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Supporting information

for

Cu-Catalyzed β-functionalization of saturated ketones with indoles: A One-Step Synthesis of C3-substituted indoles

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Ⅰ, General experimental information

Reagents and solvents: Commercially available reagents were used without any further purification. All organic solvents were also of reagent grade quality without any further purification.

Chromatography: Flash column chromatography was performed using silicycle silica gel (200-300 mesh).

Analytical thin-layer chromatography (TLC) was performed on 0.2 mm coated silica gel plates (HSGF 254) and visualized using a UV lamp (254 nm or 365 nm).

Nuclear Magnetic Resonance Spectroscopy:

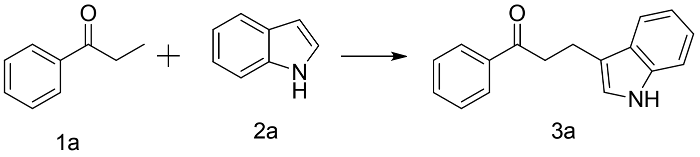
^{1}H NMR was recorded on magnet system 400'54 ascend purchased from Bruker Biospin AG.

^{1}H NMR spectra chemical shifts (δ) are reported in parts per million (ppm) referenced to TMS (0 ppm).

^{13}C NMR spectra chemical shifts (δ) are reported in parts per million (ppm) were referenced to carbon resonances in the NMR solvent.

ESI-MS spectra were recorded on Agilent Q-TOF 6520.

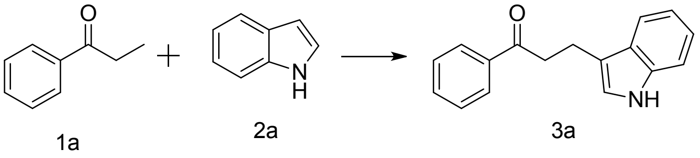
Ⅱ, Table S1: the solvent screening



entry	solvent	t (h)	Yield (%)[b]
1	DMSO	24	65
2	DMF	24	9
3	NMP	24	trace
4	*p*-xylene	12	86

[a]Reaction condition: 1a (3 mmol), 2a (1 mmol), $Cu(OAc)_2$ (0.2 mmol), L2 (0.2 mmol) and TEMPO (1 mmol) in solvent (3 mL) were heated at 100℃ under Ar (Ar balloon). [b]Yield of isolated product.

Ⅲ, Table S2: the temperature screening



entry	T (℃)	t (h)	Yield (%)[b]
1	120	4	86
2	110	6	84
3	100	12	86
4	90	24	65
5	80	24	Trace

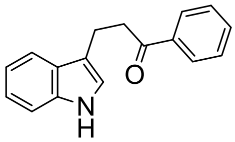
[a]Reaction condition: 1a (3 mmol), 2a (1 mmol), $Cu(OAc)_2$ (0.1 mmol), L2 (0.1 mmol) and TEMPO (1 mmol) in *p*-xylene (3 mL) were heated under Ar (Ar balloon). [b]Yield of isolated product.

Ⅳ, Experimental details for the synthesis of alkylated indole derivatives

To a mixture of saturated ketones (3 mmol, 3 eq) and indoles (1 mmol, 1 eq) in pxylene (3 mL) $Cu(OAc)_2$ (0.1 mmol, 0.1 eq), TMEDA (0.1 mmol, 0.1 eq) and TEMPO (1 mmol, 1 eq) were added and stirred at 120℃ under Ar atmosphere for 4-8 h. The progress of the reaction was monitored by TLC. After complete conversion, the mixture was cooled down to room temperature. Then, the reaction mixture was diluted with H_2O (30 mL) and extracted by ethyl acetate (30 mL). The separated organic layers were dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexane/ethyl acetate to afford the desired product.

1,

3-(1*H*-indol-3-yl)-1-phenylpropan-1-one(3a)

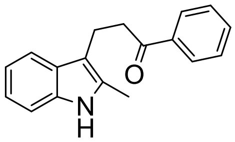


To a mixture of propiophenone (3 mmol, 402.5 mg) and indole (1 mmol, 117.2 mg) in pxylene (3 mL) $Cu(OAc)_2$ (0.1 mmol, 18.2mg), TMEDA (0.1 mmol, 11.6 mg) and TEMPO (1 mmol, 156.2 mg) were added and stirred at 120℃ under Ar atmosphere for 5 h. The progress of the reaction was monitored by TLC. After complete conversion, the mixture was cooled down to room temperature. Then, the reaction mixture was diluted with H_2O (30 mL) and extracted by ethyl acetate (30 mL). The separated organic layers were dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexane/ethyl acetate (10:1) to afford the desired product.

Orange solid (214.2 mg, 86%)

2,

3-(2-methyl-1*H*-indol-3-yl)-1-phenylpropan-1-one(3b)

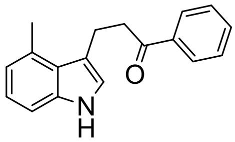


To a mixture of propiophenone (3 mmol, 402.5 mg) and 2-methylindole (1 mmol, 131.2 mg) in pxylene (3 mL) $Cu(OAc)_2$ (0.1 mmol, 18.2mg), TMEDA (0.1 mmol, 11.6 mg) and TEMPO (1 mmol, 156.2 mg) were added and stirred at 120℃ under Ar atmosphere for 5 h. The progress of the reaction was monitored by TLC. After complete conversion, the mixture was cooled down to room temperature. Then, the reaction mixture was diluted with H_2O (30 mL) and extracted by ethyl acetate (30 mL). The separated organic layers were dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexane/ethyl acetate (10:1) to afford the desired product.

White solid (228.9 mg, 87%)

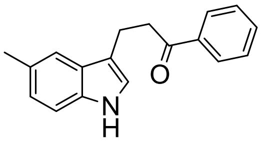
3,

3-(4-methyl-1*H*-indol-3-yl)-1-phenylpropan-1-one(3c)



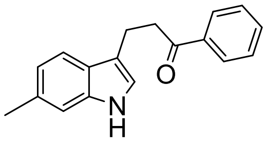
To a mixture of propiophenone (3 mmol, 402.5 mg) and 4-methylindole (1 mmol, 131.2 mg) in pxylene (3 mL) $Cu(OAc)_2$ (0.1 mmol, 18.2mg), TMEDA (0.1 mmol, 11.6 mg) and TEMPO (1 mmol, 156.2 mg) were added and stirred at 120℃ under Ar atmosphere for 5 h. The progress of the reaction was monitored by TLC. After complete conversion, the mixture was cooled down to room temperature. Then, the reaction mixture was diluted with H_2O (30 mL) and extracted by ethyl acetate (30 mL). The separated organic layers were dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexane/ethyl acetate (10:1) to afford the desired product.
Yellow solid (221.0 mg, 84%)

4,
3-(5-methyl-1*H*-indol-3-yl)-1-phenylpropan-1-one(3d)



To a mixture of propiophenone (3 mmol, 402.5 mg) and 5-methylindole (1 mmol, 131.2 mg) in pxylene (3 mL) $Cu(OAc)_2$ (0.1 mmol, 18.2mg), TMEDA (0.1 mmol, 11.6 mg) and TEMPO (1 mmol, 156.2 mg) were added and stirred at 120℃ under Ar atmosphere for 5 h. The progress of the reaction was monitored by TLC. After complete conversion, the mixture was cooled down to room temperature. Then, the reaction mixture was diluted with H_2O (30 mL) and extracted by ethyl acetate (30 mL). The separated organic layers were dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexane/ethyl acetate (10:1) to afford the desired product.
Black solid (189.4 mg, 72%)

5,
3-(6-methyl-1*H*-indol-3-yl)-1-phenylpropan-1-one(3e)

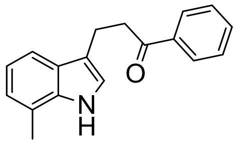


To a mixture of propiophenone (3 mmol, 402.5 mg) and 6-methylindole (1 mmol, 131.2 mg) in pxylene (3 mL) $Cu(OAc)_2$ (0.1 mmol, 18.2mg), TMEDA (0.1 mmol, 11.6 mg) and TEMPO (1 mmol, 156.2 mg) were added and stirred at 120℃ under Ar atmosphere for 5 h. The progress of the reaction was monitored by TLC. After complete conversion, the mixture was cooled down to room temperature. Then, the reaction mixture was diluted with H_2O (30 mL) and extracted by ethyl acetate (30 mL). The separated organic layers were dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexane/ethyl acetate (10:1) to afford

the desired product.
Pale red solid (223.7 mg, 85%)

6,

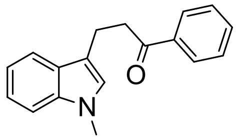
3-(7-methyl-1*H*-indol-3-yl)-1-phenylpropan-1-one(3f)



To a mixture of propiophenone (3 mmol, 402.5 mg) and 7-methylindole (1 mmol, 131.2 mg) in pxylene (3 mL) $Cu(OAc)_2$ (0.1 mmol, 18.2mg), TMEDA (0.1 mmol, 11.6 mg) and TEMPO (1 mmol, 156.2 mg) were added and stirred at 120℃ under Ar atmosphere for 5 h. The progress of the reaction was monitored by TLC. After complete conversion, the mixture was cooled down to room temperature. Then, the reaction mixture was diluted with H_2O (30 mL) and extracted by ethyl acetate (30 mL). The separated organic layers were dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexane/ethyl acetate (10:1) to afford the desired product.
White solid (218.4 mg, 83%)

7,

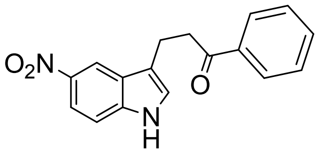
3-(1-methyl-1*H*-indol-3-yl)-1-phenylpropan-1-one(3g)



To a mixture of propiophenone (3 mmol, 402.5 mg) and 1-methylindole (1 mmol, 131.2 mg) in pxylene (3 mL) $Cu(OAc)_2$ (0.1 mmol, 18.2mg), TMEDA (0.1 mmol, 11.6 mg) and TEMPO (1 mmol, 156.2 mg) were added and stirred at 120℃ under Ar atmosphere for 5 h. The progress of the reaction was monitored by TLC. After complete conversion, the mixture was cooled down to room temperature. Then, the reaction mixture was diluted with H_2O (30 mL) and extracted by ethyl acetate (30 mL). The separated organic layers were dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexane/ethyl acetate (10:1) to afford the desired product.
Pale yellow oil (178.9 mg, 68%)

8,

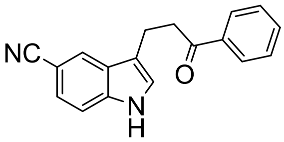
3-(5-nitro-1*H*-indol-3-yl)-1-phenylpropan-1-one(3h)



To a mixture of propiophenone (3 mmol, 402.5 mg) and 5-nitroindole (1 mmol, 162.2 mg) in pxylene (3 mL) $Cu(OAc)_2$ (0.1 mmol, 18.2mg), TMEDA (0.1 mmol, 11.6 mg) and TEMPO (1 mmol, 156.2 mg) were added and stirred at 120℃ under Ar atmosphere for 8 h. The progress of the reaction was monitored by TLC. After complete conversion, the mixture was cooled down to room temperature. Then, the reaction mixture was diluted with H_2O (30 mL) and extracted by ethyl acetate (30 mL). The separated organic layers were dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexane/ethyl acetate (7:1) to afford the desired product.

Yellow solid (241.2 mg, 82%)

9

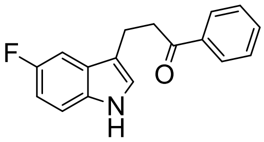


3-(5-cyano-1*H*-indol-3-yl)-1-phenylpropan-1-one(3i)

To a mixture of propiophenone (3 mmol, 402.5 mg) and 5-cyanoindole (1 mmol, 142.2 mg) in pxylene (3 mL) $Cu(OAc)_2$ (0.1 mmol, 18.2mg), TMEDA (0.1 mmol, 11.6 mg) and TEMPO (1 mmol, 156.2 mg) were added and stirred at 120℃ under Ar atmosphere for 7 h. The progress of the reaction was monitored by TLC.

10,

3-(5-fluoro-1*H*-indol-3-yl)-1-phenylpropan-1-one(3j)

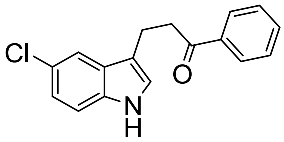


To a mixture of propiophenone (3 mmol, 402.5 mg) and 5-fluoroindole (1 mmol, 135.1 mg) in pxylene (3 mL) $Cu(oAc)_2$ (0.1 mmol, 18.2mg), TMEDA (0.1 mmol, 11.6 mg) and TEMPO (1 mmol, 156.2 mg) were added and stirred at 120℃ under Ar atmosphere for 5 h. The progress of the reaction was monitored by TLC. After complete conversion, the mixture was cooled down to room temperature. Then, the reaction mixture was diluted with H_2O (30 mL) and extracted by ethyl acetate (30 mL). The separated organic layers were dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexane/ethyl acetate (9:1) to afford the desired product.

Blue solid (213.7 mg, 80%)

11,

3-(5- chloro-1*H*-indol-3-yl)-1-phenylpropan-1-one(3k)

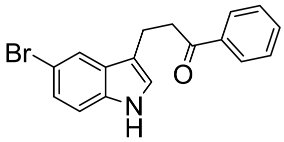


To a mixture of propiophenone (3 mmol, 402.5 mg) and 5-chloroindole (1 mmol, 151.6 mg) in pxylene (3 mL) Cu(OAc)$_2$ (0.1 mmol, 18.2mg), TMEDA (0.1 mmol, 11.6 mg) and TEMPO (1 mmol, 156.2 mg) were added and stirred at 120℃ under Ar atmosphere for 5 h. The progress of the reaction was monitored by TLC. After complete conversion, the mixture was cooled down to room temperature. Then, the reaction mixture was diluted with H_2O (30 mL) and extracted by ethyl acetate (30 mL). The separated organic layers were dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexane/ethyl acetate (9:1) to afford the desired product.

Pale purple solid (229.3 mg, 81%)

12,

3-(5-bromo-1*H*-indol-3-yl)-1-phenylpropan-1-one(3l)

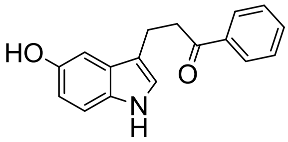


To a mixture of propiophenone (3 mmol, 402.5 mg) and 5-bromoindole (1 mmol, 196.4 mg) in pxylene (3 mL) Cu(OAc)$_2$ (0.1 mmol, 18.2mg), TMEDA (0.1 mmol, 11.6 mg) and TEMPO (1 mmol, 156.2 mg) were added and stirred at 120℃ under Ar atmosphere for 5 h. The progress of the reaction was monitored by TLC. After complete conversion, the mixture was cooled down to room temperature. Then, the reaction mixture was diluted with H_2O (30 mL) and extracted by ethyl acetate (30 mL). The separated organic layers were dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexane/ethyl acetate (9:1) to afford the desired product.

Blue solid (278.0 mg, 85%)

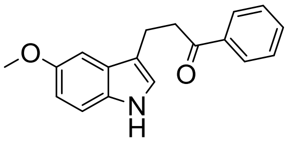
13,

3-(5-hydroxy-1*H*-indol-3-yl)-1-phenylpropan-1-one(3m)



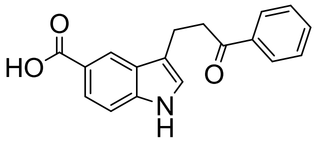
To a mixture of propiophenone (3 mmol, 402.5 mg) and 5-hydroxyindole (1 mmol, 133.2 mg) in pxylene (3 mL) $Cu(OAc)_2$ (0.1 mmol, 18.2mg), TMEDA (0.1 mmol, 11.6 mg) and TEMPO (1 mmol, 156.2 mg) were added and stirred at 120℃ under Ar atmosphere for 4 h. The progress of the reaction was monitored by TLC. After complete conversion, the mixture was cooled down to room temperature. Then, the reaction mixture was diluted with H_2O (30 mL) and extracted by ethyl acetate (30 mL). The separated organic layers were dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexane/ethyl acetate (7:1) to afford the desired product.
Pale yellow solid (172.3 mg, 65%)

14,
3-(5-methoxy-1*H*-indol-3-yl)-1-phenylpropan-1-one(3n)



To a mixture of propiophenone (3 mmol, 402.5 mg) and 5-methoxyindole (1 mmol, 147.2 mg) in pxylene (3 mL) $Cu(OAc)_2$ (0.1 mmol, 18.2mg), TMEDA (0.1 mmol, 11.6 mg) and TEMPO (1 mmol, 156.2 mg) were added and stirred at 120℃ under Ar atmosphere for 4 h. The progress of the reaction was monitored by TLC. After complete conversion, the mixture was cooled down to room temperature. Then, the reaction mixture was diluted with H_2O (30 mL) and extracted by ethyl acetate (30 mL). The separated organic layers were dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexane/ethyl acetate (9:1) to afford the desired product.
Pale yellow solid (240.0 mg, 86%)

15,
3-(5-carboxy-1*H*-indol-3-yl)-1-phenylpropan-1-one(3o)

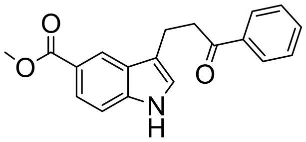


To a mixture of propiophenone (3 mmol, 402.5 mg) and indole-5-carboxylic acid (1 mmol, 161.2 mg) in pxylene/DMSO (3 mL, 1.5+1.5) $Cu(OAc)_2$ (0.1 mmol, 18.2mg), TMEDA (0.1 mmol, 11.6 mg) and TEMPO (1 mmol, 156.2 mg) were added and stirred at 120℃ under Ar atmosphere for 8 h. The progress of the reaction was monitored by TLC. After complete conversion, the mixture was cooled down to room temperature. Then, the reaction mixture was diluted with H_2O (30 mL) and extracted by ethyl acetate (30 mL). The separated organic layers were dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using

hexane/ethyl acetate (5:1) to afford the desired product.
Yellow solid (228.6 mg, 78%)

16,

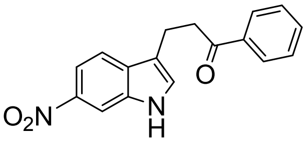
3-(5- methoxycarbonyl-1*H*-indol-3-yl)-1-phenylpropan-1-one(3p)



To a mixture of propiophenone (3 mmol, 402.5 mg) and methyl indole-5-carboxylate (1 mmol, 175.2 mg) in pxylene (3 mL) $Cu(OAc)_2$ (0.1 mmol, 18.2mg), TMEDA (0.1 mmol, 11.6 mg) and TEMPO (1 mmol, 156.2 mg) were added and stirred at 120℃ under Ar atmosphere for 6 h. The progress of the reaction was monitored by TLC. After complete conversion, the mixture was cooled down to room temperature. Then, the reaction mixture was diluted with H_2O (30 mL) and extracted by ethyl acetate (30 mL). The separated organic layers were dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexane/ethyl acetate (7:1) to afford the desired product.
Pale yellow solid (254.9 mg, 83%)

17

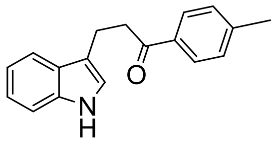
3-(6-nitro-1*H*-indol-3-yl)-1-phenylpropan-1-one(3q)



To a mixture of propiophenone (3 mmol, 402.5 mg) and 6-nitroindole (1 mmol, 162.2 mg) in pxylene (3 mL) $Cu(OAc)_2$ (0.1 mmol, 18.2mg), TMEDA (0.1 mmol, 11.6 mg) and TEMPO (1 mmol, 156.2 mg) were added and stirred at 120℃ under Ar atmosphere for 8 h. The progress of the reaction was monitored by TLC. After complete conversion, the mixture was cooled down to room temperature. Then, the reaction mixture was diluted with H_2O (30 mL) and extracted by ethyl acetate (30 mL). The separated organic layers were dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexane/ethyl acetate (7:1) to afford the desired product.
Yellow solid (220.6 mg, 75%)

18

3-(1H-indol-3-yl)-1-(4-methylphenyl)propan-1-one(3r)

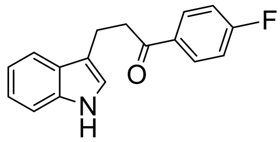


To a mixture of 4'-methylpropiophenone (3 mmol, 444.6 mg) and indole (1 mmol, 117.2 mg) in pxylene (3 mL) $Cu(OAc)_2$ (0.1 mmol, 18.2mg), TMEDA (0.1 mmol, 11.6 mg) and TEMPO (1 mmol, 156.2 mg) were added and stirred at 120℃ under Ar atmosphere for 5 h. The progress of the reaction was monitored by TLC. After complete conversion, the mixture was cooled down to room temperature. Then, the reaction mixture was diluted with H_2O (30 mL) and extracted by ethyl acetate (30 mL). The separated organic layers were dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexane/ethyl acetate (10:1) to afford the desired product.

White solid (228.9 mg, 87%)

19

3-(1H-indol-3-yl)-1-(4-fluorophenyl)propan-1-one(3s)

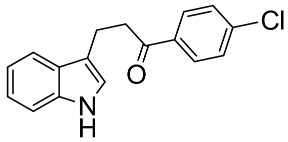


To a mixture of 4'-fluoropropiophenone (3 mmol, 456.5 mg) and indole (1 mmol, 117.2 mg) in pxylene (3 mL) $Cu(OAc)_2$ (0.1 mmol, 18.2mg), TMEDA (0.1 mmol, 11.6 mg) and TEMPO (1 mmol, 156.2 mg) were added and stirred at 120℃ under Ar atmosphere for 5 h. The progress of the reaction was monitored by TLC. After complete conversion, the mixture was cooled down to room temperature. Then, the reaction mixture was diluted with H_2O (30 mL) and extracted by ethyl acetate (30 mL). The separated organic layers were dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexane/ethyl acetate (9:1) to afford the desired product.

Pink solid (213.7 mg, 80%)

20

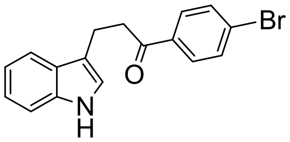
3-(1H-indol-3-yl)-1-(4-chlorophenyl)propan-1-one(3t)



To a mixture of 4'-chloropropiophenone (3 mmol, 505.8 mg) and indole (1 mmol, 117.2 mg) in pxylene (3 mL) $Cu(OAc)_2$ (0.1 mmol, 18.2mg), TMEDA (0.1 mmol, 11.6 mg) and TEMPO (1 mmol, 156.2 mg) were added and stirred at 120℃ under Ar atmosphere for 5 h. The progress of the reaction was monitored by TLC. After complete conversion, the mixture was

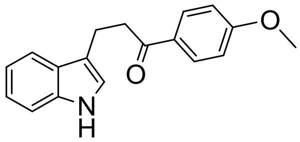
cooled down to room temperature. Then, the reaction mixture was diluted with H_2O (30 mL) and extracted by ethyl acetate (30 mL). The separated organic layers were dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexane/ethyl acetate (9:1) to afford the desired product.
Pale yellow solid (246.3.9 mg, 87%)

21
3-(1H-indol-3-yl)-1-(4-bromophenyl)propan-1-one(3u)



To a mixture of 4'-bromopropiophenone (3 mmol, 639.2 mg) and indole (1 mmol, 117.2 mg) in pxylene (3 mL) $Cu(OAc)_2$ (0.1 mmol, 18.2mg), TMEDA (0.1 mmol, 11.6 mg) and TEMPO (1 mmol, 156.2 mg) were added and stirred at 120℃ under Ar atmosphere for 5 h. The progress of the reaction was monitored by TLC. After complete conversion, the mixture was cooled down to room temperature. Then, the reaction mixture was diluted with H_2O (30 mL) and extracted by ethyl acetate (30 mL). The separated organic layers were dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexane/ethyl acetate (9:1) to afford the desired product.
Brown yellow solid (278.0 mg, 85%)

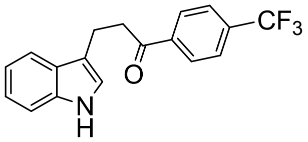
22
3-(1H-indol-3-yl)-1-(4-methoxyphenyl)propan-1-one(3v)



To a mixture of methoxypropiophenone (3 mmol, 492.6 mg) and indole (1 mmol, 117.2 mg) in pxylene (3 mL) $Cu(OAc)_2$ (0.1 mmol, 18.2mg), TMEDA (0.1 mmol, 11.6 mg) and TEMPO (1 mmol, 156.2 mg) were added and stirred at 120℃ under Ar atmosphere for 5 h. The progress of the reaction was monitored by TLC. After complete conversion, the mixture was cooled down to room temperature. Then, the reaction mixture was diluted with H_2O (30 mL) and extracted by ethyl acetate (30 mL). The separated organic layers were dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexane/ethyl acetate (10:1) to afford the desired product.
Red solid (237.3mg, 85%)

23

3-(1H-indol-3-yl)-1-(4-(trifluoromethyl)phenyl)propan-1-one(3w)

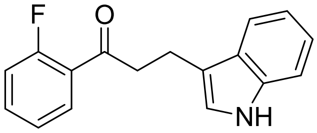


To a mixture of 4'-(trifluoromethyl)propiophenone (3 mmol, 606.5 mg) and indole (1 mmol, 117.2 mg) in pxylene (3 mL) $Cu(OAc)_2$ (0.1 mmol, 18.2mg), TMEDA (0.1 mmol, 11.6 mg) and TEMPO (1 mmol, 156.2 mg) were added and stirred at 120℃ under Ar atmosphere for 5 h. The progress of the reaction was monitored by TLC. After complete conversion, the mixture was cooled down to room temperature. Then, the reaction mixture was diluted with H_2O (30 mL) and extracted by ethyl acetate (30 mL). The separated organic layers were dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexane/ethyl acetate (8:1) to afford the desired product.

Pale yellow solid (279.0mg, 88%)

24

3-(1H-indol-3-yl)-1-(2-fluorophenyl)propan-1-one(3y)



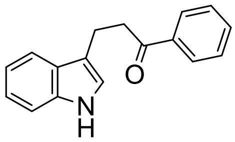
To a mixture of 2'-fluoropropiophenone (3 mmol, 456.5 mg) and indole (1 mmol, 117.2 mg) in pxylene (3 mL) $Cu(OAc)_2$ (0.1 mmol, 18.2mg), TMEDA (0.1 mmol, 11.6 mg) and TEMPO (1 mmol, 156.2 mg) were added and stirred at 120℃ under Ar atmosphere for 5 h. The progress of the reaction was monitored by TLC. After complete conversion, the mixture was cooled down to room temperature. Then, the reaction mixture was diluted with H_2O (30 mL) and extracted by ethyl acetate (30 mL). The separated organic layers were dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexane/ethyl acetate (9:1) to afford the desired product.

White solid (235.7 mg, 88%)

Ⅴ, Analytical data for compounds 3

1,

3-(1*H*-indol-3-yl)-1-phenylpropan-1-one(3a)



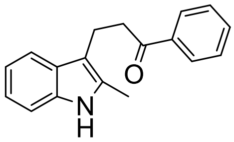
^{1}H NMR (400 MHz, DMSO) δ 10.79 (s, 1H), 8.04 – 7.97 (m, 2H), 7.65 – 7.55 (m, 2H), 7.51 (t, *J* = 7.7 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.17 (s, 1H), 7.08 (t, *J* = 7.5 Hz, 1H), 6.99 (t, *J* = 7.4 Hz, 1H), 3.41 (t, 2H), 3.07 (t, *J* = 8.0 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 199.66 (s), 136.73, 136.26, 132.99, 128.65, 127.89, 127.06, 122.35, 120.89, 118.29, 118.19, 113.62, 111.30, 38.71, 19.36

HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{17}H_{15}NO$ 272.1046 found 272.1061.

2,

3-(2-methyl-1*H*-indol-3-yl)-1-phenylpropan-1-one(3b)



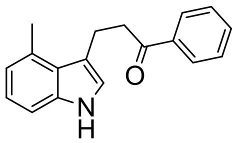
^{1}H NMR (400 MHz, DMSO) δ 10.68 (s, 1H), 7.96 – 7.91 (m, 2H), 7.59 (t, *J* = 7.4 Hz, 1H), 7.47 (dd, *J* = 16.3, 8.3 Hz, 3H), 7.23 (d, *J* = 7.7 Hz, 1H), 7.01 – 6.89 (m, 2H), 3.27 (t, *J* = 7.4 Hz, 2H), 3.01 (t, *J* = 7.4 Hz, 2H), 2.31 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ 199.78, 136.66, 135.19, 132.95, 131.62, 128.62, 128.00, 127.85, 119.85, 118.07, 117.39, 110.32, 109.07, 39.09, 18.61, 11.21

HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{18}H_{17}NO$ 286.1202 found 286.1211.

3,

3-(4-methyl-1*H*-indol-3-yl)-1-phenylpropan-1-one(3c)



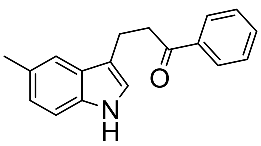
^{1}H NMR (400 MHz, DMSO) δ 10.76 (s, 1H), 8.06 – 8.01 (m, 2H), 7.63 (t, *J* = 7.3 Hz, 1H), 7.52 (t, *J* = 7.6 Hz, 2H), 7.16 (d, *J* = 8.1 Hz, 1H), 7.11 (d, *J* = 1.9 Hz, 1H), 6.92 (t, *J* = 7.6 Hz, 1H), 6.70 (d, *J* = 7.0 Hz, 1H), 3.41 (t, *J* = 7.2 Hz, 2H), 3.24 (t, *J* = 7.6 Hz, 2H), 2.64 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ 199.54, 136.72 (d, *J* = 2.9 Hz), 133.04, 129.54, 128.67, 127.93, 125.54, 122.33, 120.88, 119.81, 114.52, 109.35, 21.28, 20.02.

HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{18}H_{17}NO$ 286.1202 found 286.1230.

4,

3-(5-methyl-1*H*-indol-3-yl)-1-phenylpropan-1-one(3d)



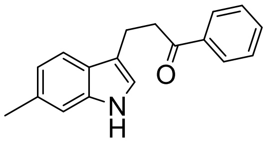
^{1}H NMR (400 MHz, DMSO) δ 10.63 (s, 1H), 8.00 (dd, *J* = 8.2, 1.1 Hz, 2H), 7.62 (tt, *J* = 7.6, 1.2 Hz 1H), 7.51 (t, *J* = 7.6 Hz, 2H), 7.33 (s, 1H), 7.22 (d, *J* = 8.2 Hz, 1H), 7.10 (d, *J* = 1.9 Hz, 1H), 6.89 (d, *J* = 8.2 Hz, 1H), 3.40 (t, *J* = 7.5 Hz, 2H), 3.02 (t, *J* = 7.5 Hz, 2H), 2.38 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ 199.70, 136.74, 134.62, 132.99, 128.66, 127.90, 127.27, 126.54, 122.48, 122.40, 117.89, 113.05, 111.00, 38.75, 21.24, 19.38

HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{18}H_{17}NO$ 286.1202 found 286.1216.

5,

3-(6-methyl-1*H*-indol-3-yl)-1-phenylpropan-1-one(3e)



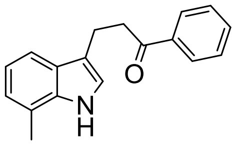
^{1}H NMR (400 MHz, DMSO) δ 10.60 (s, 1H), 8.01 – 7.97 (m, 2H), 7.62 (tt, *J* = 7.6, 1.2 Hz, 1H), 7.51 ((tt, *J* = 8.0, 1.6 Hz, 2H), 7.42 (d, *J* = 8.0 Hz, 1H), 7.12 (s, 1H), 7.06 (d, *J* = 2.1 Hz, 1H), 6.81 (dd, *J* = 8.0, 0.9 Hz, 1H), 3.39 (t, *J* = 7.5 Hz, 2H), 3.02 (t, *J* = 7.4 Hz, 2H), 2.38 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ 199.69, 136.71 (d, *J* = 3.9 Hz), 133.00, 129.81, 128.66, 127.88, 125.02, 121.58, 119.94, 117.99, 113.43, 111.11, 38.68, 21.36, 19.43.

HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{18}H_{17}NO$ 286.1202 found 286.1232.

6,

3-(7-methyl-1*H*-indol-3-yl)-1-phenylpropan-1-one(3f)



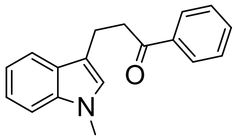
^{1}H NMR (400 MHz, DMSO) δ 10.75 (s, 1H), 8.00 (d, *J* = 7.4 Hz, 2H), 7.62 (t, *J* = 7.3 Hz, 1H), 7.51 (t, *J* = 7.5 Hz, 2H), 7.39 (d, *J* = 7.2 Hz, 1H), 7.16 (d, *J* = 2.1 Hz, 1H), 6.918- 6.858(m, 2H), 3.41 (t, *J* = 7.5 Hz, 2H), 3.05 (t, *J* = 7.3 Hz, 2H), 2.44 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ 199.66, 136.73, 135.77, 133.00, 128.66, 127.89, 126.72, 122.07, 121.40, 120.34, 118.42, 115.90, 114.04, 38.70, 19.48, 16.74

HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{18}H_{17}NO$ 286.1202 found 286.1225.

7,

3-(1-methyl-1*H*-indol-3-yl)-1-phenylpropan-1-one(3g)



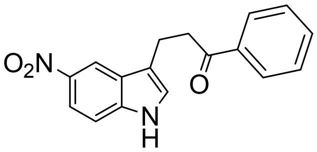
^{1}H NMR (400 MHz, DMSO) δ 7.99 (tt, *J* = 8.3, 1.2 Hz, 2H), 7.62 (tt, *J* = 7.2, 1.2 Hz, 1H), 7.57 (d, *J* = 7.7 Hz, 1H), 7.54 – 7.49 (m, 2H), 7.36 (d, *J* = 8.2 Hz, 1H), 7.17 – 7.10 (m, 2H), 7.05 – 6.99 (m, 1H), 3.71 (s, 3H), 3.40 (t, *J* = 7.6 Hz, 2H), 3.04 (t, *J* = 7.4 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 199.50, 136.68, 136.63, 133.02, 128.66, 127.88, 127.35, 126.81, 121.02, 118.53, 118.27, 113.01, 109.45, 38.73, 32.16, 19.11

HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{18}H_{17}NO$ 264.1383 found 264.1372.

8,

3-(5-nitro-1*H*-indol-3-yl)-1-phenylpropan-1-one(3h)

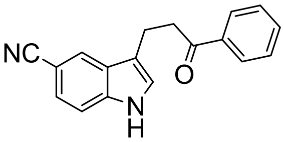


^{1}H NMR (400 MHz, DMSO) δ 11.57 (s, 1H), 8.57 (d, *J* = 1.9 Hz, 1H), 8.01-7.95 (m, 3H), 7.62 (t, *J* = 7.3 Hz, 1H), 7.51 (t, *J* = 8.5 Hz, 3H), 7.44 (s, 1H), 3.45 (t, *J* = 7.3 Hz, 2H), 3.12 (t, *J* = 7.2 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 199.41, 140.19, 139.31, 136.66, 133.06, 128.65, 127.90, 126.41 (d, *J* = 3.6 Hz), 116.92, 116.37, 115.77, 111.72, 38.64, 18.77

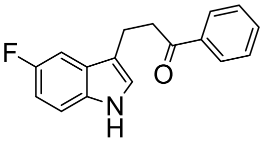
HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{17}H_{14}N_2O_3$ 317.0897 found 317.0907.

9



10,

3-(5-fluoro-1*H*-indol-3-yl)-1-phenylpropan-1-one(3j)



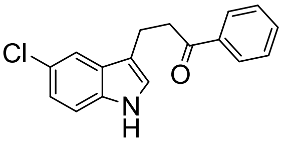
^{1}H NMR (400 MHz, DMSO) δ 10.89 (s, 1H), 8.00 (d, *J* = 7.4 Hz, 2H), 7.62 (t, *J* = 7.3 Hz, 1H), 7.51 (t, *J* = 7.5 Hz, 2H), 7.32 (dd, *J* = 8.5, 4.5 Hz, 2H), 7.25 (s, 1H), 6.90 (td, *J* = 9.3, 2.4 Hz, 1H), 3.41 (t, *J* = 7.4 Hz, 2H), 3.02 (t, *J* = 7.4 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 199.60, 157.76, 155.46, 136.72, 132.93 (d, *J* = 12.1 Hz), 128.63, 127.89, 127.26 (d, *J* = 10.0 Hz), 124.58, 113.97 (d, *J* = 4.8 Hz), 112.15 (d, *J* = 9.6 Hz), 109.06, 108.80, 103.19, 102.96, 38.55, 19.19.

HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{17}H_{14}NOF$ 290.0952 found 290.0960.

11,

3-(5- chloro-1*H*-indol-3-yl)-1-phenylpropan-1-one(3k)



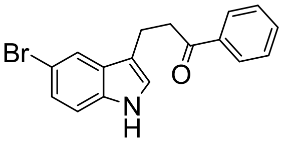
^{1}H NMR (400 MHz, DMSO) δ 10.99 (s, 1H), 8.03 – 7.96 (m, 2H), 7.64 – 7.58 (m, 2H), 7.51 (tt, *J* = 7.6, 1.6 Hz, 2H), 7.34 (d, *J* = 8.6 Hz, 1H), 7.24 (d, *J* = 2.2 Hz, 1H), 7.05 (dd, *J* = 8.6, 2.0 Hz, 1H), 3.40 (t, *J* = 7.6 Hz, 2H), 3.02 (t, *J* = 7.3 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 199.57, 136.70, 134.65, 133.01, 128.64, 128.20, 127.89, 124.34, 122.94, 120.79, 117.66, 113.68, 112.79, 38.68, 19.03

HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{17}H_{14}NOCl$ 306.0656 found 306.0659.

12,

3-(5-bromo-1*H*-indol-3-yl)-1-phenylpropan-1-one(3l)



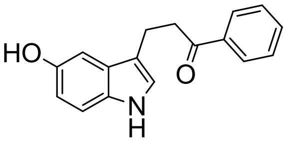
^{1}H NMR (400 MHz, DMSO) δ 11.01 (s, 1H), 7.98 (d, *J* =4 Hz, 2H), 7.75 (s, 1H), 7.62 (t, *J* =6.4 Hz, 1H), 7.51 (t, *J* =7.2 Hz, 2H), 7.31 (d, *J* = 6.1 Hz, 1H), 7.23 (s, 1H), 7.18 (d, *J* =7.6 Hz, 1H), 3.40 (t, *J* =7.4 Hz, 2H), 3.03 (t, *J* =7.2 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 199.52, 136.71, 134.88, 132.99, 128.93, 128.63, 127.89, 124.18, 123.32, 120.69, 113.62, 113.28, 110.92, 38.71, 19.02

HRMS (TOF) m/z [M - H]$^-$ Calcd for $C_{17}H_{14}NOBr$ 326.0186 found 326.0156.

13,

3-(5-hydroxy-1*H*-indol-3-yl)-1-phenylpropan-1-one(3m)



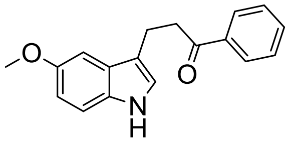
^{1}H NMR (400 MHz, DMSO) δ 10.46 (s, 1H), 8.60 (s, 1H), 7.99 (dt, *J* = 7.2, 1.2 Hz, 2H), 7.62 (tt, *J* = 7.4 0.8 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 2H), 7.14 (d, *J* = 8.6 Hz, 1H), 7.06 (d, *J* = 2.1 Hz, 1H), 6.86 (d, *J* = 2.2 Hz, 1H), 6.61 (dd, *J* = 8.6, 2.3 Hz, 1H), 3.36 (t, *J* = 7.7 Hz, 2H), 2.96 (t, *J* = 7.4 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 199.74, 150.15, 136.72, 133.01, 130.82, 128.67, 127.88, 127.71, 122.79, 112.62, 111.63, 111.24, 102.19, 38.60, 19.48

HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{17}H_{15}NO_2$ 288.0995 found 288.0995.

14,

3-(5-methoxy-1*H*-indol-3-yl)-1-phenylpropan-1-one(3n)



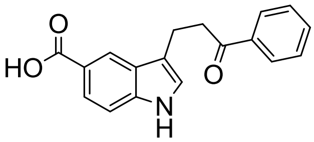
^{1}H NMR (400 MHz, DMSO) δ 10.61 (s, 1H), 8.00 (d, *J* = 7.5 Hz, 2H), 7.63 (t, *J* = 7.2 Hz, 1H), 7.52 (t, *J* = 7.5 Hz, 2H), 7.22 (d, *J* = 8.7 Hz, 1H), 7.12 (s, 1H), 7.03 (s, 1H), 6.71 (dd, *J* = 8.6, 1.8 Hz, 1H), 3.76 (s, 3H), 3.41 (t, *J* = 7.4 Hz, 2H), 3.02 (t, *J* = 7.3 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 199.76, 152.93, 136.75, 133.00, 131.36, 128.66, 127.90, 127.33, 123.02, 113.38, 111.92, 111.05, 100.14, 55.32, 38.64, 19.38

HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{18}H_{17}NO_2$ 302.1151 found 302.1191.

15,

3-(5-carboxy-1*H*-indol-3-yl)-1-phenylpropan-1-one(3o)



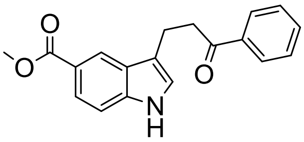
^{1}H NMR (400 MHz, DMSO) δ 11.18 (s, 1H), 8.29 (s, 1H), 7.98 (d, *J* = 7.6 Hz, 2H), 7.75 (dd, *J* = 8.5, 1.4 Hz, 1H), 7.61 (t, *J* = 7.3 Hz, 1H), 7.50 (t, *J* = 7.6 Hz, 2H), 7.42 (d, *J* = 8.5 Hz, 1H), 7.30 (s, 1H), 3.43 (t, *J* = 7.3 Hz, 2H), 3.11 (t, *J* = 7.3 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 199.49, 168.52, 138.70, 136.67, 133.01, 128.63, 127.88, 126.64, 124.04, 122.30, 121.05, 120.87, 115.25, 111.06, 38.65, 19.02

HRMS (TOF) m/z $[M - H]^-$ Calcd for $C_{18}H_{15}NO_3$ 292.0979 found 292.0988.

16,

3-(5- methoxycarbonyl-1*H*-indol-3-yl)-1-phenylpropan-1-one(3p)



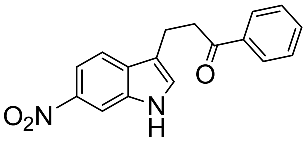
^{1}H NMR (400 MHz, DMSO) δ 11.23 (s, 1H), 8.27 (s, 1H), 8.00 (d, *J* = 7.3 Hz, 2H), 7.73 (dd, *J* = 8.6, 1.4 Hz, 1H), 7.62 (t, *J* = 7.3 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 2H), 7.42 (d, *J* = 8.6 Hz, 1H), 7.31 (d, *J* = 1.6 Hz, 1H), 3.84 (s, 3H), 3.43 (t, *J* = 7.4 Hz, 2H), 3.10 (t, *J* = 7.3 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 199.45, 167.32, 138.81, 136.67, 133.03, 128.64, 127.90, 126.67, 124.29, 121.98, 120.92, 119.78, 115.36, 111.27, 51.56, 38.66, 18.98

HRMS (TOF) m/z $[M + Na]^+$ Calcd for $C_{19}H_{17}NO_3$ 330.1101 found 330.1092.

17

3-(6-nitro-1*H*-indol-3-yl)-1-phenylpropan-1-one(3q)



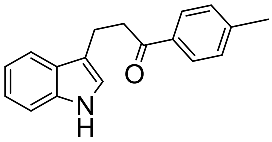
^{1}H NMR (400 MHz, DMSO) δ 11.61 (s, 1H), 8.30 (d, *J* = 7.6 Hz, 1H), 8.03 – 7.96 (m, 2H), 7.90 – 7.84 (m, 1H), 7.79-7.74 (m, 1H), 7.66-7.59 (m, 2H), 7.55 – 7.46 (m, 2H), 3.44 (m, 2H), 3.10 (t, *J* = 7.1 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 199.28, 141.78, 136.62, 134.48, 133.03, 131.75, 129.80, 128.61, 127.87, 118.59, 115.29, 113.42, 108.14, 38.52, 18.84

HRMS (TOF) m/z $[M + K]^+$ Calcd for $C_{17}H_{14}N_2O_3$ 333.0636 found 333.0618.

18

3-(1H-indol-3-yl)-1-(4-methylphenyl)propan-1-one(3r)



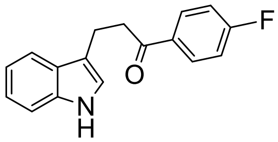
^{1}H NMR (400 MHz, DMSO) δ 10.77 (s, 1H), 7.90 (d, *J* = 8.2 Hz, 2H), 7.55 (d, *J* = 7.8 Hz, 1H), 7.35- 7.30 (m, 3H), 7.16 (d, *J* = 2.1 Hz, 1H), 7.10 – 7.04 (m, 1H), 7.01 – 6.95 (m, 1H), 3.37 (dd, *J* = 12.8, 5.0 Hz, 2H), 3.04 (t, *J* = 7.4 Hz, 2H), 2.36 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ 199.17, 143.30, 136.24, 134.27, 129.19, 128.01, 127.05, 122.33, 120.86, 118.27, 118.17, 113.65, 111.29, 38.56, 21.09, 19.42

HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{18}H_{17}NO$ 286.1202 found 286.1203.

19

3-(1H-indol-3-yl)-1-(4-fluorophenyl)propan-1-one(3s)



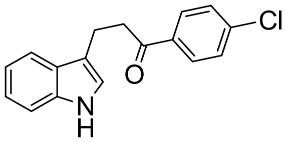
^{1}H NMR (400 MHz, DMSO) δ 10.79 (s, 1H), 8.07 (dd, *J* = 8.5, 5.7 Hz, 2H), 7.56 (d, *J* = 7.8 Hz, 1H), 7.37-7.28 (m, 3H), 7.17 (d, *J* = 1.4 Hz, 1H), 7.08 (t, *J* = 7.5 Hz, 1H), 6.98 (t, *J* = 7.4 Hz, 1H), 3.39 (t, *J* = 7.6 Hz, 2H), 3.06 (t, *J* = 7.4 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 198.24, 166.17, 163.67, 136.26, 133.45 (d, *J* = 2.7 Hz), 130.85 (d, *J* = 9.5 Hz), 127.05, 122.35, 120.89, 118.24 (d, *J* = 9.3 Hz), 115.69, 115.47, 113.56, 111.30, 38.65, 19.31

HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{17}H_{14}NOF$ 290.0952 found 290.0964 .

20

3-(1H-indol-3-yl)-1-(4-chlorophenyl)propan-1-one(3t)



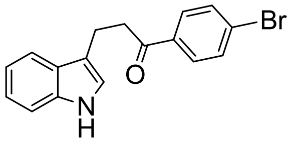
^{1}H NMR (400 MHz, DMSO) δ 10.77 (s, 1H), 8.03 – 7.98 (m, 2H), 7.61 – 7.52 (m, 3H), 7.33 (d, *J* = 8.1 Hz, 1H), 7.15 (d, *J* = 2.2 Hz, 1H), 7.09 – 7.03 (m, 1H), 7.00 – 6.94 (m, 1H), 3.41 (t, *J* = 7.5 Hz, 2H), 3.04 (t, *J* = 7.4 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 198.72, 137.92, 136.22, 135.37, 129.84, 128.76, 127.01, 122.36, 120.88, 118.22 (d, *J* = 10.8 Hz), 113.47, 111.28,38.70, 19.24.

HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{17}H_{14}NOCl$ 306.0656 found 306.0665.

21

3-(1H-indol-3-yl)-1-(4-bromophenyl)propan-1-one(3u)



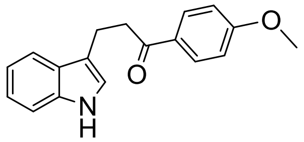
^{1}H NMR (400 MHz, DMSO) δ 10.77 (s, 1H), 7.92 (d, *J* = 8.3 Hz, 2H), 7.71 (d, *J* = 8.2 Hz, 2H), 7.55 (d, *J* = 7.8 Hz, 1H), 7.33 (d, *J* = 8.0 Hz, 1H), 7.16 (d, *J* = 1.6 Hz, 1H), 7.06 (t, *J* = 7.5 Hz, 1H), 6.97 (t, *J* = 7.4 Hz, 1H), 3.40 (t, *J* = 7.4 Hz, 2H), 3.04 (t, *J* = 7.4 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 198.88, 136.24, 135.69, 131.70, 129.94, 127.08, 127.02, 122.36, 120.88, 118.28, 118.18, 113.47, 111.29, 38.70, 19.24

HRMS (TOF) m/z $[M + H]^+$Calcd for $C_{17}H_{14}NOBr$ 328.0332 found 328.0301.

22

3-(1H-indol-3-yl)-1-(4-methoxyphenyl)propan-1-one(3v)



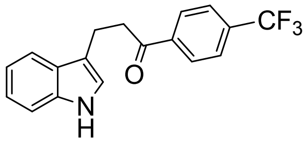
^{1}H NMR (400 MHz, DMSO) δ 10.78 (s, 1H), 7.98 (d, *J* = 8.8 Hz, 2H), 7.55 (d, *J* = 7.8 Hz, 1H), 7.34 (d, *J* = 8.0 Hz, 1H), 7.16 (d, *J* = 2.0 Hz, 1H), 7.09-6.96 (m, 4H), 3.83 (s, 3H), 3.35 (t, *J* = 7.6 Hz, 2H), 3.04 (t, *J* = 7.4 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 198.02, 162.98, 136.24, 130.19, 129.70, 127.06, 122.32, 120.86, 118.27, 118.17, 113.81, 113.73, 111.29, 55.45, 38.31, 19.53

HRMS (TOF) m/z $[M + Na]^+$ Calcd for $C_{18}H_{17}NO_2$ 302.1151 found 302.1181.

23

3-(1H-indol-3-yl)-1-(4-(trifluoromethyl)phenyl)propan-1-one(3w)



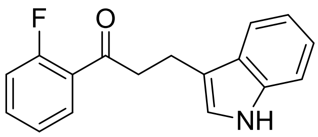
^{1}H NMR (400 MHz, DMSO) δ 10.79 (s, 1H), 8.17 (d, *J* = 8.1 Hz, 2H), 7.87 (d, *J* = 8.2 Hz, 2H), 7.57 (d, *J* = 7.8 Hz, 1H), 7.34 (d, *J* = 8.1 Hz, 1H), 7.17 (d, *J* = 2.2 Hz, 1H), 7.11 – 7.03 (m, 1H), 7.02 – 6.94 (m, 1H), 3.48 (t, *J* = 7.5 Hz, 2H), 3.07 (t, *J* = 7.4 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 199.13, 139.83, 136.25, 132.54, 132.22, 128.70, 127.01, 125.62 (d, *J* = 3.7 Hz), 125.13, 122.37, 120.89, 118.29, 118.18, 113.38, 111.29, 19.14.

HRMS (TOF) m/z $[M - H]^-$ Calcd for $C_{18}H_{14}NOF_3$ 316.0955 found 316.0969.

24

3-(1H-indol-3-yl)-1-(2-fluorophenyl)propan-1-one(3y)

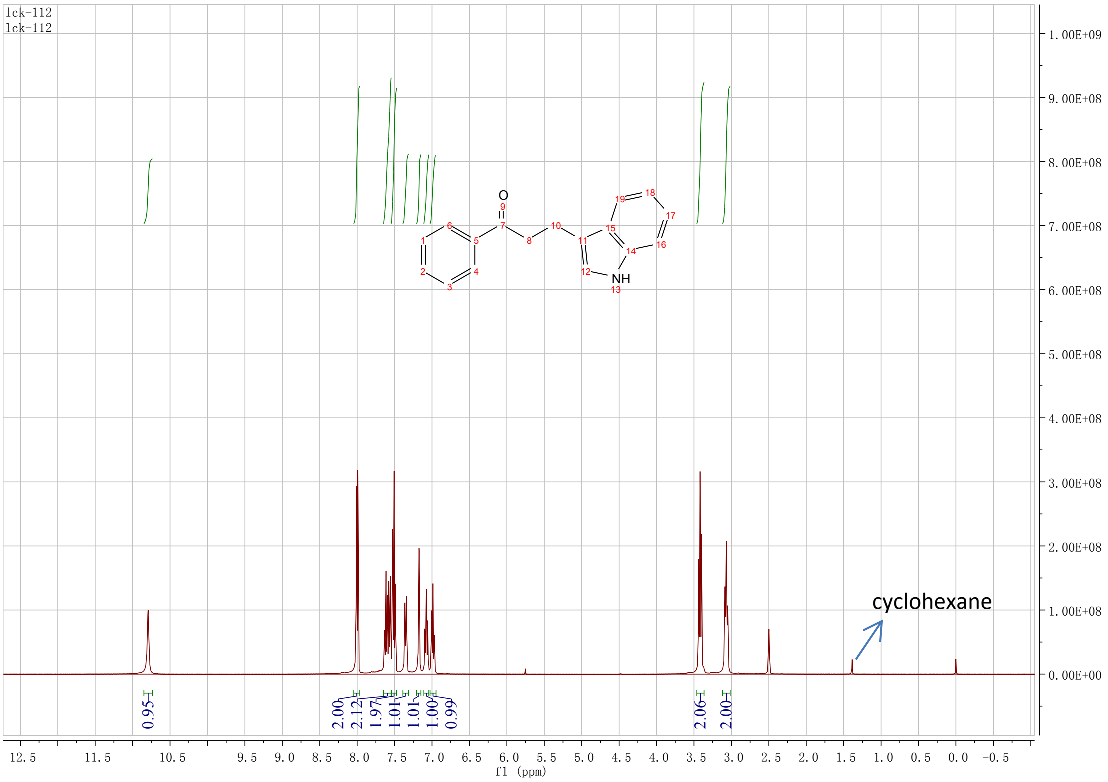


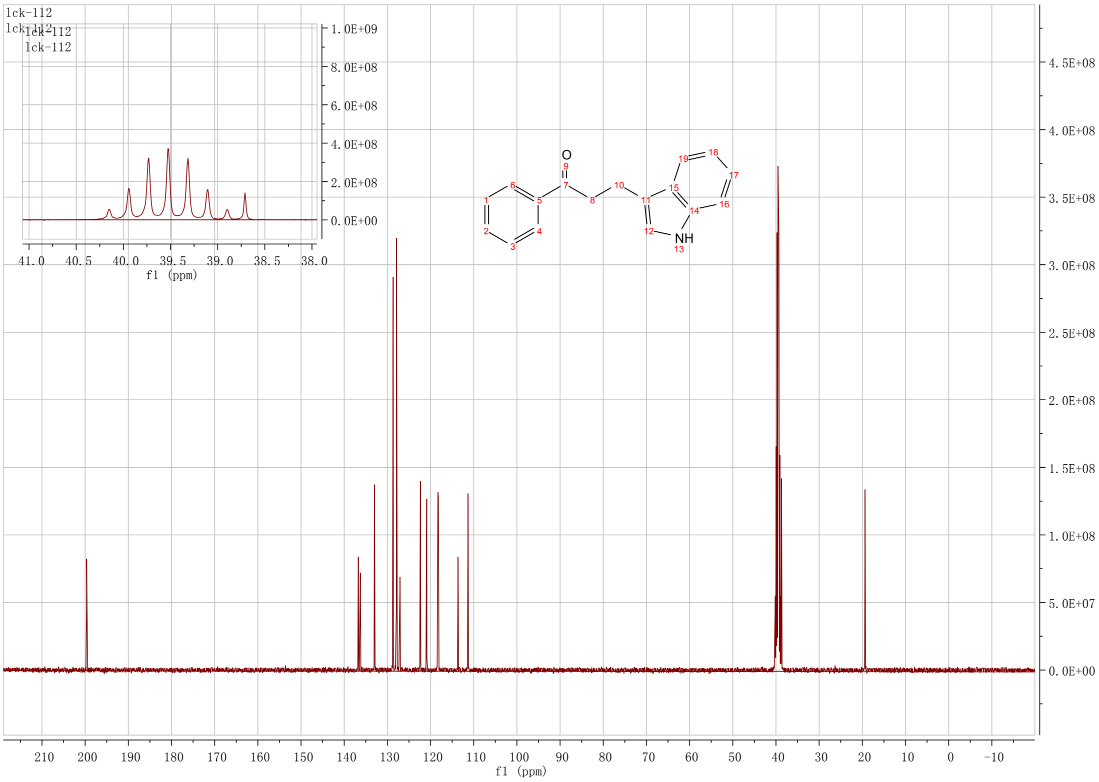
^{1}H NMR (400 MHz, DMSO) δ 10.79 (s, 1H), 7.83 (td, *J* = 7.7, 1.7 Hz, 1H), 7.67 – 7.61 (m, 1H), 7.54 (d, *J* = 7.8 Hz, 1H), 7.36-7.30 (m, 3H), 7.12 (d, *J* = 1.8 Hz, 1H), 7.07 (t, *J* = 7.5 Hz, 1H), 6.97 (t, *J* = 7.4 Hz, 1H), 3.35 (td, *J* = 7.6, 2.4 Hz, 2H), 3.05 (t, *J* = 7.4 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 197.81 (d, *J* = 3.4 Hz), 162.16, 159.64, 136.24, 134.78 (d, *J* = 9.1 Hz), 130.20 (d, *J* = 2.4 Hz), 126.96, 125.61, 125.48, 124.75 (d, *J* = 3.2 Hz), 122.31, 120.89, 118.20 (d, *J* = 1.4 Hz), 116.91, 116.68, 113.36, 111.32, 43.36 (d, *J* = 5.7 Hz), 19.19.

HRMS (TOF) m/z [M + Na]$^{+}$ Calcd for $C_{17}H_{14}NOF$ 290.0952 found 290.0948 .

Ⅵ, ^{1}H NMR and ^{13}C NMR spectra of compounds 3

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lck-112
lck-112
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4.0E+08
2.0E+08
0.0E+00
41.0 40.5 40.0 39.5 39.0 38.5 38.0
f1 (ppm)
O
NH
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
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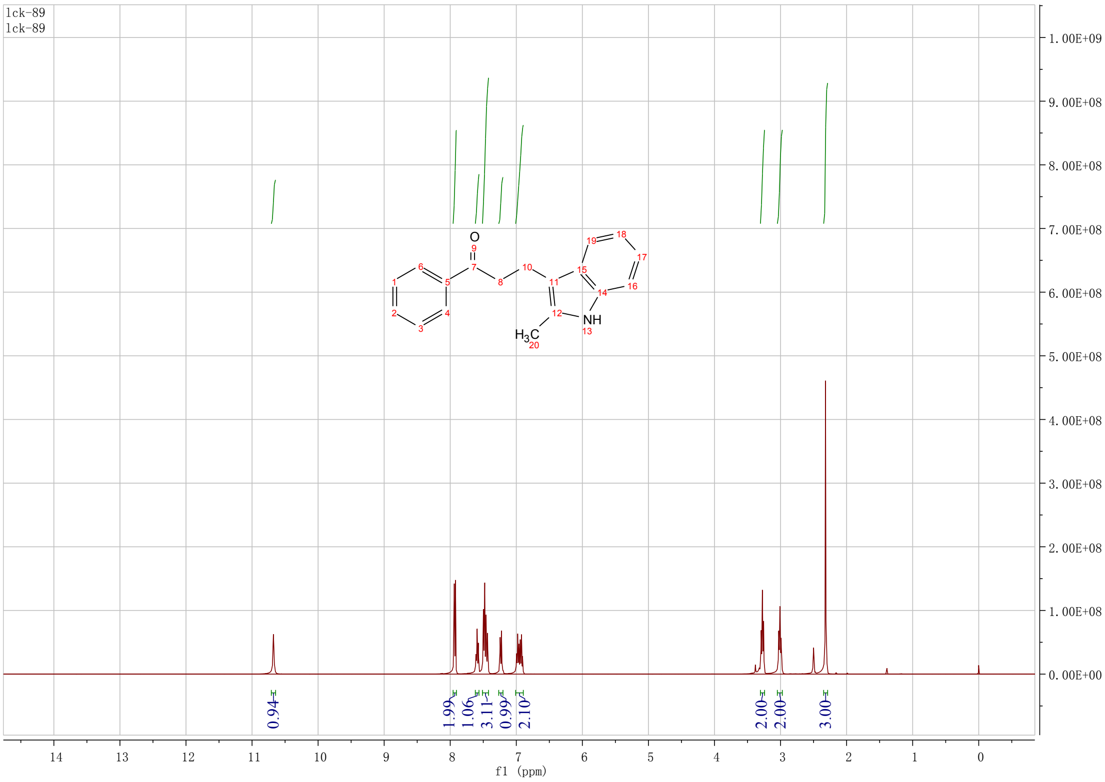
f1 (ppm)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lck-89
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6.00E+08
5.00E+08
4.00E+08
3.00E+08
2.00E+08
1.00E+08
0.00E+00
0.94
1.99
1.06
3.11
0.99
2.10
2.00
2.00
3.00
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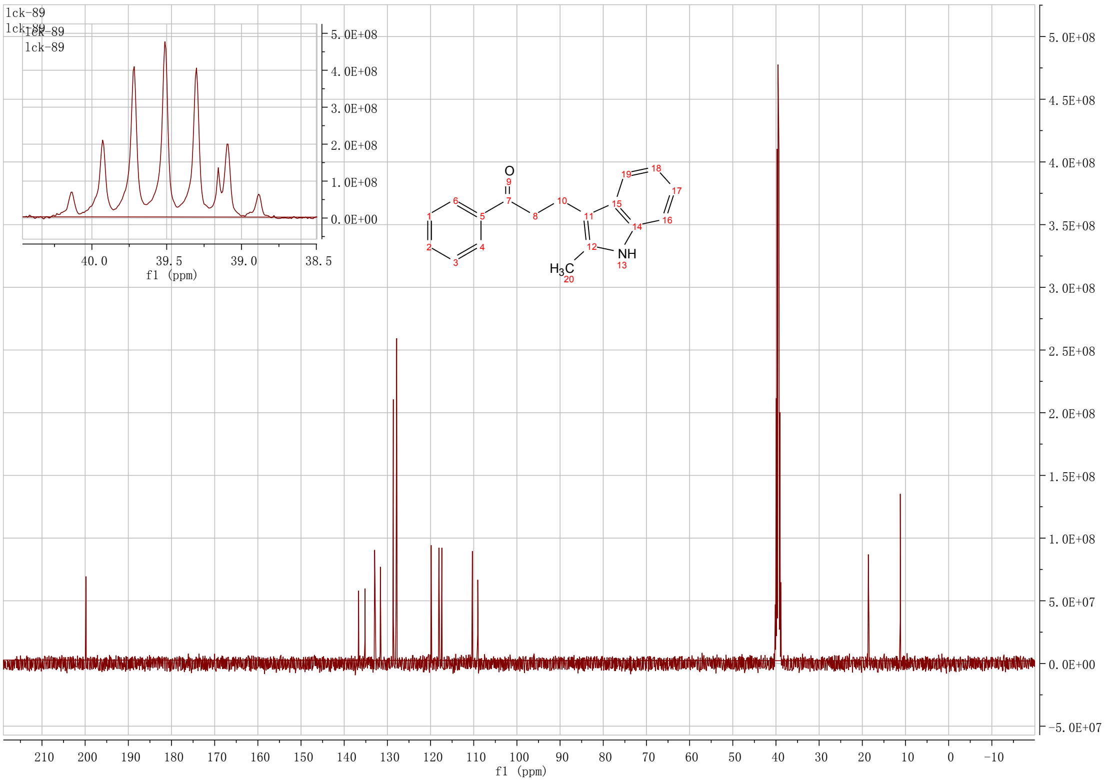
f1 (ppm)


lck-89
lck-89
lck-89
f1 (ppm)
f1 (ppm)
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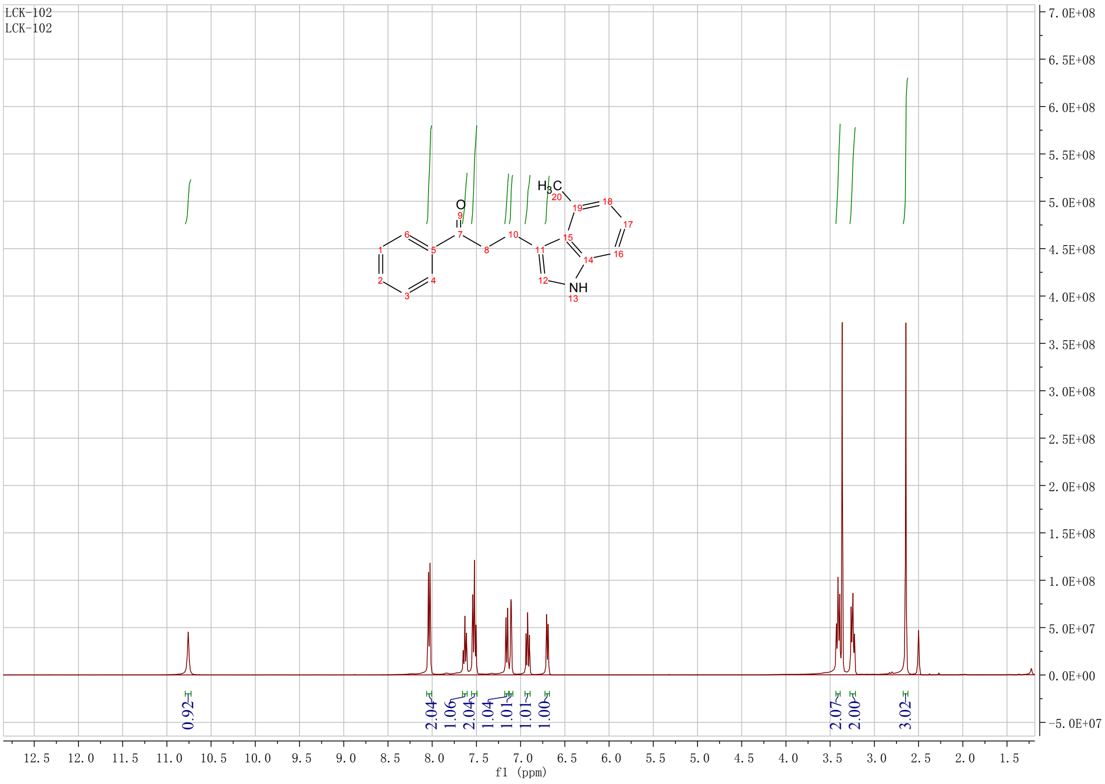
H3C
NH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LCK-102
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1.06
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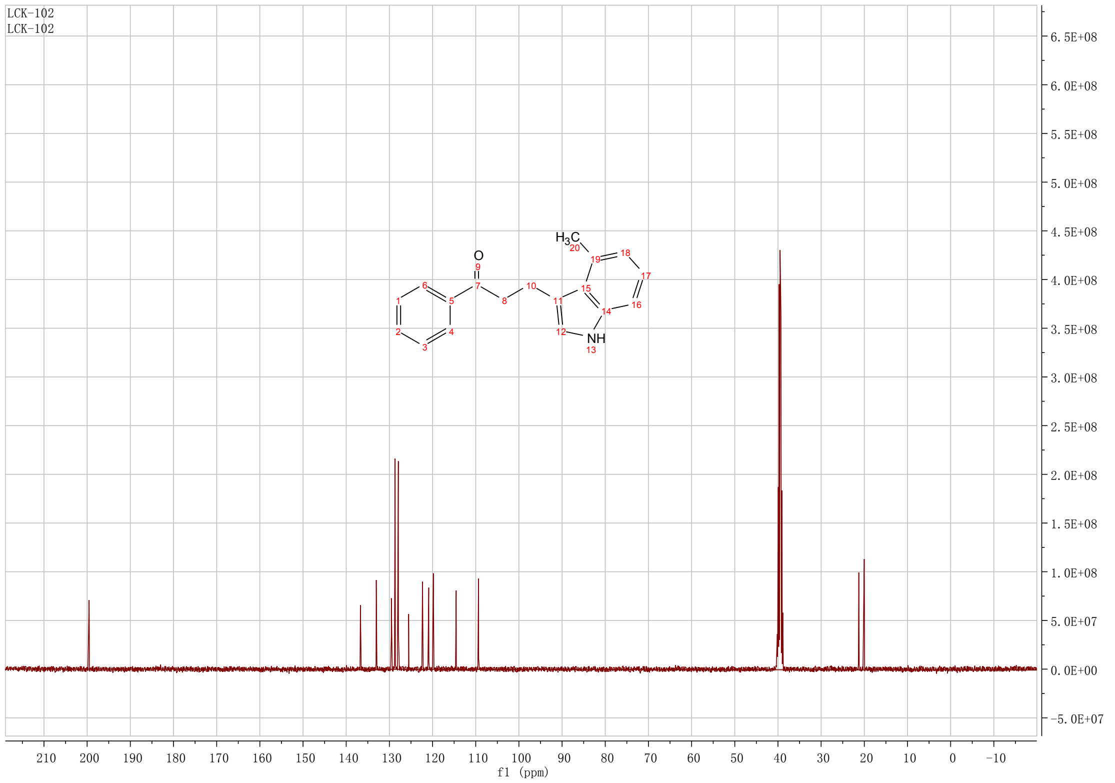
1.01
1.01
1.00
2.07
2.00
3.02
f1 (ppm)
O
H3C
NH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LCK-102
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7
8
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12
NH
13
14
15
16
17
18
19
20
H_3C
1
2
3
4
5
6
6.5E+08
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
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0.0E+00
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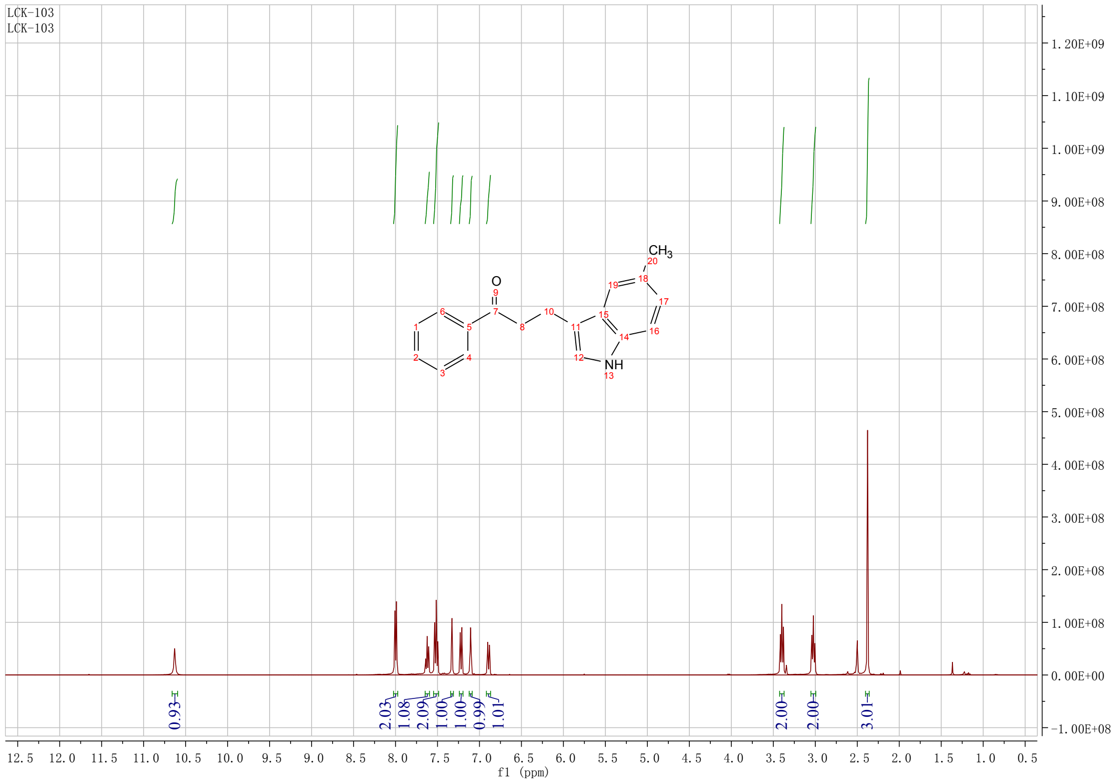
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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LCK-103
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20
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9
7
8
10
11
12
NH
13
14
15
16
17
18
19
1
2
3
4
5
6
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1.10E+09
1.00E+09
9.00E+08
8.00E+08
7.00E+08
6.00E+08
5.00E+08
4.00E+08
3.00E+08
2.00E+08
1.00E+08
0.00E+00
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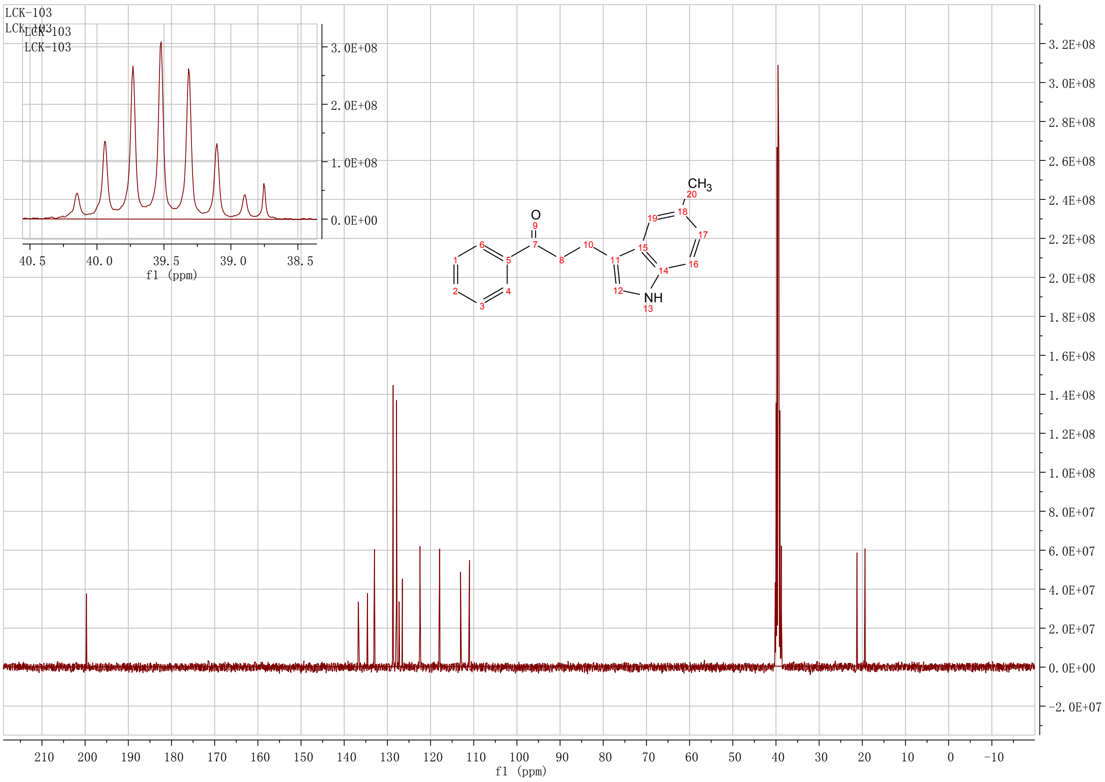
0.93
2.03
1.08
2.09
1.00
1.00
0.99
1.01
2.00
2.00
3.01
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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LCK-103
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39.5
39.0
38.5
f1 (ppm)
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CH3
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
NH
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3.0E+08
2.8E+08
2.6E+08
2.4E+08
2.2E+08
2.0E+08
1.8E+08
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1.4E+08
1.2E+08
1.0E+08
8.0E+07
6.0E+07
4.0E+07
2.0E+07
0.0E+00
-2.0E+07
210
200
190
180
170
160
150
140
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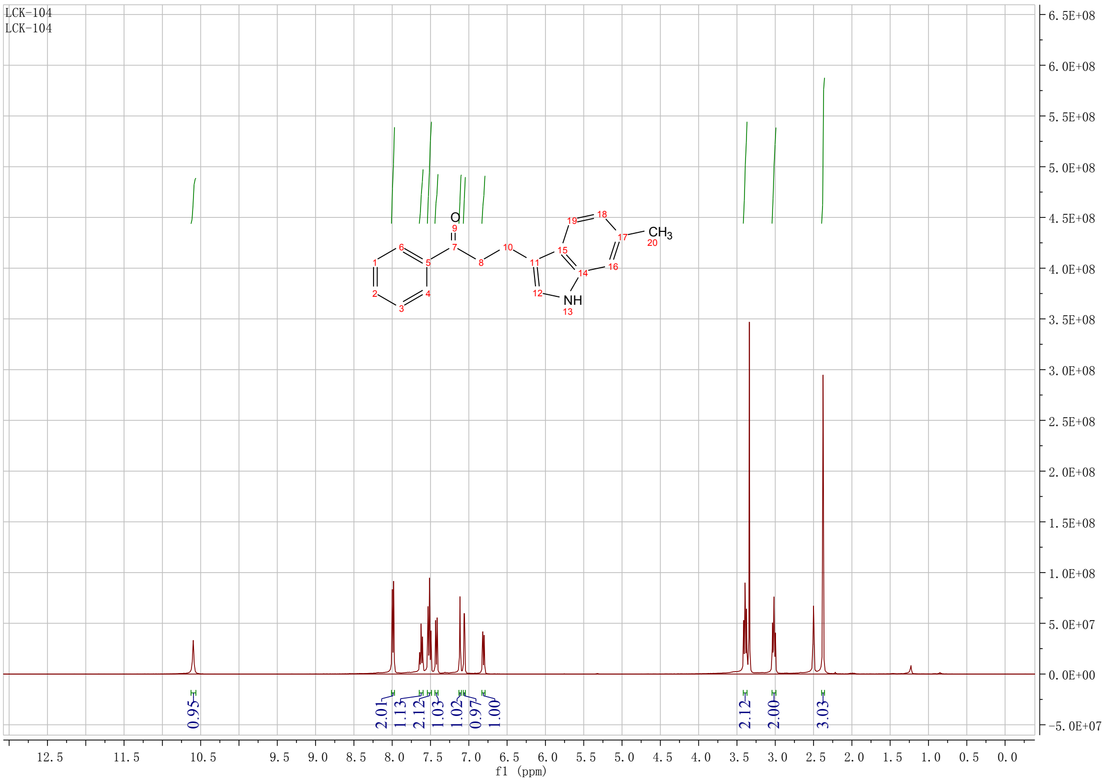
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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LCK-104
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4
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6
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8
9
10
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12
13
14
15
16
17
18
19
20
NH
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2.12
1.03
1.02
0.97
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2.12
2.00
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5.5E+08
5.0E+08
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4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.0
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2.0
1.5
1.0
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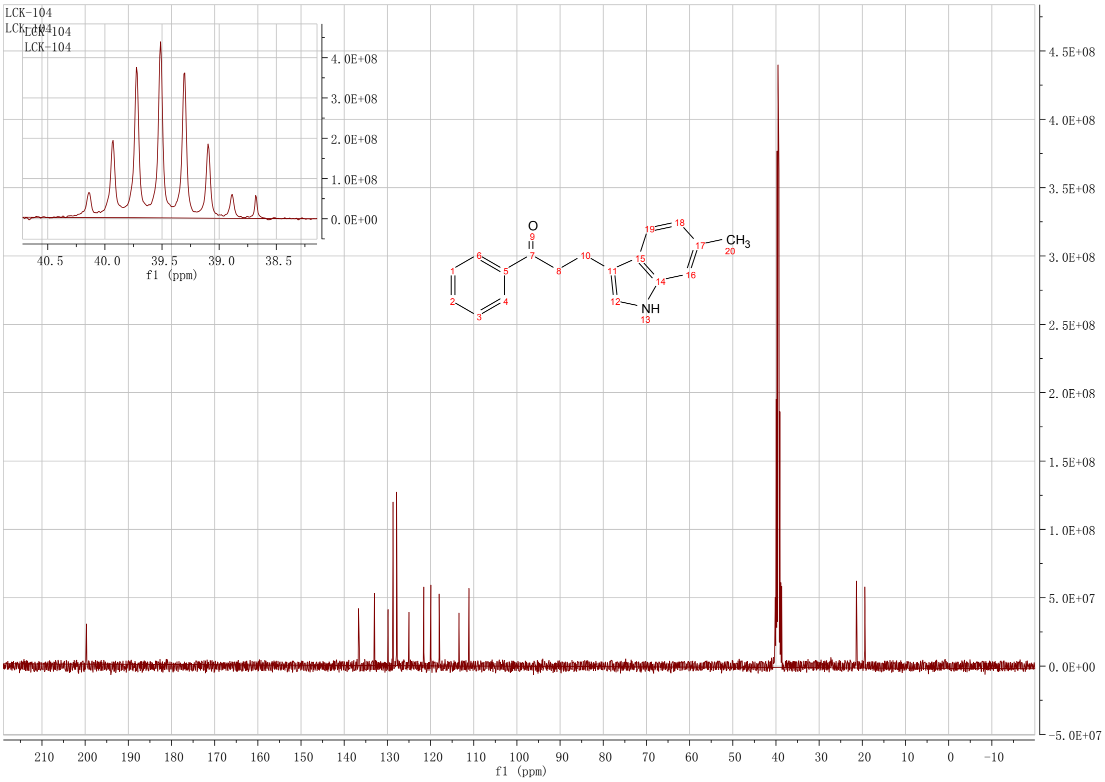
0.0
f1 (ppm)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LCK-104
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40.5
40.0
39.5
39.0
38.5
f1 (ppm)
O
9
7
5
6
1
2
3
4
8
10
11
12
NH
13
14
15
16
17
18
19
CH3
20
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3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
210
200
190
180
170
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120
110
100
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40
30
20
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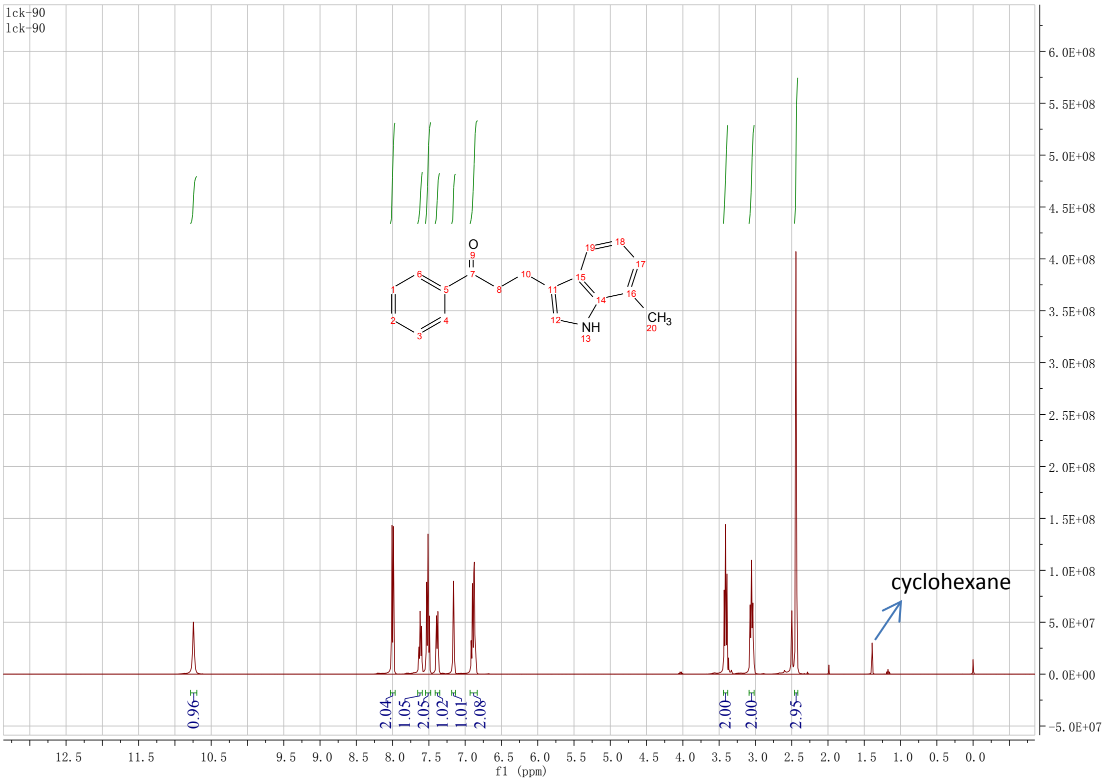
0
-10
f1 (ppm)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9
7
5
6
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2
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4
8
10
11
12
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13
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15
16
17
18
19
CH3
20
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0.96
2.04
1.05
2.05
1.02
1.01
2.08
2.00
2.00
2.95
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5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
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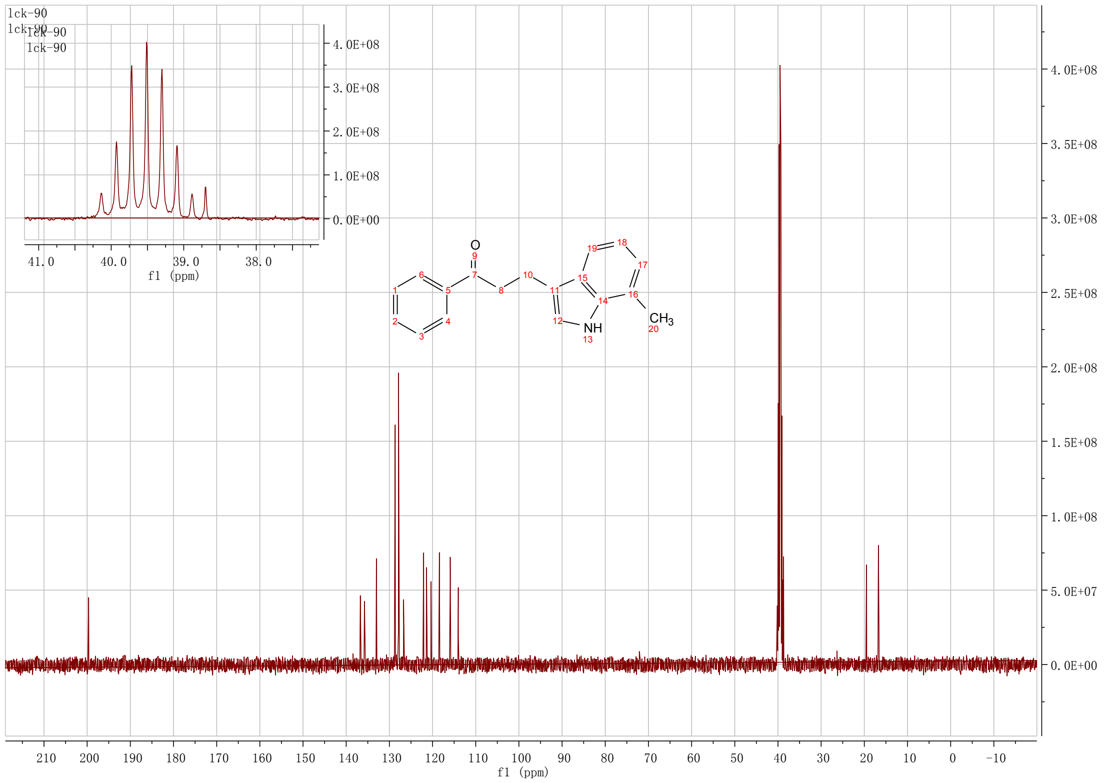
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


lck-90
lck-90
lck-90
lck-90
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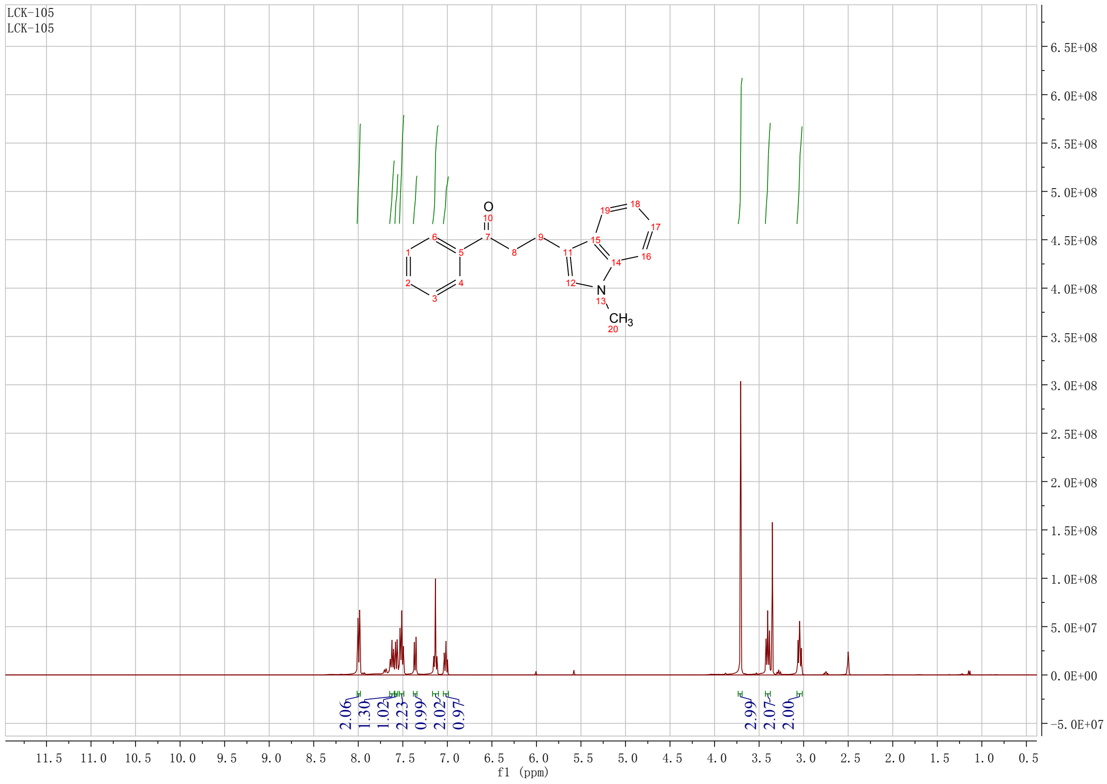
3.0E+08
2.0E+08
1.0E+08
0.0E+00
41.0
40.0
39.0
38.0
f1 (ppm)
O
CH3
NH
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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N
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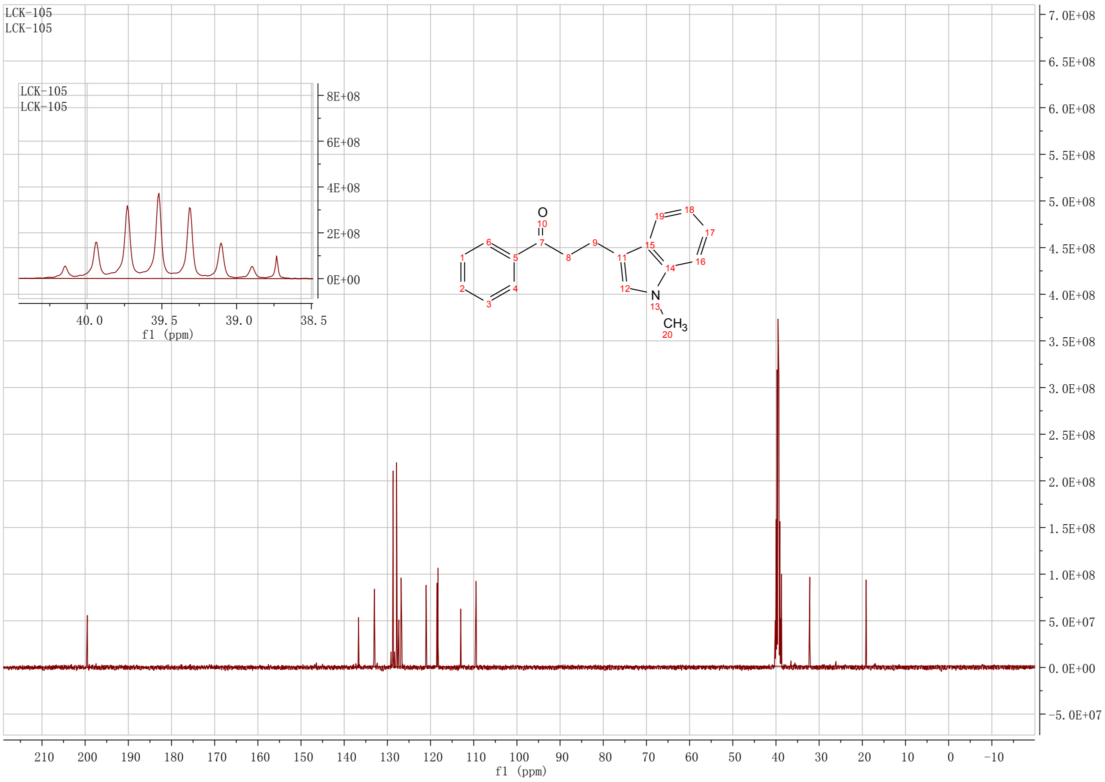
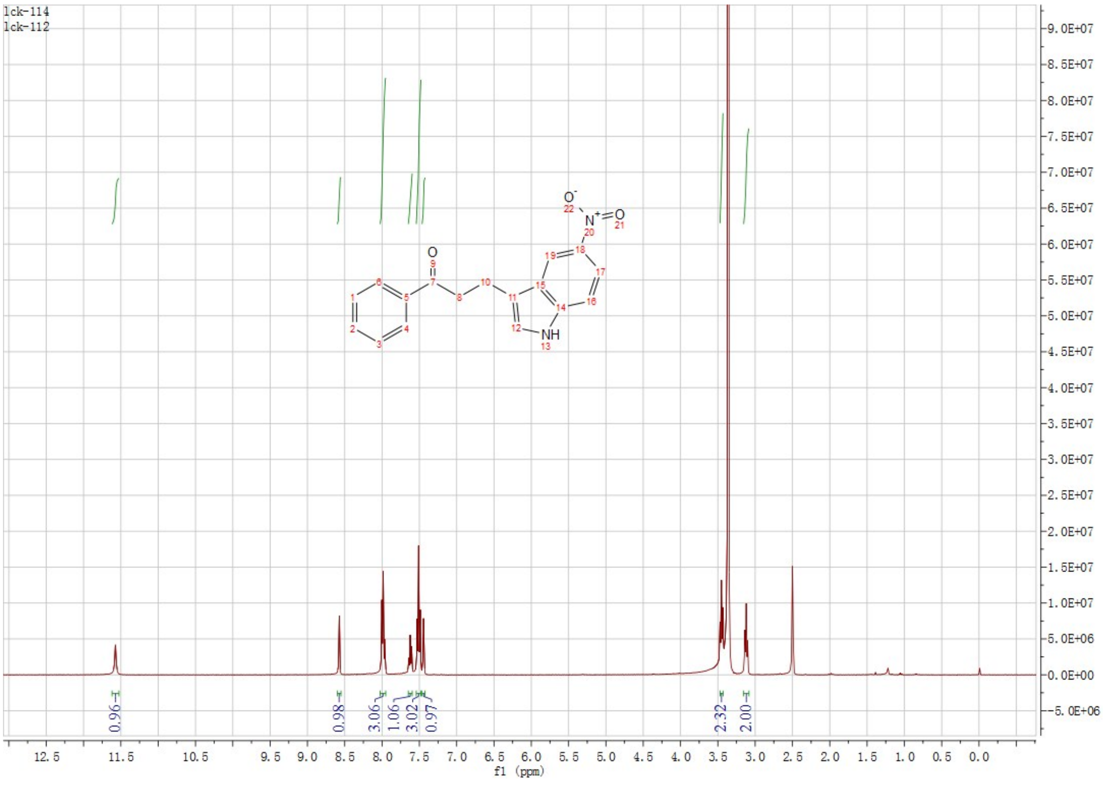
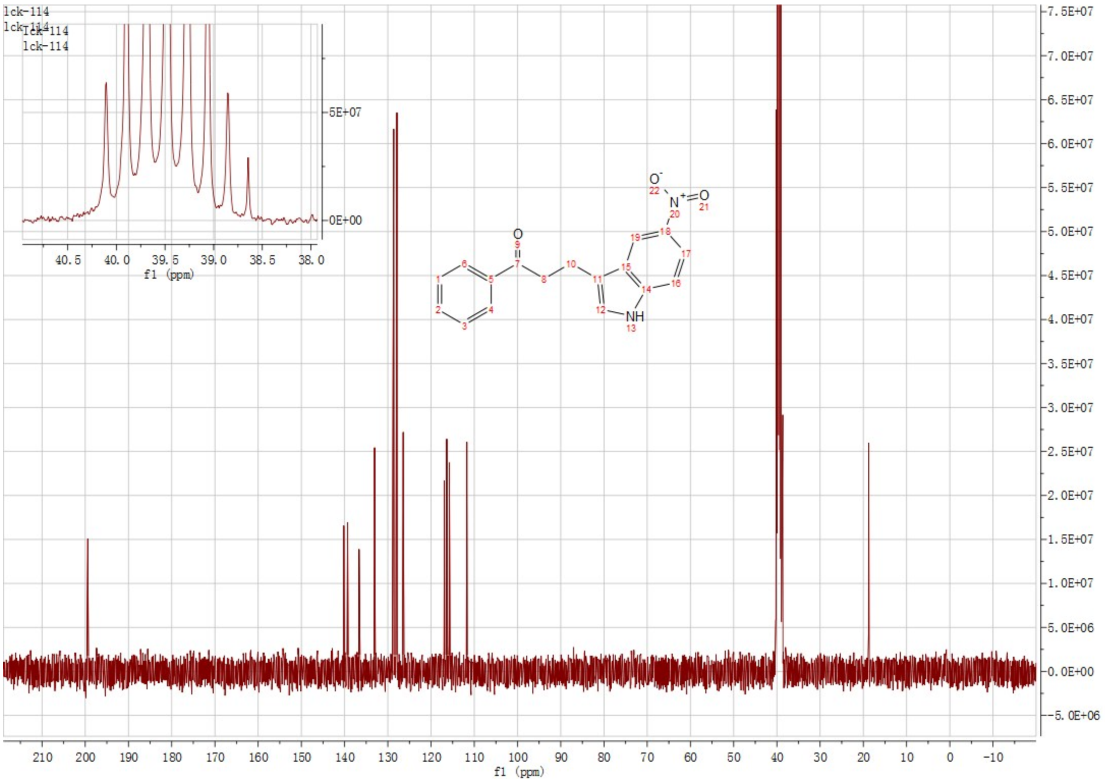
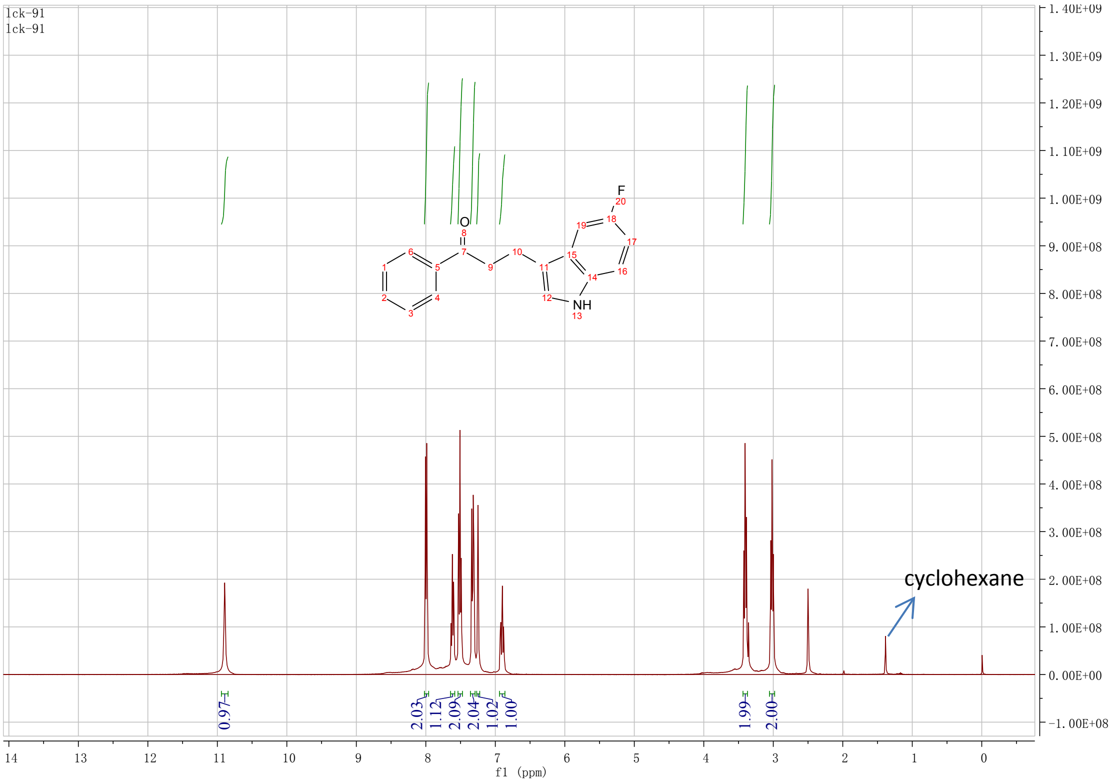
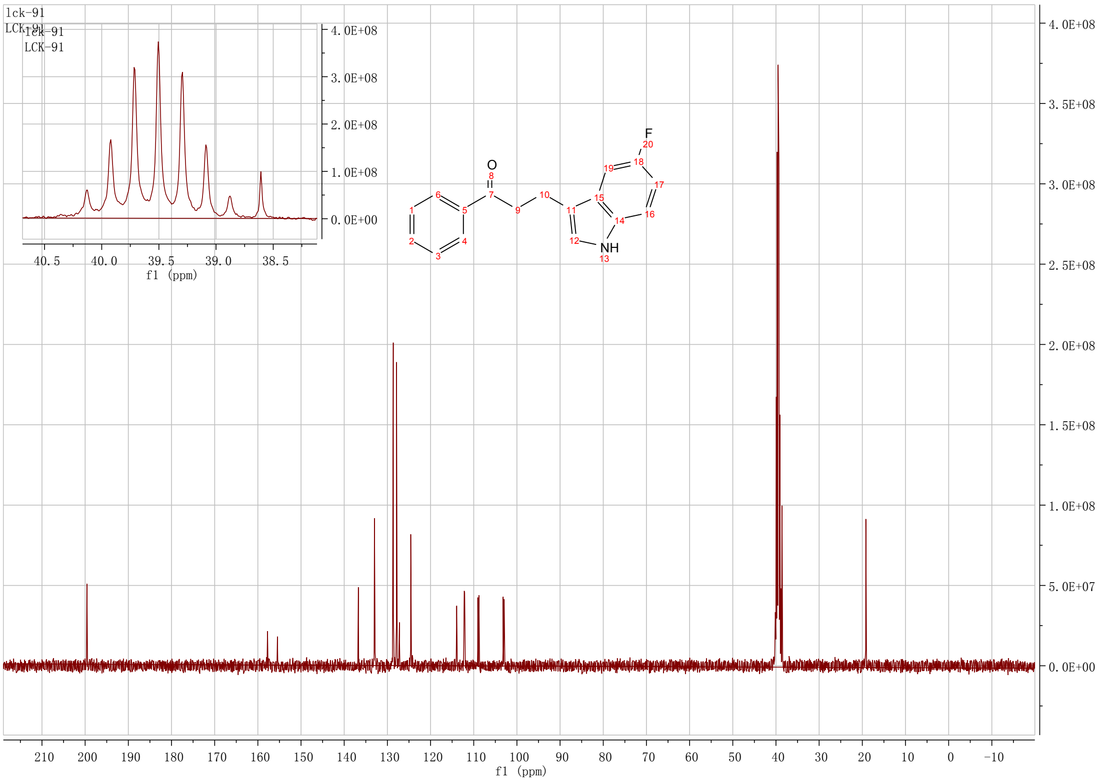
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
2.06
1.30
1.02
2.23
0.99
2.02
0.97
2.99
2.07
2.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

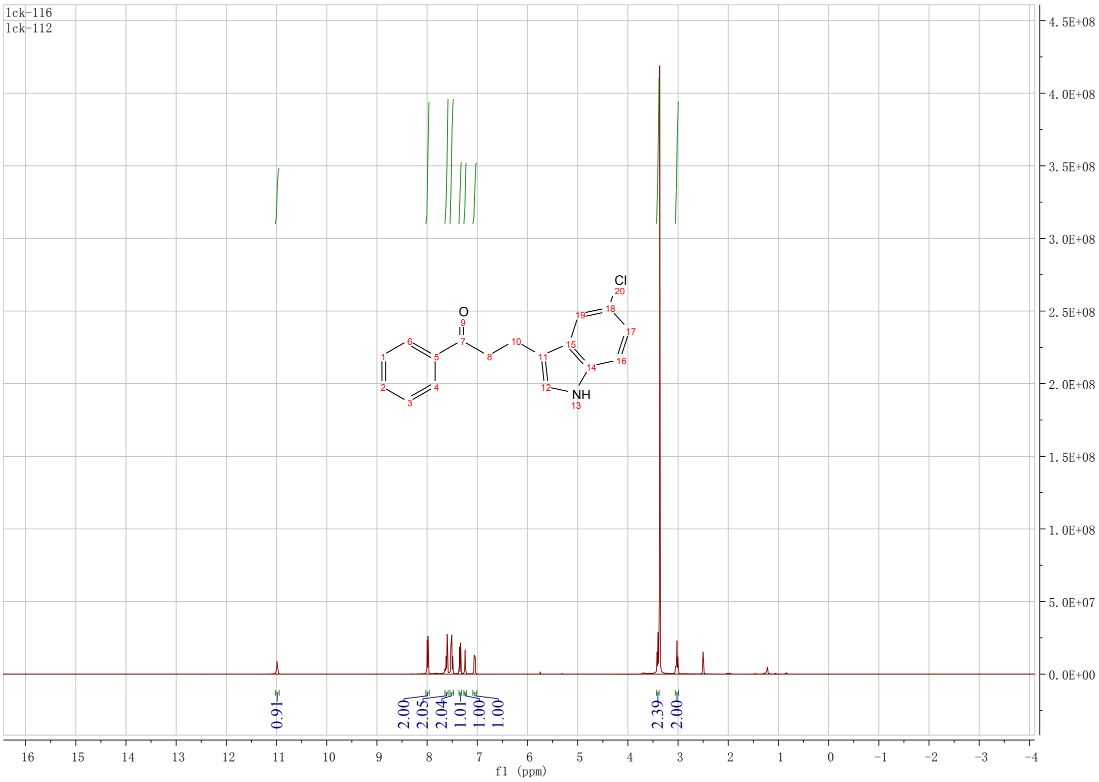

LCK-105
LCK-105
LCK-105
LCK-105
8E+08
6E+08
4E+08
2E+08
0E+00
40.0
39.5
39.0
38.5
f1 (ppm)
O
10
7
6
5
4
3
2
1
8
9
11
12
13
N
CH3
20
14
15
16
17
18
19
7.0E+08
6.5E+08
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
−5.0E+07
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

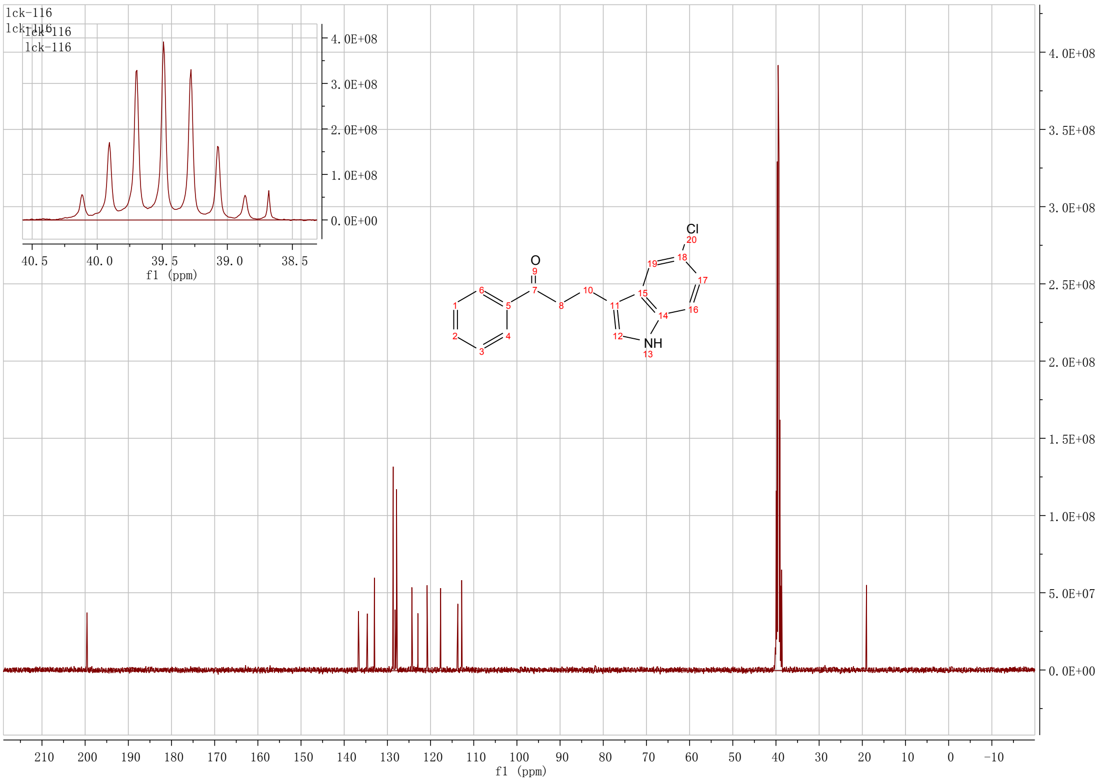

lck-114
lck-112
O
22
N+
21
20
18
19
17
16
15
14
O
9
7
6
5
4
3
2
1
8
10
11
12
NH
13
9.0E+07
8.5E+07
8.0E+07
7.5E+07
7.0E+07
6.5E+07
6.0E+07
5.5E+07
5.0E+07
4.5E+07
4.0E+07
3.5E+07
3.0E+07
2.5E+07
2.0E+07
1.5E+07
1.0E+07
5.0E+06
0.0E+00
−5.0E+06
0.96
0.98
3.06
1.06
3.02
0.97
2.32
2.00
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

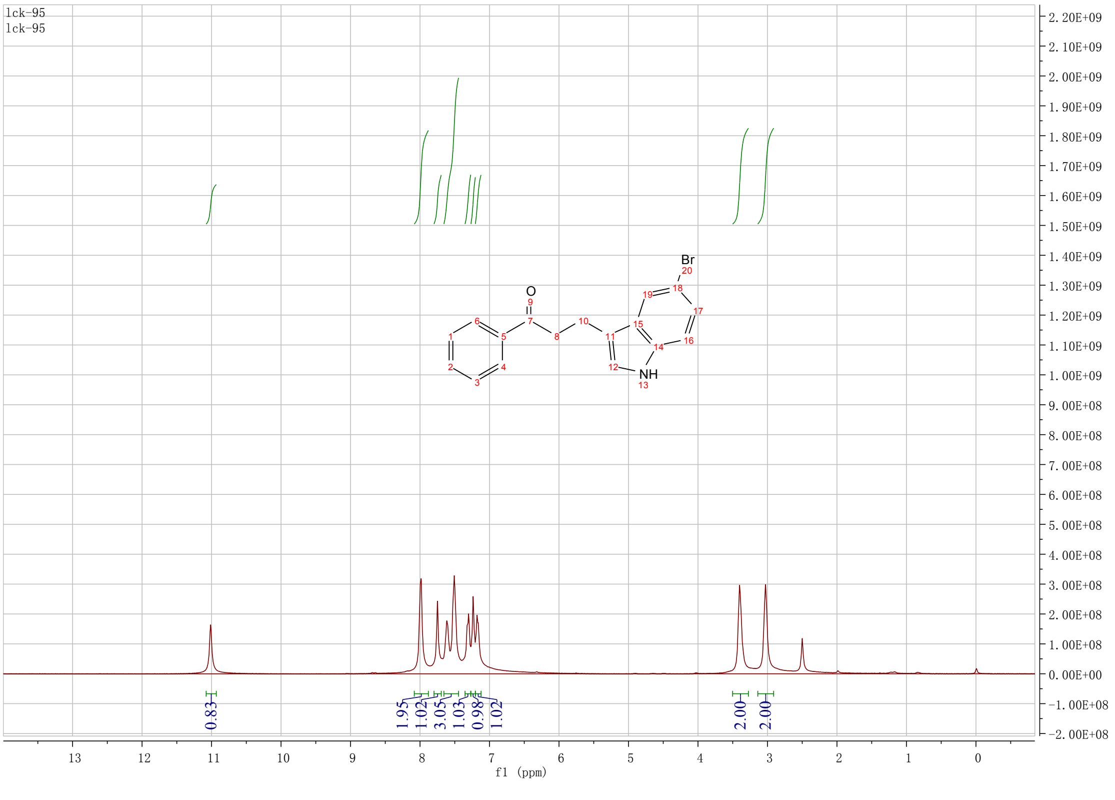

lck-114
lck-114
lck-114
lck-114
5E+07
0E+00
40.5
40.0
39.5
39.0
38.5
38.0
f1 (ppm)
O-
22
N+
20
O
21
19
18
17
16
15
14
11
12
NH
13
10
8
7
O
9
6
5
4
3
2
1
7.5E+07
7.0E+07
6.5E+07
6.0E+07
5.5E+07
5.0E+07
4.5E+07
4.0E+07
3.5E+07
3.0E+07
2.5E+07
2.0E+07
1.5E+07
1.0E+07
5.0E+06
0.0E+00
-5.0E+06
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

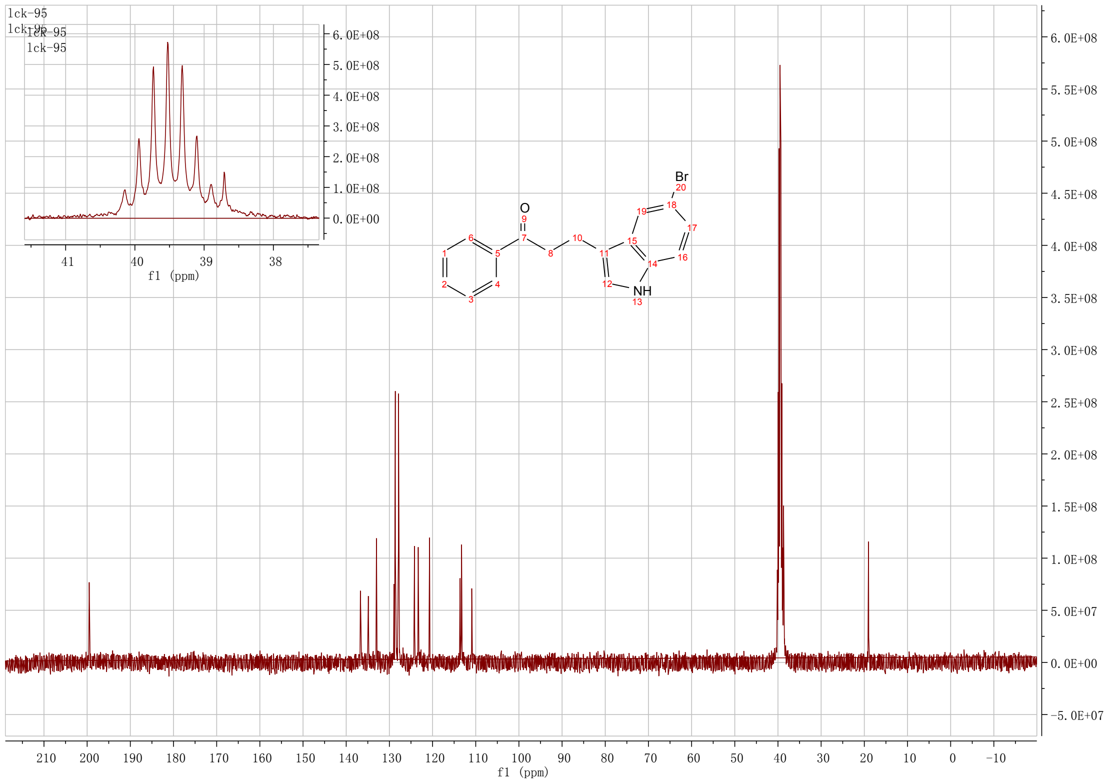

lck-91
lck-91
F
20
19
18
17
16
15
14
11
12
NH
13
10
9
7
O
8
6
5
4
3
2
1
cyclohexane
0.97
2.03
1.12
2.09
2.04
1.02
1.00
1.99
2.00
1.40E+09
1.30E+09
1.20E+09
1.10E+09
1.00E+09
9.00E+08
8.00E+08
7.00E+08
6.00E+08
5.00E+08
4.00E+08
3.00E+08
2.00E+08
1.00E+08
0.00E+00
-1.00E+08
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

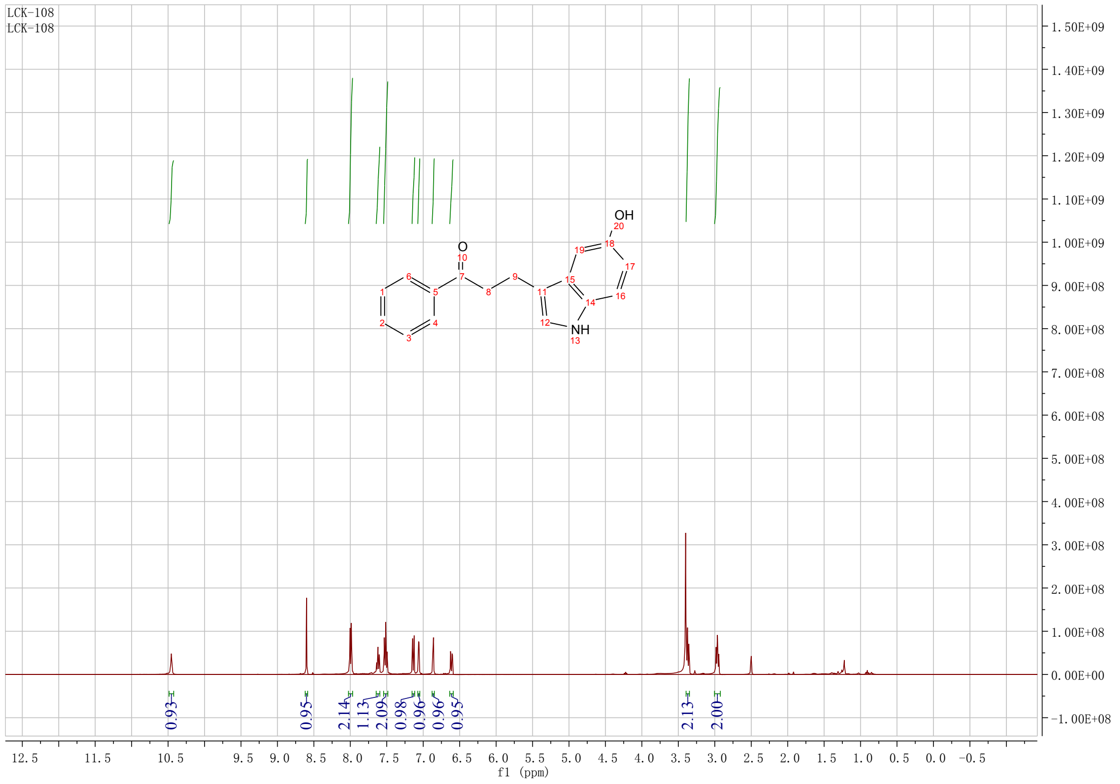

lck-91
LCK-91
lck-91
LCK-91
4.0E+08
3.0E+08
2.0E+08
1.0E+08
0.0E+00
40.5
40.0
39.5
39.0
38.5
f1 (ppm)
O
F
NH
3.5E+08
2.5E+08
1.5E+08
5.0E+07
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

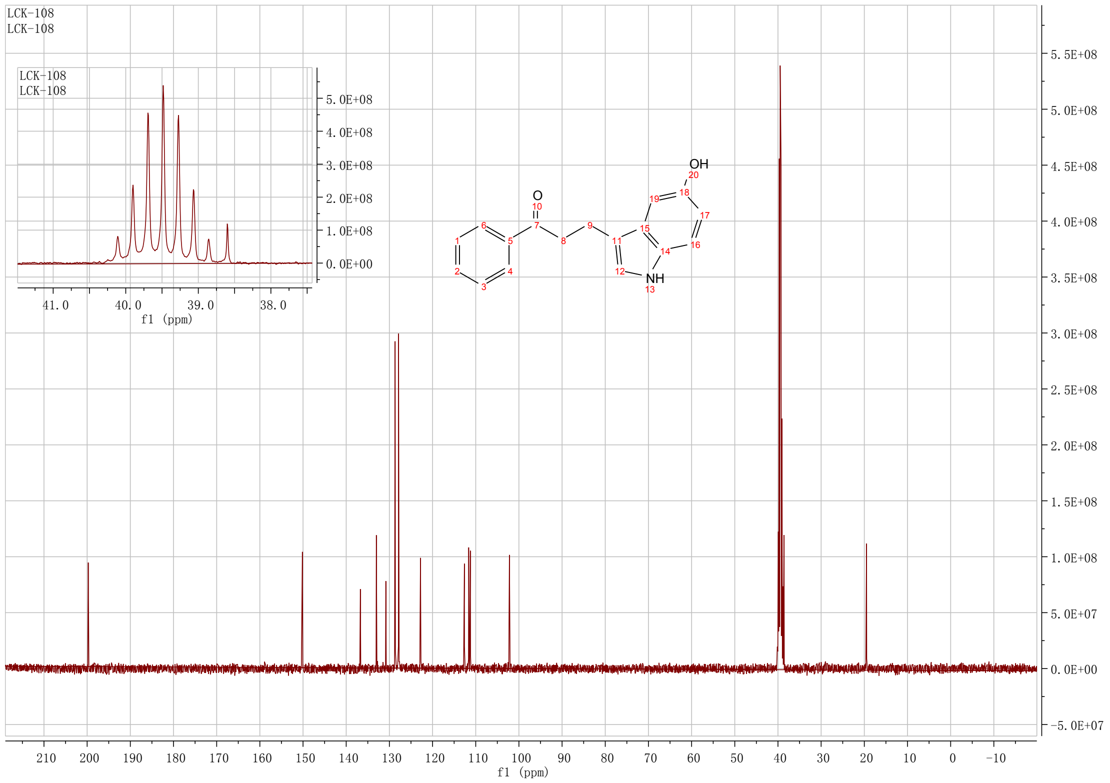

lck-116
lck-112
Cl
O
NH
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
0.91
2.00
2.05
2.04
1.01
1.00
1.00
2.39
2.00
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)

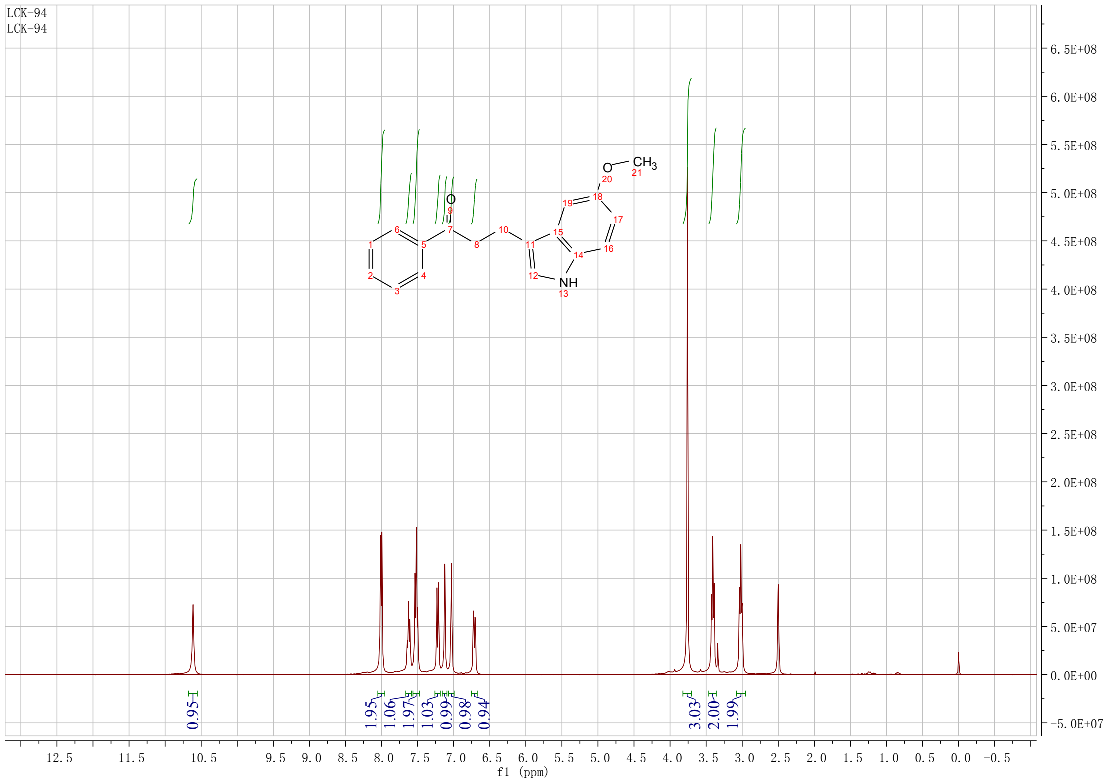

lck-116
lck-116
lck-116
lck-116
Cl
f1 (ppm)
f1 (ppm)

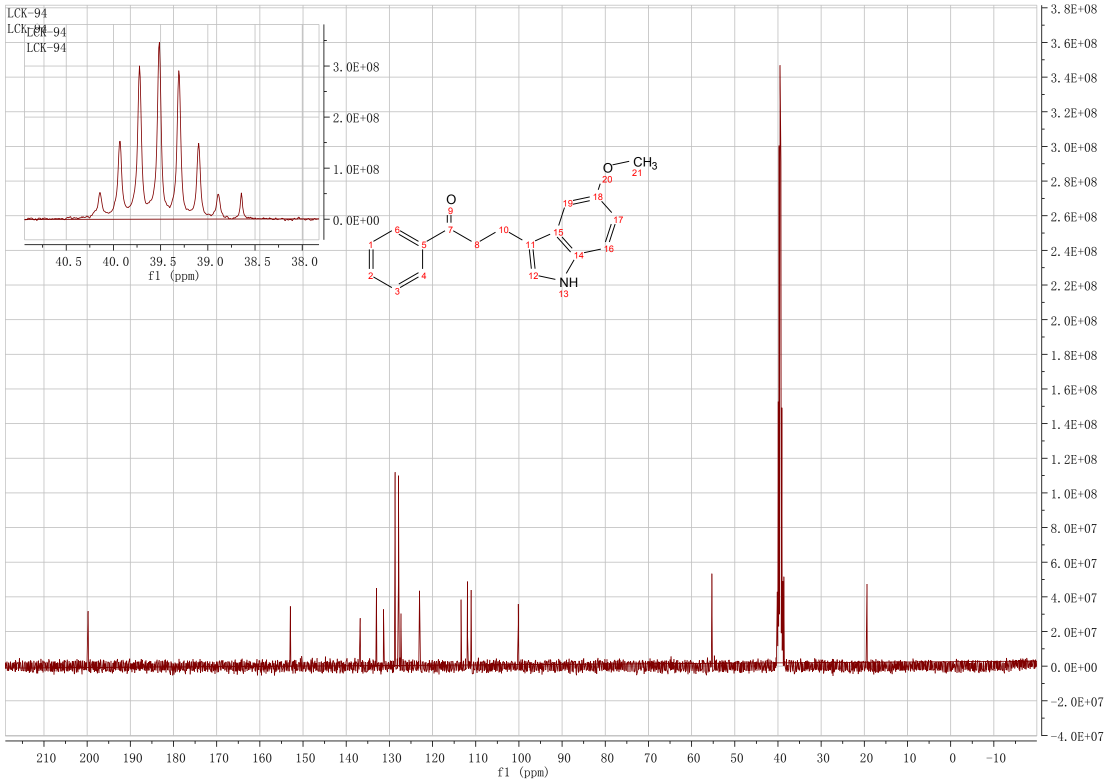

lck-95
lck-95
Br
0.83
1.95
1.02
3.05
1.03
0.98
1.02
2.00
2.00
f1 (ppm)

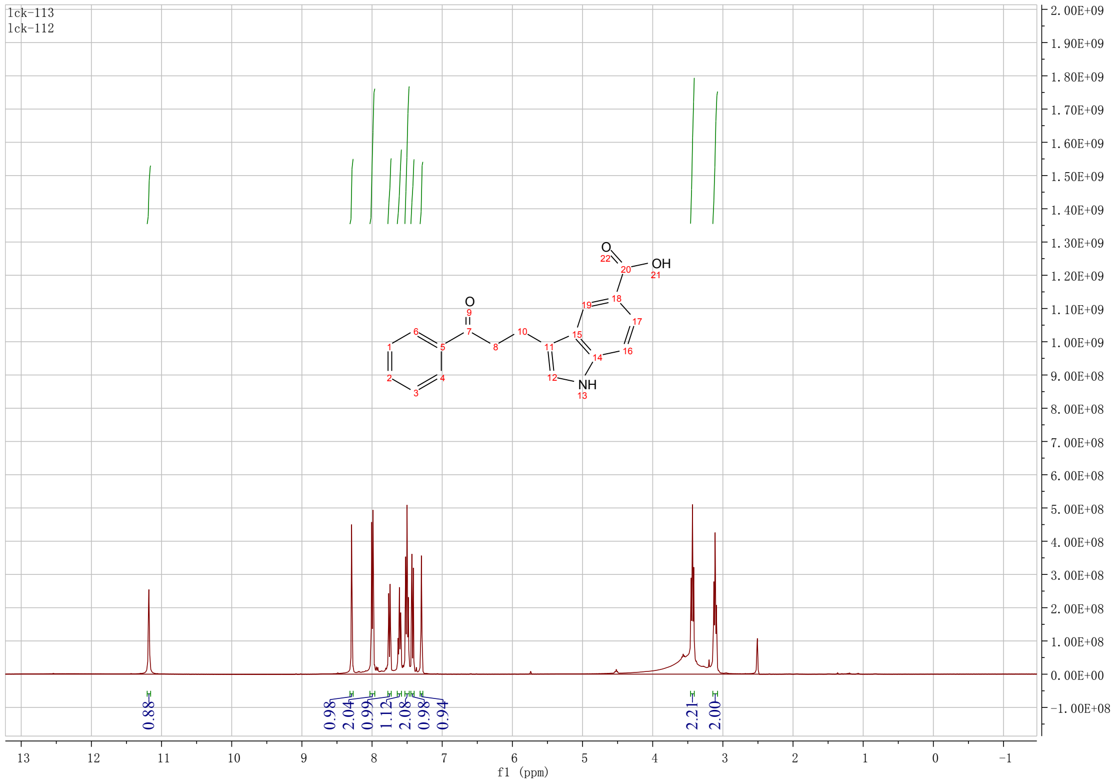

lck-95
lck-95
lck-95
41
40
39
38
f1 (ppm)
6.0E+08
5.0E+08
4.0E+08
3.0E+08
2.0E+08
1.0E+08
0.0E+00
O
Br
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07

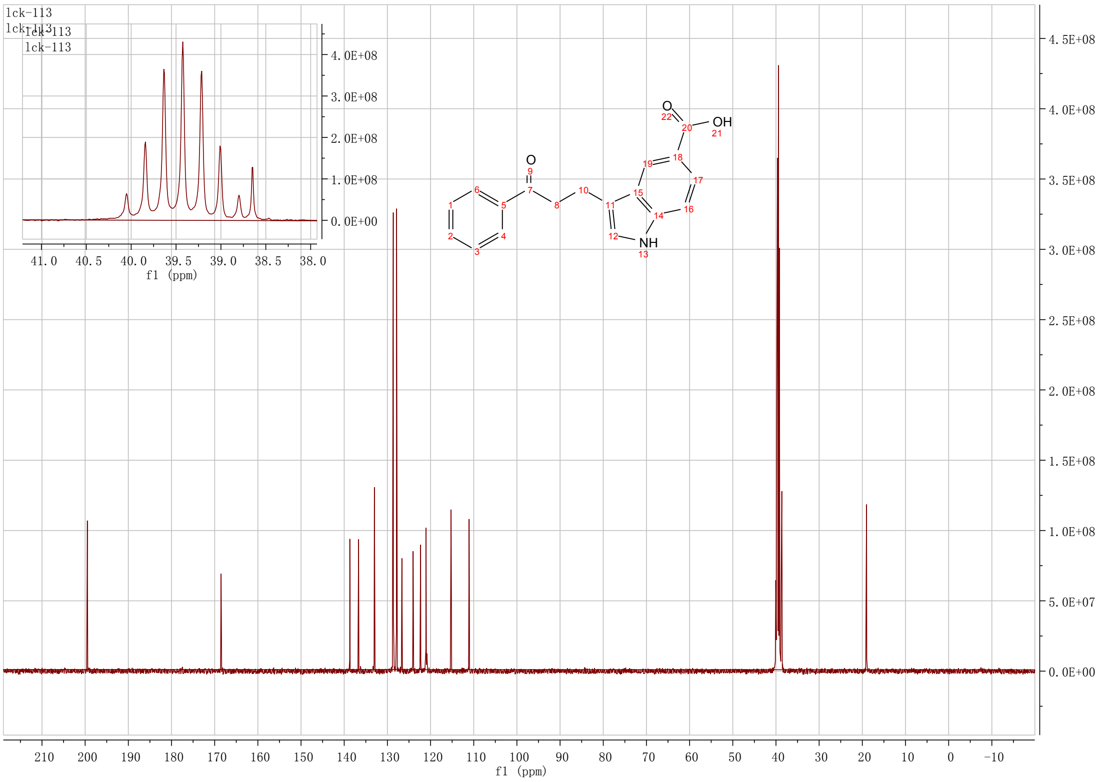

LCK-108
LCK-108
OH
O
NH
0.93
0.95
2.14
1.13
2.09
0.98
0.96
0.96
0.95
2.13
2.00
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)
1.50E+09
1.40E+09
1.30E+09
1.20E+09
1.10E+09
1.00E+09
9.00E+08
8.00E+08
7.00E+08
6.00E+08
5.00E+08
4.00E+08
3.00E+08
2.00E+08
1.00E+08
0.00E+00
-1.00E+08

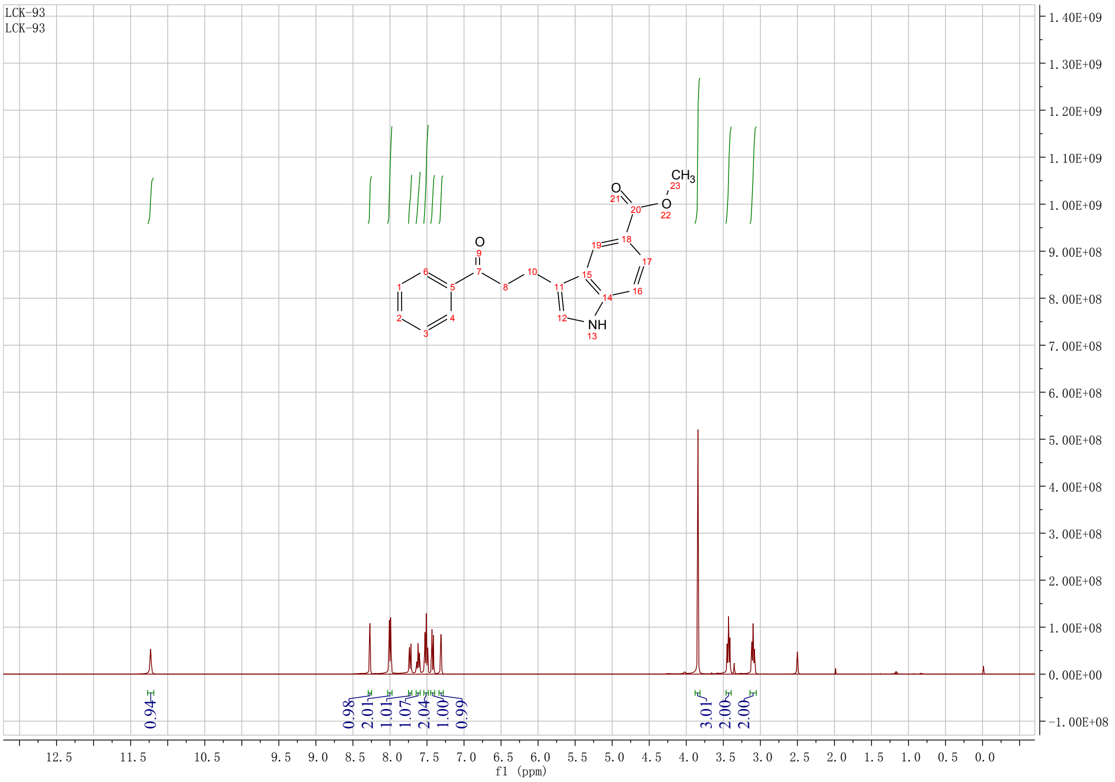

LCK-108
LCK-108
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
5.5E+08 5.0E+08 4.5E+08 4.0E+08 3.5E+08 3.0E+08 2.5E+08 2.0E+08 1.5E+08 1.0E+08 5.0E+07 0.0E+00 -5.0E+07
41.0 40.0 39.0 38.0
5.0E+08 4.0E+08 3.0E+08 2.0E+08 1.0E+08 0.0E+00
O
OH
NH

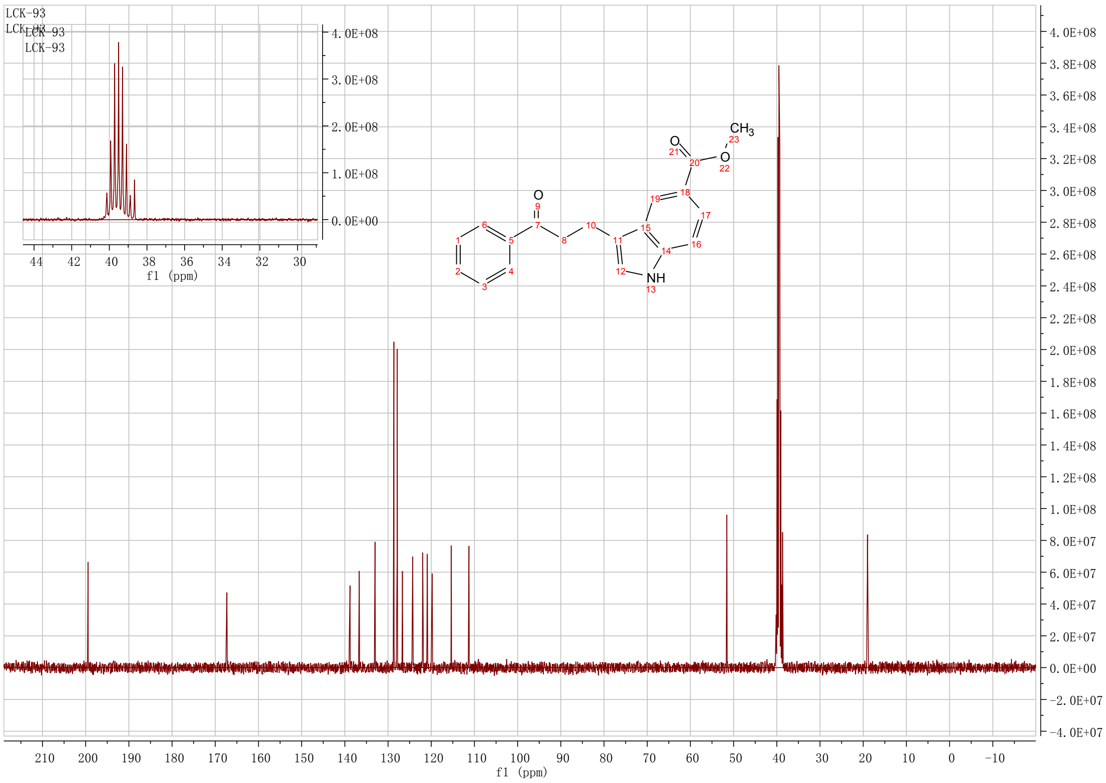

LCK-94
LCK-94
f1 (ppm)
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
6.5E+08 6.0E+08 5.5E+08 5.0E+08 4.5E+08 4.0E+08 3.5E+08 3.0E+08 2.5E+08 2.0E+08 1.5E+08 1.0E+08 5.0E+07 0.0E+00 -5.0E+07
0.95
1.95
1.06
1.97
1.03
0.99
0.98
0.94
3.03
2.00
1.99
O
O
CH3
NH

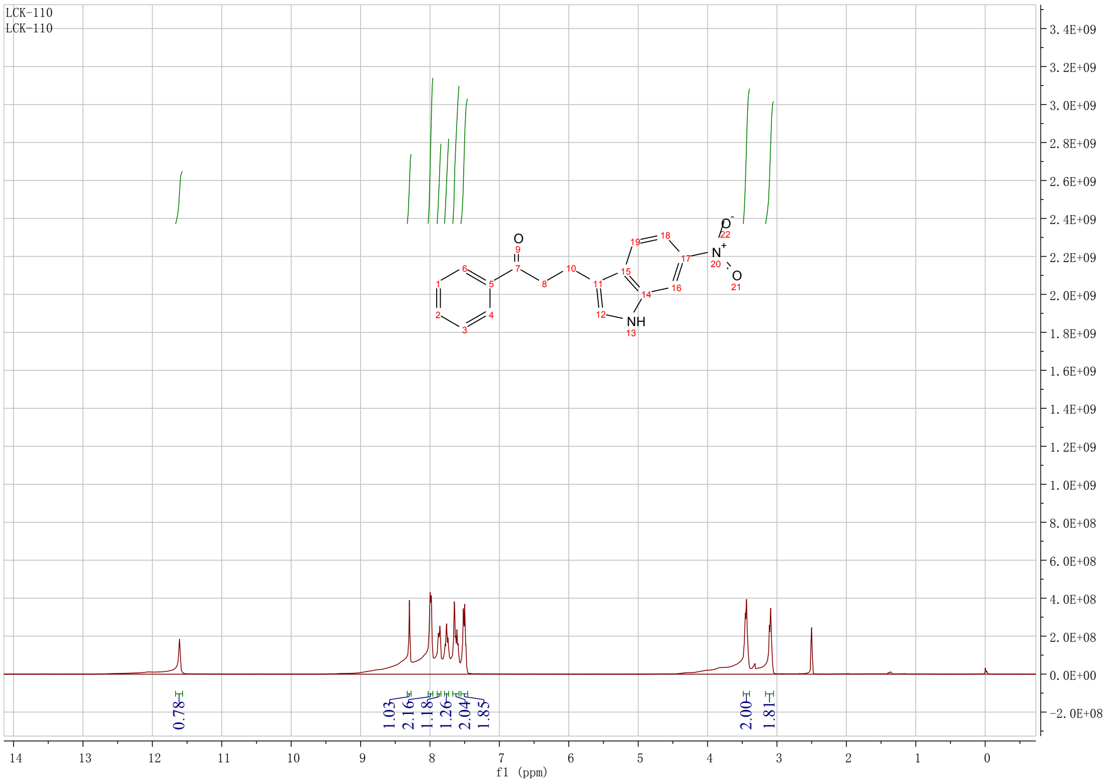

LCK-94
LCK-94
LCK-94
40.5
40.0
39.5
39.0
38.5
38.0
f1 (ppm)
3.0E+08
2.0E+08
1.0E+08
0.0E+00
O
CH3
1
2
3
4
5
6
7
8
9
10
11
12
NH
13
14
15
16
17
18
19
20
21
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)
3.8E+08
3.6E+08
3.4E+08
3.2E+08
3.0E+08
2.8E+08
2.6E+08
2.4E+08
2.2E+08
2.0E+08
1.8E+08
1.6E+08
1.4E+08
1.2E+08
1.0E+08
8.0E+07
6.0E+07
4.0E+07
2.0E+07
0.0E+00
-2.0E+07
-4.0E+07

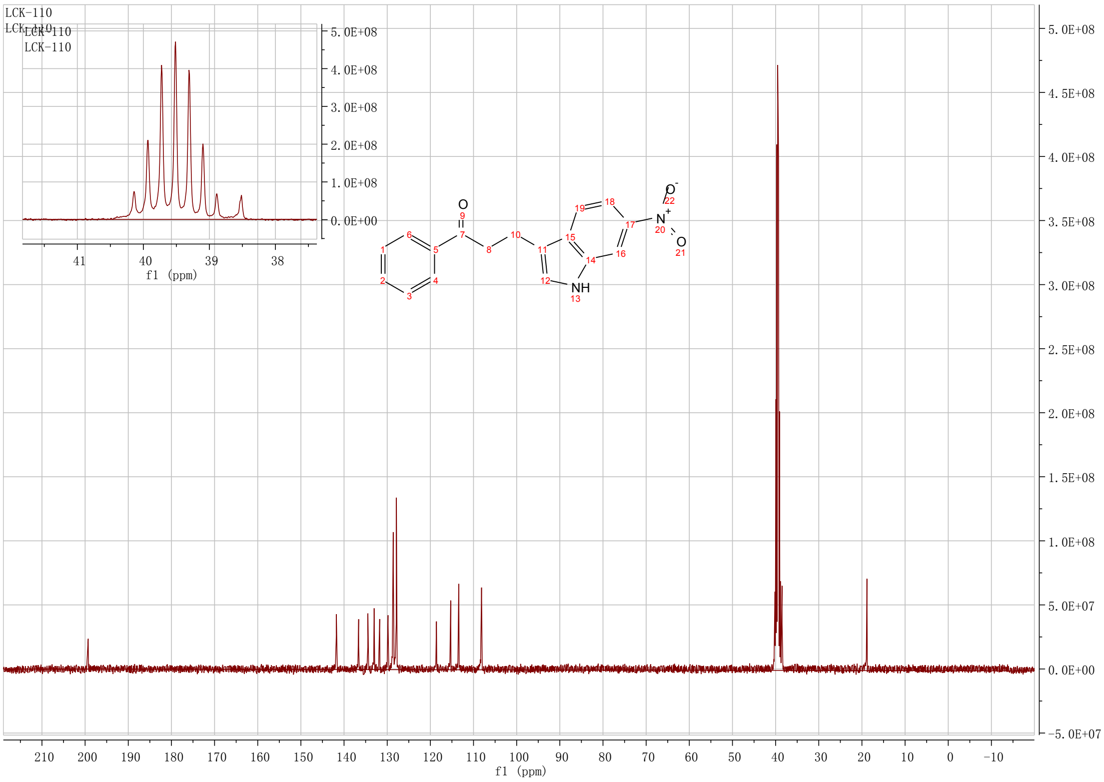

lck-113
lck-112
O
OH
1
2
3
4
5
6
7
8
9
10
11
12
NH
13
14
15
16
17
18
19
20
21
22
0.88
0.98
2.04
0.99
1.12
2.08
0.98
0.94
2.21
2.00
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)
2.00E+09
1.90E+09
1.80E+09
1.70E+09
1.60E+09
1.50E+09
1.40E+09
1.30E+09
1.20E+09
1.10E+09
1.00E+09
9.00E+08
8.00E+08
7.00E+08
6.00E+08
5.00E+08
4.00E+08
3.00E+08
2.00E+08
1.00E+08
0.00E+00
-1.00E+08

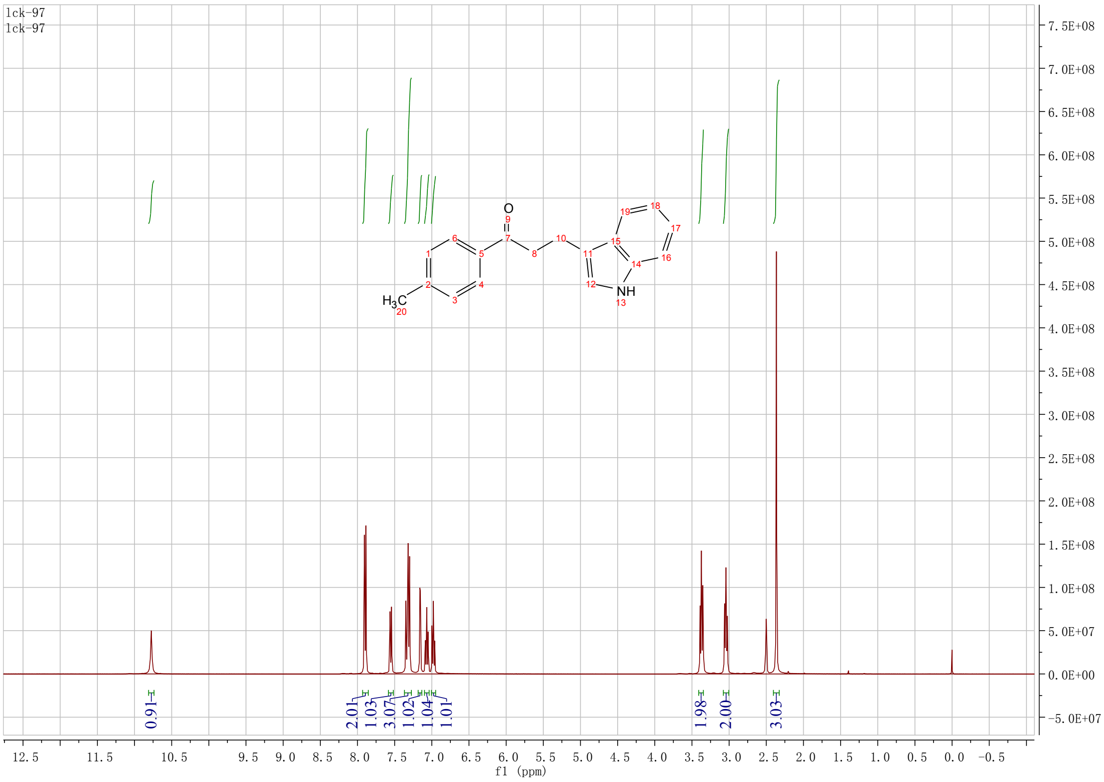

lck-113
lck-113
lck-113
4.0E+08
3.0E+08
2.0E+08
1.0E+08
0.0E+00
41.0 40.5 40.0 39.5 39.0 38.5 38.0
f1 (ppm)
O
OH
NH
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

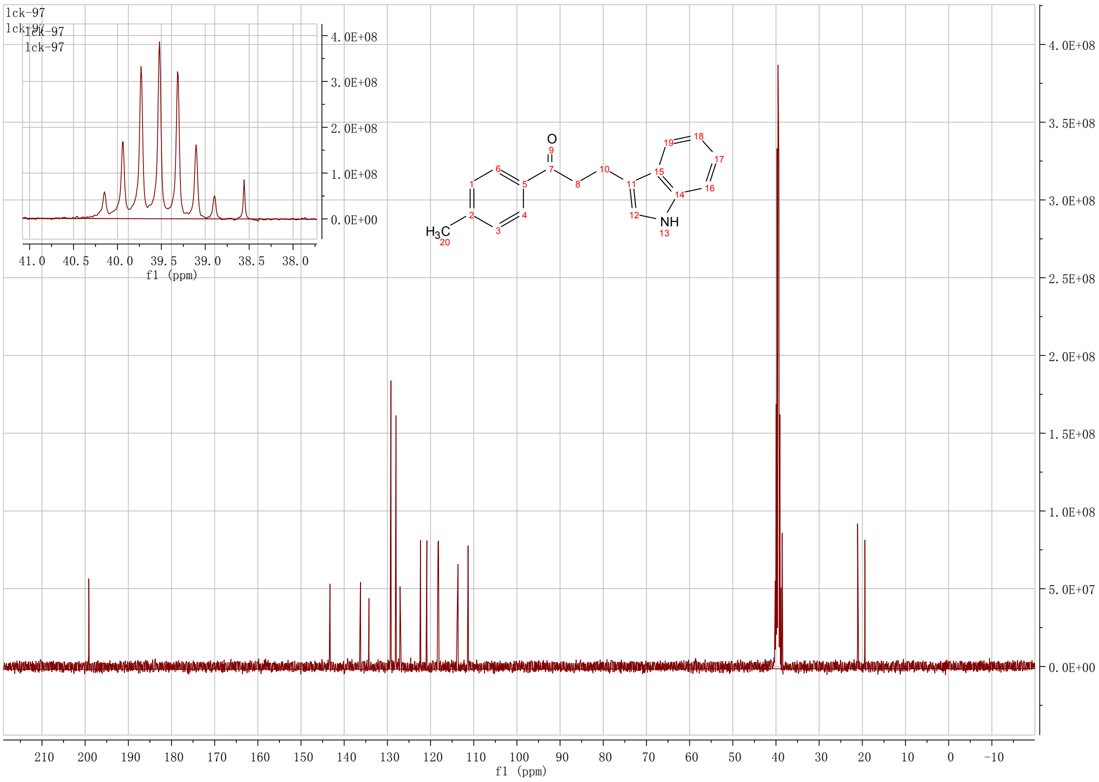

LCK-93
LCK-93
CH3
O
O
O
NH
0.94
0.98
2.01
1.01
1.07
2.04
1.00
0.99
3.01
2.00
2.00
1.40E+09
1.30E+09
1.20E+09
1.10E+09
1.00E+09
9.00E+08
8.00E+08
7.00E+08
6.00E+08
5.00E+08
4.00E+08
3.00E+08
2.00E+08
1.00E+08
0.00E+00
-1.00E+08
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

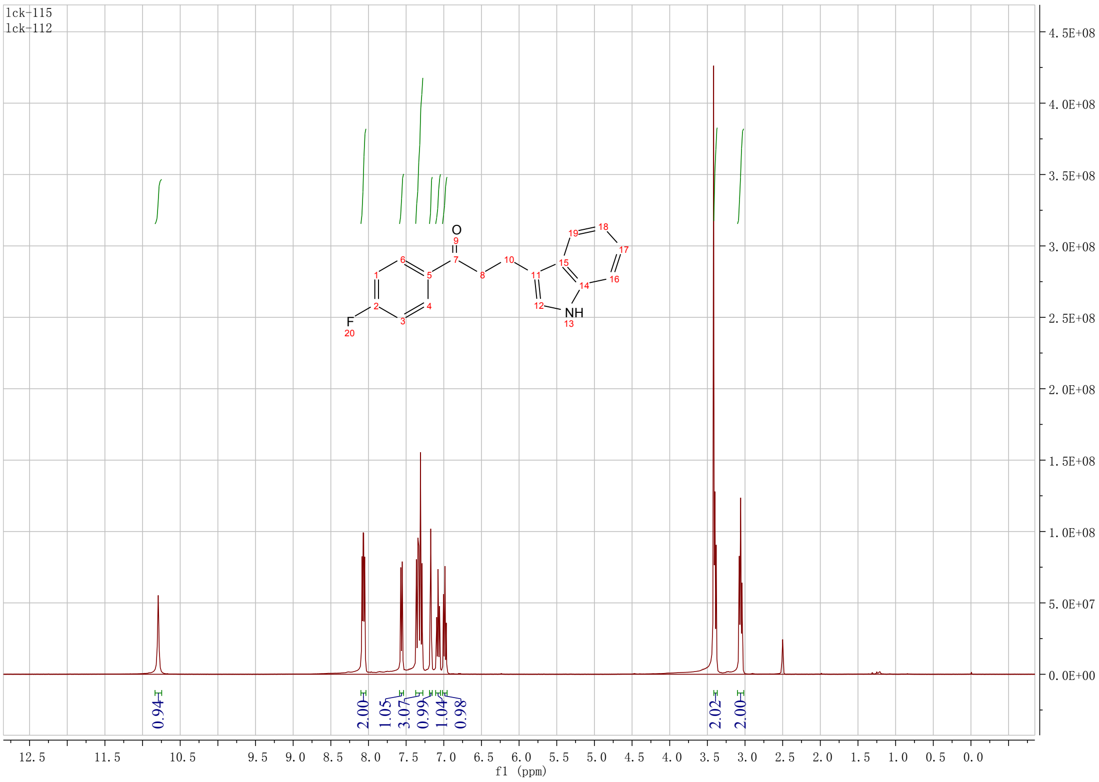

LCK-93
LCK-93
LCK-93
O
9
7
8
10
11
12
NH
13
14
15
16
17
18
19
20
O
21
O
22
CH3
23
1
2
3
4
5
6
f1 (ppm)
f1 (ppm)

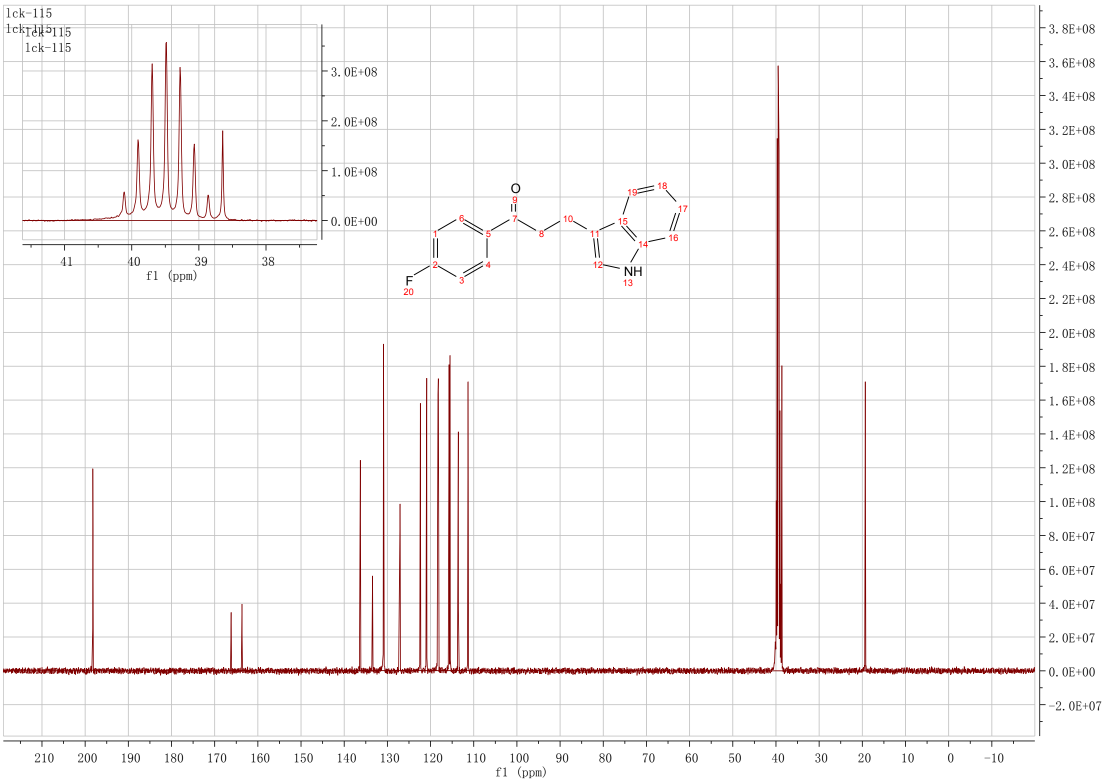

LCK-110
LCK-110
O
9
7
8
10
11
12
NH
13
14
15
16
17
18
19
N+
20
O-
22
O
21
1
2
3
4
5
6
0.78
1.03
2.16
1.18
1.26
2.04
1.85
2.00
1.81
f1 (ppm)

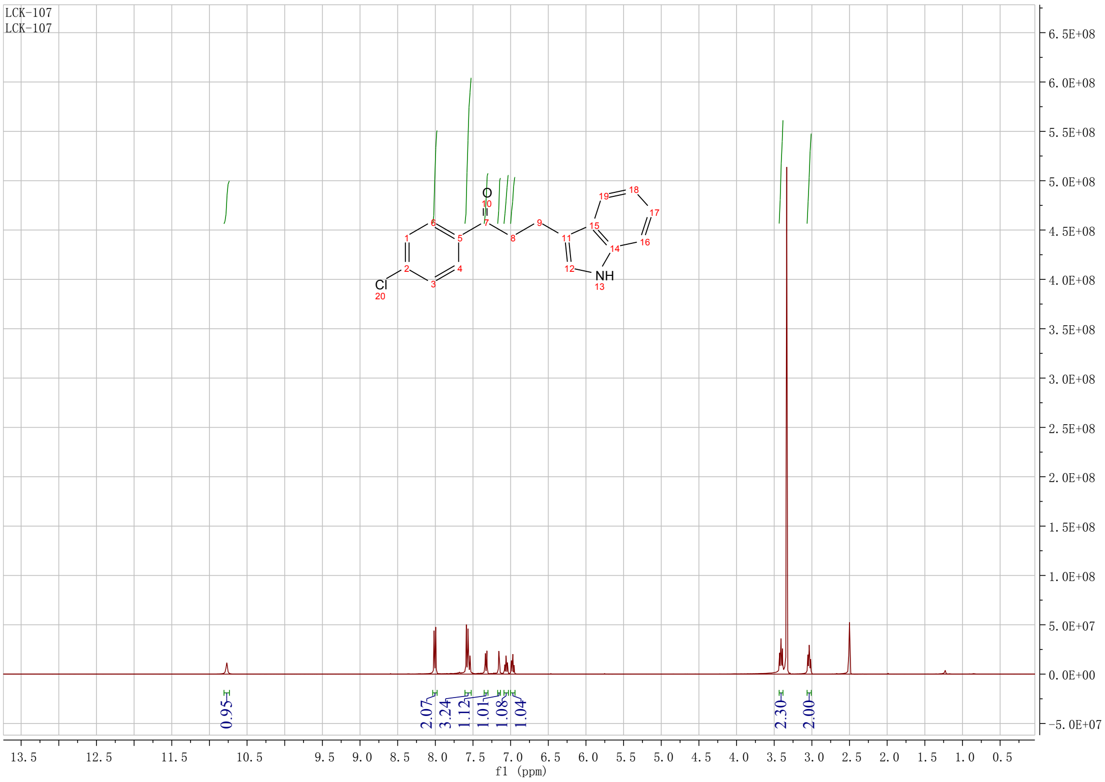

LCK-110
LCK-110
LCK-110
5.0E+08
4.0E+08
3.0E+08
2.0E+08
1.0E+08
0.0E+00
41
40
39
38
f1 (ppm)
O
9
7
6
5
1
2
3
4
8
10
11
12
NH
13
14
15
16
17
18
19
N
20
+
O
22
-
O
21
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

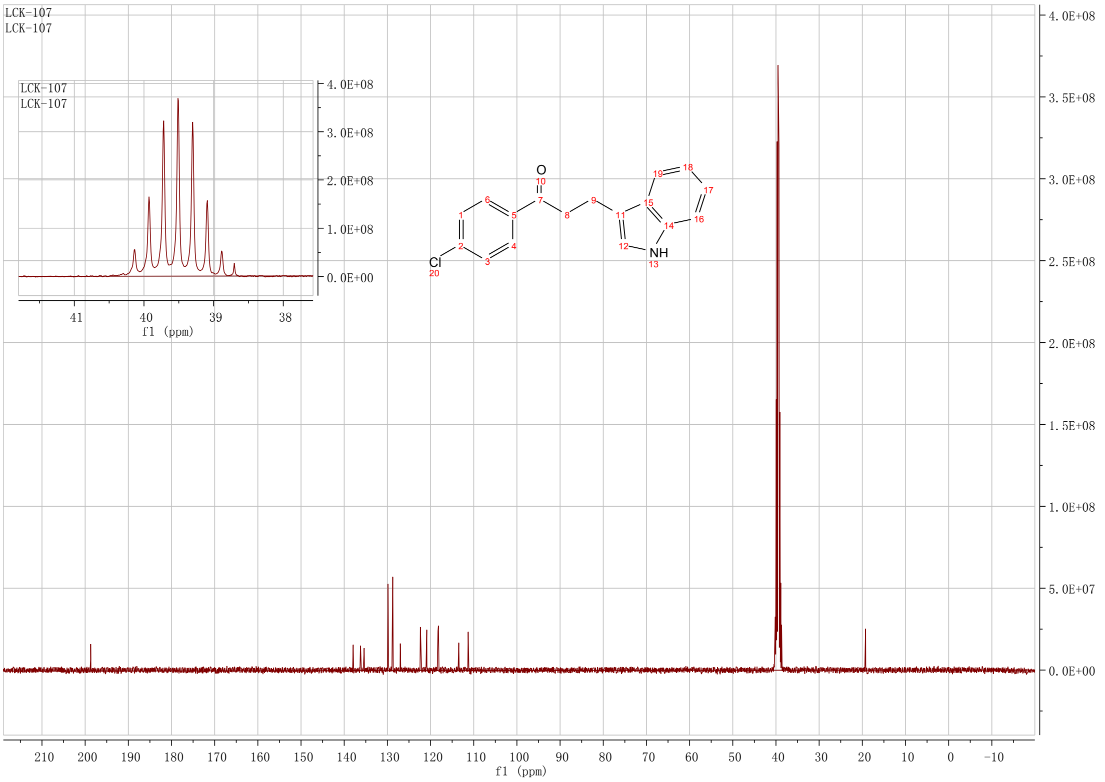

lck-97
lck-97
O
9
7
6
5
1
2
4
3
H3C
20
8
10
11
12
NH
13
14
15
16
17
18
19
7.5E+08
7.0E+08
6.5E+08
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
0.91
2.01
1.03
3.07
1.02
1.04
1.01
1.98
2.00
3.03
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

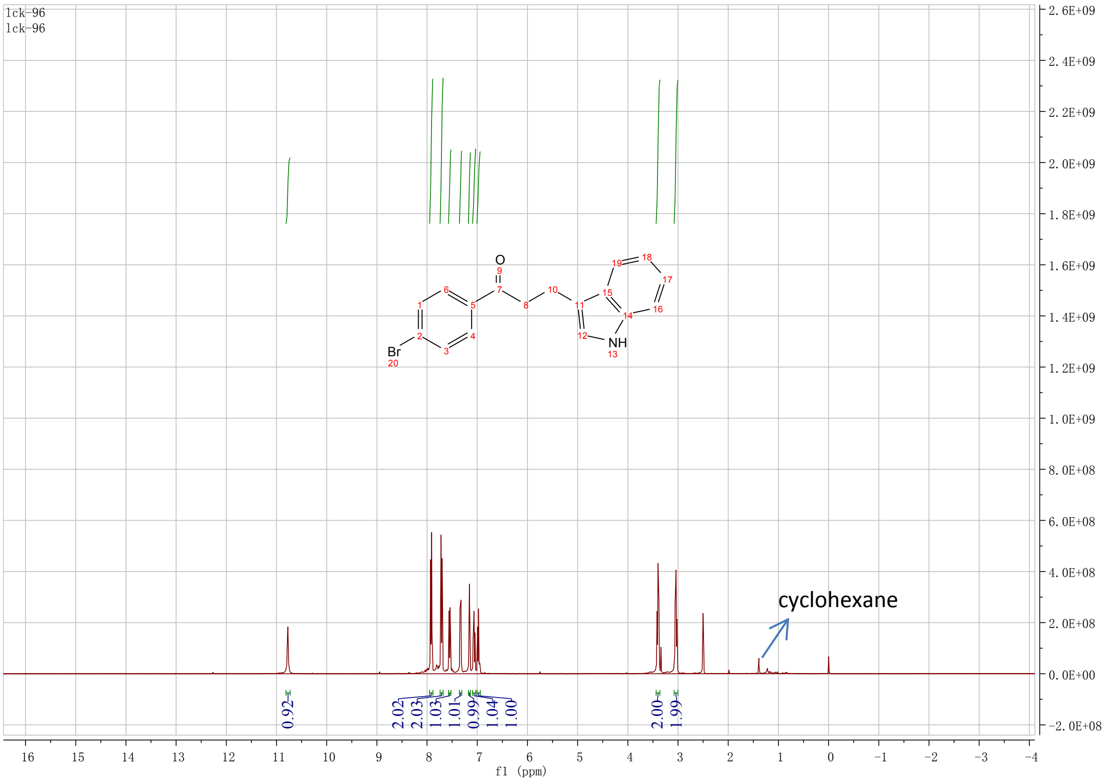

lck-97
lck-97
lck-97
4.0E+08
3.0E+08
2.0E+08
1.0E+08
0.0E+00
41.0
40.5
40.0
39.5
39.0
38.5
38.0
f1 (ppm)
O
H$_3$C
NH
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

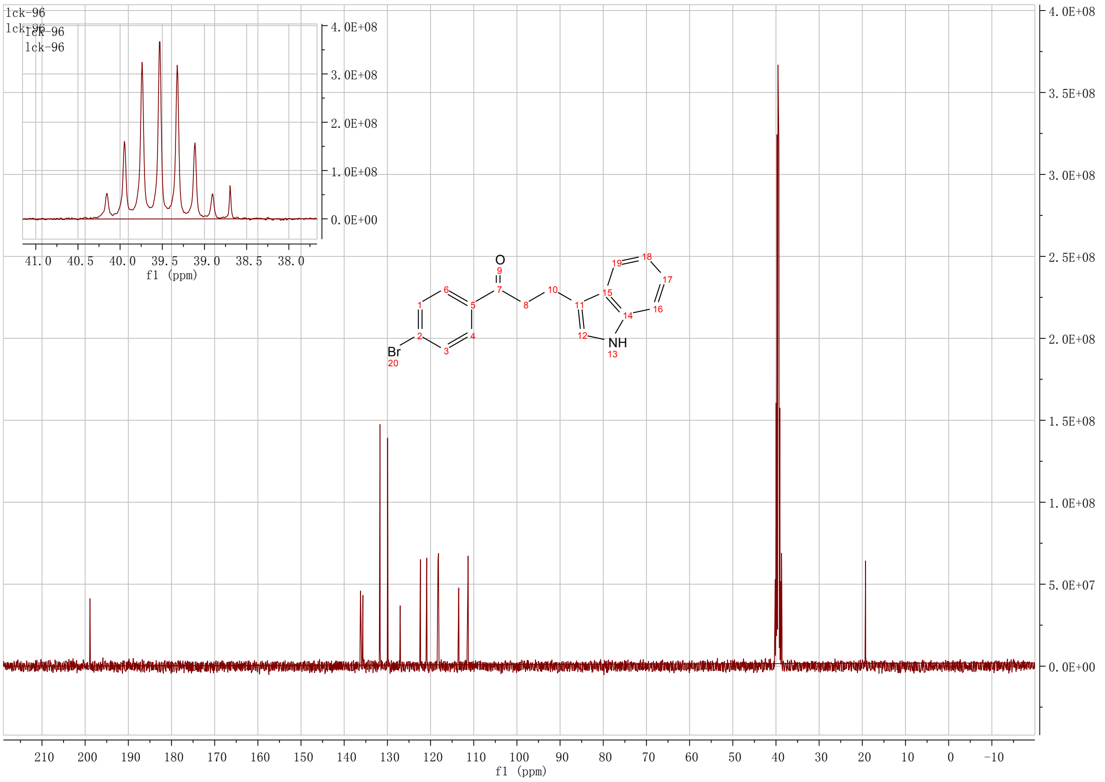

lck-115
lck-112
O
F
NH
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
0.94
2.00
1.05
3.07
0.99
1.04
0.98
2.02
2.00
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

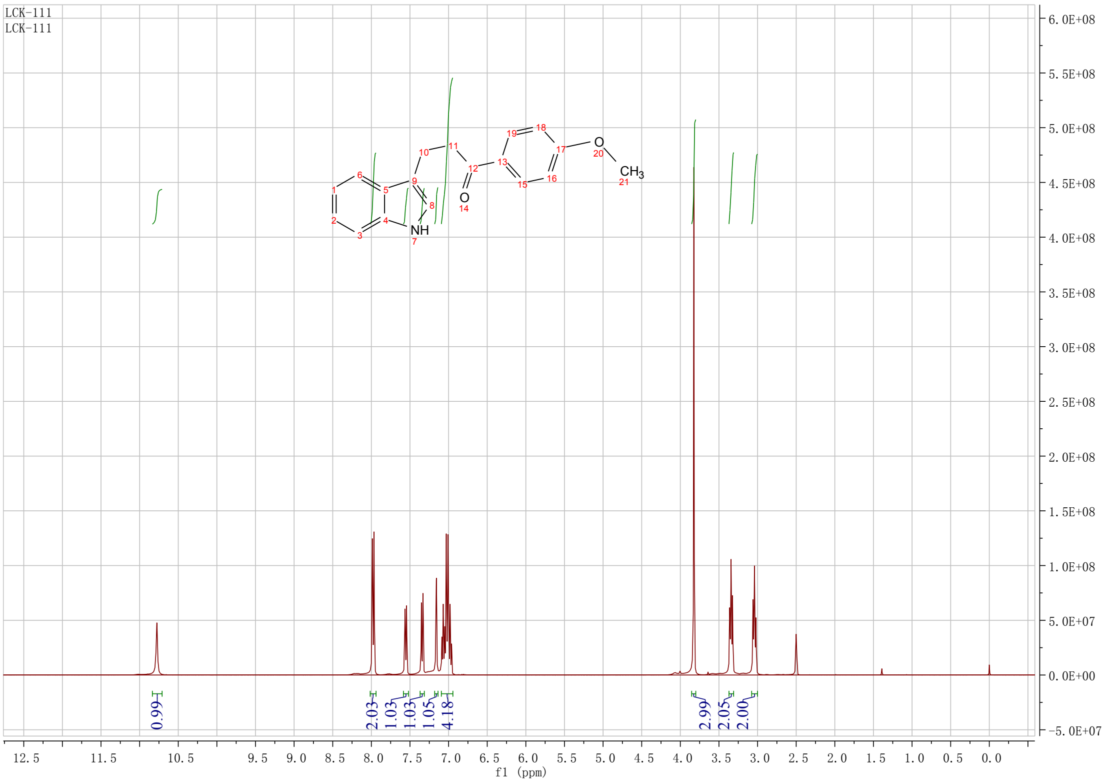

lck-115
lck-115
lck-115
lck-115
3.0E+08
2.0E+08
1.0E+08
0.0E+00
41
40
39
38
f1 (ppm)
O
F
NH
3.8E+08
3.6E+08
3.4E+08
3.2E+08
3.0E+08
2.8E+08
2.6E+08
2.4E+08
2.2E+08
2.0E+08
1.8E+08
1.6E+08
1.4E+08
1.2E+08
1.0E+08
8.0E+07
6.0E+07
4.0E+07
2.0E+07
0.0E+00
-2.0E+07
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

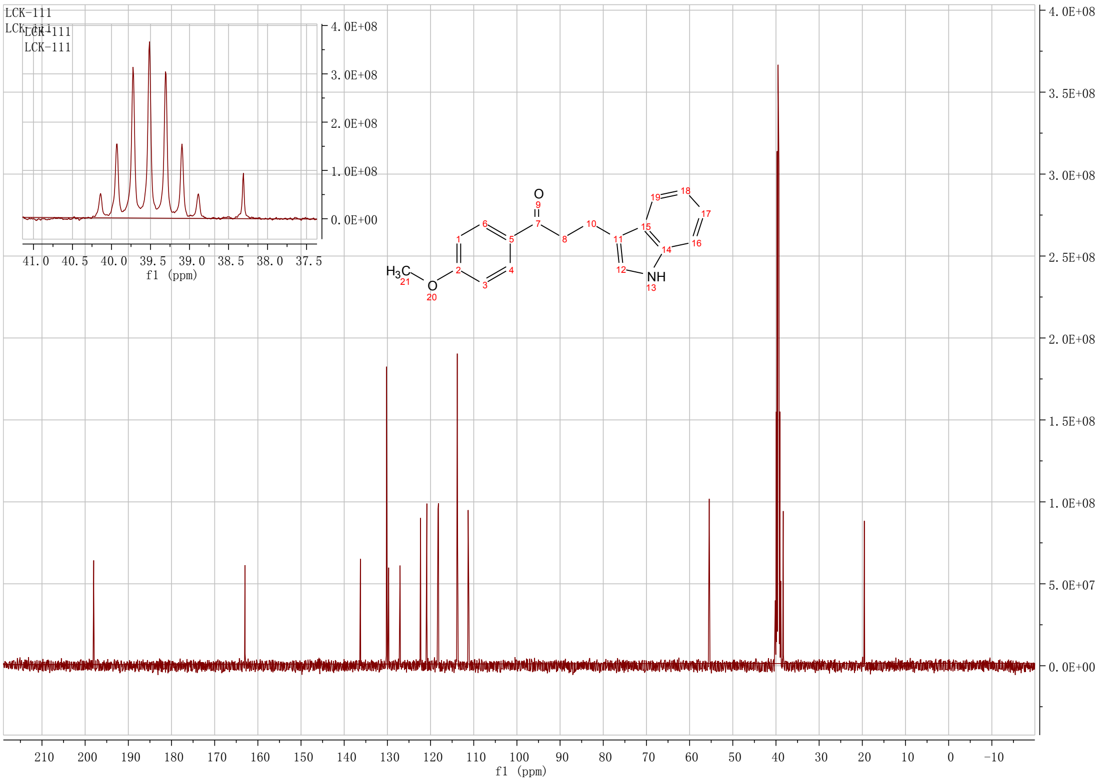

LCK-107
LCK-107
O
Cl
NH
0.95
2.07
3.24
1.12
1.01
1.08
1.04
2.30
2.00
6.5E+08
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

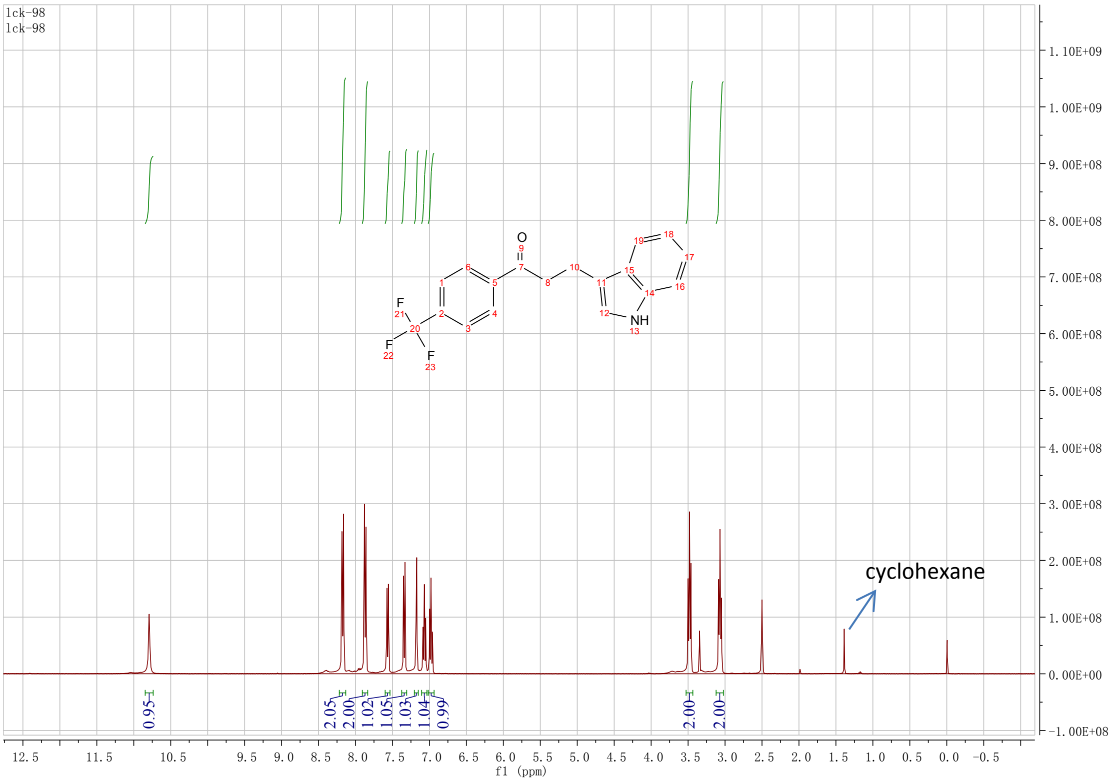

LCK-107
LCK-107
LCK-107
LCK-107
4.0E+08
3.0E+08
2.0E+08
1.0E+08
0.0E+00
41
40
39
38
f1 (ppm)
O
10
7
6
5
1
2
3
4
8
9
11
12
13
NH
14
15
16
17
18
19
Cl
20
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

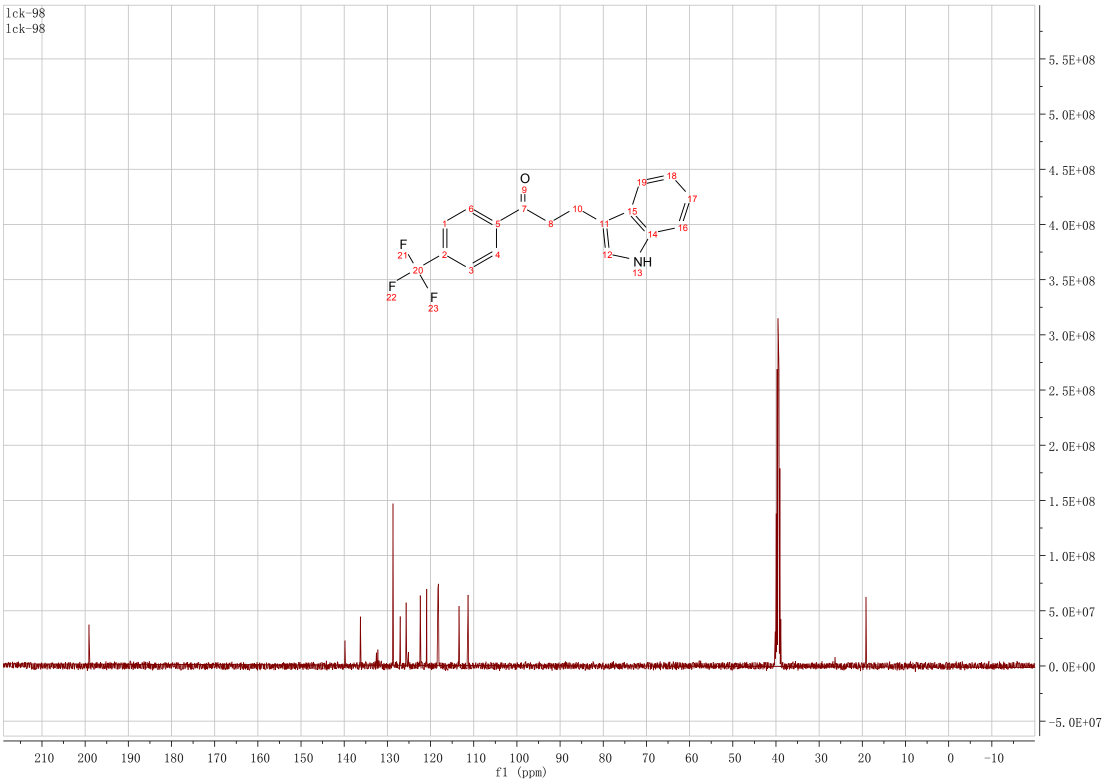

lck-96
lck-96
O
9
7
6
5
1
2
3
4
8
10
11
12
NH
13
14
15
16
17
18
19
Br
20
cyclohexane
0.92
2.02
2.03
1.03
1.01
0.99
1.04
1.00
2.00
1.99
2.6E+09
2.4E+09
2.2E+09
2.0E+09
1.8E+09
1.6E+09
1.4E+09
1.2E+09
1.0E+09
8.0E+08
6.0E+08
4.0E+08
2.0E+08
0.0E+00
-2.0E+08
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)


lck-96
lck-96
lck-96
f1 (ppm)
f1 (ppm)
Br
O
NH

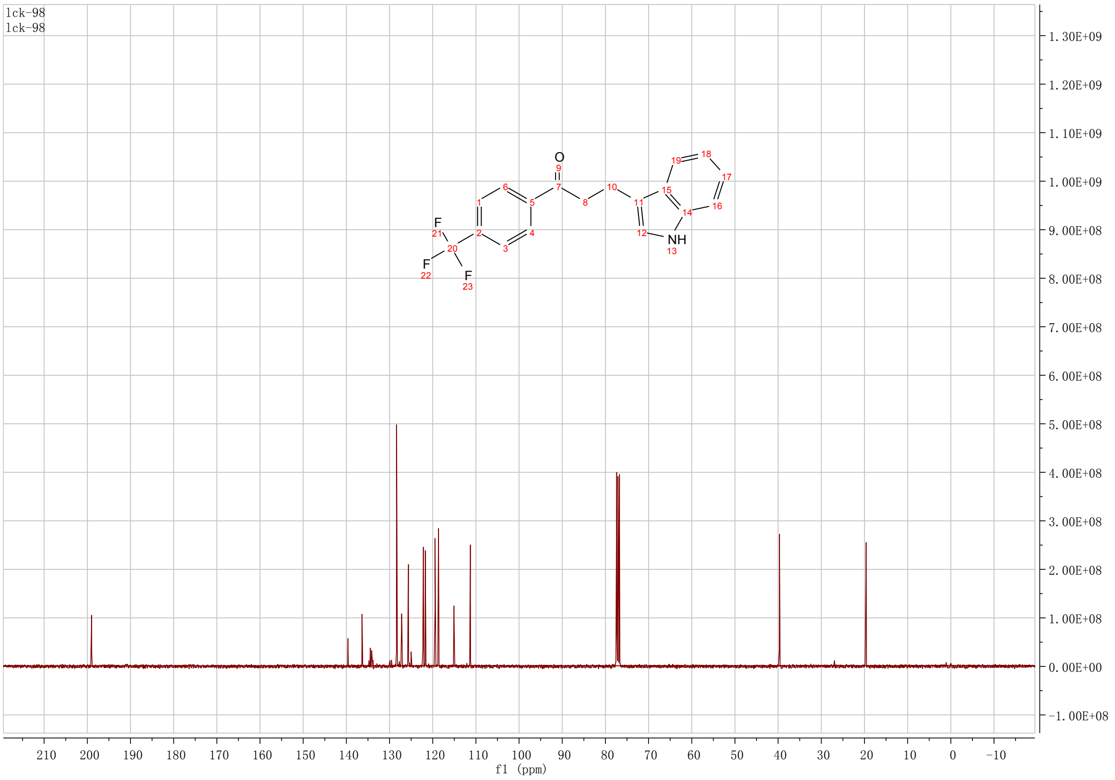

LCK-111
LCK-111
0.99
2.03
1.03
1.03
1.05
4.18
2.99
2.05
2.00
f1 (ppm)
NH
O
O
CH3

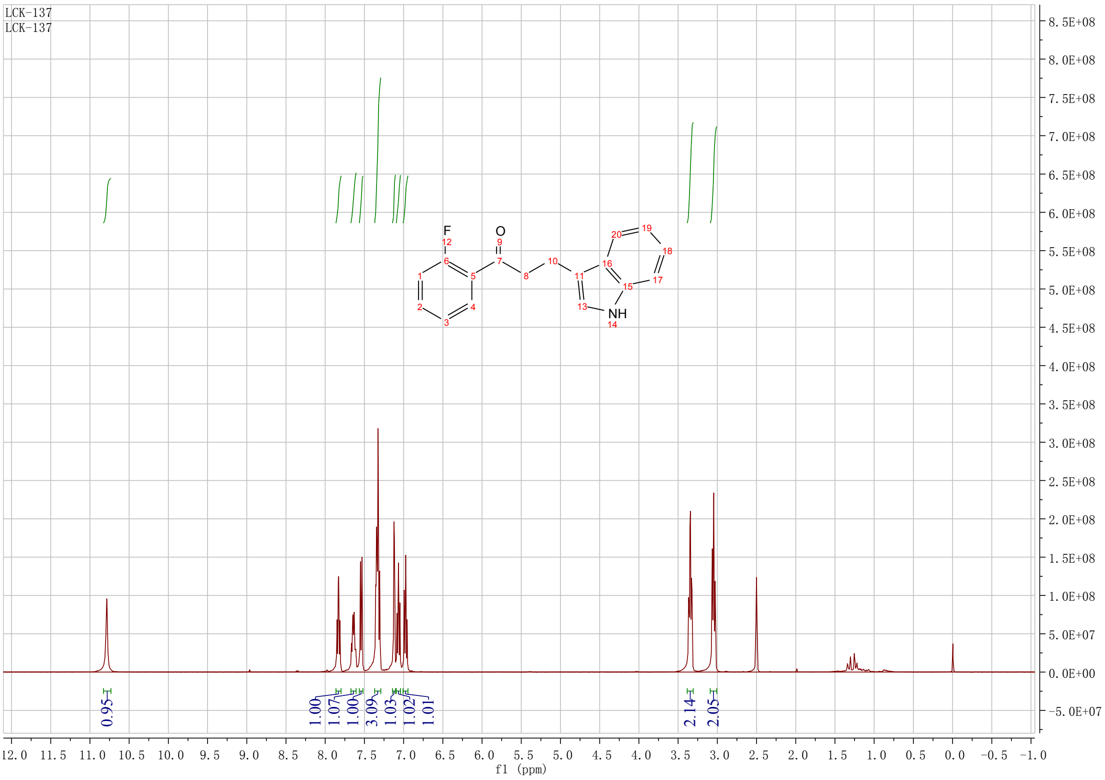

LCK-111
LCK-111
LCK-111
41.0 40.5 40.0 39.5 39.0 38.5 38.0 37.5
f1 (ppm)
4.0E+08
3.0E+08
2.0E+08
1.0E+08
0.0E+00
H3C
21
O
20
O
9
7
8
10
11
12
NH
13
14
15
16
17
18
19
1
2
3
4
5
6
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

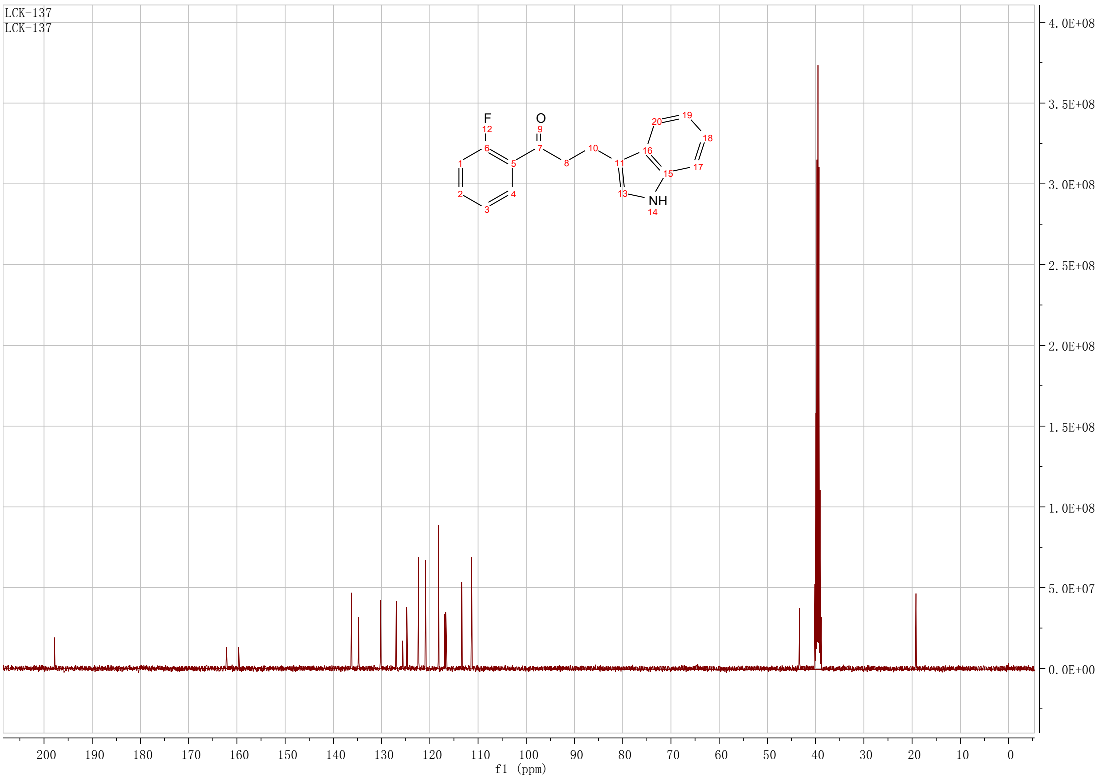

lck-98
lck-98
O
9
7
8
10
11
12
NH
13
14
15
16
17
18
19
1
2
3
4
5
6
F
21
20
F
22
F
23
cyclohexane
0.95
2.05
2.00
1.02
1.05
1.03
1.04
0.99
2.00
2.00
1.10E+09
1.00E+09
9.00E+08
8.00E+08
7.00E+08
6.00E+08
5.00E+08
4.00E+08
3.00E+08
2.00E+08
1.00E+08
0.00E+00
-1.00E+08
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)



In this ^{13}C NMR spectra, α-C of carbonyl was wrapped in the solvent peak. To prove it, $CDCl_3$ was used instead of DMSO-D_6 shown in the following ^{13}C NMR spectra. And, the missing the peak of α-C of carbonyl was appeared obviously.




LCK-137
LCK-137
F
12
O
9
6
7
1
5
8
10
11
16
20
19
18
17
15
13
NH
14
2
4
3
0.95
1.00
1.07
1.00
3.09
1.03
1.02
1.01
2.14
2.05
8.5E+08
8.0E+08
7.5E+08
7.0E+08
6.5E+08
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


LCK-137
LCK-137
F
12
O
9
6
7
1
5
8
10
11
16
20
19
18
17
15
13
NH
14
2
4
3
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)