

## Supporting Information

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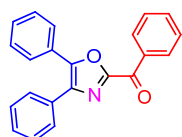
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## 1. General

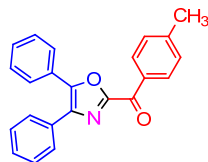
All starting materials and catalysts were obtained commercially, and used without further purification. Whenever possible, reactions were monitored by thin-layer chromatography using polygram SIL G/UV254 0.2 mm silica gel plates with fluorescent indicator. Column chromatography: silica gel 200–300 mesh.

NMR spectra were measured on Varian Mercury 400 spectrometer operating at 400 MHz for  $^1\text{H}$  and 100 MHz for  $^{13}\text{C}$  relative to tetramethylsilane as internal standard. NMR spectra were measured on Varian NMR System 600MHz operating at 600 MHz for  $^1\text{H}$  and 125 MHz for  $^{13}\text{C}$  relative to tetramethylsilane as internal standard. HRMS were carried out on an apex-Ultra spectrometer. IR spectra were recorded on a Tensor 27 infrared spectrometer as KBr pellets with absorption reported in  $\text{cm}^{-1}$ . The X-ray crystal structures were obtained on a Bruker SMART APEX CCD system. GC-MS were recorded on a Termo DSQ II. Melting points were determined using a melting point apparatus and are uncorrected.

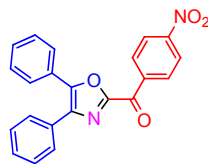
## 2. General procedure for the synthesis of polysubstituted oxazoles (3)



**(4,5-diphenyloxazol-2-yl)(phenyl)methanone (3a).** To a stirred solution of acetophenone (120mg, 1mmol), benzoin (233mg, 1.1mmol) and  $\text{CH}_3\text{COONH}_4$  (154 mg, 2mmol) in DMSO (3mL) were added  $\text{I}_2$  (635mg, 2.5mmol). The reaction mixture was stirred at  $120^\circ\text{C}$  for 5 h. EtOAc and  $\text{H}_2\text{O}/\text{Na}_2\text{S}_2\text{O}_3$  saturated solution were added, and the organic layer was separated, dried ( $\text{Na}_2\text{SO}_4$ ), and concentrated under reduced pressure. The residue was purified by flash chromatography (silica gel, 100/1=petroleum ether/ethylacetate) to give **3a** (237mg, 73% yield): mp=121.2-124.8; IR spectrum (KBr  $\text{cm}^{-1}$ ) 1655, 1513, 1477, 1335, 1204, 1181, 913, 767;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 8.70 (d,  $J = 8$  Hz, 2H), 8.71 (q,  $J = 2.4$  Hz, 4H), 7.61 (t,  $J = 7.2$  Hz, 1H), 7.51 (t,  $J = 8$  Hz, 2H), 7.38 (t,  $J = 5.6$  Hz, 6H);  $^{13}\text{C}$  NMR (100MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 178.5, 155.8, 148.5, 137.2, 135.2, 133.7, 131.5, 130.9, 129.8, 128.7, 128.6 128.4, 128.1, 127.6, 127.3. HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{22}\text{H}_{16}\text{NO}_2$ : 326.11756; found: 326.11734.

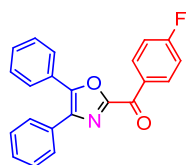


**(4,5-diphenyloxazol-2-yl)(p-tolyl)methanone (3b)** (251mg, 74% yield): mp=157.7-160.2; IR spectrum (KBr  $\text{cm}^{-1}$ ) 1650, 1604, 1510, 1477, 1445, 1334, 1178, 911, 767;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 8.49 (d,  $J = 8$  Hz, 2H), 7.75-7.72 (m, 4H), 7.42(t,  $J = 6$  Hz, 6H), 7.33 (d,  $J = 8$  Hz, 2H), 2.45(s, 3H);  $^{13}\text{C}$  NMR (100MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 178.3, 156.1, 148.4, 144.9, 137.2, 132.8, 131.6, 131.1, 129.7, 129.2, 128.8, 128.7, 128.2, 127.7, 127.3, 21.8. HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{23}\text{H}_{18}\text{NO}_2$ : 340.13321; found: 340.13296.



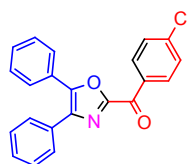
**(4,5-diphenyloxazol-2-yl)(4-nitrophenyl)methanone (3c)** (259mg, 70%

yield): mp=154.6-158.8; IR spectrum (KBr  $\text{cm}^{-1}$ ) 1657, 1599, 1580, 1521, 1445, 1346, 1333, 1207, 916, 850, 769, 696;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 8.77 (d,  $J = 8$  Hz, 2H), 8.37 (d,  $J = 8$  Hz, 2H) 7.76-7.70 (m, 4H), 7.44(q,  $J = 4.8$  Hz, 6H);  $^{13}\text{C}$  NMR (100MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 176.6, 155.4, 150.5, 149.5, 139.9, 137.8, 132.0, 131.1, 130.2, 129.1, 128.9, 128.8, 128.2, 127.4, 127.2, 123.5. HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{22}\text{H}_{15}\text{N}_2\text{O}_4$ : 371.10263; found: 371.10230.



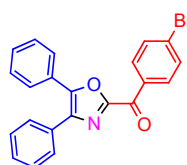
**(4,5-diphenyloxazol-2-yl)(4-fluorophenyl)methanone (3d)** (257mg, 75%

yield): mp=149.6-152.4; IR spectrum (KBr  $\text{cm}^{-1}$ ) 1656, 1593, 1502, 1477, 1336, 1202, 1155, 915, 767, 693;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 8.70-8.66 (m, 2H), 7.75-7.71 (m, 4H) 7.46-7.40 (m, 6H), 7.21 (t,  $J = 7.2$  Hz, 2H);  $^{13}\text{C}$  NMR (100MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 176.9, 167.6, 165.0, 155.7, 148.7, 137.3, 133.9, 133.8, 131.6, 131.4, 129.9, 128.8, 128.7, 128.2, 127.6, 127.3, 115.8, 115.6. HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{22}\text{H}_{15}\text{FNO}_2$ : 344.10813; found: 344.10793.



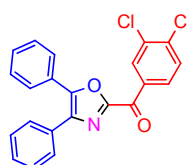
**(4-chlorophenyl)(4,5-diphenyloxazol-2-yl)methanone (3e)** (273mg, 76%

yield): mp=155.2-157.5; IR spectrum (KBr  $\text{cm}^{-1}$ ) 1649, 1584, 1476, 1335, 1210, 1090, 910, 768, 698;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 8.56 (d,  $J = 8$  Hz, 2H), 7.74-7.70 (m, 4H), 7.50 (d,  $J = 8$  Hz, 2H), 7.45-7.40 (m, 6H);  $^{13}\text{C}$  NMR (100MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 177.2, 155.7, 148.8, 140.5, 137.4, 133.5, 132.4, 131.4, 129.9, 128.8, 128.8, 128.7, 128.2, 127.5, 127.3. HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{22}\text{H}_{15}\text{ClNO}_2$ : 360.07858; found: 360.07840.



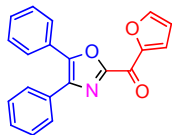
**(4-bromophenyl)(4,5-diphenyloxazol-2-yl)methanone (3f)** (323mg, 80%

yield): mp=149.5-152.6; IR spectrum (KBr  $\text{cm}^{-1}$ ) 1648, 1581, 1476, 1335, 1211, 909, 767, 698;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 8.48 (d,  $J = 8$  Hz, 2H), 7.75-7.67 (m, 6H), 7.45-7.41 (m, 6H);  $^{13}\text{C}$  NMR (100MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 177.4, 155.7, 148.9, 137.4, 133.9, 132.4, 131.8, 131.4, 129.9, 129.4, 128.8, 128.7, 128.2, 127.5, 127.4. HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{22}\text{H}_{15}\text{BrNO}_2$ : 404.02807; found: 404.02773.

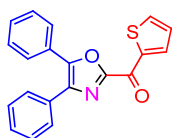


**(3,4-dichlorophenyl)(4,5-diphenyloxazol-2-yl)methanone (3g)** (264mg, 67%

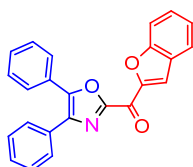
yield): mp=138.7-141.3; IR spectrum (KBr  $\text{cm}^{-1}$ ) 1650, 1552, 1509, 1445, 1337, 1206, 1187, 928, 768, 697;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 8.71 (d,  $J = 2$  Hz, 1H), 8.51 (q,  $J = 2$  Hz, 1H), 7.72 (t,  $J = 8$  Hz, 4H), 7.61 (d,  $J = 8$  Hz, 1H), 7.43 (t,  $J = 6$  Hz, 6H);  $^{13}\text{C}$  NMR (100MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 175.9, 155.3, 149.2, 138.5, 137.5, 134.8, 134.7, 133.1, 132.7, 131.2, 130.6, 130.1, 129.9, 128.9, 128.8, 128.7, 128.4, 128.2, 127.4. HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{22}\text{H}_{14}\text{Cl}_2\text{NO}_2$ : 394.03961; found: 394.03928.



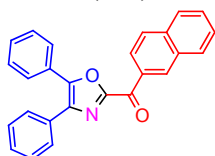
**(4,5-diphenyloxazol-2-yl)(furan-2-yl)methanone (3h)** (268mg, 85% yield): mp=167.1-169.4; IR spectrum (KBr  $\text{cm}^{-1}$ ) 1648, 1519, 1460, 1393, 1022, 864, 772, 696;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 8.24 (d,  $J = 3.2$  Hz, 1H), 7.80 (s, 1H), 7.75-7.72 (m, 4H), 7.42 (t,  $J = 6.4$  Hz, 6H), 6.66 (q,  $J = 1.6$  Hz, 1H);  $^{13}\text{C}$  NMR (100MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 165.6, 155.1, 150.2, 148.8, 148.7, 137.3, 131.4, 129.8, 128.8, 128.7, 128.1, 127.5, 127.3, 124.1, 112.7. HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{20}\text{H}_{14}\text{NO}_3$ : 316.09682; found: 316.09656.



**(4,5-diphenyloxazol-2-yl)(thiophen-2-yl)methanone (3i)** (275mg, 83% yield): mp=163.7-165.8; IR spectrum (KBr  $\text{cm}^{-1}$ ) 1631, 1514, 1412, 1356, 1215, 1048, 831, 772, 697;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 8.70 (d,  $J = 4$  Hz, 1H), 7.79 (d,  $J = 4.8$  Hz, 1H), 7.75 (d,  $J = 6.4$  Hz, 4H), 7.43 (q,  $J = 6$  Hz, 6H), 7.23 (t,  $J = 4$  Hz, 1H);  $^{13}\text{C}$  NMR (100MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 170.6, 155.5, 148.8, 140.8, 137.3, 137.0, 136.2, 131.5, 129.9, 128.8, 128.7, 128.5, 128.1, 127.7, 127.4. HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{20}\text{H}_{14}\text{NO}_2\text{S}$ : 332.07398; found: 332.07382.

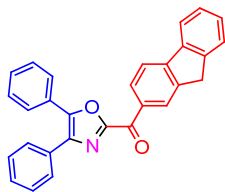


**benzofuran-2-yl(4,5-diphenyloxazol-2-yl)methanone (3j)** (183mg, 50% yield): mp=181.3-186.2; IR spectrum (KBr  $\text{cm}^{-1}$ ) 1649, 1547, 1519, 1445, 1340, 1120, 890, 753, 664;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 8.65 (s, 1H), 7.79 (d,  $J = 4.8$  Hz, 1H), 7.81 (d,  $J = 8$  Hz, 1H), 7.72 (d,  $J = 6$  Hz, 4H), 7.67 (d,  $J = 8$  Hz, 1H), 7.40 (t,  $J = 8$  Hz, 1H), 7.49-7.42 (m, 6H), 7.36 (t,  $J = 8$  Hz, 1H);  $^{13}\text{C}$  NMR (100MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 167.3, 156.4, 155.2, 150.3, 149.2, 137.5, 131.4, 130.0, 129.2, 128.9, 128.8, 128.7, 128.2, 127.5, 127.4, 127.3, 124.1, 124.0, 120.1, 112.6. HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{24}\text{H}_{16}\text{NO}_3$ : 366.11247; found: 366.11189.

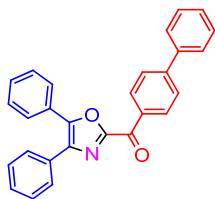


**(4,5-diphenyloxazol-2-yl)(naphthalen-2-yl)methanone (3l)** (233mg, 64% yield): mp=178.1-181.7; IR spectrum (KBr  $\text{cm}^{-1}$ ) 1646, 1513, 1443, 1332, 1180, 1119, 763, 691;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 9.33 (s, 1H), 8.48 (q,  $J = 1.6$  Hz, 1H), 8.50 (d,  $J = 8$  Hz, 1H), 7.96 (d,  $J = 8$  Hz, 1H), 7.90 (d,  $J = 8$  Hz, 1H), 7.77 (q,  $J = 2$  Hz, 4H), 7.63 (t,  $J = 8$  Hz, 1H), 7.57 (d,  $J = 8$  Hz, 1H), 7.47-7.42 (m, 6H);  $^{13}\text{C}$  NMR (100MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 178.4, 156.1, 148.6, 137.3, 135.9, 133.9, 132.5, 132.4, 131.6, 130.2, 129.8, 128.9, 128.8, 128.7, 128.6, 128.2, 127.7, 127.4.

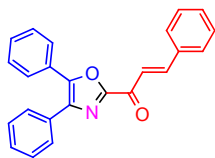
126.7, 125.6. HRMS (ESI):  $m/z$   $[M+H]^+$  calcd for  $C_{26}H_{18}NO_2$ : 376.13321; found: 376.13307.



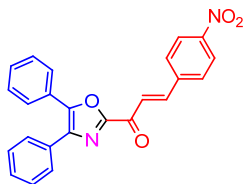
**(4,5-diphenyloxazol-2-yl)(9H-fluoren-2-yl)methanone (3m)** (214mg, 52% yield): mp=201.8-203.7; IR spectrum (KBr  $cm^{-1}$ ) 1645, 1611, 1511, 1476, 1444, 1334, 1203, 1124, 766, 693;  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  (ppm) 8.71 (q,  $J = 8$  Hz, 2H), 7.87 (q,  $J = 8$  Hz, 2H), 7.74 (s, 4H), 7.58 (d,  $J = 7.2$  Hz, 1H), 7.40 (d,  $J = 6.4$  Hz, 8H), 3.98 (s, 2H);  $^{13}C$  NMR (100MHz,  $CDCl_3$ )  $\delta$  (ppm) 178.3, 156.2, 148.5, 147.2, 144.8, 143.1, 140.4, 137.2, 133.6, 131.7, 130.6, 129.7, 128.8, 128.7, 128.6, 127.7, 127.5, 127.3, 127.0, 125.2, 121.1, 119.6, 37.0. HRMS (ESI):  $m/z$   $[M+H]^+$  calcd for  $C_{29}H_{20}NO_2$ : 414.14886; found: 414.14872.



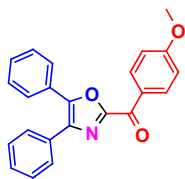
**[1,1'-biphenyl]-4-yl(4,5-diphenyloxazol-2-yl)methanone (3n)** (208mg, 52% yield): mp=166.8-171.3; IR spectrum (KBr  $cm^{-1}$ ) 1646, 1601, 1512, 1477, 1444, 1336, 1181, 913, 771, 749, 694;  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  (ppm) 8.67 (d,  $J = 8$  Hz, 2H), 7.76 (t,  $J = 8$  Hz, 6H), 7.67 (d,  $J = 8$  Hz, 2H), 7.51-7.43 (m, 9H);  $^{13}C$  NMR (100MHz,  $CDCl_3$ )  $\delta$  (ppm) 178.1, 156.0, 148.6, 146.4, 139.8, 137.3, 134.0, 131.6, 129.8, 128.9, 128.8, 128.7, 128.3, 128.2, 127.7, 127.3, 127.1. HRMS (ESI):  $m/z$   $[M+H]^+$  calcd for  $C_{28}H_{20}NO_2$ : 402.14886; found: 402.14862.



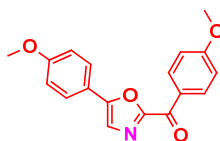
**(E)-1-(4,5-diphenyloxazol-2-yl)-3-phenylprop-2-en-1-one (3o)** (246mg, 70% yield): mp=154.0-157.5; IR spectrum (KBr  $cm^{-1}$ ) 1665, , 1605, 1574, 1511, 1475, 1444, 1352, 1077, 1049, 771, 693;  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  (ppm) 8.05 (d,  $J = 16$  Hz, 1H), 7.91 (d,  $J = 16$  Hz, 1H), 7.73 (t,  $J = 6$  Hz, 6H), 7.47-7.40 (m, 9H);  $^{13}C$  NMR (100MHz,  $CDCl_3$ )  $\delta$  (ppm) 176.1, 157.2, 149.0, 145.8, 137.5, 134.4, 131.5, 131.1, 130.4, 129.8, 128.9, 128.8, 128.7, 128.2, 127.6, 127.3, 121.3. HRMS (ESI):  $m/z$   $[M+H]^+$  calcd for  $C_{24}H_{18}NO_2$ : 352.13321; found: 352.13298.



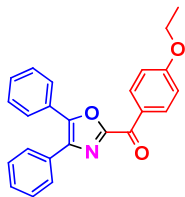
**(E)-1-(4,5-diphenyloxazol-2-yl)-3-(4-nitrophenyl)prop-2-en-1-one (3p)** (293mg, 74% yield): mp=162.1-166.1; IR spectrum (KBr  $cm^{-1}$ ) 1669, 1612, 1593, 1519, 1476, 1445, 1342, 1048, 778, 691;  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  (ppm) 8.29 (d,  $J = 8$  Hz, 2H), 8.03 (s, 2H), 7.86 (d,  $J = 8$  Hz, 2H), 7.72 (t,  $J = 8$  Hz, 4H), 7.47-7.41(m, 6H);  $^{13}C$  NMR (100MHz,  $CDCl_3$ )  $\delta$  (ppm) 175.4, 156.8, 149.6, 148.7, 142.2, 140.4, 137.8, 131.2, 130.1, 129.4, 129.0, 128.9, 128.8, 128.2, 127.3, 127.2, 125.1, 124.1. HRMS (ESI):  $m/z$   $[M+H]^+$  calcd for  $C_{24}H_{17}N_2O_4$ : 397.11828 ; found: 397.11771.



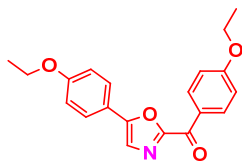
**(4,5-diphenyloxazol-2-yl)(4-methoxyphenyl)methanone (3q)** (188mg, 53% yield): mp=144.2-148.4; IR spectrum (KBr  $\text{cm}^{-1}$ ) 1646, 1592, 1506, 1338, 1260, 1213, 1169, 913, 771, 697;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 8.64 (d,  $J = 8$  Hz, 2H), 7.73 (d,  $J = 5.2$  Hz, 4H), 7.45-7.40 (m, 6H), 7.01 (d,  $J = 8$  Hz, 2H), 3.90 (s, 3H);  $^{13}\text{C}$  NMR (100MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 177.0, 164.2, 156.1, 148.2, 137.0, 133.4, 131.6, 129.7, 128.7, 128.6, 128.2, 127.7, 127.3, 113.7, 55.5. HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{23}\text{H}_{18}\text{NO}_3$ : 356.12812 ; found: 356.12787.



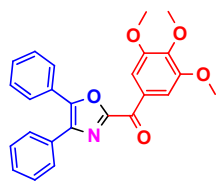
**(4-methoxyphenyl)(5-(4-methoxyphenyl)oxazol-2-yl)methanone (4q)** (59mg, 38% yield): mp=151.0-153.5; IR spectrum (KBr  $\text{cm}^{-1}$ ) 1644, 1599, 1566, 1482, 1424, 1306, 1248, 1158, 1023, 905, 828, 634;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 8.53 (d,  $J = 8.8$  Hz, 2H), 7.76 (d,  $J = 8.8$  Hz, 2H), 7.47 (s, 1H), 7.00 (t,  $J = 8.8$  Hz, 4H), 3.90 (s, 3H), 3.86(s, 3H);  $^{13}\text{C}$  NMR (100MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 177.0, 164.1, 160.1, 156.8, 154.0, 133.2, 128.3, 127.0, 122.3, 119.5, 114.5, 113.7, 55.5, 55.4. HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{18}\text{H}_{16}\text{NO}_4$ : 310.10738 ; found: 310.10709.



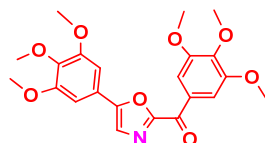
**(4,5-diphenyloxazol-2-yl)(4-ethoxyphenyl)methanone (3r)** (203mg, 55% yield): mp=141.8-144.7; IR spectrum (KBr  $\text{cm}^{-1}$ ) 1649, 1601, 1572, 1259, 1171, 1156, 913, 772, 694;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 8.63 (d,  $J = 8.8$  Hz, 2H), 7.73 (d,  $J = 5.6$  Hz, 4H), 7.44-7.40 (m, 6H), 7.00 (d,  $J = 8.8$  Hz, 2H), 4.15 (d,  $J = 7.6$  Hz, 2H), 1.47 (t,  $J = 6.8$  Hz, 3H);  $^{13}\text{C}$  NMR (100MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 177.0, 163.7, 156.2, 148.2, 137.0, 133.5, 131.7, 129.7, 128.8, 128.7, 128.2, 128.0, 127.8, 127.3, 114.2, 63.8, 14.6. HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{24}\text{H}_{20}\text{NO}_3$ : 370.14377 ; found: 370.14344.



**(4-ethoxyphenyl)(5-(4-ethoxyphenyl)oxazol-2-yl)methanone (4r)** (67mg, 40% yield): mp=128.1-135.4; IR spectrum (KBr  $\text{cm}^{-1}$ ) 1638, 1613, 1590, 1476, 1360, 1248, 1157, 1046, 1027, 1004, 829, 636;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 8.43 (d,  $J = 8.4$  Hz, 2H), 7.64 (d,  $J = 8.8$  Hz, 2H), 6.87 (t,  $J = 8.8$  Hz, 4H), 4.04-3.97 (m, 4H), 1.34(q,  $J = 6.4$  Hz, 6H);  $^{13}\text{C}$  NMR (100MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 176.9, 163.5, 160.2, 156.7, 154.0, 133.2, 128.0, 126.9, 122.2, 119.2, 114.9, 114.1, 63.7, 63.5, 14.6, 14.5. HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{20}\text{H}_{20}\text{NO}_4$ : 338.13868 ; found: 338.13844.

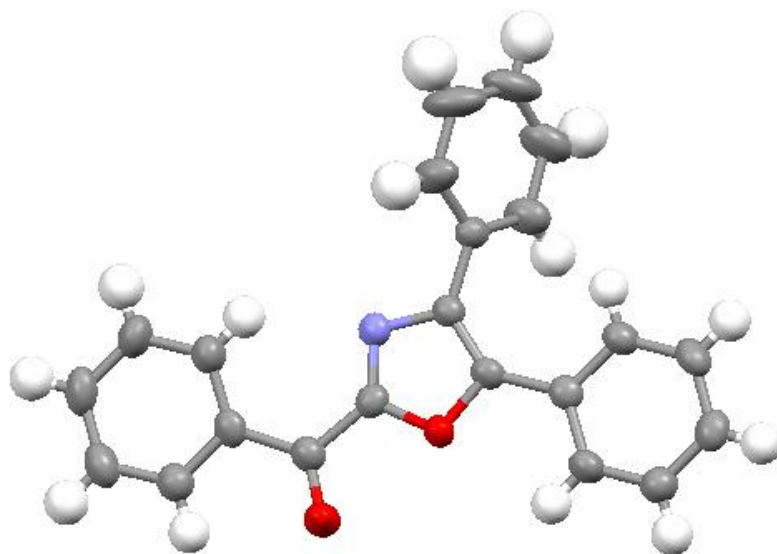


**(4,5-diphenyloxazol-2-yl)(3,4,5-trimethoxyphenyl)methanone (3s)** (207mg, 50% yield): mp=155.1-159.4; IR spectrum (KBr  $\text{cm}^{-1}$ ) 1656, 1582, 1503, 1474, 1416, 1372, 1344, 1244, 1167, 1126, 995, 771, 698;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 8.01 (s, 2H), 7.73 (t,  $J = 9$  Hz, 4H), 7.35 (t,  $J = 7.8$  Hz, 6H), 3.97 (d,  $J = 3$  Hz, 9H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 177.0, 156.0, 152.8, 148.5, 143.4, 137.0, 131.6, 130.1, 129.9, 128.8, 128.7, 128.0, 127.9, 127.7, 127.5, 127.3, 108.6, 60.9, 56.3, 56.2. HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{25}\text{H}_{22}\text{NO}_5$ : 416.14925 ; found: 416.15032.

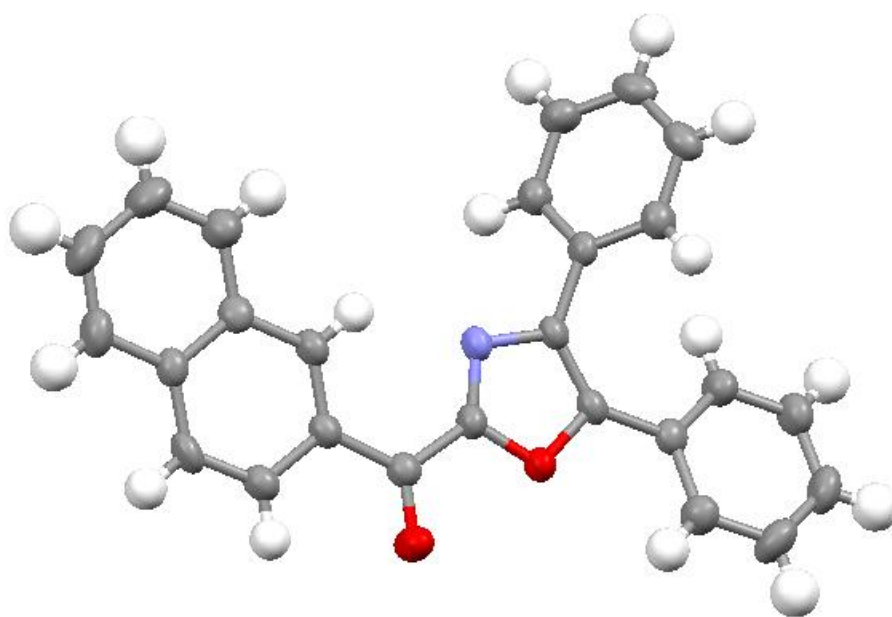


**(3,4,5-trimethoxyphenyl)(4-(3,4,5-trimethoxyphenyl)oxazol-2-yl)methanone (4s)** (88mg, 41% yield): mp=192.9-194.4; IR spectrum (KBr  $\text{cm}^{-1}$ ) 1644, 1583, 1486, 1454, 1416, 1356, 1321, 1238, 1131, 991, 770, 662;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 7.89 (s, 2H), 7.55 (s, 1H), 7.03 (s, 2H), 3.97 (t,  $J = 6$  Hz, 12H), 3.92 (s, 6H);  $^{13}\text{C}$  NMR (100MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 177.0, 156.9, 154.0, 153.8, 152.8, 143.4, 139.7, 130.1, 123.5, 122.1, 108.4, 102.6, 61.0, 56.3, 56.2. HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{22}\text{H}_{24}\text{NO}_8$ : 430.14964 ; found: 430.15036.

### 3. The X-ray crystal structures

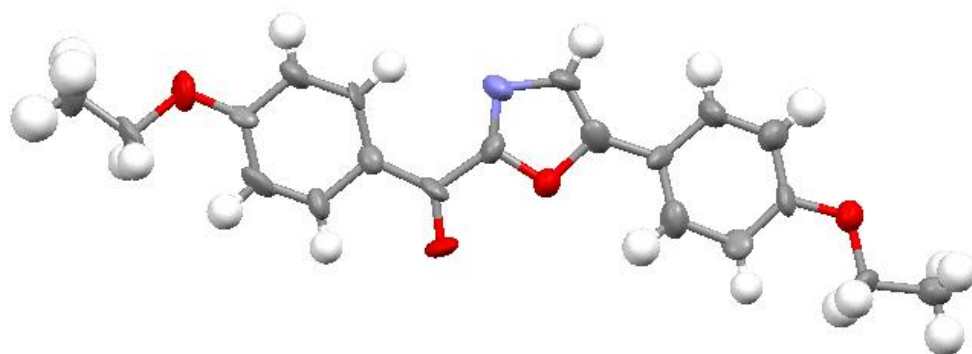


**Figure S 1.** Crystal structure of **3a** (some disordered parts were omitted for clarity).



**Figure S 2.** Crystal structure of **3l**.





**Figure S 3.** Crystal structure of **4r**.

#### 4. Mechanism for the for the formation of two types of oxazoles

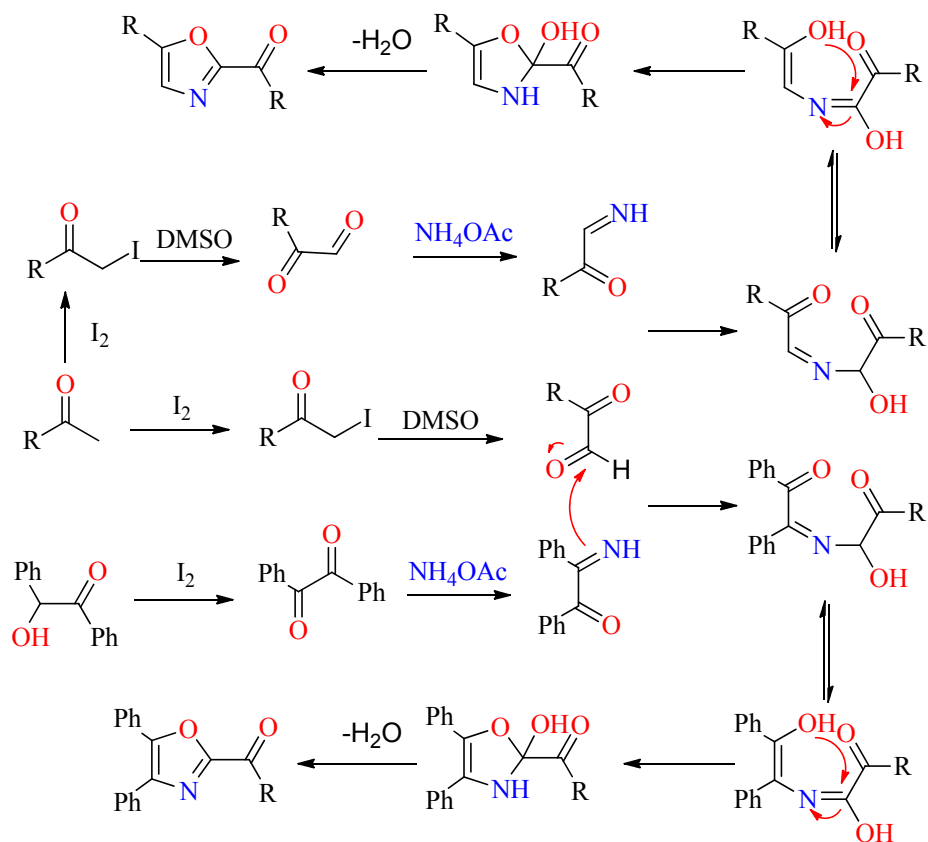


Figure S 4 Mechanism for the for the formation of two types of oxazoles.

When the aromatic rings bind electron-donating groups, aryl methyl ketones are faster to transform into phenylglyoxal than the formation of **7**. Phenylglyoxal can react with itself and **7** for the formation of oxazoles **4** and **3**. Contrary to this, when the aromatic rings don't bind electron-donating groups, the formation of **7** is faster than phenylglyoxal. Phenylglyoxal can react with **7** for the formation of oxazoles **3**. Yet **4** is less for isolated.

## 5. Intermediates reaction

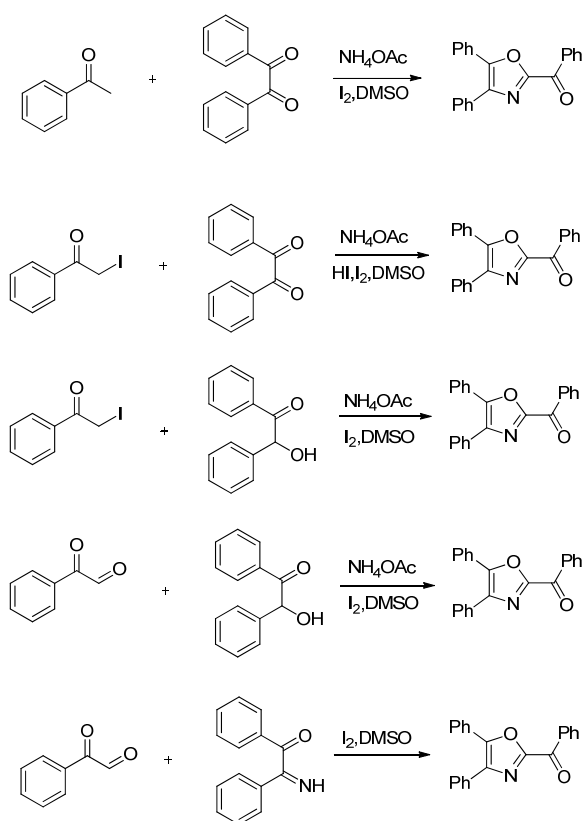


Figure S 5 Intermediates reaction

In order to prove that the reaction mechanism, we used **1a** with **5**, **6a** and **5**, **6a** with **2**, **8a** with **2** and **8a** with **7** to synthesize **3a**. Fortunately, we get **3a** from the above reactions.

## 6. The spectra of GC-MS

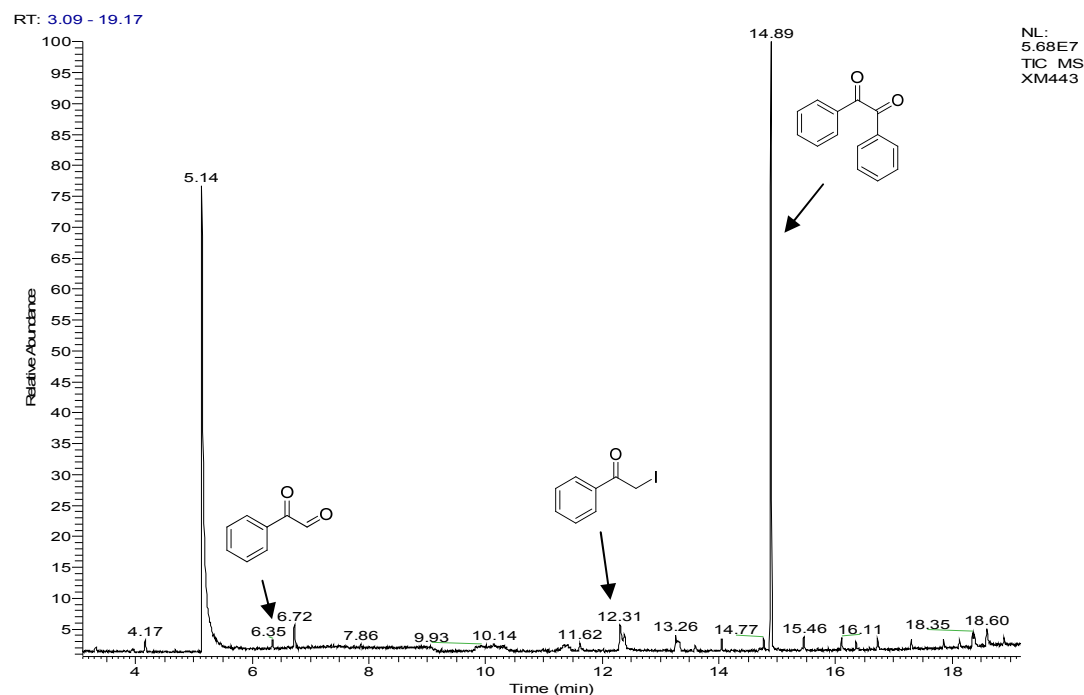


Figure S 6 GC-MS of the reaction.

The reaction mixture was stirred at 120 °C for 0.5h, CHCl<sub>3</sub> and H<sub>2</sub>O/Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> saturated solution were added, and the organic layer was separated to detect intermediates. From the spectrogram, we get the peaks of 4a, 6a and 5 which prove the reaction mechanism.

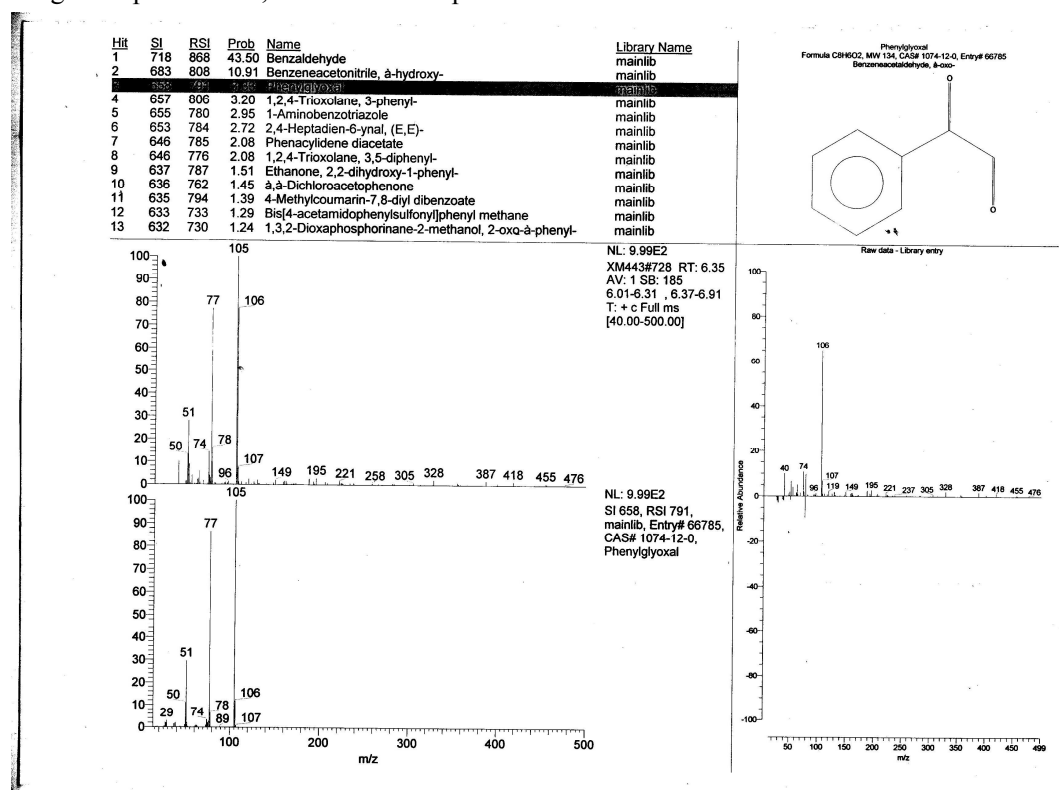


Figure S 7 GC-MS of the reaction.

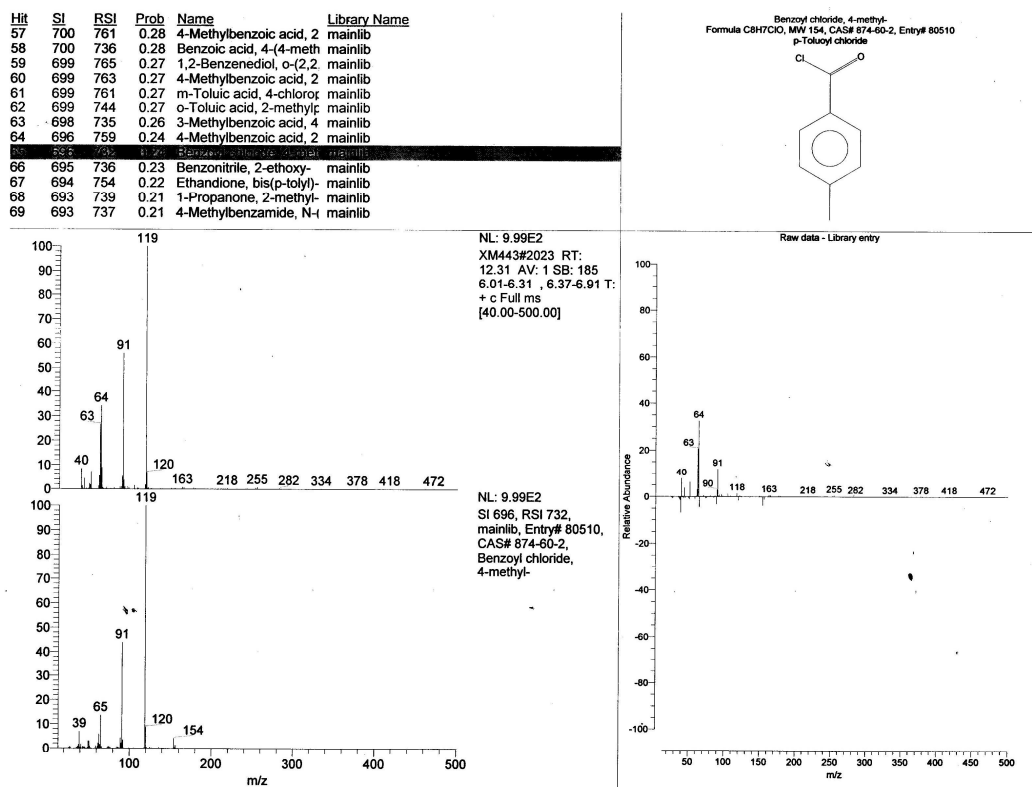


Figure S 8 GC-MS of the reaction.

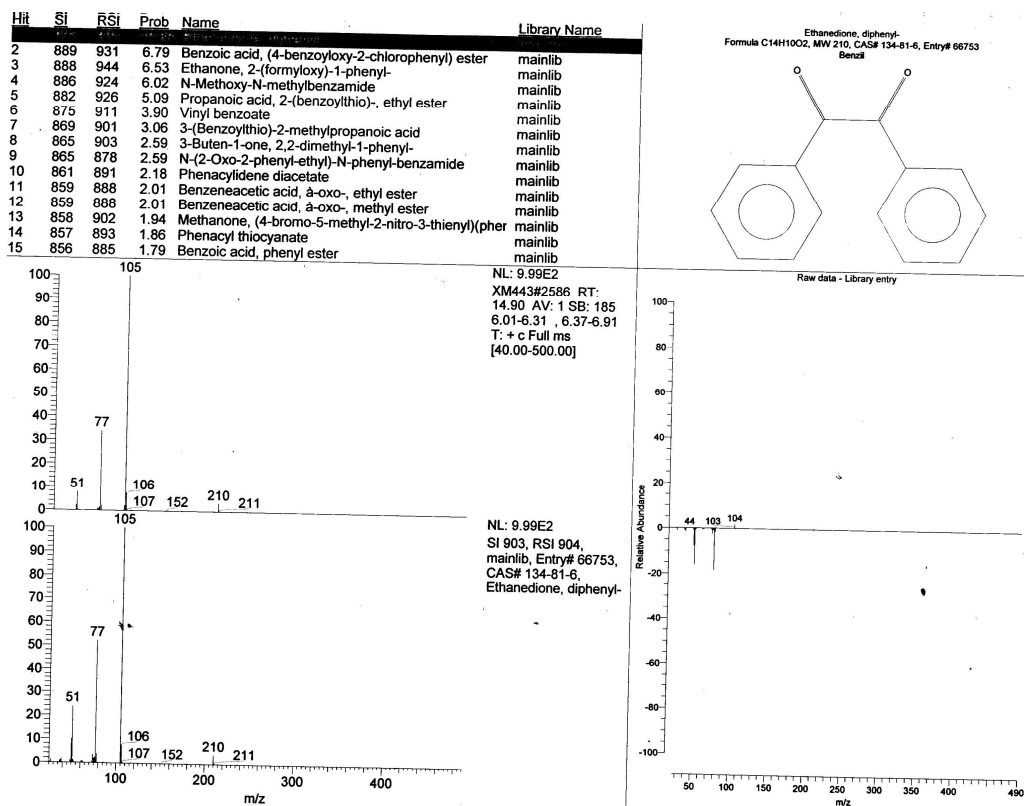
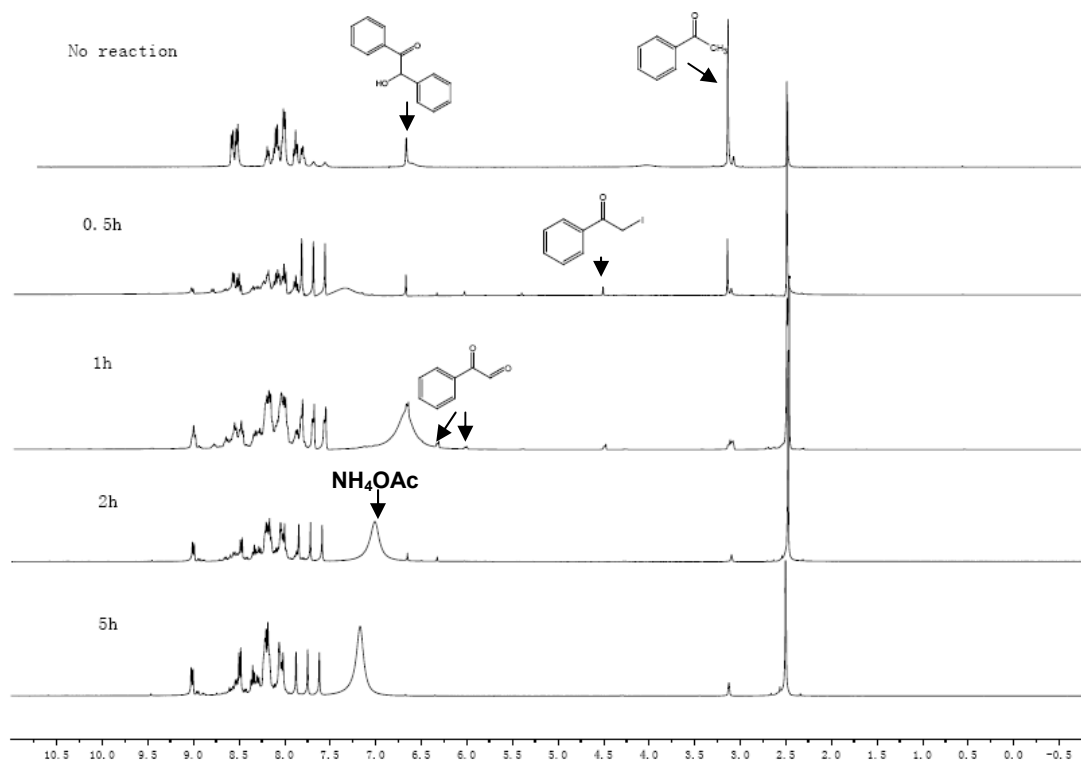


Figure S 9 GC-MS of the reaction.

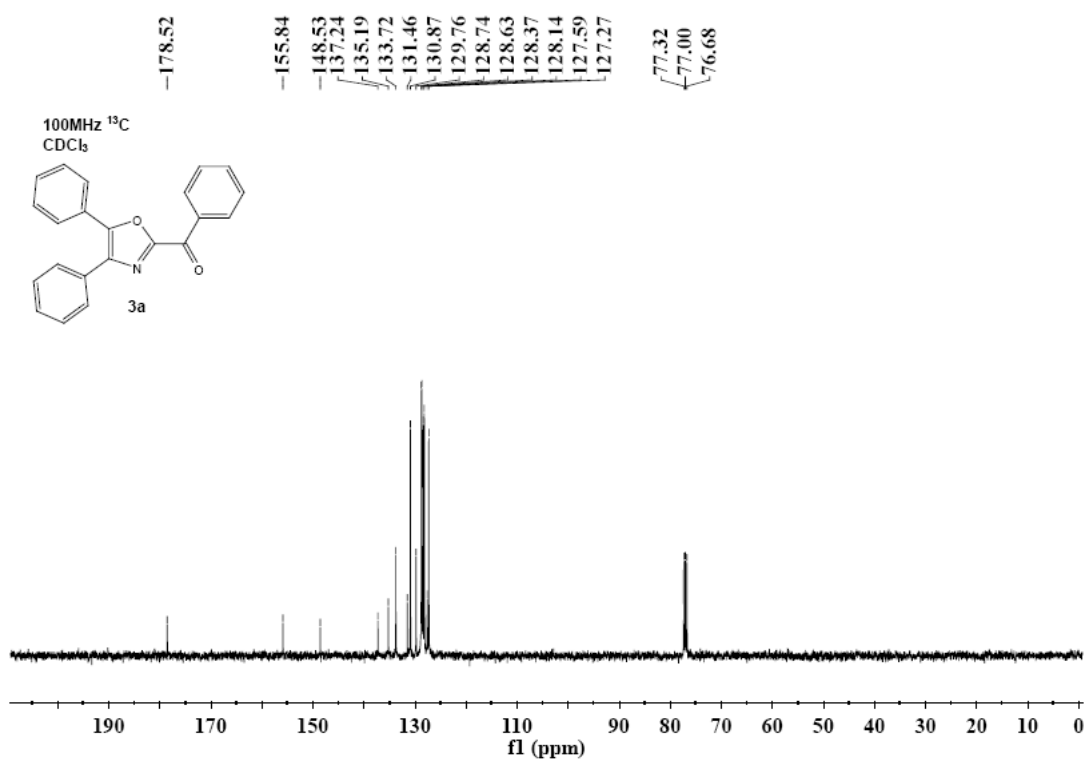
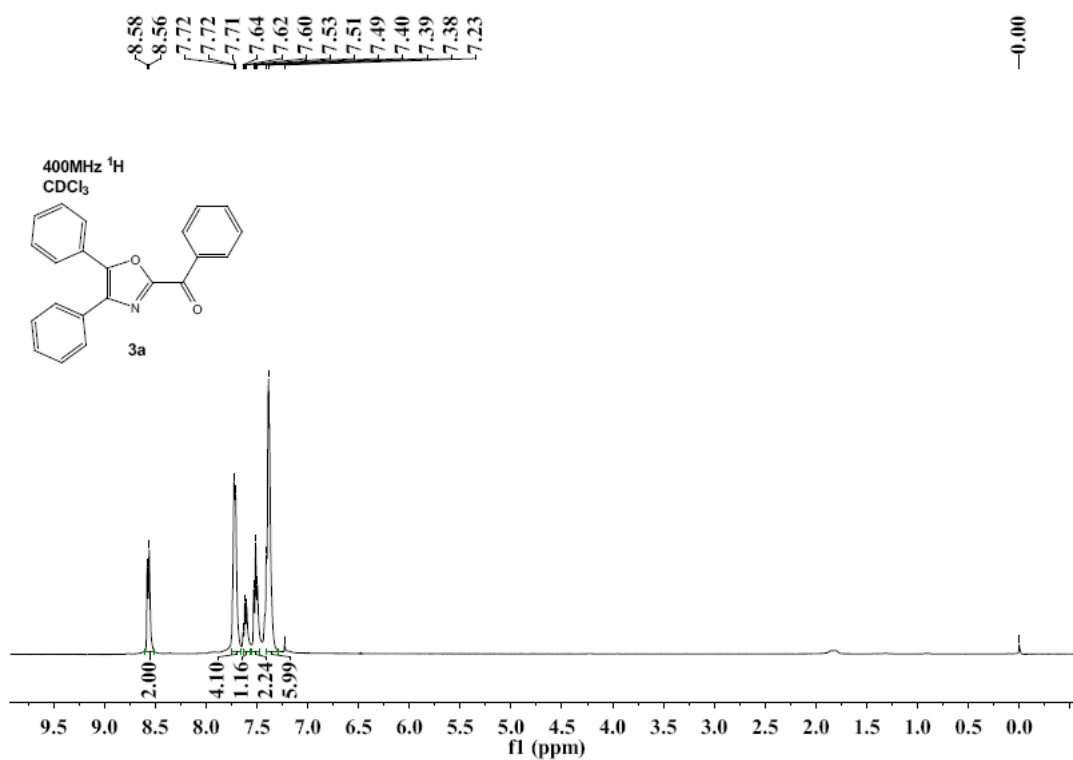
## 7. NMR analysis

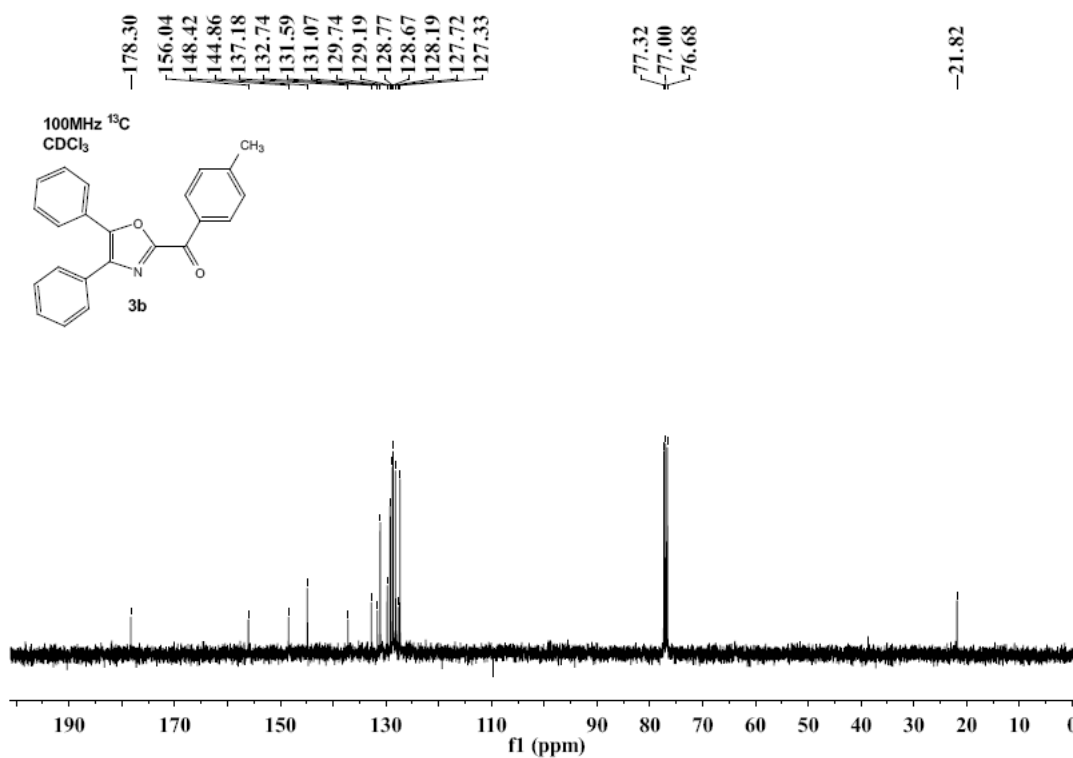
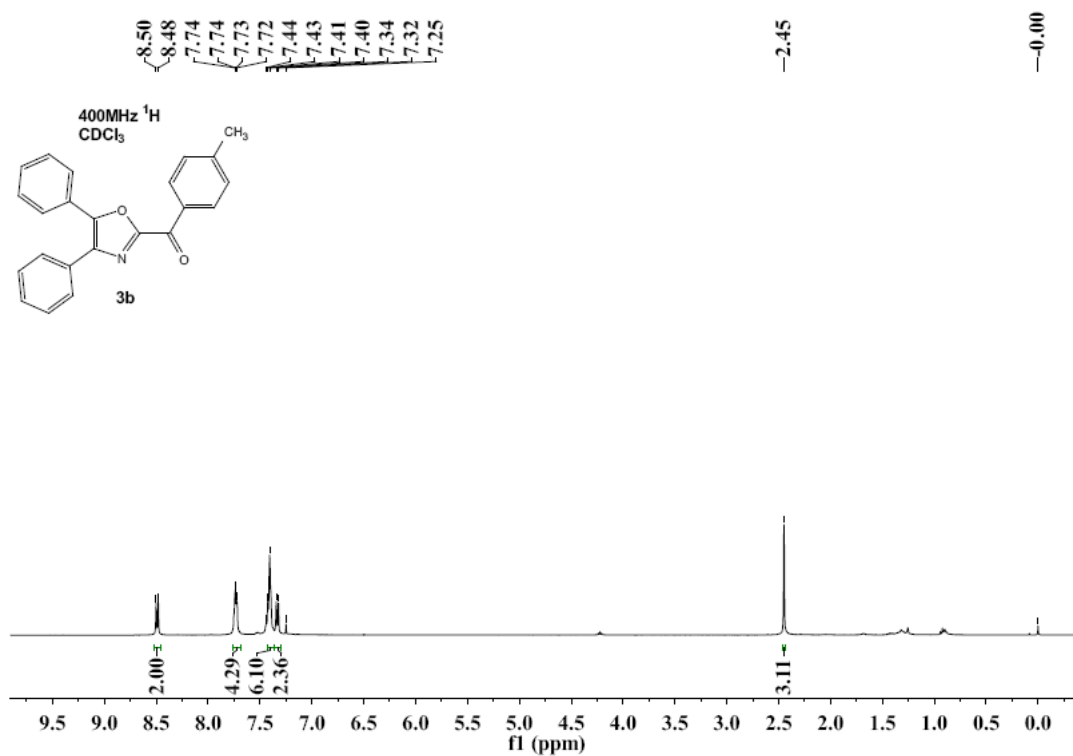


**Figure S 10** NMR of the reaction.

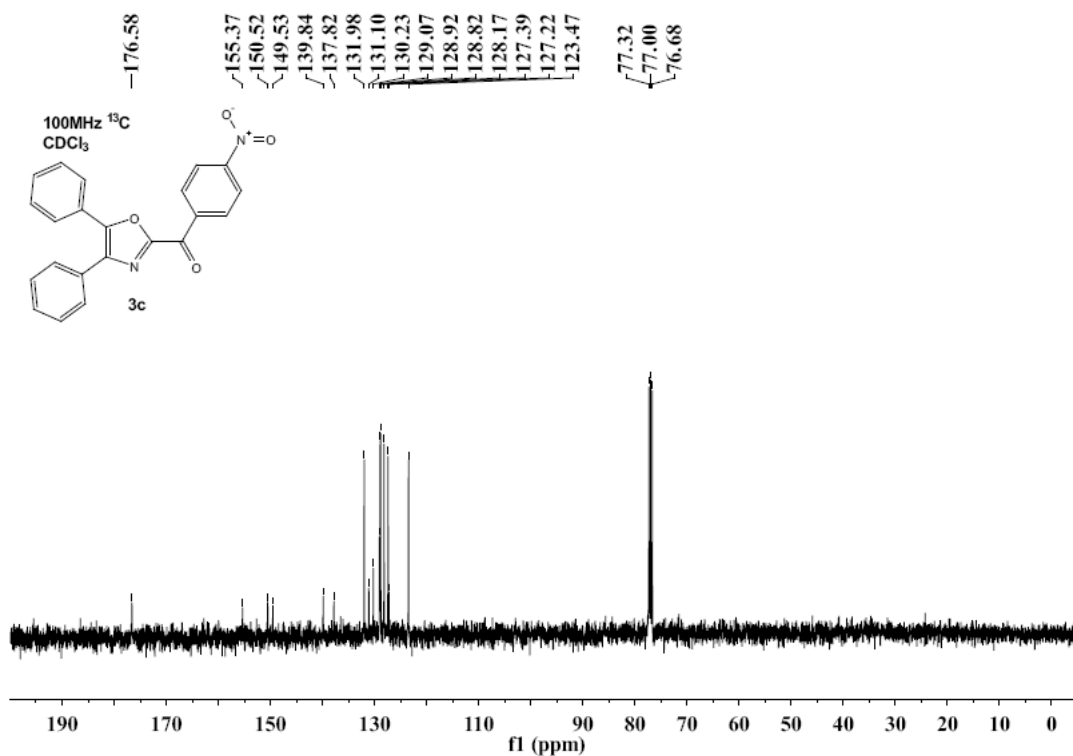
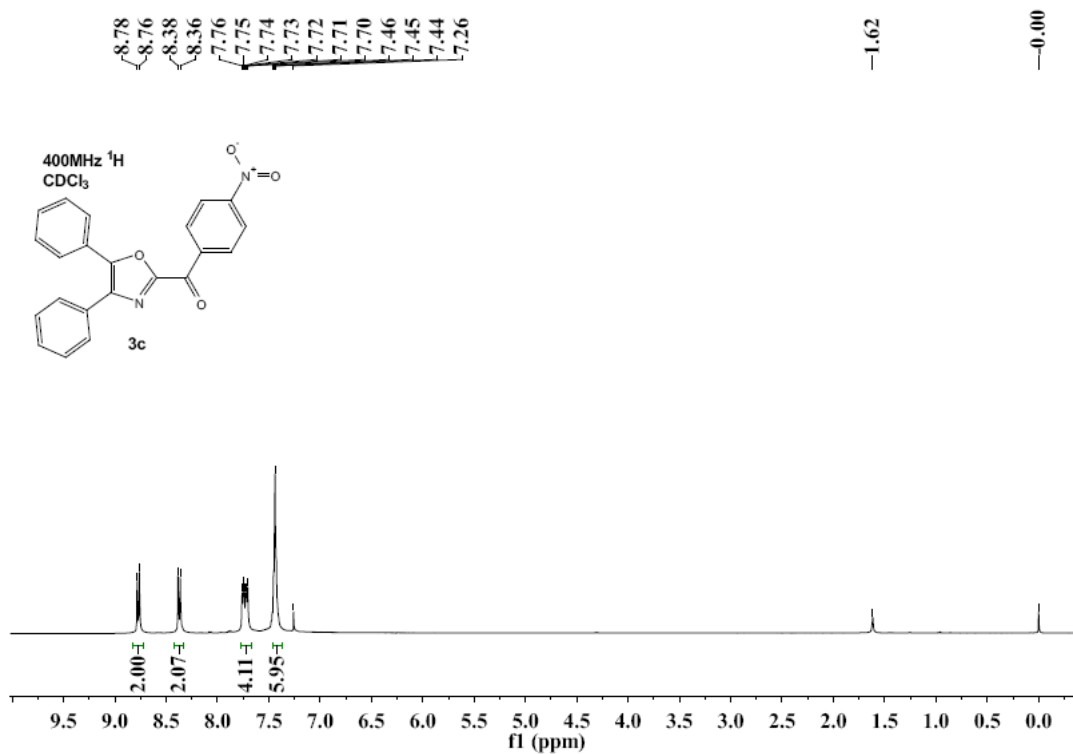
From the NMR of the reaction, we also get the peaks of 6a and 8a which prove the reaction mechanism.

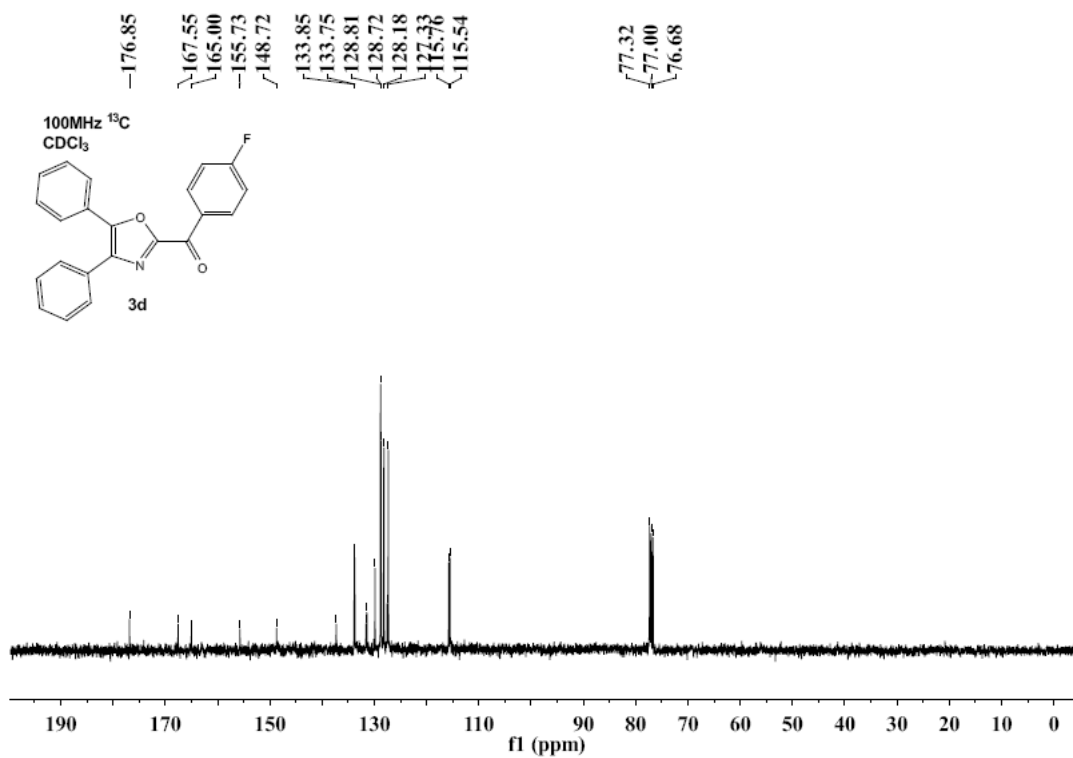
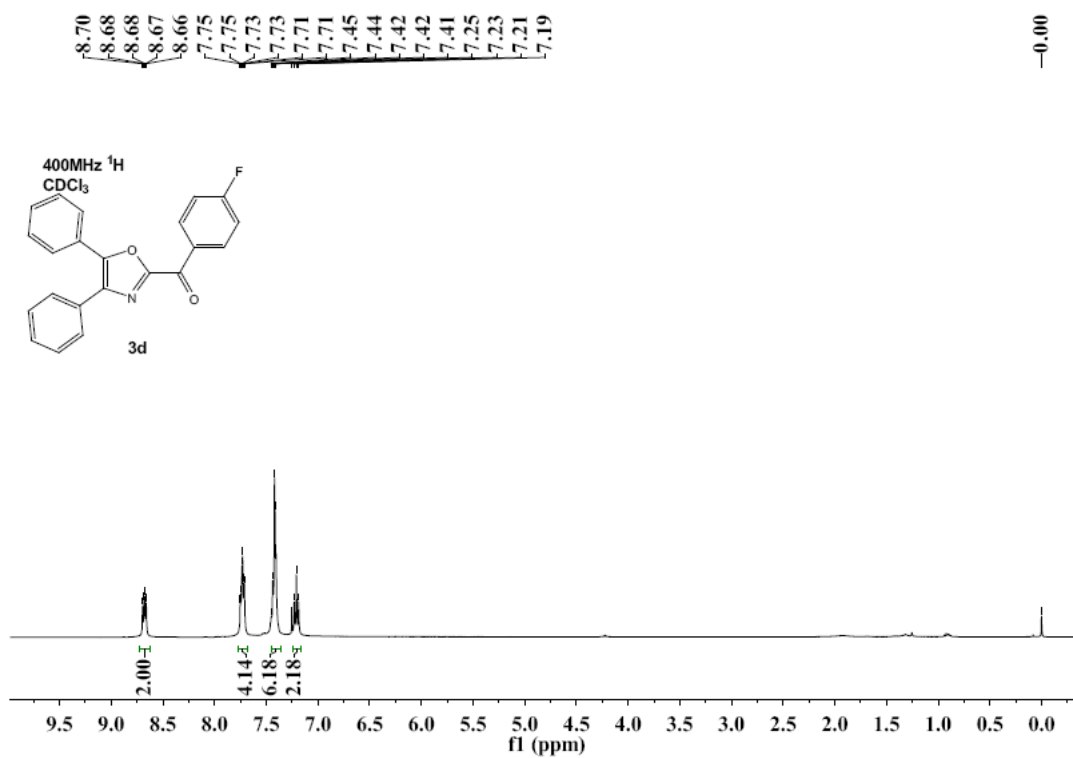
### 8. $^1\text{H}$ and $^{13}\text{C}$ NMR spectra $^1\text{H}$ and $^{13}\text{C}$ NMR spectra

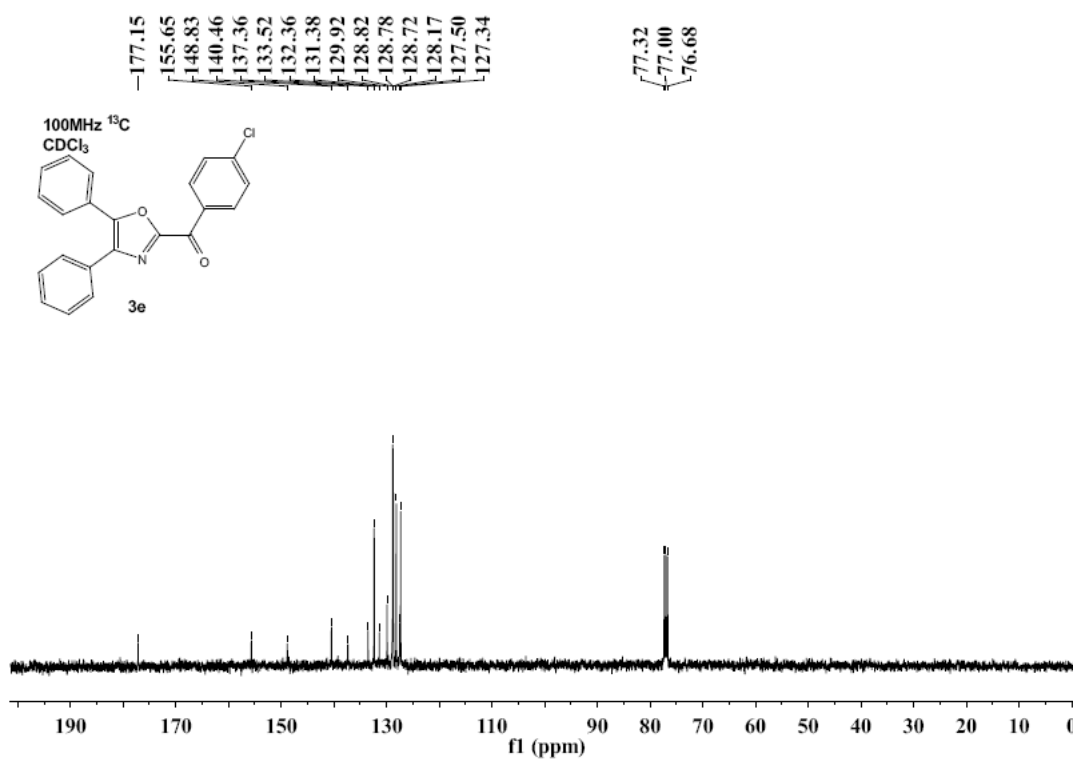
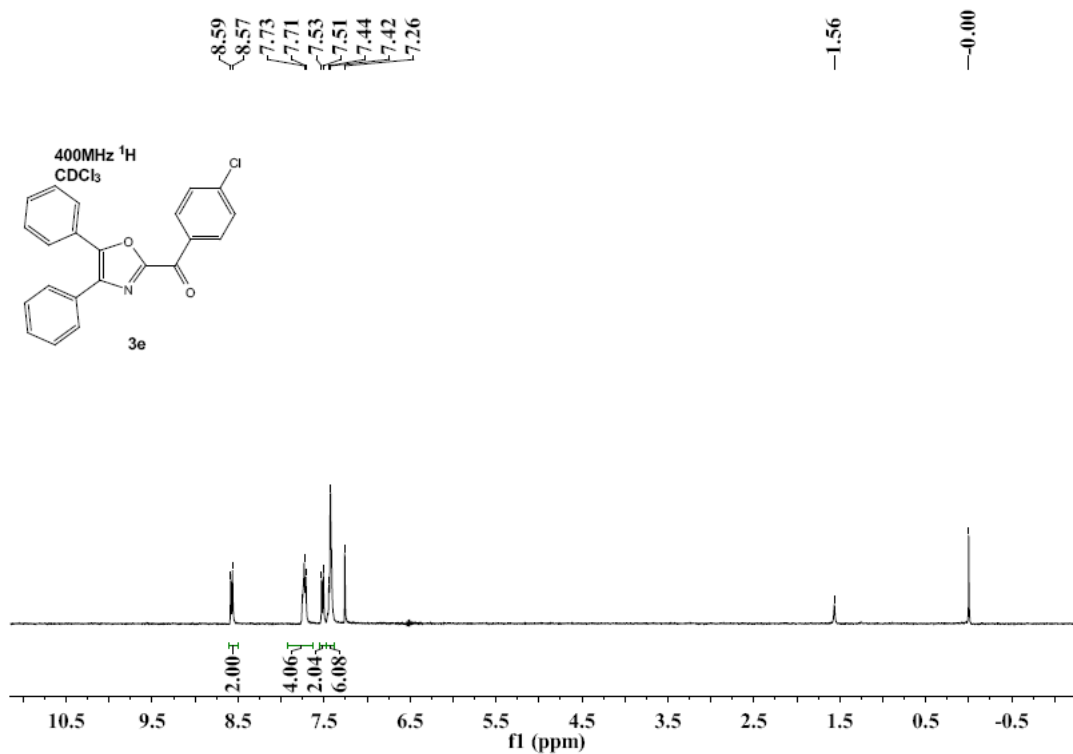


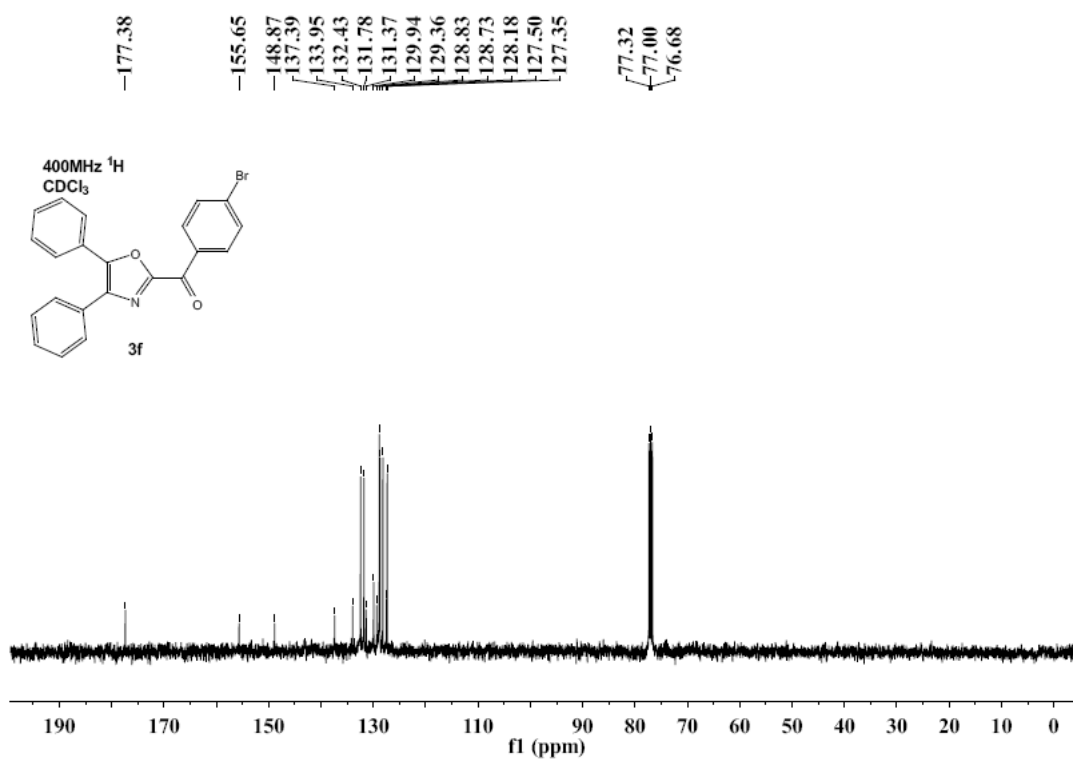
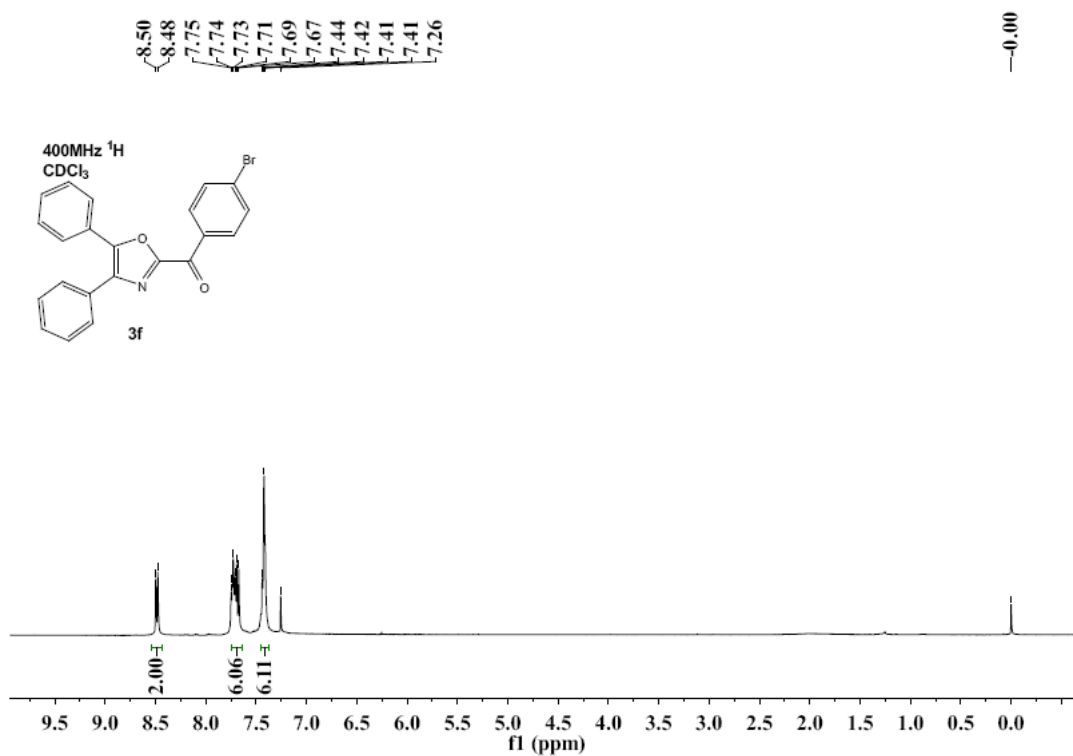


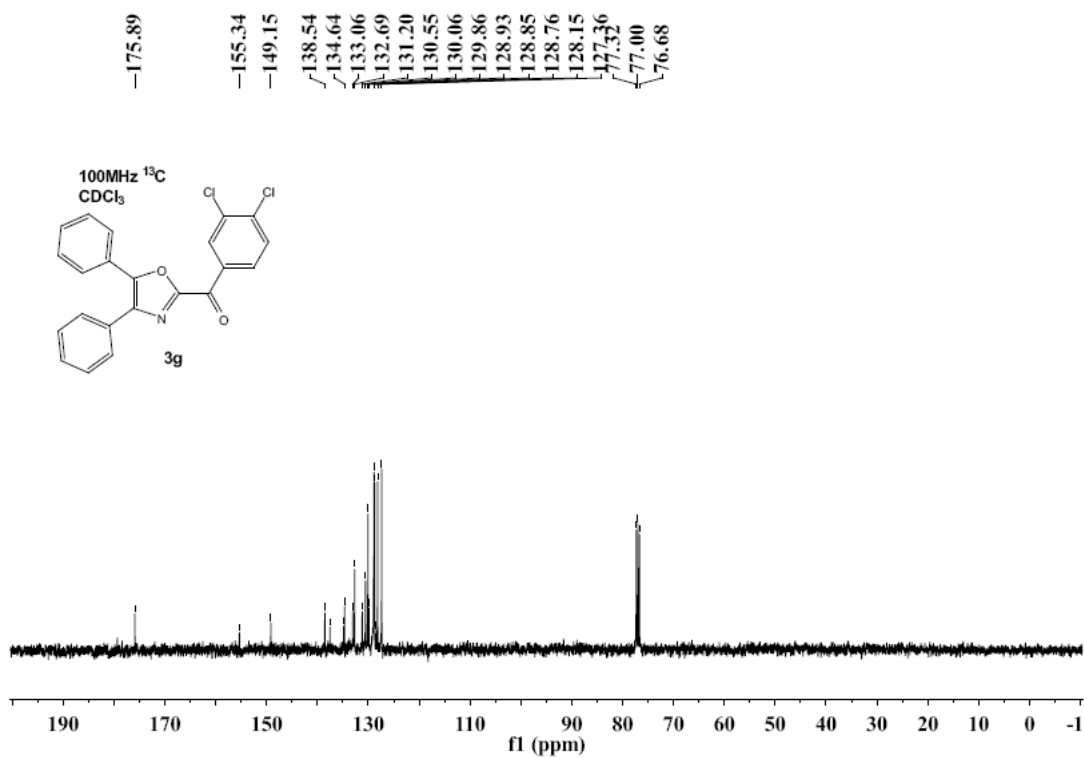
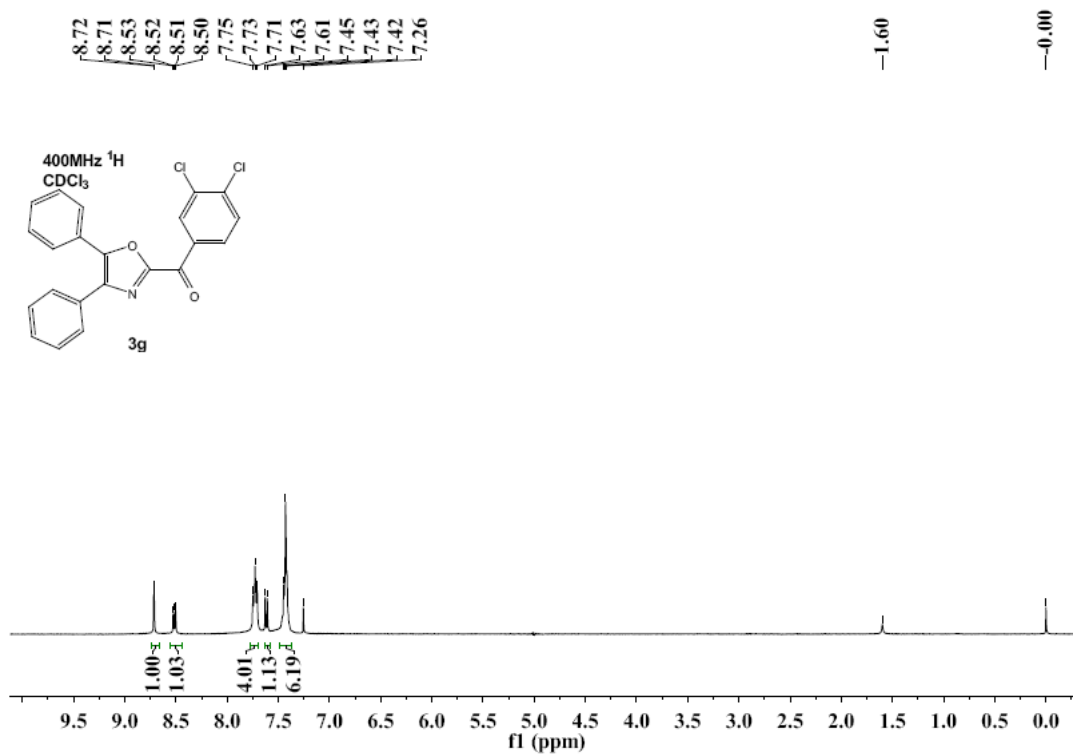


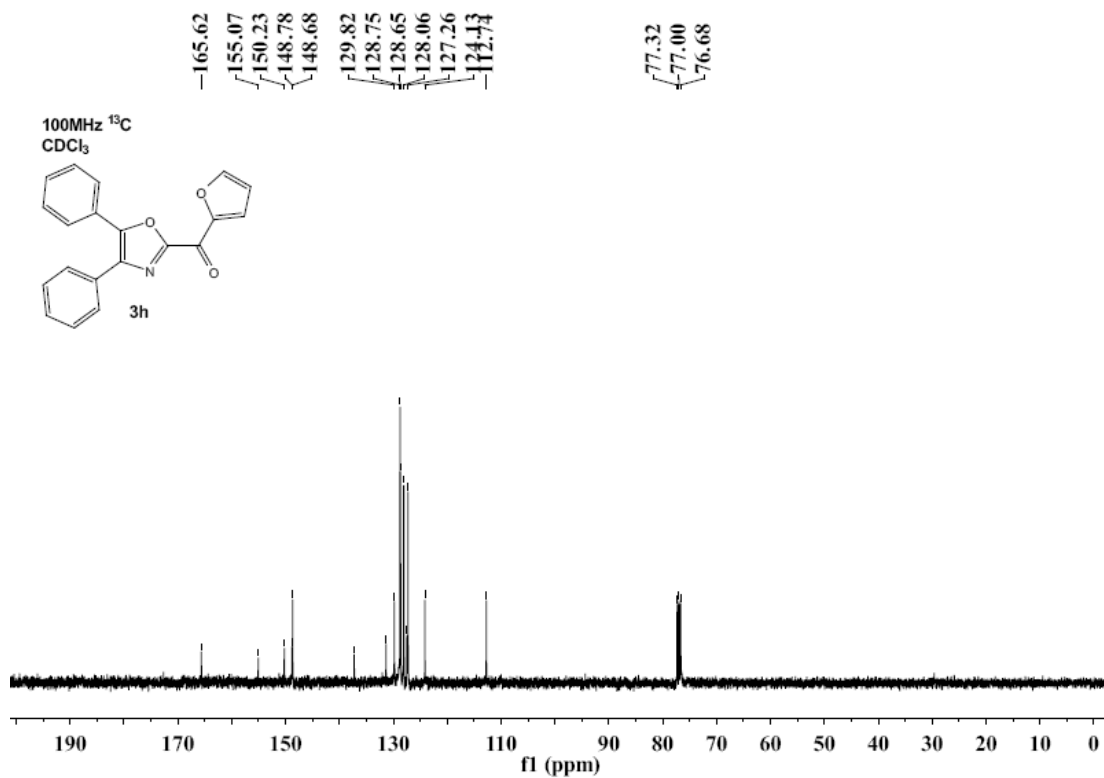
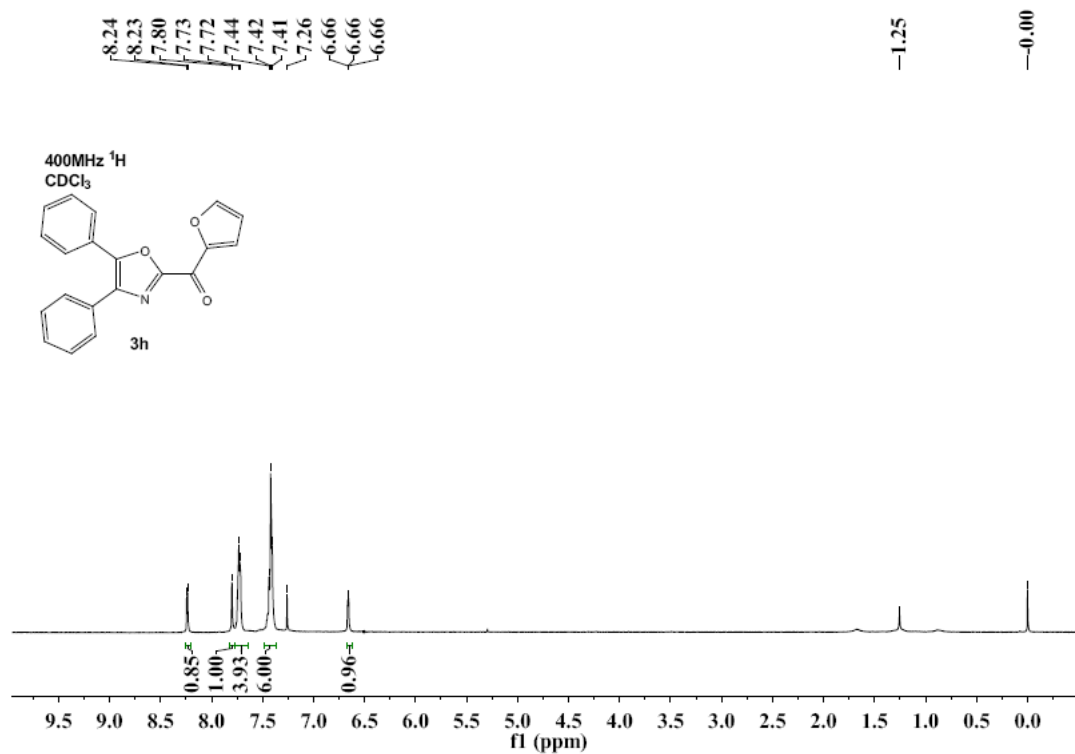


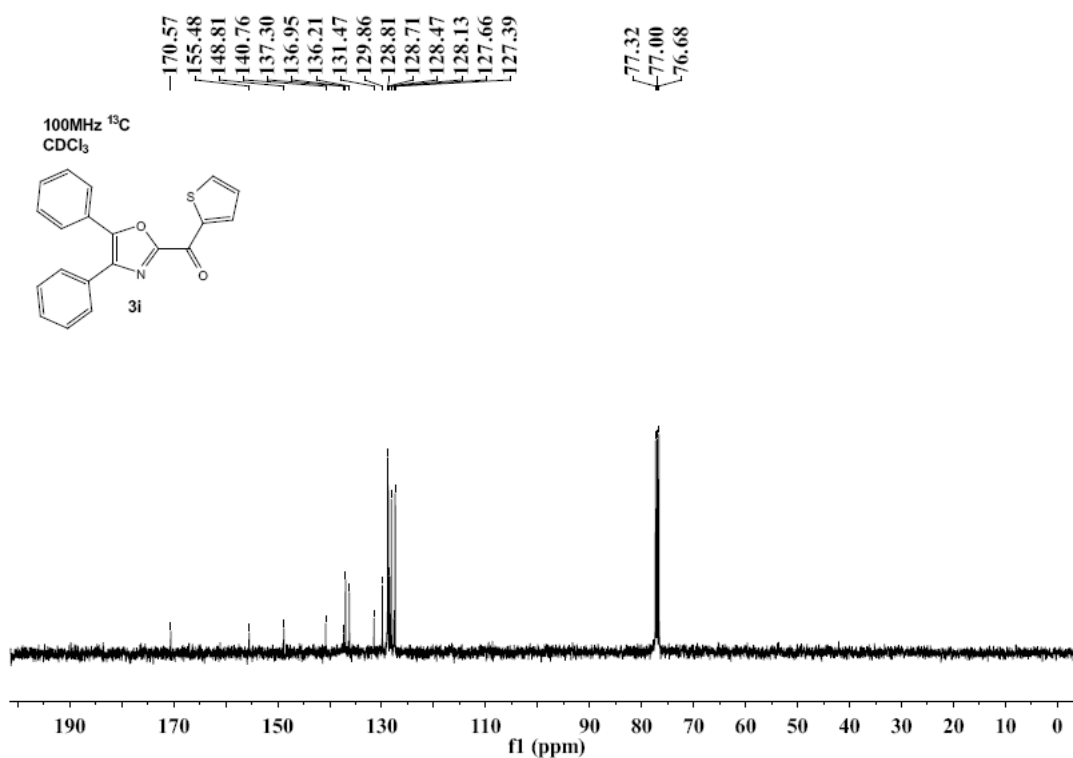
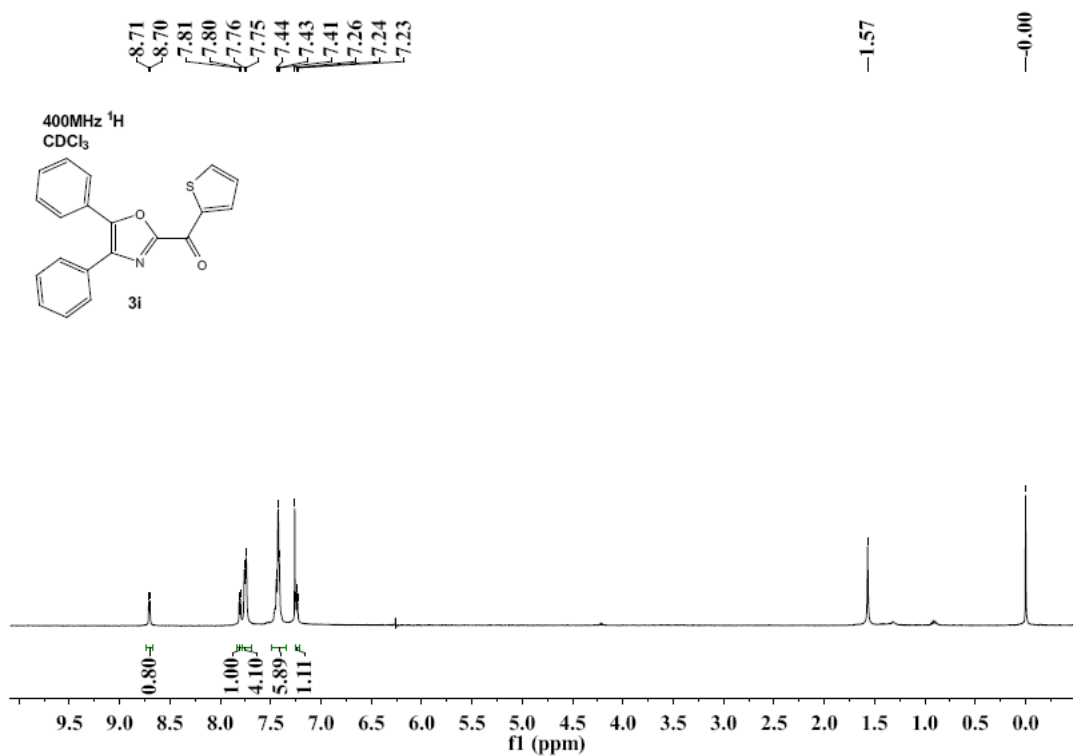


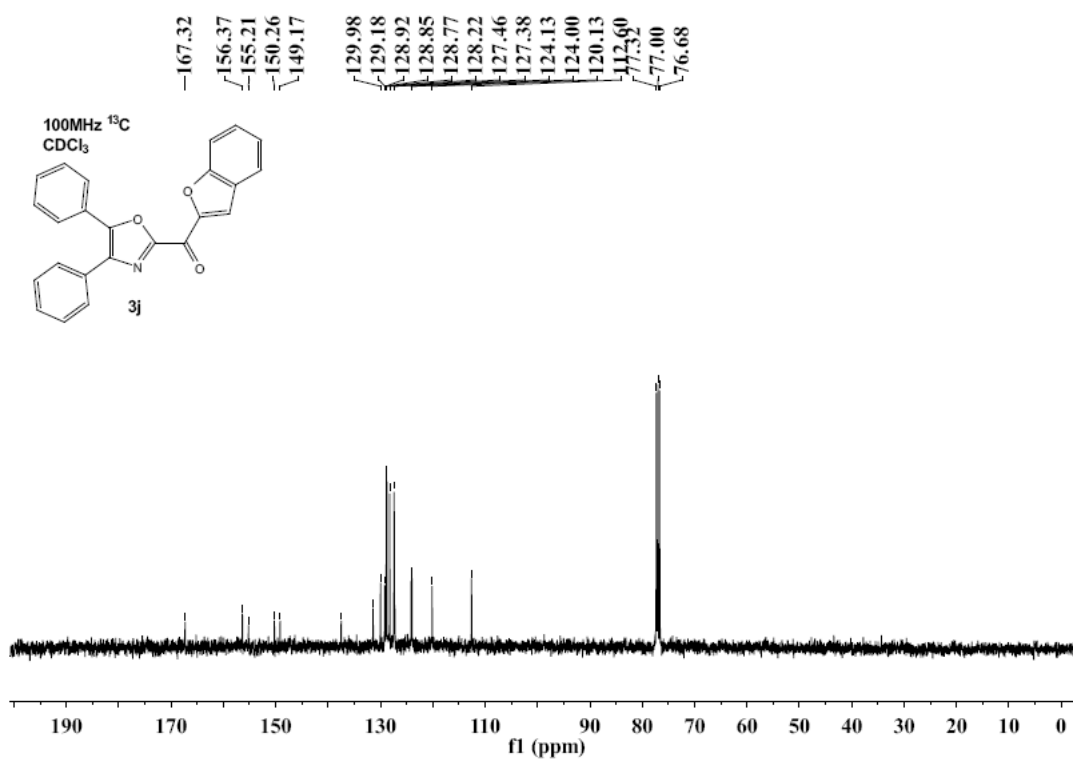
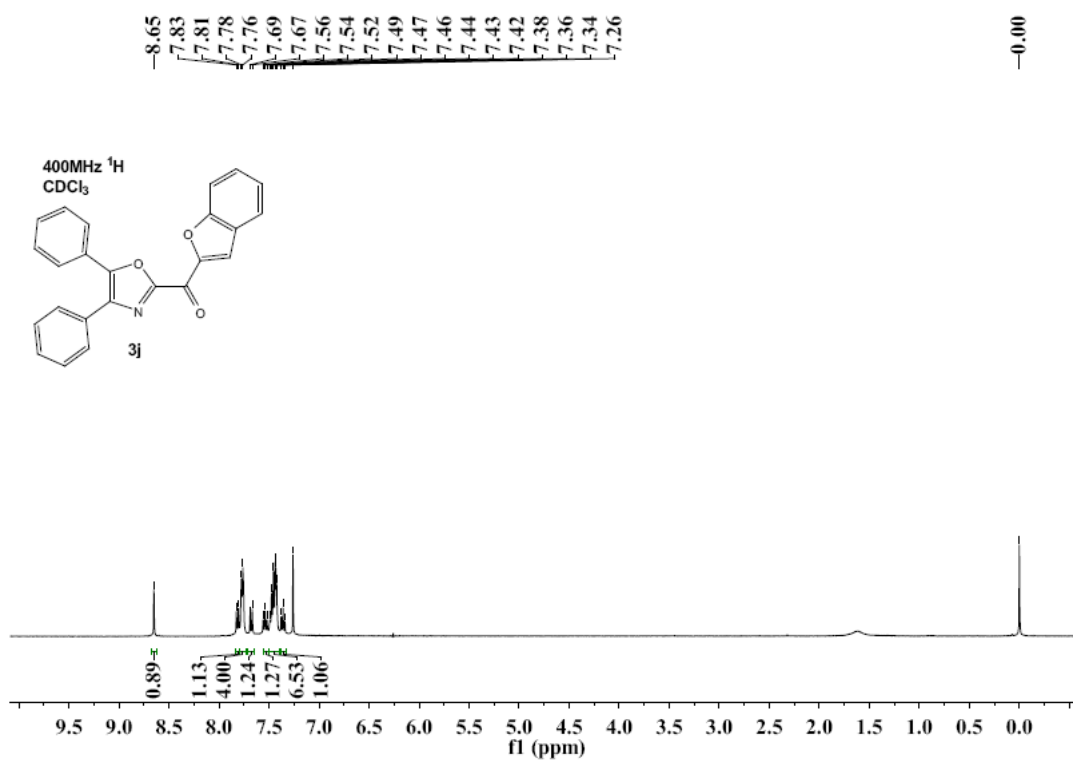






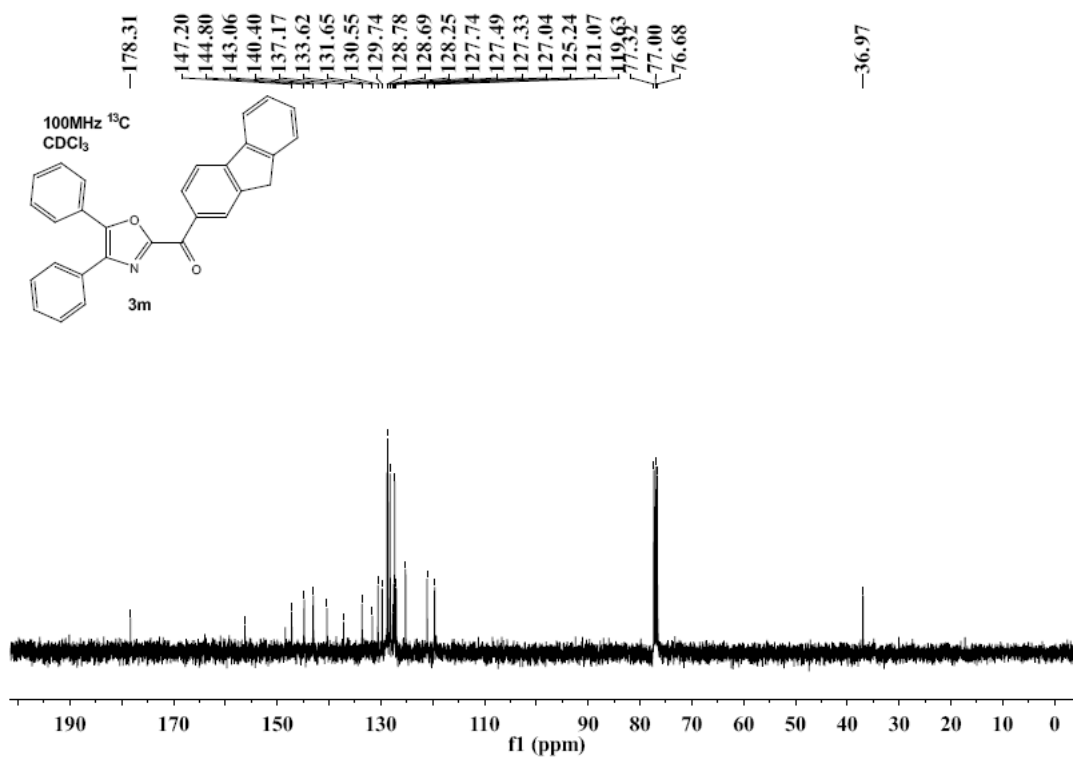
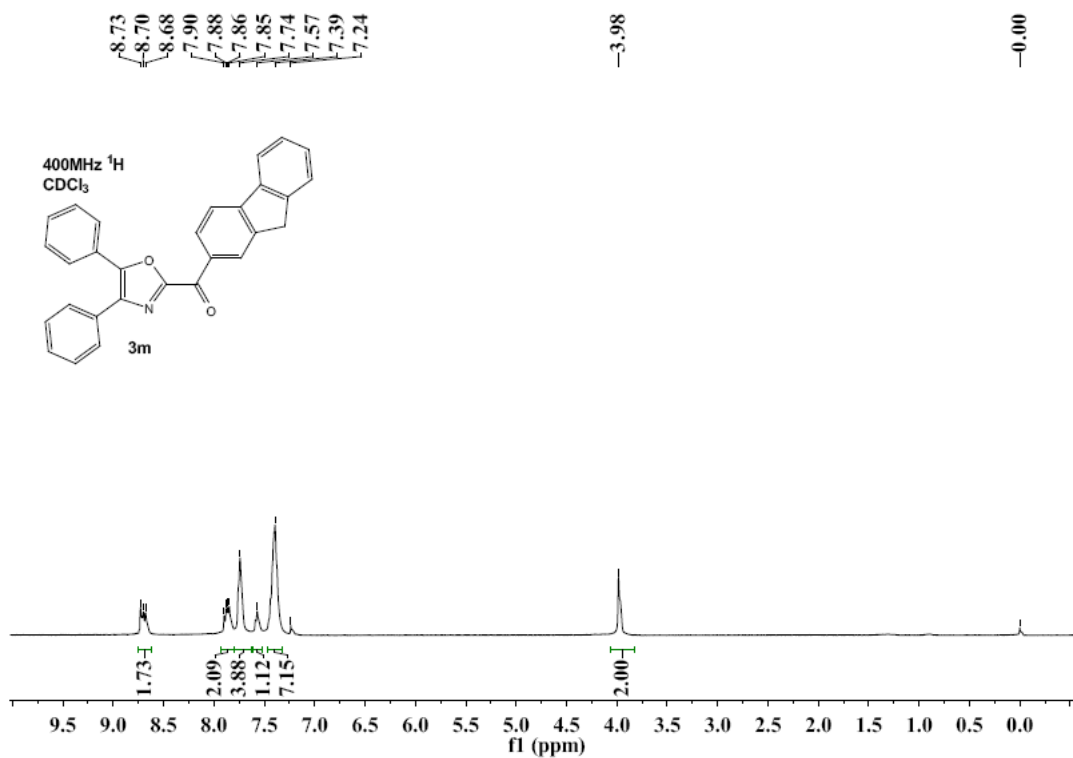


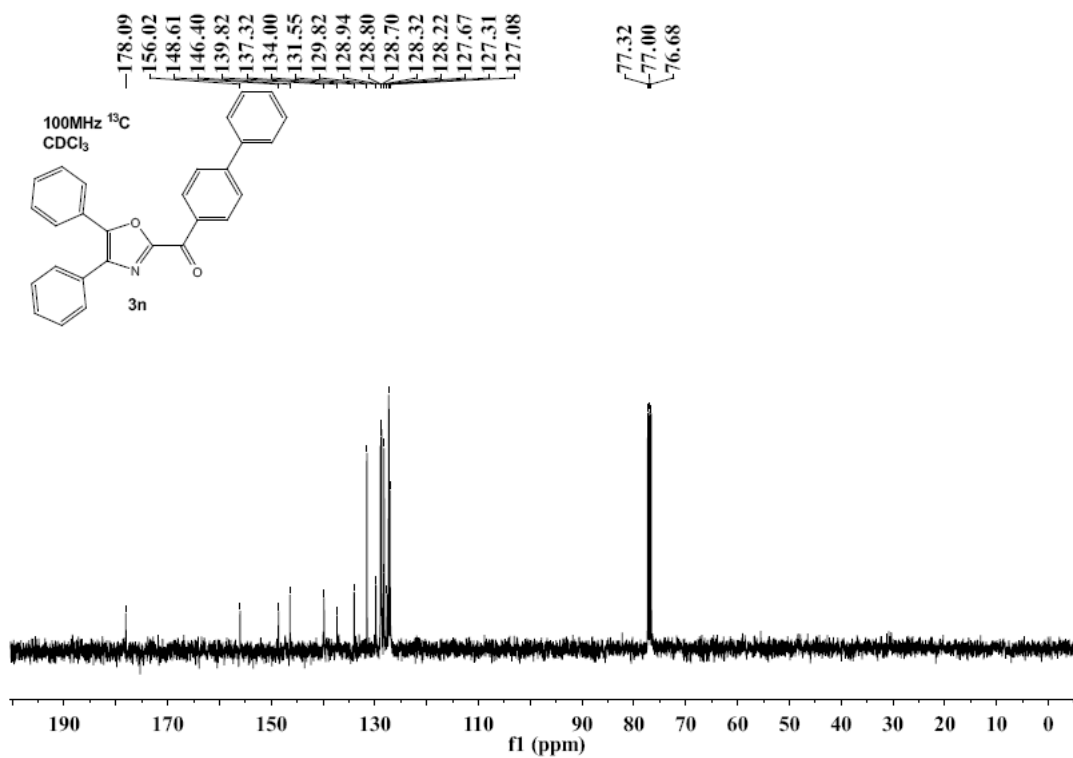
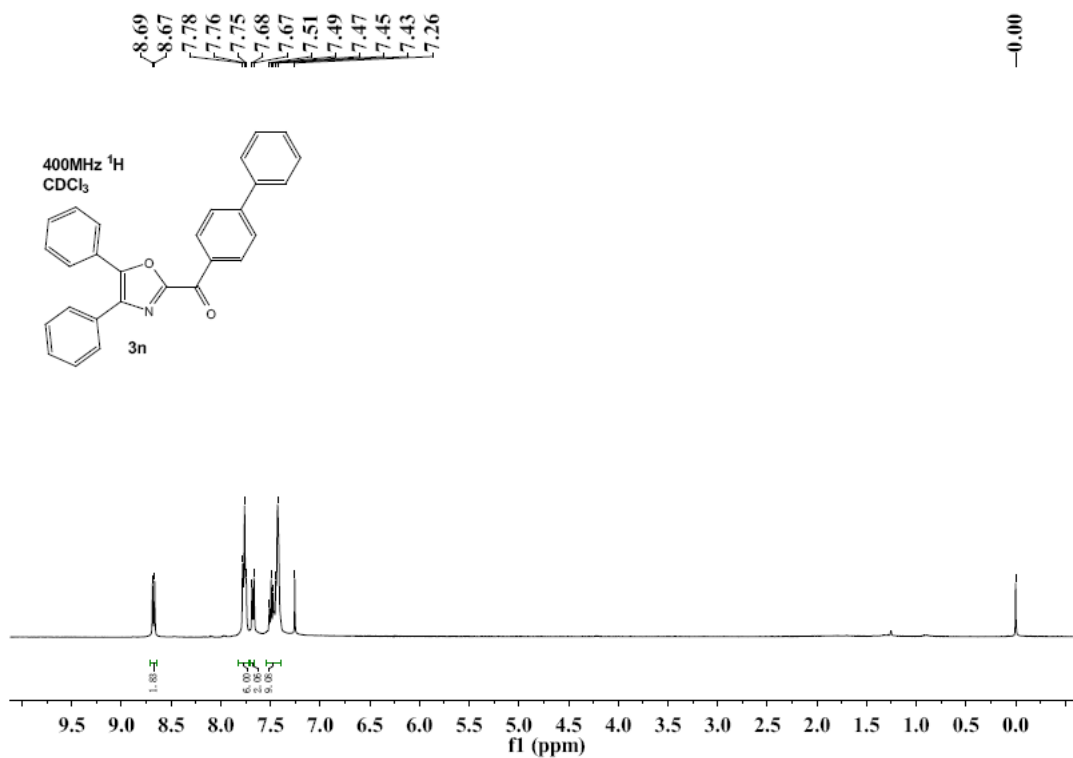


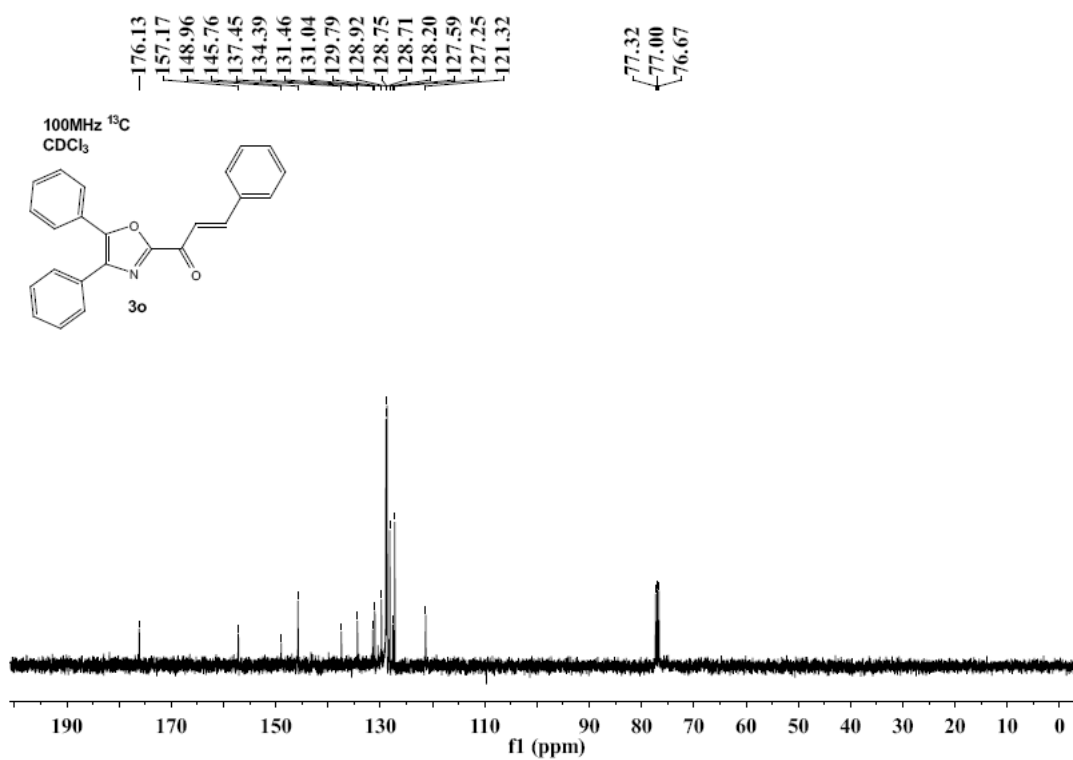
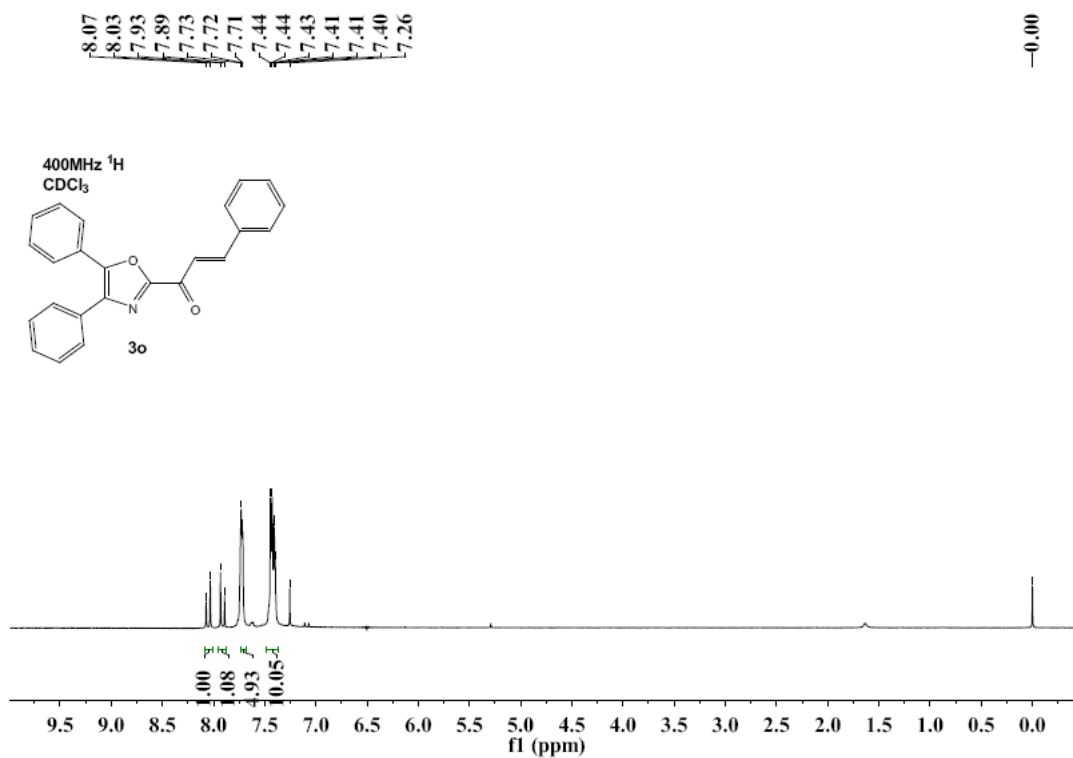


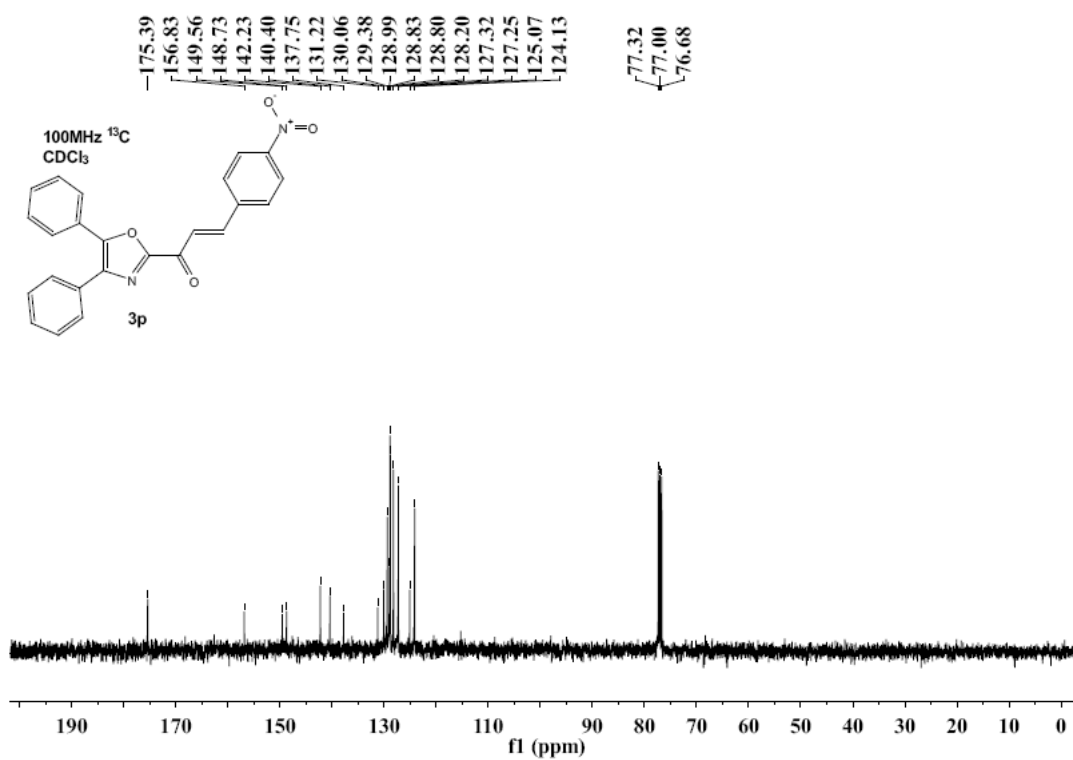
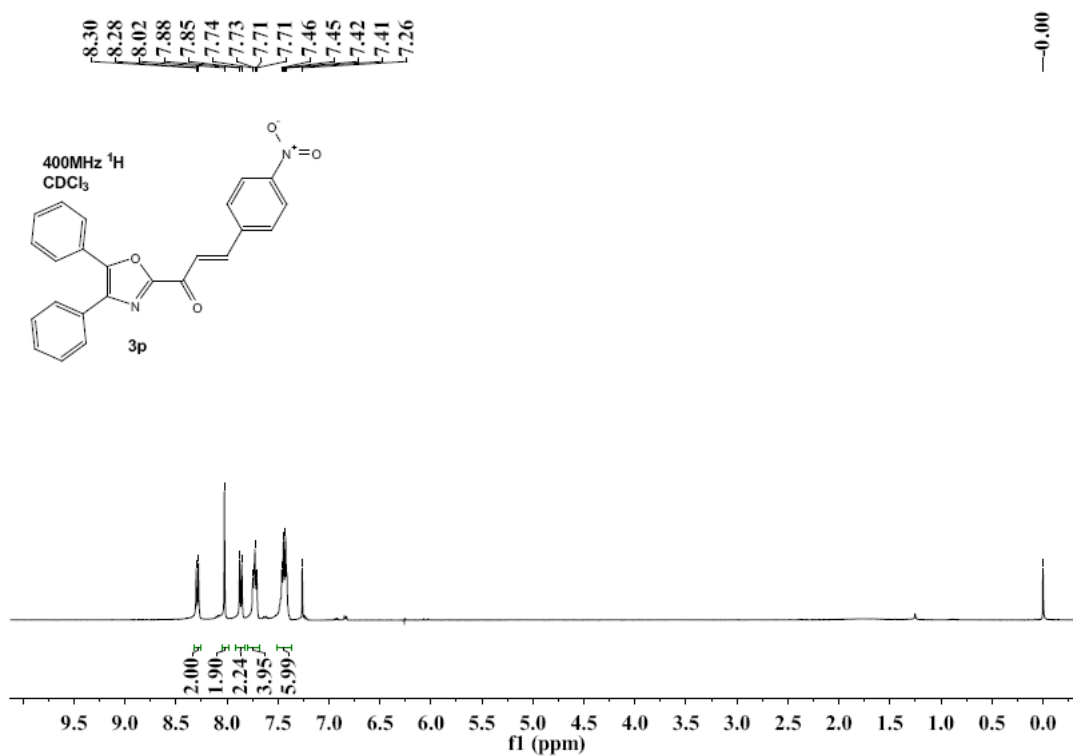


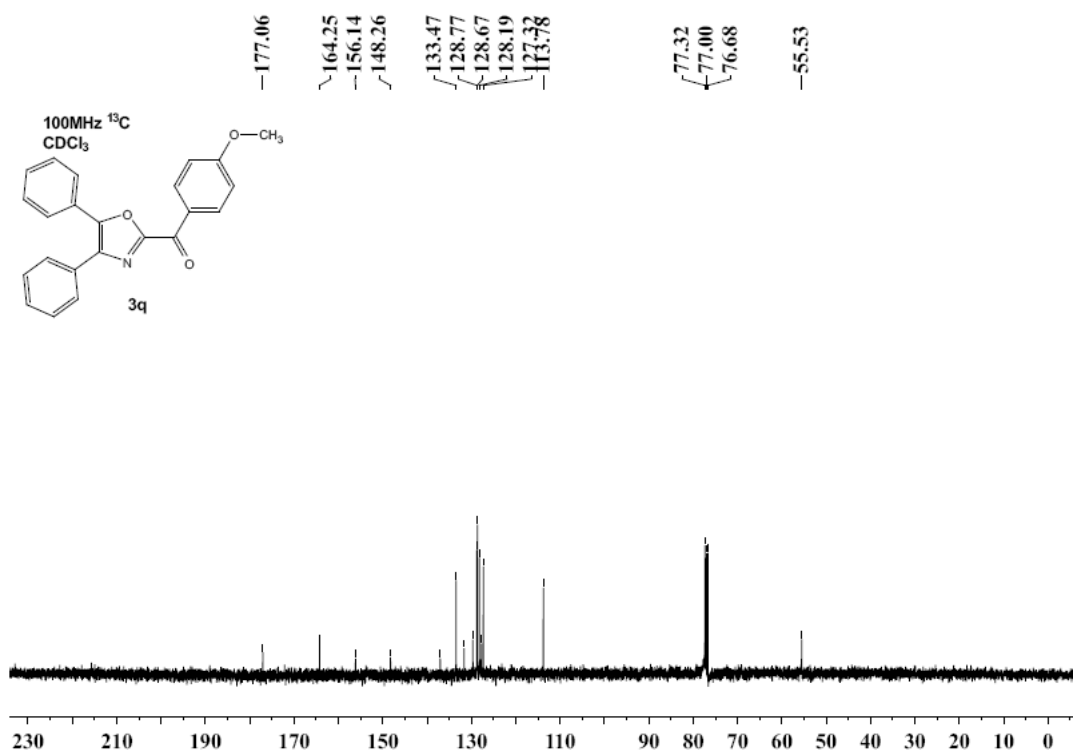
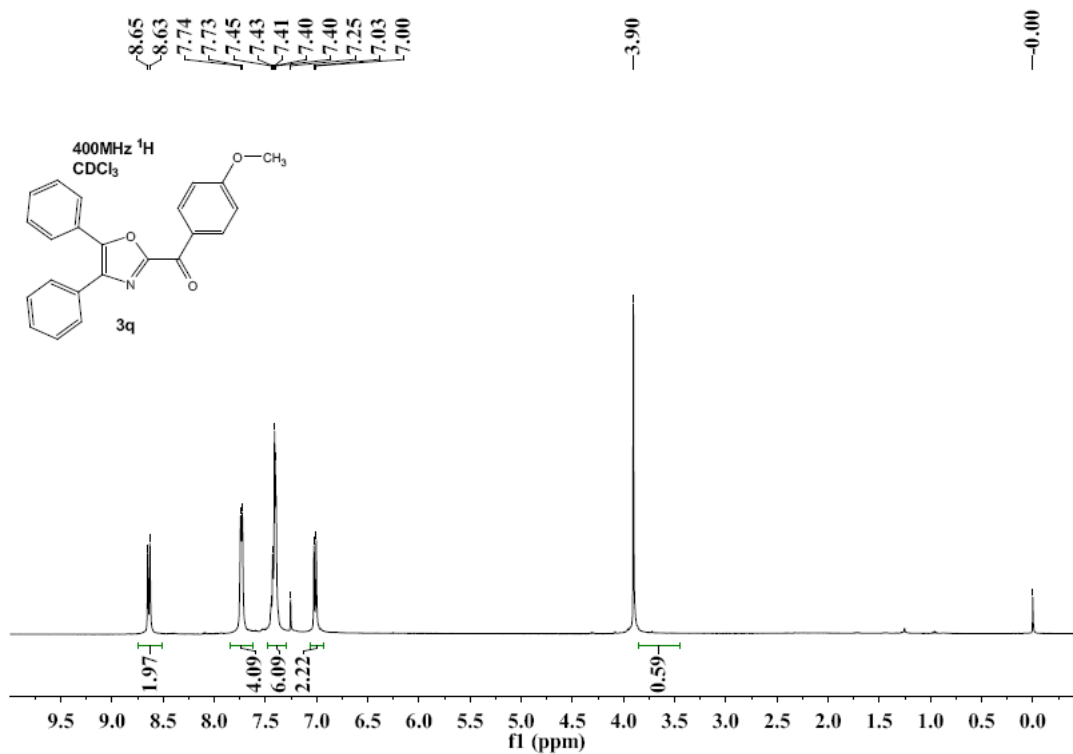


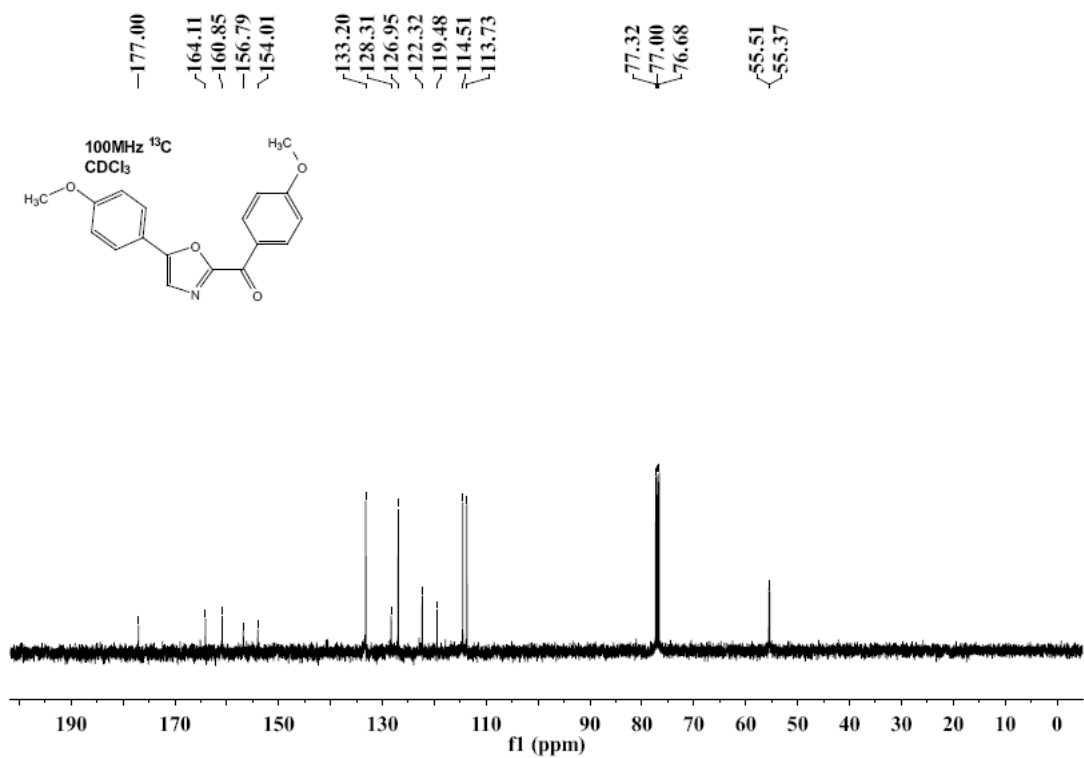
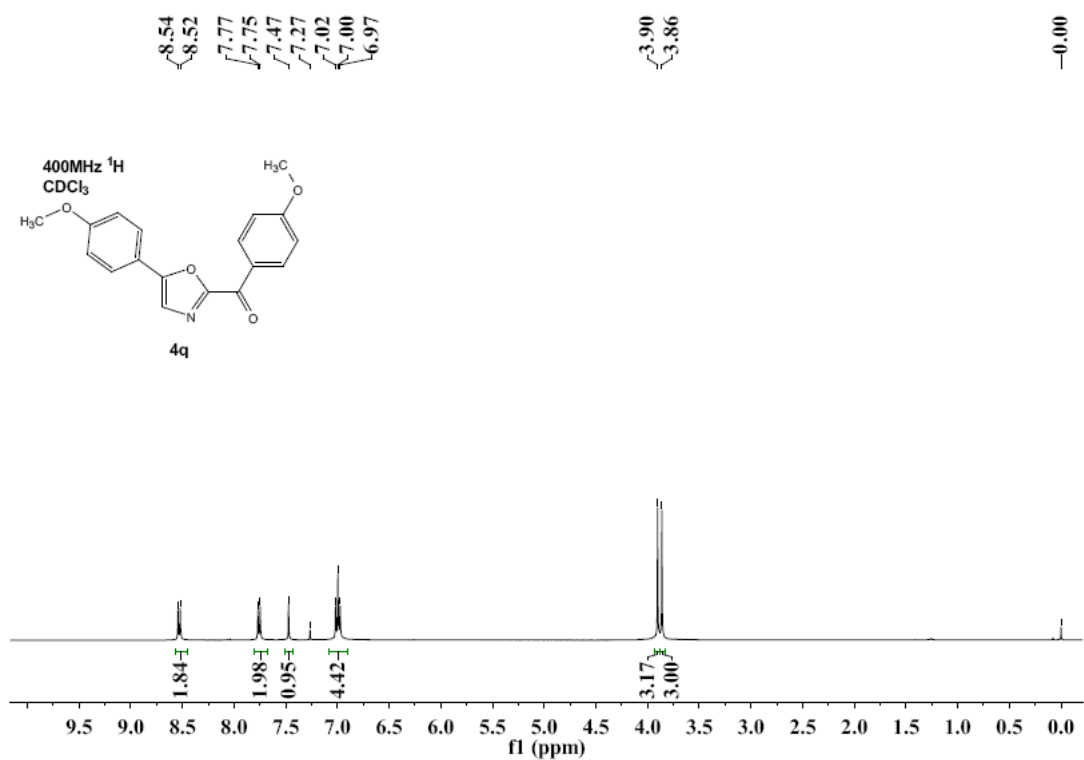


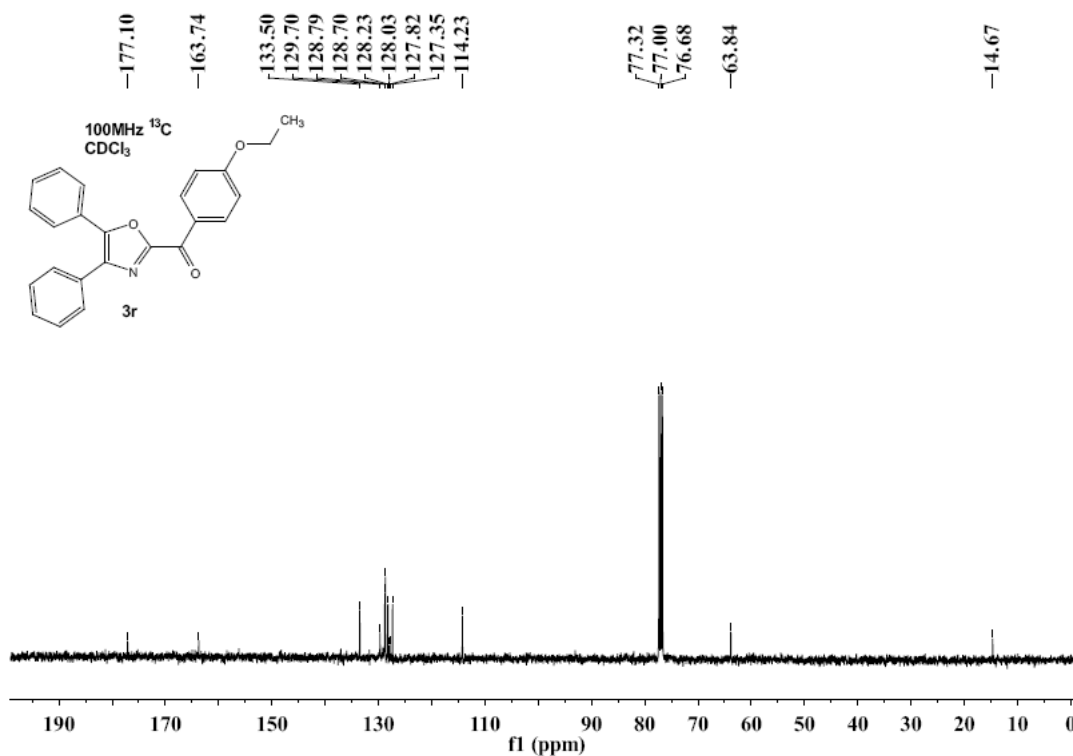
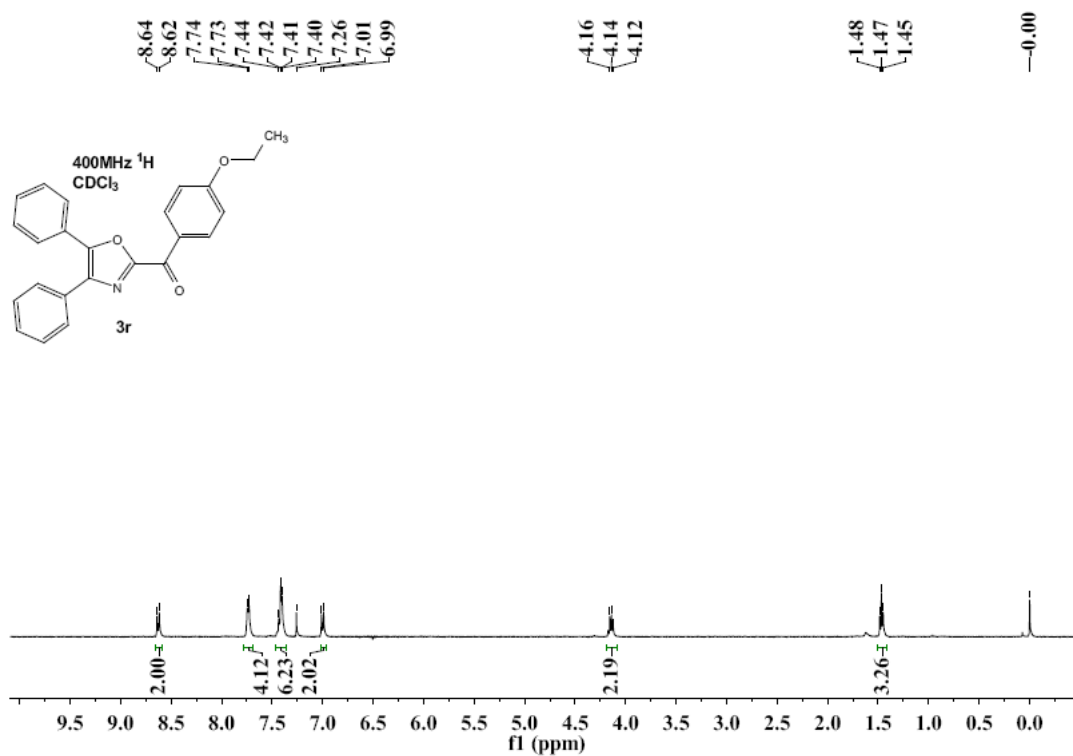




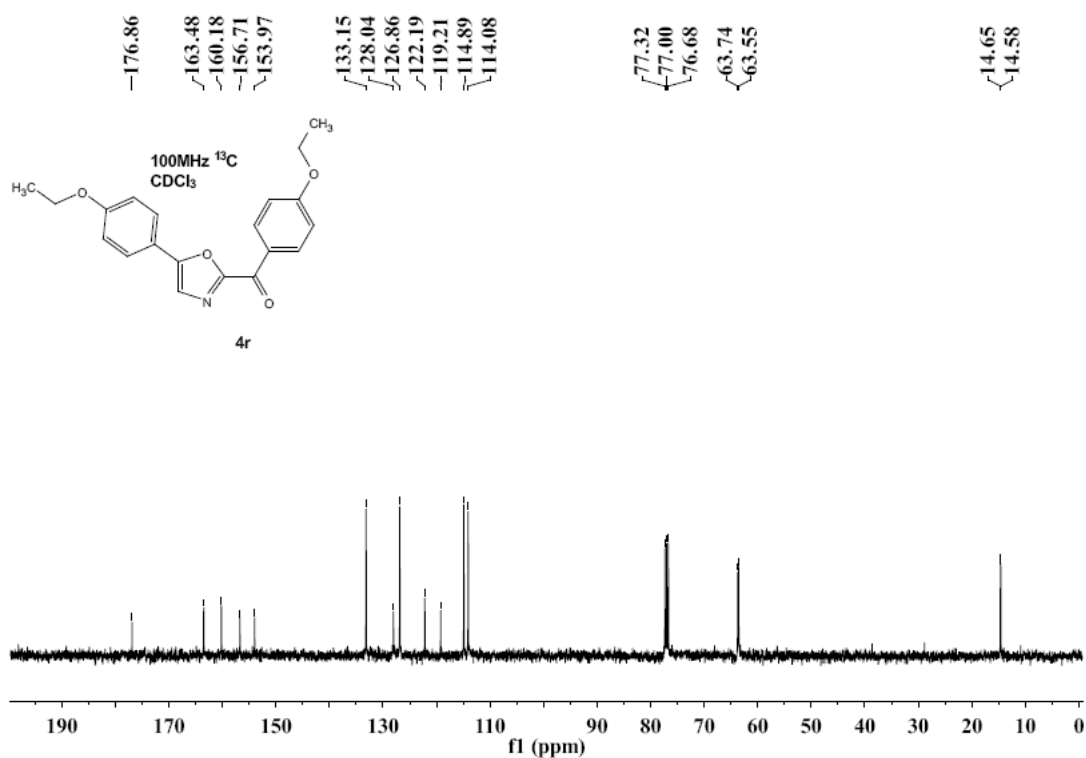
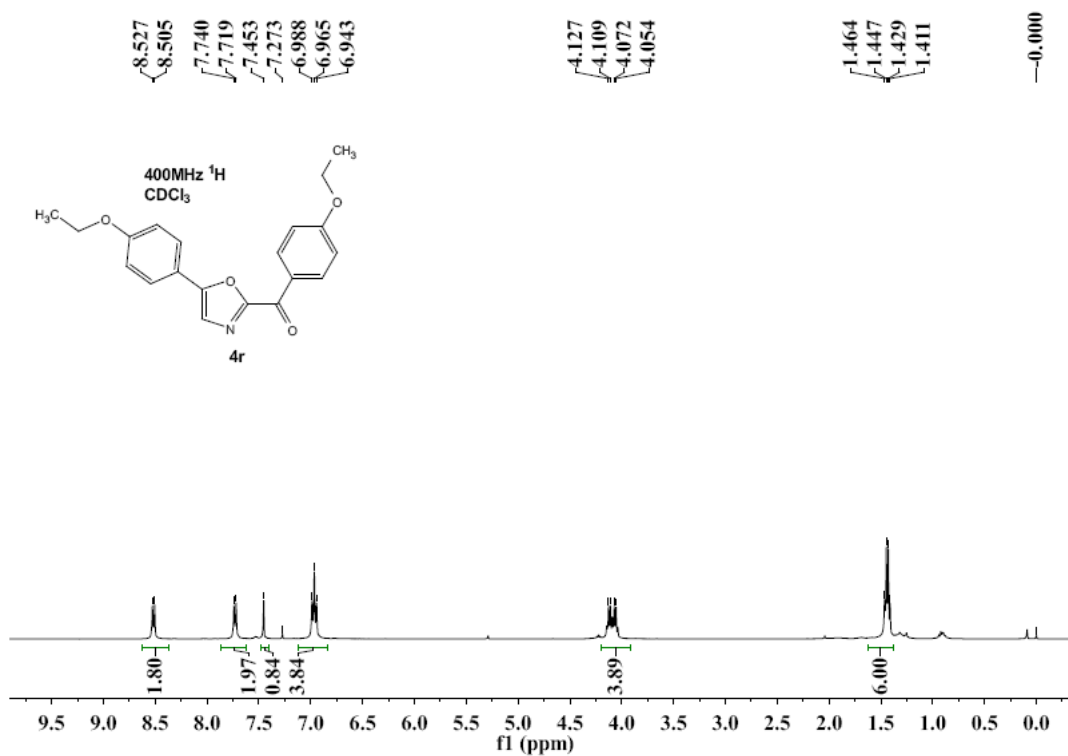


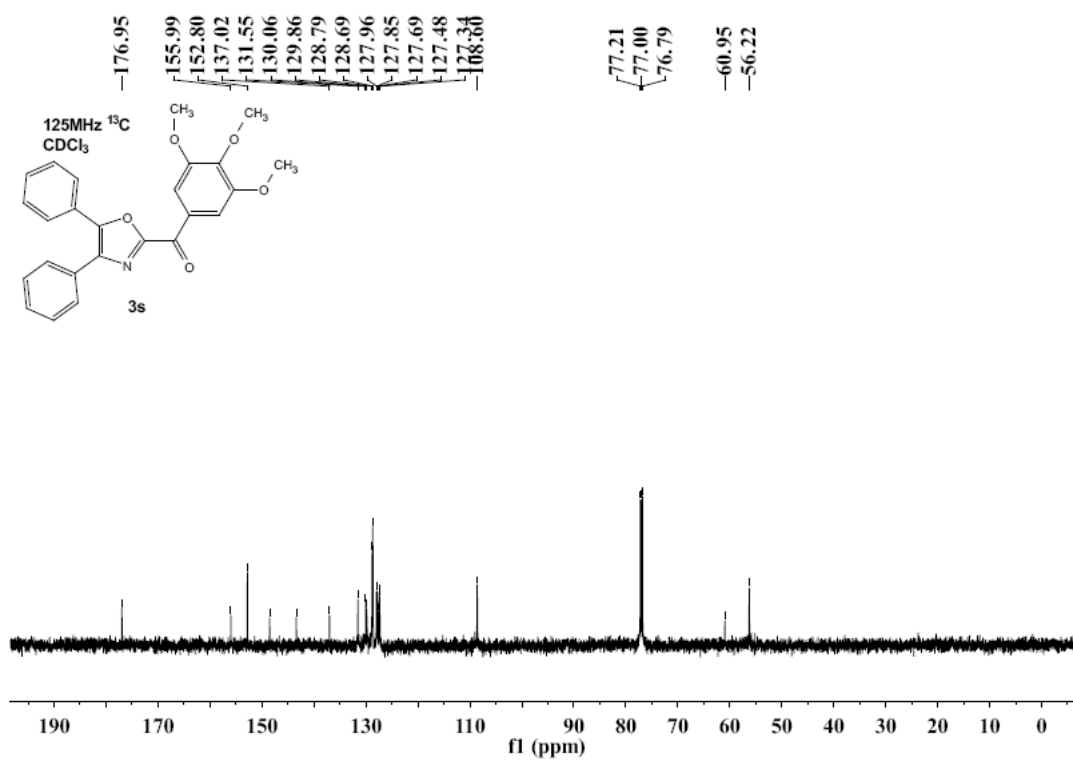
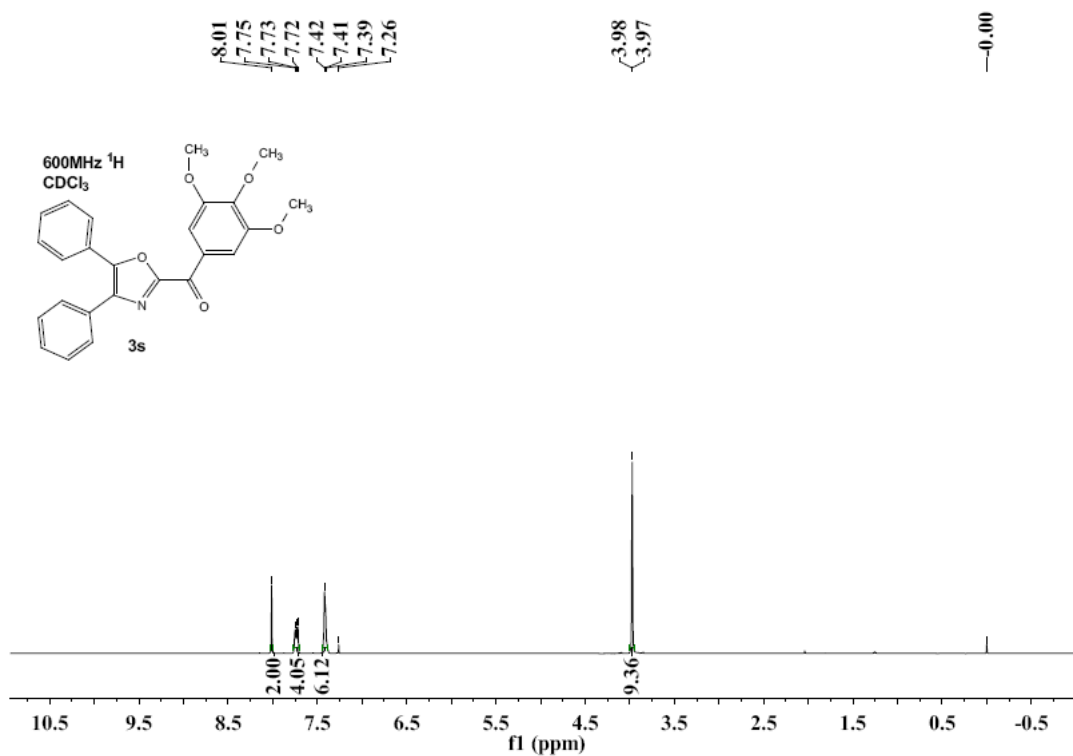


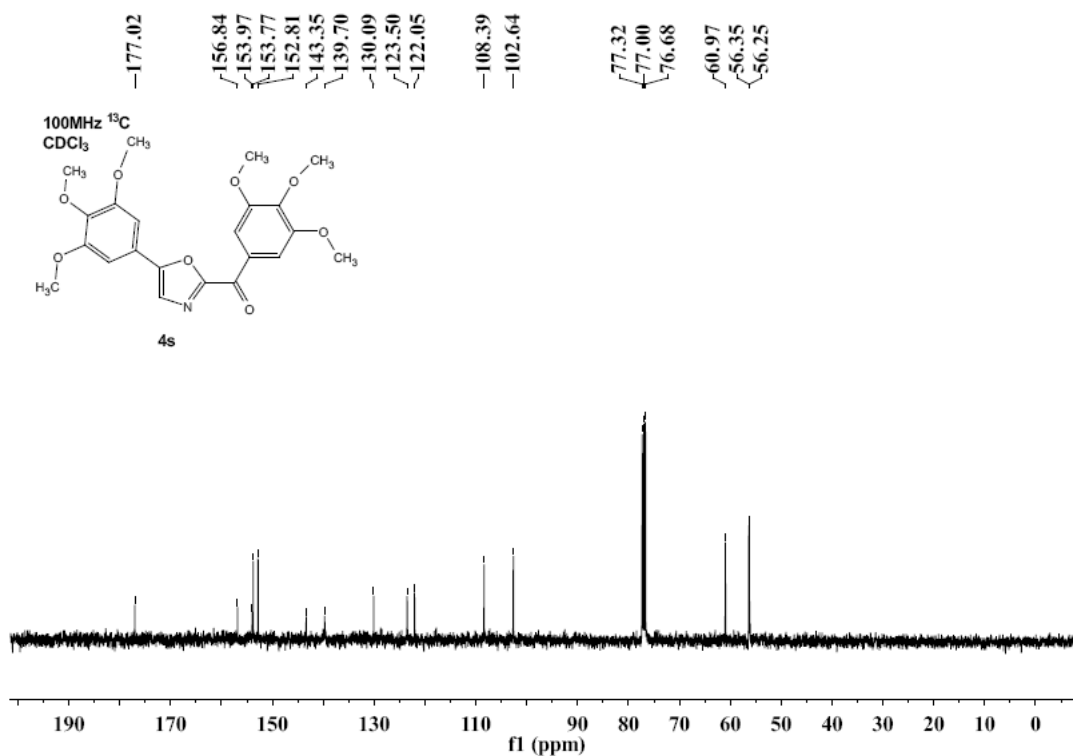
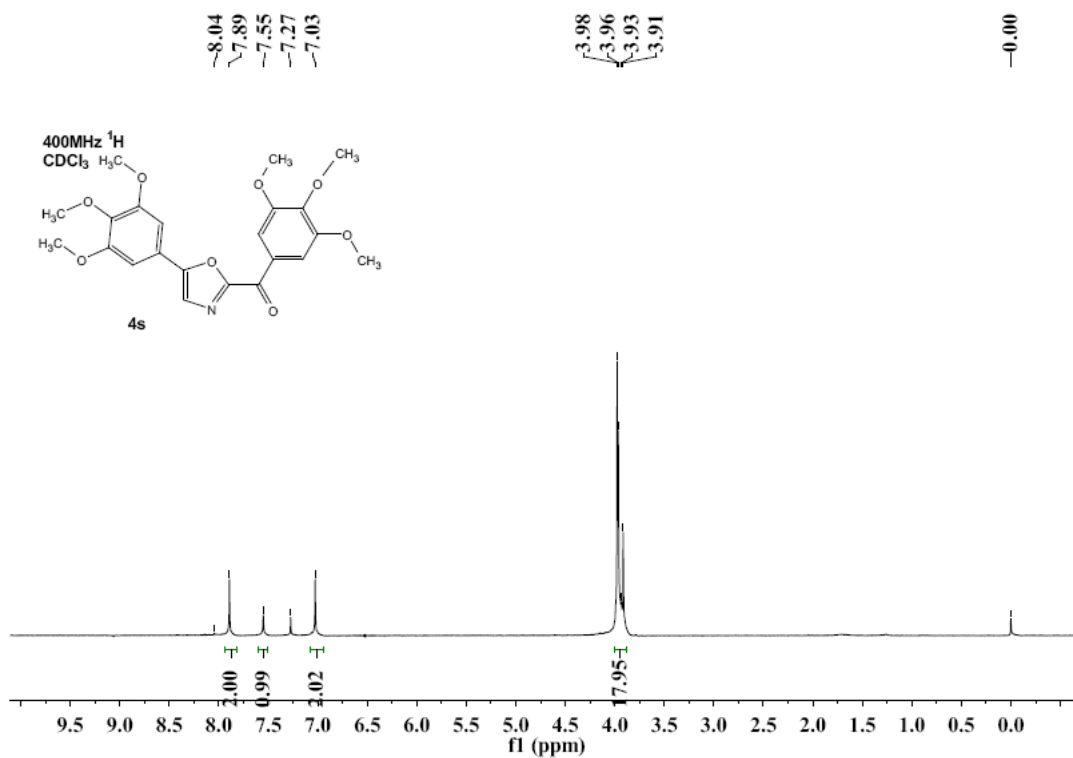




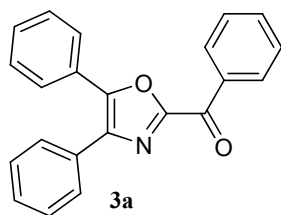








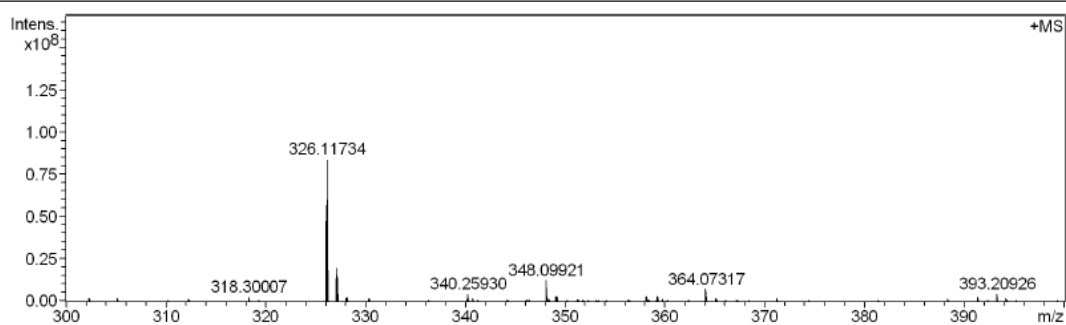
## 9. HRMS spectra



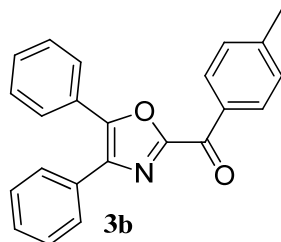
Chemical Formula: C<sub>22</sub>H<sub>15</sub>NO<sub>2</sub>  
 Molecular Weight: 325.36

### Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	4	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	2000.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 μm
Acquisition Mode	Single MS	Skimmer 1	20.0 V	Calibration Date	Mon Sep 19 06:39:58
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Data Acquisition Size	101072
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.0 sec	Nebulizer Gas Flow Rate	1.0 L/min		
Flight Time to Acq. Cell	0.0 sec				



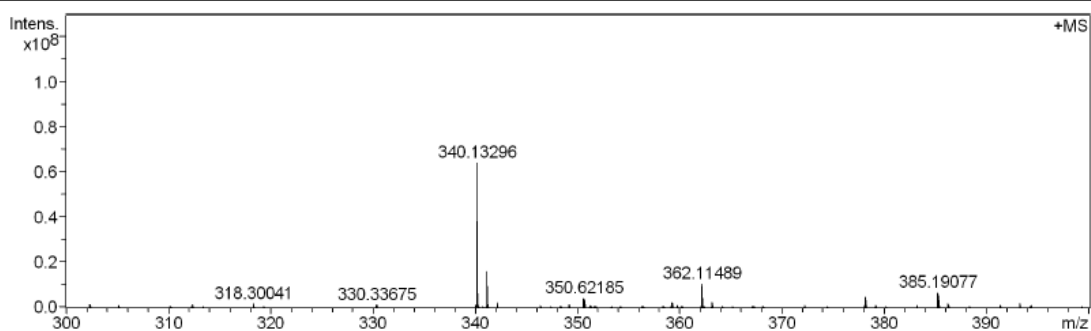
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e <sub>1</sub>	Conf	N-Rule
326.11734	1	C <sub>22</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>	100.00	326.11756	0.2	0.7	3.9	15.5	even		ok
	2	C <sub>17</sub> H <sub>16</sub> N <sub>3</sub> O <sub>4</sub>	4.26	326.11353	-3.8	-11.7	23.3	11.5	even		ok
	3	C <sub>16</sub> H <sub>16</sub> N <sub>5</sub> O <sub>3</sub>	0.01	326.12477	7.4	22.8	25.6	11.5	even		ok
	4	C <sub>15</sub> H <sub>20</sub> N <sub>2</sub> O <sub>7</sub>	0.12	326.12343	6.1	18.7	39.9	6.5	even		ok
	5	C <sub>15</sub> H <sub>18</sub> N <sub>2</sub> O <sub>7</sub>	0.00	324.10778	-4.2	-12.9	97.1	7.5	even		ok
	6	C <sub>15</sub> H <sub>14</sub> N <sub>7</sub> O <sub>2</sub>	0.00	324.12035	7.9	24.1	109.2	12.5	even		ok
	7	C <sub>16</sub> H <sub>14</sub> N <sub>5</sub> O <sub>3</sub>	0.00	324.10912	-3.0	-9.3	111.4	12.5	even		ok
	8	C <sub>18</sub> H <sub>17</sub> N <sub>2</sub> O <sub>4</sub>	0.00	325.11828	4.1	12.6	117.7	11.5	even		ok
	9	C <sub>22</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>	0.00	324.10191	-9.2	-28.1	140.7	16.5	even		ok



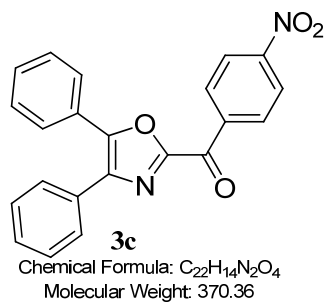
Chemical Formula:  $C_{23}H_{17}NO_2$   
 Molecular Weight: 339.39

**Acquisition Parameter**

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	4	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	2000.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 $\mu$ m
Acquisition Mode	Single MS	Skimmer 1	20.0 V	Calibration Date	Mon Sep 19 06:39:58
Pulse Program	basic	Drying Gas Temperature	180.0 $^{\circ}$ C	Data Acquisition Size	201072
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.0 sec	Nebulizer Gas Flow Rate	1.0 L/min		
Flight Time to Acq. Cell	0.0 sec				

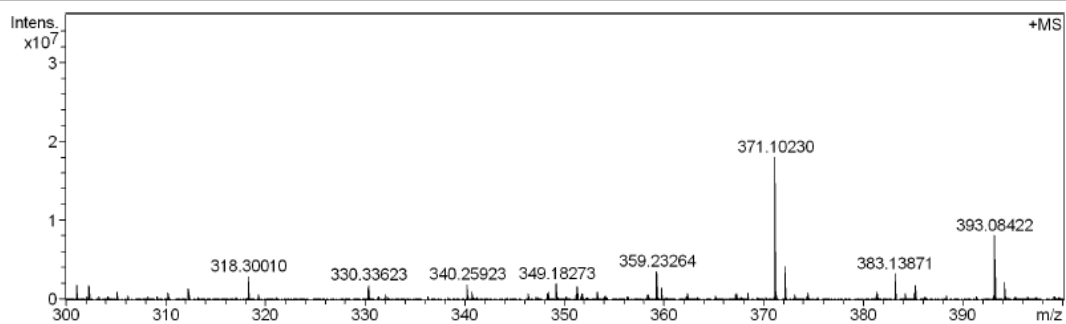


Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	ej*Conf	N-Rule
340.13296	1	C <sub>23</sub> H <sub>18</sub> NO <sub>2</sub>	100.00	340.13321	0.2	0.7	1.0	15.5	even	ok
	2	C <sub>23</sub> H <sub>16</sub> NO <sub>2</sub>	0.00	338.11756	-9.1	-26.8	147.1	16.5	even	ok

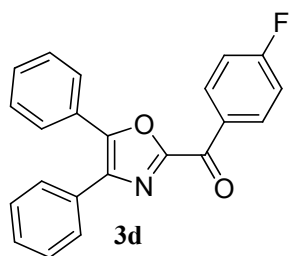


**Acquisition Parameter**

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	4	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	2000.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 μm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Mon Sep 19 06:39:58
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	101072
Ion Accumulation Time	0.0 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



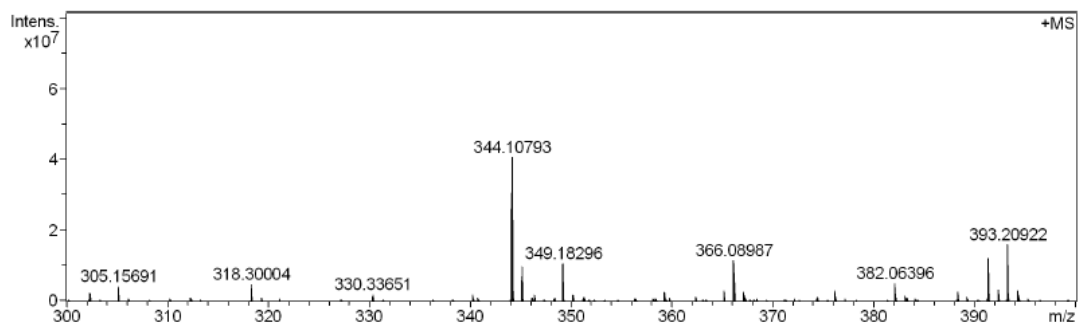
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e <sub>1</sub> Conf	N-Rule
371.10230	1	C <sub>22</sub> H <sub>15</sub> N <sub>2</sub> O <sub>4</sub>	100.00	371.10263	0.3	0.9	4.7	16.5	even	ok
	2	C <sub>17</sub> H <sub>15</sub> N <sub>4</sub> O <sub>6</sub>	5.28	371.09861	-3.7	-9.9	22.5	12.5	even	ok
	3	C <sub>16</sub> H <sub>15</sub> N <sub>6</sub> O <sub>5</sub>	0.01	371.10984	7.5	20.3	24.7	12.5	even	ok
	4	C <sub>15</sub> H <sub>19</sub> N <sub>2</sub> O <sub>9</sub>	0.10	371.10851	6.2	16.7	39.2	7.5	even	ok
	5	C <sub>18</sub> H <sub>16</sub> N <sub>3</sub> O <sub>6</sub>	0.00	370.10336	4.1	11.1	746.7	12.5	even	ok
	6	C <sub>15</sub> H <sub>17</sub> N <sub>2</sub> O <sub>9</sub>	0.00	369.09286	-4.3	-11.6	809.5	8.5	even	ok
	7	C <sub>16</sub> H <sub>13</sub> N <sub>6</sub> O <sub>5</sub>	0.00	369.09419	-3.2	-8.5	812.9	13.5	even	ok
	8	C <sub>15</sub> H <sub>13</sub> N <sub>8</sub> O <sub>4</sub>	0.00	369.10543	7.7	20.9	813.8	13.5	even	ok
	9	C <sub>22</sub> H <sub>13</sub> N <sub>2</sub> O <sub>4</sub>	0.00	369.08698	-9.4	-25.4	814.0	17.5	even	ok



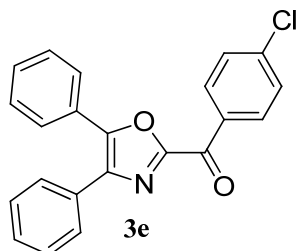
Chemical Formula: C<sub>22</sub>H<sub>14</sub>FNO<sub>2</sub>  
 Molecular Weight: 343.35

**Acquisition Parameter**

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	4	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	2000.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 μm
Acquisition Mode	Single MS	Skimmer 1	20.0 V	Calibration Date	Mon Sep 19 06:39:58
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Data Acquisition Size	101072
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.0 sec	Nebulizer Gas Flow Rate	1.0 L/min		
Flight Time to Acq. Cell	0.0 sec				



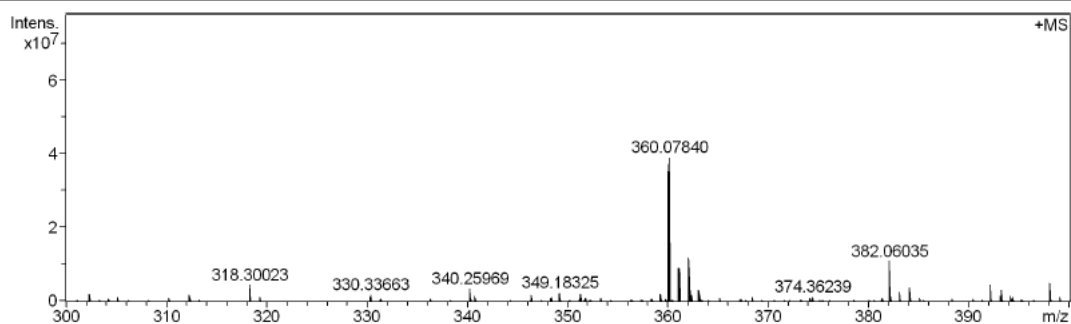
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	ej*	Conf	N-Rule
344.10793	1	C 22 H 15 F N O 2	100.00	344.10813	0.2	0.6	3.9	15.5	even		ok
	2	C 19 H 16 F 2 N O 3	40.10	344.10928	1.3	3.9	19.9	11.5	even		ok
	3	C 17 H 15 F N 3 O 4	3.75	344.10411	-3.8	-11.1	28.1	11.5	even		ok
	4	C 16 H 15 F N 5 O 3	0.01	344.11534	7.4	21.6	30.1	11.5	even		ok
	5	C 16 H 17 F 3 N O 4	10.87	344.11042	2.5	7.2	38.6	7.5	even		ok



Chemical Formula: C<sub>22</sub>H<sub>14</sub>ClNO<sub>2</sub>  
 Molecular Weight: 359.81

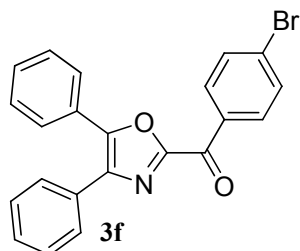
**Acquisition Parameter**

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	4	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	2000.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 μm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Mon Sep 19 06:39:58
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	101072
Ion Accumulation Time	0.0 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e <sub>j</sub>	Conf	N-Rule
360.07840	1	C <sub>22</sub> H <sub>15</sub> ClNO <sub>2</sub>	100.00	360.07858	0.2	0.5	21.5	15.5	even	ok	
	2	C <sub>17</sub> H <sub>15</sub> ClN <sub>3</sub> O <sub>4</sub>	5.31	360.07456	-3.8	-10.7	26.0	11.5	even	ok	
	3	C <sub>16</sub> H <sub>15</sub> ClN <sub>5</sub> O <sub>3</sub>	0.02	360.08579	7.4	20.5	26.4	11.5	even	ok	
	4	C <sub>15</sub> H <sub>19</sub> ClNO <sub>7</sub>	0.18	360.08446	6.1	16.8	37.0	6.5	even	ok	
	5	C <sub>15</sub> H <sub>20</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>3</sub>	0.00	360.08762	9.2	25.6	153.8	6.5	even	ok	
	6	C <sub>16</sub> H <sub>20</sub> Cl <sub>2</sub> N <sub>4</sub> O <sub>4</sub>	0.10	360.07639	-2.0	-5.6	154.9	6.5	even	ok	

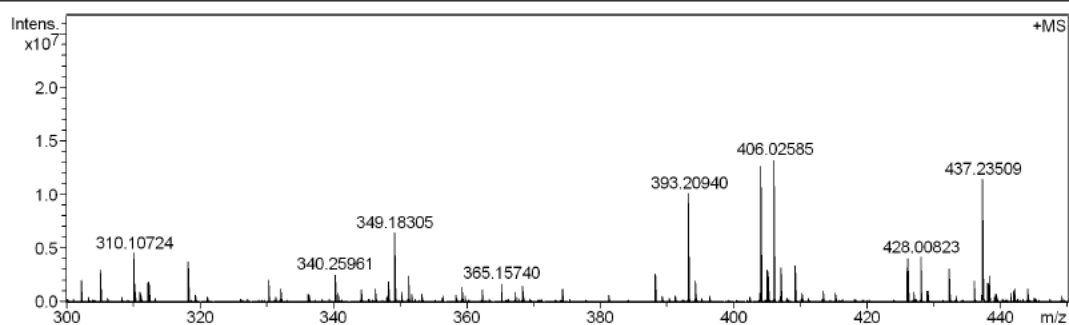




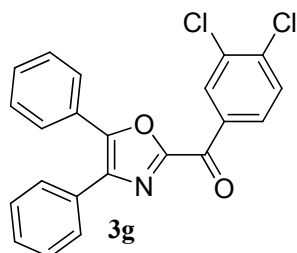
Chemical Formula:  $C_{22}H_{14}BrNO_2$   
 Molecular Weight: 404.26

#### Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	4	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	2000.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 $\mu$ m
Acquisition Mode	Single MS	Skimmer 1	20.0 V	Calibration Date	Mon Sep 19 06:39:58
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Data Acquisition Size	201072
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.0 sec	Nebulizer Gas Flow Rate	1.0 L/min		
Flight Time to Acq. Cell	0.0 sec				



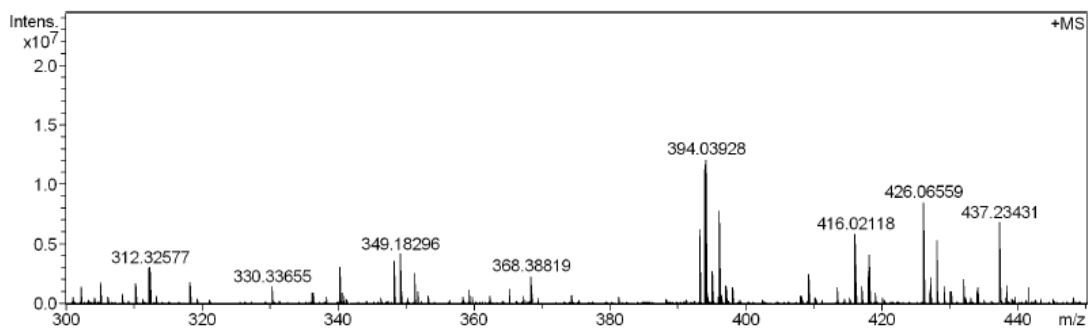
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	ej%	Conf	N-Rule
404.02773	1	C 22 H 15 Br N O 2	100.00	404.02807	0.3	0.8	14.4	15.5	even	ok	ok
	2	C 17 H 15 Br N 3 O 4	5.13	404.02405	-3.7	-9.1	31.7	11.5	even	ok	ok
	3	C 16 H 15 Br N 5 O 3	0.01	404.03528	7.5	18.7	33.8	11.5	even	ok	ok
	4	C 15 H 19 Br N O 7	0.10	404.03394	6.2	15.4	48.0	6.5	even	ok	ok



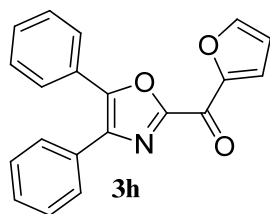
Chemical Formula: C<sub>22</sub>H<sub>13</sub>Cl<sub>2</sub>NO<sub>2</sub>  
 Molecular Weight: 394.25

#### Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	4	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	2000.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 μm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Mon Sep 19 06:39:58
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	201072
Ion Accumulation Time	0.0 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



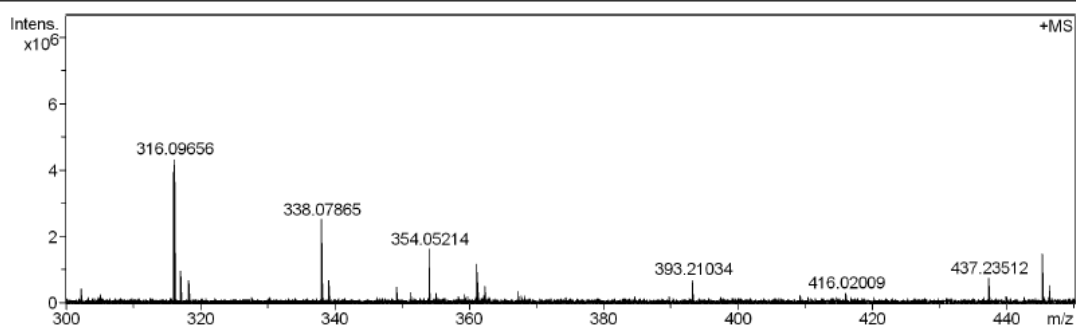
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	ej*Conf	N-Rule
394.03928	1	C <sub>22</sub> H <sub>14</sub> Cl <sub>2</sub> NO <sub>2</sub>	100.00	394.03961	0.3	0.8	16.9	15.5	even	ok



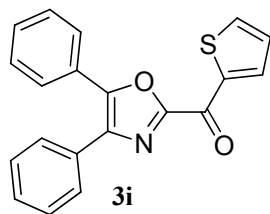
Chemical Formula: C<sub>20</sub>H<sub>13</sub>NO<sub>3</sub>  
 Molecular Weight: 315.32

**Acquisition Parameter**

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	4	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	2000.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 μm
Acquisition Mode	Single MS	Skimmer 1	20.0 V	Calibration Date	Mon Sep 19 06:39:58
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Data Acquisition Size	101072
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.0 sec	Nebulizer Gas Flow Rate	1.0 L/min		
Flight Time to Acq. Cell	0.0 sec				



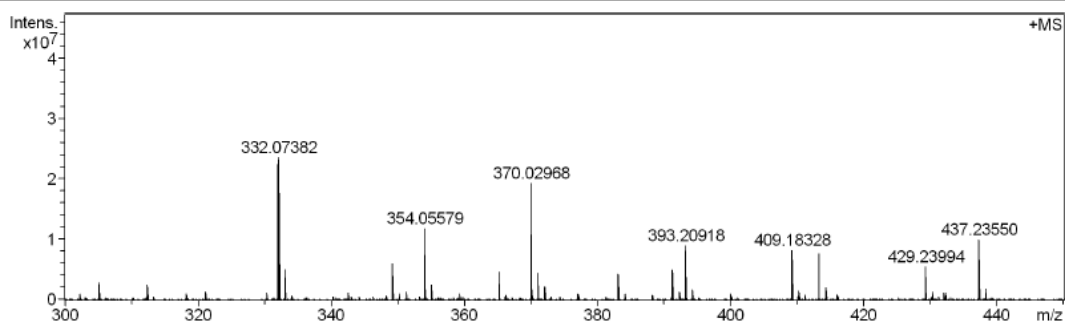
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e <sub>i</sub> Conf	N-Rule
316.09656	1	C 20 H 14 N O 3	100.00	316.09682	0.3	0.8	17.6	14.5	even	ok
	2	C 15 H 14 N 3 O 5	4.46	316.09280	-3.8	-11.9	35.1	10.5	even	ok
	3	C 16 H 15 N 2 O 5	0.00	315.09755	4.1	13.1	105.2	10.5	even	ok
	4	C 18 H 11 N 4 O 2	0.00	315.08765	-6.0	-18.9	121.8	15.5	even	ok
	5	C 19 H 12 N 3 O 2	0.00	314.09240	1.7	5.2	126.0	15.5	even	ok
	6	C 20 H 12 N O 3	0.00	314.08117	-9.3	-29.5	128.1	15.5	even	ok



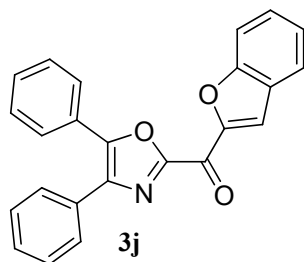
Chemical Formula: C<sub>20</sub>H<sub>13</sub>NO<sub>2</sub>S  
 Molecular Weight: 331.39

**Acquisition Parameter**

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	4	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	2000.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 μm
Acquisition Mode	Single MS	Skimmer 1	20.0 V	Calibration Date	Mon Sep 19 06:39:58
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Data Acquisition Size	101072
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.0 sec	Nebulizer Gas Flow Rate	1.0 L/min		
Flight Time to Acq. Cell	0.0 sec				



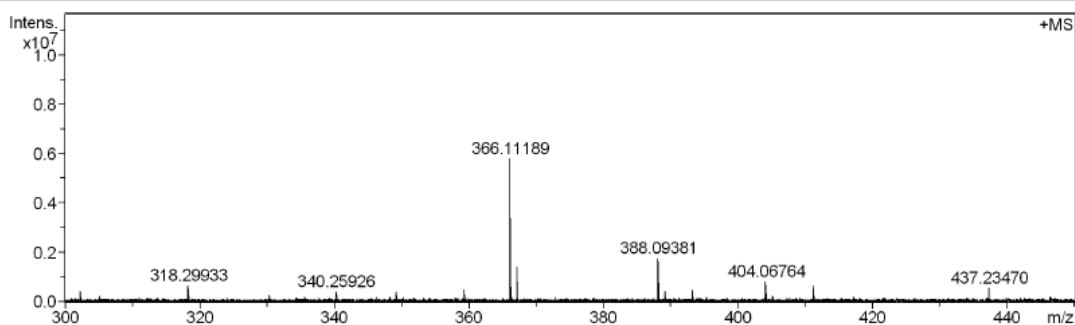
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	ej#Conf	N-Rule
332.07382	1	C <sub>20</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> S	100.00	332.07398	0.2	0.5	21.9	14.5	even	ok
	2	C <sub>15</sub> H <sub>14</sub> N <sub>3</sub> O <sub>4</sub> S	5.11	332.06995	-3.9	-11.7	26.2	10.5	even	ok
	3	C <sub>14</sub> H <sub>14</sub> N <sub>5</sub> O <sub>3</sub> S	0.02	332.08119	7.4	22.2	26.5	10.5	even	ok
	4	C <sub>17</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub> S <sub>2</sub>	5.01	332.07735	3.5	10.6	42.2	9.5	even	ok
	5	C <sub>14</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub> S <sub>3</sub>	0.02	332.08072	6.9	20.8	58.2	4.5	even	ok
	6	C <sub>16</sub> H <sub>15</sub> N <sub>2</sub> O <sub>4</sub> S	0.00	331.07470	3.9	11.6	648.3	10.5	even	ok
	7	C <sub>14</sub> H <sub>20</sub> N <sub>4</sub> O <sub>4</sub> S <sub>2</sub>	0.00	330.08283	6.7	20.1	681.6	5.5	even	ok
	8	C <sub>17</sub> H <sub>16</sub> N <sub>4</sub> O <sub>4</sub> S	0.00	330.07946	5.1	15.3	697.1	10.5	even	ok
	9	C <sub>14</sub> H <sub>12</sub> N <sub>5</sub> O <sub>3</sub> S	0.00	330.06554	-9.6	-28.8	697.8	11.5	even	ok
	10	C <sub>15</sub> H <sub>13</sub> N <sub>4</sub> O <sub>3</sub> S	0.00	329.07029	-3.1	-9.3	710.6	11.5	even	ok



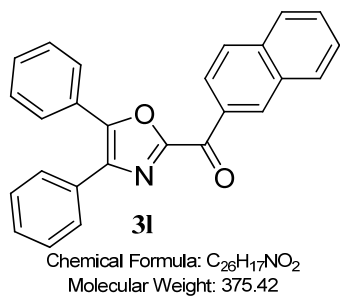
Chemical Formula: C<sub>24</sub>H<sub>15</sub>NO<sub>3</sub>  
 Molecular Weight: 365.38

**Acquisition Parameter**

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	4	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	2000.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 μm
Acquisition Mode	Single MS	Skimmer 1	20.0 V	Calibration Date	Mon Sep 19 06:39:58
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Data Acquisition Size	101072
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.0 sec	Nebulizer Gas Flow Rate	1.0 L/min		
Flight Time to Acq. Cell	0.0 sec				

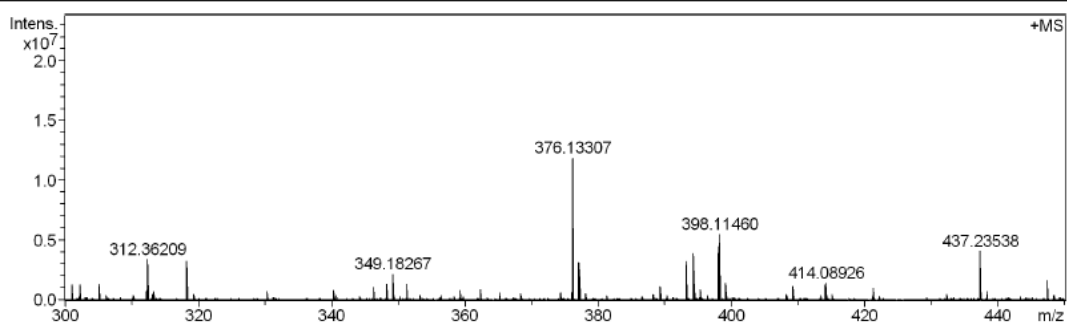


Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e <sub>i</sub> Conf	N-Rule
366.11189	1	C <sub>24</sub> H <sub>16</sub> N <sub>1</sub> O <sub>3</sub>	100.00	366.11247	0.6	1.6	24.0	17.5	even	ok
	2	C <sub>19</sub> H <sub>16</sub> N <sub>3</sub> O <sub>5</sub>	10.29	366.10845	-3.4	-9.4	26.9	13.5	even	ok
	3	C <sub>18</sub> H <sub>16</sub> N <sub>5</sub> O <sub>4</sub>	0.01	366.11968	7.8	21.3	27.3	13.5	even	ok
	4	C <sub>17</sub> H <sub>20</sub> N <sub>1</sub> O <sub>8</sub>	0.11	366.11834	6.5	17.6	40.7	8.5	even	ok
	5	C <sub>20</sub> H <sub>17</sub> N <sub>2</sub> O <sub>5</sub>	0.00	365.11320	4.5	12.3	741.4	13.5	even	ok
	6	C <sub>17</sub> H <sub>13</sub> N <sub>6</sub> O <sub>4</sub>	0.00	365.09928	-9.9	-27.0	748.2	14.5	even	ok
	7	C <sub>16</sub> H <sub>13</sub> N <sub>8</sub> O <sub>3</sub>	0.00	365.11051	1.1	3.0	749.7	14.5	even	ok
	8	C <sub>17</sub> H <sub>18</sub> N <sub>1</sub> O <sub>8</sub>	0.00	364.10269	-3.8	-10.3	810.4	9.5	even	ok
	9	C <sub>16</sub> H <sub>18</sub> N <sub>3</sub> O <sub>7</sub>	0.00	364.11393	7.2	19.8	811.2	9.5	even	ok
	10	C <sub>18</sub> H <sub>14</sub> N <sub>5</sub> O <sub>4</sub>	0.00	364.10403	-2.6	-7.1	813.8	14.5	even	ok
	11	C <sub>17</sub> H <sub>14</sub> N <sub>7</sub> O <sub>3</sub>	0.00	364.11526	8.3	22.8	814.7	14.5	even	ok
	12	C <sub>24</sub> H <sub>14</sub> N <sub>1</sub> O <sub>3</sub>	0.00	364.09682	-8.9	-24.2	814.9	18.5	even	ok

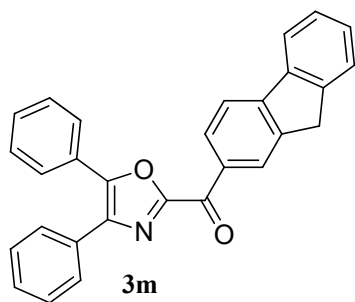


**Acquisition Parameter**

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	4	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	2000.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 μm
Acquisition Mode	Single MS	Skimmer 1	20.0 V	Calibration Date	Mon Sep 19 06:39:58
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Data Acquisition Size	181072
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.0 sec	Nebulizer Gas Flow Rate	1.0 L/min		
Flight Time to Acq. Cell	0.0 sec				



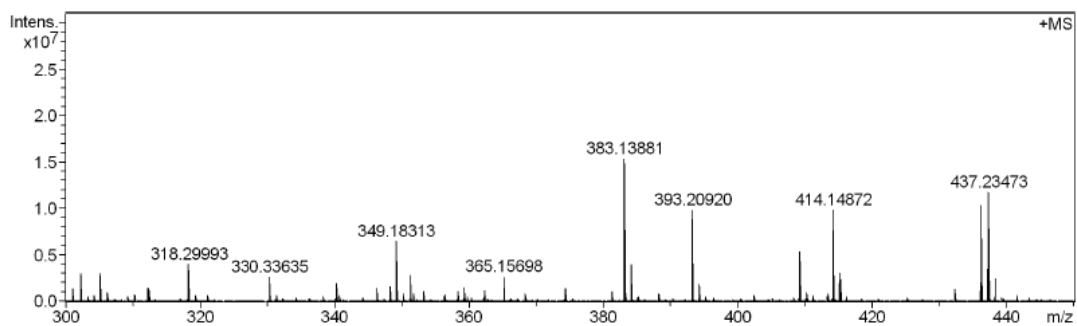
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e <sub>i</sub> Conf	N-Rule
376.13307	1	C <sub>26</sub> H <sub>18</sub> NO <sub>2</sub>	100.00	376.13321	0.1	0.3	10.4	18.5	even	ok



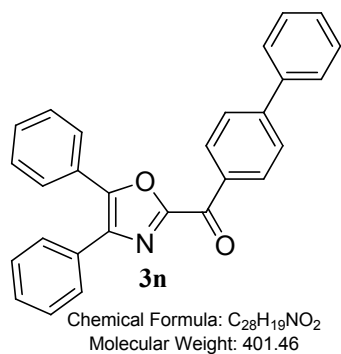
Chemical Formula: C<sub>29</sub>H<sub>19</sub>NO<sub>2</sub>  
 Molecular Weight: 413.47

**Acquisition Parameter**

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	4	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	2000.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 μm
Acquisition Mode	Single MS	Skimmer 1	20.0 V	Calibration Date	Mon Sep 19 06:39:58
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Data Acquisition Size	101072
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.0 sec	Nebulizer Gas Flow Rate	1.0 L/min		
Flight Time to Acq. Cell	0.0 sec				

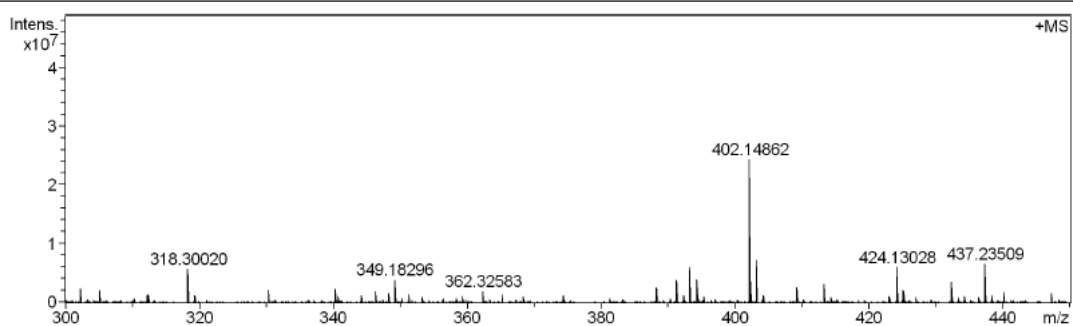


Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	ej*Conf	N-Rule
414.14872	1	C <sub>29</sub> H <sub>20</sub> NO <sub>2</sub>	100.00	414.14886	0.1	0.3	5.2	20.5	even	ok
	2	C <sub>24</sub> H <sub>20</sub> N <sub>3</sub> O <sub>4</sub>	3.46	414.14483	-3.9	-9.4	27.6	16.5	even	ok
	3	C <sub>23</sub> H <sub>20</sub> N <sub>5</sub> O <sub>3</sub>	0.02	414.15607	7.3	17.7	30.0	16.5	even	ok
	4	C <sub>22</sub> H <sub>24</sub> NO <sub>7</sub>	0.12	414.15473	6.0	14.5	43.7	11.5	even	ok



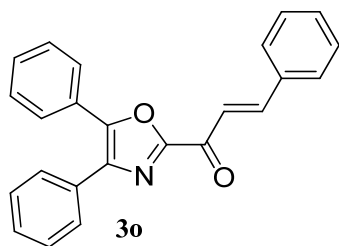
**Acquisition Parameter**

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	4	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	2000.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 μm
Acquisition Mode	Single MS	Skimmer 1	20.0 V	Calibration Date	Mon Sep 19 06:39:58
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Data Acquisition Size	101072
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.0 sec	Nebulizer Gas Flow Rate	1.0 L/min		
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e <sub>i</sub>	Conf	N-Rule
402.14862	1	C <sub>28</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>	100.00	402.14886	0.2	0.6	4.7	19.5	even		ok
	2	C <sub>23</sub> H <sub>20</sub> N <sub>3</sub> O <sub>4</sub>	4.45	402.14483	-3.8	-9.4	23.1	15.5	even		ok
	3	C <sub>22</sub> H <sub>20</sub> N <sub>5</sub> O <sub>3</sub>	0.01	402.15607	7.4	18.5	25.5	15.5	even		ok
	4	C <sub>21</sub> H <sub>24</sub> N <sub>2</sub> O <sub>7</sub>	0.12	402.15473	6.1	15.2	39.7	10.5	even		ok

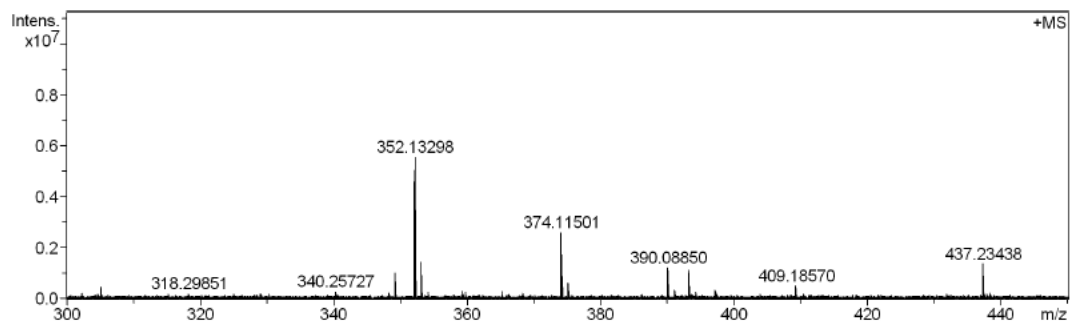




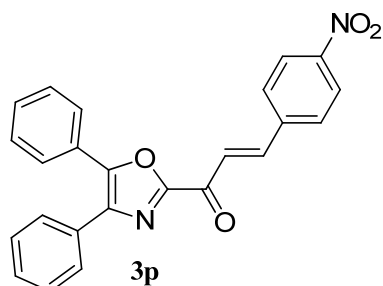
Chemical Formula: C<sub>24</sub>H<sub>17</sub>NO<sub>2</sub>  
 Molecular Weight: 351.40

**Acquisition Parameter**

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	4	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	2000.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 μm
Acquisition Mode	Single MS	Skimmer 1	20.0 V	Calibration Date	Mon Sep 19 06:39:58
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Data Acquisition Size	201072
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.0 sec	Nebulizer Gas Flow Rate	1.0 L/min		
Flight Time to Acq. Cell	0.0 sec				



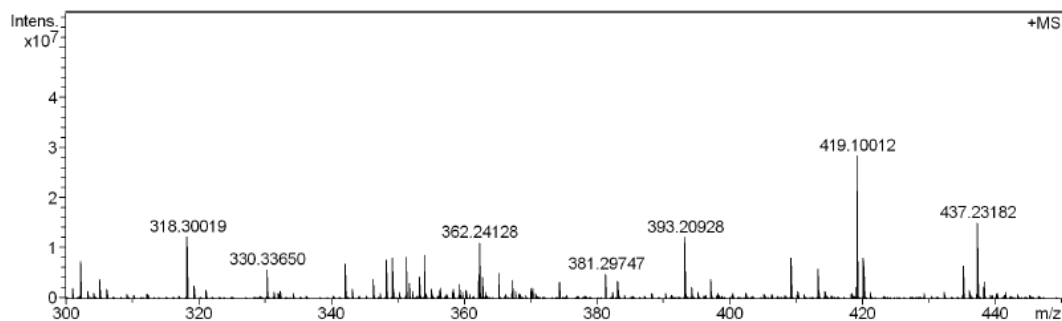
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	ej	Conf	N-Rule
352.13298	1	C <sub>24</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>	100.00	352.13321	0.2	0.6	7.8	16.5	even	ok	
	2	C <sub>19</sub> H <sub>18</sub> N <sub>3</sub> O <sub>4</sub>	4.00	352.12918	-3.8	-10.8	29.8	12.5	even	ok	
	3	C <sub>18</sub> H <sub>18</sub> N <sub>5</sub> O <sub>3</sub>	0.01	352.14042	7.4	21.1	32.2	12.5	even	ok	
	4	C <sub>17</sub> H <sub>22</sub> N <sub>2</sub> O <sub>7</sub>	0.10	352.13908	6.1	17.3	45.6	7.5	even	ok	



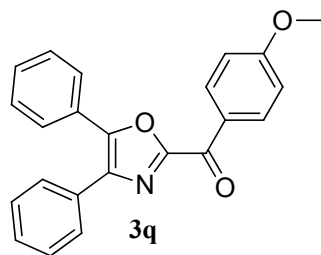
Chemical Formula: C<sub>24</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>  
 Molecular Weight: 396.39

**Acquisition Parameter**

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	4	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	2000.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 μm
Acquisition Mode	Single MS	Skimmer 1	20.0 V	Calibration Date	Mon Sep 19 06:39:58
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Data Acquisition Size	101072
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.1 sec	Nebulizer Gas Flow Rate	1.0 L/min		
Flight Time to Acq. Cell	0.0 sec				



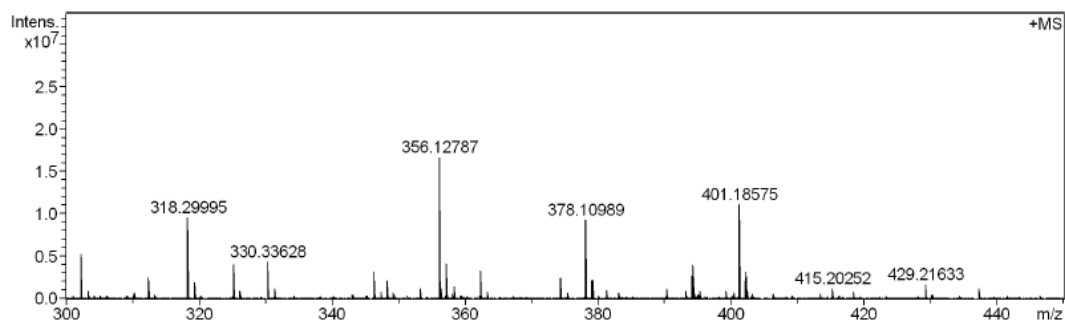
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
397.11771	1	C <sub>24</sub> H <sub>17</sub> N <sub>2</sub> O <sub>4</sub>	100.00	397.11828	0.6	1.4	27.0	17.5	even	ok



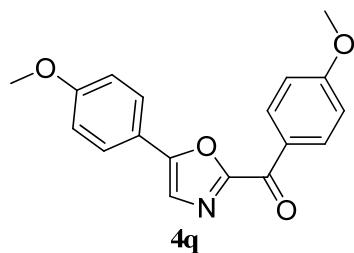
Chemical Formula: C<sub>23</sub>H<sub>17</sub>NO<sub>3</sub>  
 Molecular Weight: 355.39

**Acquisition Parameter**

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	4	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	2000.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 μm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Mon Sep 19 06:39:58
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	101072
Ion Accumulation Time	0.0 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



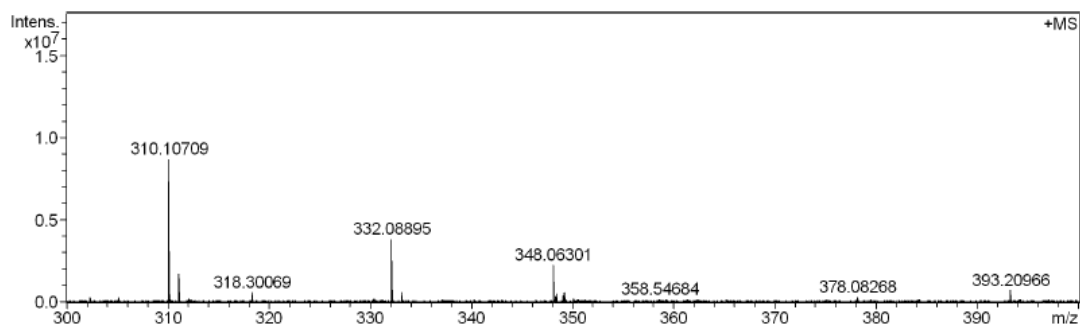
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	ej*Conf	N-Rule
356.12787	1	C <sub>23</sub> H <sub>18</sub> N <sub>1</sub> O <sub>3</sub>	100.00	356.12812	0.3	0.7	0.7	15.5	even	ok
	2	C <sub>18</sub> H <sub>18</sub> N <sub>3</sub> O <sub>5</sub>	3.96	356.12410	-3.8	-10.6	26.7	11.5	even	ok
	3	C <sub>17</sub> H <sub>18</sub> N <sub>5</sub> O <sub>4</sub>	0.01	356.13533	7.5	21.0	28.9	11.5	even	ok
	4	C <sub>16</sub> H <sub>22</sub> N <sub>1</sub> O <sub>8</sub>	0.10	356.13399	6.1	17.2	43.3	6.5	even	ok



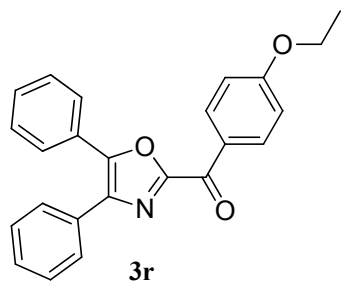
Chemical Formula: C<sub>18</sub>H<sub>15</sub>NO<sub>4</sub>  
 Molecular Weight: 309.32

**Acquisition Parameter**

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	4	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	2000.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 μm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Mon Sep 19 06:39:58
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	201072
Ion Accumulation Time	0.0 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



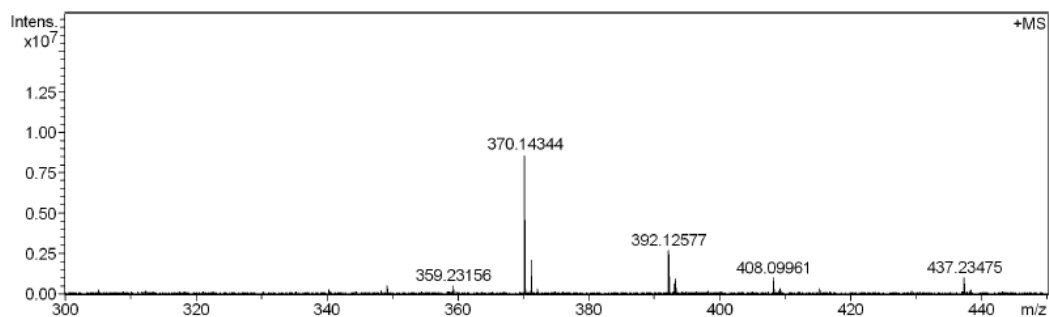
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	ej	Conf	N-Rule
310.10709	1	C <sub>18</sub> H <sub>16</sub> N <sub>1</sub> O <sub>4</sub>	100.00	310.10738	0.3	1.0	1.6	11.5	even		ok
	2	C <sub>13</sub> H <sub>16</sub> N <sub>3</sub> O <sub>6</sub>	4.13	310.10336	-3.7	-12.0	28.4	7.5	even		ok
	3	C <sub>12</sub> H <sub>16</sub> N <sub>5</sub> O <sub>5</sub>	0.01	310.11460	7.5	24.2	30.6	7.5	even		ok
	4	C <sub>12</sub> H <sub>14</sub> N <sub>5</sub> O <sub>5</sub>	0.00	308.09895	-3.4	-11.0	86.4	8.5	even		ok
	5	C <sub>14</sub> H <sub>17</sub> N <sub>2</sub> O <sub>6</sub>	0.00	309.10811	4.1	13.3	92.7	7.5	even		ok
	6	C <sub>18</sub> H <sub>14</sub> N <sub>1</sub> O <sub>4</sub>	0.00	308.09173	-9.5	-30.7	115.6	12.5	even		ok



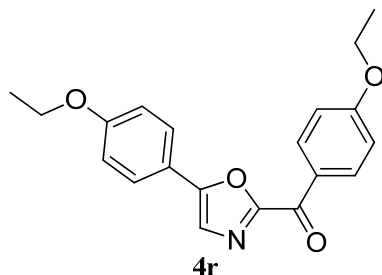
Chemical Formula: C<sub>24</sub>H<sub>19</sub>NO<sub>3</sub>  
 Molecular Weight: 369.41

**Acquisition Parameter**

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	4	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	2000.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 μm
Acquisition Mode	Single MS	Skimmer 1	20.0 V	Calibration Date	Mon Sep 19 06:39:58
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Data Acquisition Size	201072
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.0 sec	Nebulizer Gas Flow Rate	1.0 L/min		
Flight Time to Acq. Cell	0.0 sec				



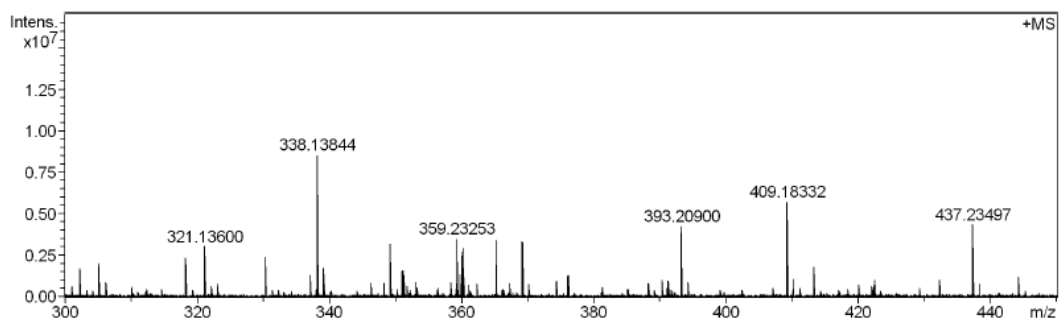
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	ej*Conf	N-Rule
370.14344	1	C <sub>24</sub> H <sub>20</sub> N <sub>3</sub> O <sub>3</sub>	100.00	370.14377	0.3	0.9	8.5	15.5	even	ok
	2	C <sub>19</sub> H <sub>20</sub> N <sub>3</sub> O <sub>5</sub>	5.91	370.13975	-3.7	-10.0	20.1	11.5	even	ok
	3	C <sub>18</sub> H <sub>20</sub> N <sub>5</sub> O <sub>4</sub>	0.01	370.15098	7.5	20.4	22.6	11.5	even	ok
	4	C <sub>17</sub> H <sub>24</sub> N <sub>3</sub> O <sub>8</sub>	0.12	370.14964	6.2	16.8	36.3	6.5	even	ok



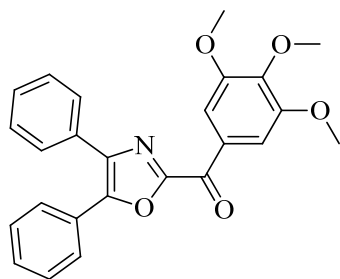
Chemical Formula: C<sub>20</sub>H<sub>19</sub>NO<sub>4</sub>  
 Molecular Weight: 337.37

**Acquisition Parameter**

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	4	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	2000.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Mon Sep 19 06:39:58
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	101072
Ion Accumulation Time	0.0 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	ejConf	N-Rule
338.13844	1	C <sub>20</sub> H <sub>20</sub> NO <sub>4</sub>	100.00	338.13868	0.2	0.7	9.2	11.5	even	ok
	2	C <sub>15</sub> H <sub>20</sub> N <sub>3</sub> O <sub>6</sub>	5.34	338.13466	-3.8	-11.2	19.3	7.5	even	ok
	3	C <sub>14</sub> H <sub>20</sub> N <sub>5</sub> O <sub>5</sub>	0.02	338.14590	7.5	22.0	21.7	7.5	even	ok
	4	C <sub>13</sub> H <sub>24</sub> NO <sub>9</sub>	0.14	338.14456	6.1	18.1	35.4	2.5	even	ok



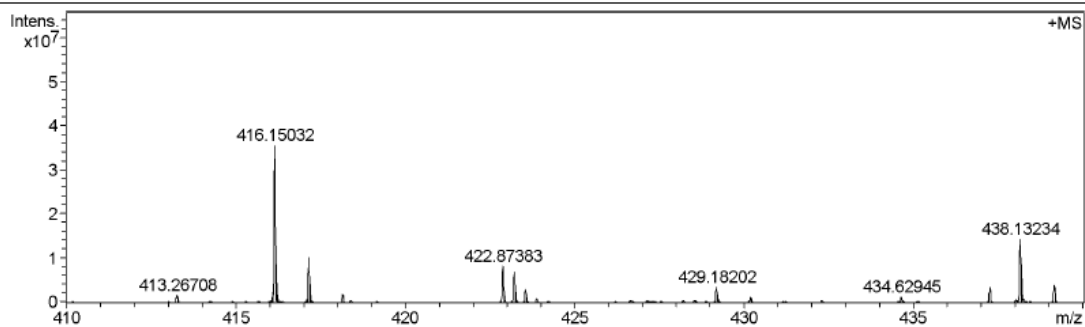
3s

Chemical Formula:  $C_{25}H_{21}NO_5$

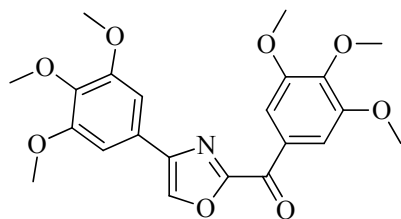
Exact Mass: 415.14

#### Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	4	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1600.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 $\mu$ m
Acquisition Mode	Single MS	Skimmer 1	20.0 V	Calibration Date	Wed Dec 7 10:47:13 2011
Pulse Program	basic	Drying Gas Temperature	180.0 $^{\circ}$ C	Data Acquisition Size	131072
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.1 sec	Nebulizer Gas Flow Rate	1.0 L/min		
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
416.15032	1	C <sub>25</sub> H <sub>22</sub> N <sub>1</sub> O <sub>5</sub>	100.00	416.14925	-1.1	-2.6	9.1	15.5	even	ok



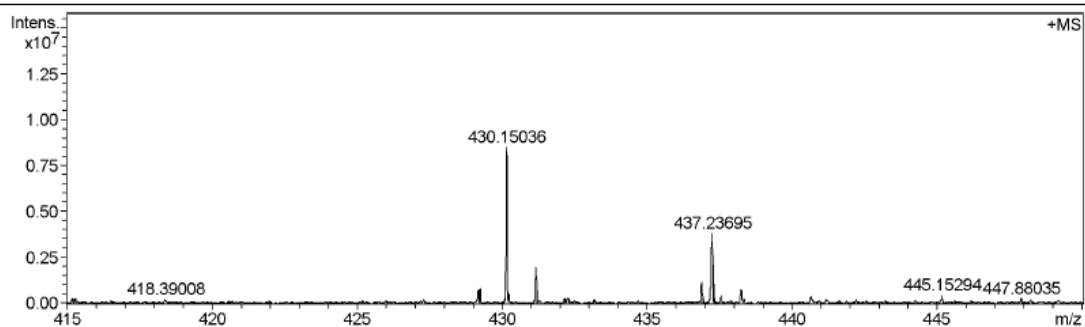
**4s**

Chemical Formula: C<sub>22</sub>H<sub>23</sub>NO<sub>8</sub>

Exact Mass: 429.14

**Acquisition Parameter**

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	4	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1600.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 μm
Acquisition Mode	Single MS	Skimmer 1	20.0 V	Calibration Date	Wed Dec 7 10:47:13 2011
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Data Acquisition Size	131072
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.1 sec	Nebulizer Gas Flow Rate	1.0 L/min		
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
430.15036	1	C <sub>22</sub> H <sub>24</sub> N <sub>1</sub> O <sub>8</sub>	100.00	430.14964	-0.7	-1.7	14.1	11.5	even	ok
	2	C <sub>23</sub> H <sub>20</sub> N <sub>5</sub> O <sub>4</sub>	96.05	430.15098	0.6	1.4	18.6	16.5	even	ok
	3	C <sub>24</sub> H <sub>16</sub> N <sub>9</sub>	29.97	430.15232	2.0	4.5	32.9	21.5	even	ok