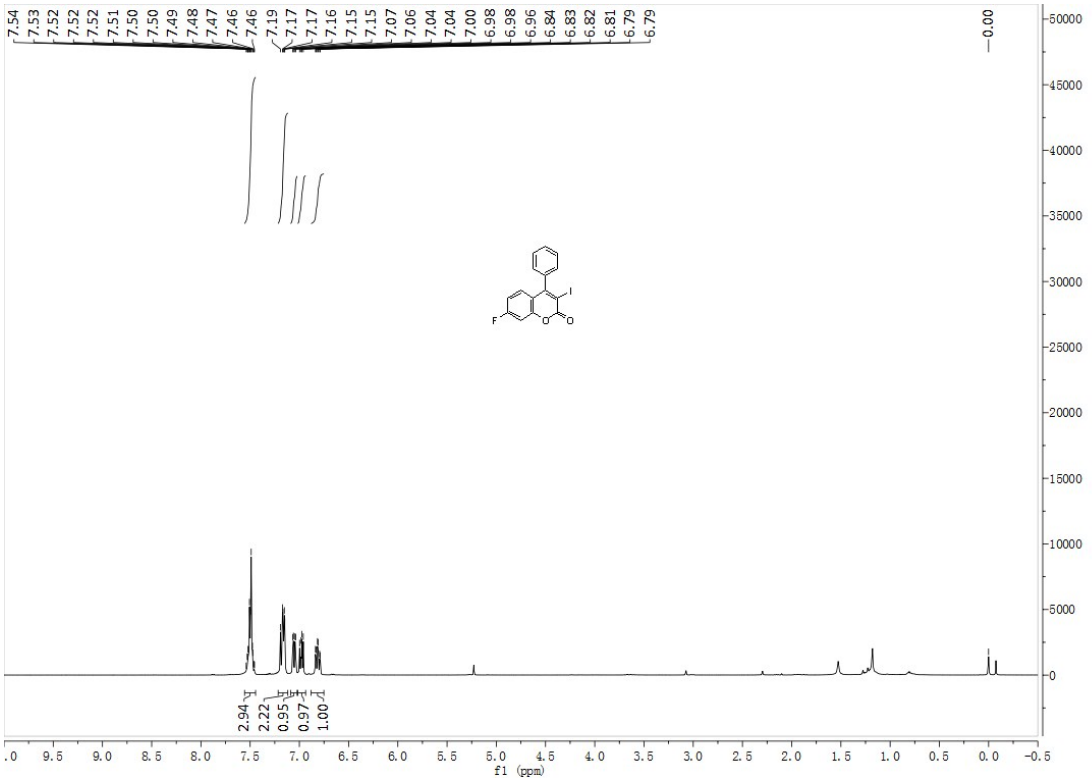


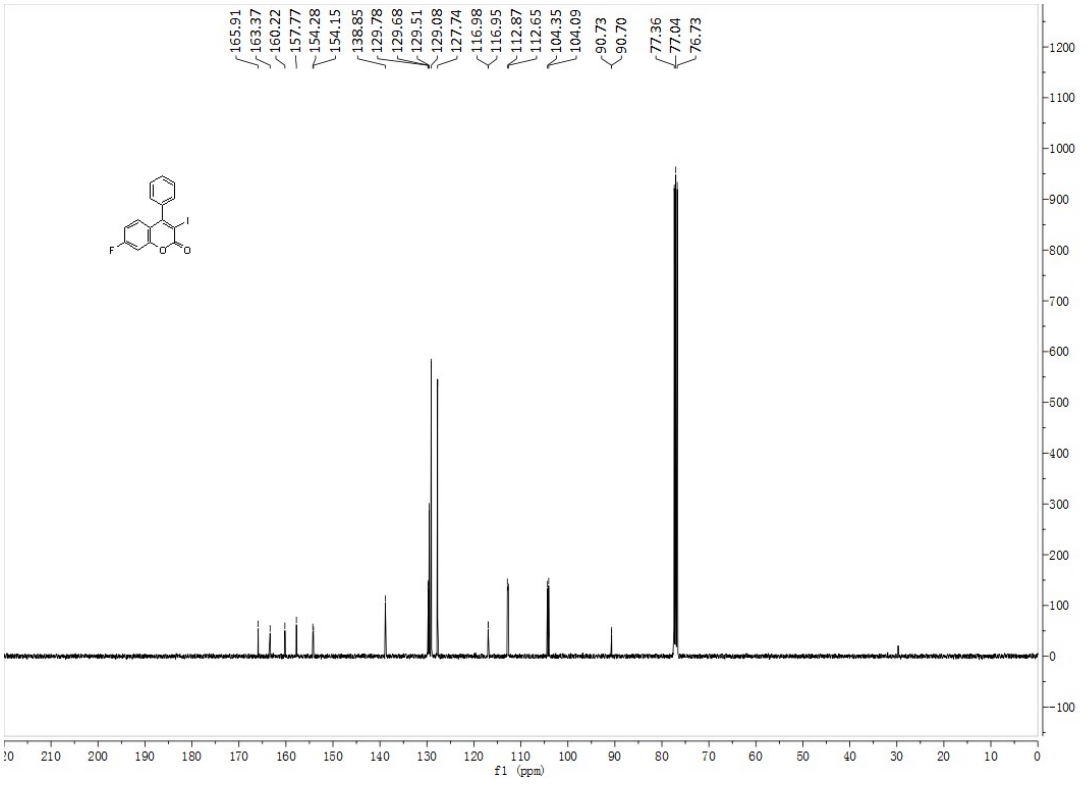
^{1}H and ^{13}C NMR spectra of **3c**



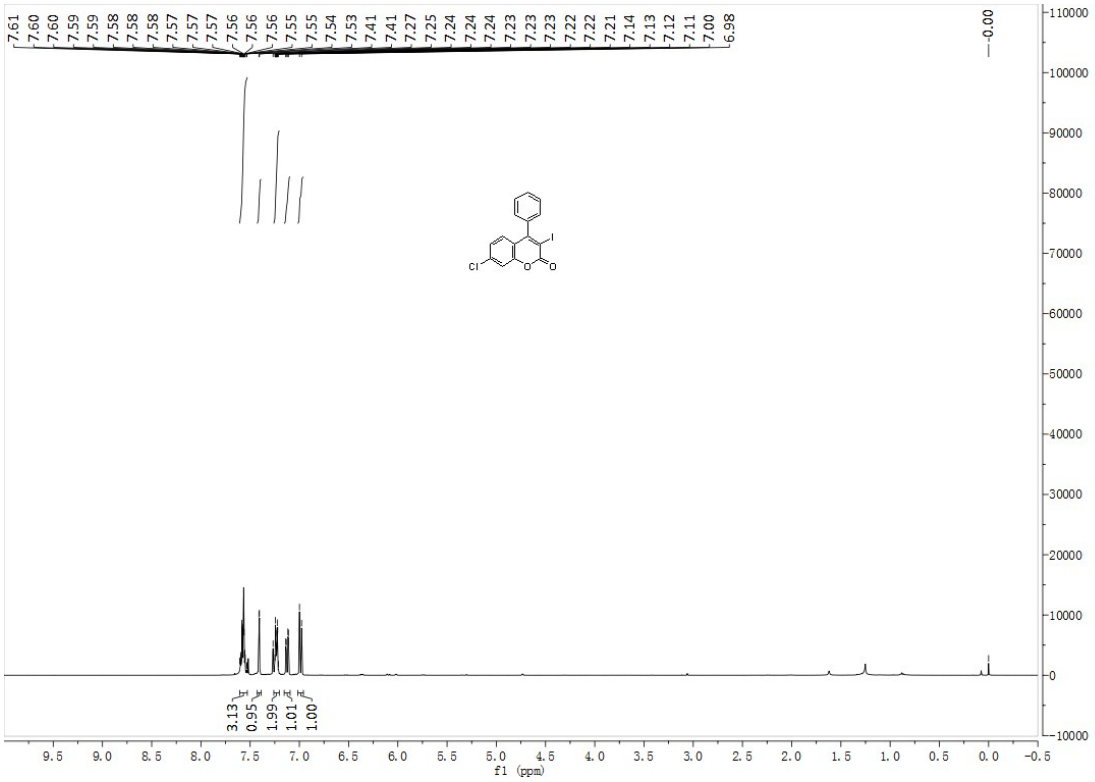


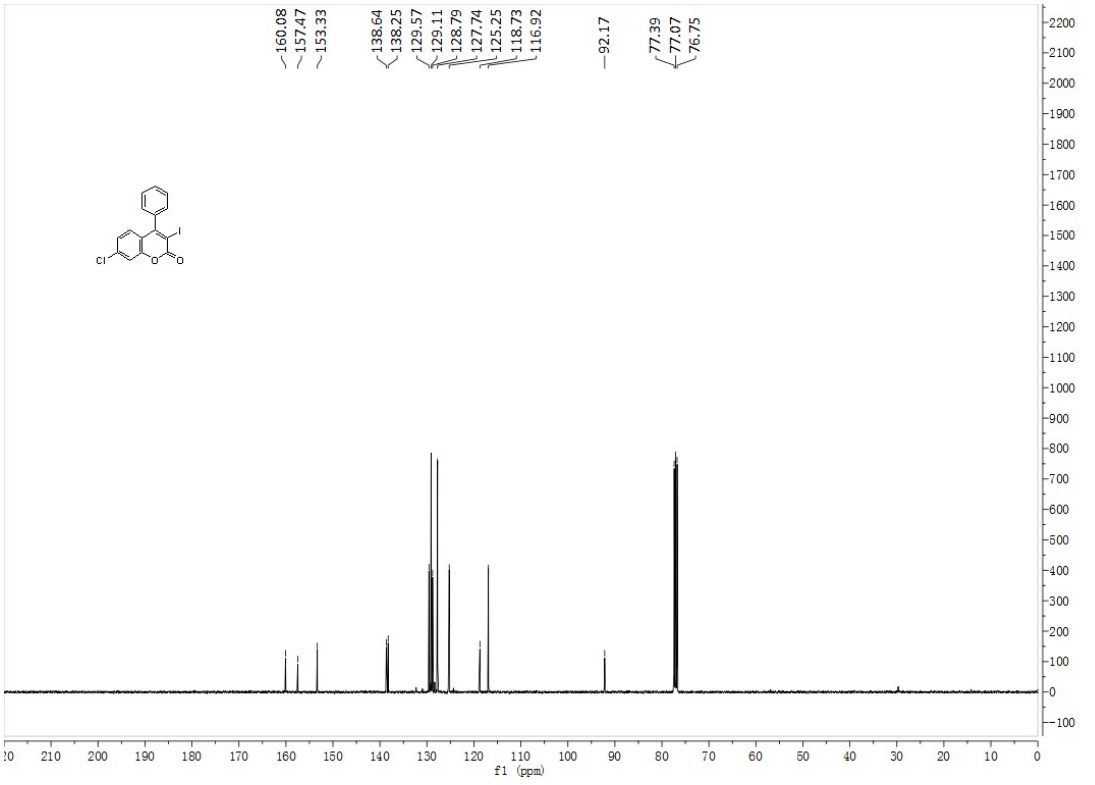
^{1}H and ^{13}C NMR spectra of **3d**



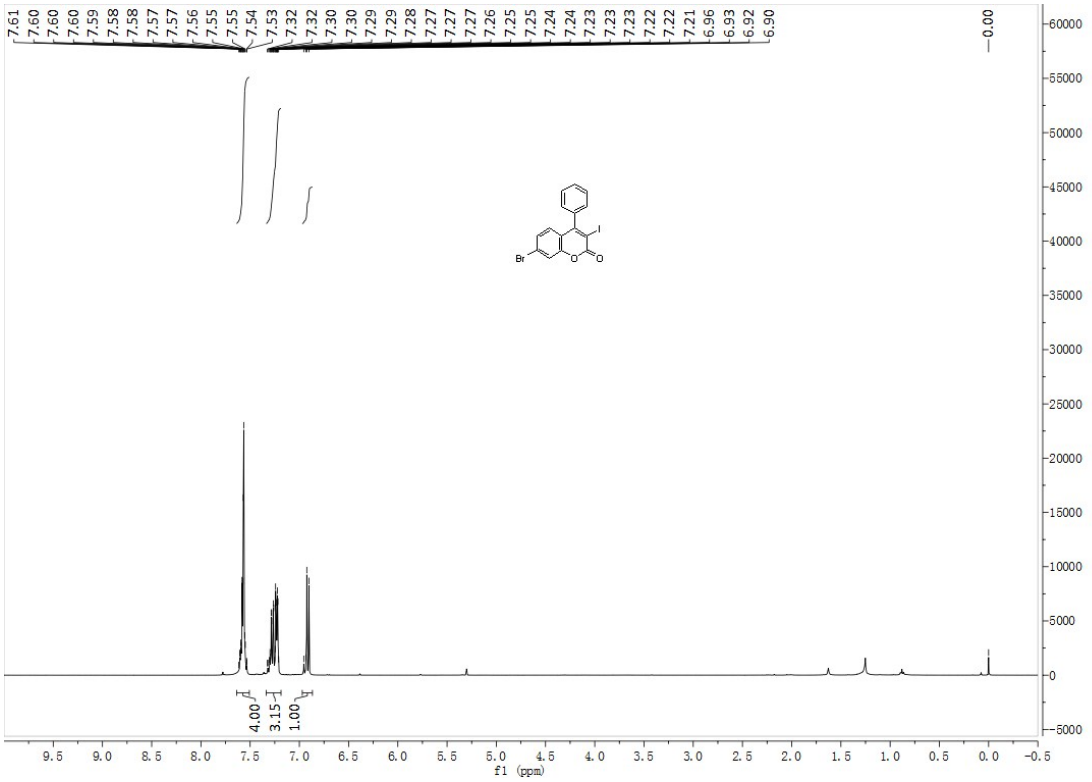


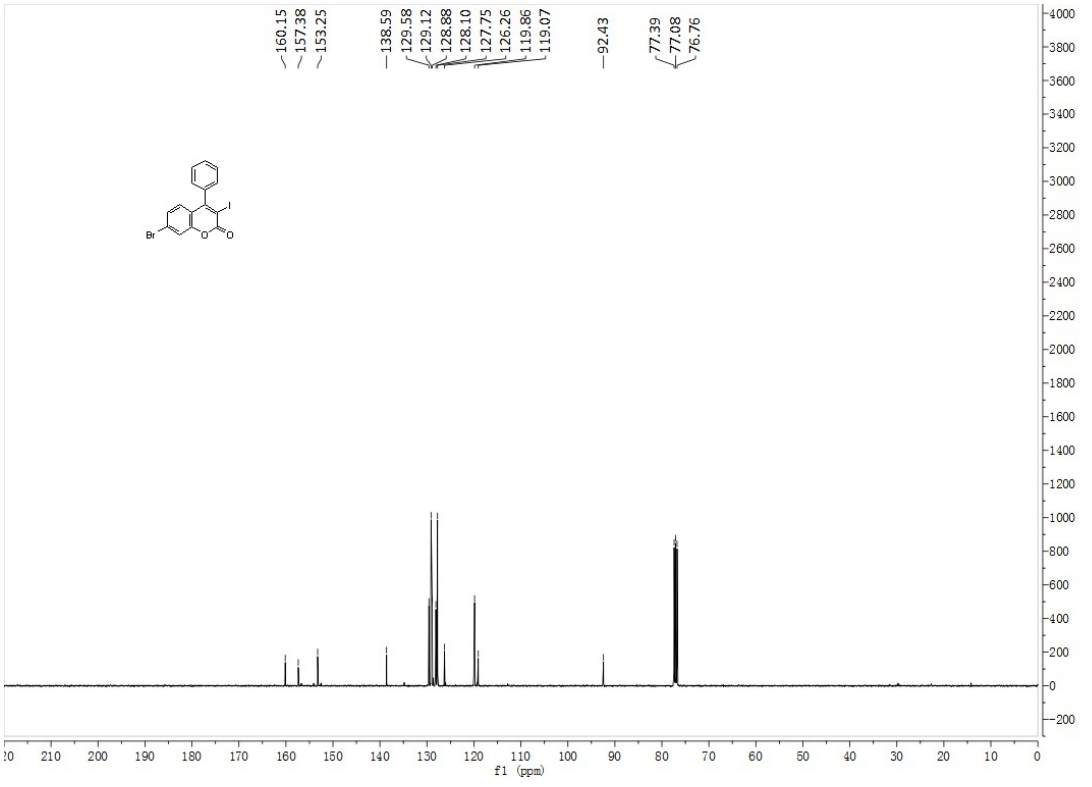
^{1}H and ^{13}C NMR spectra of **3e**



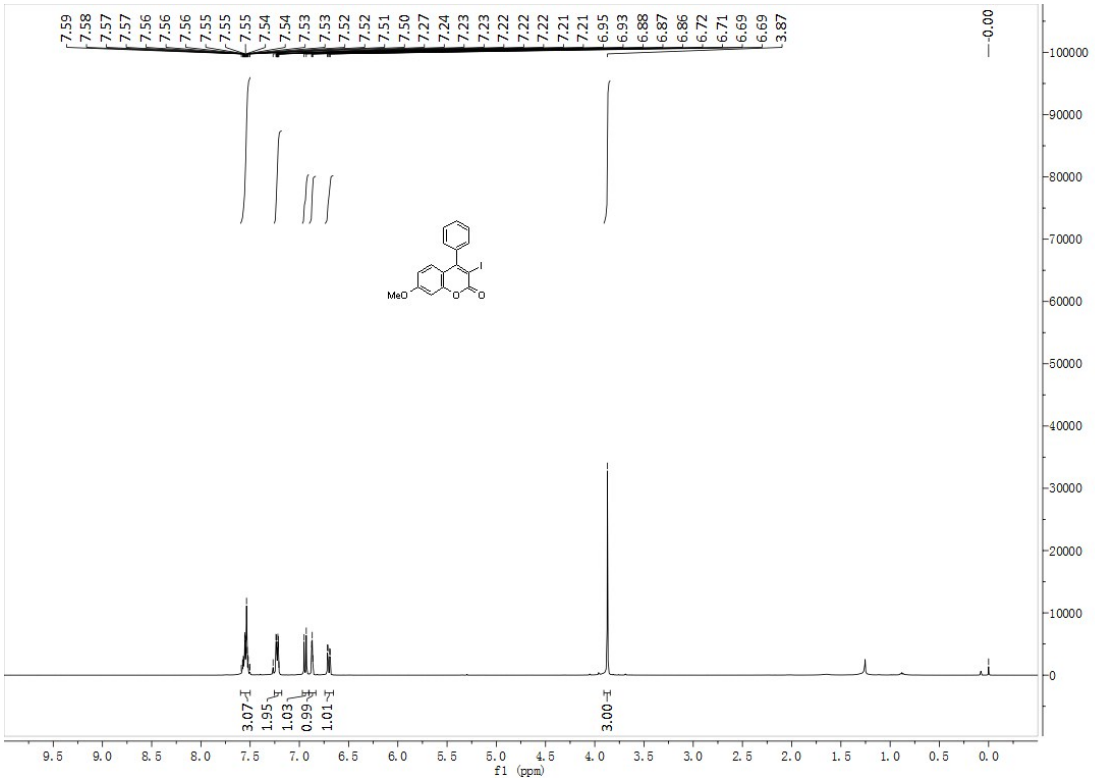


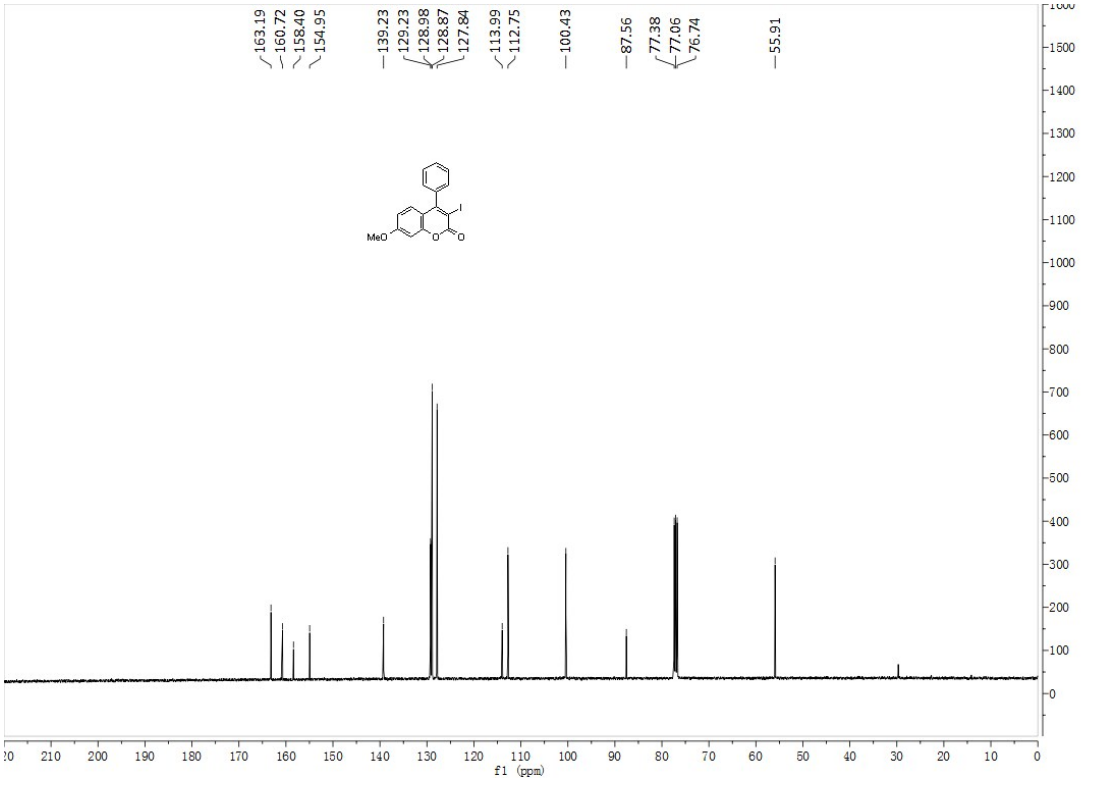
^{1}H and ^{13}C NMR spectra of **3f**



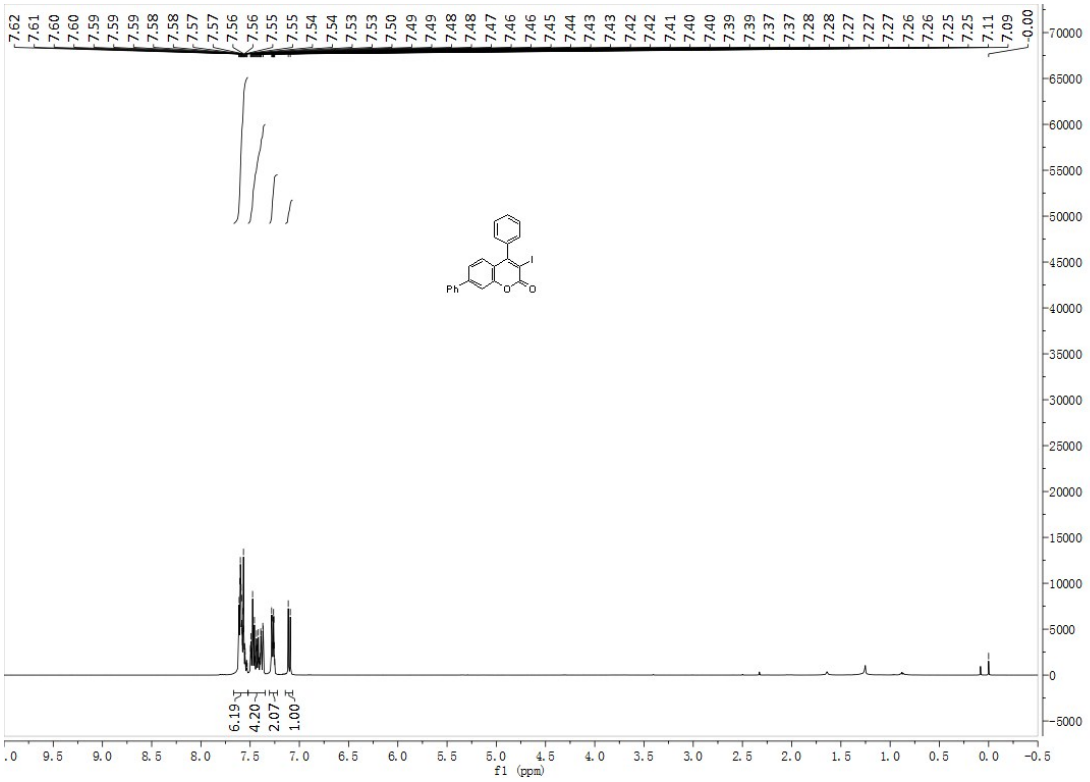


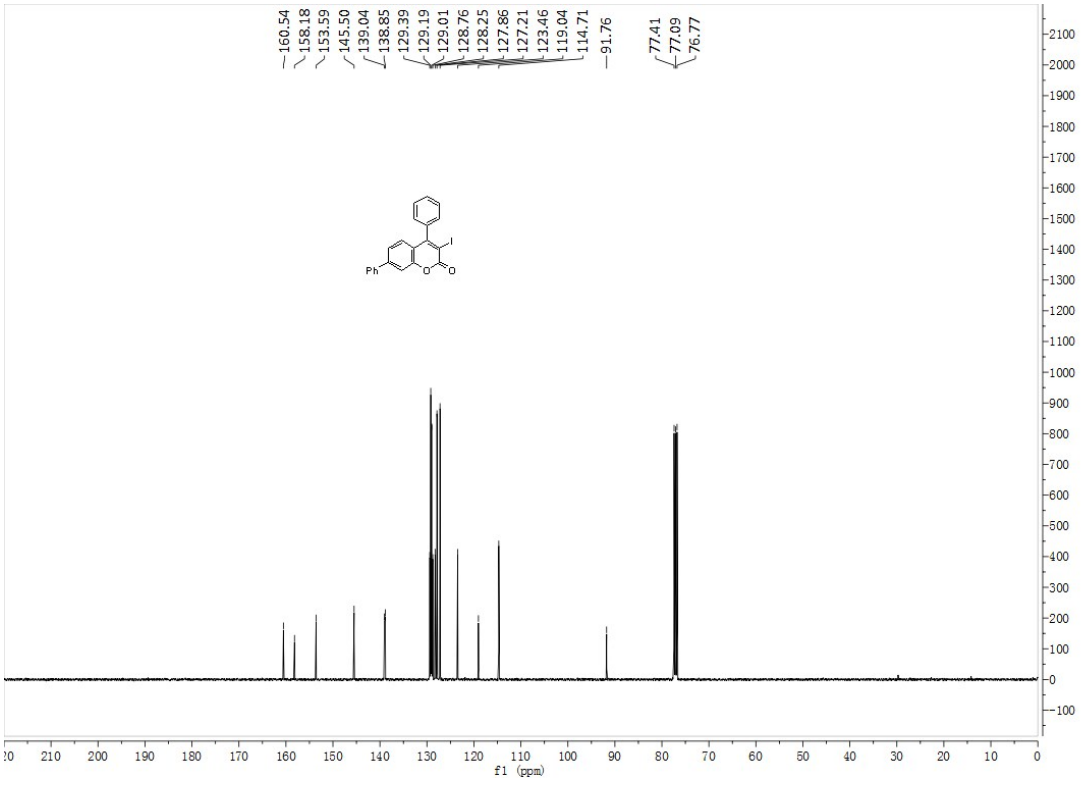
^{1}H and ^{13}C NMR spectra of **3g**



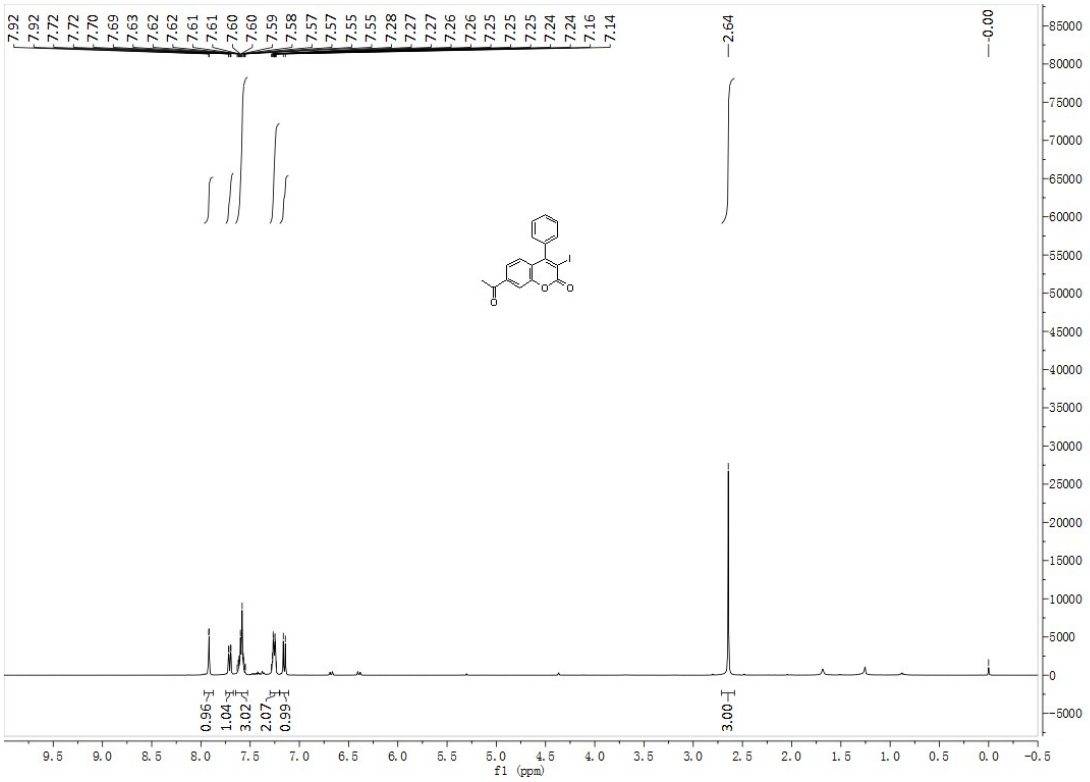


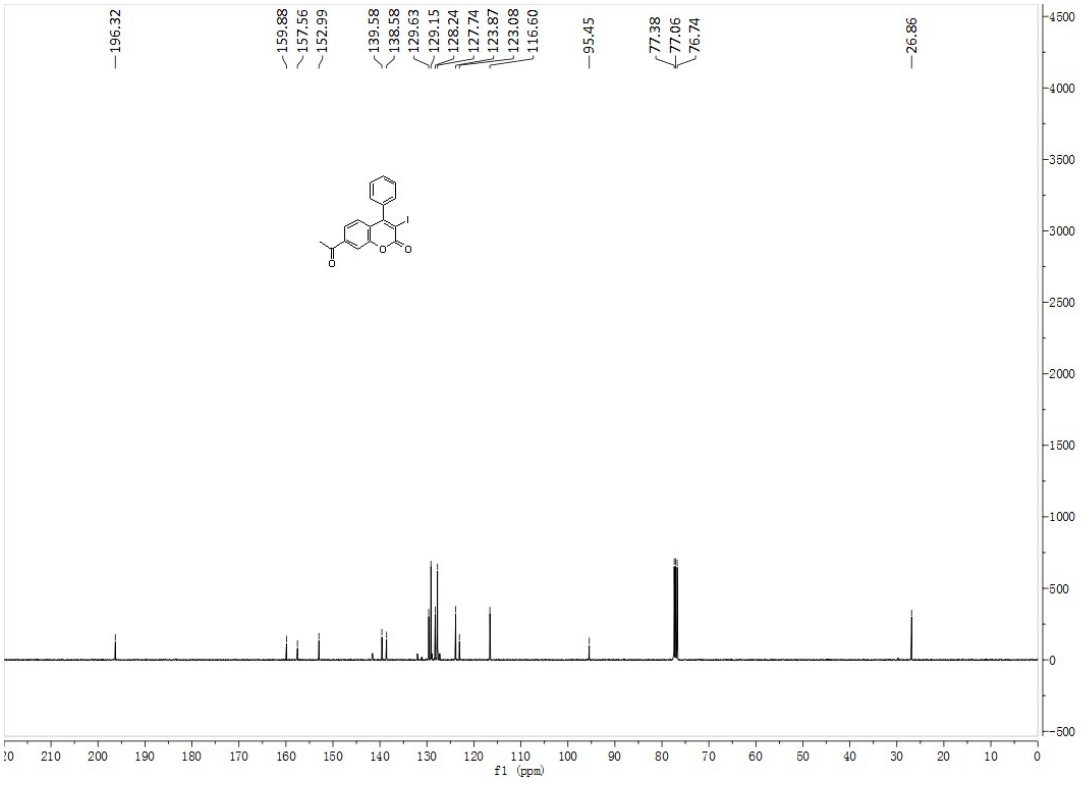
^{1}H and ^{13}C NMR spectra of **3h**



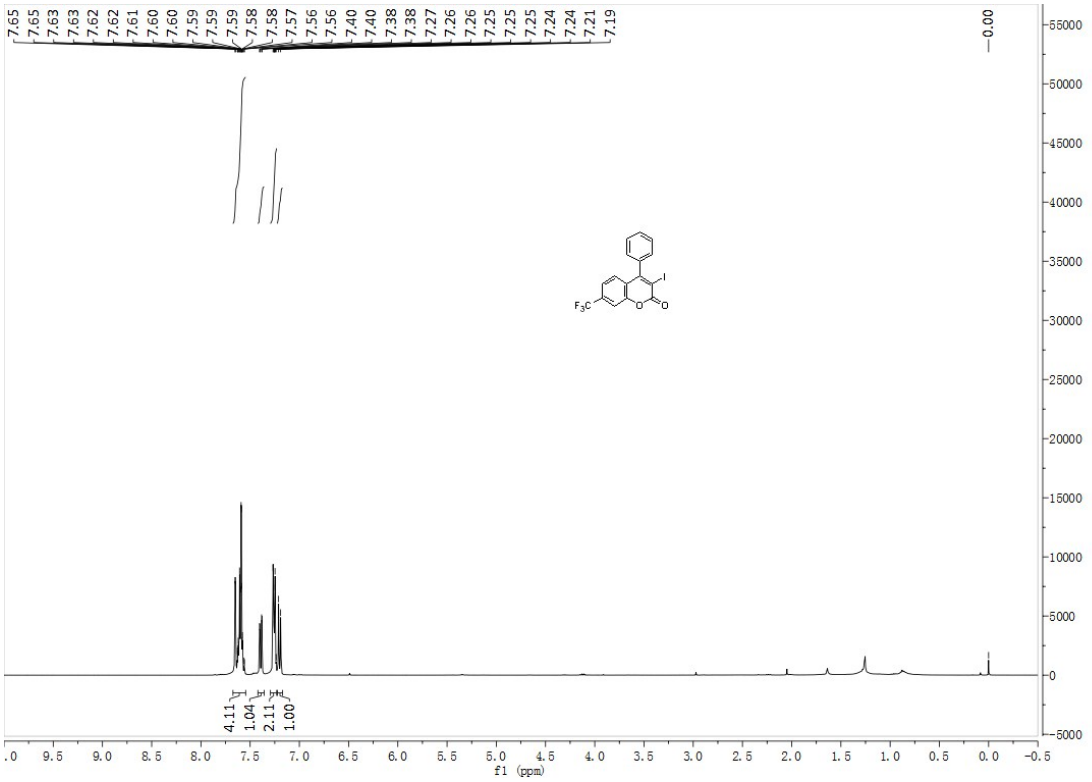


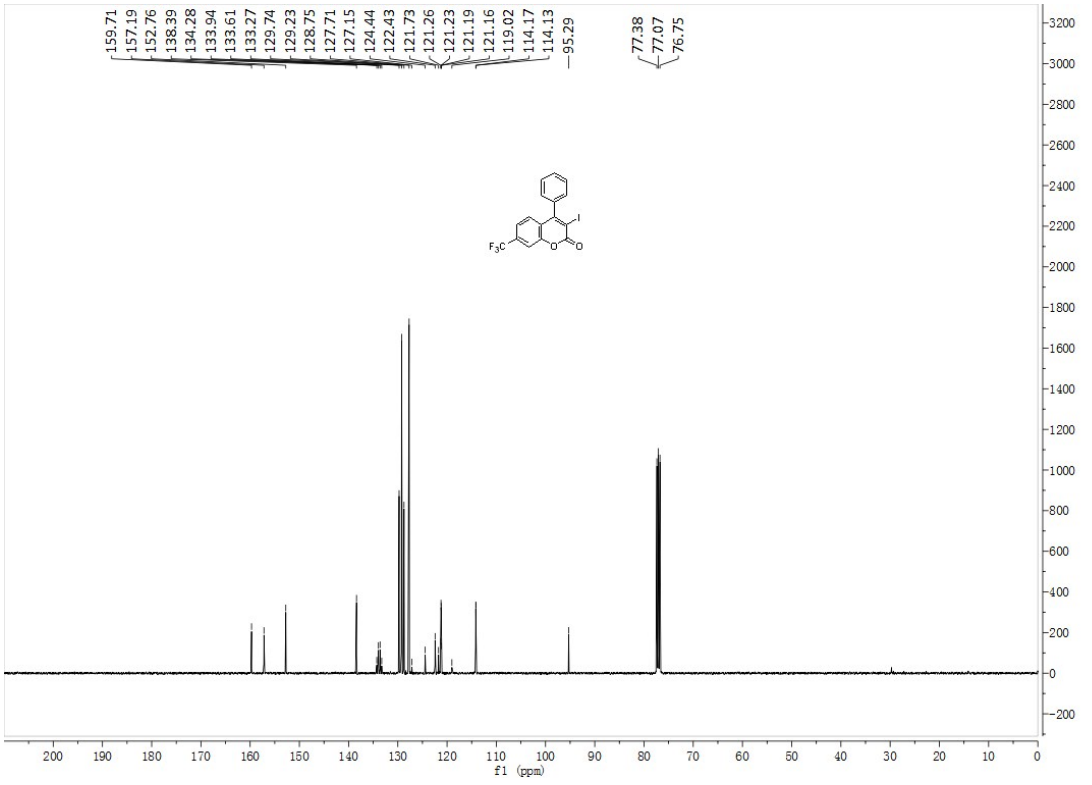
^{1}H and ^{13}C NMR spectra of **3i**



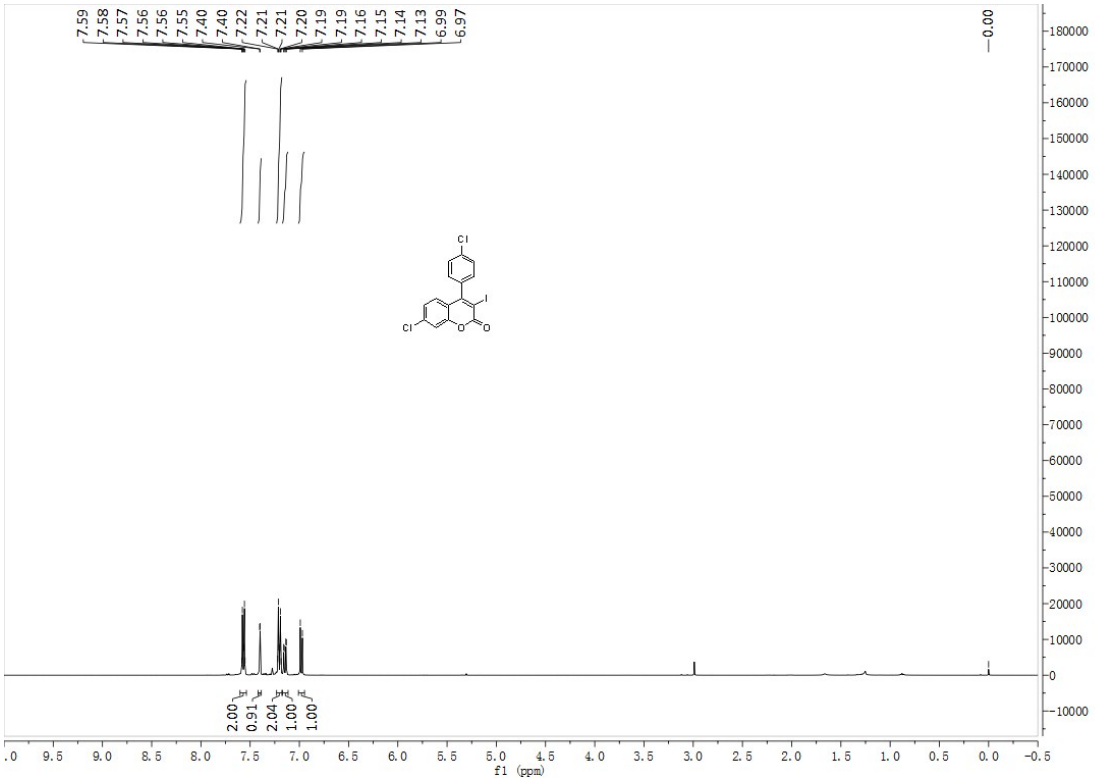


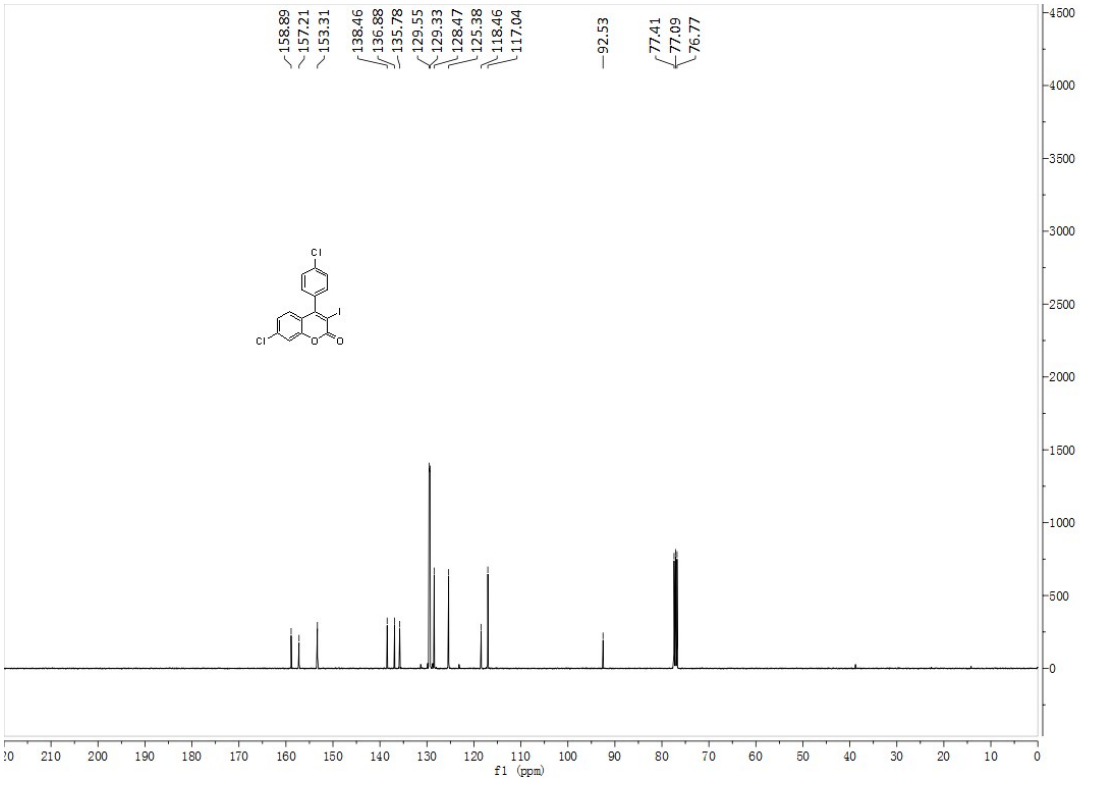
^{1}H and ^{13}C NMR spectra of **3j**



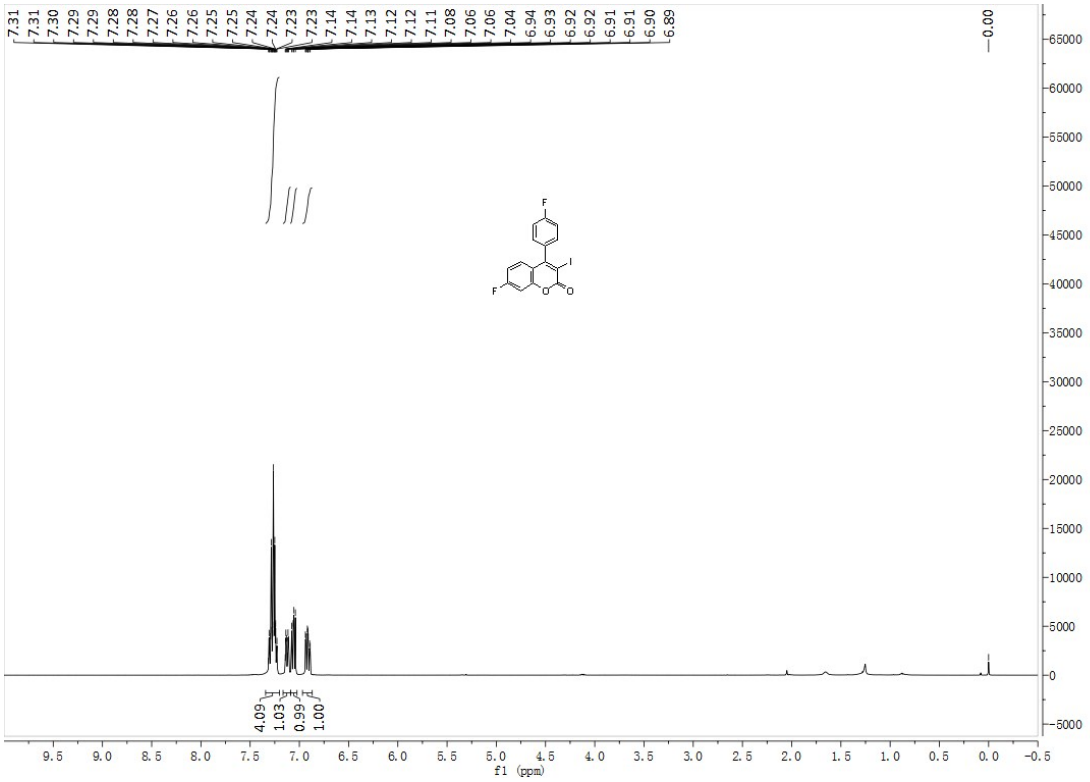


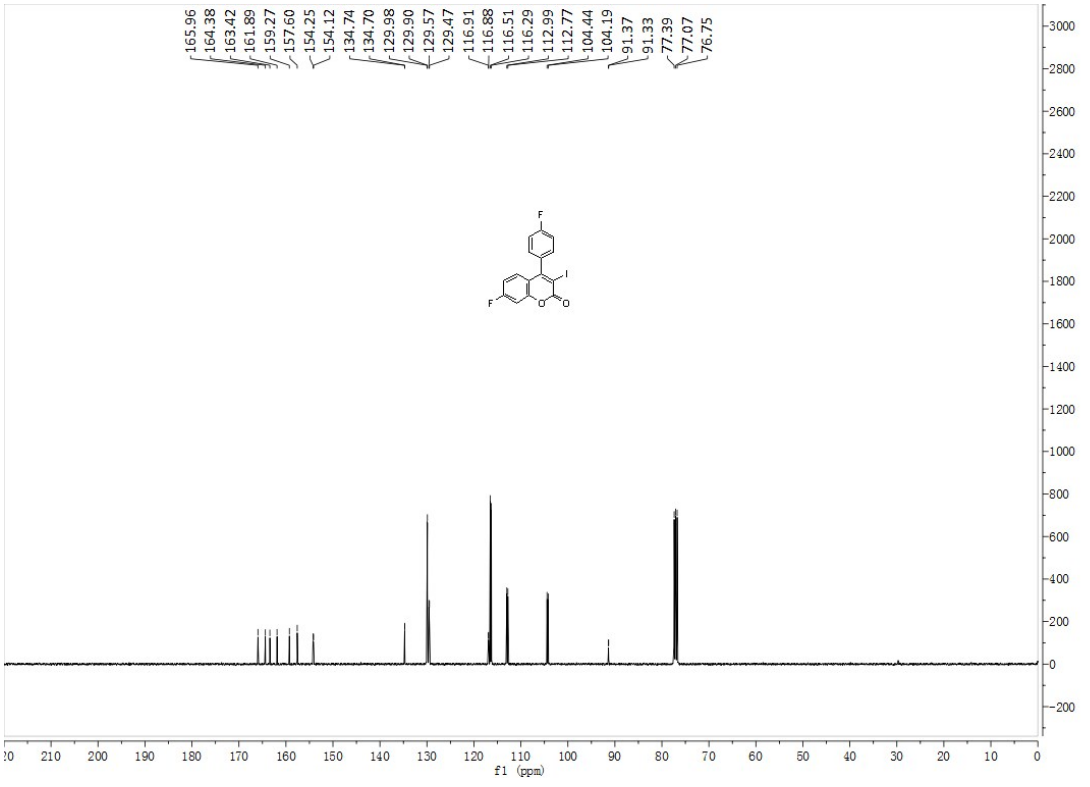
^{1}H and ^{13}C NMR spectra of **3k**



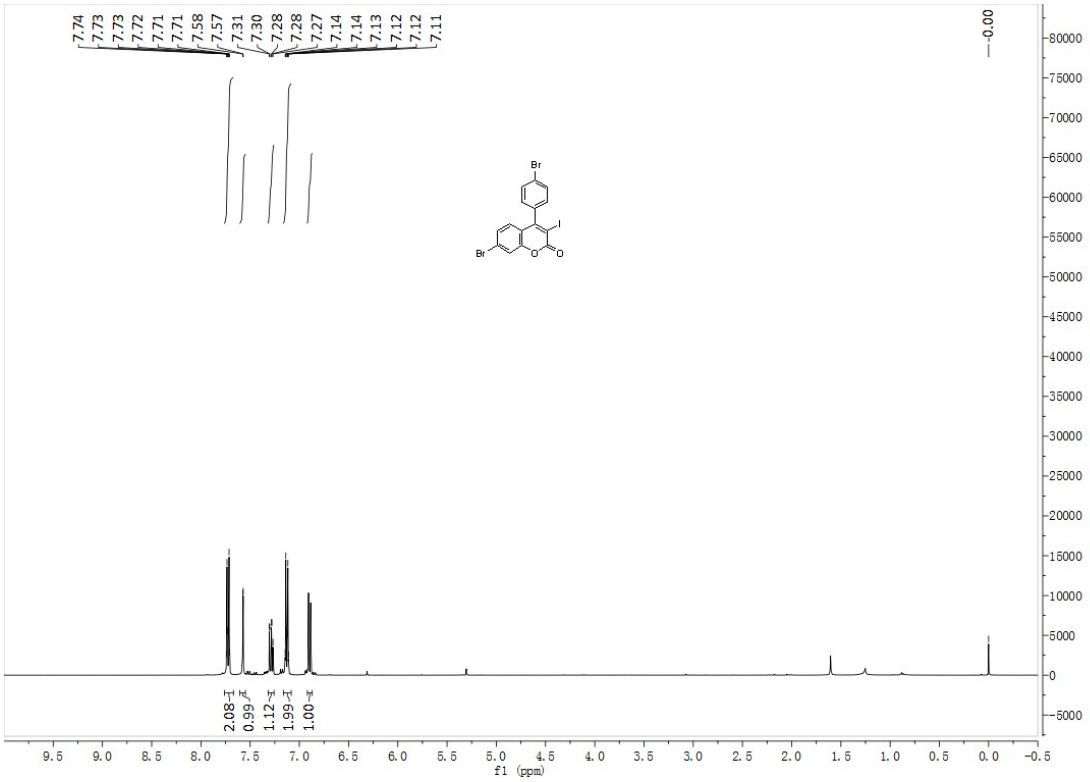


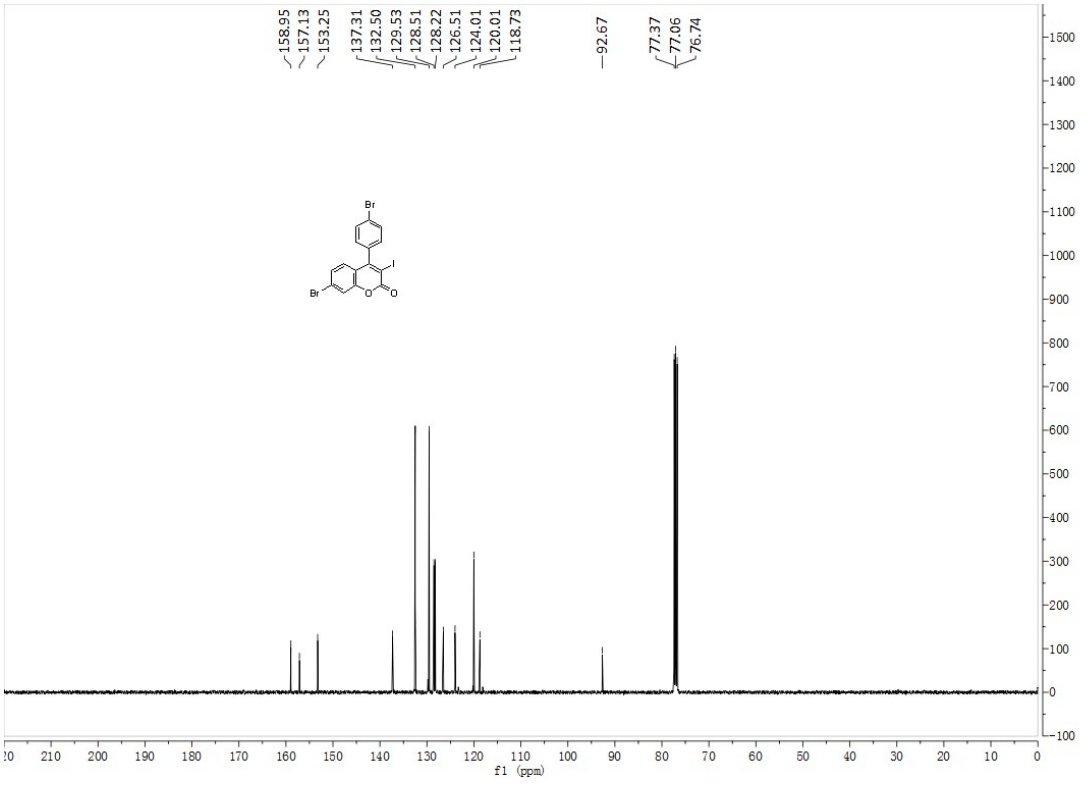
^{1}H and ^{13}C NMR spectra of **3l**



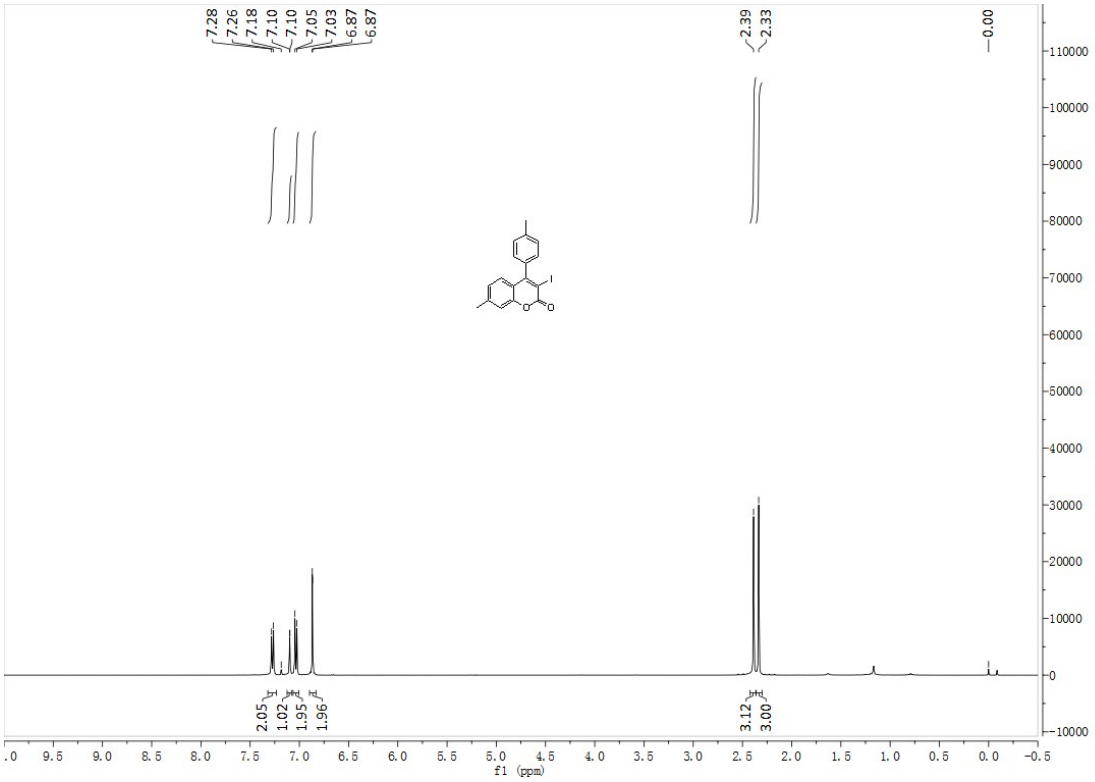


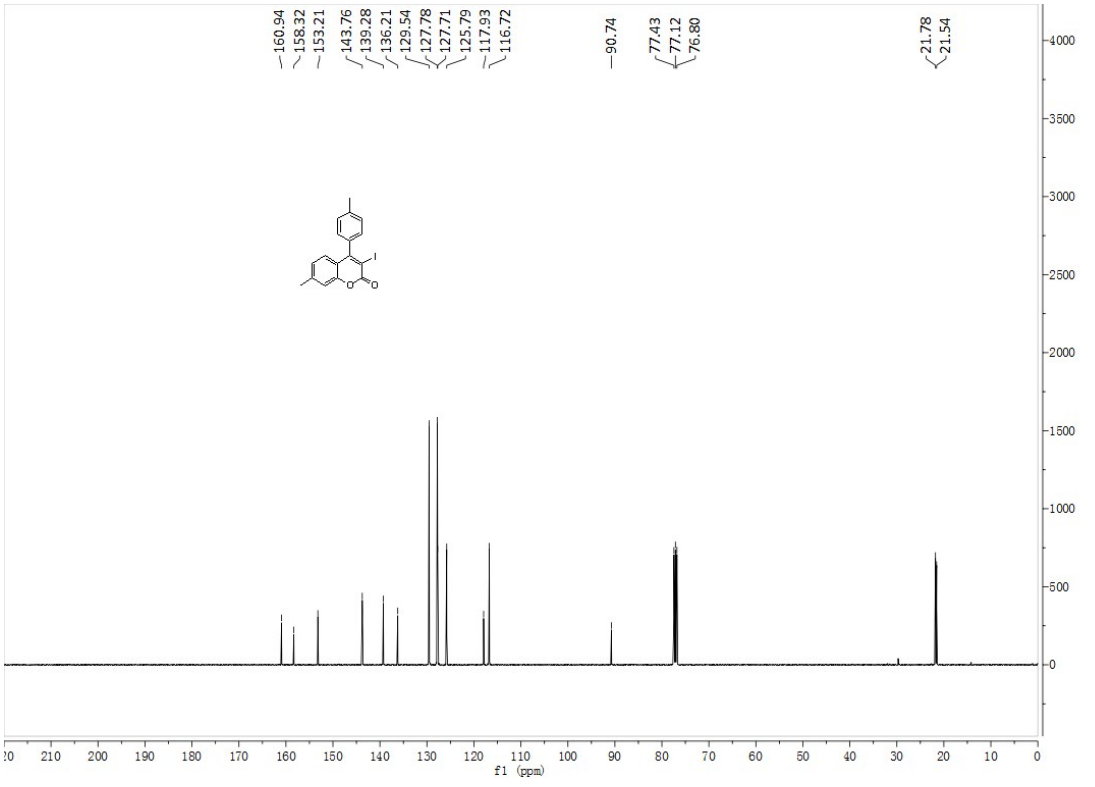
^{1}H and ^{13}C NMR spectra of **3m**



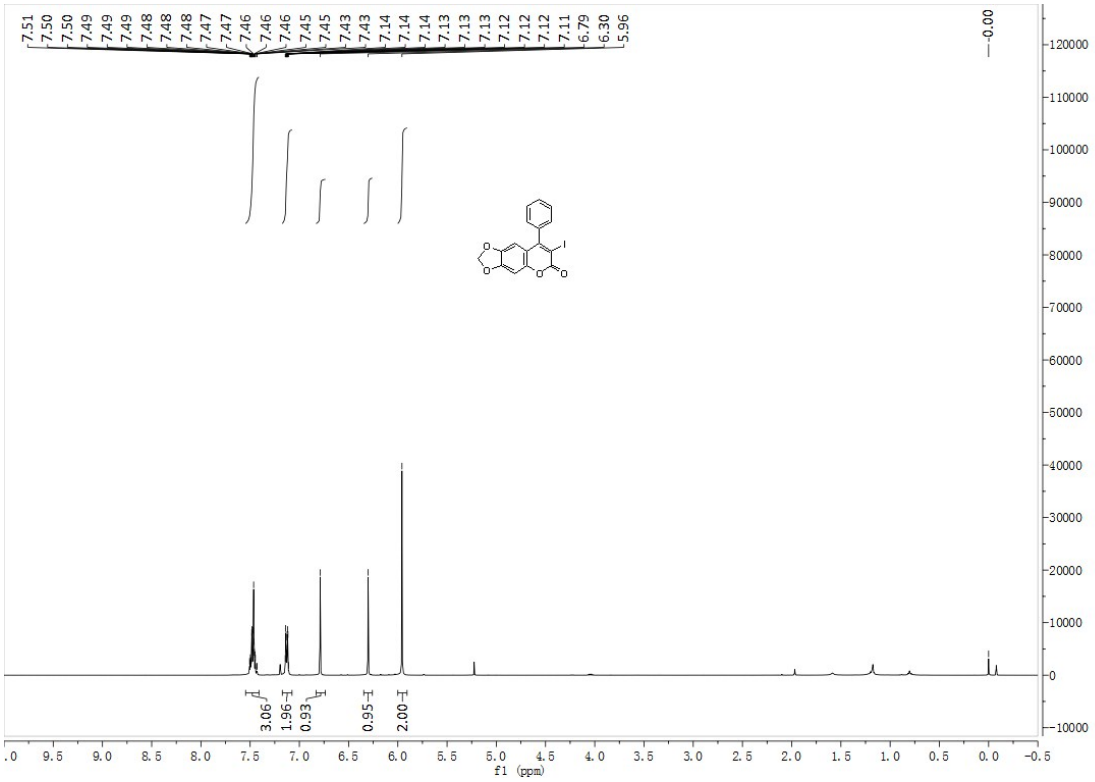


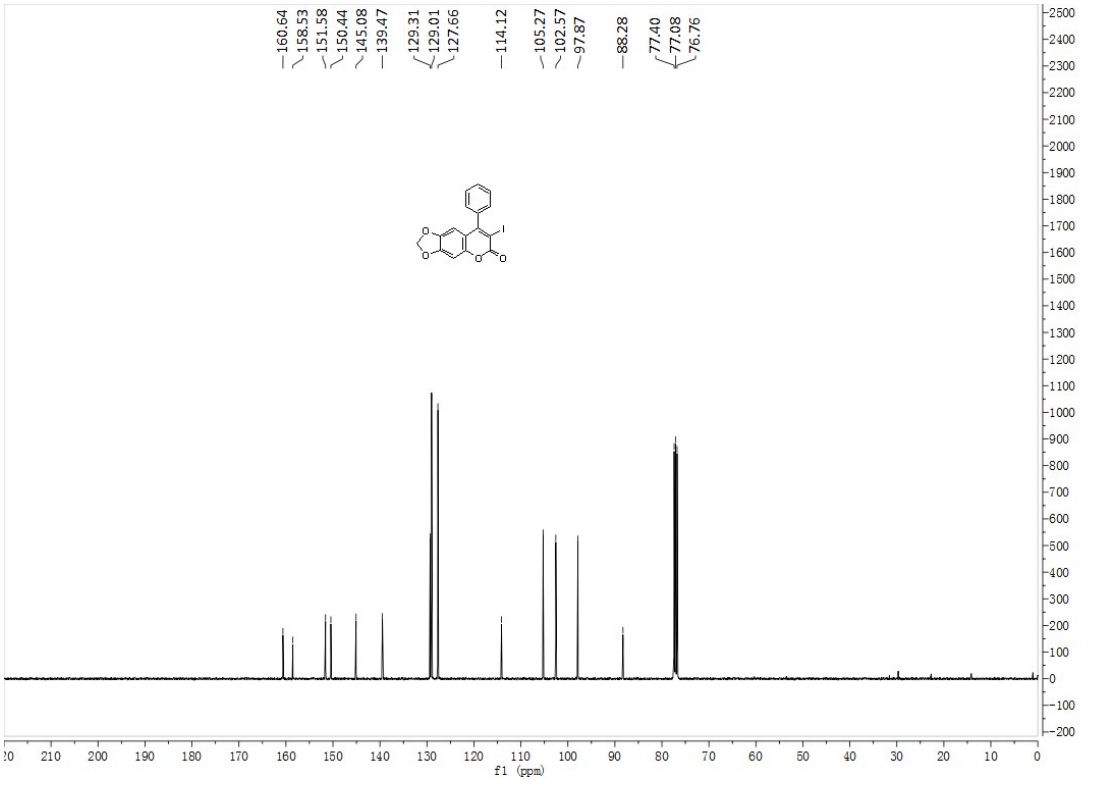
^{1}H and ^{13}C NMR spectra of **3n**



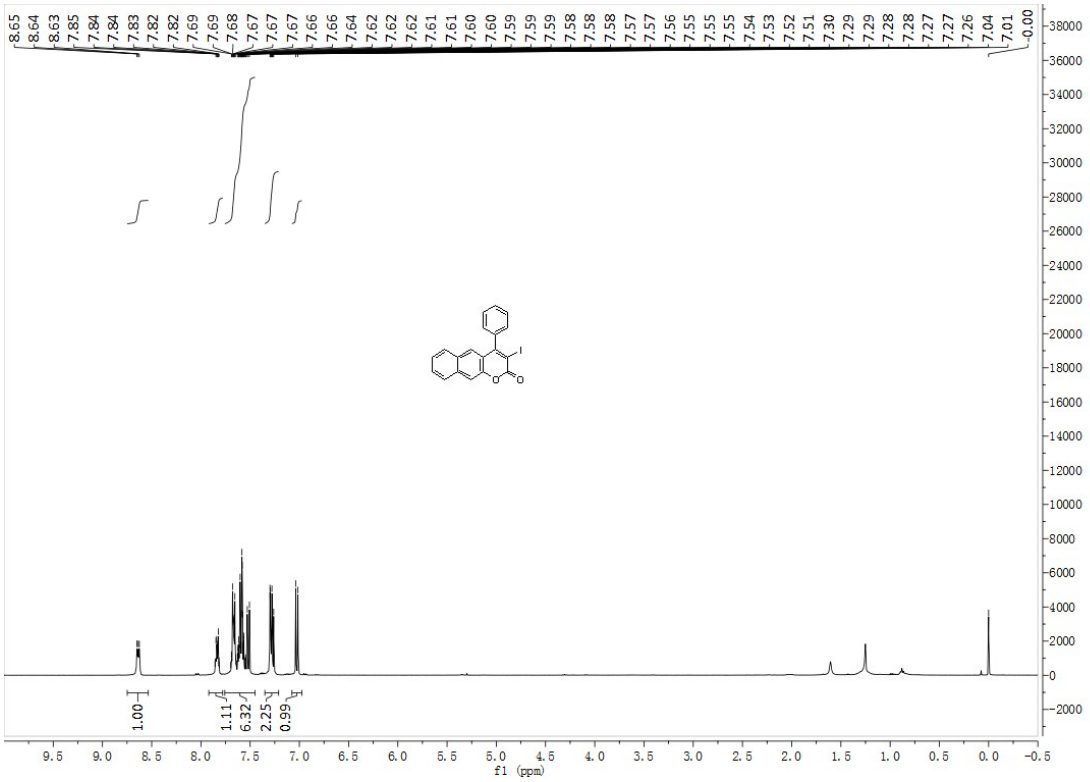


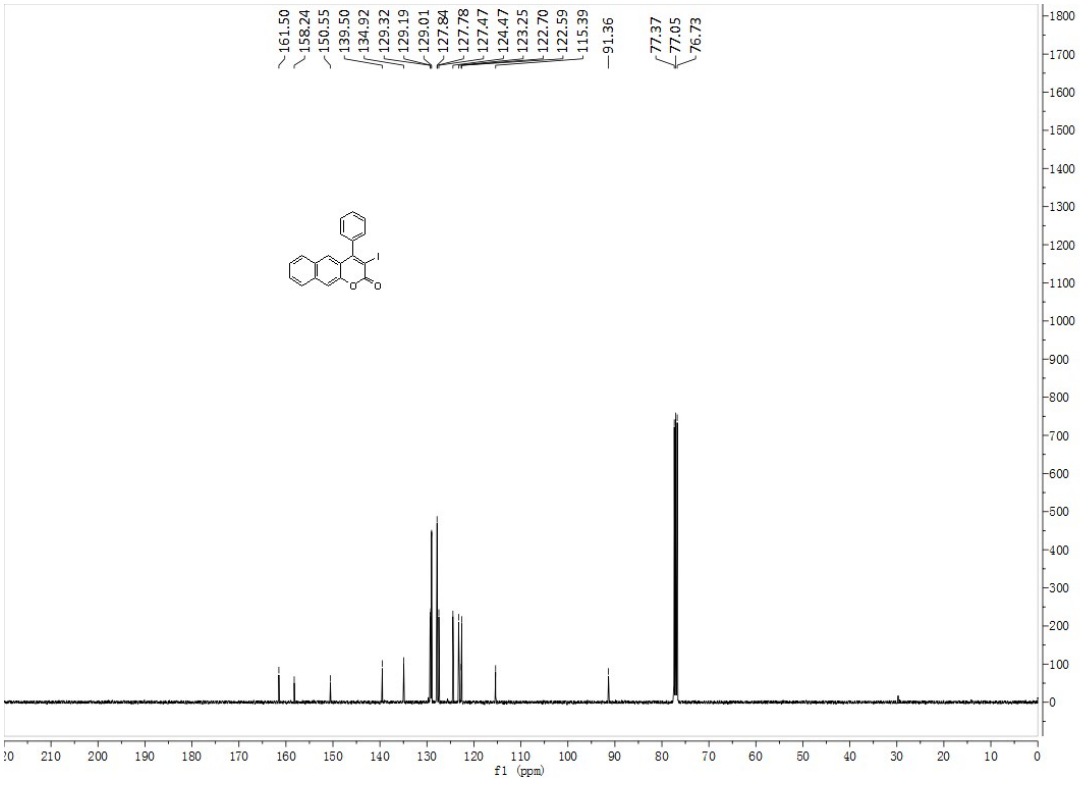
^{1}H and ^{13}C NMR spectra of **3o**



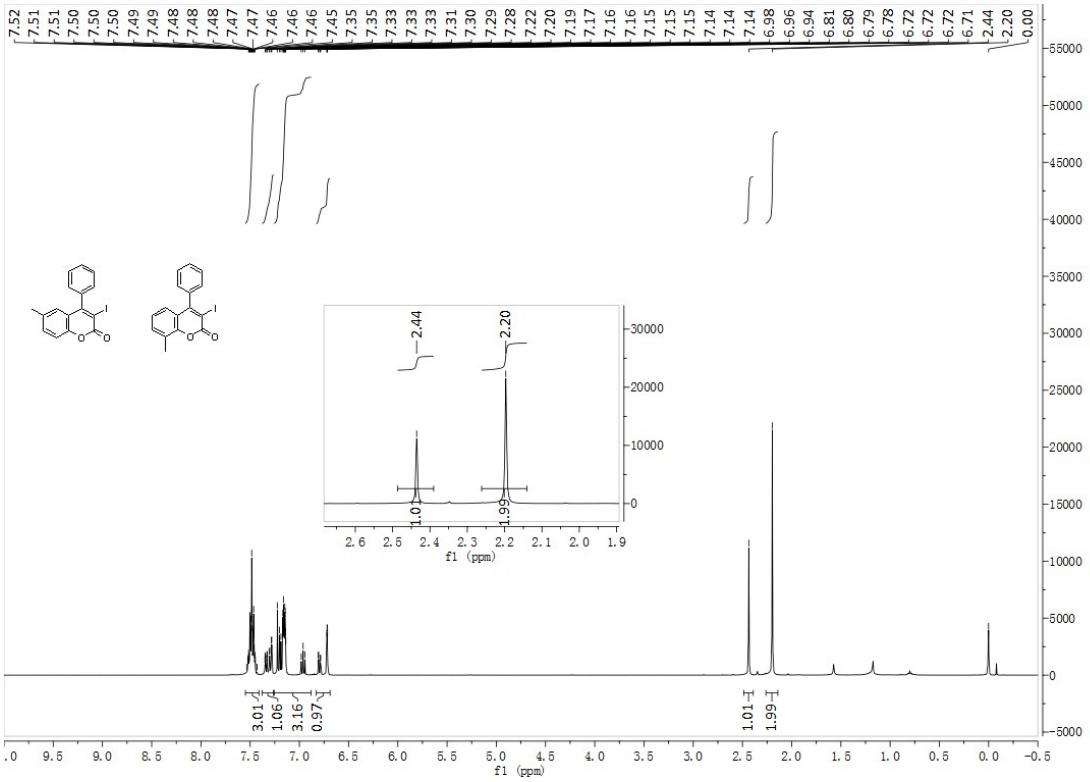


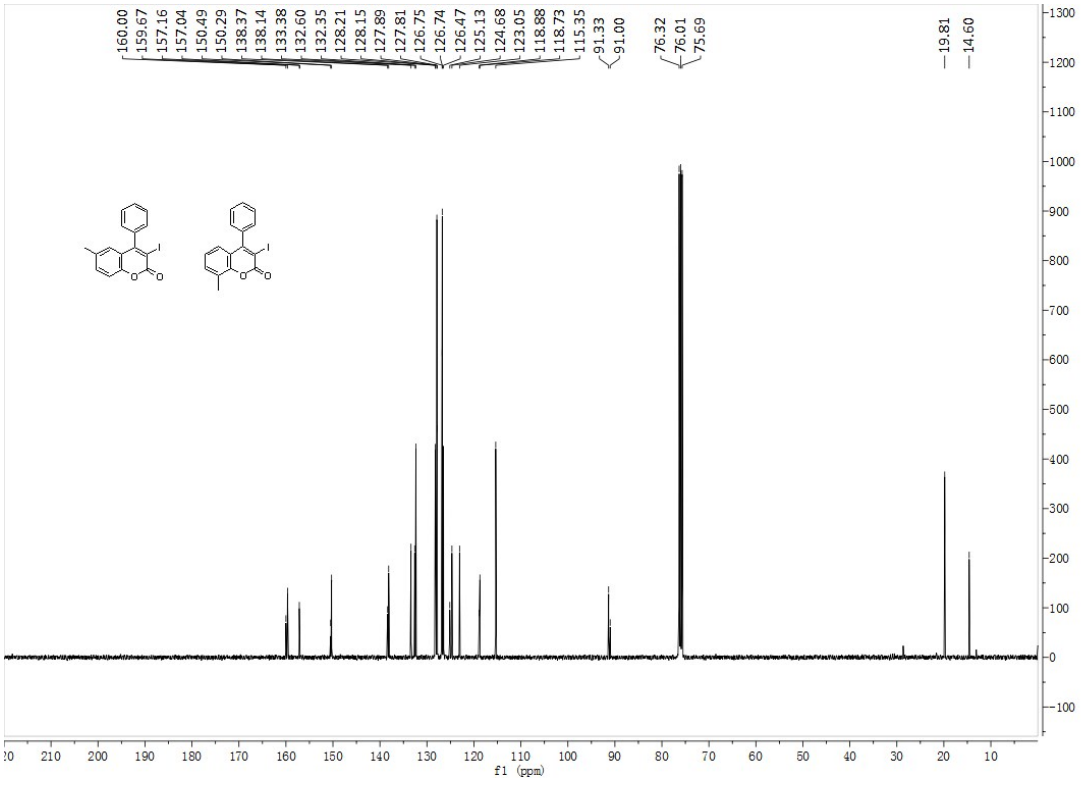
^{1}H and ^{13}C NMR spectra of **3p**



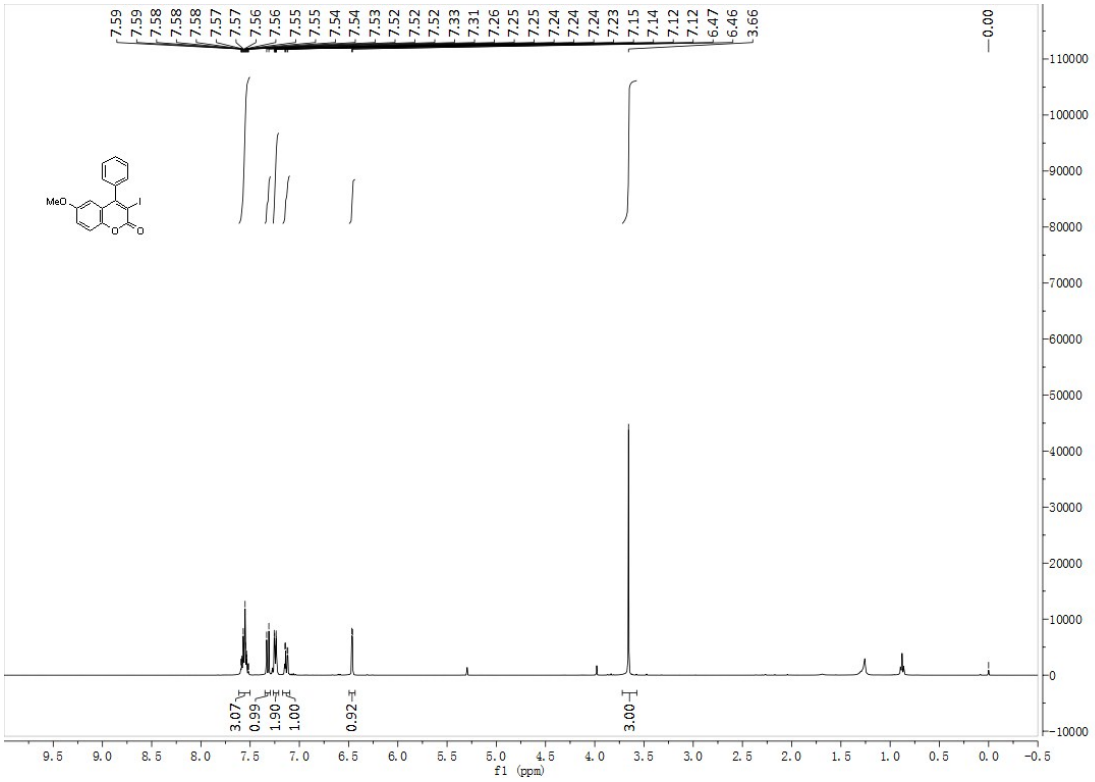


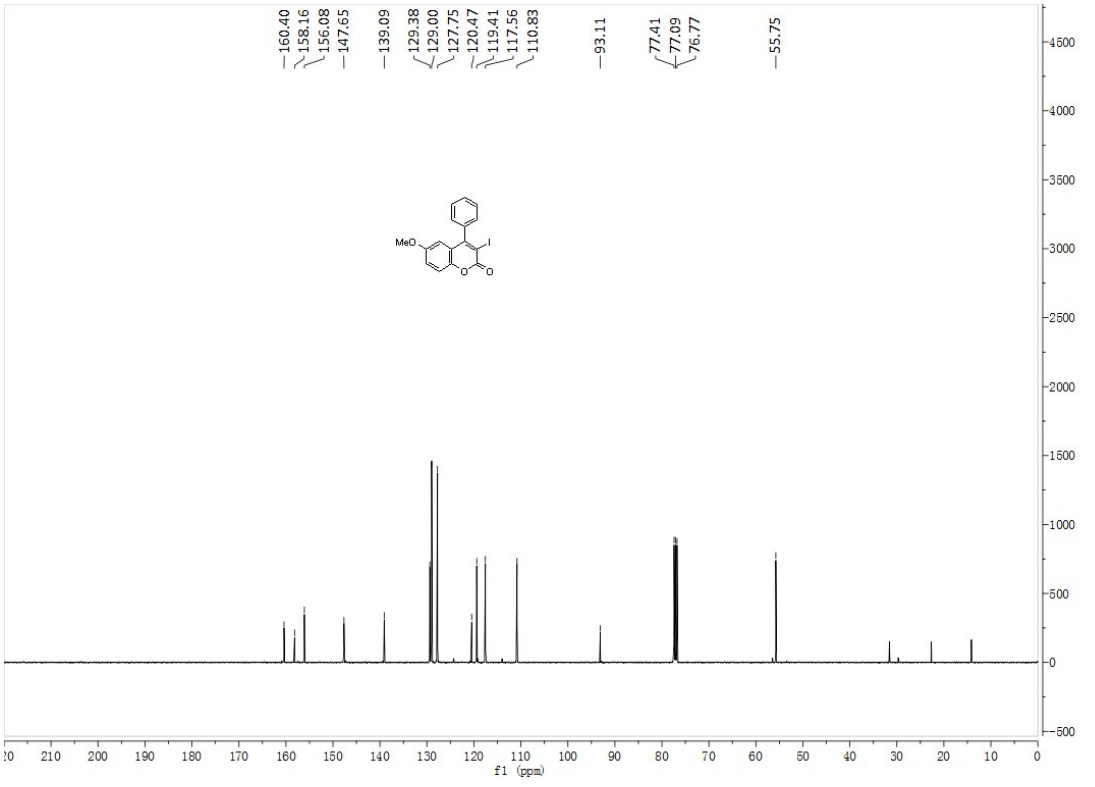
^{1}H and ^{13}C NMR spectra of **3q**



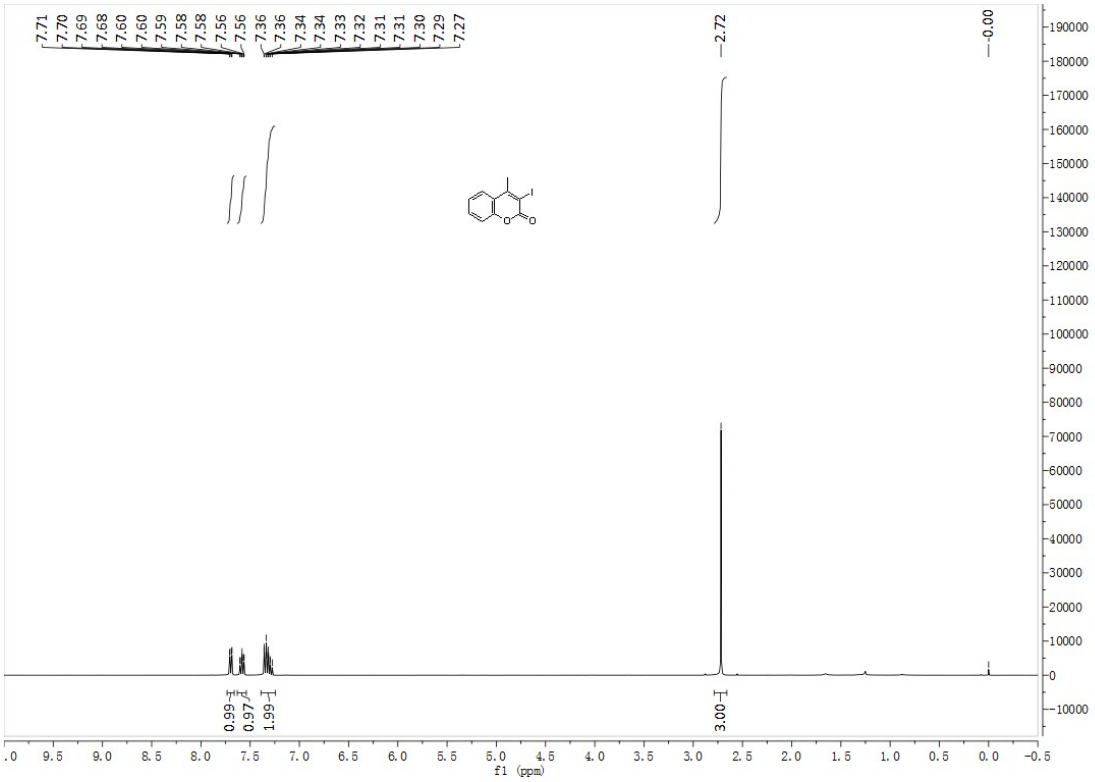


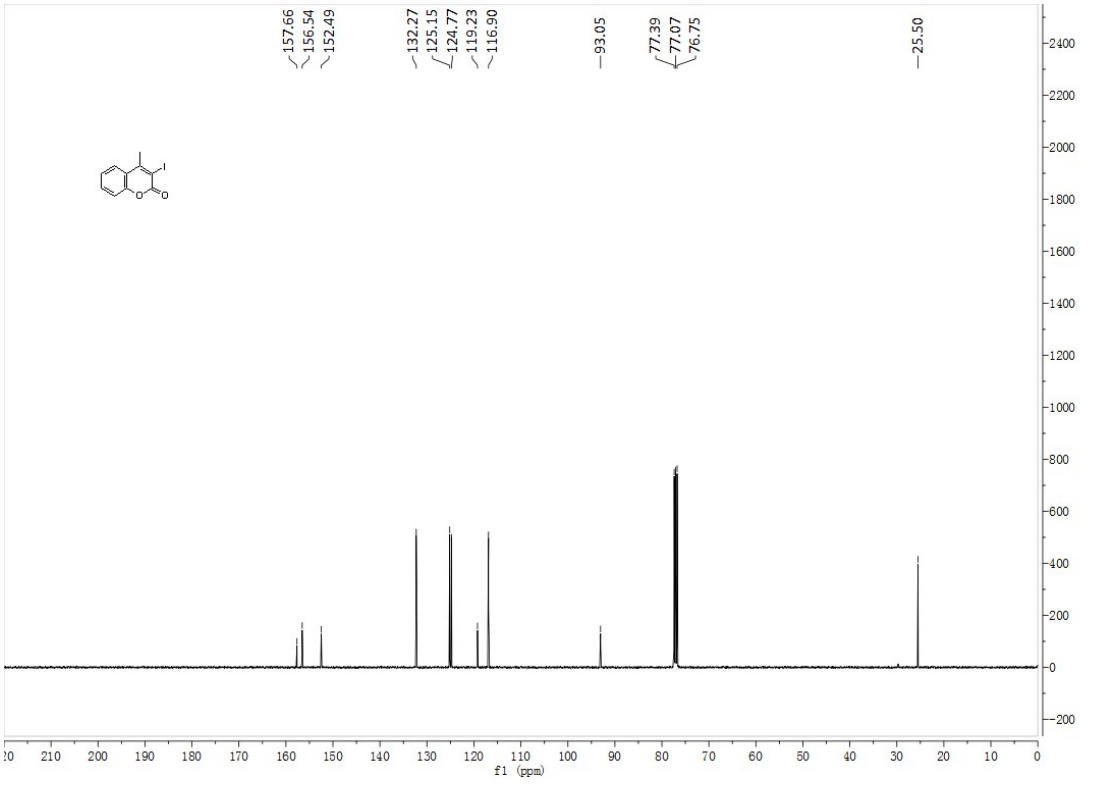
^{1}H and ^{13}C NMR spectra of **3r**



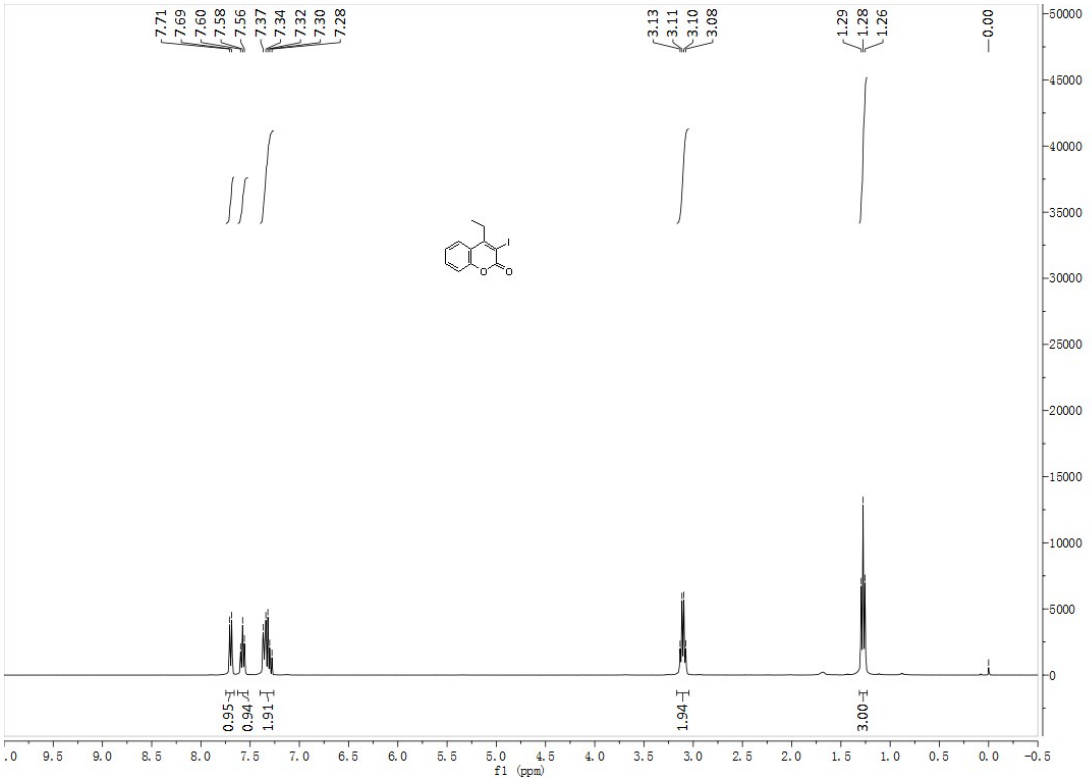


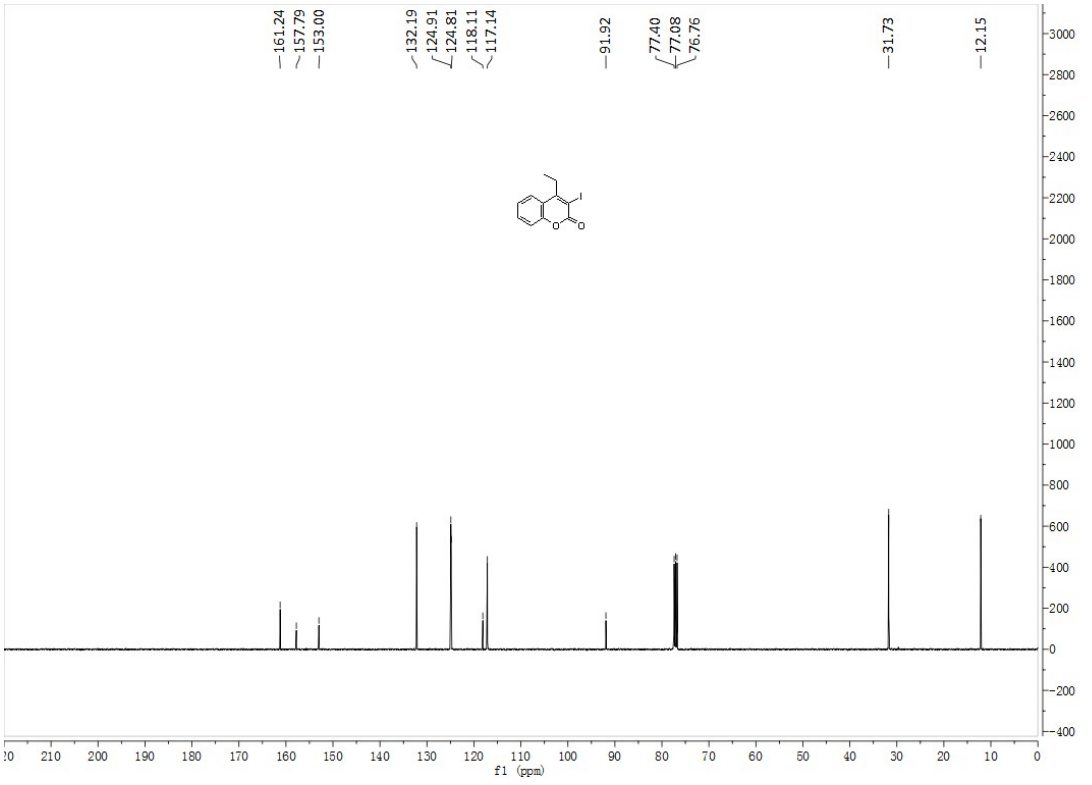
^{1}H and ^{13}C NMR spectra of **3t**





^{1}H and ^{13}C NMR spectra of **3u**





^{1}H and ^{13}C NMR spectra of **4a**