

# **Palladium-Catalyzed Intramolecular Addition of C-N Bond to Alkynes: A Novel Approach to 3-Diketoindoles**

## **Supporting Information**

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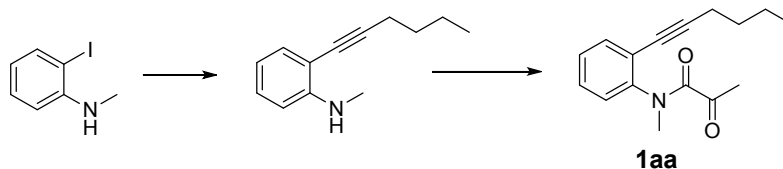
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## **General Information**

The reagents were purchased from commercial suppliers and used without further purification. Analytical thin-layer chromatography (TLC) was performed on HSGF 254 (0.15-0.2 mm thickness), visualized by irradiation with UV light (254 nm). Column chromatography was performed using silica gel FCP 200-300. Melting points were measured with a micro melting point apparatus. Nuclear magnetic resonance spectra were recorded on a Bruker AMX-400MHz instrument (TMS as IS). Chemical shifts were reported in parts per million (ppm,  $\delta$ ) downfield from tetramethylsilane. Proton coupling patterns were described as singlet (s), doublet (d), triplet (t), quartet (q), multiplet (m), and broad (br). Low and high resolution mass were measured by the EI method with a Tsou-EI mass spectrometer.

## Preparation and Characterization data of the materials

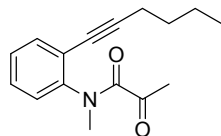
### Procedure for the preparation of *N*-(2-(hex-1-yn-1-yl)phenyl)-*N*-methyl-2-oxopropanamide (**1aa**)



To a solution of 2-iodo-*N*-methylaniline (3.8 mmol, 885 mg) in DMF (5 ml) and Et<sub>3</sub>N (5 ml) was added PdCl<sub>2</sub>(PPh<sub>3</sub>)<sub>2</sub> (0.38 mmol), CuI (0.38 mmol), and 1-hexyne (3.99 mmol, 455 μl), and the resulting mixture was stirred at room temperature for 6 hours. Then water was added and the reaction mixture was extracted with ethyl acetate. The organic extracts were washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, and concentrated. The residue was purified by flash chromatography to give 2-(hex-1-yn-1-yl)-*N*-methylaniline (683 mg, 96%). To a solution of 2-(hex-1-yn-1-yl)-*N*-methylaniline (683 mg, 3.65 mmol) in anhydrous CH<sub>2</sub>Cl<sub>2</sub> (25 mL) was added 2-oxopropanoyl chloride (7.3 mmol) and pyridine (882 μl, 10.95 mmol). The resulting mixture was stirred under nitrogen at 0 °C for 4 hours. Then 1 mol/L HCl was added and the reaction mixture was extracted with CH<sub>2</sub>Cl<sub>2</sub>. The organic extracts were washed with saturated aqueous NaHCO<sub>3</sub> solution, dried over Na<sub>2</sub>SO<sub>4</sub> and concentrated. The residue was purified by flash chromatography to give *N*-(2-(hex-1-yn-1-yl)phenyl)-*N*-methyl-2-oxopropanamide (**1aa**) (930 mg, 99%).

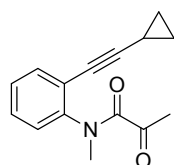
Compounds 1ab-1ay were prepared following the similar procedure carried out for 1aa.

***N*-(2-(hex-1-yn-1-yl) phenyl)-*N*-methyl-2-oxopropanamide (1aa)**



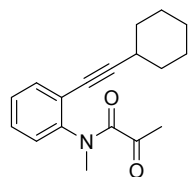
$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.41(dd,  $J = 7.6, 1.6$  Hz, 1H), 7.30 (dd,  $J = 7.6, 1.8$  Hz, 1H), 7.26 (dd,  $J = 7.6, 1.6$  Hz, 1H), 7.24-7.20 (m, 1H), 3.30 (s, 3H), 2.42 (t,  $J = 7.1$  Hz, 2H), 2.30 (s, 3H), 1.63-1.52 (m, 2H), 1.49-1.41 (m, 2H), 0.94 (t,  $J = 7.3$  Hz, 3H); EI-MS ( $m/z$ ): 257 ( $\text{M}^+$ ).

***N*-(2-(cyclopropylethynyl) phenyl)-*N*-methyl-2-oxopropanamide (1ab)**



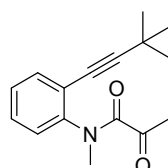
$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.39-7.34 (m, 1H), 7.29 (dd,  $J = 7.6, 1.7$  Hz, 1H), 7.26-7.19 (m, 2H), 3.28 (s, 3H), 2.32 (s, 3H), 1.48-1.37 (m, 1H), 0.95-0.89 (m, 2H), 0.86-0.79 (m, 2H); EI-MS ( $m/z$ ): 241 ( $\text{M}^+$ ).

***N*-(2-(cyclohexylethynyl) phenyl)-*N*-methyl-2-oxopropanamide (1ac)**



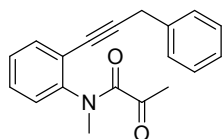
$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.38 (d,  $J = 7.8$  Hz, 1H), 7.31-7.26 (m, 1H), 7.25-7.18 (m, 2H), 3.27 (s, 3H), 2.63-2.51 (m, 1H), 2.27 (s, 3H), 1.89-1.82 (m, 2H), 1.73-1.69 (m, 2H), 1.55-1.44 (m, 3H), 1.37-1.28 (m, 3H); EI-MS ( $m/z$ ): 283 ( $\text{M}^+$ ).

***N*-(2-(3,3-dimethylbut-1-yn-1-yl) phenyl)-*N*-methyl-2-oxopropanamide (1ad)**



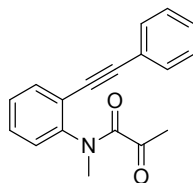
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.39 (dd,  $J = 7.4, 1.8$  Hz, 1H), 7.33-7.28 (m, 1H), 7.28-7.26 (m, 1H), 7.25-7.22 (dd,  $J = 1.7$  Hz, 1H), 3.29 (s, 3H), 2.29 (s, 3H), 1.32 (s, 9H); EI-MS ( $m/z$ ): 257 ( $\text{M}^+$ ).

***N*-methyl-2-oxo-*N*-(2-(3-phenylprop-1-yn-1-yl) phenyl)propanamide (1ae)**



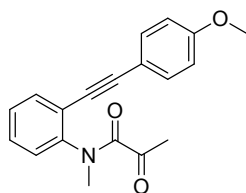
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.47 (dd,  $J = 7.6, 1.6$  Hz, 1H), 7.38-7.32 (m, 5H), 7.30-7.26 (m, 2H), 7.24 (dd,  $J = 7.8, 1.3$  Hz, 1H), 3.84 (s, 2H), 3.31 (s, 3H), 2.21 (s, 3H); EI-MS ( $m/z$ ): 291 ( $\text{M}^+$ ).

***N*-methyl-2-oxo-*N*-(2-(phenylethynyl) phenyl) propanamide (1af)**



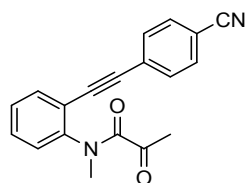
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.59-7.42 (m, 3H), 7.42-7.35 (m, 4H), 7.35-7.31 (m, 2H), 3.38 (s, 3H), 2.31 (s, 3H); EI-MS ( $m/z$ ): 277 ( $\text{M}^+$ ).

***N*-(2-((4-methoxyphenyl) ethynyl) phenyl)-*N*-methyl-2-oxopropanamide (1ag)**



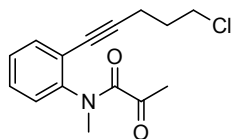
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.52-7.45 (m, 3H), 7.39-7.34 (m, 1H), 7.33-7.28 (m, 2H), 6.92-6.88 (m, 2H), 3.84 (s, 3H), 3.37 (s, 3H), 2.30 (s, 3H); EI-MS ( $m/z$ ): 307 ( $\text{M}^+$ ).

***N*-(2-((4-cyanophenyl) ethynyl) phenyl)-*N*-methyl-2-oxopropanamide (1ah)**



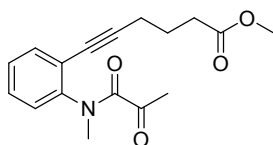
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.69-7.65 (m, 2H), 7.62-7.59 (m, 2H), 7.56 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.46 (m, 1H), 7.39-7.32 (m, 2H), 3.37 (s, 3H), 2.29 (s, 3H); EI-MS (*m/z*): 302 (M<sup>+</sup>).

***N*-(2-(5-chloropent-1-yn-1-yl) phenyl)-*N*-methyl-2-oxopropanamide (1ai)**



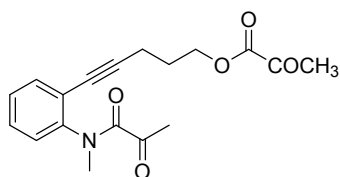
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.39 (dd, *J* = 7.5 Hz, 1H), 7.36-7.28 (m, 1H), 7.25 (dd, *J* = 7.5 Hz, 1H), 7.20 (d, *J* = 7.8 Hz, 1H), 3.66 (t, *J* = 6.2 Hz, 2H), 3.28 (s, 3H), 2.61 (t, *J* = 6.8 Hz, 2H), 2.27 (s, 3H), 2.05-2.00 (m, 2H); EI-MS (*m/z*): 279 (M<sup>+</sup>, (Cl<sup>37</sup>)), 277 (M<sup>+</sup>, (Cl<sup>35</sup>)).

**Methyl 6-(2-(*N*-methyl-2-oxopropanamido) phenyl) hex-5-ynoate (1aj)**



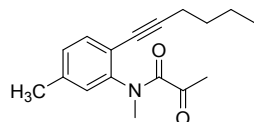
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.40 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.35-7.28 (m, 1H), 7.27-7.22 (m, 1H), 7.22-7.19 (m, 1H), 3.67 (s, 3H), 3.28 (s, 3H), 2.51-2.44 (m, 4H), 2.28 (s, 3H), 1.95-1.88 (m, 2H); EI-MS (*m/z*): 301 (M<sup>+</sup>).

**5-(2-(*N*-methyl-2-oxopropanamido) phenyl) pent-4-yn-1-yl 2-oxopropanoate (1ak)**



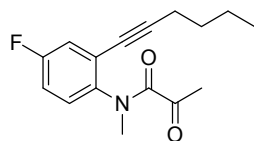
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.49-7.37 (d, *J* = 7.6 Hz, 1H), 7.35-7.32 (m, 1H), 7.27-7.24 (m, 1H), 7.21-7.18 (m, 1H), 4.36 (t, *J* = 6.3 Hz, 2H), 3.27 (s, 3H), 2.56 (t, *J* = 7.0 Hz, 2H), 2.47 (s, 3H), 2.26 (s, 3H), 2.04-1.99 (m, 2H); EI-MS (*m/z*): 329 (M<sup>+</sup>).

***N*-(2-(hex-1-yn-1-yl)-5-methylphenyl)-*N*-methyl-2-oxopropanamide (1al)**



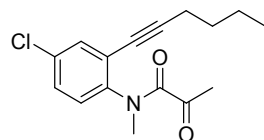
$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.27 (d,  $J = 7.8$  Hz, 1H), 7.06-7.03 (m, 2H), 3.28 (s, 3H), 2.40 (t,  $J = 7.1$  Hz, 2H), 2.33 (s, 3H), 2.29 (s, 3H), 1.60-1.53 (m, 2H), 1.47-1.41 (m, 2H), 0.93 (t,  $J = 7.3$  Hz, 3H); EI-MS ( $m/z$ ): 271 ( $\text{M}^+$ ).

***N*-(4-fluoro-2-(hex-1-yn-1-yl)phenyl)-*N*-methyl-2-oxopropanamide (1am)**



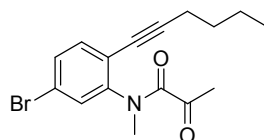
$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.19 (dd,  $J = 8.8, 5.2$  Hz, 1H), 7.08 (dd,  $J = 8.7, 2.9$  Hz, 1H), 7.03-6.97 (m, 1H), 3.27 (s, 3H), 2.41 (t,  $J = 7.1$  Hz, 2H), 2.30 (s, 3H), 1.60-1.54 (m, 2H), 1.47-1.41 (m, 2H), 0.94 (t,  $J = 7.3$  Hz, 3H); EI-MS ( $m/z$ ): 275 ( $\text{M}^+$ ).

***N*-(4-chloro-2-(hex-1-yn-1-yl)phenyl)-*N*-methyl-2-oxopropanamide (1an)**



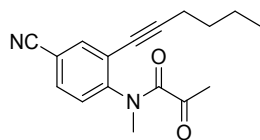
$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.37 (d,  $J = 2.4$  Hz, 1H), 7.28 (dd,  $J = 8.5, 2.4$  Hz, 1H), 7.15 (d,  $J = 8.5$  Hz, 1H), 3.27 (s, 3H), 2.41 (t,  $J = 7.1$  Hz, 2H), 2.32 (s, 3H), 1.61-1.54 (m, 2H), 1.47-1.41 (m, 2H), 0.94 (t,  $J = 7.3$  Hz, 3H); EI-MS ( $m/z$ ): 293 ( $\text{M}^+$ , ( $\text{Cl}^{37}$ )), 291 ( $\text{M}^+$ , ( $\text{Cl}^{35}$ )).

***N*-(5-bromo-2-(hex-1-yn-1-yl)phenyl)-*N*-methyl-2-oxopropanamide (1ao)**



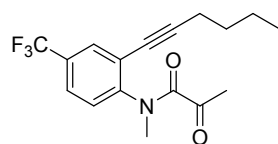
$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.53 (d,  $J = 2.3$  Hz, 1H), 7.42 (dd,  $J = 8.5, 2.3$  Hz, 1H), 7.09 (d,  $J = 8.5$  Hz, 1H), 3.27 (s, 3H), 2.41 (t,  $J = 7.1$  Hz, 2H), 2.32 (s, 3H), 1.60-1.54 (m, 2H), 1.47-1.41 (m, 2H), 0.94 (t,  $J = 7.3$  Hz, 3H); EI-MS ( $m/z$ ): 337 ( $\text{M}^+$ , ( $\text{Br}^{81}$ )), 335 ( $\text{M}^+$ , ( $\text{Br}^{79}$ )).

***N*-(4-cyano-2-(hex-1-yn-1-yl) phenyl)-*N*-methyl-2-oxopropanamide (1ap)**



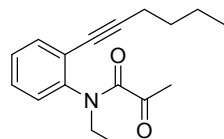
$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.67 (s, 1H), 7.58 (dd,  $J = 8.2, 1.7$  Hz, 1H), 7.33 (d,  $J = 8.3$  Hz, 1H), 3.30 (s, 3H), 2.41 (t,  $J = 7.1$  Hz, 2H), 2.37 (s, 3H), 1.61-1.54 (m, 2H), 1.48-1.40 (m, 2H), 0.94 (t,  $J = 7.3$  Hz, 3H); EI-MS ( $m/z$ ): 282 ( $\text{M}^+$ ).

***N*-(2-(hex-1-yn-1-yl)-4-(trifluoromethyl) phenyl)-*N*-methyl-2-oxopropanamide (1aq)**



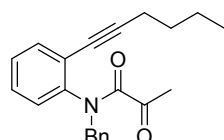
$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.65 (s, 1H), 7.55 (d,  $J = 8.3, 1.6$  Hz, 1H), 7.34 (d,  $J = 8.3$  Hz, 1H), 3.31 (s, 3H), 2.42 (t,  $J = 7.1$  Hz, 2H), 2.36 (s, 3H), 1.61-1.56 (m, 2H), 1.49-1.40 (m, 2H), 0.94 (t,  $J = 7.3$  Hz, 3H); EI-MS ( $m/z$ ): 325 ( $\text{M}^+$ ).

***N*-ethyl-*N*-(2-(hex-1-yn-1-yl) phenyl)-2-oxopropanamide (1ar)**



$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.40 (d,  $J = 7.6$  Hz, 1H), 7.33-7.29 (m, 1H), 7.25-7.23 (m, 1H), 7.20 (d,  $J = 7.7$  Hz, 1H), 3.92-3.83 (m, 1H), 3.80-3.71 (m, 1H), 2.40 (t,  $J = 7.1$  Hz, 2H), 2.29 (s, 3H), 1.61-1.54 (m, 2H), 1.49-1.41 (m, 2H), 1.15 (t,  $J = 7.2$  Hz, 3H), 0.93 (t,  $J = 7.3$  Hz, 3H); EI-MS ( $m/z$ ): 271 ( $\text{M}^+$ ).

**Methyl 6-(2-(*N*-benzyl-2-oxopropanamido) phenyl) hex-5-ynoate (1as)**

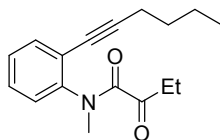


$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.38 (dd,  $J = 7.6, 1.7$  Hz, 1H), 7.29-7.26 (m, 1H), 7.26-7.24 (m, 2H), 7.24-7.18 (m, 3H), 7.18-7.13 (m, 1H), 6.89 (dd,  $J = 7.8, 1.3$  Hz, 1H), 5.36 (d,  $J = 14.3$  Hz, 1H), 4.50 (d,



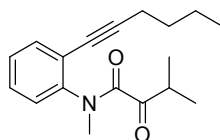
$J = 14.3$  Hz, 1H), 2.40 (t,  $J = 7.1$  Hz, 2H), 2.32 (s, 3H), 1.61-1.54 (m, 2H), 1.49-1.40 (m, 2H), 0.96 (t,  $J = 7.3$  Hz, 3H); EI-MS ( $m/z$ ): 333 ( $M^+$ ).

***N*-(2-(hex-1-yn-1-yl) phenyl)-*N*-methyl-2-oxobutanamide (1at)**



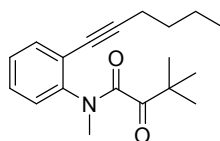
$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.40 (dd,  $J = 7.4, 1.1$  Hz, 1H), 7.32-7.27 (m, 1H), 7.25-7.19 (m, 1H), 3.30 (s, 3H), 2.88-2.76 (m, 1H), 2.66-2.55 (m, 1H), 2.41 (t,  $J = 7.1$  Hz, 2H), 1.61-1.54 (m, 2H), 1.48-1.42 (m, 2H), 0.94 (t,  $J = 5.2$  Hz, 3H), 0.91 (t,  $J = 5.2$  Hz, 3H); EI-MS ( $m/z$ ): 271 ( $M^+$ ).

***N*-(2-(hex-1-yn-1-yl) phenyl)-*N*, 3-dimethyl-2-oxobutanamide (1au)**



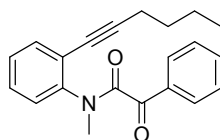
$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.45-7.37 (m, 1H), 7.29-7.26 (m, 1H), 7.26-7.21 (m, 1H), 7.19-7.15 (m, 1H), 3.31 (s, 3H), 2.99-2.85 (m, 1H), 2.41 (t,  $J = 7.1$  Hz, 2H), 1.60-1.53 (m, 2H), 1.48-1.41 (m, 2H), 1.08 (d,  $J = 6.9$  Hz, 3H), 0.95-0.84 (m, 6H); EI-MS ( $m/z$ ): 285 ( $M^+$ ).

***N*-(2-(hex-1-yn-1-yl) phenyl)-*N*, 3, 3-trimethyl-2-oxobutanamide (1av)**



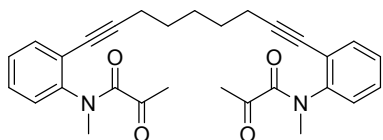
$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.46-7.42 (m, 1H), 7.28-7.23 (m, 3H), 3.36 (s, 3H), 2.44 (t,  $J = 7.0$  Hz, 2H), 1.62-1.57 (m, 2H), 1.50-1.45 (m, 2H), 1.05 (s, 9H), 0.94 (t,  $J = 7.2$  Hz, 3H); EI-MS ( $m/z$ ): 299 ( $M^+$ ).

***N*-(2-(hex-1-yn-1-yl) phenyl)-*N*-methyl-2-oxo-2-phenylacetamide (1aw)**



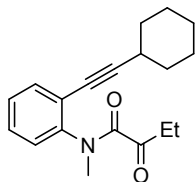
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.89 (dd,  $J = 8.2, 1.0$  Hz, 2H), 7.56-7.51 (m, 1H), 7.40-7.35 (m, 2H), 7.31-7.27 (m, 1H), 7.22-7.13 (m, 3H), 3.46 (s, 3H), 2.45-2.40 (m, 2H), 1.64-1.57 (m, 2H), 1.53-1.45 (m, 2H), 0.96 (t,  $J = 7.3$  Hz, 3H); EI-MS ( $m/z$ ): 319 ( $\text{M}^+$ ).

***N, N'*-(nona-1, 8-diyne-1, 9-diylbis(2,1-phenylene))bis(*N*-methyl-2-oxopropanamide) (1ax)**



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.39 (dd,  $J = 7.5, 1.5$  Hz, 2H), 7.33-7.28 (m, 2H), 7.25-7.19 (m, 4H), 3.28 (s, 6H), 2.45 (t,  $J = 6.8$  Hz, 4H), 2.29 (s, 6H), 1.71-1.58 (m, 6H); EI-MS ( $m/z$ ): 470 ( $\text{M}^+$ ).

***N*-(2-(cyclohexylethynyl) phenyl)-*N*-methyl-2-oxobutanamide (1ay)**



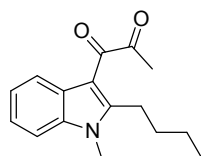
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.40 (dd,  $J = 7.4, 1.8$  Hz, 1H), 7.33-7.18 (m, 3H), 3.29 (s, 3H), 2.89-2.75 (m, 1H), 2.65-2.53 (m, 2H), 1.87 (d,  $J = 11.3$  Hz, 2H), 1.77-1.69 (m, 2H), 1.57-1.45 (m, 3H), 1.38-1.30 (m, 3H), 0.90 (t,  $J = 7.3$  Hz, 3H); EI-MS ( $m/z$ ): 297 ( $\text{M}^+$ ).

## Preparation and Characterization data of compounds 2

### General procedure for the preparation of 2

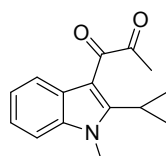
A vial equipped with a magnetic stir bar was charged with **1** (0.5 mmol), PdCl<sub>2</sub>(CH<sub>3</sub>CN)<sub>2</sub> (0.05 mmol, 12.9 mg), and solvent indicated (2.0 ml) and capped with septa. Then the vial was evacuated and backfilled with argon. After that, the vial was kept in the pre-heated oil bath at the temperature indicated for indicated time. After removal of the solvent, the residue was purified by flash chromatography on silica gel to give the desired product.

### 1-(2-butyl-1-methyl-1H-indol-3-yl) propane-1, 2-dione (2aa)



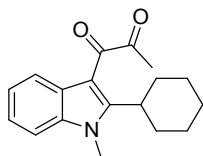
Yellow solid (125.9 mg, yield 98%), mp 44-45 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.81-7.74 (m, 1H), 7.34-7.30 (m, 1H), 7.30-7.26 (m, 1H), 7.26-7.23 (m, 1H), 3.73 (s, 3H), 3.11-3.06 (m, 2H), 2.55 (s, 3H), 1.65-1.58 (m, 2H), 1.51-1.43 (m, 2H), 0.98 (t, *J* = 7.3 Hz, 3H); <sup>13</sup>C NMR (151 MHz, CDCl<sub>3</sub>) δ 203.12, 189.28, 152.38, 137.09, 126.14, 122.94, 122.88, 120.46, 109.85, 107.86, 31.21, 29.76, 26.40, 26.03, 22.83, 13.81; EI-MS (*m/z*): 257(M<sup>+</sup>); HRMS (EI) calcd for C<sub>16</sub>H<sub>19</sub>NO<sub>2</sub> (M<sup>+</sup>) 257.1416, found: 257.1411.

### 1-(2-cyclopropyl-1-methyl-1H-indol-3-yl) propane-1, 2-dione (2ab)



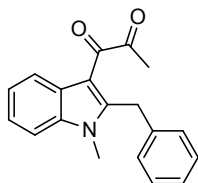
Yellow solid (108.5 mg, yield 90%), mp 108-109 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.22-8.15 (m, 1H), 7.32-7.26 (m, 3H), 3.85 (s, 3H), 2.59 (s, 3H), 2.00-1.94 (m, 1H), 1.16-1.10 (m, 2H), 0.68-0.64 (m, 2H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 201.24, 189.41, 150.93, 136.90, 126.77, 123.58, 123.23, 121.65, 110.30, 109.56, 30.97, 25.58, 9.11, 7.96; EI-MS (*m/z*): 241(M<sup>+</sup>); HRMS (EI) calcd for C<sub>15</sub>H<sub>15</sub>NO<sub>2</sub> (M<sup>+</sup>) 241.1103, found: 241.1097.

### 1-(2-cyclohexyl-1-methyl-1H-indol-3-yl) propane-1, 2-dione (2ac)



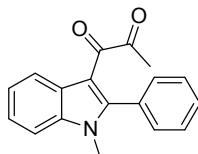
Yellow Solid (131.6 mg, yield 93%), mp 56-58 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.69 (d, *J* = 7.8 Hz, 1H), 7.32 (d, *J* = 7.8 Hz, 1H), 7.29-7.20 (m, 2H), 3.87 (s, 3H), 3.65-3.51 (m, 1H), 2.58 (s, 3H), 2.07-1.96 (m, 2H), 1.92-1.89 (m, 2H), 1.94-1.78 (m, 3H), 1.49-1.33 (m, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 203.06, 190.05, 154.99, 137.51, 126.44, 123.00, 122.87, 120.32, 109.84, 108.15, 37.68, 32.14, 29.42, 26.86, 26.40, 25.83; EI-MS (*m/z*): 283 (M<sup>+</sup>); HRMS (EI) calcd for C<sub>18</sub>H<sub>21</sub>NO<sub>2</sub> (M<sup>+</sup>) 283.1572, found: 283.1566.

#### 1-(2-benzyl-1-methyl-1H-indol-3-yl) propane-1, 2-dione (2ae)



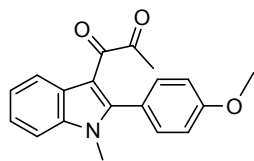
White solid (128.0 mg, yield 88%), mp 106-107 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.93-7.86 (m, 1H), 7.36-7.26 (m, 5H), 7.24-7.19 (m, 1H), 7.12 (d, *J* = 7.5 Hz, 2H), 4.59 (s, 2H), 3.63 (s, 3H), 2.45 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 202.94, 189.54, 148.72, 137.35, 136.82, 129.01, 128.32, 126.95, 126.33, 123.44, 123.20, 121.07, 109.95, 109.55, 31.87, 30.33, 26.33; EI-MS (*m/z*): 291 (M<sup>+</sup>); HRMS (EI) calcd for C<sub>19</sub>H<sub>17</sub>NO<sub>2</sub> (M<sup>+</sup>) 291.1259, found: 291.1253.

#### 1-(1-methyl-2-phenyl-1H-indol-3-yl) propane-1, 2-dione (2af)



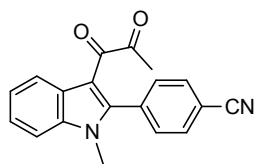
Yellow solid (83.1 mg, yield 60%), mp 165-166 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.36 (dd, *J* = 7.7, 4.1 Hz, 1H), 7.55-7.49 (m, 3H), 7.41-7.36 (m, 5H), 3.61 (s, 3H), 2.07 (s, 3H); <sup>13</sup>C NMR (151 MHz, CDCl<sub>3</sub>) δ 201.29, 190.93, 149.23, 137.49, 130.92, 130.38, 130.25, 128.66, 126.87, 124.22, 123.67, 122.36, 110.97, 110.08, 31.19, 26.02; EI-MS (*m/z*): 277 (M<sup>+</sup>); HRMS (EI) calcd for C<sub>18</sub>H<sub>15</sub>NO<sub>2</sub> (M<sup>+</sup>) 277.1103, found: 277.1096.

**1-(2-(4-methoxyphenyl)-1-methyl-1H-indol-3-yl) propane-1, 2-dione (2ag)**



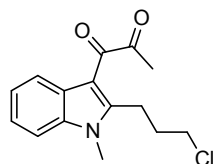
Yellow solid (99.8 mg, yield 65%), mp 159-160 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.38-8.33 (m, 1H), 7.40-7.35 (m, 3H), 7.31-7.27 (m, 2H), 7.03-6.99 (m, 2H), 3.89 (s, 3H), 3.59 (s, 3H), 2.08 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 201.62, 191.11, 161.02, 149.41, 137.47, 132.30, 126.83, 124.09, 123.55, 122.22, 122.11, 114.08, 110.92, 110.05, 55.50, 31.08, 26.12; EI-MS (*m/z*): 307 (M<sup>+</sup>); HRMS (EI) calcd for C<sub>19</sub>H<sub>17</sub>NO<sub>3</sub> (M<sup>+</sup>) 307.1208, found: 307.1201.

**4-(1-methyl-3-(2-oxopropanoyl)-1H-indol-2-yl) benzonitrile (2ah)**



Pale Yellow solid (93.6 mg, yield 62%), mp 196-198 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.26-8.24 (m, 1H), 7.84-7.77 (m, 2H), 7.53-7.51 (m, 2H), 7.44-7.42 (m, 2H), 7.41-7.37 (m, 1H), 3.61 (s, 3H), 2.20 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 200.90, 189.45, 146.19, 137.58, 135.54, 132.30, 131.54, 126.63, 124.73, 124.02, 122.31, 118.12, 114.06, 111.05, 110.27, 31.39, 26.04; EI-MS (*m/z*): 302 (M<sup>+</sup>); HRMS (EI) calcd for C<sub>19</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub>(M<sup>+</sup>) 302.1055, found: 302.1052.

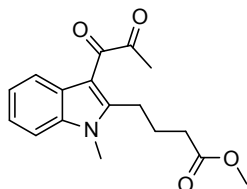
**1-(2-(3-chloropropyl)-1-methyl-1H-indol-3-yl) propane-1, 2-dione (2ai)**



Pale Yellow solid (131.6 mg, yield 95%), mp 108-109 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.72-7.70 (d, *J* = 7.6 Hz, 1H), 7.38-7.35 (m, 1H), 7.32 (dd, *J* = 7.1, 1.3 Hz, 1H), 7.29-7.26 (m, 1H), 3.81 (s, 3H), 3.67 (t, *J* = 6.1 Hz, 2H), 3.35-3.28 (m, 2H), 2.56 (s, 3H), 2.21-2.12 (m, 2H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 203.12, 189.15, 150.64, 137.24, 126.06, 123.34, 123.24, 120.55, 110.11, 108.52, 44.79, 31.74,

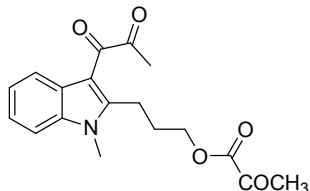
30.05, 26.45, 23.98; EI-MS ( $m/z$ ): 279 ( $M^+$ , ( $Cl^{37}$ )), 277( $M^+$ , ( $Cl^{35}$ )); HRMS (EI) calcd for  $C_{15}H_{16}ClNO_2$  ( $M^+$ ) 277.0870, found: 277.0865.

**Methyl 4-(1-methyl-3-(2-oxopropanoyl)-1H-indol-2-yl) butanoate (2aj)**



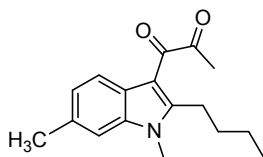
Yellow solid (135.5 mg, yield 90%), mp 92-93 °C.  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.72 (d,  $J = 7.9$  Hz, 1H), 7.35 (d,  $J = 7.9$  Hz, 1H), 7.31-7.21 (m, 2H), 3.81 (s, 3H), 3.68 (s, 3H), 3.22-3.16 (t,  $J = 8.0$  Hz, 2H), 2.55 (s, 3H), 2.52-2.48 (t,  $J = 6.8$  Hz, 2H), 2.02-1.93 (m, 2H);  $^{13}C$  NMR (126 MHz,  $CDCl_3$ )  $\delta$  203.17, 189.24, 173.81, 151.13, 137.26, 126.07, 123.23, 123.12, 120.54, 110.04, 108.31, 51.79, 33.11, 29.94, 26.46, 25.60, 23.92; EI-MS ( $m/z$ ): 301 ( $M^+$ ); HRMS (EI) calcd for  $C_{17}H_{19}NO_4$  ( $M^+$ ) 301.1314, found: 301.1318.

**2-(1-methyl-3-(2-oxopropanoyl)-1H-indol-2-yl) ethyl 2-oxopropanoate (2ak)**



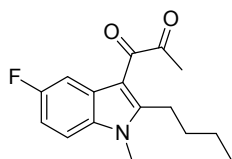
Yellow oil (149.7 mg, yield 91%).  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.69 (d,  $J = 8.0$  Hz, 1H), 7.33 (d,  $J = 7.8$  Hz, 1H), 7.29 (d,  $J = 7.0$  Hz, 1H), 7.23 (d,  $J = 7.3$  Hz, 1H), 4.34 (t,  $J = 6.0$  Hz, 2H), 3.75 (s, 3H), 3.23 (t,  $J = 7.6$  Hz, 2H), 2.53 (s, 3H), 2.46 (s, 3H), 2.10 (m, 2H);  $^{13}C$  NMR (126 MHz,  $CDCl_3$ )  $\delta$  203.13, 191.86, 189.10, 160.76, 150.32, 137.16, 125.91, 123.30, 123.16, 120.48, 110.09, 108.35, 65.43, 29.89, 27.62, 26.72, 26.35, 22.88; EI-MS ( $m/z$ ): 329 ( $M^+$ ); HRMS (EI) calcd for  $C_{18}H_{19}NO_5$  ( $M^+$ ) 329.1263, found: 329.1259.

**1-(2-butyl-1, 6-dimethyl-1H-indol-3-yl) propane-1, 2-dione (2al)**



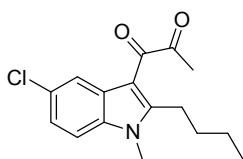
Yellow solid (134.1 mg, yield 99%), mp 78-80 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.64 (d, *J* = 8.2 Hz, 1H), 7.12 (s, 1H), 7.07 (d, *J* = 8.2 Hz, 1H), 3.71 (s, 3H), 3.08 (t, *J* = 8.0 Hz, 2H), 2.54 (s, 3H), 2.48 (s, 3H), 1.64-1.58 (m, 2H), 1.46 (m, 2H), 0.97 (t, *J* = 7.3 Hz, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 203.29, 189.29, 152.08, 137.63, 133.08, 124.58, 123.99, 120.34, 109.98, 107.96, 31.39, 29.83, 26.50, 26.19, 22.94, 21.82, 13.93; EI-MS (*m/z*): 271(M<sup>+</sup>); HRMS (EI) calcd for C<sub>17</sub>H<sub>21</sub>NO<sub>2</sub> (M<sup>+</sup>) 271.1572, found: 271.1566.

**1-(2-butyl-5-fluoro-1-methyl-1H-indol-3-yl) propane-1, 2-dione (2am)**



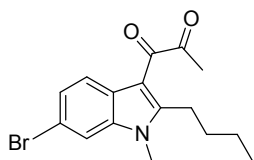
Yellow solid (130.6 mg, yield 95%), mp 62-63 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.52-7.45 (m, 1H), 7.19-7.13 (m, 1H), 6.96-6.87 (m, 1H), 3.65 (s, 3H), 3.01-2.94 (m, 2H), 2.51 (s, 3H), 1.60-1.52 (m, 2H), 1.48-1.39 (m, 2H), 0.94 (t, *J* = 7.2 Hz, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 202.75, 188.82, 160.69, 158.80, 153.41, 133.60, 127.01, 126.92, 111.05, 110.84, 110.61, 110.53, 108.05, 106.54, 106.34, 31.21, 29.99, 26.31, 26.18, 22.81, 13.75; EI-MS (*m/z*): 275(M<sup>+</sup>); HRMS (EI) calcd for C<sub>16</sub>H<sub>18</sub>FNO<sub>2</sub> (M<sup>+</sup>) 275.1322, found: 275.1317.

**1-(2-butyl-5-chloro-1-methyl-1H-indol-3-yl) propane-1, 2-dione (2an)**



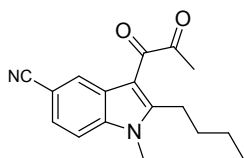
Yellow solid (135.3 mg, yield 93%), mp 77-78 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.82-7.80 (m, 1H), 7.21-7.18 (m, 2H), 3.70 (s, 3H), 3.05-2.99 (m, 2H), 2.55 (s, 3H), 1.63-1.56 (m, 2H), 1.50-1.42 (m, 2H), 0.97 (t, *J* = 7.3 Hz, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 202.62, 188.85, 153.23, 135.61, 128.93, 127.38, 123.35, 120.55, 110.78, 107.88, 31.34, 30.10, 26.40, 26.26, 22.93, 13.86; EI-MS (*m/z*): 293 (M<sup>+</sup>, (Cl<sup>37</sup>)), 291 (M<sup>+</sup>, (Cl<sup>35</sup>)); HRMS (EI) calcd for C<sub>16</sub>H<sub>18</sub>ClNO<sub>2</sub> (M<sup>+</sup>) 291.1026, found: 291.1021.

**1-(6-bromo-2-butyl-1-methyl-1H-indol-3-yl) propane-1, 2-dione (2ao)**



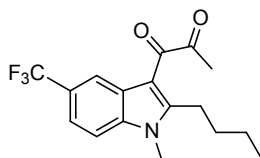
Pale Yellow solid (148.3 mg, yield 88%), mp 95-96 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.98 (d, *J* = 1.7 Hz, 1H), 7.35 (dd, *J* = 8.7, 1.9 Hz, 1H), 7.17 (d, *J* = 8.6 Hz, 1H), 3.71 (s, 3H), 3.05-3.00 (m, 2H), 2.55 (s, 3H), 1.63-1.57 (m, 2H), 1.51-1.43 (m, 2H), 0.97 (t, *J* = 7.3 Hz, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 202.56, 188.85, 153.05, 135.94, 127.97, 126.05, 123.62, 116.69, 111.17, 107.87, 31.38, 30.10, 26.40, 26.26, 22.94, 13.88; EI-MS (*m/z*): 337 (M<sup>+</sup>, (Br<sup>81</sup>)), 335 (M<sup>+</sup>, (Br<sup>79</sup>)); HRMS (EI) calcd for C<sub>16</sub>H<sub>18</sub>BrNO<sub>2</sub> (M<sup>+</sup>) 335.0521, found: 335.0516.

### 2-butyl-1-methyl-3-(2-oxopropanoyl)-1H-indole-5-carbonitrile (2ap)



White solid (114.2 mg, yield 81%), mp 116-117 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.98 (d, *J* = 1.7 Hz, 1H), 7.34 (dd, *J* = 8.7, 1.9 Hz, 1H), 7.17 (d, *J* = 8.6 Hz, 1H), 3.71 (s, 3H), 2.55 (s, 3H), 1.64-1.56 (m, 2H), 1.50-1.43 (m, 2H), 0.97 (t, *J* = 7.3 Hz, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 202.01, 188.57, 154.28, 138.80, 126.34, 126.29, 126.24, 120.10, 110.69, 108.74, 106.19, 77.41, 77.16, 76.91, 31.37, 30.29, 26.27, 22.94, 13.84; EI-MS (*m/z*): 282(M<sup>+</sup>); HRMS (EI) calcd for C<sub>17</sub>H<sub>18</sub>N<sub>2</sub>O<sub>2</sub> (M<sup>+</sup>) 282.1368, found: 282.1366.

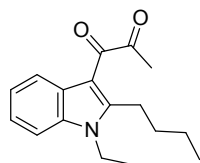
### 1-(2-butyl-1-methyl-5-(trifluoromethyl)-1H-indol-3-yl) propane-1, 2-dione (2aq)



Pale Yellow solid (134.8 mg, yield 83%), mp 86-87 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.19 (s, 1H), 7.52 (d, *J* = 8.5 Hz, 1H), 7.40 (d, *J* = 8.5 Hz, 1H), 3.79 (s, 3H), 3.06 (t, *J* = 8.0 Hz, 2H), 2.57 (s, 3H), 1.65-1.59 (m, 2H), 1.51-1.45 (m, 2H), 0.98 (t, *J* = 7.3 Hz, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 202.28, 188.92, 153.78, 138.64, 126.02, 125.71, 125.46, 125.20, 124.95, 123.93, 120.04, 120.01, 118.85, 118.82, 110.09, 108.96, 31.48, 30.24, 26.33, 26.30, 22.95, 13.88; EI-MS (*m/z*): 325(M<sup>+</sup>); HRMS (EI) calcd for C<sub>17</sub>H<sub>18</sub>F<sub>3</sub>NO<sub>2</sub> (M<sup>+</sup>) 325.1290, found: 325.1295.

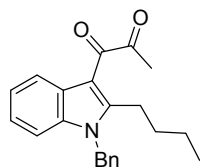


### 1-(2-butyl-1-ethyl-1H-indol-3-yl) propane-1, 2-dione (2ar)



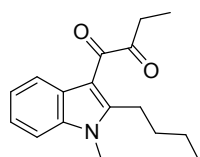
Gray solid (126.0 mg, yield 93%), mp 42-43 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.78-7.72 (m, 1H), 7.37-7.32 (m, 1H), 7.29-7.20 (m, 2H), 4.21 (q, *J* = 7.3 Hz, 2H), 3.11-3.05 (m, 2H), 2.56 (s, 3H), 1.67-1.60 (m, 2H), 1.55-1.48 (m, 2H), 1.42 (t, *J* = 7.3 Hz, 3H), 0.98 (t, *J* = 7.4 Hz, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 203.24, 189.24, 151.97, 135.94, 126.49, 122.93, 122.85, 120.58, 110.08, 107.91, 38.21, 31.77, 26.42, 26.11, 23.03, 15.11, 13.85; EI-MS (*m/z*): 271(M<sup>+</sup>); HRMS (EI) calcd for C<sub>17</sub>H<sub>21</sub>NO<sub>2</sub> (M<sup>+</sup>) 271.1572, found: 271.1568.

### 1-(1-benzyl-2-butyl-1H-indol-3-yl) propane-1, 2-dione (2as)



Yellow oil (146.5 mg, yield 88%). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 7.76 (dd, *J* = 6.6, 2.0 Hz, 1H), 7.25-7.08 (m, 6H), 6.94 (dd, *J* = 7.7, 2.4 Hz, 2H), 5.33 (s, 2H), 3.06-2.97 (m, 2H), 2.53 (s, 3H), 1.53-1.43 (m, 2H), 1.42-1.31 (m, 2H), 0.85 (t, *J* = 7.2 Hz, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 203.09, 189.46, 152.61, 136.86, 135.84, 129.14, 128.02, 126.36, 125.99, 123.28, 123.10, 120.64, 110.59, 108.47, 46.82, 31.54, 26.47, 26.35, 22.97, 13.79; EI-MS (*m/z*): 333 (M<sup>+</sup>); HRMS (EI) calcd for C<sub>22</sub>H<sub>23</sub>NO<sub>2</sub> (M<sup>+</sup>) 333.1729, found: 333.1723.

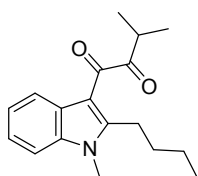
### 1-(2-butyl-1-methyl-1H-indol-3-yl) butane-1, 2-dione (2at)



Yellow Solid (121.9 mg, yield 90%), mp 80-82 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.74 (d, *J* = 7.3 Hz, 1H), 7.32 (d, *J* = 7.6 Hz, 1H), 7.29-7.27 (m, 1H), 7.25-7.21 (m, 1H), 3.73 (s, 3H), 3.10-3.05 (m, 2H), 2.94 (q, *J* = 7.3 Hz, 2H), 1.65-1.58 (m, 2H), 1.51-1.44 (m, 2H), 1.26 (t, *J* = 7.3 Hz, 3H), 0.98 (t, *J*

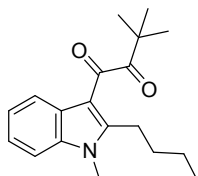
= 7.3 Hz, 3H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  206.34, 190.25, 152.28, 137.15, 126.25, 122.99, 120.47, 109.87, 108.30, 32.16, 31.30, 29.85, 26.16, 22.95, 13.90, 7.09; EI-MS ( $m/z$ ): 271( $\text{M}^+$ ); HRMS (EI) calcd for  $\text{C}_{17}\text{H}_{21}\text{NO}_2$  ( $\text{M}^+$ ) 271.1572, found: 271.1565.

**1-(2-butyl-1-methyl-1H-indol-3-yl)-3-methylbutane-1, 2-dione (2au)**



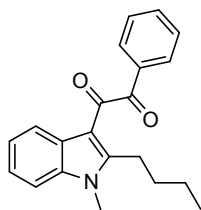
Yellow oil (123.9 mg, yield 87%).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.74-7.68 (m, 1H), 7.33-7.29 (m, 1H), 7.28-7.26 (m, 1H), 7.27-7.20 (m, 1H), 3.70 (s, 3H), 3.42-3.29 (m, 1H), 3.13-3.04 (m, 2H), 1.67-1.59 (m, 2H), 1.53-1.45 (m, 2H), 1.28 (d,  $J = 7.1$  Hz, 6H), 0.98 (t,  $J = 7.3$  Hz, 3H);  $^{13}\text{C}$  NMR (151 MHz,  $\text{CDCl}_3$ )  $\delta$  208.51, 190.51, 152.25, 137.12, 126.16, 122.88, 122.85, 120.42, 109.86, 108.91, 36.75, 31.12, 29.77, 26.15, 22.94, 17.19, 13.89; EI-MS ( $m/z$ ): 285( $\text{M}^+$ ); HRMS (EI) calcd for  $\text{C}_{18}\text{H}_{23}\text{NO}_2$  ( $\text{M}^+$ ) 285.1729, found: 285.1727.

**1-(2-butyl-1-methyl-1H-indol-3-yl)-3, 3-dimethylbutane-1, 2-dione (2av)**



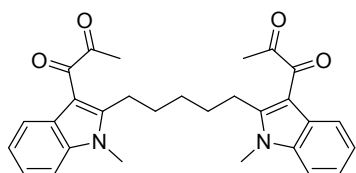
Pale Yellow solid (127.1 mg, yield 85%), mp 64-66 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.66 (d,  $J = 7.5$  Hz, 1H), 7.33 (d,  $J = 7.6$  Hz, 1H), 7.28 (dd,  $J = 7.0, 1.2$  Hz, 1H), 7.25-7.20 (m, 1H), 3.75 (s, 3H), 3.15 (t,  $J = 7.9$  Hz, 2H), 1.68-1.60 (m, 2H), 1.53-1.46 (m, 2H), 1.36 (s, 9H), 0.98 (t,  $J = 7.3$  Hz, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  211.98, 190.94, 151.91, 137.16, 126.10, 122.90, 120.25, 109.88, 109.22, 42.68, 31.16, 29.80, 27.01, 26.26, 23.01, 14.02; EI-MS ( $m/z$ ): 299( $\text{M}^+$ ); HRMS (EI) calcd for  $\text{C}_{19}\text{H}_{25}\text{NO}_2$  ( $\text{M}^+$ ) 299.1885, found: 299.1882.

**1-(2-butyl-1-methyl-1H-indol-3-yl)-2-phenylethane-1, 2-dione (2aw)**



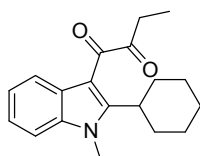
White solid (140.4 mg, yield 88%), mp 109-110 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.06 (d, *J* = 7.8 Hz, 2H), 7.89 (d, *J* = 7.8 Hz, 1H), 7.62 (m, 1H), 7.49 (m, 2H), 7.33 (d, *J* = 8.0 Hz, 1H), 7.28-7.20 (m, 2H), 3.74 (s, 3H), 3.06 (t, 2H), 1.62-1.52 (m, 2H), 1.44-1.34 (m, 2H), 0.89 (t, *J* = 7.3 Hz, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 195.31, 190.06, 152.14, 137.25, 134.47, 133.49, 130.16, 129.05, 126.33, 123.19, 121.09, 110.05, 109.79, 31.42, 29.92, 26.23, 22.94, 13.79; EI-MS (*m/z*): 319 (M<sup>+</sup>); HRMS (EI) calcd for C<sub>21</sub>H<sub>21</sub>NO<sub>2</sub> (M<sup>+</sup>) 319.1572, found: 319.1567.

**1, 1'-(2, 2'-(pentane-1, 5-diyl) bis (1-methyl-1H-indole-3,2-diyl) bis (propane-1,2-dione) (2ax)**



Yellow solid (211.5 mg, yield 90%), mp 125-126 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.71 (d, *J* = 7.7 Hz, 2H), 7.34 (d, *J* = 7.7 Hz, 2H), 7.31-7.22 (m, 4H), 3.75 (s, 6H), 3.15 (t, *J* = 7.7 Hz, 4H), 2.55 (s, 6H), 1.77-1.69 (m, 4H), 1.66-1.60 (m, 2H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 203.34, 189.33, 152.22, 137.21, 126.10, 123.13, 123.09, 120.42, 110.04, 108.01, 29.98, 29.50, 28.65, 26.50, 26.25; EI-MS (*m/z*): 470 (M<sup>+</sup>); HRMS (EI) calcd for C<sub>29</sub>H<sub>30</sub>N<sub>2</sub>O<sub>4</sub> (M<sup>+</sup>) 470.2206, found: 470.2201.

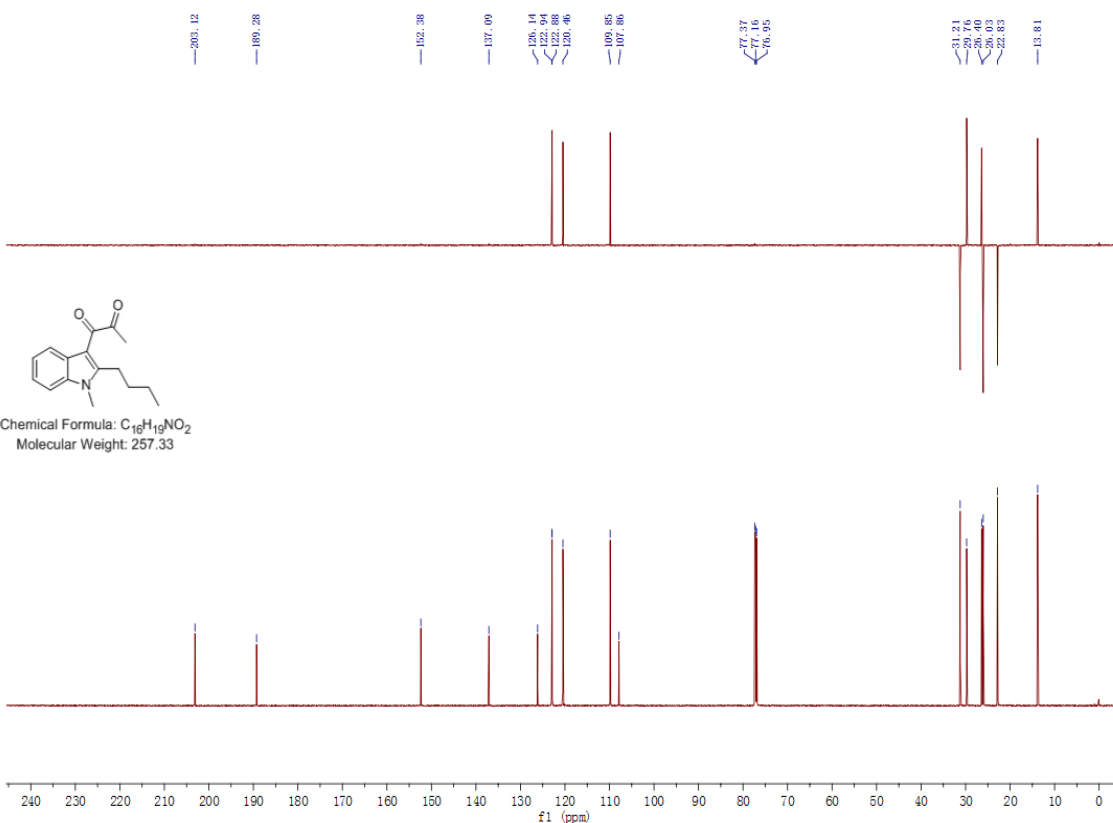
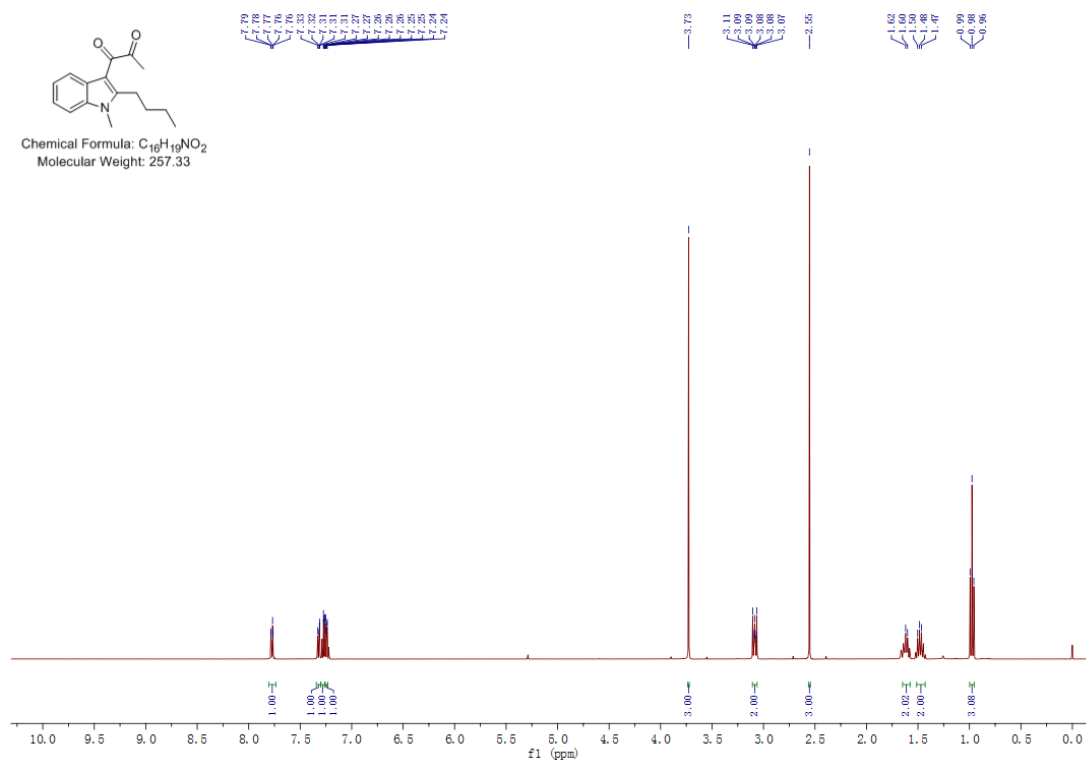
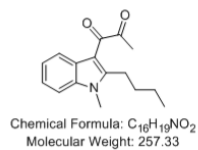
**1-(2-cyclohexyl-1-methyl-1H-indol-3-yl) butane-1, 2-dione (2ay)**



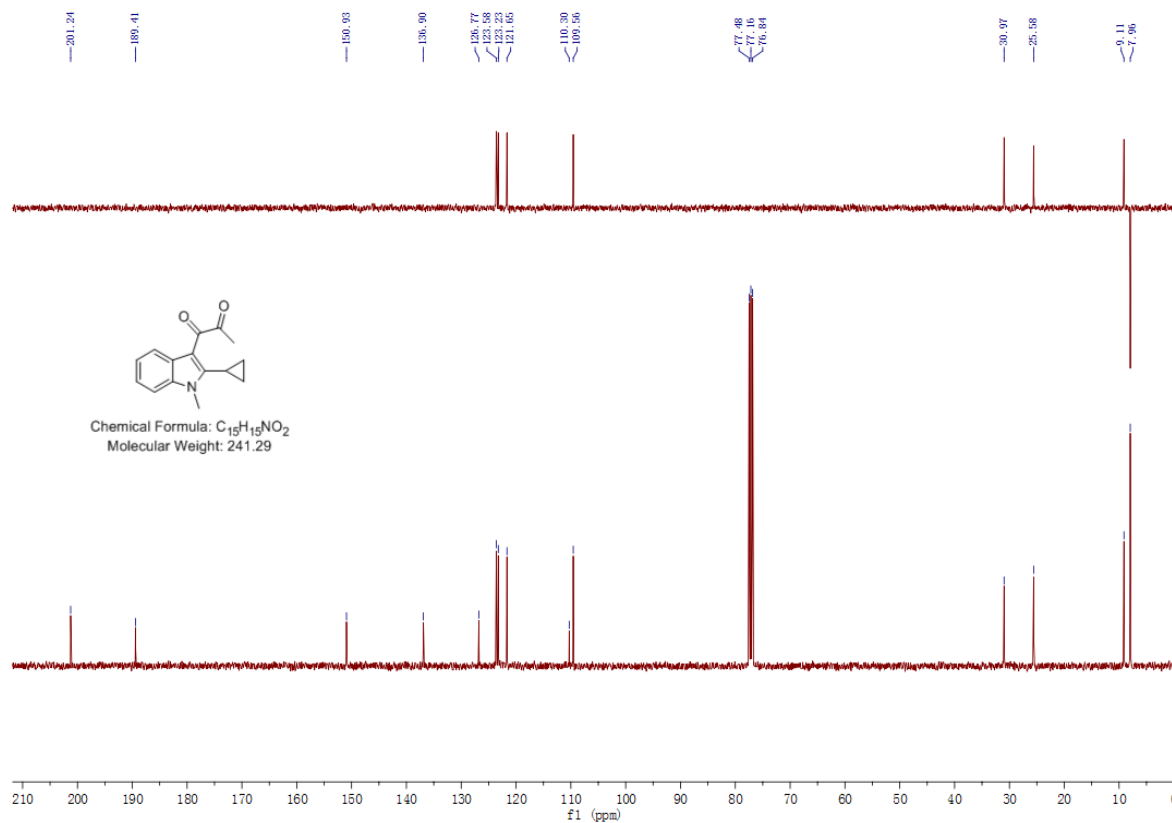
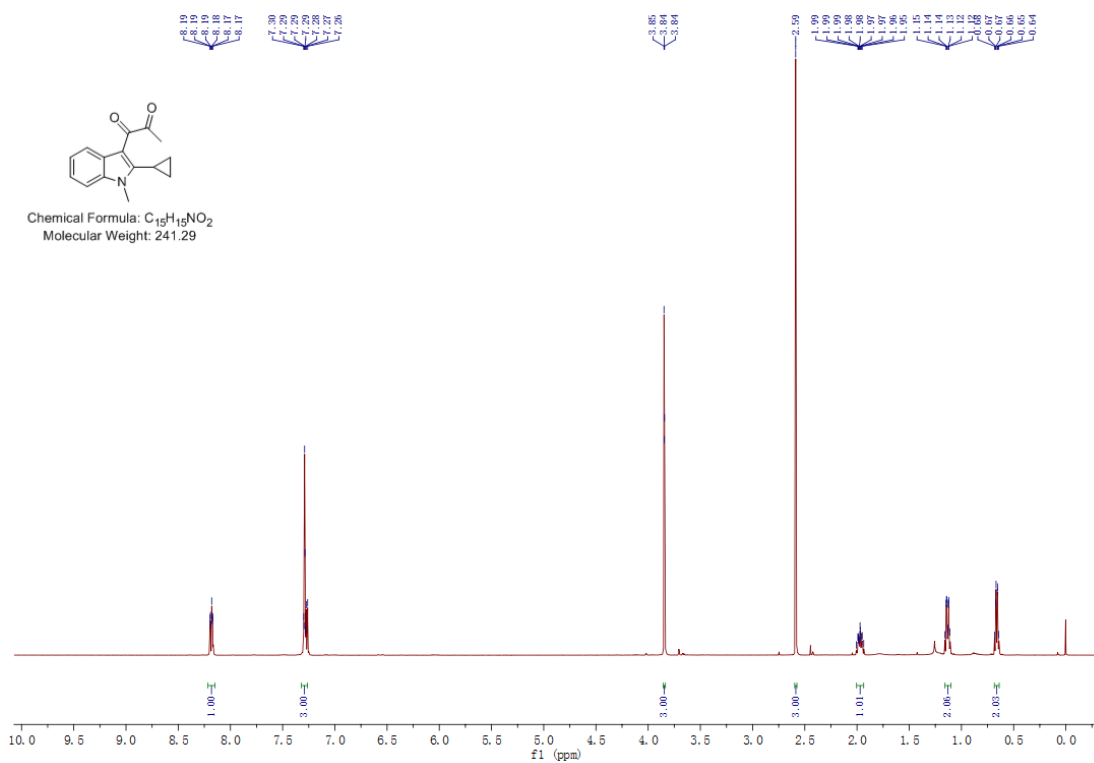
Yellow solid (133.6 mg, yield 90%), mp 88-90 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.74-7.67 (m, 1H), 7.35-7.31 (m, 1H), 7.28 (dd, *J* = 7.0, 1.3 Hz, 1H), 7.26-7.20 (m, 1H), 3.88 (s, 3H), 3.59-3.48 (m, 1H), 2.95 (q, *J* = 7.3 Hz, 2H), 2.06-1.79 (m, 7H), 1.46-1.33 (m, 3H), 1.28 (t, *J* = 7.3 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 206.24, 191.00, 154.79, 137.59, 126.56, 123.05, 122.95, 120.46, 109.79, 108.64, 37.77, 32.23, 32.20, 29.49, 26.92, 25.88, 7.20; EI-MS (*m/z*): 297 (M<sup>+</sup>); HRMS (EI) calcd for C<sub>19</sub>H<sub>23</sub>NO<sub>2</sub> (M<sup>+</sup>) 297.1729, found: 297.1723.

# <sup>1</sup>H and <sup>13</sup>C NMR Spectra

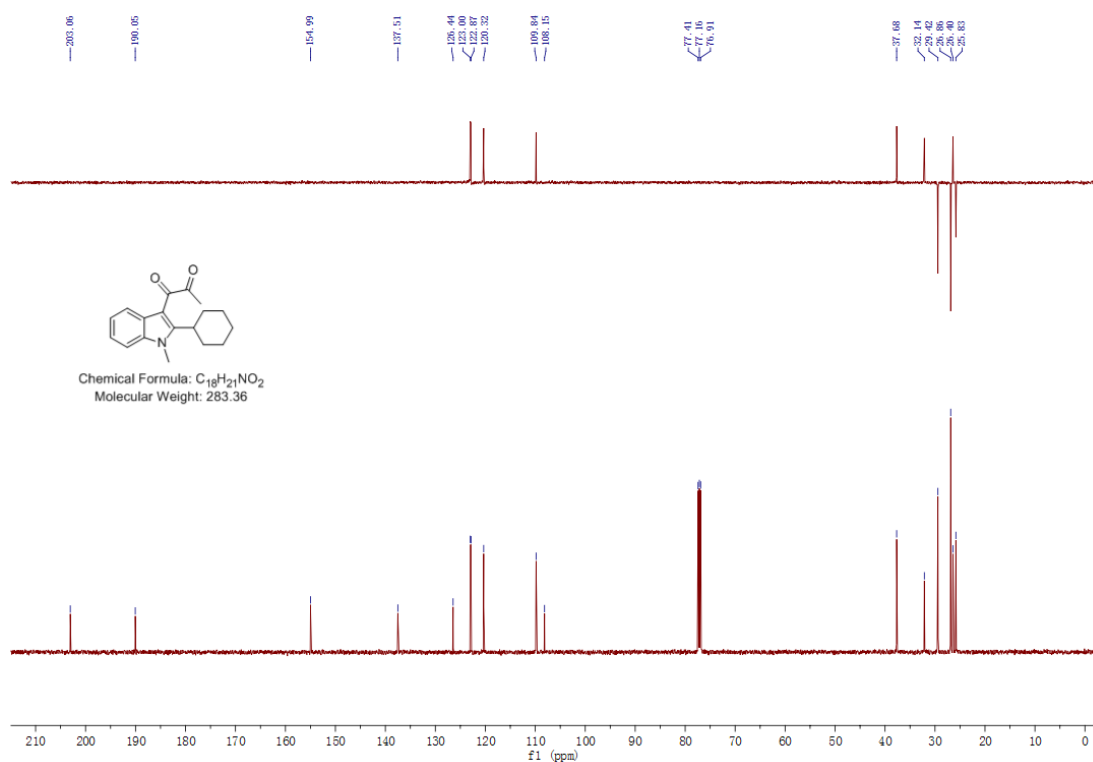
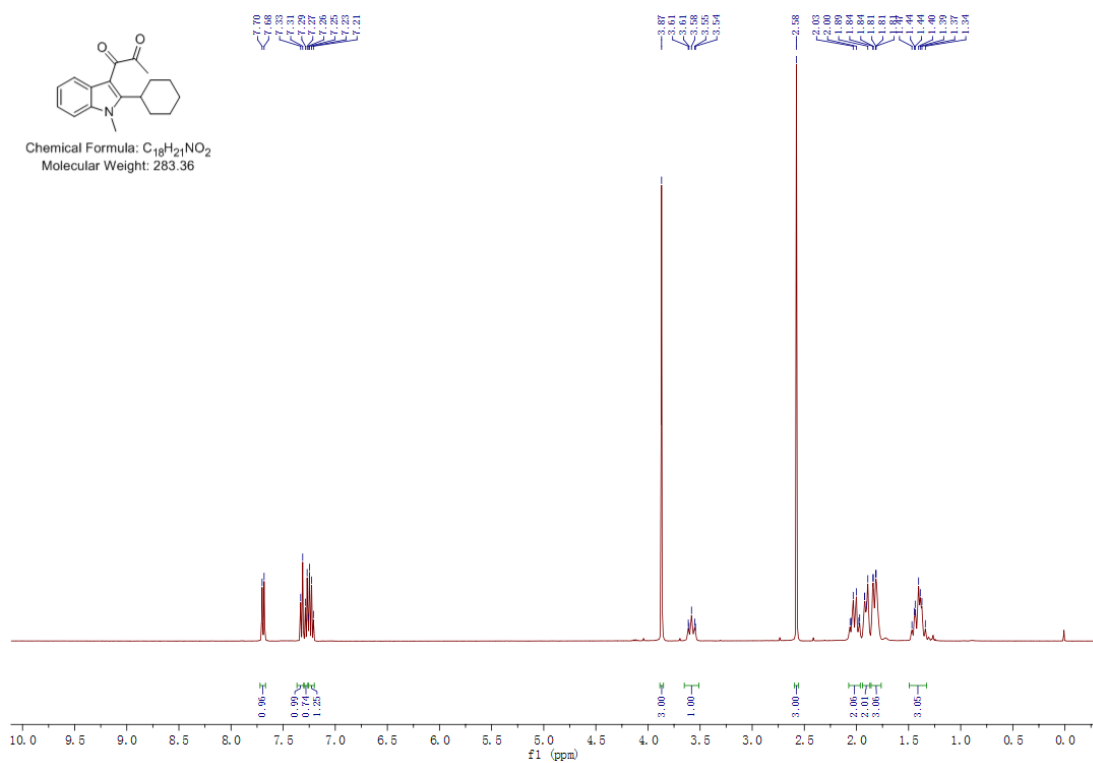
## 1-(2-butyl-1-methyl-1H-indol-3-yl) propane-1,2-dione(2aa)



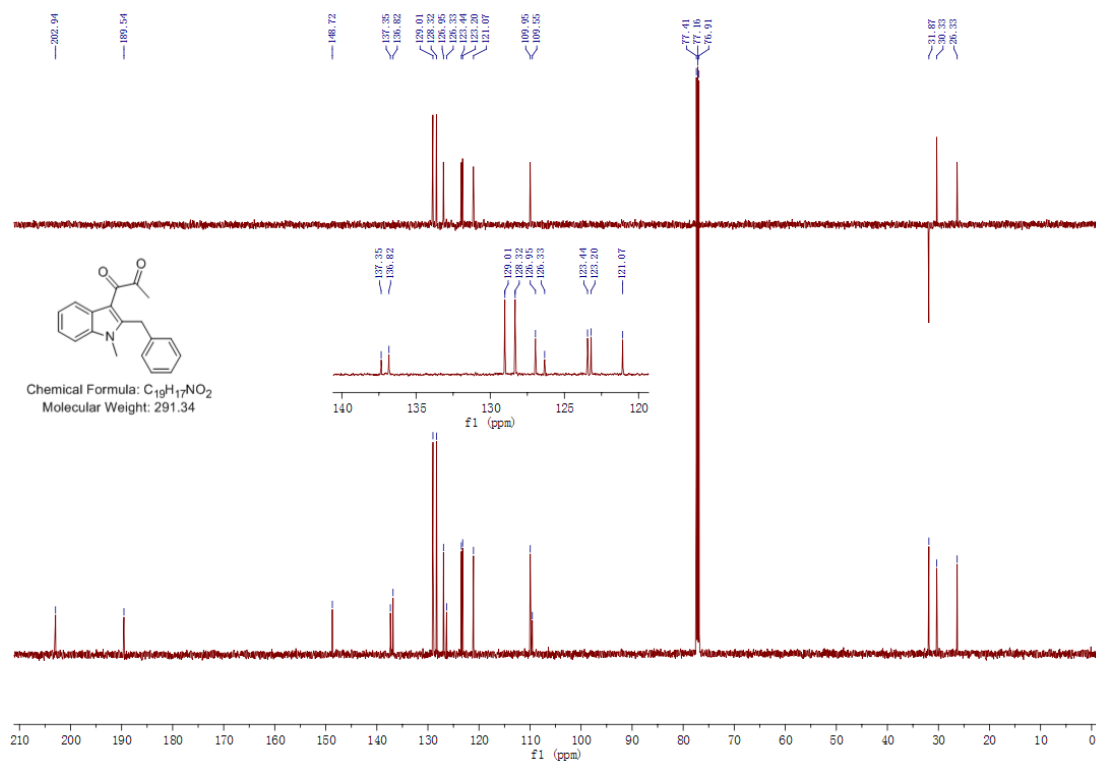
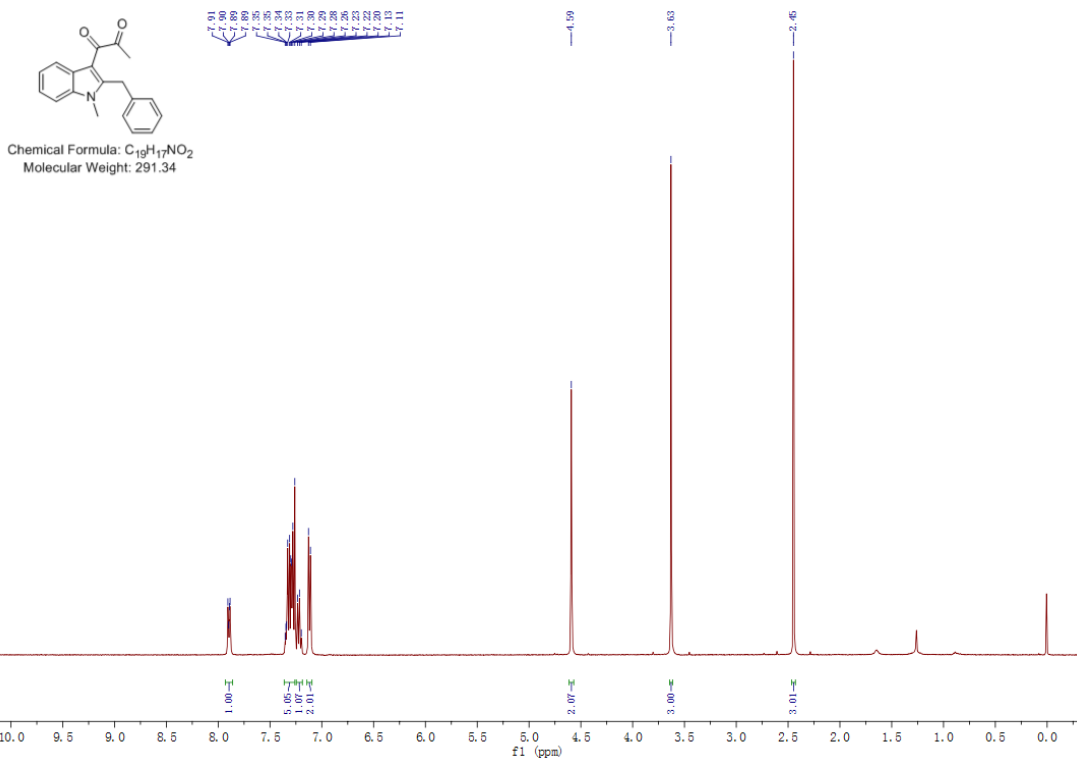
# 1-(2-cyclopropyl-1-methyl-1H-indol-3-yl) propane-1,2-dione(2ab)



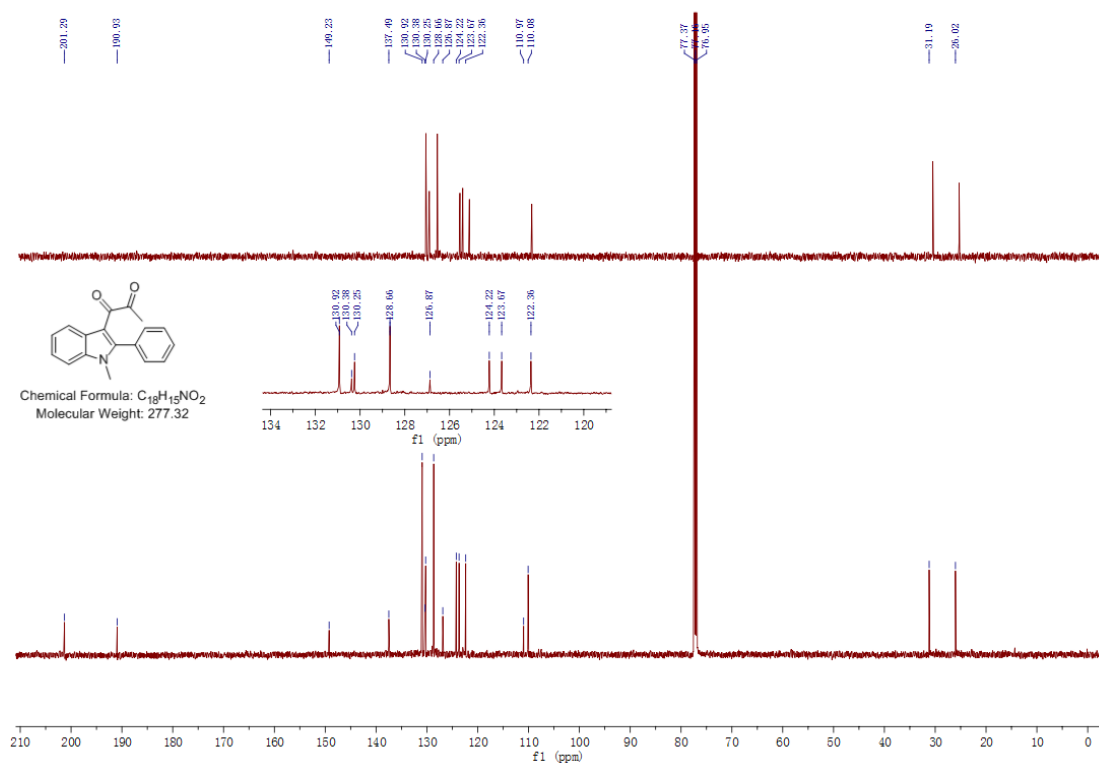
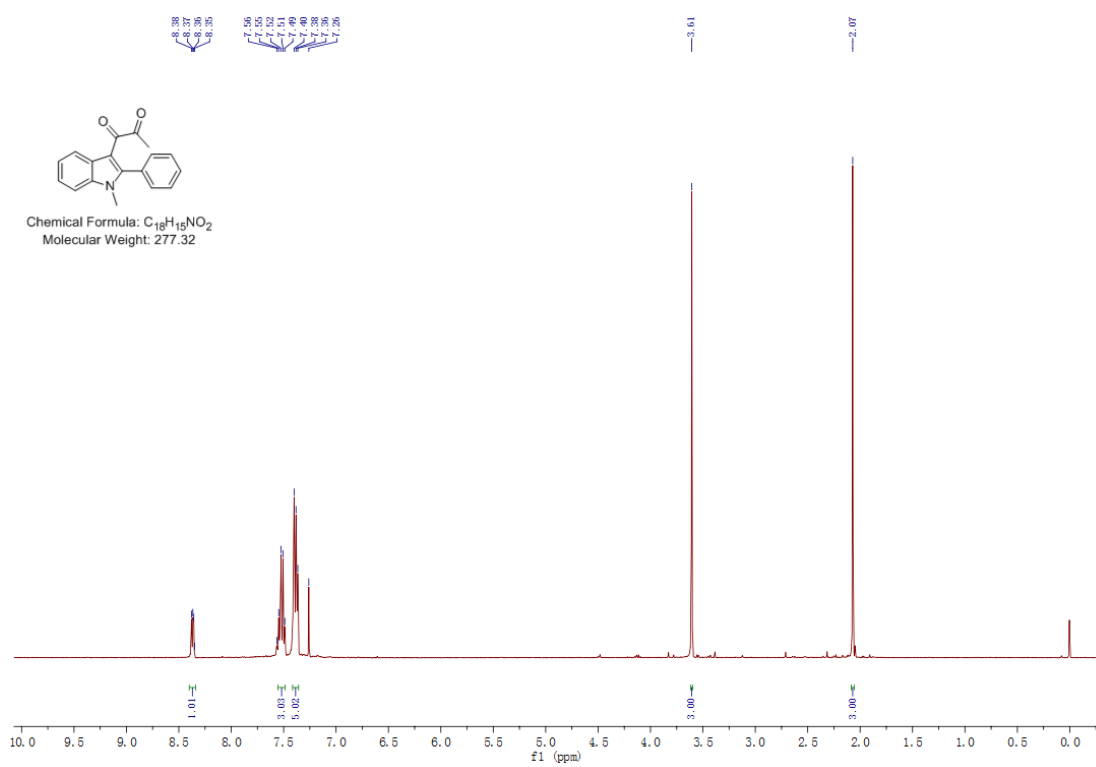
# 1-(2-cyclohexyl-1-methyl-1H-indol-3-yl) propane-1,2-dione(2ac)



# 1-(2-benzyl-1-methyl-1H-indol-3-yl) propane-1,2-dione(2ae)

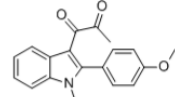


# 1-(1-methyl-2-phenyl-1H-indol-3-yl) propane-1,2-dione(2af)

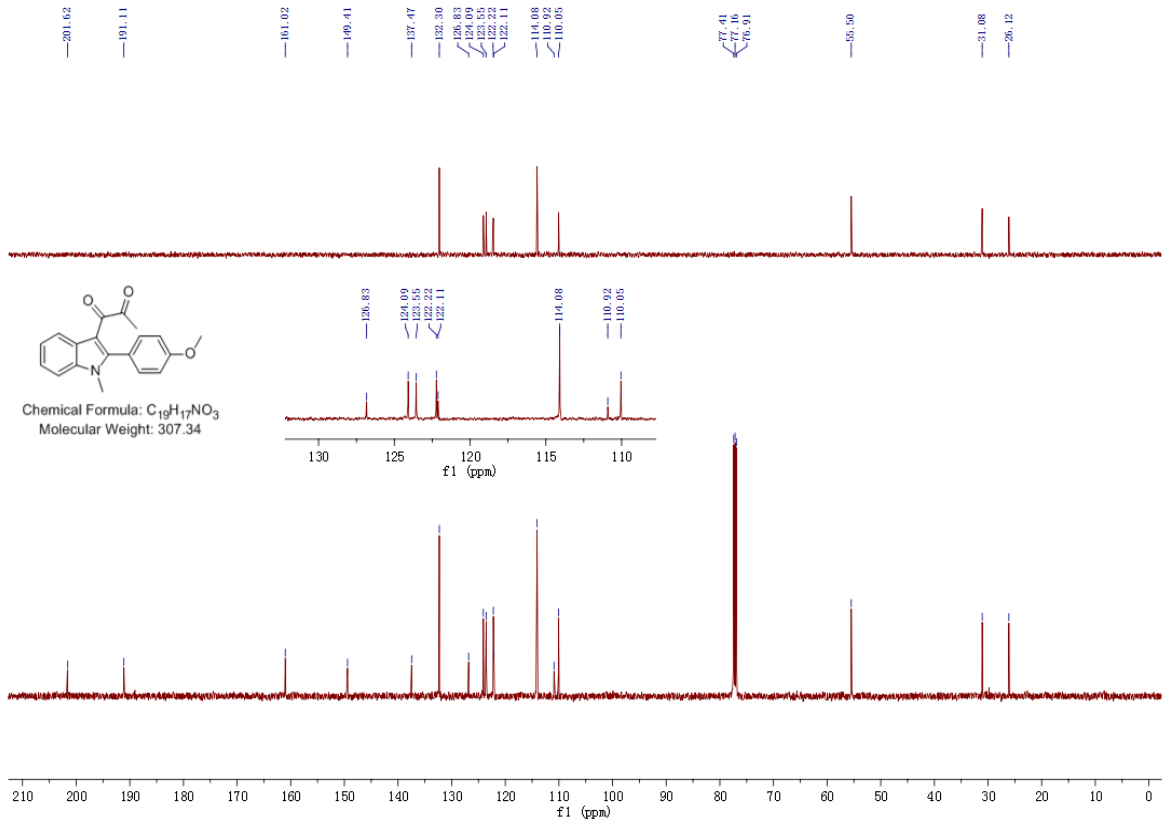
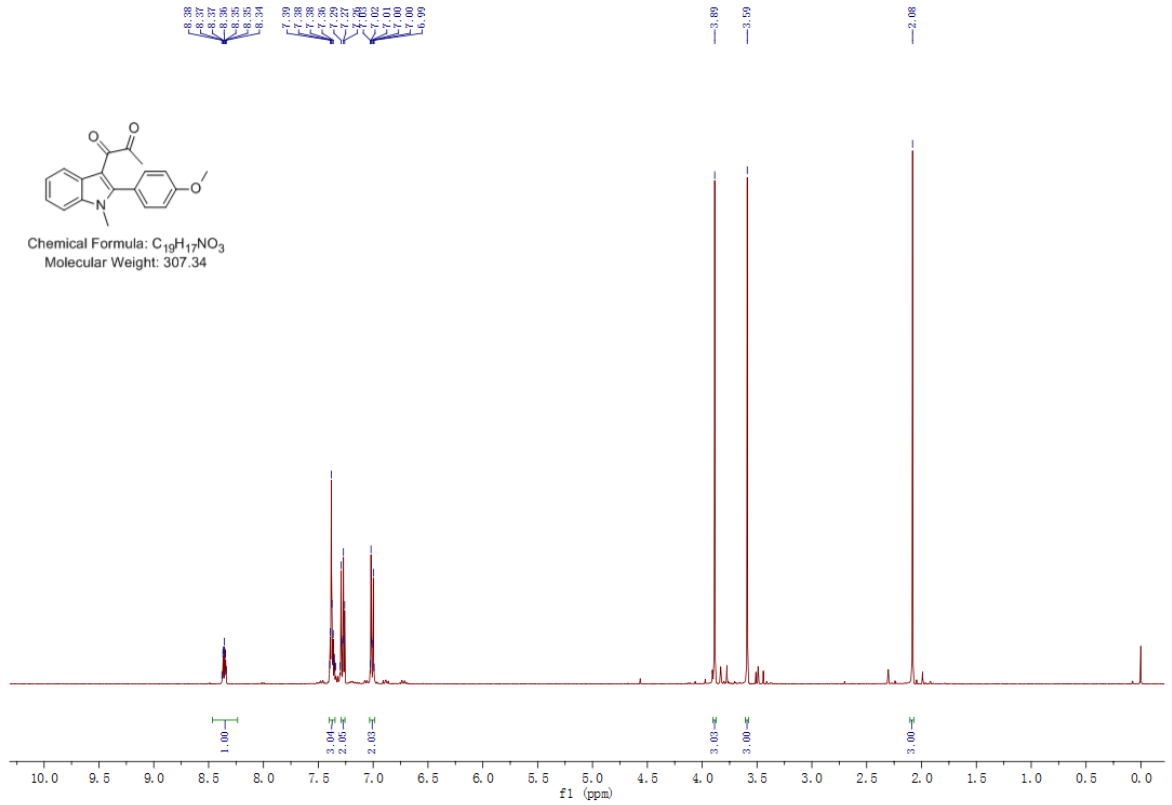




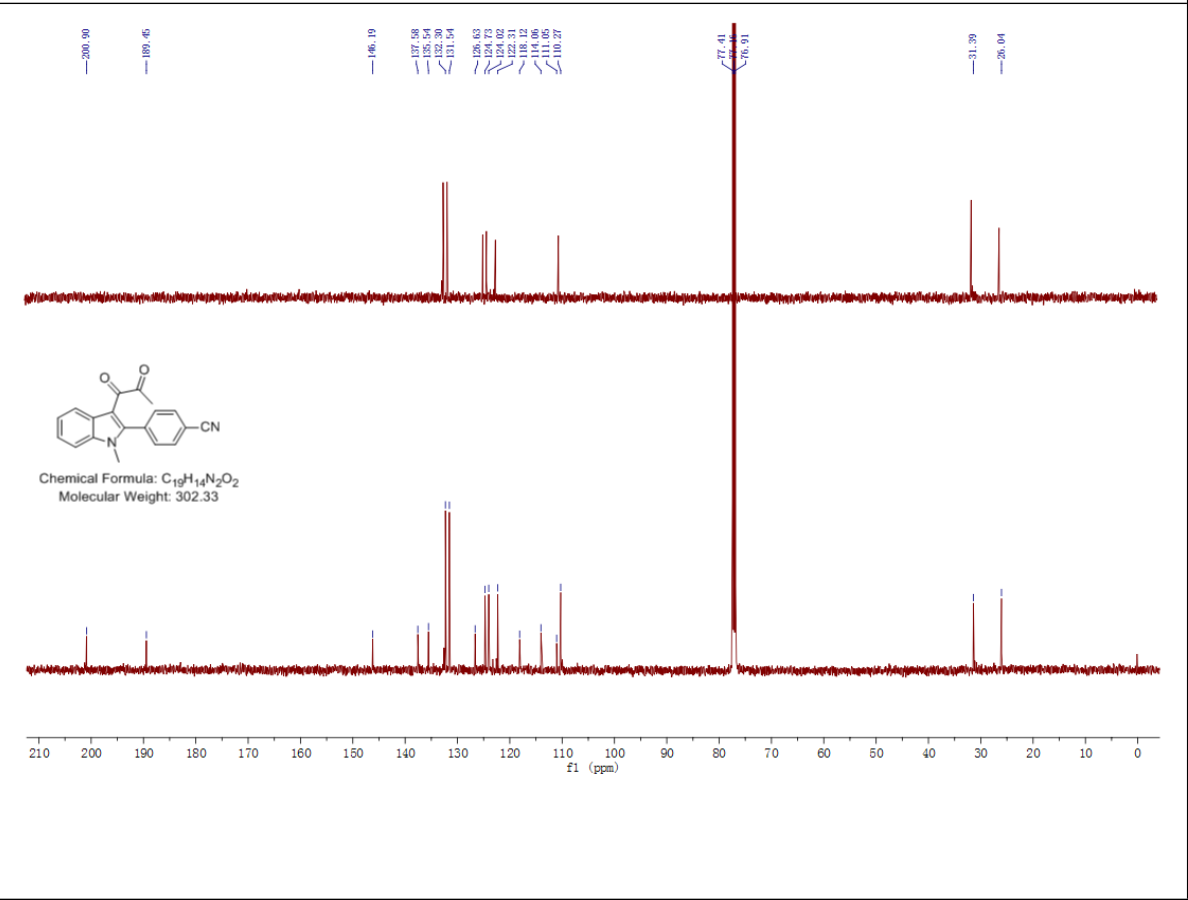
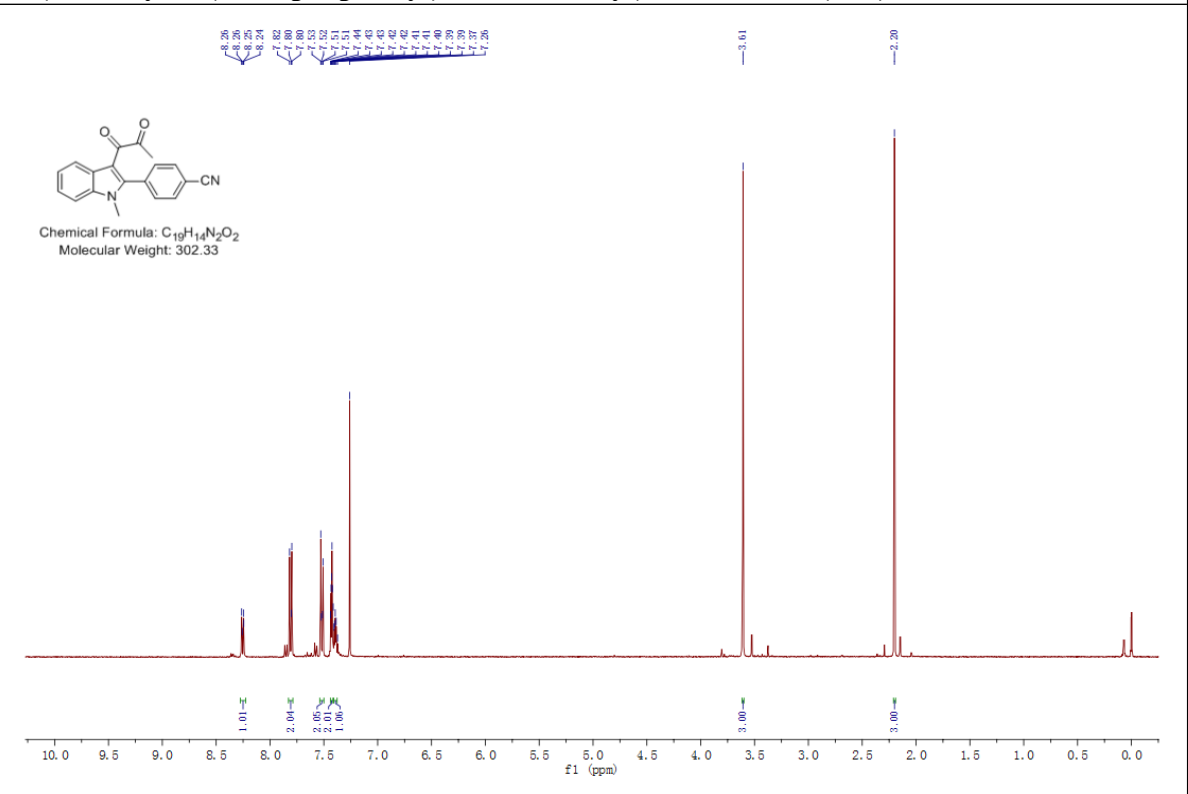
# 1-(2-(4-methoxyphenyl)-1-methyl-1H-indol-3-yl) propane-1,2-dione(2ag)



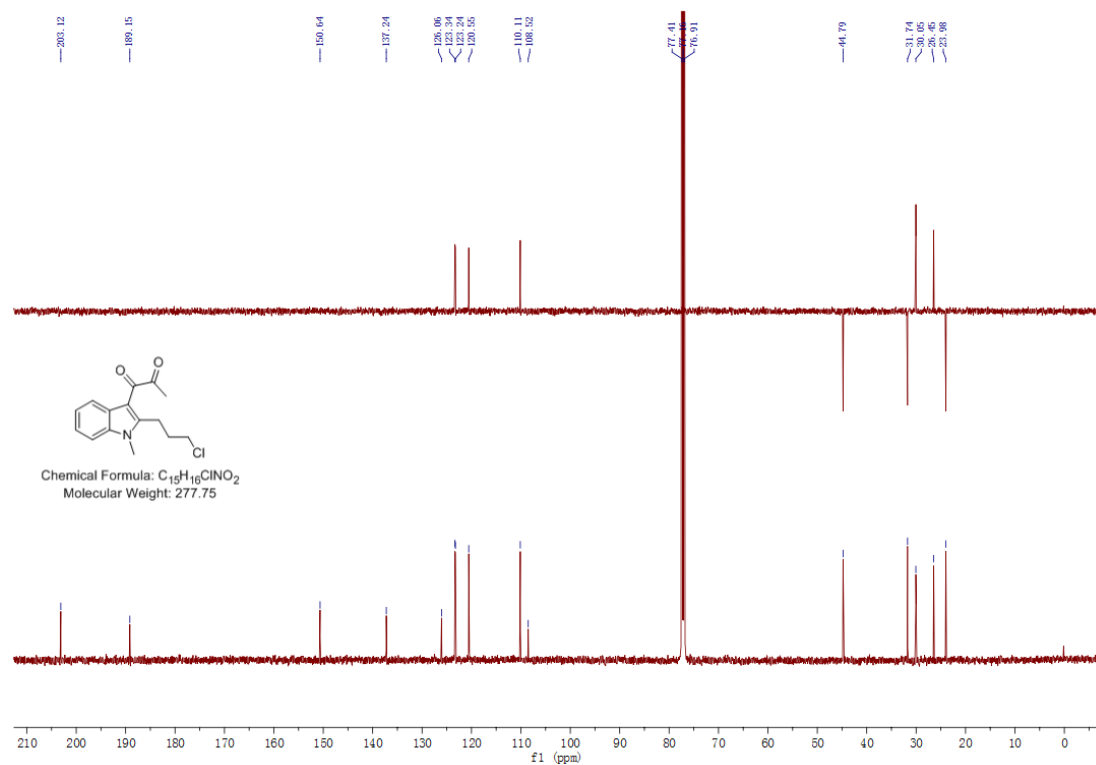
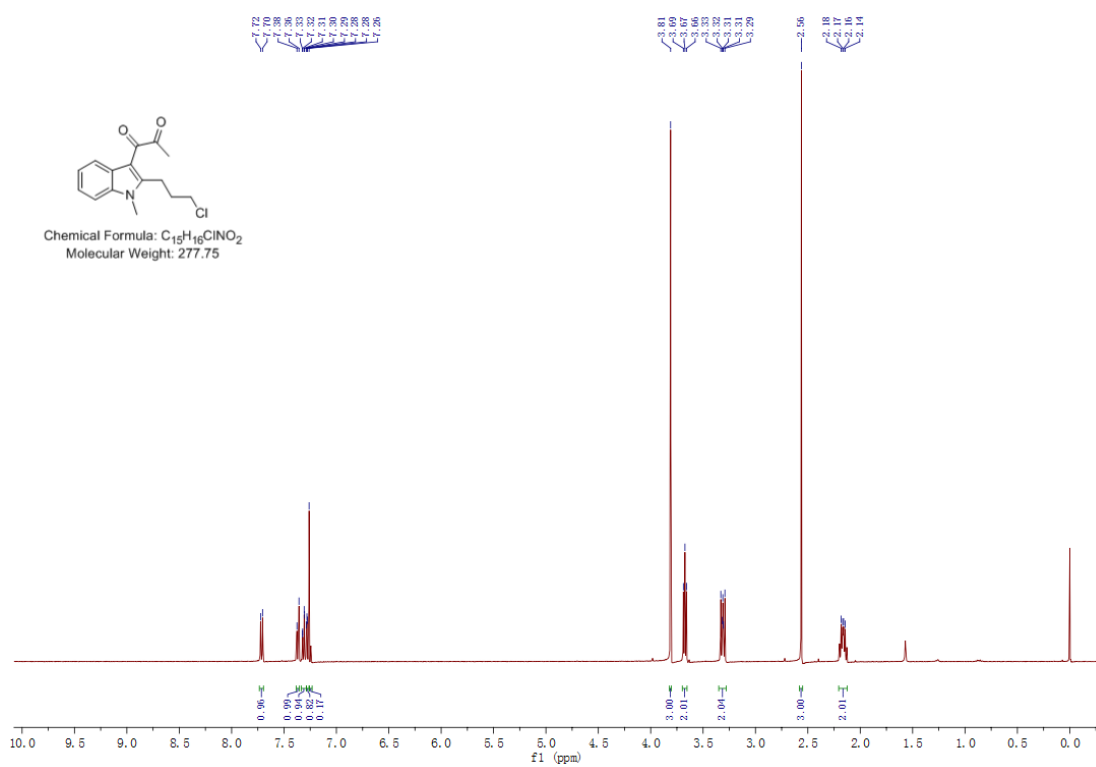
Chemical Formula: C<sub>19</sub>H<sub>17</sub>NO<sub>3</sub>  
Molecular Weight: 307.34



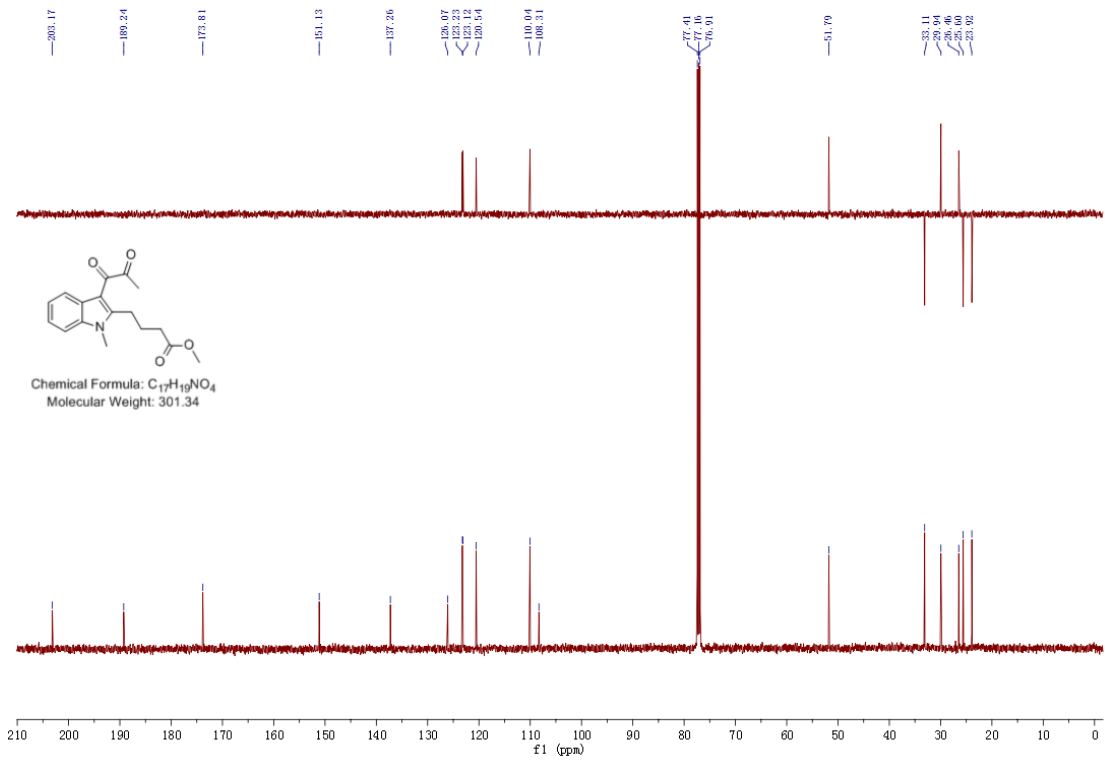
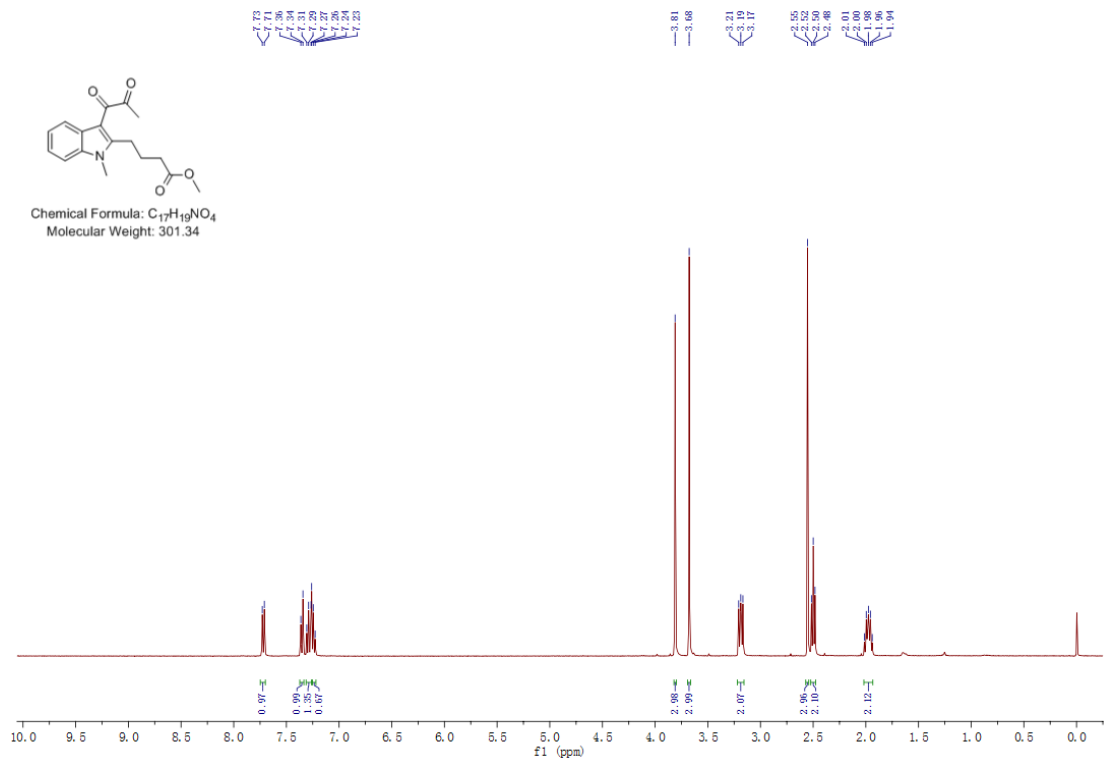
### 4-(1-methyl-3-(2-oxopropanoyl)-1H-indol-2-yl) benzonitrile(2ah)



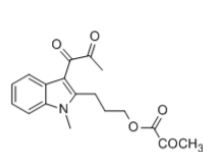
# 1-(2-(3-chloropropyl)-1-methyl-1H-indol-3-yl) propane-1,2-dione(2ai)



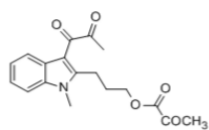
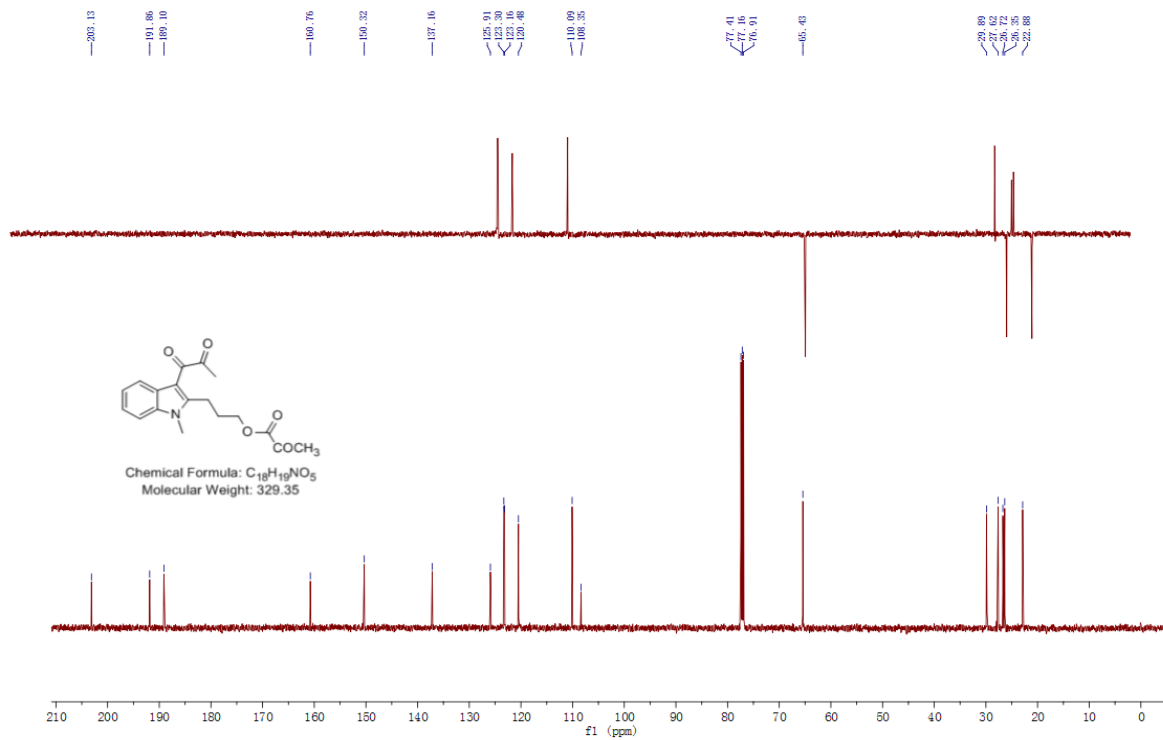
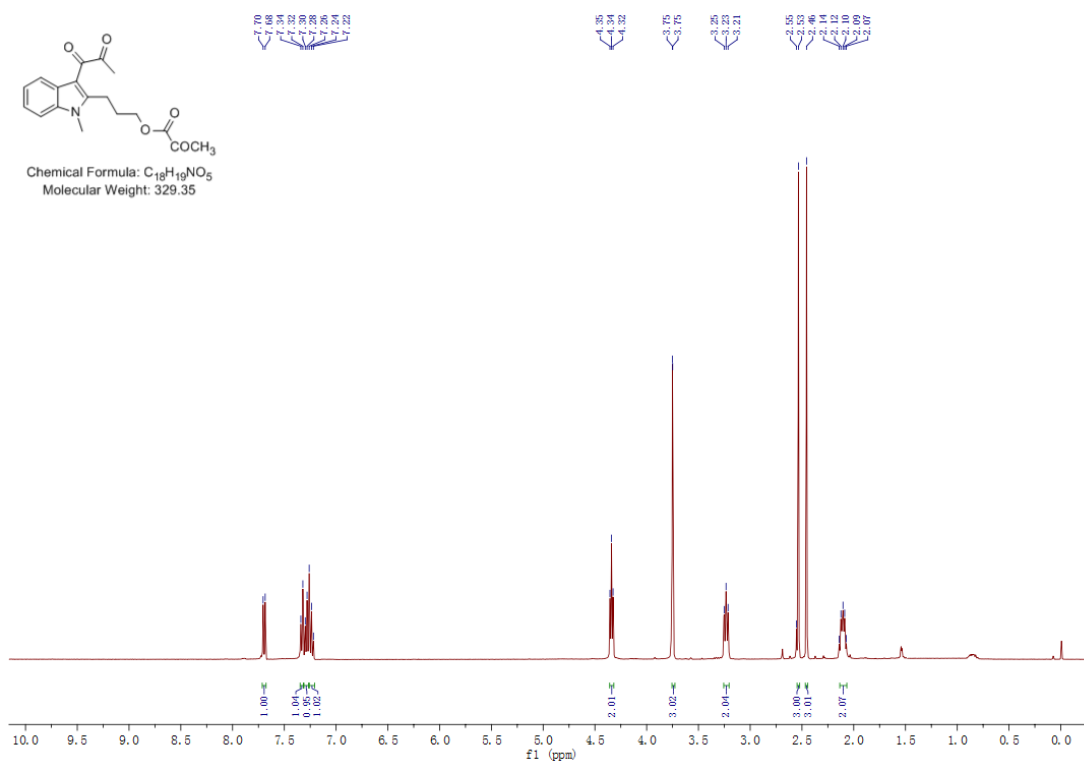
**methyl 4-(1-methyl-3-(2-oxopropanoyl)-1H-indol-2-yl) butanoate(2aj)**



## 2-(1-methyl-3-(2-oxopropanoyl)-1H-indol-2-yl)ethyl 2-oxopropanoate(2ak)

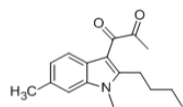


Chemical Formula: C<sub>18</sub>H<sub>19</sub>NO<sub>5</sub>  
Molecular Weight: 329.35

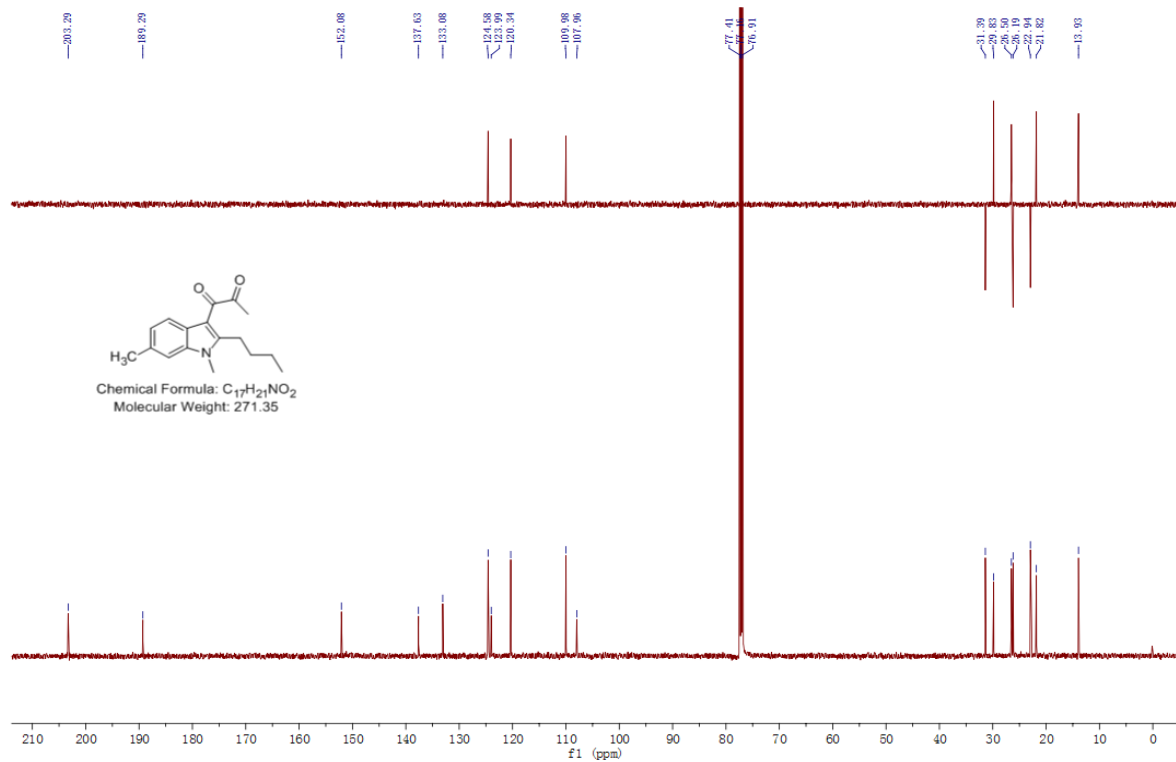
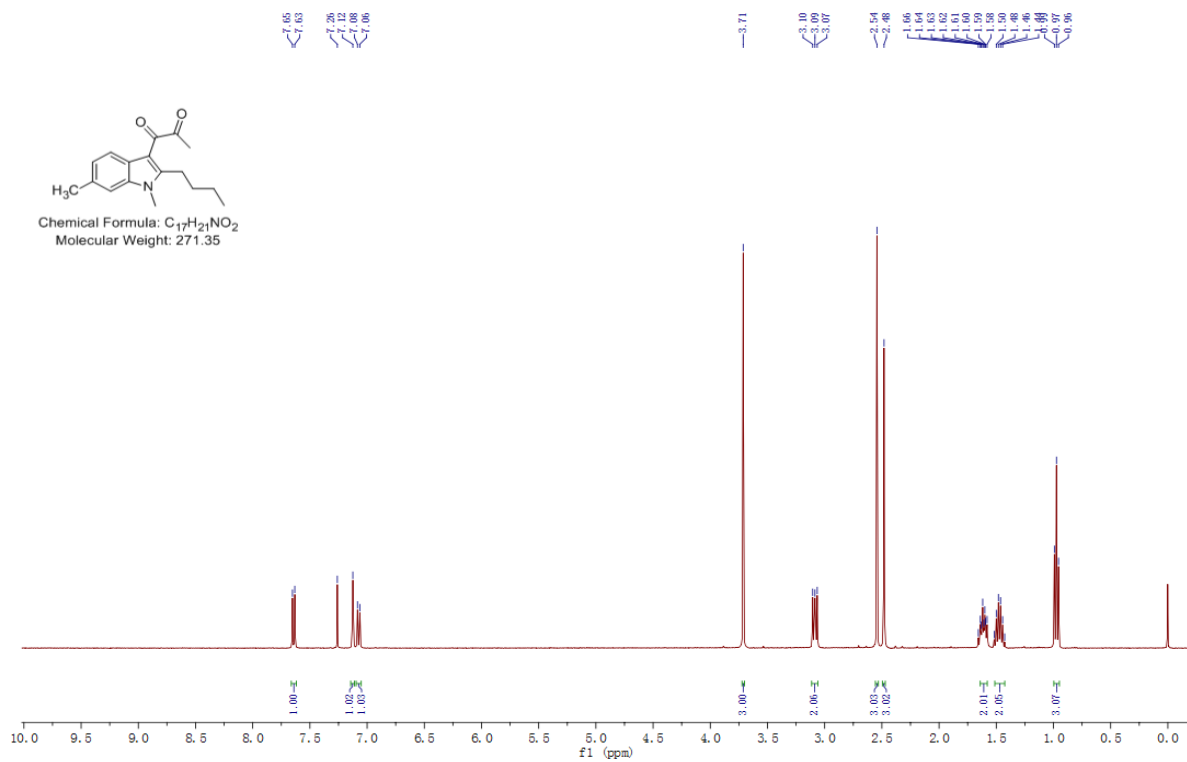


Chemical Formula: C<sub>18</sub>H<sub>19</sub>NO<sub>5</sub>  
Molecular Weight: 329.35

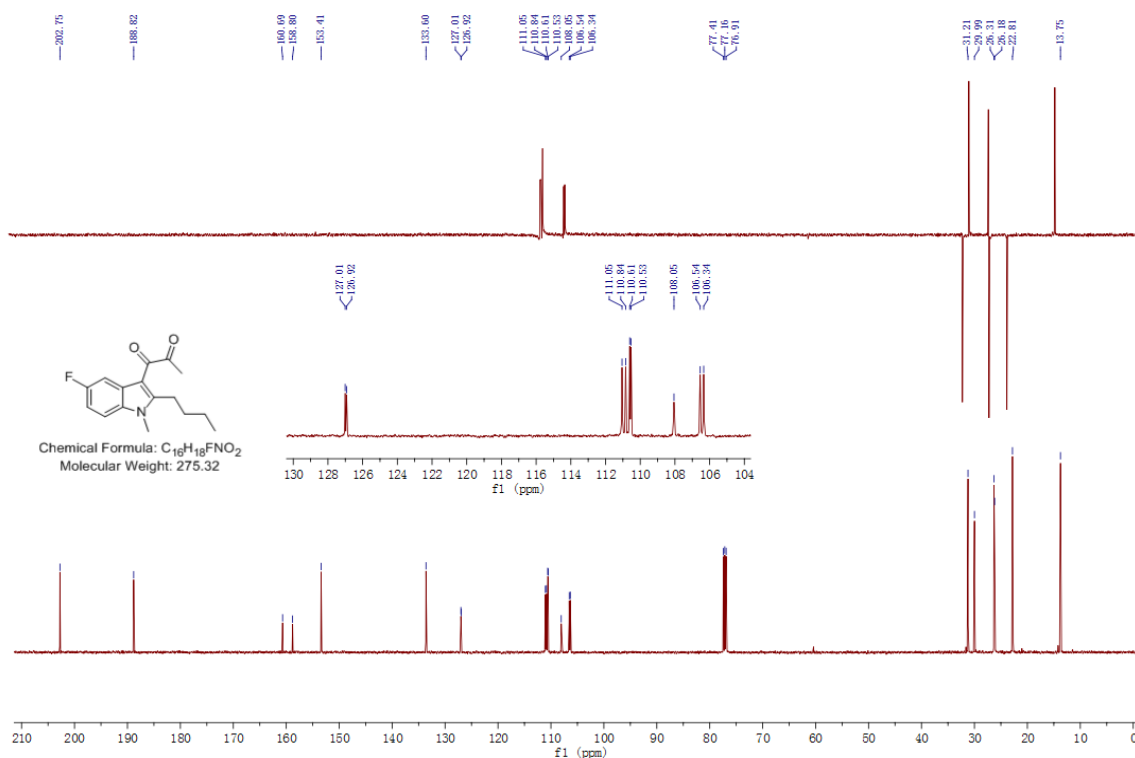
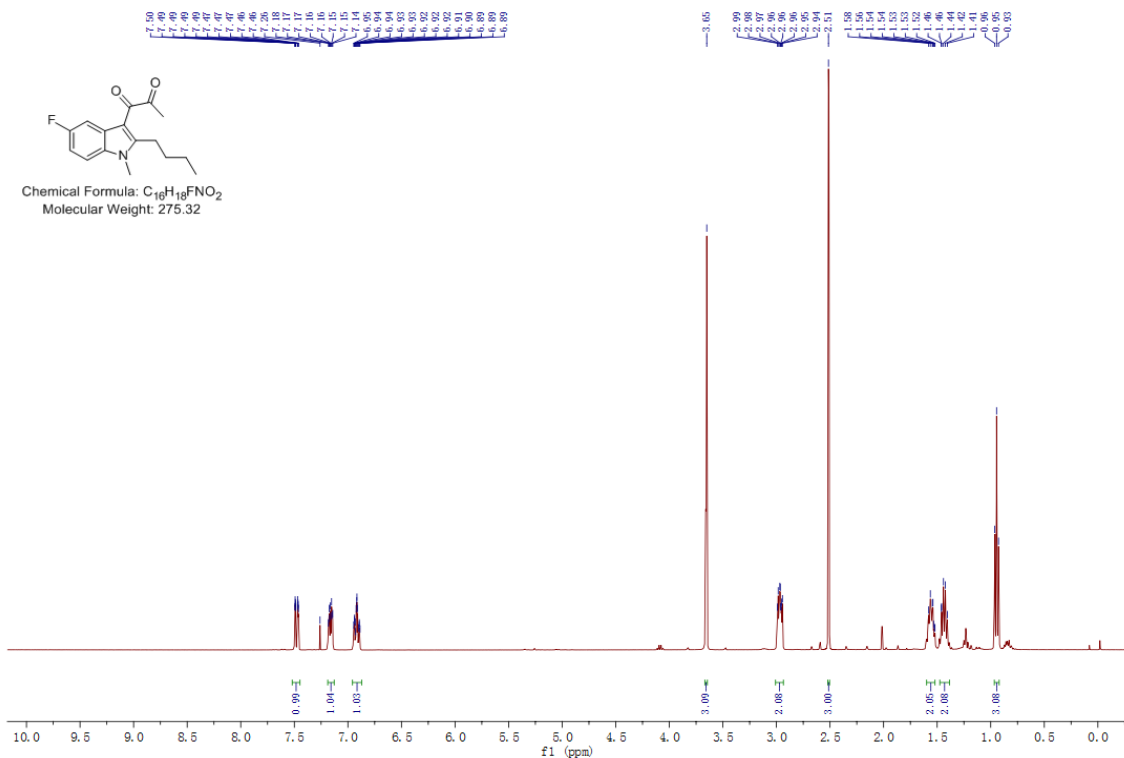
# 1-(2-butyl-1,6-dimethyl-1H-indol-3-yl)propane-1,2-dione(2a)



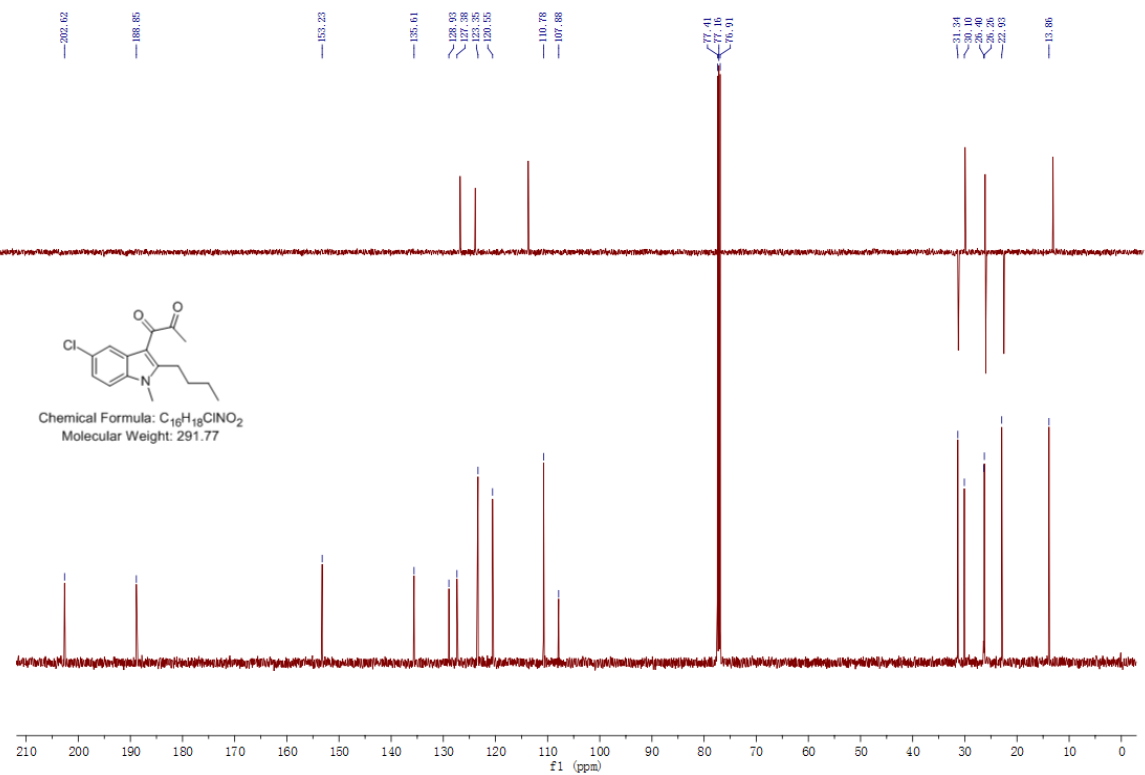
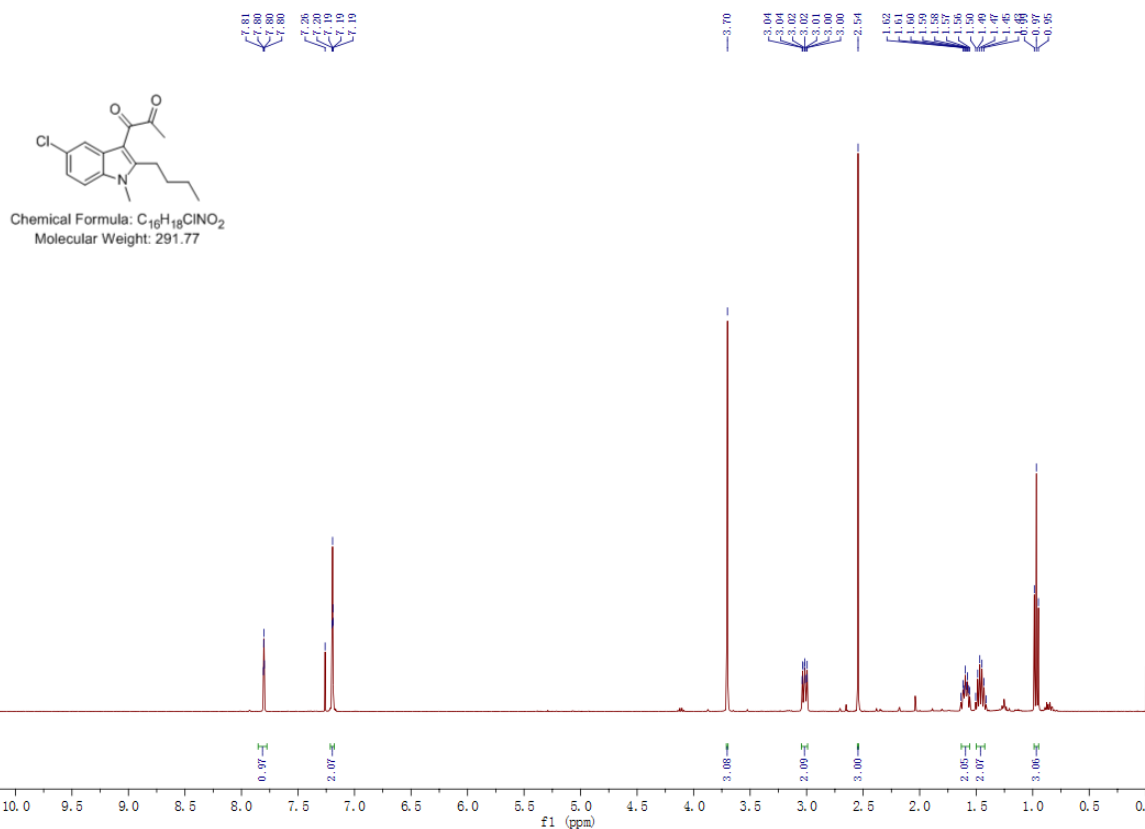
Chemical Formula: C<sub>17</sub>H<sub>21</sub>NO<sub>2</sub>  
Molecular Weight: 271.35



# 1-(2-butyl-5-fluoro-1-methyl-1H-indol-3-yl)propane-1,2-dione(2am)

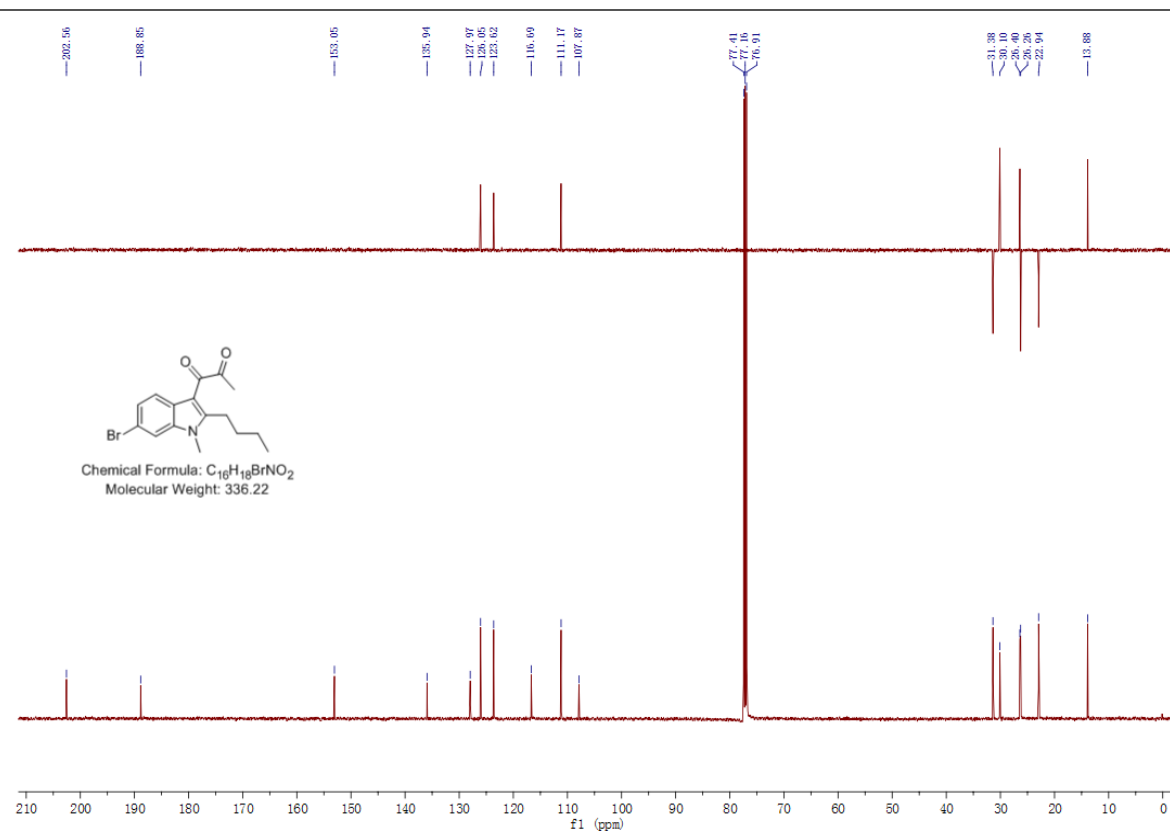
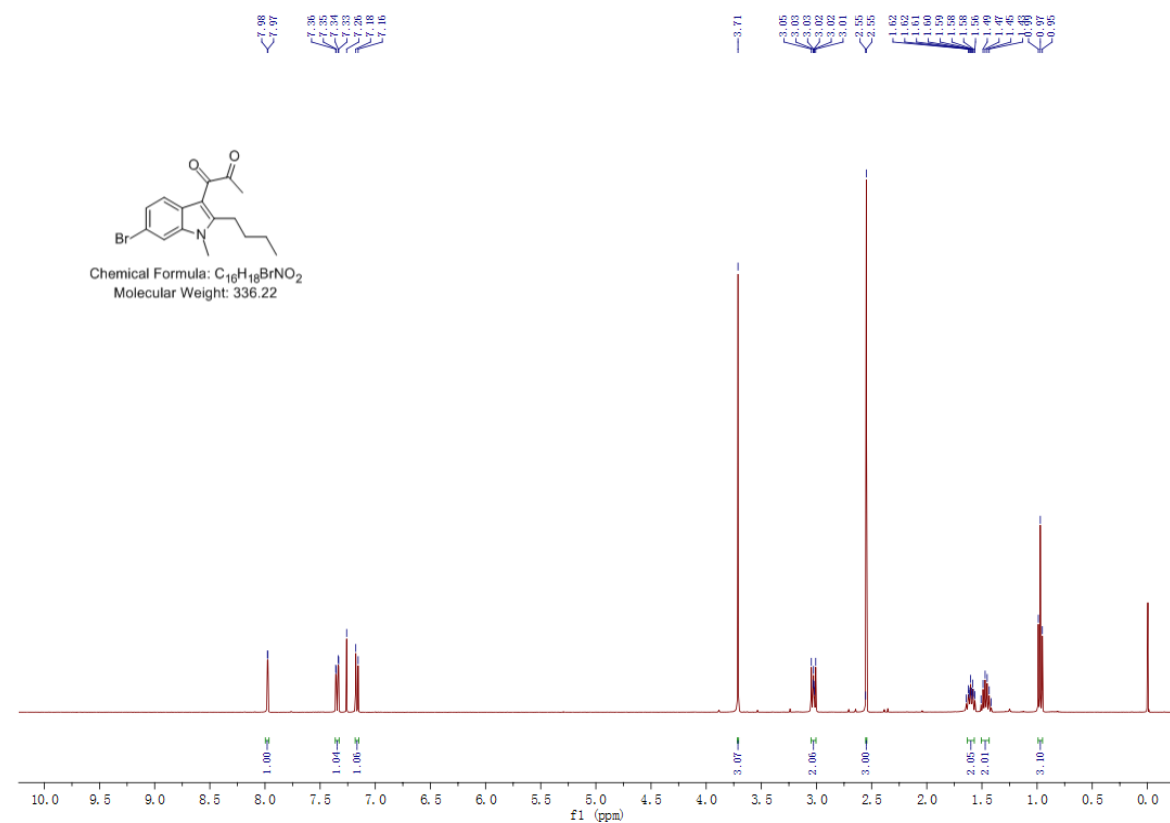


# 1-(2-butyl-5-chloro-1-methyl-1H-indol-3-yl)propane-1,2-dione(2a)

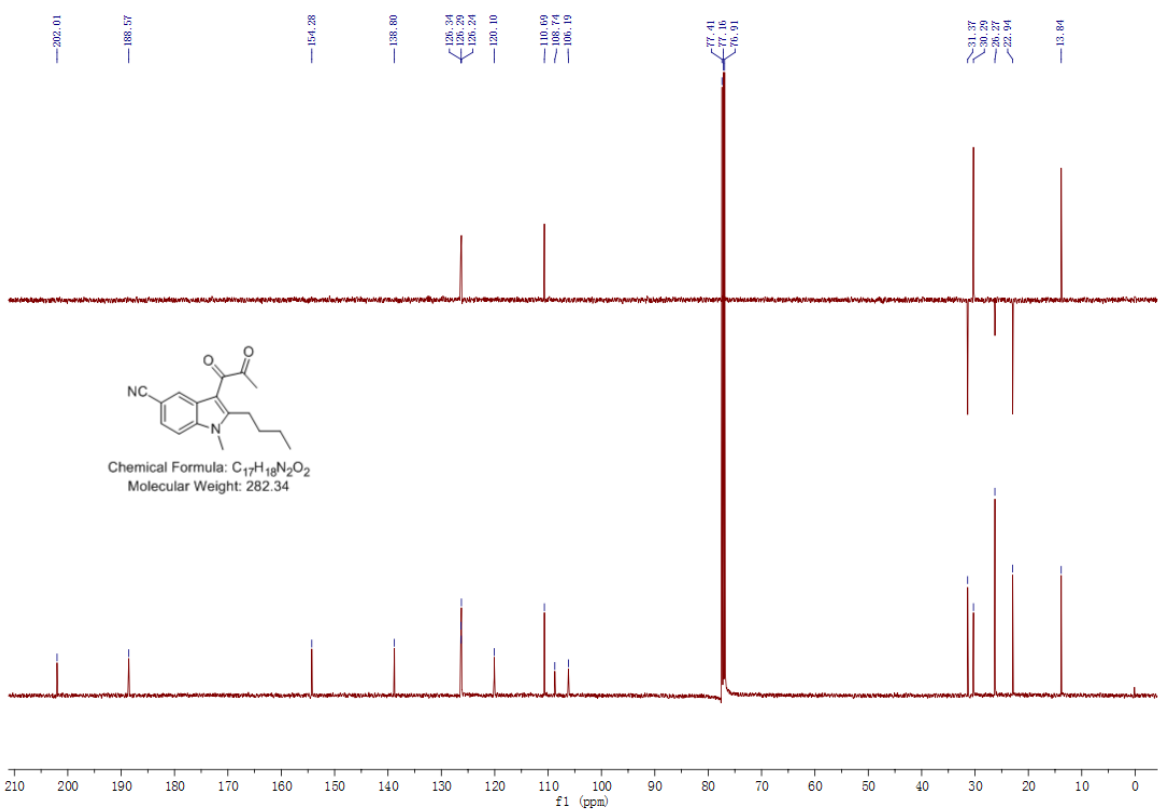
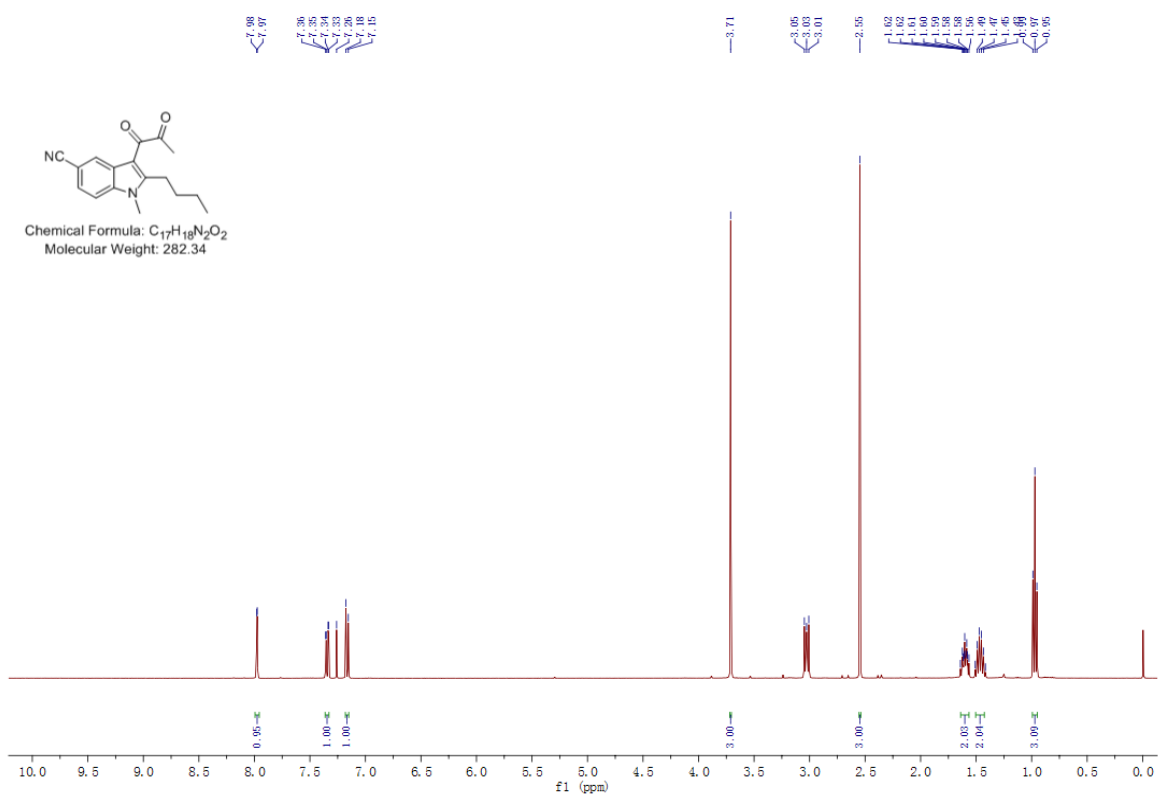




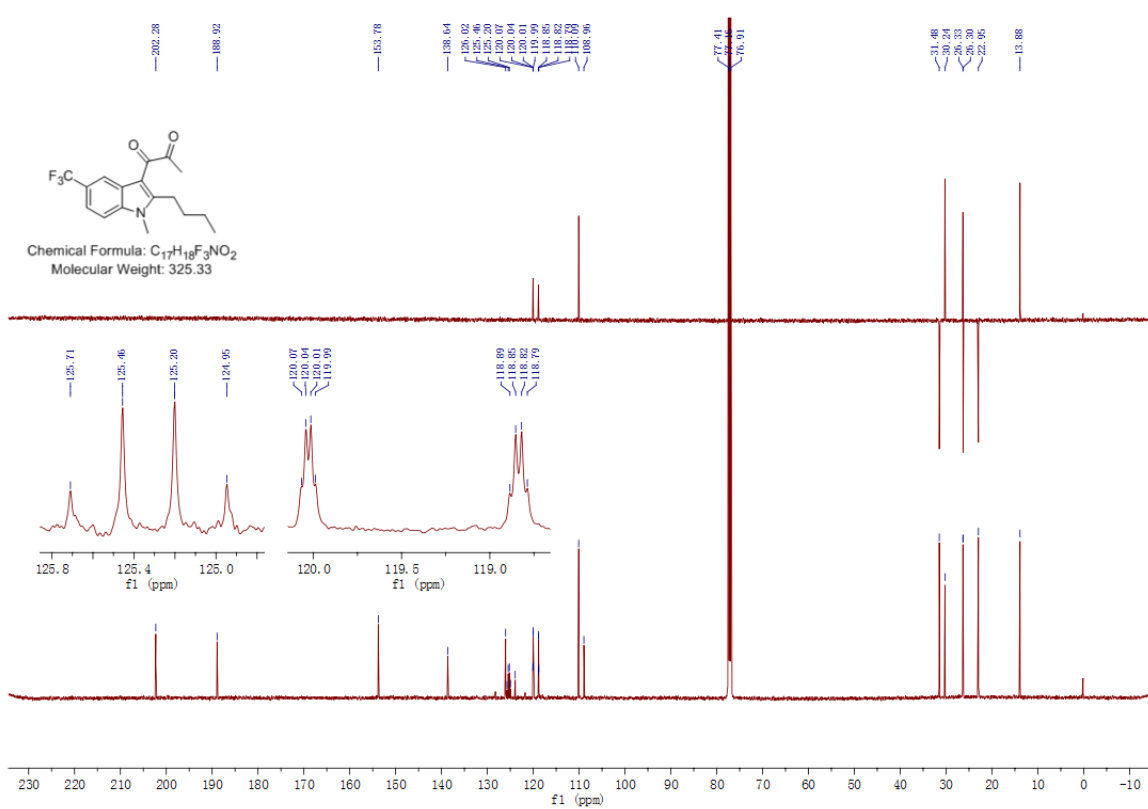
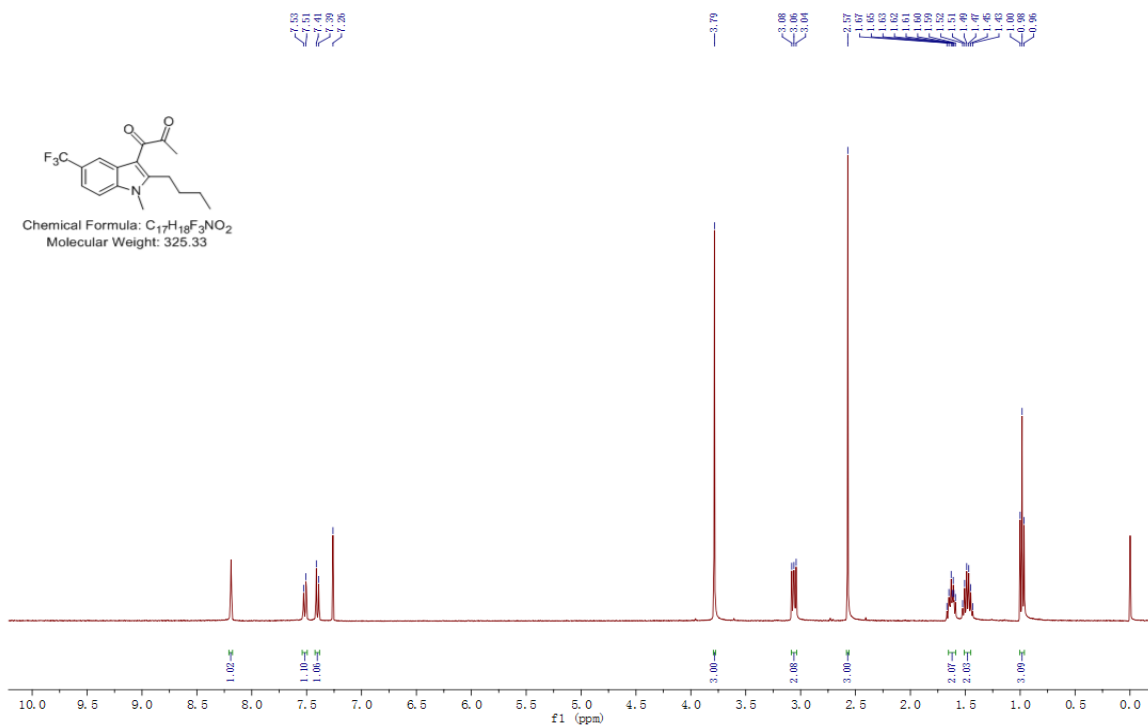
# 1-(6-bromo-2-butyl-1-methyl-1H-indol-3-yl)propane-1,2-dione(2ao)



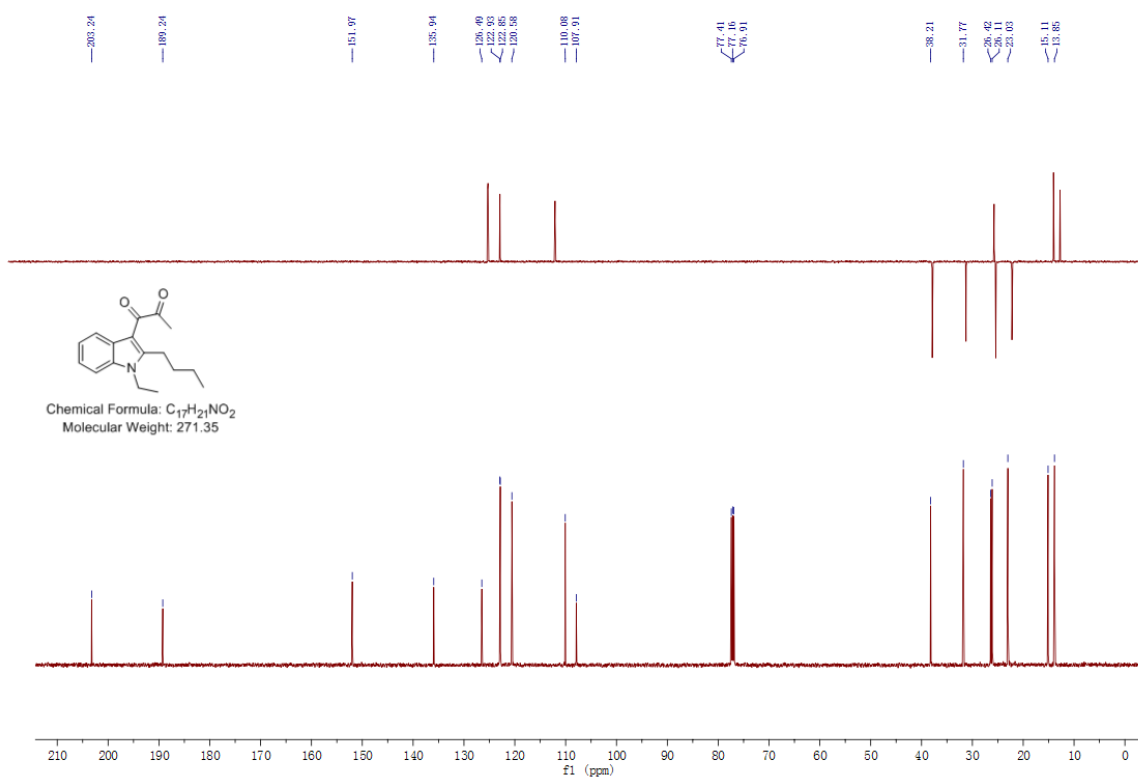
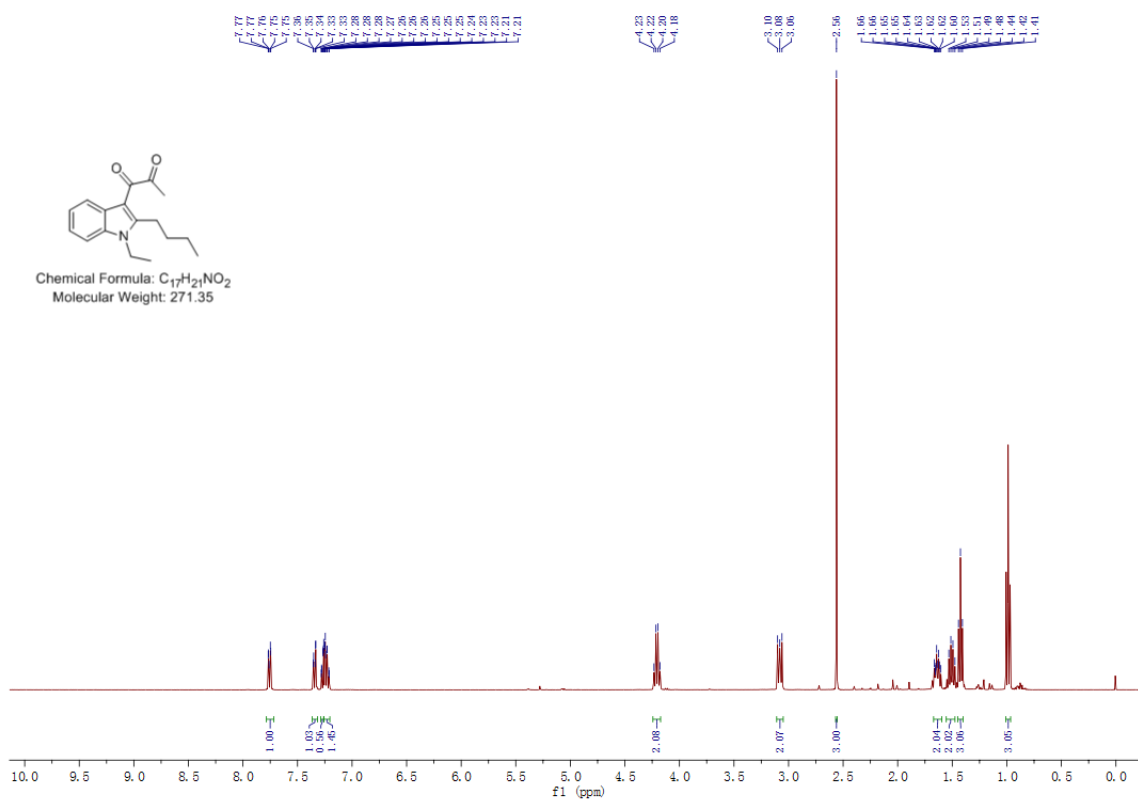
## 2-butyl-1-methyl-3-(2-oxopropanoyl)-1H-indole-5-carbonitrile(2ap)



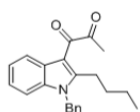
# 1-(2-butyl-1-methyl-5-(trifluoromethyl)-1H-indol-3-yl) propane-1,2-dione(2aq)



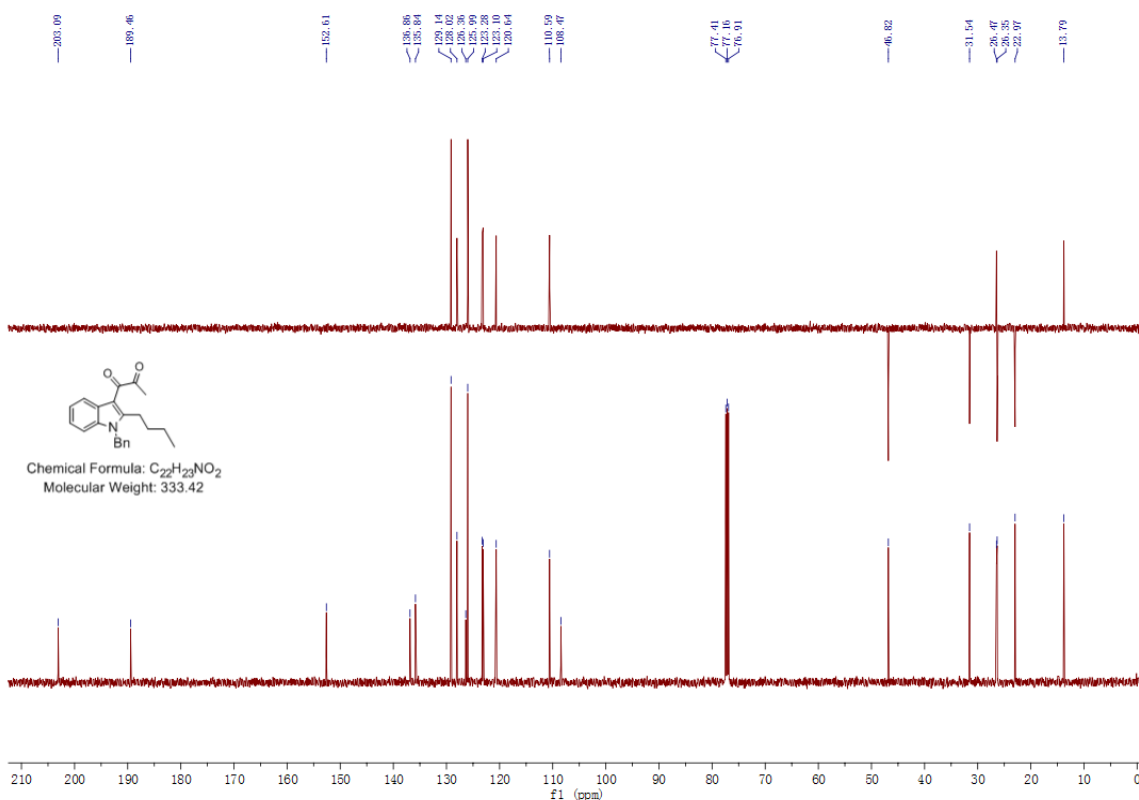
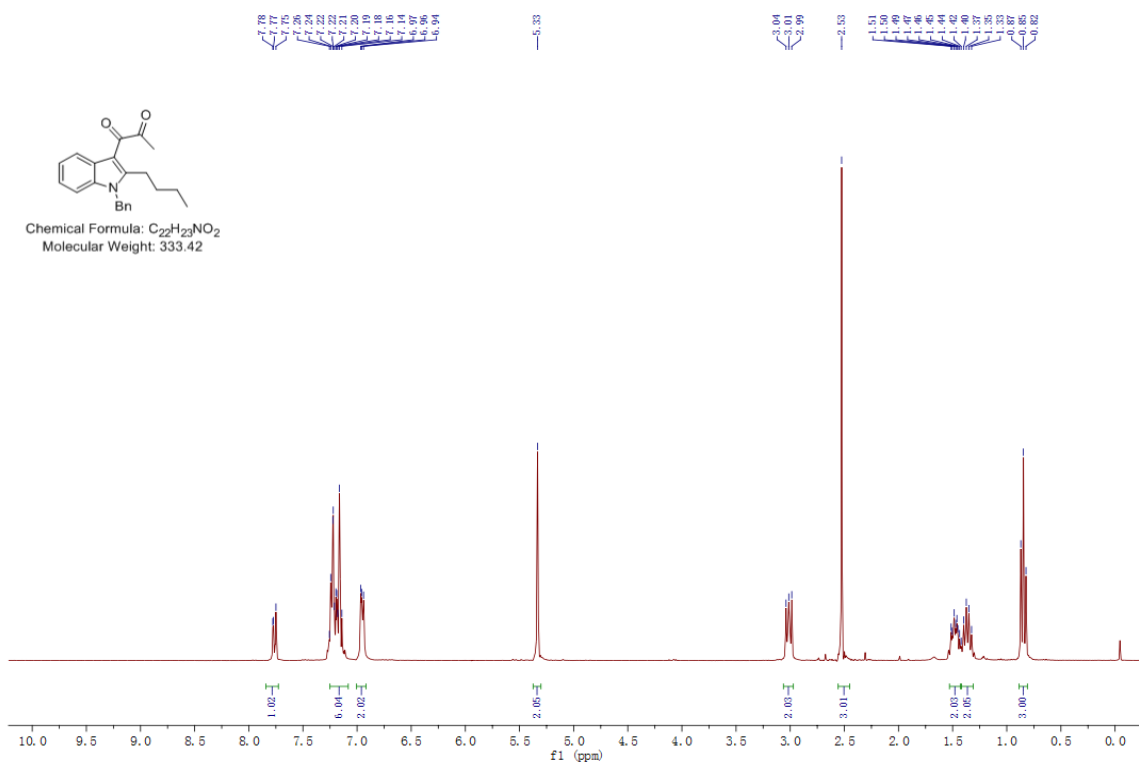
# 1-(2-butyl-1-ethyl-1H-indol-3-yl)propane-1,2-dione(2ar)



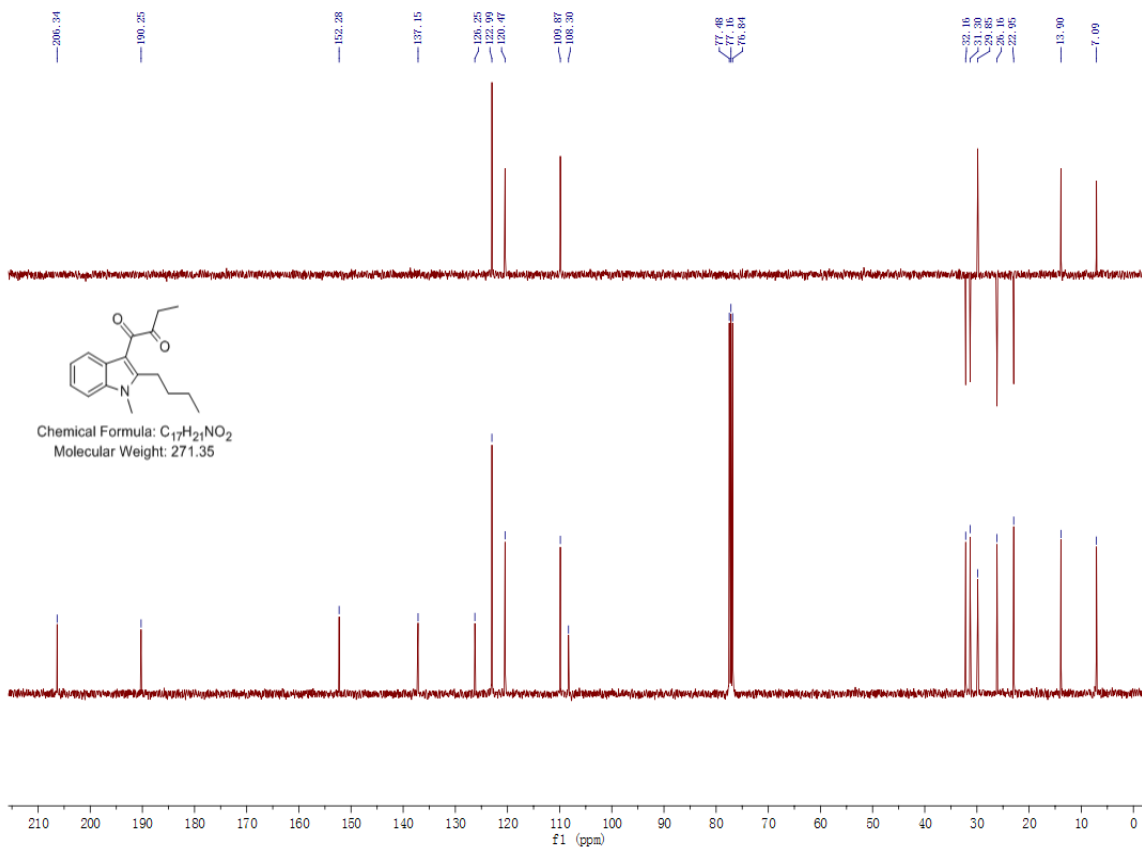
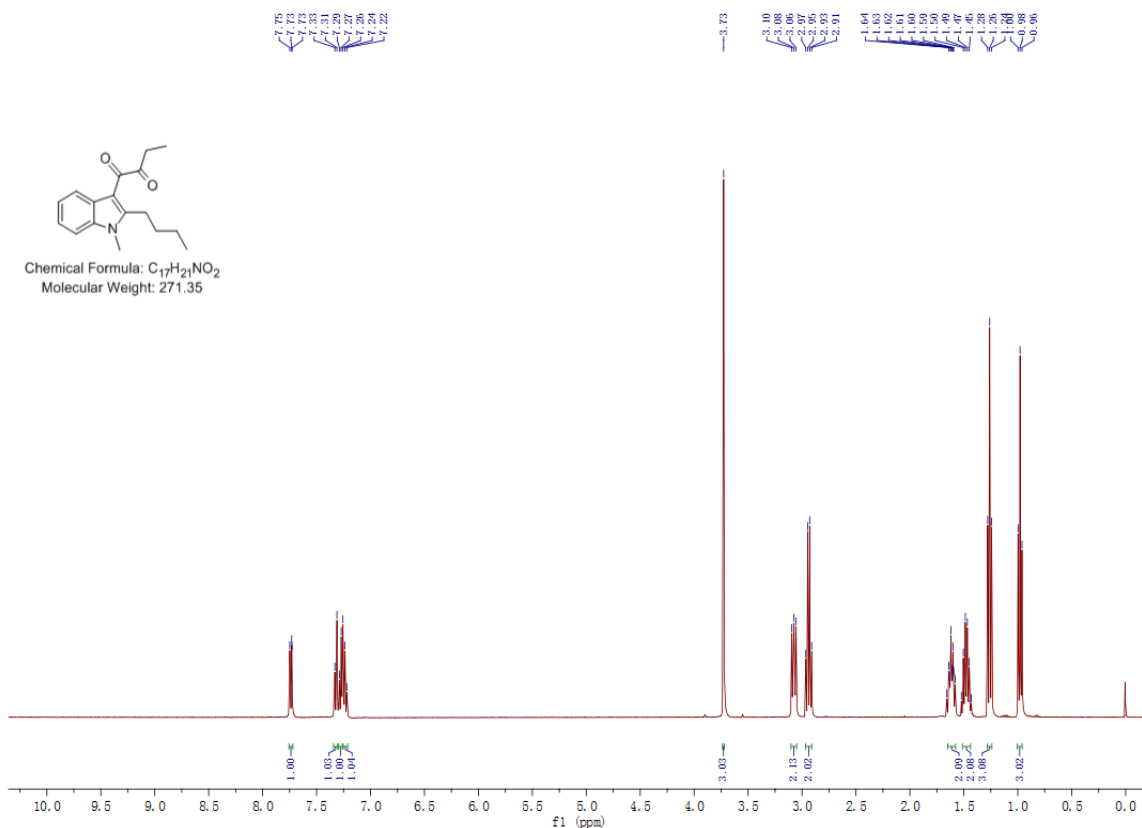
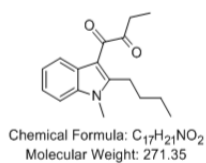
# 1-(1-benzyl-2-butyl-1H-indol-3-yl)propane-1,2-dione(2as)



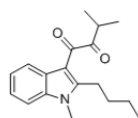
Chemical Formula:  $C_{22}H_{23}NO_2$   
Molecular Weight: 333.42



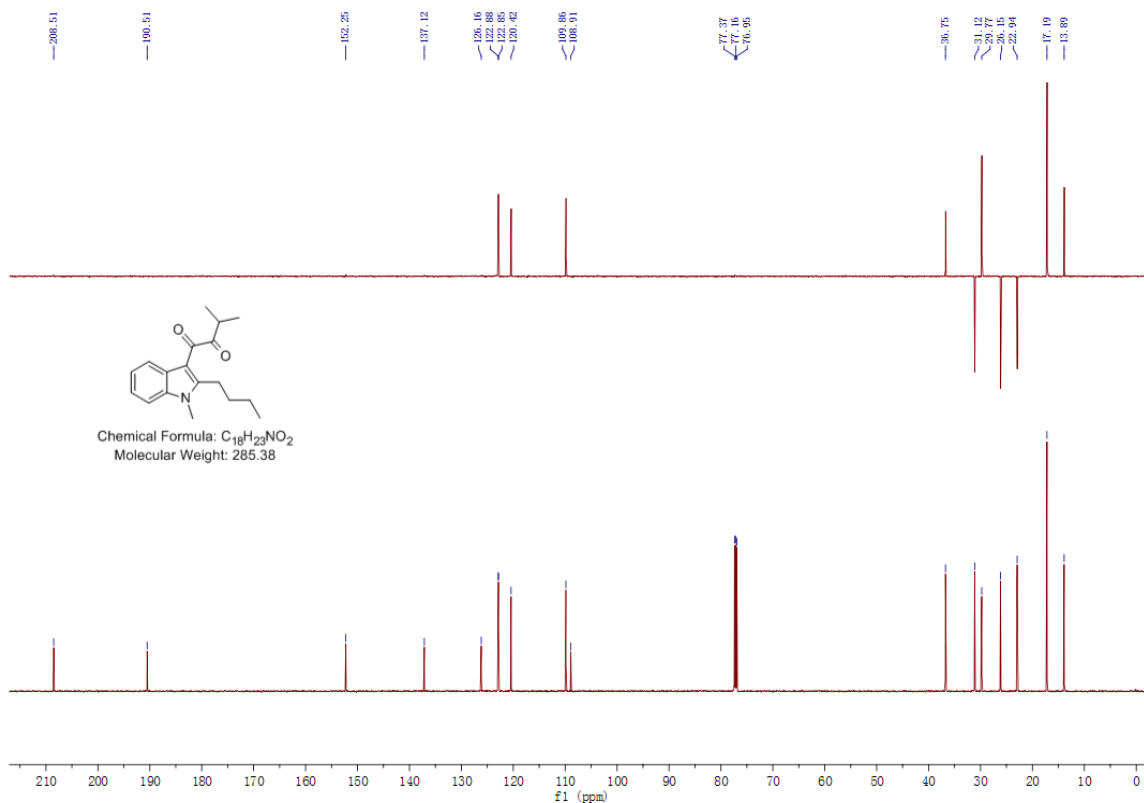
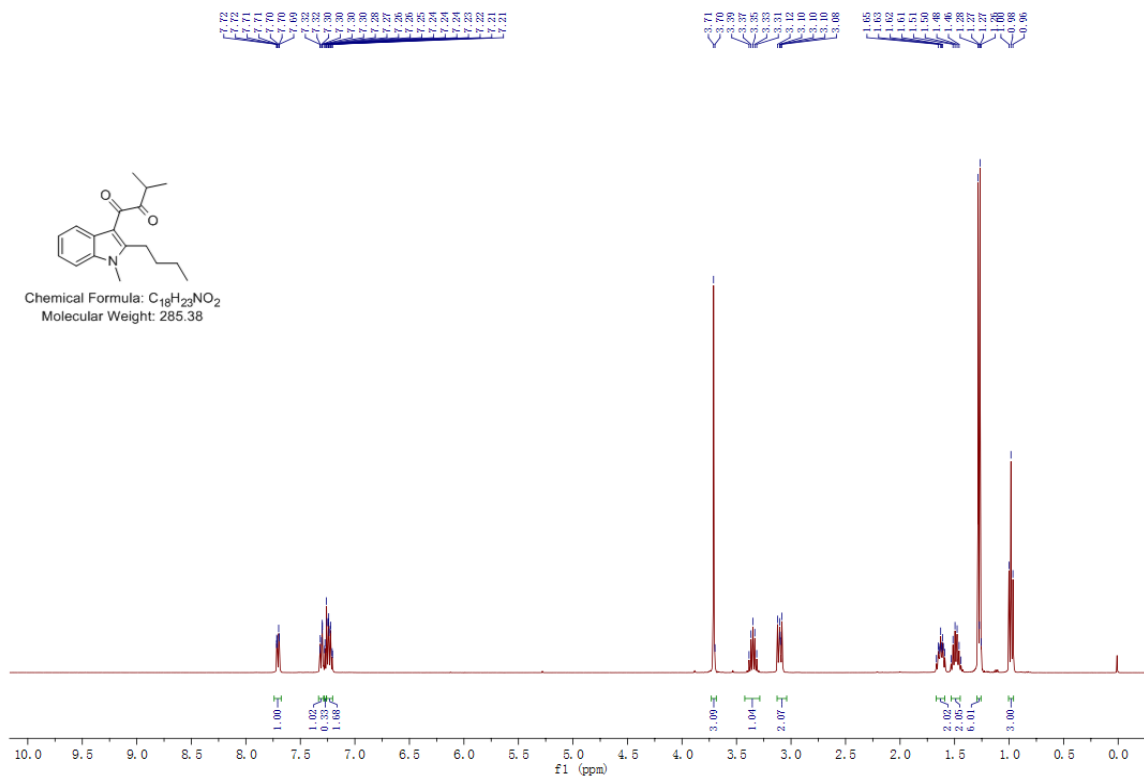
# 1-(2-butyl-1-methyl-1H-indol-3-yl)butane-1,2-dione(2at)



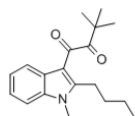
# 1-(2-butyl-1-methyl-1H-indol-3-yl)-3-methylbutane-1,2-dione(2au)



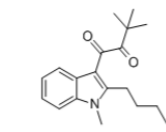
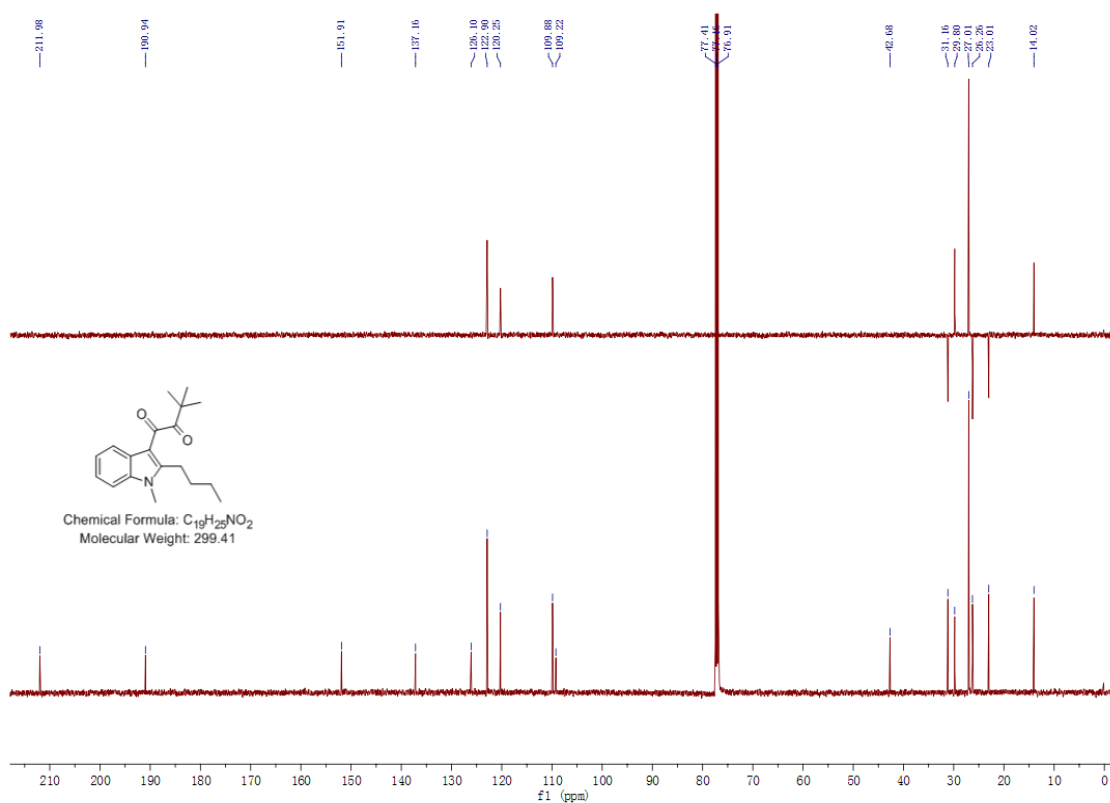
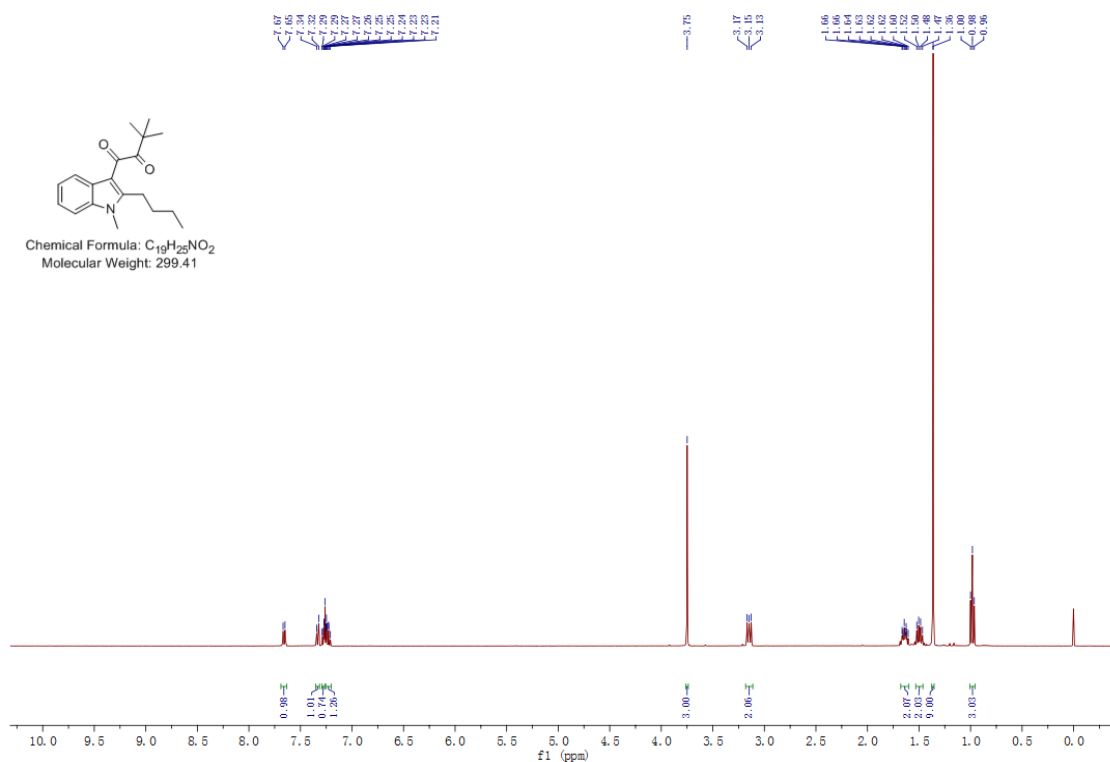
Chemical Formula: C<sub>18</sub>H<sub>23</sub>NO<sub>2</sub>  
Molecular Weight: 285.38



# 1-(2-butyl-1-methyl-1H-indol-3-yl)-3,3-dimethylbutane-1,2-dione(2av)



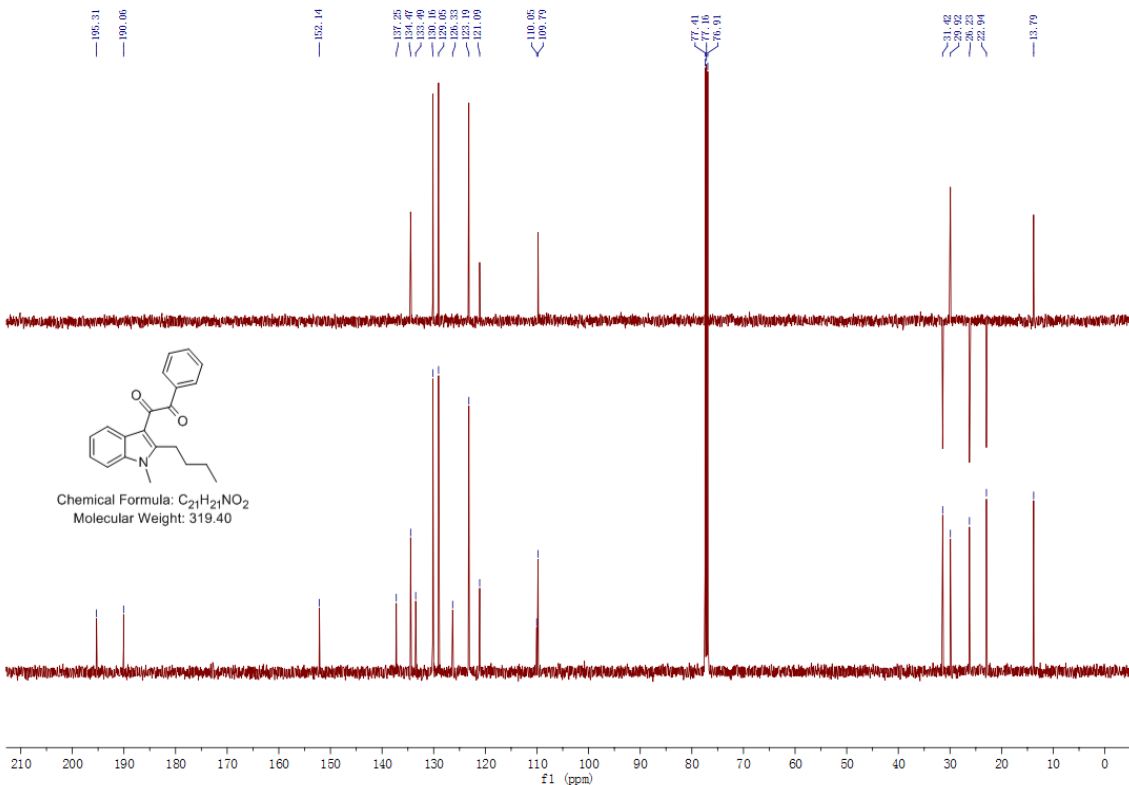
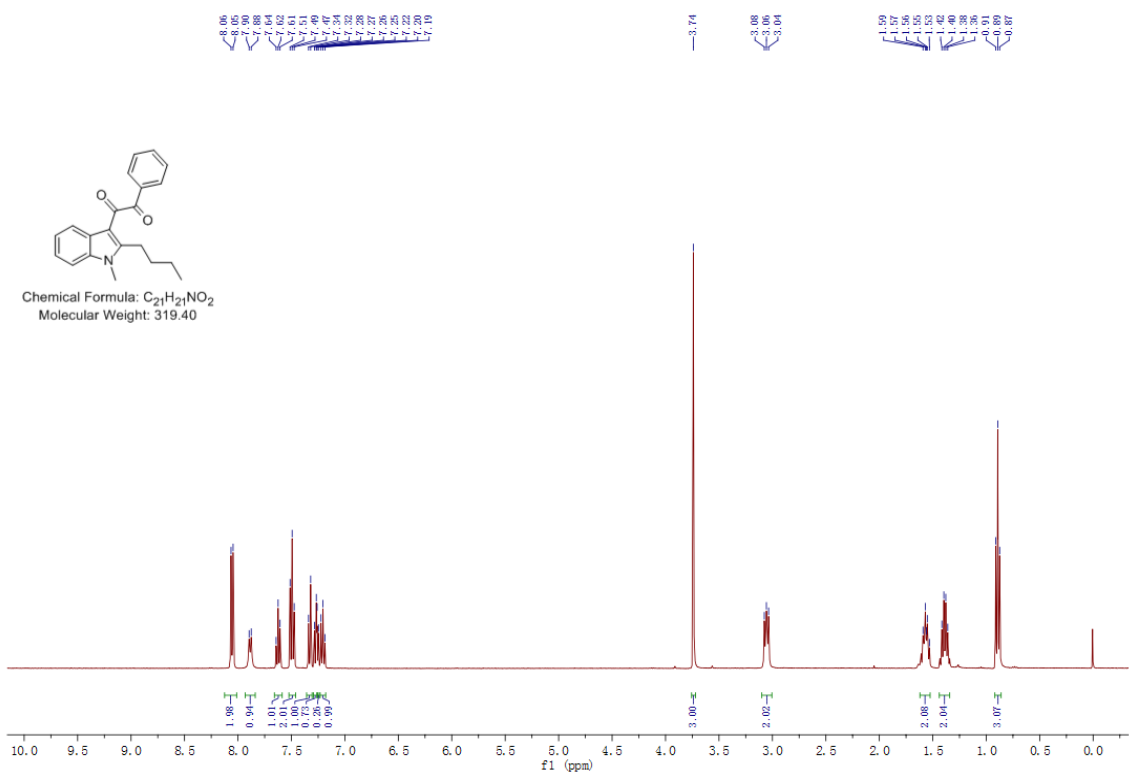
Chemical Formula: C<sub>19</sub>H<sub>25</sub>NO<sub>2</sub>  
Molecular Weight: 299.41



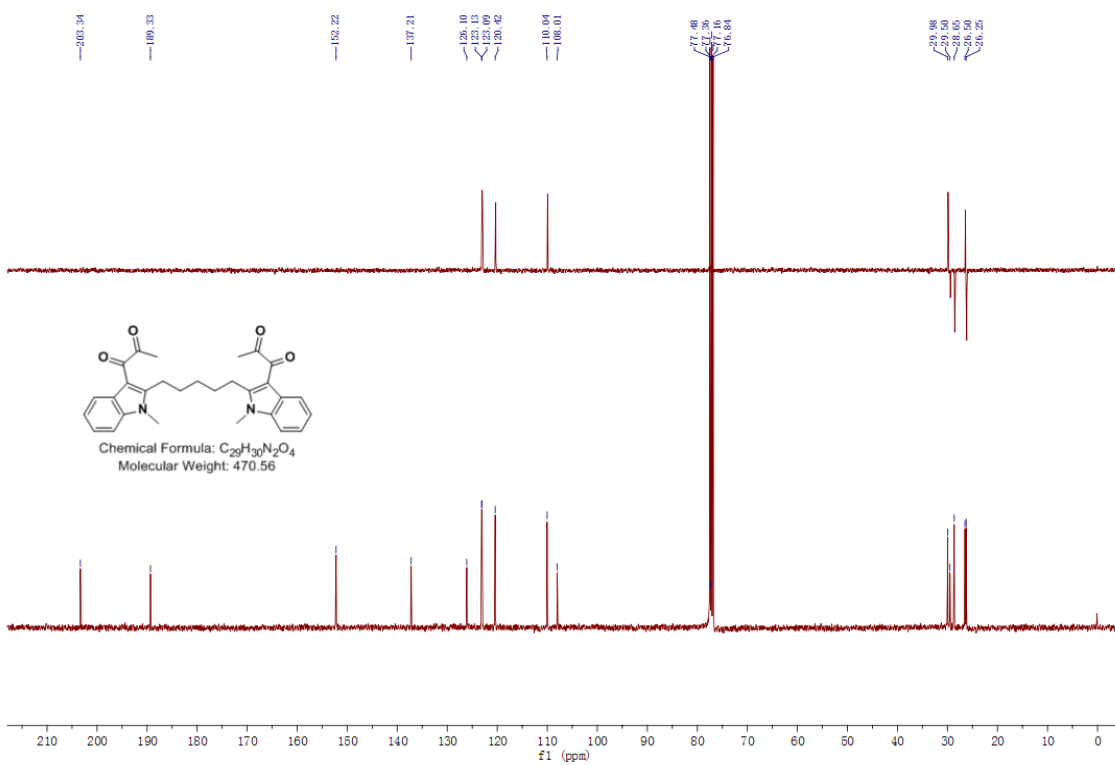
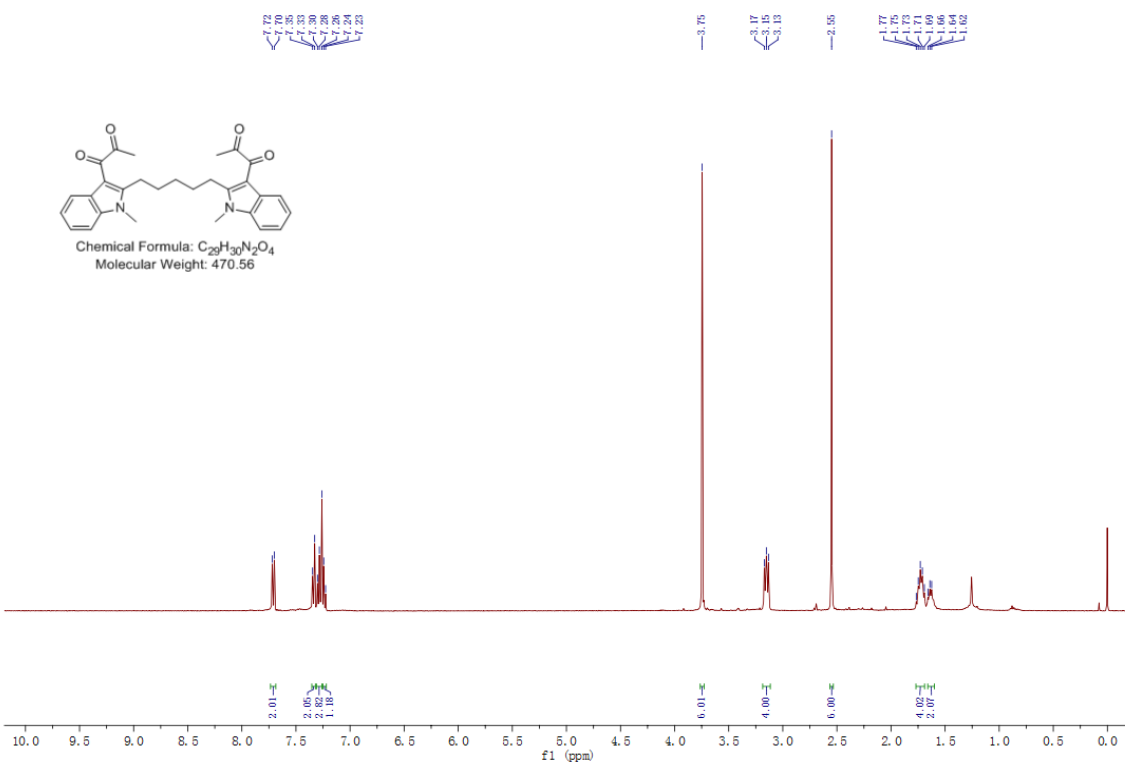
Chemical Formula: C<sub>19</sub>H<sub>25</sub>NO<sub>2</sub>  
Molecular Weight: 299.41



# 1-(2-butyl-1-methyl-1H-indol-3-yl)-2-phenylethane-1,2-dione(2aw)



# 1,1'-(2,2'-(pentane-1,5-diyl)bis(1-methyl-1H-indole-3,2-diyl))bis(propane-1,2-dione)(2ax)



# 1-(2-cyclohexyl-1-methyl-1H-indol-3-yl)butane-1,2-dione(2ay)

