Ruthenium- and rhodium -catalyzed oxidative alkylation of C-H bonds: efficient access to β-aryl ketones

Ji Qi,[a] Liangbin Huang,[b] Zhaoyang Wang*[a] and Huanfeng Jiang*[b]

[a] *School of Chemistry and Environment, South China Normal University*

Guangzhou 510004, PR China *wangzy@scnu.edu.cn*

[b] *School of Chemistry and Chemical Engineering, South China University of Technology*

Guangzhou 510640, PR China *jianghf@scut.edu.cn*

Electronic Supplementary Information

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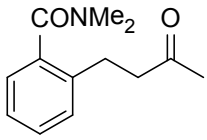
A. General procedure for 3a-3o

To a Schlenk tube were added *N*,*N*-dimethylbenzamide (1 mmol), but-3-en-2-ol (1.2 mmol), $RuCl_2$(*p*-cymene)]$_2$ (5 mol%), $AgSbF_6$ (15 mol%), $Cu(OAc)_2$ (1.1 equiv) HOAc (2 equiv) and CH_2Cl_2 2 mL at 140 ^oC stirred for 16 h. After the reaction was finished, the reaction mixture was cooled to room temperature, diluted in diethyl ether, and wash with $NaHCO_3$. The aqueous phase was re-extracted with diethyl ether. The combined organic extracts were dried over $MgSO_4$ and concentrated in vacuum, and the resulting residue was purified by silica gel column chromatography using light petroleum ether/ethyl acetate as eluent to afford the desired product.

B. Analytical data for 3a-o, 4a-ad, 5a, 6a

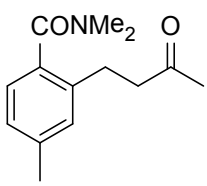
N,N-dimethyl-2-(3-oxobutyl)benzamide (3a)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.28 (m, 1H), 7.24 - 7.21 (m, 2H), 7.16 - 7.14 (m, 1H), 3.12 (s, 3H), 2.83 (s, 3H), 2.81(s, 4H), 2.12 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 207.7, 171.1, 137.2, 136.3, 129.3, 128.8, 126.2, 125.9, 44.7, 38.5, 34.5, 29.7, 27.0 ppm; IR *v* (neat, cm^{-1}) 2933, 2361, 1765, 1636, 1765, 1393, 1163, 753; MS (EI, 70 eV) m/z (%): 219 (M+, 8.5), 176 (100.0), 131 (61.1), 103 (20.8), 77 (18.9).

HRMS (ESI): m/z calcd for $C_{13}H_{17}NO_2$ $[M+H]^+$: 220.1332; found: 220.1327.

N,N,4-trimethyl-2-(3-oxobutyl)benzamide (3b)

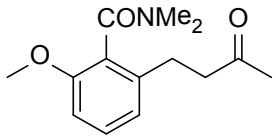


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.09 (d, *J* = 8.0 HZ, 1H), 6.76 - 6.75 (m, 2H), 3.80 (s,

3H), 3.10 (s, 3H), 2.85 (s, 3H), 2.80 (s, 4H), 2.13 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 207.8, 171.3, 159.9, 139.5, 128.9, 127.5, 115.0, 111.5, 55.2, 44.9, 38.8, 34.7, 29.8, 27.4 ppm; IR *v* (neat, cm^{-1}) 2927, 2358, 1718, 1498, 1392, 1069, 817, 651; MS (EI, 70 eV) *m/z* (%): 233 (M^+, 7.5), 190 (84.3), 145 (100.0), 117 (43.2), 91 (42.5), 77 (28.7).

HRMS (ESI): m/z calcd for $C_{14}H_{19}NO_2$ [M+Na] : 256.1308; found: 256.1314.

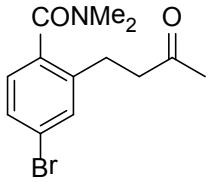
2-methoxy-N,N-dimethyl-6-(3-oxobutyl)benzamide (3c)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 (t, *J* = 8.0 HZ, 1H), 6.81 (d, *J* = 8.0 HZ, 1H), 6.76 (d, *J* = 8.0 HZ, 1H), 3.80 (s, 3H), 3.12 (s, 3H), 2.95 - 2.84 (m, 2H), 2.80 (s, 3H), 2.72 - 2.62 (m, 2H), 2.12 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 208.0, 168.9, 155.4, 138.9, 129.6, 126.0, 121.6, 108.6, 55.7, 44.9, 37.8, 34.5, 29.9, 27.1 ppm; IR *v* (neat, cm^{-1}) 2993, 1765, 171, 1635, 1468, 1376, 1243, 1058, 767; MS (EI, 70 eV) *m/z* (%): 249 (M^+, 3.2), 206 (34.4), 161 (100.0), 133 (19.4), 105 (20.1), 77 (20.2).

HRMS (ESI): m/z calcd for $C_{14}H_{19}NO_3$ [M+Na] : 272.1257; found: 272.1257.

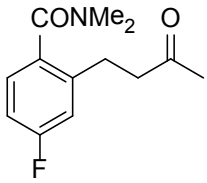
4-bromo-N,N-dimethyl-2-(3-oxobutyl)benzamide (3d)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (dd, *J* = 17.1, 9.0 HZ, 2H), 7.04 (d, *J* = 8.0 HZ, 1H), 3.11 (s, 3H), 2.84 (s, 3H), 2.80 (d, *J* = 12.0 HZ, 4H), 2.13 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 207.3, 170.2, 140.0, 135.4, 132.5, 129.5, 127.7, 122.9, 44.5, 38.7, 34.7, 29.8, 26.8 ppm; IR *v* (neat, cm^{-1}) 2930, 1714, 1636, 1587, 1394, 1265, 1088, 1063, 917, 827; MS (EI, 70 eV) *m/z* (%): 297 (M^+, 9.5), 254 (100.0), 211 (56.2), 183 (11.0), 130 (43.7), 102 (75.6), 89 (34.2) 77 (25.8), 72 (60.6).

HRMS (ESI): m/z calcd for $C_{13}H_{16}BrNO_2$ [M+Na] : 320.0257; found: 320.0242.

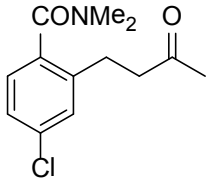
4-fluoro-N,N-dimethyl-2-(3-oxobutyl)benzamide (3e)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14 (dd, *J* = 8.2, 5.8 HZ, 1H), 6.96 - 6.90 (m, 2H), 3.12 (s, 3H), 2.84 (s, 3H), 2.81 (s, 4H), 2.14 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 207.09, 170.03, 139.59, 134.78, 134.49, 129.44, 127.31, 126.38, 44.29, 38.53, 34.53, 29.68, 26.72 ppm; IR *v* (neat, cm^{-1}) 2991, 2361, 1765, 1715, 1637, 1392, 1243, 1098, 1060, 831; MS (EI, 70 eV) *m/z* (%): 237 (M^+, 8.0), 194 (88.8), 149 (100.0), 121 (31.9), 72 (45.5).

HRMS (ESI): m/z calcd for $C_{13}H_{16}FNO_2$ [M+Na] : 260.1057; found: 260.1054.

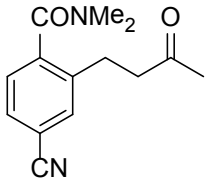
4-chloro-N,N-dimethyl-2-(3-oxobutyl)benzamide (3f)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 - 7.20 (m, 2H), 7.10 (d, *J* = 8.0 HZ, 1H), 3.11 (s, 3H), 2.84 (s, 3H), 2.81 (d, *J* = 8.0 HZ, 4H), 2.13 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 207.1, 170.0, 139.6, 134.8, 134.5, 129.4, 127.3, 126.4, 44.3, 38.5, 34.5, 29.7, 26.7 ppm; IR *v* (neat, cm^{-1}) 2937, 2361, 1765, 1716, 1637, 1395, 1242, 1160, 1062, 828, 581; MS (EI, 70 eV) *m/z* (%): 253 (M^+, 11.0), 210 (100.0), 165 (72.3), 131 (14.5), 89 (21.8), 72 (49.4).

HRMS (ESI): m/z calcd for $C_{13}H_{16}ClNO_2$ [M+Na] : 276.0762; found: 276.0769.

4-cyano-N,N-dimethyl-2-(3-oxobutyl)benzamide (3g)

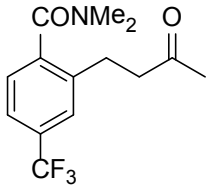


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (dd, *J* = 10.0, 2.1 HZ, 2H), 7.28 (d, *J* = 1.0 HZ, 1H), 3.13 (s, 3H), 2.82 (d, *J* = 8.0 HZ, 7H), 2.15 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 206.8, 169.2, 141.0, 139.2, 133.2, 130.1, 126.8, 118.1, 112.9, 44.0, 38.5, 34.6, 29.8,

26.6 ppm; IR v (neat, cm-1) 2932, 2230, 1766, 1715, 1638, 1398, 1244, 1063,842; MS (EI, 70 eV) m/z (%): 244 (M+, 6.0), 243 (6.9), 201 (100), 156 (58.0), 128 (21.5), 116 (8.7), 101 (16.7), 77 (12.1).

HRMS (ESI): m/z calcd for $C_{14}H_{16}N_2O_2$ [M+Na] : 267.1104; found: 267.1099.

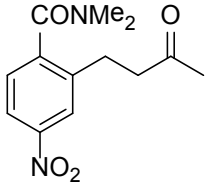
N,N-dimethyl-2-(3-oxobutyl)-4-(trifluoromethyl)benzamide (3h)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 4.0 HZ, 2H), 7.30 (d, *J* = 4.0 HZ, 1H), 3.14 (s, 3H), 2.84 (s, 7H), 2.15 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 207.1, 169.8, 140.1, 138.6, 131.3, 131.0, 126.6, 126.5, 126.4, 125.1, 123.41, 123.38, 122.4, 44.5, 38.6, 34.7, 29.8, 27.0 ppm; IR *v* (neat, cm^{-1}) 2935, 1761, 1713, 1640, 1333, 1246, 1167, 1124, 1085, 839; MS (EI, 70 eV) m/z (%): 287 (M+, 8.9), 244 (100.0), 199 (74.4), 151 (48.3), 103 (21.5), 77 (14.2).

HRMS (ESI): m/z calcd for $C_{14}H_{16}F_3NO_2$ $[M+H]^+$: 288.1206; found: 288.1200.

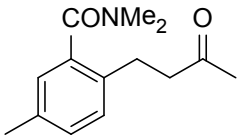
N,N-dimethyl-4-nitro-2-(3-oxobutyl)benzamide (3i)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 - 8.09 (m, 2H), 7.35 (d, *J* = 8.0 HZ, 1H), 3.15 (s, 3H), 2.89 (s, 4H), 2.85 (s, 3H), 2.16 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 206.7, 168.9, 148.0, 142.7, 139.8, 127.1, 124.4, 121.6, 43.9, 38.5, 34.7, 29.8, 26.8 ppm; IR *v* (neat, cm^{-1}) 2991, 1765, 1716, 1639, 1523, 1349, 1243, 1060, 846, 741; MS (EI, 70 eV) *m/z* (%): 264 (M^+, 17.0), 221 (84.0), 207 (76.0), 191 (46.4), 176 (60.6) 103 (95.3), 89 (39.2), 77 (24.8).

HRMS (ESI): m/z calcd for $C_{13}H_{16}N_2O_4$ [M+Na] : 287.1002; found: 287.1000.

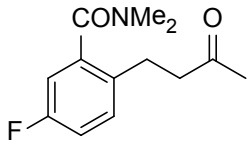
N,N,5-trimethyl-2-(3-oxobutyl)benzamide (3j)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.10 (t, *J* = 8.0 HZ, 2H), 6.97 (s, 1H), 3.11 (s, 3H), 2.84 (s, 3H), 2.77 (s, 4H), 2.31 (s, 3H), 2.11 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 207.9, 171.3, 136.3, 136.0, 134.1, 129.7, 129.3, 126.5, 44.9, 38.6, 34.5, 29.8, 26.7, 20.8 ppm; IR *v* (neat, cm^{-1}) 2928, 2362, 1714, 1636, 1498, 1392, 1243, 1167, 1068, 817, 649; MS (EI, 70 eV) *m/z* (%): 233 (M^+, 7.5), 190 (93.6), 145 (100.0), 117 (33.8), 91 (36.4), 77 (30.4).

HRMS (ESI): m/z calcd for $C_{14}H_{19}NO_2$ [M+Na] : 256.1308; found: 256.1314.

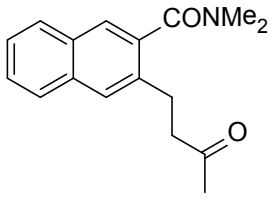
5-fluoro-N,N-dimethyl-2-(3-oxobutyl)benzamide (3k)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 - 7.20 (m, 1H), 7.04 (t, *J* = 8.0 HZ, 1H), 6.96 (d, *J* = 8.0 HZ, 1H), 3.12 (s, 3H), 2.84 (s, 3H), 2.79 (s, 4H), 2.14 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 207.3, 169.52, 169.49, 162.4, 160.0, 138.7, 138.6, 127.94, 127.85, 125.0, 124.8, 121.59, 121.55, 115.7, 115.4, 43.4, 38.6, 34.5, 29.5, 20.80, 20.77 ppm; IR *v* (neat, cm^{-1}) 2933, 2361, 1765, 1751, 1639, 1456, 1395, 1244, 1053, 799, 751; MS (EI, 70 eV) *m/z* (%): 237 (M^+, 18.1), 149 (100.0), 121 (42.2), 101 (52.9), 96 (20.3), 75 (40.1).

HRMS (ESI): m/z calcd for $C_{13}H_{16}FNO_2$ [M+Na] : 260.1057; found: 260.1059.

N,N-dimethyl-3-(3-oxobutyl)-2-naphthamide (3l)

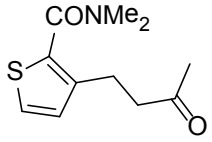


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 - 7.75 (m, 2H), 7.67 (d, *J* = 12.0 HZ, 2H), 7.51-7.43 (m, 2H), 3.17 (s, 3H), 2.93 (m, 4H), 2.86 (s, 3H), 2.14 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 207.8, 171.0, 135.04, 134.97, 133.4, 131.5, 128.0, 127.7, 127.3,

126.7, 126.0, 125.4, 44.8, 38.8, 34.7, 29.9, 27.3 ppm; IR *v* (neat, cm^{-1}) 2993, 1765, 1712, 1633, 1496, 1389, 1243, 1119, 1052; MS (EI, 70 eV) *m/z* (%): 269 (M^+, 18.6), 226 (93.6), 181 (100.0), 153 (4.1), 72 (25.9).

HRMS (ESI): m/z calcd for $C_{17}H_{19}NO_2$ [M+Na] : 292.1308; found: 292.1296.

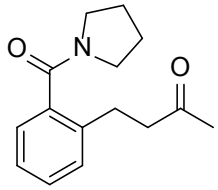
N,N-dimethyl-3-(3-oxobutyl)thiophene-2-carboxamide (3m)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (s, 1H), 6.87 (d, *J* = 4.0 HZ, 1H), 3.06 (s, 6H), 2.87 (t, *J* = 8.0 HZ, 2H), 2.77 (t, *J* = 8.0 HZ, 2H), 2.13 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 207.7, 165.7, 140.7, 130.8, 128.4, 125.8, 44.1, 29.9, 23.0 ppm; MS (EI, 70 eV) *m/z* (%): 225 (M^+, 9.1), 182 (79.6), 137 (100.0), 109 (17.4), 72 (36.8).

HRMS (ESI): m/z calcd for $C_{11}H_{15}NO_2S$ [M+Na] : 249.9873; found: 249.9872.

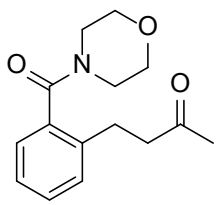
4-(2-(pyrrolidine-1-carbonyl)phenyl)butan-2-one (3n)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31-7.27 (m, 1H), 7.24 - 7.18 (m, 3H), 3.64 (t, *J* = 8.0 HZ, 2H), 3.15 (t, *J* = 8.0 HZ, 2H), 2.83 (s, 4H), 2.12 (s, 3H), 2.00 - 1.93 (m, 2H), 1.90 - 1.84 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 207.7, 169.4, 137.4, 137.0, 129.4, 128.8, 126.2, 125.7, 48.5, 45.2, 44.9, 29.7, 27.1, 25.8, 24.4 ppm; IR *v* (neat, cm^{-1}) 2984, 2362, 1750, 1628, 1421, 1373, 1242, 1049, 753, 608; MS (EI, 70 eV) *m/z* (%): 245 (M^+, 7.0), 202 (100.0), 131 (79.5), 103 (35.4), 77 (44.5).

HRMS (ESI): m/z calcd for $C_{15}H_{19}NO_2$ [M+Na] : 268.1308; found: 268.1303.

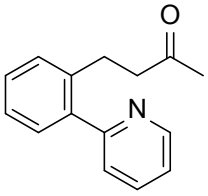
4-(2-(morpholine-4-carbonyl)phenyl)butan-2-one (3o)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (t, *J* = 8.0 HZ, 1H), 7.23 (t, *J* = 8.0 HZ, 2H), 7.15 (d, *J* = 8.0 HZ, 1H), 3.78 (t, *J* = 8.0 HZ, 4H), 3.59 (t, *J* = 4.0 HZ, 2H), 3.25 (d, *J* = 4.0 HZ, 2H), 2.90 (s, 2H), 2.76 (s, 2H), 2.13 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 207.5, 169.7, 137.6, 135.3, 129.5, 129.2, 126.3, 125.9, 66.7, 47.3, 44.7, 41.8, 29.8, 26.9 ppm; IR *v* (neat, cm^{-1}) 2965, 2855, 2362, 1765, 1713, 1634, 1428, 1364, 1250, 1114, 1016, 754, 558; MS (EI, 70 eV) *m/z* (%): 261 (M^+, 8.5), 218 (22.0), 175 (34.4), 103 (40.2), 91 (28.2), 77 (50.5).

HRMS (ESI): m/z calcd for $C_{15}H_{19}NO_3$ $[M+H]^+$: 262.1438; found: 262.1435.

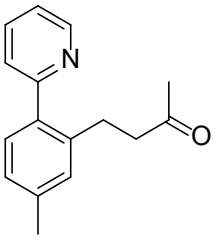
4-(2-(pyridin-2-yl)phenyl)butan-2-one (4a)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (d, *J* = 4.2 Hz, 1H), 7.74 (t, *J* = 7.6 Hz, 1H), 7.39 (d, *J* = 7.8 Hz, 1H), 7.33 (t, *J* = 7.2 Hz, 2H), 7.25 (dd, *J* = 11.1, 6.0 Hz, 2H), 2.95 (t, J = 7.8 Hz, 2H), 2.80 – 2.53 (m, 2H), 2.03 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 208.26, 159.98, 149.06, 140.34, 139.12, 136.46, 129.92, 129.82, 128.55, 126.31, 124.02, 121.85, 45.42, 29.81, 27.48.

HRMS (ESI): m/z calcd for $C_{15}H_{15}NO$ $[M+H]^+$: 226.1226; found: 226.1229.

4-(5-methyl-2-(pyridin-2-yl)phenyl)butan-2-one (4b)

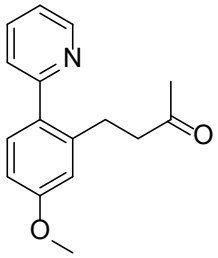


^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (d, *J* = 4.0 HZ, 1H), 7.73 (td, *J* = 7.7, 1.8 HZ, 1H), 7.37 (d, *J* = 4.0 HZ, 1H), 7.26 - 7.21 (m, 2H), 7.09 (d, *J* = 8.0 HZ, 2H), 2.93 (t, *J* = 8.0 HZ, 2H), 2.68 (t, *J* = 8.0 HZ, 2H), 2.36 (s, 3H), 2.04 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 208.4, 160.0, 149.0, 139.0, 138.3, 137.5, 136.4, 130.6, 129.9, 127.1, 124.0, 121.6, 45.6, 29.8, 27.5, 21.2 ppm; IR *v* (neat, cm^{-1}) 2923, 1713, 1584, 1359, 1158, 787. MS (EI, 70 eV) *m/z* (%): 239 (M^+) (1.3%), 196 (94.4%), 181 (100%), 167 (7.2%), 152

(13.6%), 139 (5.5%), 115 (8.5%), 90 (12.5%), 77 (13.4%), 51 (8.1%).

HRMS (ESI): m/z calcd for $C_{16}H_{17}NO$ $[M+H]^+$: 240.1383; found: 240.1382.

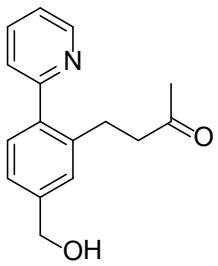
4-(5-methoxy-2-(pyridin-2-yl)phenyl)butan-2-one (4c)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (d, *J* = 4.0 HZ, 1H), 7.73 (td, *J* = 7.7, 1.7 HZ, 1H), 7.37 (d, *J* = 8.0 HZ, 1H), 7.29 (dd, *J* = 9.3, 4.6 HZ, 1H), 7.22 (dd, *J* = 6.6, 5.1 HZ, 1H), 6.83 - 6.81 (m, 2H), 3.83 (s, 3H), 2.96 (t, *J* = 8.0 HZ, 2H), 2.69 (t, *J* = 8.0 HZ, 2H), 2.05 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 208.3, 159.7, 149.0, 140.8, 136.5, 133.0, 131.3, 124.1, 121.5, 115.4, 111.6, 55.3, 45.4, 29.8, 27.7 ppm; MS (EI, 70 eV) *m/z* (%): 255 (M^+) (2.3%), 212 (100%), 197 (73.9%), 168 (34.7%), 154 (45.4%), 127 (10.0%), 84 (10.1%), 77 (9.2%), 63 (6.3%).

HRMS (ESI): m/z calcd for $C_{16}H_{17}NO_2$ $[M+H]^+$: 256.1332; found: 256.1329.

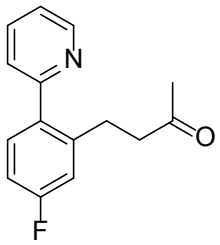
4-(5-(hydroxymethyl)-2-(pyridin-2-yl)phenyl)butan-2-one (4d)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 (d, *J* = 8.0 HZ, 1H), 7.75 (td, *J* = 7.7, 1.8 HZ, 1H), 7.37 (d, *J* = 8.0 HZ, 1H), 7.29 - 7.24 (m, 2H), 7.19 (t, *J* = 8.0 HZ, 2H), 4.61 (s, 2H), 3.60 (s, 1H), 2.91 (t, *J* = 8.0 HZ, 2H), 2.63 (t, *J* = 8.0 HZ, 2H), 2.01 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 208.5, 159.7, 148.9, 142.0, 139.0, 136.7, 132.1, 130.0, 127.9, 124.5, 124.2, 122.0, 64.2, 45.2, 29.8, 27.3 ppm; IR *v* (neat, cm^{-1}) 3389, 3007, 1711, 1587, 1162, 790.

HRMS (ESI): m/z calcd for $C_{16}H_{17}NO_2$ $[M+H]^+$: 256.1332; found: 256.1328.

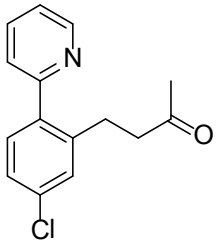
4-(5-fluoro-2-(pyridin-2-yl)phenyl)butan-2-one (4e)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (d, *J* = 8.0 HZ, 1H), 7.75 (td, *J* = 7.7, 1.8 HZ, 1H), 7.37 (d, *J* = 8.0 HZ, 1H), 7.31 (dd, *J* = 8.3, 6.0 HZ, 1H), 7.28 - 7.24 (m, 1H), 6.98 (ddd, *J* = 10.9, 8.8, 2.5 HZ, 2H), 2.94 (t, *J* = 8.0 HZ, 2H), 2.70 (t, *J* = 8.0 HZ, 2H), 2.06 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ ppm; IR *v* (neat, cm^{-1}) 3006, 1714, 1592, 1465, 1103, 788. MS (EI, 70 eV) *m/z* (%): 243 (M^+) (0.8%), 200 (100%), 185 (87.5%), 157 (4.8%), 133 (2.8%), 99 (2.9%), 78 (6.6%).

HRMS (ESI): m/z calcd for $C_{15}H_{14}FNO$ $[M+H]^+$: 244.1132; found: 244.1130.

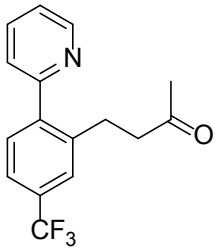
4-(5-chloro-2-(pyridin-2-yl)phenyl)butan-2-one (4f)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (d, *J* = 4.0 HZ, 1H), 7.76 (td, *J* = 7.7, 1.8 HZ, 1H), 7.37 (d, *J* = 8.0 HZ, 1H), 7.29 - 7.24 (m, 4H), 2.93 (t, *J* = 8.0 HZ, 2H), 2.70 (t, *J* = 8.0 HZ, 2H), 2.06 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 207.6, 158.9, 149.2, 141.2, 138.7, 136.6, 134.3, 131.3, 129.8, 126.4, 124.0, 122.1, 45.0, 29.8, 27.2 ppm; IR *v* (neat, cm^{-1}) 2928, 1713, 1590, 1463, 1360, 787. MS (EI, 70 eV) *m/z* (%): 259 (M^+) (0.9%), 216 (100%), 201 (60.2%), 181 (27.7%), 166 (17.8%), 152 (15.2%), 139 (7.1%), 89 (6.5%), 78 (9.0%), 77 (4.8%).

HRMS (ESI): m/z calcd for $C_{15}H_{14}ClNO$ $[M+H]^+$: 260.0837; found: 260.0834.

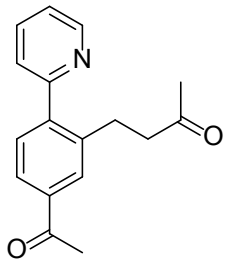
4-(2-(pyridin-2-yl)-5-(trifluoromethyl)phenyl)butan-2-one (4g)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (d, *J* = 4.0 HZ, 1H), 7.80 (td, *J* = 7.7, 1.8 HZ, 1H), 7.55 (d, *J* = 8.0 HZ, 2H), 7.46 (d, *J* = 8.0 HZ, 1H), 7.41 (d, *J* = 8.0 HZ, 1H), 7.32 (ddd, *J* = 7.6, 4.9, 1.0 HZ, 1H), 2.99 (t, *J* = 8.0 HZ, 2H), 2.73 (t, *J* = 8.0 HZ, 2H), 2.07 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 207.5, 158.6, 149.3, 143.7, 140.3, 136.8, 130.4, 126.63, 126.59, 124.0, 123.13, 123.09, 122.5, 45.0, 29.8, 27.2 ppm; IR *v* (neat, cm^{-1}) 2929, 1716, 1332, 1164, 1124, 791. MS (EI, 70 eV) *m/z* (%): 293 (M^+) (0.7%), 274 (3.7%), 250 (100%), 235 (86.0%), 216 (6.6%), 180 (7.5%), 166 (12.5%), 139 (6.9%), 89 (4.9%), 78 (11.4%), 75 (6.2%).

HRMS (ESI): m/z calcd for $C_{16}H_{14}F_3NO$ $[M+H]^+$: 294.1100; found: 294.1096.

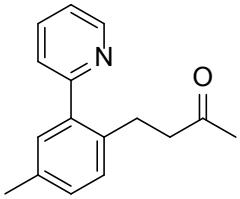
4-(5-acetyl-2-(pyridin-2-yl)phenyl)butan-2-one (4h)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 4.0 HZ, 1H), 7.91 (d, *J* = 1.6 HZ, 1H), 7.87 (dd, *J* = 8.0, 4.0 HZ, 1H), 7.80 (td, *J* = 7.7, 1.8 HZ, 1H), 7.46 - 7.41 (m, 2H), 7.32 - 7.29 (m, 1H), 3.01 (t, *J* = 8.0 HZ, 2H), 2.74 (t, *J* = 8.0 HZ, 2H), 2.63 (s, 3H), 2.07 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 207.7, 197.9, 158.8, 149.2, 144.8, 139.8, 136.9, 136.7, 130.3, 129.7, 126.3, 124.0, 122.4, 45.1, 29.8, 27.3, 26.7 ppm; IR *v* (neat, cm^{-1}) 2997, 1764, 1682, 1583, 1360, 1245, 751. MS (EI, 70 eV) *m/z* (%): 267 (M^+) (1.0%), 224 (100%), 209 (45.5%), 194 (9.1%), 181 (45.9%), 166 (39.9%), 152 (16.3%), 139 (13.4%), 89 (9.8%), 78 (14.0%), 77 (10.4%), 63 (7.7%).

HRMS (ESI): m/z calcd for $C_{17}H_{17}NO_2$ $[M+H]^+$: 268.1332; found: 268.1329.

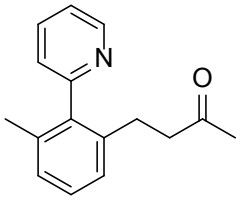
4-(4-methyl-2-(pyridin-2-yl)phenyl)butan-2-one (4i)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (d, *J* = 4.0 HZ, 1H), 7.76 (td, *J* = 7.7, 1.8 HZ, 1H), 7.41 (d, *J* = 8.0 HZ, 1H), 2.28 - 2.25 (m, 1H), 7.20 - 7.15 (m, 3H), 2.94 (t, *J* = 8.0 HZ, 2H), 2.67 (t, *J* = 8.0 HZ, 2H), 2.37 (s, 3H), 2.05 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 208.4, 160.1, 149.1, 140.2, 136.4, 135.9, 135.8, 130.6, 129.7, 129.3, 124.0, 121.8, 45.5, 29.8, 27.1, 20.9 ppm; IR *v* (neat, cm^{-1}) 2998, 2927, 1764, 1712, 1586, 1242, 993, 795. MS (EI, 70 eV) *m/z* (%): 239 (M^+) (2.0%), 197 (14.2%), 181 (100%), 152 (12.1%), 139 (5.1%), 115 (6.3%), 77 (9.5%).

HRMS (ESI): m/z calcd for $C_{16}H_{17}NO$ $[M+H]^+$: 240.1383; found: 240.1382.

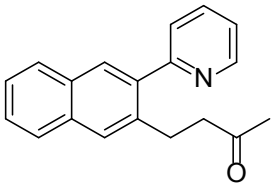
4-(3-methyl-2-(pyridin-2-yl)phenyl)butan-2-one (4j)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (d, *J* = 8.0 HZ, 1H), 7.76 (td, *J* = 7.7, 1.8 HZ, 1H), 7.28 - 7.24 (m, 3H), 7.11 (t, *J* = 8.0 HZ, 2H), 2.59 (s, 4H), 2.02 (s, 3H), 1.99 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 208.1, 159.4, 149.6, 140.2, 138.8, 136.4, 136.2, 128.2, 128.1, 126.6, 124.7, 122.0, 45.2, 29.8, 27.7, 20.3 ppm; IR *v* (neat, cm^{-1}) 2926, 1714, 1585, 1460,1360, 1091, 784. MS (EI, 70 eV) *m/z* (%): 239 (M^+) (7.9%), 196 (80.0%), 181 (100%), 167 (10.2%), 152 (8.9%), 115 (4.7%), 78 (4.7%), 77 (4.0%).

HRMS (ESI): m/z calcd for $C_{16}H_{17}NO$ $[M+H]^+$: 240.1383; found: 240.1384.

4-(2-(pyridin-2-yl)naphthalen-1-yl)butan-2-one (4k)

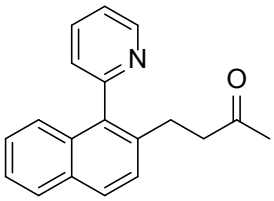


^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (d, *J* = 4.0 HZ, 1H), 7.81 (t, *J* = 4.0 HZ, 3H), 7.79-7.76 (m, 1H), 7.73 (s, 1H), 7.51 - 7.42 (m, 3H), 7.30 - 7.27 (m, 1H), 3.14 (t, *J* =

8.0 HZ, 2H), 2.70 (t, *J* = 8.0 HZ, 2H), 2.03 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 208.2, 160.0, 149.1, 138.9, 137.1, 136.6, 133.4, 132.0, 129.4, 128.3, 127.9, 127.2, 126.5, 125.8, 124.3, 122.0, 45.3, 29.9, 27.8 ppm; IR *v* (neat, cm^{-1}) 3054, 2929, 1712, 1586, 1279, 1159, 756. MS (EI, 70 eV) *m/z* (%): 275 (M^+) (5.4%), 232 (98.4%), 217 (100%), 189 (9.6%), 176 (4.3%), 152 (5.3%), 115 (11.3%), 109 (17.0%), 78 (5.7%).

HRMS (ESI): m/z calcd for $C_{19}H_{17}NO$ $[M+H]^+$: 276.1383; found: 276.1380.

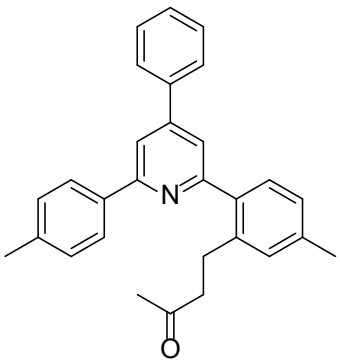
4-(1-(pyridin-2-yl)naphthalen-2-yl)butan-2-one (4l)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.76 (d, *J* = 4.0 HZ, 1H), 7.79 (ddd, *J* = 9.4, 8.5, 2.2 HZ, 3H), 7.40 - 7.37 (m, 2H), 7.35 - 7.29 (m, 3H), 7.25 (t, *J* = 4.0 HZ, 1H), 2.85 - 2.61 (m, 4H), 1.99 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 207.9, 158.4, 149.8, 136.9, 136.6, 136.4, 132.5, 132.2, 128.7, 127.9, 127.4, 126.3, 125.8, 125.6, 125.3, 122.3, 45.3, 29.8, 27.9 ppm; IR *v* (neat, cm^{-1}) 3054, 2931, 1713, 1587, 1362, 1160, 751. MS (EI, 70 eV) *m/z* (%): 275 (M^+) (2.8%), 232 (71.3%), 217 (100%), 202 (5.7%), 189 (11.5%), 176 (4.2%), 152 (4.9%), 109 (8.2%), 78 (5.4%).

HRMS (ESI): m/z calcd for $C_{19}H_{17}NO$ $[M+H]^+$: 276.1383; found: 276.1379.

4-(5-methyl-2-(4-phenyl-6-(p-tolyl)pyridin-2-yl)phenyl)butan-2-one (4m)

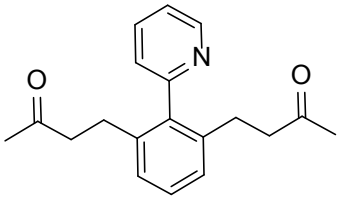


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.0 HZ, 2H), 7.86 (d, *J* = 4.0 HZ, 1H), 7.72 (d, *J* = 8.0 HZ, 2H), 7.53 (d, *J* = 4.0 HZ, 1H), 7.52 - 7.49 (m, 2H), 7.47 - 7.43 (m,

1H), 7.39 (d, *J* = 8.0 HZ, 1H), 7.27 (t, *J* = 8.0 HZ, 2H), 7.13 (d, *J* = 8.0 HZ, 2H), 3.06 (t, *J* = 8.0 HZ, 2H), 2.85 (t, *J* = 8.0 HZ, 2H), 2.40 (d, *J* = 4.0 HZ, 6H), 1.96 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 208.6, 160.4, 157.2, 149.8, 139.5, 139.0, 138.8, 138.4, 130.9, 130.1, 129.4, 129.1, 129.0, 127.2, 127.11, 127.09, 120.4, 116.5, 46.1, 29.7, 28.0, 21.3, 21.2 ppm; IR *v* (neat, cm^{-1}) 2922, 1713, 1596, 1545, 881, 821. MS (EI, 70 eV) *m/z* (%): 253 (M^+) (0.5%), 210 (1.2%), 182 (100%), 167 (58.7%), 139 (3.7%), 115 (1.9%), 90 (2.5%), 78 (2.7%), 77 (2.3%).

HRMS (ESI): m/z calcd for $C_{29}H_{27}NO$ $[M+H]^+$: 406.2165; found: 406.2163.

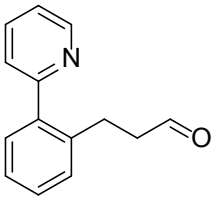
4,4'-(2-(pyridin-2-yl)-1,3-phenylene)bis(butan-2-one) (4n)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 4.0 HZ, 1H), 7.78 (td, *J* = 7.7, 1.7 HZ, 1H), 7.30 (d, *J* = 4.0 HZ, 1H), 7.29 - 7.24 (m, 2H), 7.12 (d, *J* = 4.0 HZ, 2H), 2.62 - 2.52 (m, 8H), 1.99 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 207.9, 158.8, 149.4, 140.0, 139.2, 136.6, 128.6, 127.1, 124.9, 122.3, 45.0, 29.8, 27.6 ppm; IR *v* (neat, cm^{-1}) 2932, 1713, 1586, 1361, 1161, 789, 756. MS (EI, 70 eV) *m/z* (%): 295 (M^+) (1.2%), 252 (100%), 237 (45.5%), 194 (67.4%), 180 (26.0%), 167 (18.5%), 152 (9.9%), 115 (4.1%);

HRMS (ESI): m/z calcd for $C_{19}H_{21}NO_2$ $[M+H]^+$: 296.1645; found: 296.1642.

3-(2-(pyridin-2-yl)phenyl)propanal (4o)

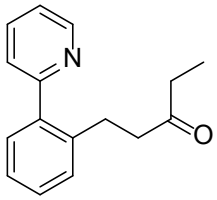


^{1}H NMR (400 MHz, $CDCl_3$) δ 9.68 (s, 1H), 8.67 (d, *J* = 4.0 HZ, 1H), 7.76 (td, *J* = 7.7, 1.7 HZ, 1H), 7.40 (d, *J* = 8.0 HZ, 1H), 7.36 - 7.33 (m, 2H), 7.31-7.28 (m, 2H), 7.26 (d, *J* = 4.0 HZ, 1H), 3.03 (t, *J* = 8.0 HZ, 2H), 2.69 (td, *J* = 7.8, 1.3 HZ, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 201.8, 159.8, 149.0, 140.2, 138.6, 136.6, 130.0, 129.8, 128.7, 126.5, 124.0, 122.0, 45.5, 25.8 ppm; IR *v* (neat, cm^{-1}) 2968, 1737, 1374, 1214, 1049,

631.

HRMS (ESI): m/z calcd for $C_{14}H_{13}NO$ $[M+H]^+$: 212.1070; found: 212.1071.

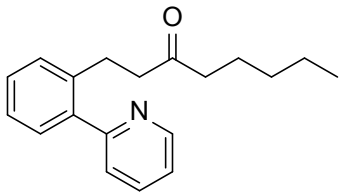
1-(2-(pyridin-2-yl)phenyl)pentan-3-one (4p)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (d, *J* = 4.0 HZ, 1H), 7.75 (td, *J* = 7.7, 1.8 HZ, 1H), 7.40 (d, *J* = 8.0 HZ, 1H), 7.35 - 7.23 (m, 5H), 2.96 (t, *J* = 8.0 HZ, 2H), 2.65 (t, *J* = 8.0 HZ, 2H), 2.31 (q, *J* = 7.3 HZ, 2H), 0.98 (t, *J* = 8.0 HZ, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 210.9, 160.0, 149.1, 140.3, 139.3, 136.4, 129.9, 129.8, 128.5, 126.3, 124.0, 121.8, 44.0, 35.9, 27.6, 7.8 ppm; IR *v* (neat, cm^{-1}) 2975, 1712, 1586, 1427, 1057, 755.

HRMS (ESI): m/z calcd for $C_{16}H_{17}NO$ $[M+H]^+$: 240.1383; found: 240.1389.

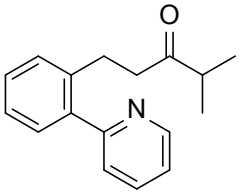
1-(2-(pyridin-2-yl)phenyl)octan-3-one (4q)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (d, *J* = 4.0 HZ, 1H), 7.75 (td, *J* = 7.7, 1.5 HZ, 1H), 7.40 (d, *J* = 8.0 HZ, 1H), 7.33 (t, *J* = 8.0 HZ, 2H), 7.29-7.23 (m, 3H), 2.95 (t, *J* = 8.0 HZ, 2H), 2.65 (t, *J* = 8.0 HZ, 2H), 2.27 (t, *J* = 8.0 HZ, 2H), 1.53 - 1.46 (m, 2H), 1.30 - 1.24 (m, 2H), 1.23 - 1.17 (m, 2H), 0.86 (t, *J* = 8.0 HZ, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 210.7, 160.0, 149.1, 140.3, 139.3, 136.4, 129.89, 129.85, 128.5, 126.3, 124.0, 121.8, 44.4, 42.8, 31.4, 27.6, 23.6, 22.4, 13.9 ppm; IR *v* (neat, cm^{-1}) 2903, 1710, 1585, 1463, 752. MS (EI, 70 eV) *m/z* (%): 281 (M^+) (0.5%), 210 (0.6%), 182 (100%), 167 (51.3%), 139 (2.6%), 90 (1.9%), 78 (2.2%), 77 (1.6%).

HRMS (ESI): m/z calcd for $C_{19}H_{23}NO$ $[M+H]^+$: 282.1582; found: 282.1581.

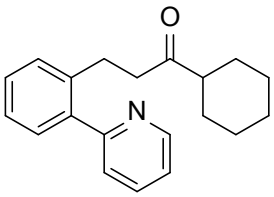
4-methyl-1-(2-(pyridin-2-yl)phenyl)pentan-3-one (4r)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (d, *J* = 8.0 HZ, 1H), 7.75 (td, *J* = 7.7, 1.5 HZ, 1H), 7.40 (d, *J* = 8.0 HZ, 1H), 7.33 (t, *J* = 8.0 HZ, 2H), 7.29 - 7.23 (m, 3H), 2.94 (t, *J* = 8.0 HZ, 2H), 2.70 (t, *J* = 8.0 HZ, 2H), 2.51 - 2.44 (m, 1H), 1.00 (d, *J* = 8.0 HZ, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 214.1, 160.0, 149.1, 140.4, 139.4, 136.5, 129.90, 129.88, 128.5, 126.3, 124.0, 121.8, 42.1, 40.8, 27.7, 18.1 ppm; IR *v* (neat, cm^{-1}) 2926, 1707, 1585, 1465, 753. MS (EI, 70 eV) *m/z* (%): 253 (M^+) (0.5%), 210 (1.2%), 182 (100%), 167 (58.7%), 139 (3.7%), 115 (1.9%), 90 (2.5%), 78 (2.7%), 77 (2.3%).

HRMS (ESI): m/z calcd for $C_{17}H_{19}NO$ $[M+H]^+$: 254.1539; found: 254.1539.

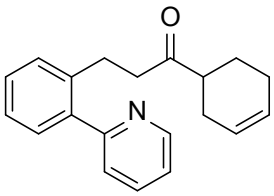
1-cyclohexyl-3-(2-(pyridin-2-yl)phenyl)propan-1-one (4s)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (d, *J* = 4.8 Hz, 1H), 7.73 (td, *J* = 7.7, 1.8 Hz, 1H), 7.39 (d, *J* = 7.8 Hz, 1H), 7.35 – 7.26 (m, 4H), 7.25 – 7.21 (m, 1H), 2.97 – 2.87 (m, 2H), 2.72 – 2.65 (m, 2H), 2.21 (dd, *J* = 13.1, 5.3 Hz, 1H), 1.74 – 1.68 (m, 4H), 1.62 (d, *J* = 10.5 Hz, 1H), 1.32 – 1.12 (m, 5H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 213.40, 160.03, 149.03, 140.35, 139.51, 136.41, 129.86, 128.51, 126.22, 124.02, 121.80, 50.70, 42.41, 28.36, 27.57, 25.85, 25.64. IR *v* (neat, cm^{-1}) 2929, 2855, 1705, 1585, 1450, 753. MS (EI, 70 eV) *m/z* (%): 293 (M^+) (0.4%), 210 (1.3%), 182 (100%), 167 (40.2%), 139 (2.0%), 115 (1.2%), 83 (2.2%), 77 (1.3%).

HRMS (ESI): m/z calcd for $C_{20}H_{23}NO$ $[M+H]^+$: 294.1852; found: 294.1855.

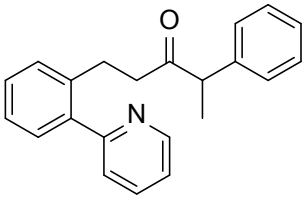
1-(cyclohex-3-en-1-yl)-3-(2-(pyridin-2-yl)phenyl)propan-1-one (4t)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (d, *J* = 4.0 HZ, 1H), 7.74 (td, *J* = 7.7, 1.8 HZ, 1H), 7.40 (d, *J* = 8.0 HZ, 1H), 7.33 (t, *J* = 8.0 HZ, 2H), 7.29-7.23 (m, 3H), 5.65 (t, *J* = 8.0 HZ, 2H), 2.95 (t, *J* = 8.0 HZ, 2H), 2.81-2.66 (m, 2H), 2.52 - 2.45 (m, 1H), 2.10 - 2.00 (m, 4H), 1.85 - 1.81 (m, 1H), 1.53 - 1.43 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 212.9, 160.0, 149.1, 140.4, 139.4, 136.4, 129.90, 129.89, 128.5, 126.6, 126.3, 125.4, 124.0, 121.8, 46.5, 42.5, 27.6, 26.7, 24.7, 24.5 ppm; IR *v* (neat, cm^{-1}) 2923, 1706, 1585, 1372, 754. MS (EI, 70 eV) *m/z* (%): 291 (M^+) (2.3%), 210 (1.5%), 182 (100%), 167 (51.0%), 139 (2.6%), 115 (1.6%), 79 (3.5%), 77 (2.7%).

HRMS (ESI): m/z calcd for $C_{20}H_{21}NO$ $[M+H]^+$: 292.1696; found: 292.1700.

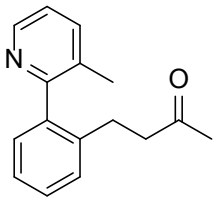
4-phenyl-1-(2-(pyridin-2-yl)phenyl)pentan-3-one (4u)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, *J* = 4.0 HZ, 1H), 7.65 (td, *J* = 7.7, 1.8 HZ, 1H), 7.27 (d, *J* = 8.0 HZ, 3H), 7.25 - 7.22 (m, 4H), 7.19 - 7.15 (m, 2H), 7.08 (d, *J* = 8.0 HZ, 2H), 3.62 (q, *J* = 7.0 HZ, 1H), 2,98 - 2.90 (m, 1H), 2.86 - 2.78 (m, 1H), 2.67 - 2.52 (m, 2H), 1.31 (d, *J* = 8.0 HZ, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 210.1, 159.9, 149.0, 140.6, 140.3, 139.2, 136.3, 129.9, 129.8, 128.9, 128.5, 127.8, 127.0, 126.2, 123.9, 121.8, 52.9, 42.7, 27.7, 17.4 ppm; IR *v* (neat, cm^{-1}) 2974, 1711, 1586, 1456, 754, 701. MS (EI, 70 eV) *m/z* (%): 315 (M^+) (0.8%), 210 (28.9%), 182 (100%), 167 (58.8%), 139 (3.6%), 105 (7.0%), 77 (5.7%).

HRMS (ESI): m/z calcd for $C_{22}H_{21}NO$ $[M+H]^+$: 316.1696; found: 316.1693.

4-(2-(3-methylpyridin-2-yl)phenyl)butan-2-one (4v)

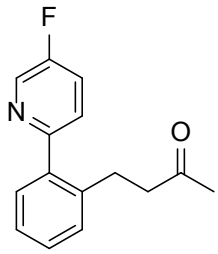


^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, *J* = 4.0 HZ, 1H), 7.59 (d, *J* = 8.0 HZ, 1H), 7.32 - 7.25 (m, 3H), 7.21 (dd, *J* = 7.6, 4.9 HZ, 1H), 7.15 (d, *J* = 8.0 HZ, 1H), 2.61 (s,

4H), 2.10 (s, 3H), 2.00 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 208.1, 159.0, 146.4, 139.8, 138.6, 138.1, 131.7, 129.3, 128.9, 128.3, 126.3, 122.5, 44.8, 29.8, 27.2, 19.2 ppm; IR *v* (neat, cm^{-1}) 2928, 1713, 1430, 1361, 1161, 758. MS (EI, 70 eV) *m/z* (%): 239 (M^+) (0.9%), 224 (2.1%), 196 (100%), 181 (63.5%), 167 (6.6%), 152 (6.5%), 115 (3.3%), 91 (4.6%), 77 (4.2%), 65 (6.2%).

HRMS (ESI): m/z calcd for $C_{16}H_{17}NO$ $[M+H]^+$: 240.1383; found: 240.1377.

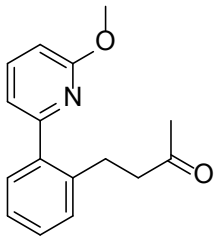
4-(2-(5-fluoropyridin-2-yl)phenyl)butan-2-one (4w)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (d, *J* = 4.0 HZ, 1H), 7.48 (td, *J* = 8.4, 2.9 HZ, 1H), 7.41 (dd, *J* = 8.6, 4.4 HZ, 1H), 7.36 - 7.31 (m, 2H), 7.29 (d, *J* = 4.0 HZ, 2H), 2.93 (t, *J* = 4.0 HZ, 2H), 2.70 (t, *J* = 8.0 HZ, 2H), 2.07 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 208.10, 159.74, 157.19, 156.11, 139.23, 137.26, 137.03, 129.91, 128.74, 126.36, 124.93, 123.36, 77.36, 77.25, 77.05, 76.73, 45.38, 29.87, 27.37. IR *v* (neat, cm^{-1}) 2991, 1764, 1712, 1241, 1056. MS (EI, 70 eV) *m/z* (%): 243 (M^+) (0.8%), 200 (90.0%), 185 (100%), 170 (3.8%), 157 (3.7%), 93 (5.0%), 77 (3.0%).

HRMS (ESI): m/z calcd for $C_{15}H_{14}FNO$ $[M+H]^+$: 244.1132; found: 244.1129.

4-(2-(6-methoxypyridin-2-yl)phenyl)butan-2-one (4x)

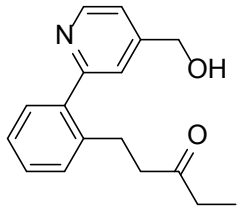


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (dd, *J* = 8.2, 7.4 HZ, 1H), 7.36 (d, *J* = 8.0 HZ, 1H), 7.32 - 7.28 (m, 2H), 7.25 (dd, *J* = 6.6, 2.1 HZ, 1H), 6.97 (d, *J* = 4.0 HZ, 1H), 6.70 (d, *J* = 8.0 HZ, 1H), 3.91 (s, 3H), 3.08 (t, *J* = 8.0 HZ, 2H), 2.69 (t, *J* = 8.0 HZ, 2H), 2.03 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 208.1, 163.3, 157.7, 140.0, 139.3, 139.0, 130.1, 130.0, 128.4, 126.3, 116.8, 109.1, 53.4, 45.4, 29.8, 27.6 ppm; MS (EI,

70 eV) *m/z* (%): 255 (M^+) (3.0%), 212 (100%), 197 (28.4%), 182 (21.3%), 154 (10.2%), 127 (6.2%), 115 (3.7%), 77 (3.4%);

HRMS (ESI): m/z calcd for $C_{16}H_{17}NO_2$ $[M+H]^+$: 256.1332; found: 256.1329.

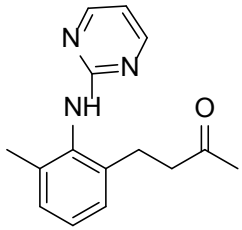
1-(2-(4-(hydroxymethyl)pyridin-2-yl)phenyl)pentan-3-one (4y)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (d, *J* = 5.1 H_Z, 1 H), 7.35 (s, 1 H), 7.32 – 7.27 (m, 2 H), 7.25 (d, *J* = 7.12 H_Z, 2H), 7.18 (d, *J* = 4.61 H_Z, 1H), 4.67 (s, 2 H), 3.35 (s, 1 H), 2.91 – 2.87 (t, *J* = 8.4 H_Z, 2H), 2.65 – 2.61 (t, *J* = 7.2 H_Z, 2H), 2.22 – 2.27 (q, *J* = 7.32 2H), 0.96 (t, *J* = 7.31, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 211.41, 159.78, 151.21, 148.78, 140.19, 139.10, 129.84, 129.66, 128.62, 126.27, 121.48, 119.44, 63.18, 43.91, 35.91, 27.45, 7.7. MS (EI, 70 eV) *m/z* (%): 269 (M^+) (0.4%), 212 (100%), 197 (33.0%), 167 (16.1%), 152 (7.8%), 139 (5.0%), 115 (4.2%), 97 (4.1%), 77 (4.8%).

HRMS (ESI): m/z calcd for $C_{17}H_{19}NO_2$ $[M+H]^+$: 270.1489; found: 270.1486.

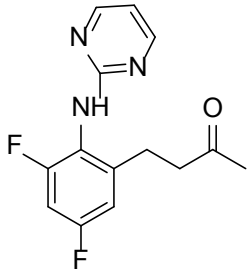
4-(3-methyl-2-(pyrimidin-2-ylamino)phenyl)butan-2-one (4z)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, *J* = 4.0 H_Z, 2H), 7.70 (s, 1H), 7.18 - 7.13 (m, 2H), 7.12 - 7.08 (m, 1H), 2.88 (t, *J* = 8.0 HZ, 2H), 2.73 (t, *J* = 8.0 H_Z, 2H), 2.22 (s, 3H), 2.05 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 208.4, 161.7, 158.4, 138.9, 137.0, 135.3, 128.9, 127.3, 127.2, 111.3, 44.5, 29.9, 25.7, 18.7 ppm; IR *v* (neat, cm^{-1}) 3750, 3682, 2981, 2365, 1709, 1570, 1420, 1254. MS (EI, 70 eV) *m/z* (%): 255 (22.2%), 212 (100%), 197 (43.7%), 184 (65.2%), 169 (25.2%), 142 (49.6%), 115 (53.6%), 91 (51.4%), 77 (41.3%).

HRMS (ESI): m/z calcd for $C_{15}H_{17}N_3O$ $[M+H]^+$: 256.1444; found: 256.1436.

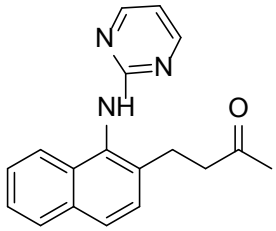
4-(3,5-difluoro-2-(pyrimidin-2-ylamino)phenyl)butan-2-one (4ab)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, *J* = 4.0 HZ, 2H), 7.43 (s, 1H), 6.80 - 6.75 (m, 2H), 6.68 (t, *J* = 8.0 HZ, 1H), 2.91 (t, *J* = 8.0 HZ, 2H), 2.79 (t, J = 8.0 HZ, 2H), 2.10 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 207.60, 162.09, 161.43, 159.75, 158.24, 157.68, 142.20, 121.26, 112.30, 111.58, 102.61, 43.79, 29.87, 25.10; IR *v* (neat, cm^{-1}) 3232, 2929, 1714, 1584, 1514, 1410, 1121, 995, 800. MS (EI, 70 eV) *m/z* (%): 277, 258, 234 (100%), 219, 206, 181, 164, 126, 79.

HRMS (ESI): m/z calcd for $C_{14}H_{13}F_2N_3O$ $[M+H]^+$: 278.1099; found: 278.1103.

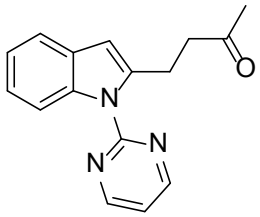
4-(1-(pyrimidin-2-ylamino)naphthalen-2-yl)butan-2-one (4ac)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (s, 2H), 8.15 (s, 1H), 7.93 (dd, *J* = 6.2, 3.4 HZ, 1H), 7.82 (dd, *J* = 6.1, 3.3 HZ, 1H), 7.76 (d, *J* = 8.0 HZ, 1H), 7.43 (dd, *J* = 6.3, 3.3 HZ, 2H), 7.38 (d, *J* = 8.0 HZ, 1H), 6.59 (t, *J* = 4.0 HZ, 1H), 3.05 (s, 2H), 2.83 (t, *J* = 8.0 HZ, 2H), 2.05 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 208.4, 162.5, 158.4, 136.1, 133.3, 131.9, 131.6, 128.2, 127.8, 127.5, 126.5, 125.6, 123.6, 111.6, 44.4, 29.9, 26.0 ppm; IR *v* (neat, cm^{-1}) 3853, 3457, 2924, 1708, 1578, 1378, 1087, 806. MS (EI, 70 eV) *m/z* (%): 291, 248 (100%), 233, 220, 205, 178, 152, 116, 96, 81.

HRMS (ESI): m/z calcd for $C_{18}H_{17}N_3O$ $[M+H]^+$: 292.1444; found: 292.1440.

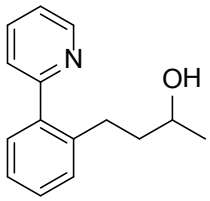
4-(1-(pyrimidin-2-yl)-1H-indol-2-yl)butan-2-one (4ad)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (d, *J* = 4.0 HZ, 2H), 8.28 (d, *J* = 8.0 HZ, 1H), 7.50 (d, *J* = 8.0 HZ, 1H), 7.24 - 7.15 (m, 2H), 7.05 (t, *J* = 8.0 HZ, 1H), 6.42 (s, 1H), 3.39 (t, *J* = 8.0 HZ, 2H), 2.85 (t, *J* = 8.0 HZ, 2H), 2.21 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 208.0, 158.2, 158.1, 140.6, 136.9, 129.2, 122.8, 122.0, 119.8, 117.2, 114.2, 106.0, 43.4, 30.0, 23.8 ppm; IR *v* (neat, cm^{-1}) 2923, 1711, 1564, 1425, 1352, 743. MS (EI, 70 eV) *m/z* (%): 265, 222 (100%), 207, 195, 154, 128, 115, 77.

HRMS (ESI): m/z calcd for $C_{16}H_{15}N_3O$ $[M+H]^+$: 266.1288; found: 266.1284.m

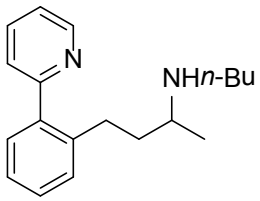
4-(2-(pyridin-2-yl)phenyl)butan-2-ol (5a)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (d, *J* = 4.0 HZ, 1H), 7.70 (t, *J* = 8.0 HZ, 1H), 7.34 (d, *J* = 8.0 HZ, 1H), 7.27 (s, 2H), 7.23 - 7.17 (m, 3H), 5.99 (s, 1H), 3.58 (s, *J* = 8.0 HZ, 1H), 2.92 (td, *J* = 14.1, 5.5 HZ, 1H), 2.60-2.54 (m, 1H), 1.86 - 1.79 (m, 1H), 1.71 - 1.63 (m, 1H), 1.06 (d, *J* = 8.0 HZ, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.7, 147.8, 139.8, 139.7, 137.4, 130.3, 129.9, 128.8, 125.9, 124.9, 122.0, 64.6, 40.4, 27.5, 23.1 ppm; IR *v* (neat, cm^{-1}) 3390, 2967, 2919, 1587, 1464, 1127, 1066, 754.

RMS (ESI): m/z calcd for $C_{15}H_{17}NO$ $[M+H]^+$: 228.1383; found: 228.1377.

N-(4-(2-(pyridin-2-yl)phenyl)butan-2-yl)butan-1-amine (6a)

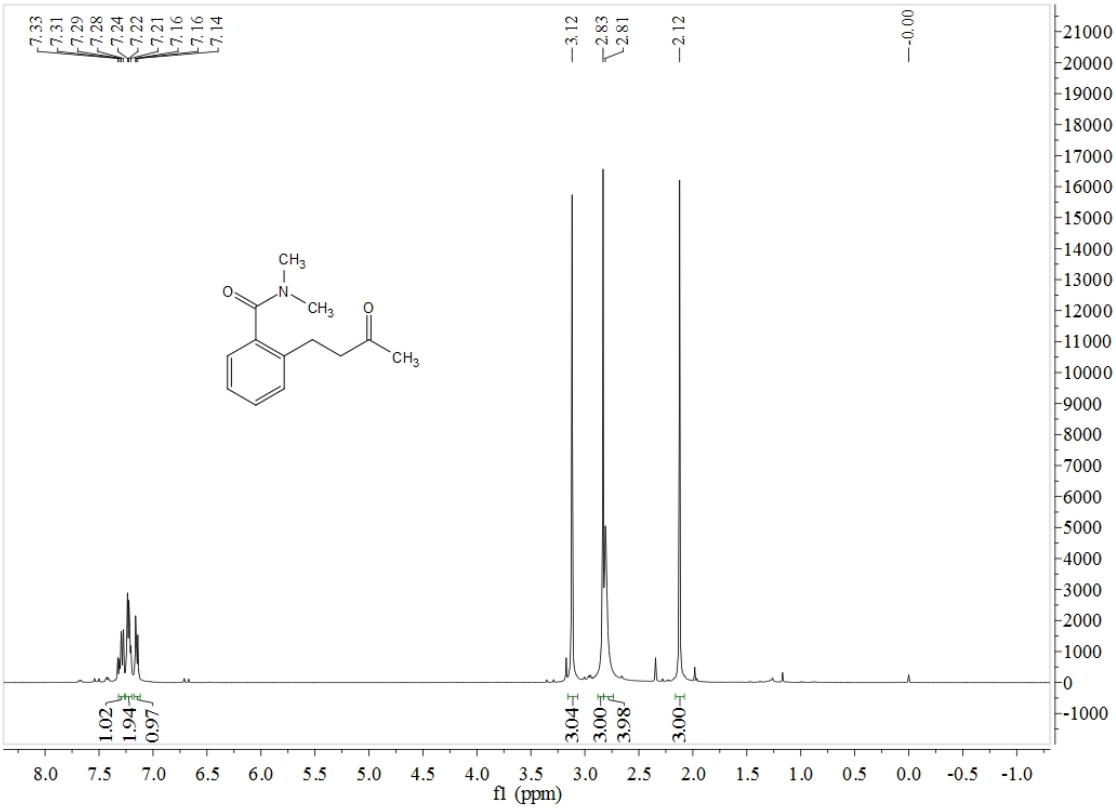


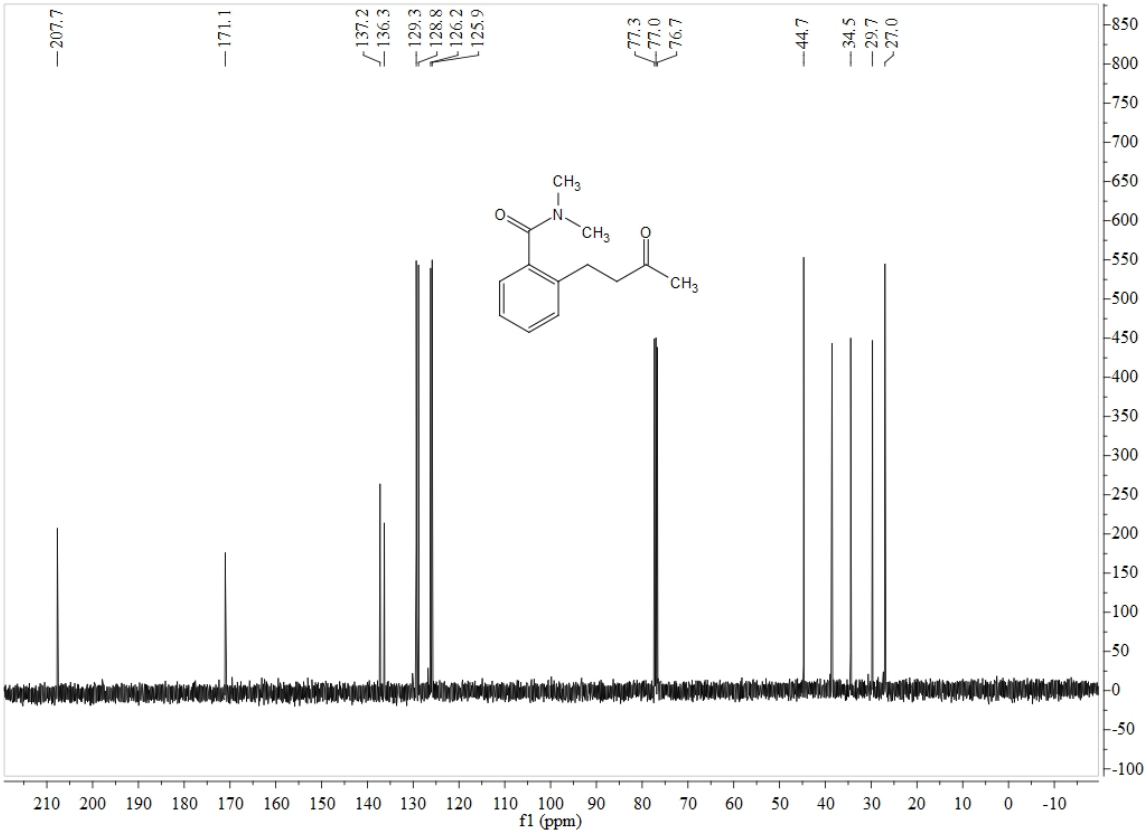
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 (d, *J* = 4.2 Hz, 1H), 7.79 (t, *J* = 7.7 Hz, 1H), 7.42 (d, J = 7.8 Hz, 1H), 7.38 – 7.28 (m, 5H), 2.92 – 2.83 (m, 2H), 2.76 – 2.65 (m, 2H),

2.56 (dd, J = 13.0, 6.0 Hz, 1H), 2.50 – 2.40 (m, 1H), 1.83 (dt, J = 14.2, 6.3 Hz, 1H), 1.67 (dt, J = 14.4, 6.9 Hz, 2H), 1.42 – 1.32 (m, 2H), 1.30 – 1.18 (m, 2H), 1.06 (d, J = 6.3 Hz, 2H), 0.84 (t, J = 7.3 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 160.03, 148.93, 140.12, 136.51, 129.89, 129.80, 128.54, 126.02, 124.23, 121.84, 52.67, 46.24, 37.70, 31.74, 28.98, 20.47, 19.69, 13.92 ppm; IR v (neat, cm^{-1}) 3853, 2974, 2374, 1659, 1242, 1061, 896. MS (EI, 70 eV) *m/z* (%): 281, 267, 239, 225, 210, 182, 168 (100%), 114, 100.

HRMS (ESI): m/z calcd for $C_{19}H_{26}N_2$ $[M+H]^+$: 283.2169; found: 283.2168.

3a





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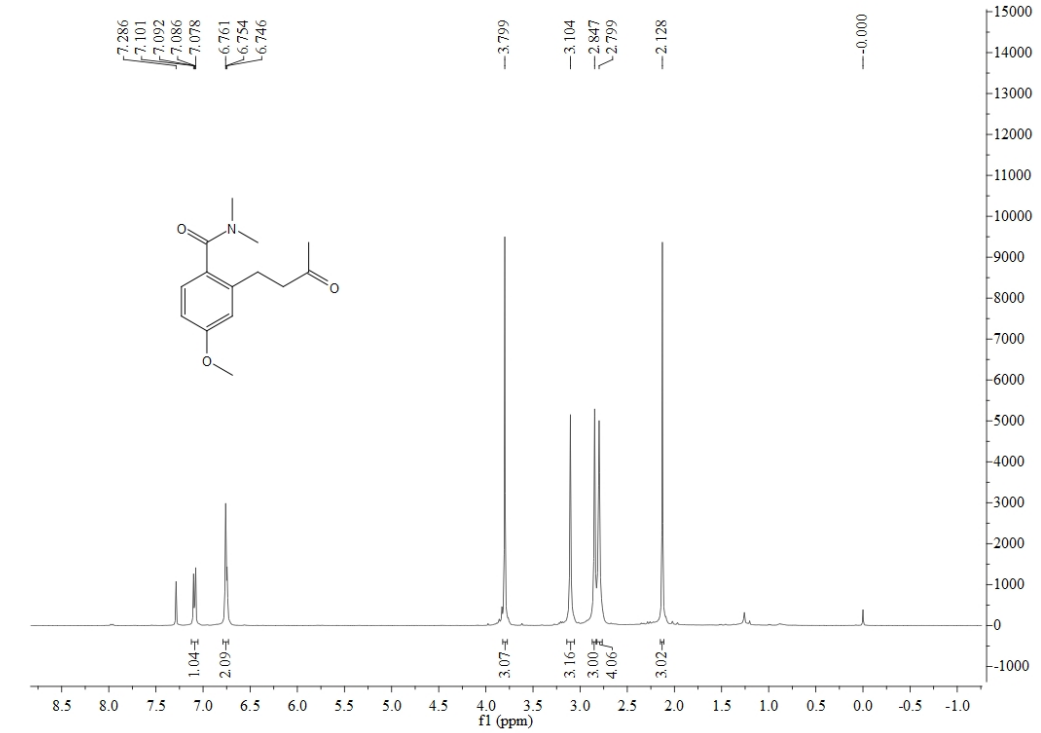

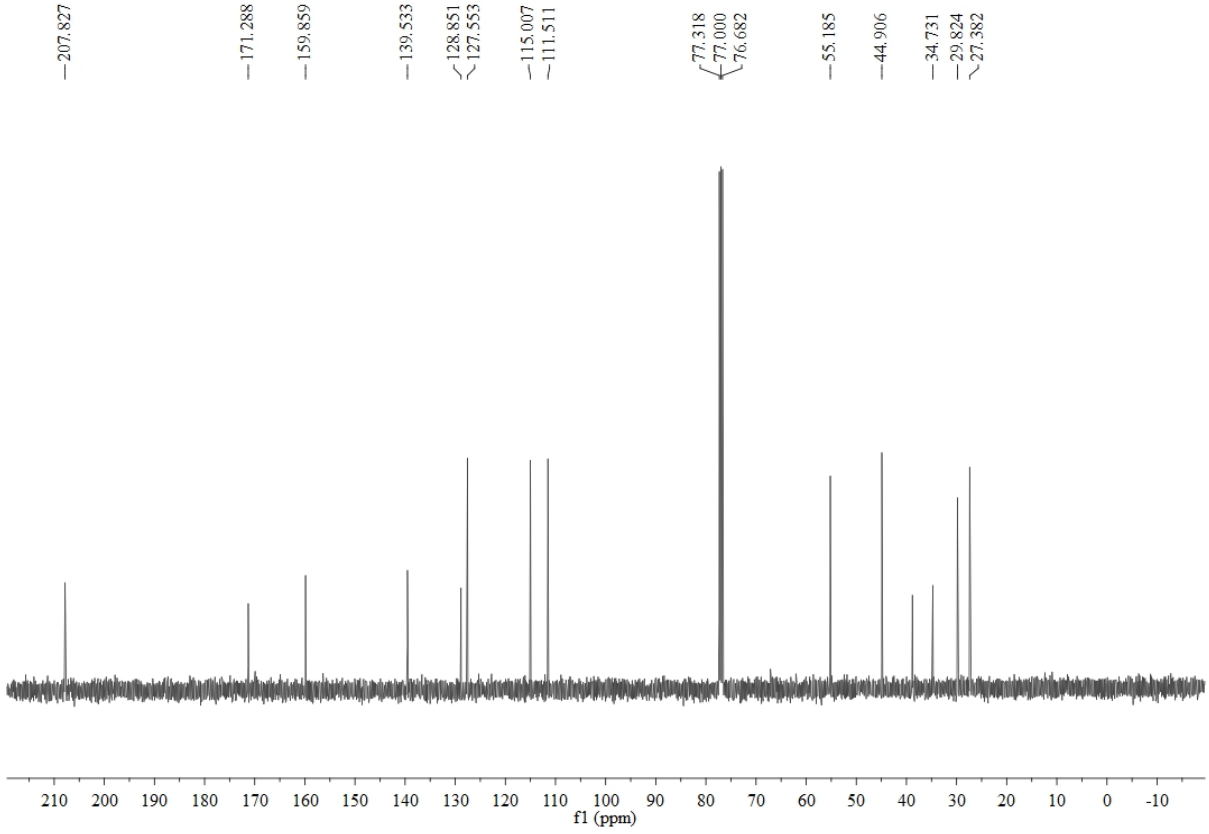

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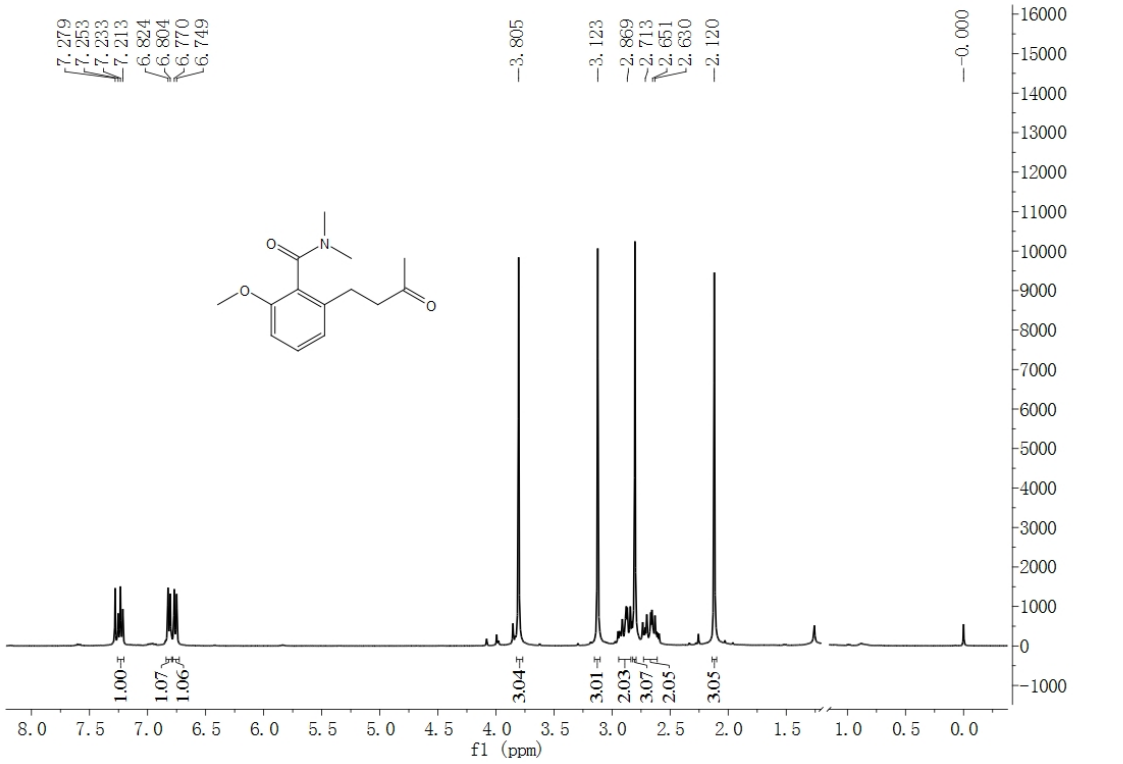

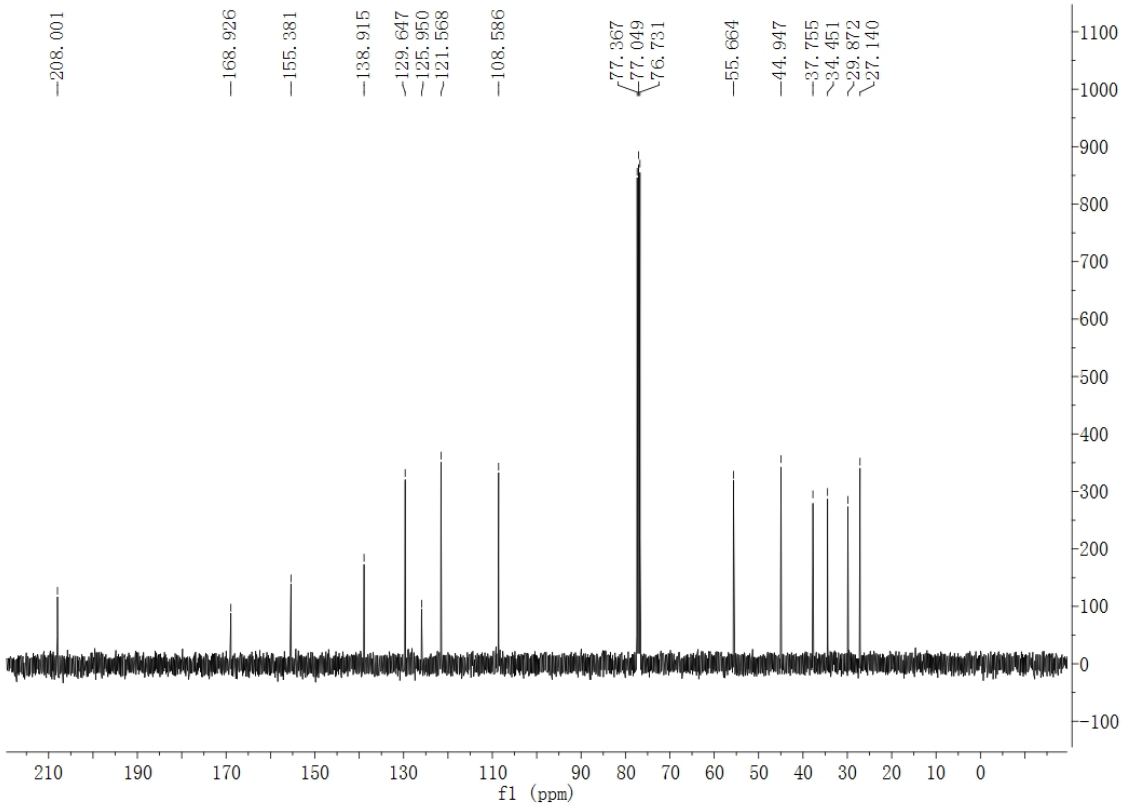

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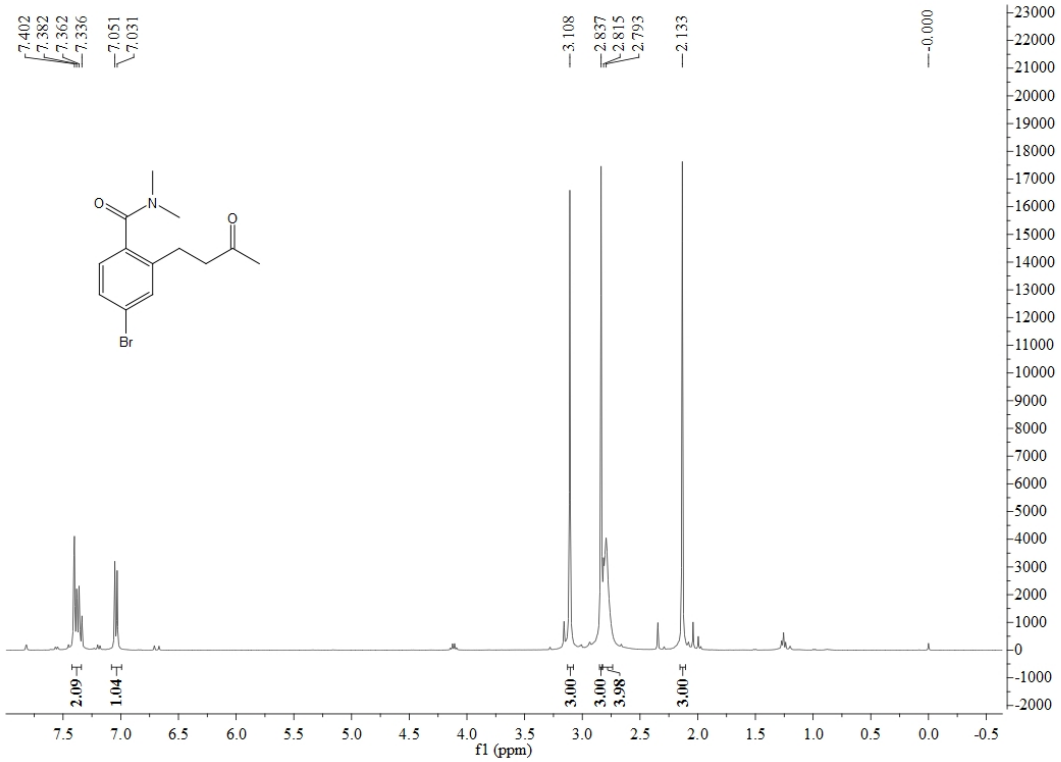

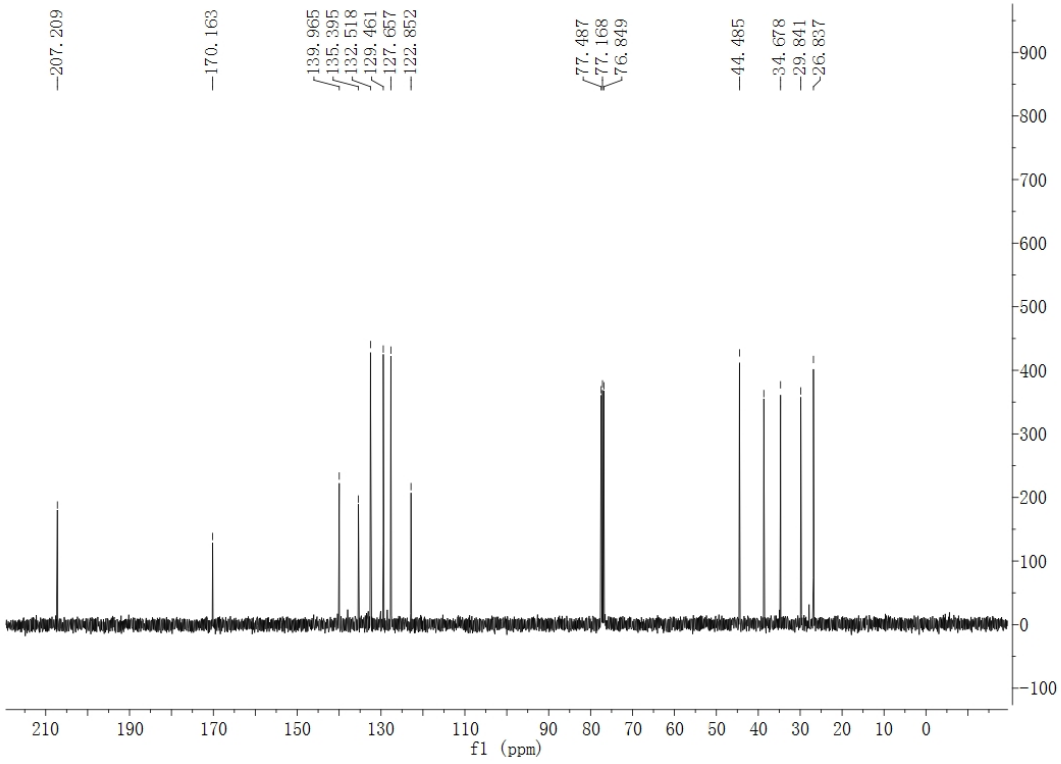

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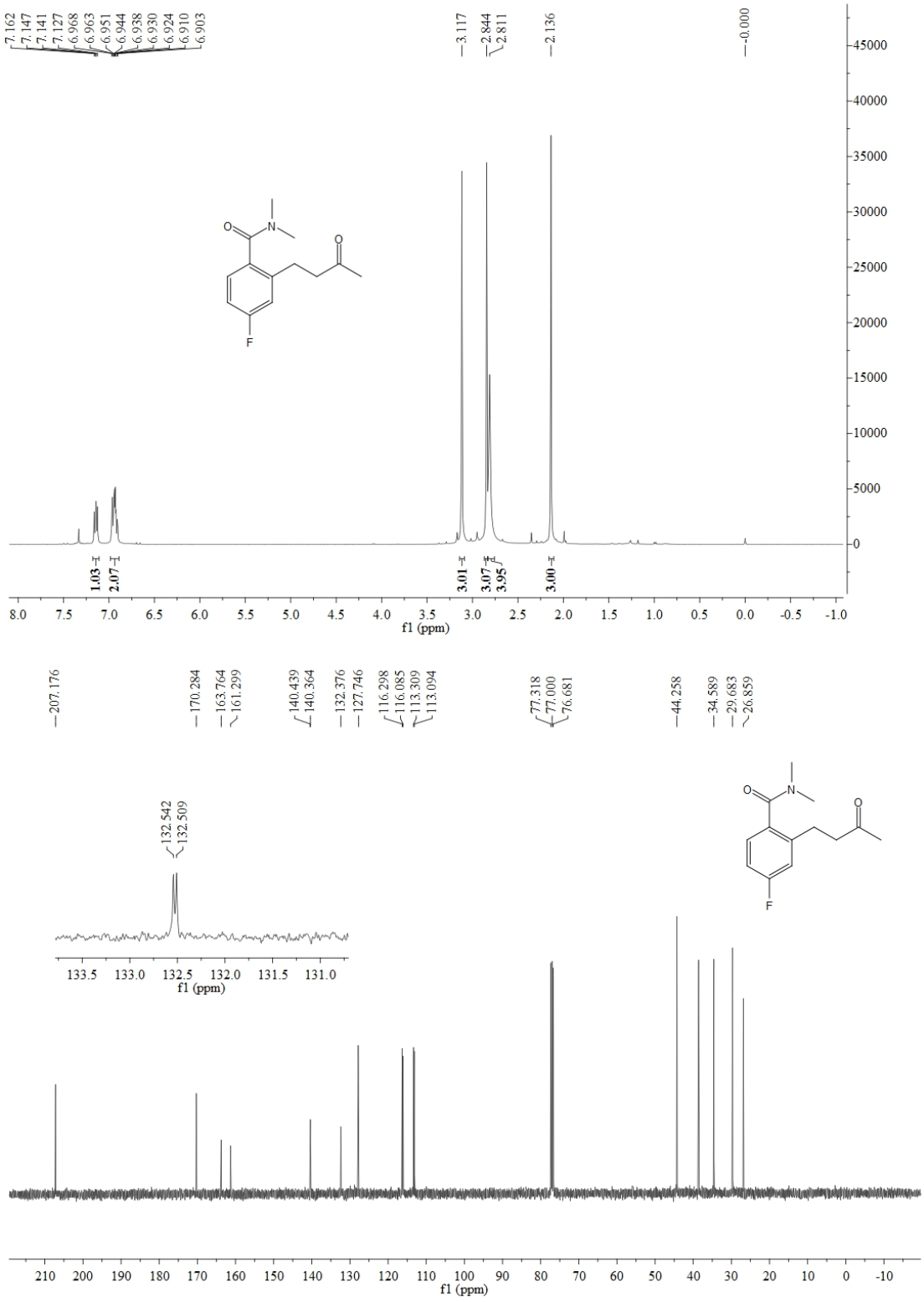

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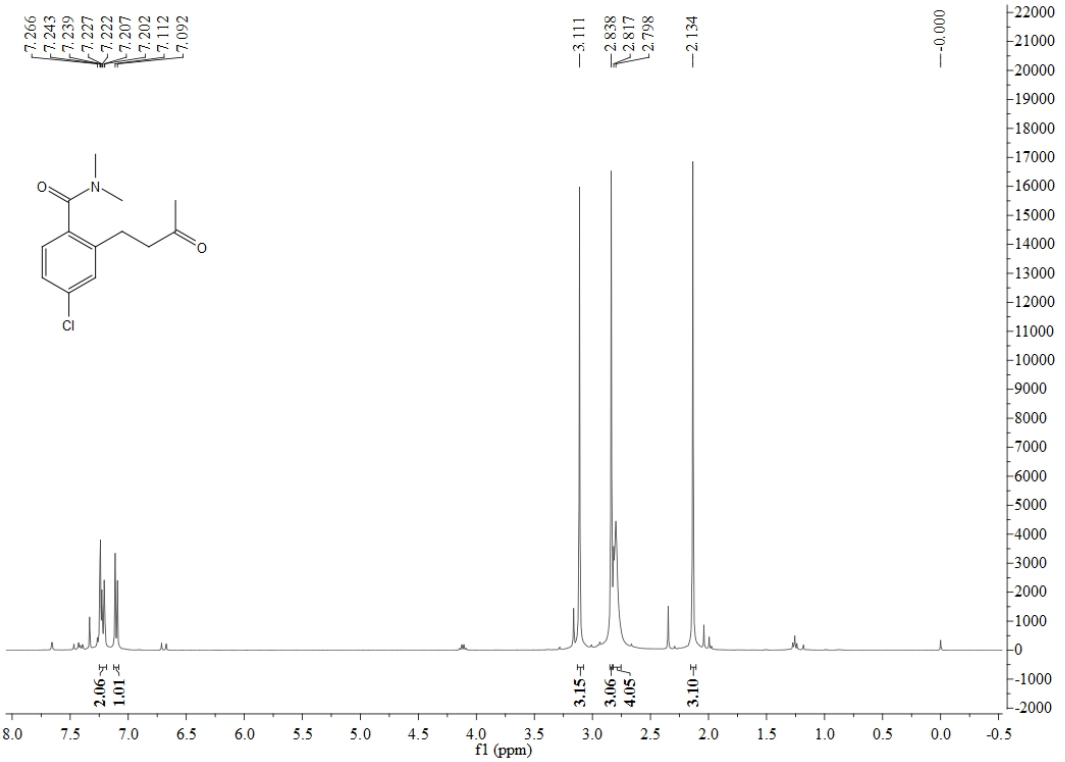

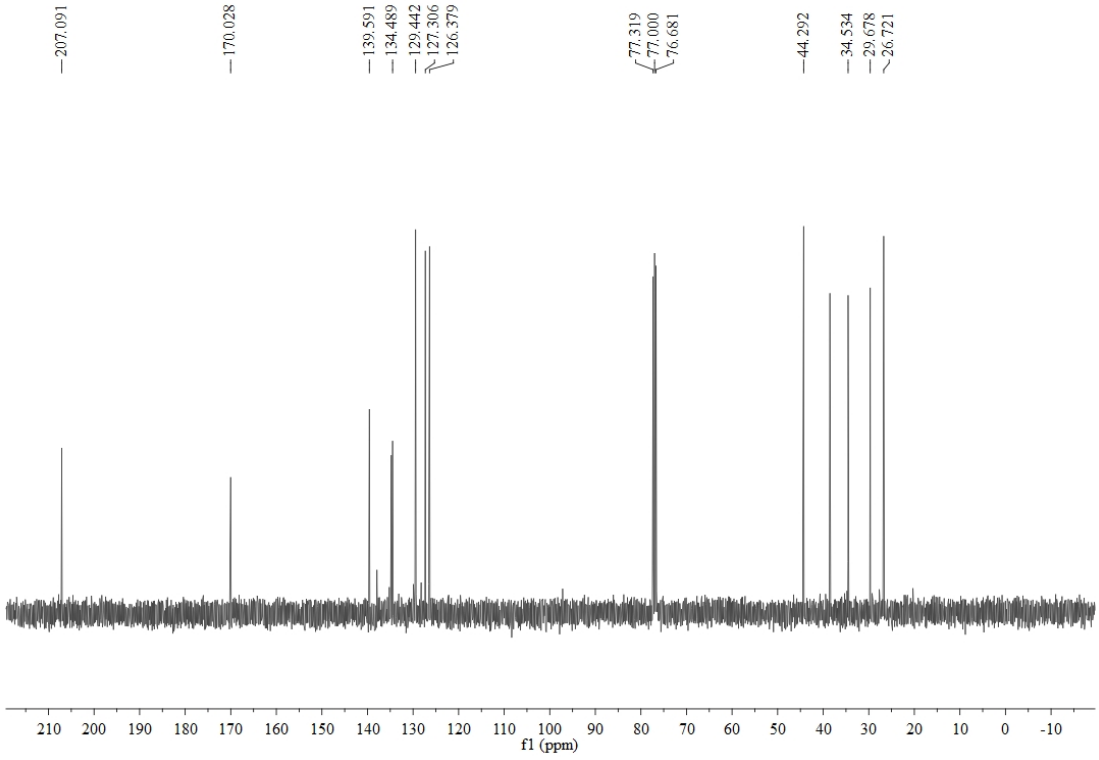

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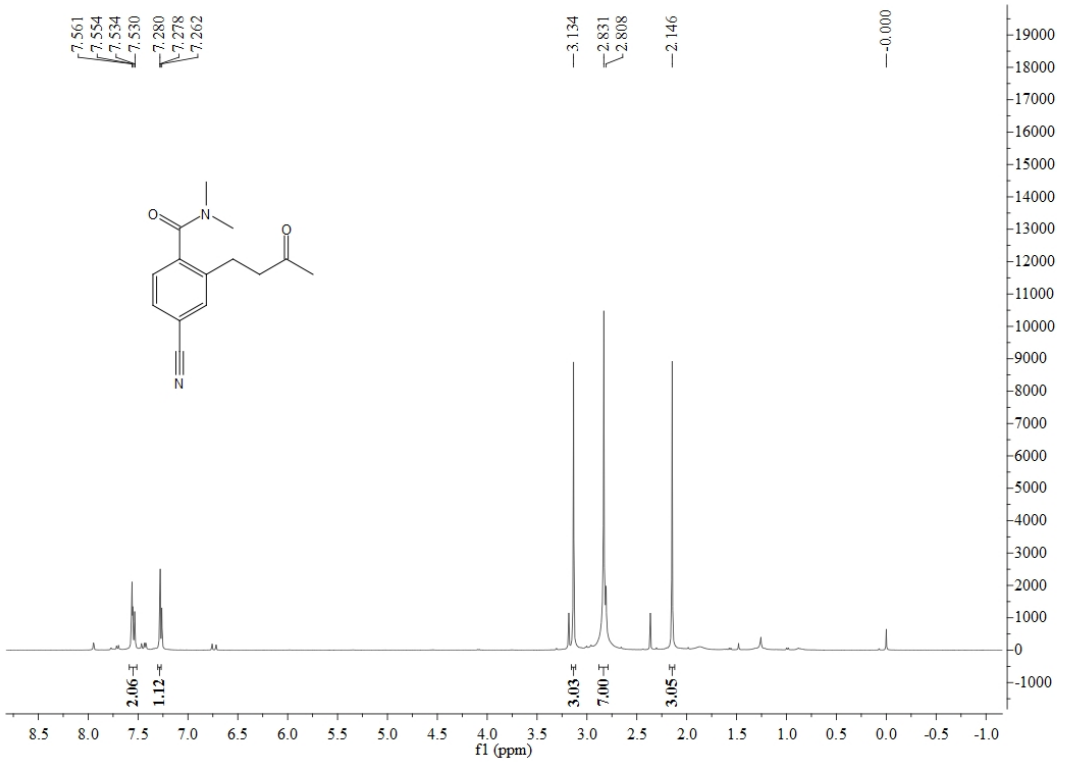

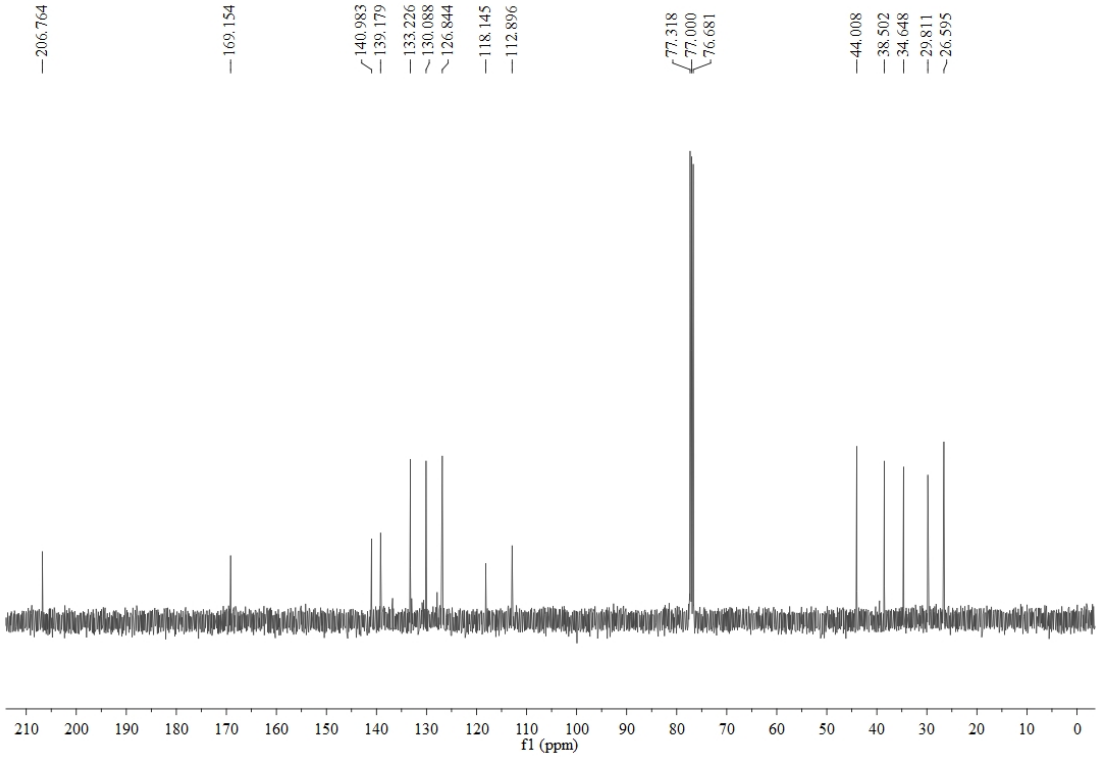

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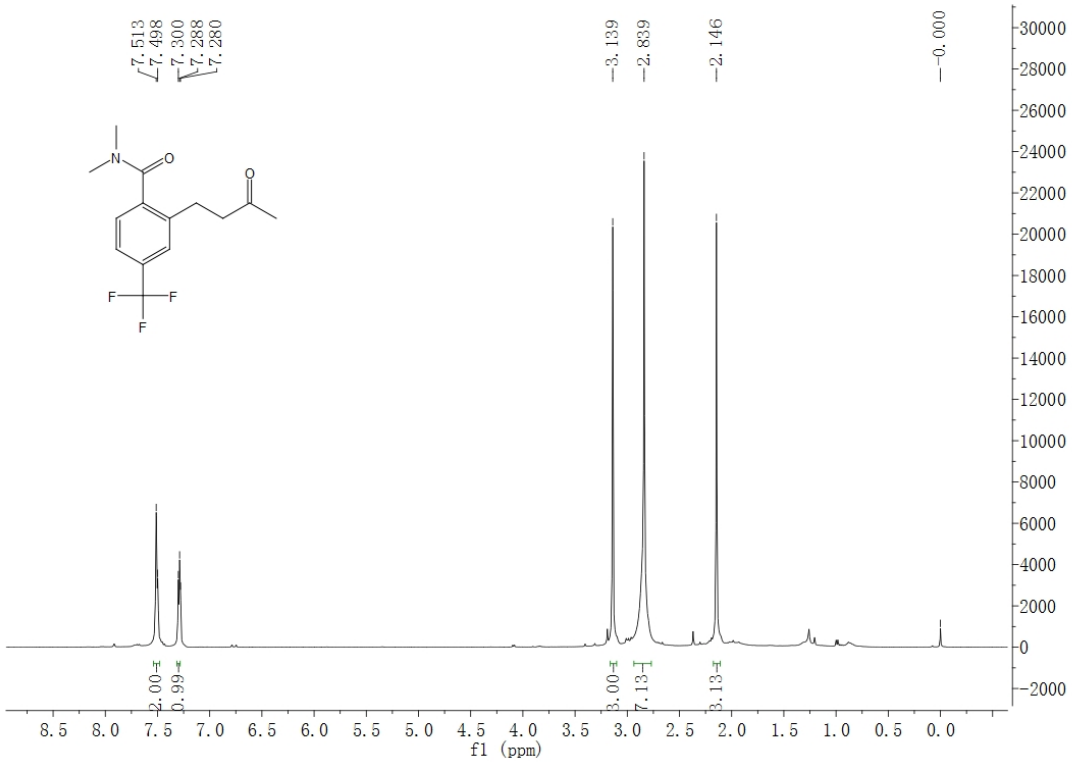

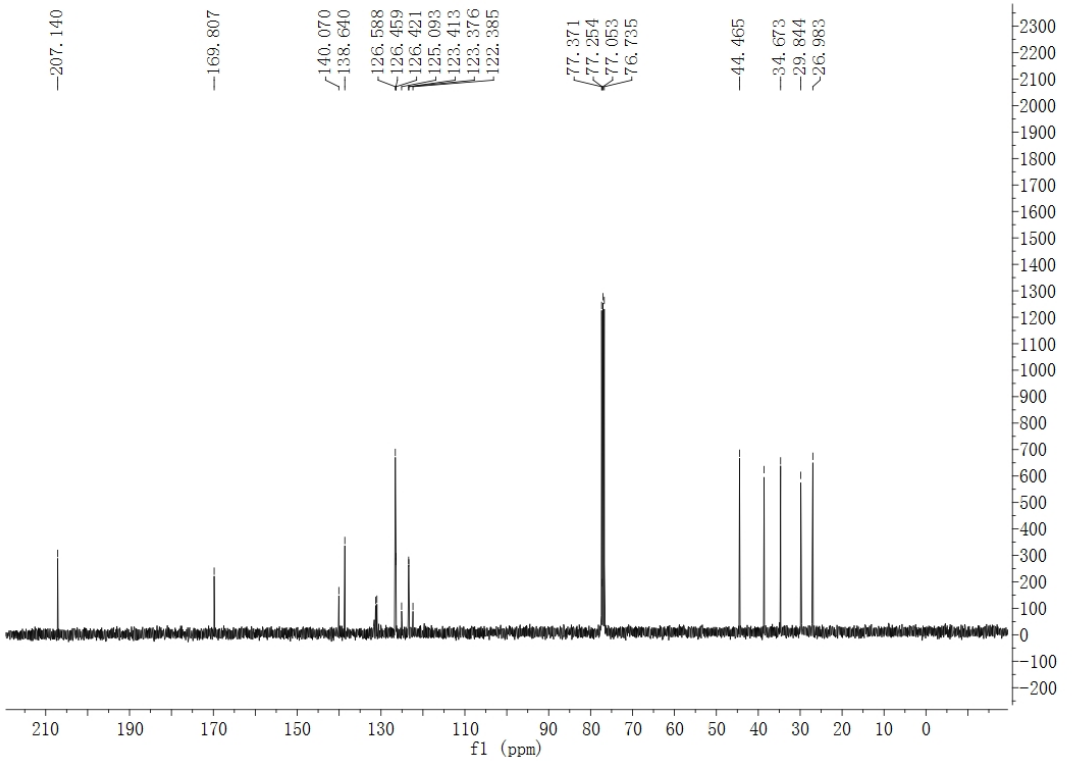

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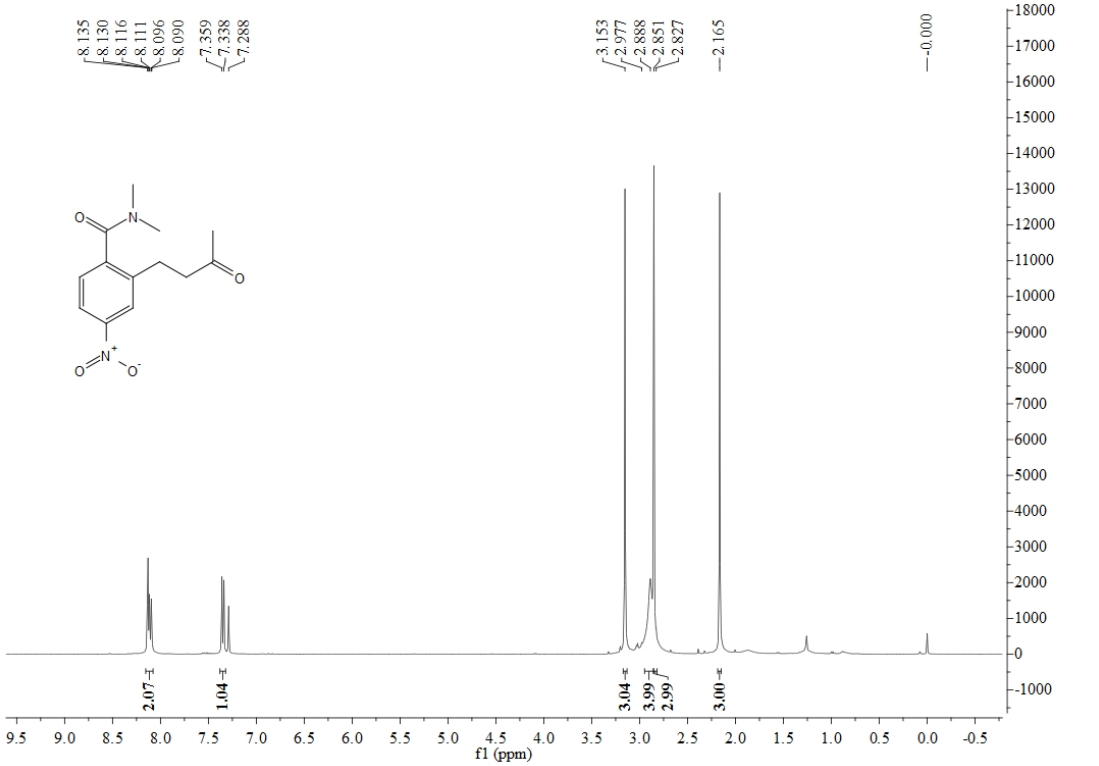

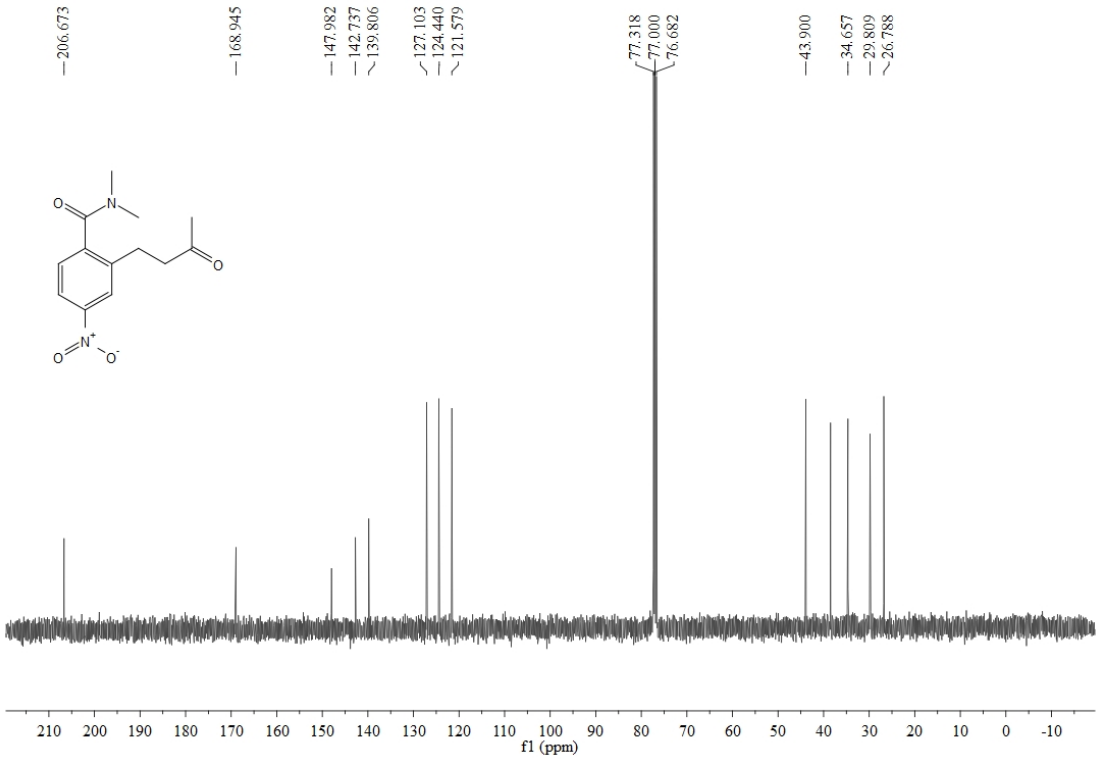

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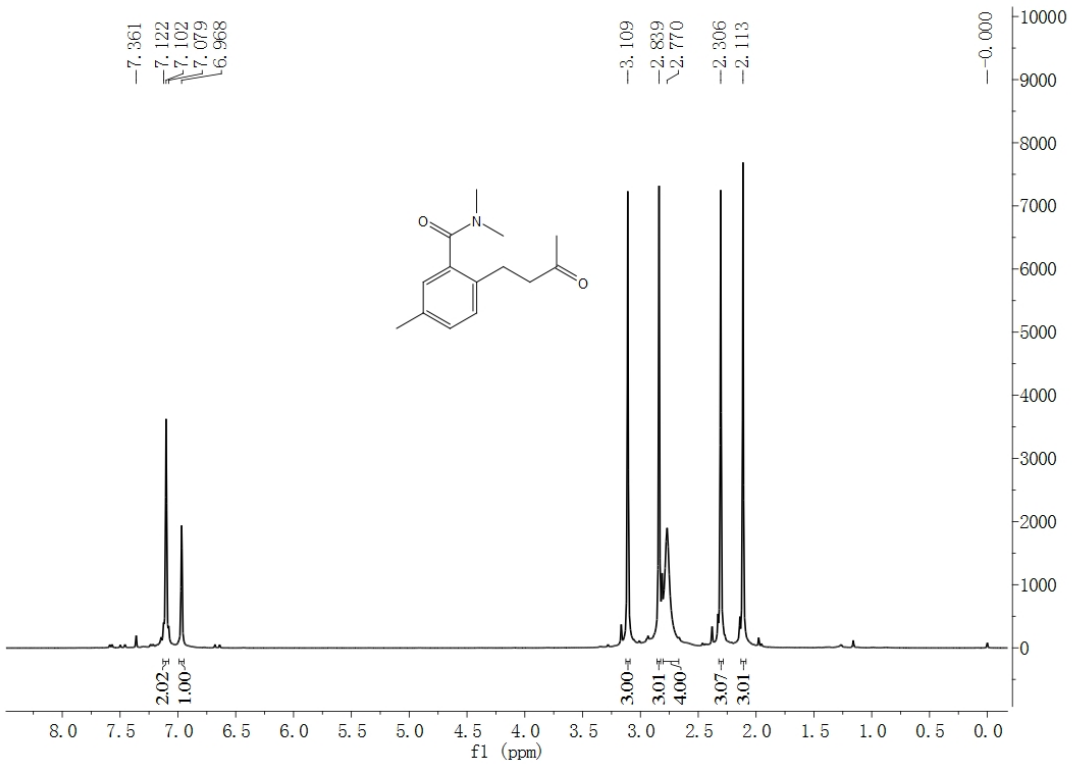

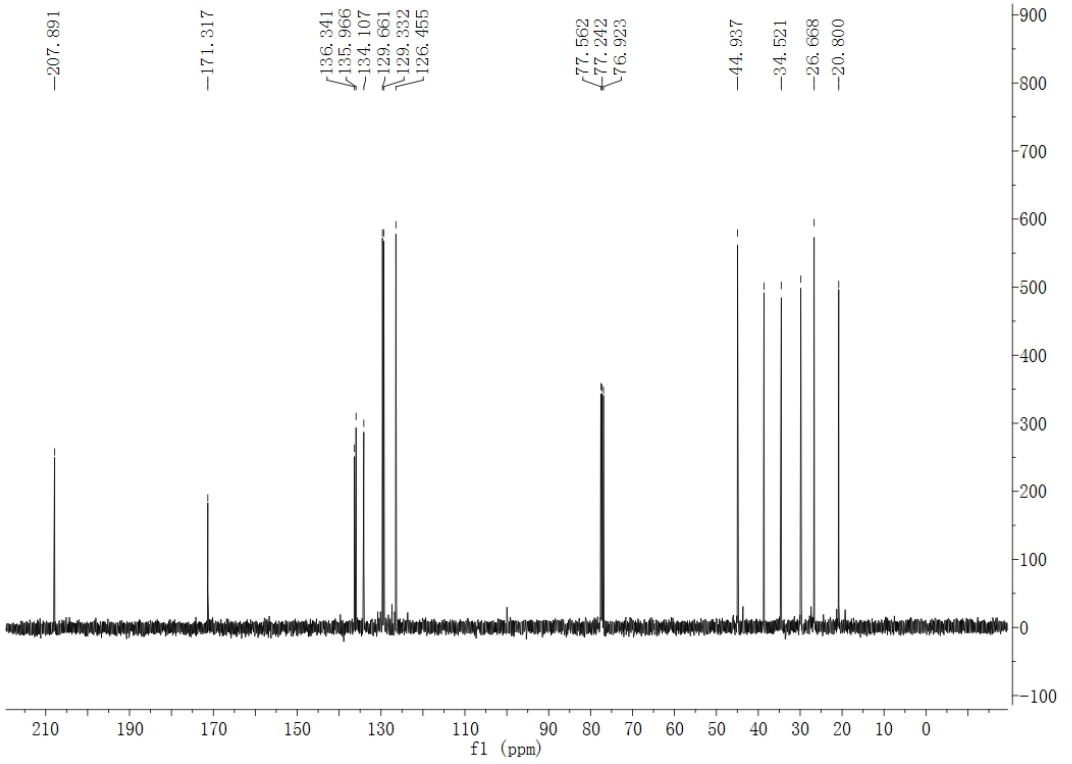

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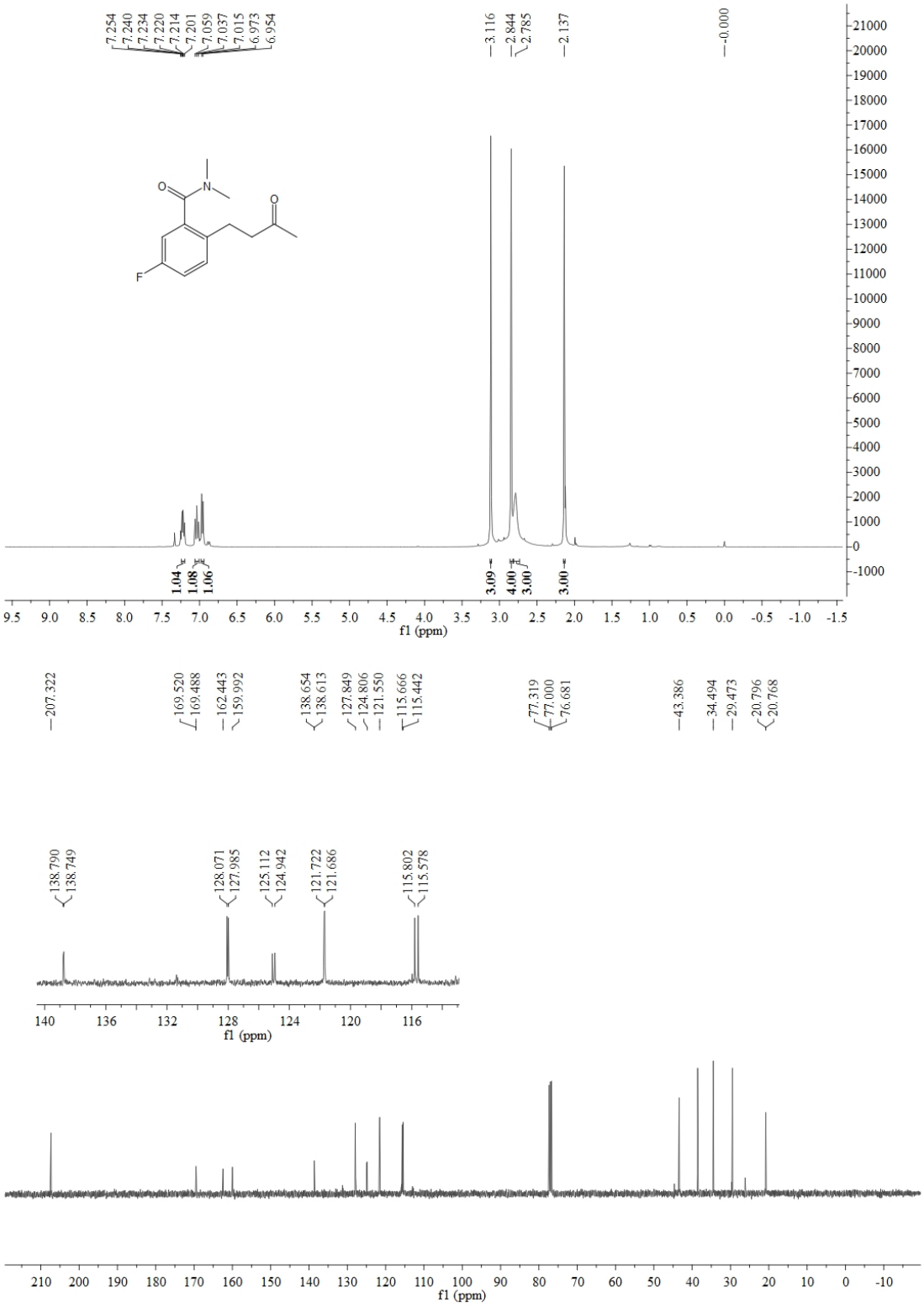

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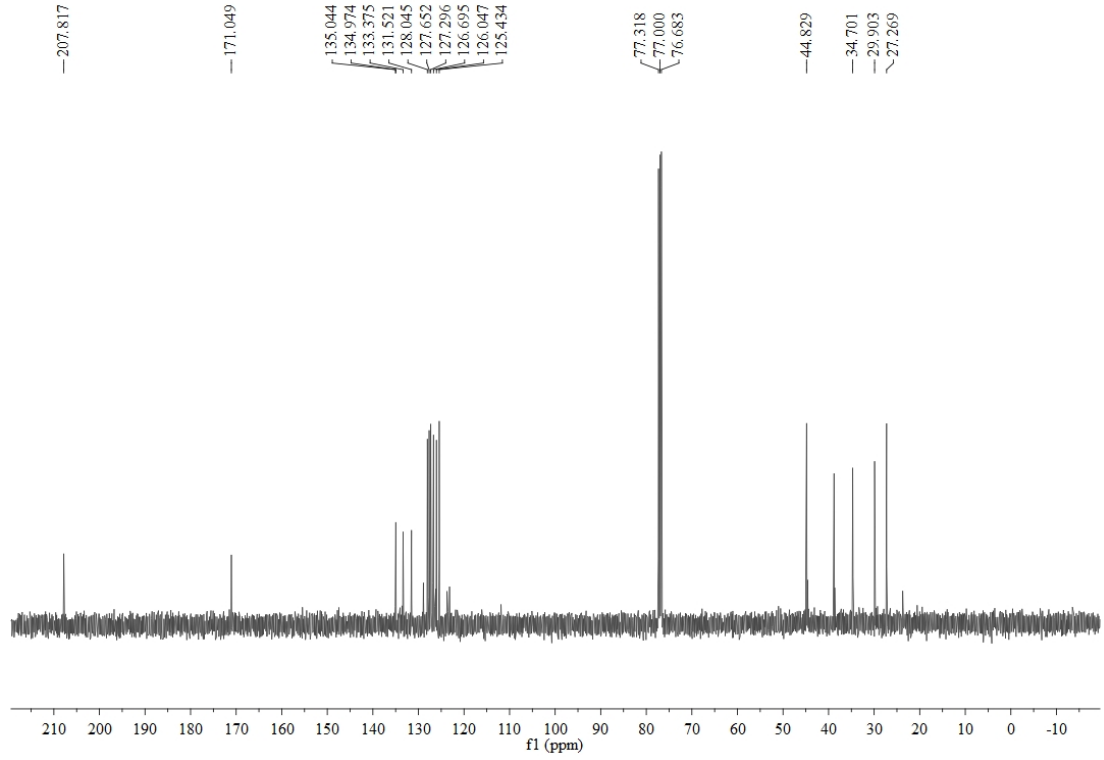

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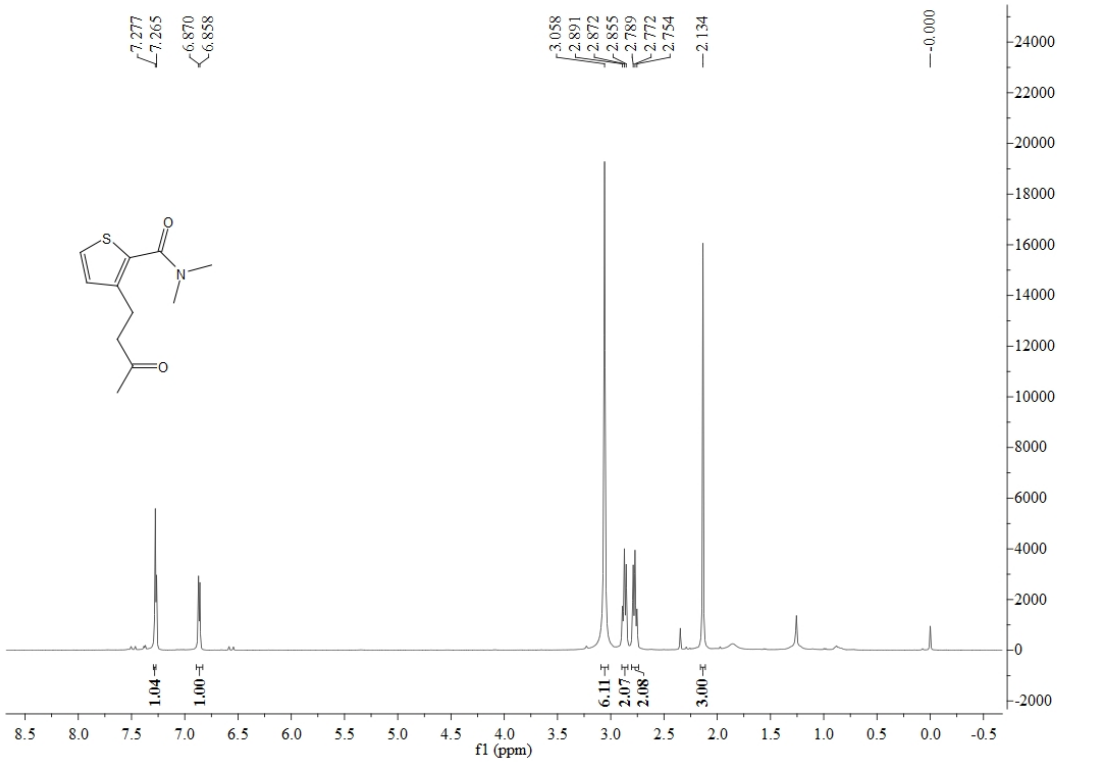

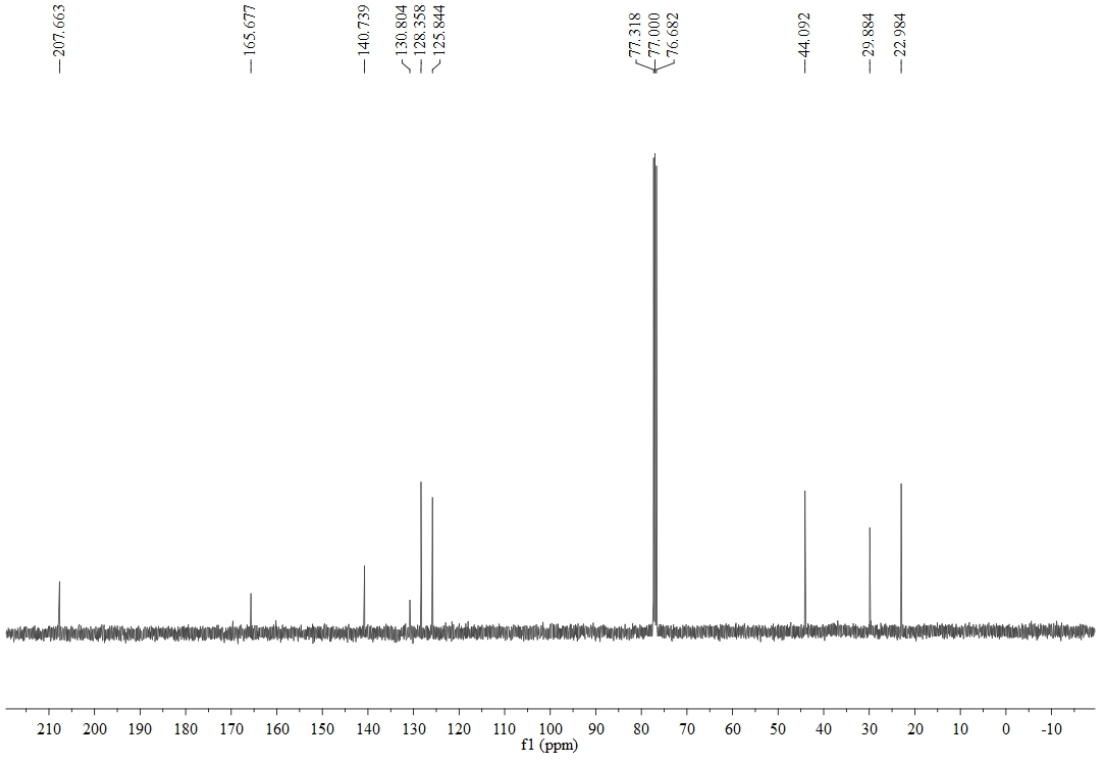

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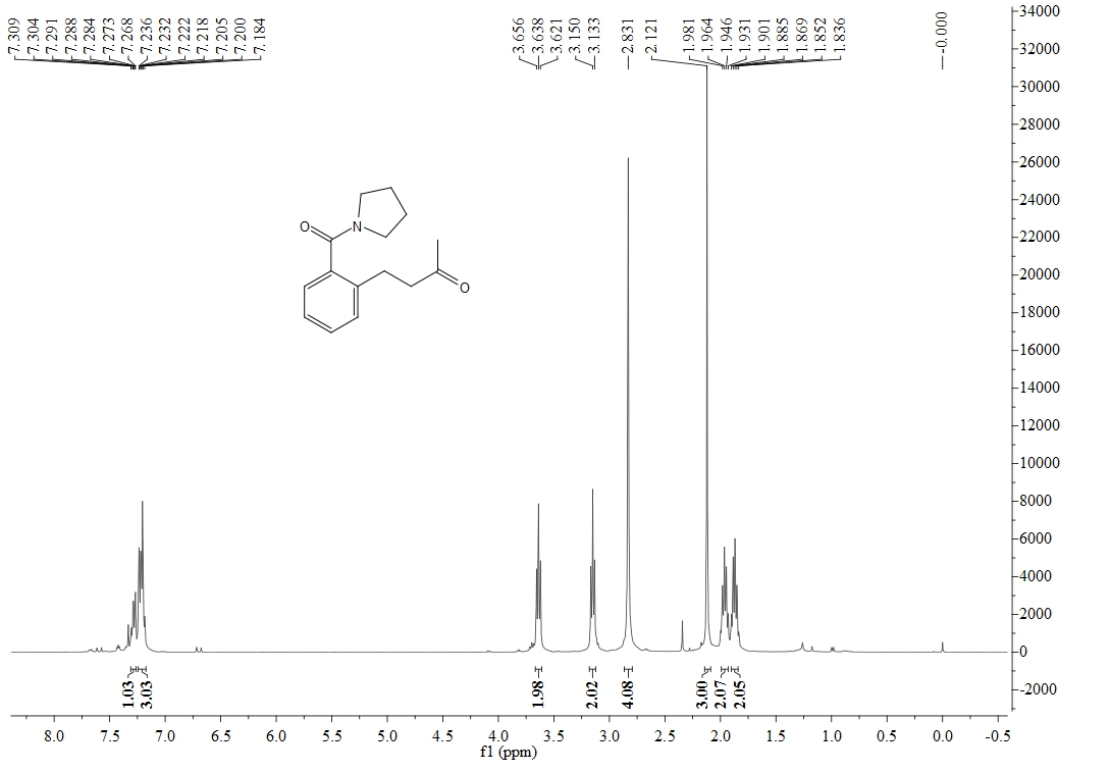

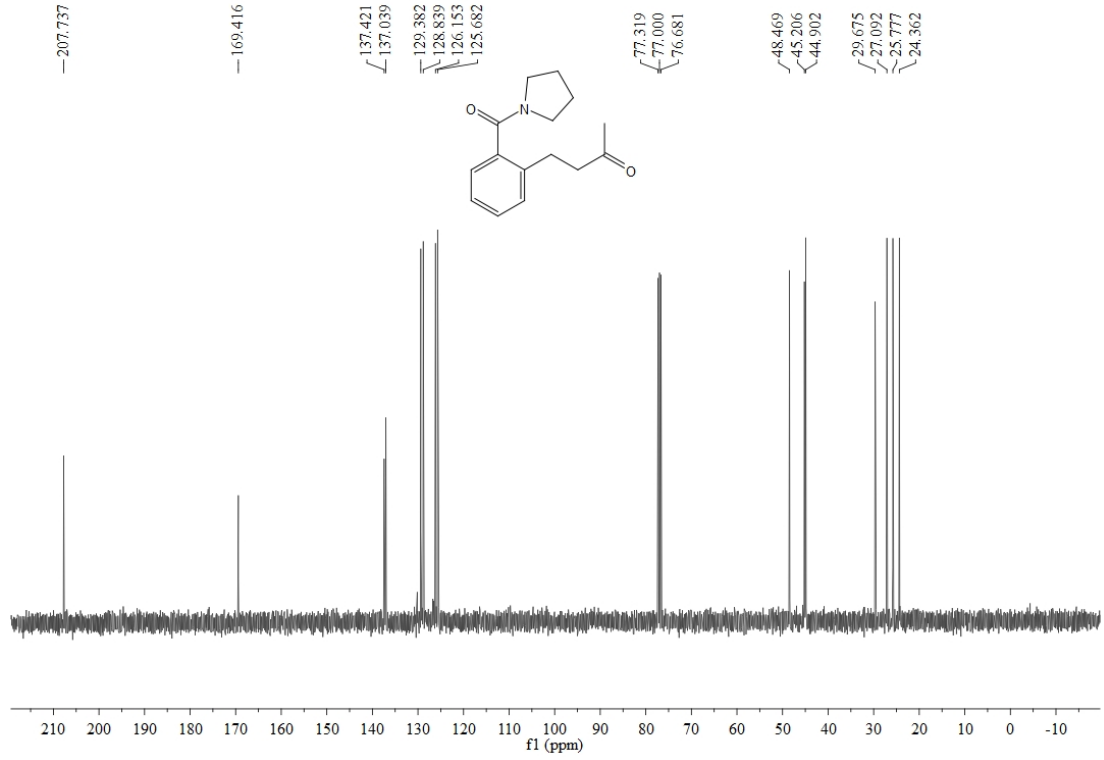

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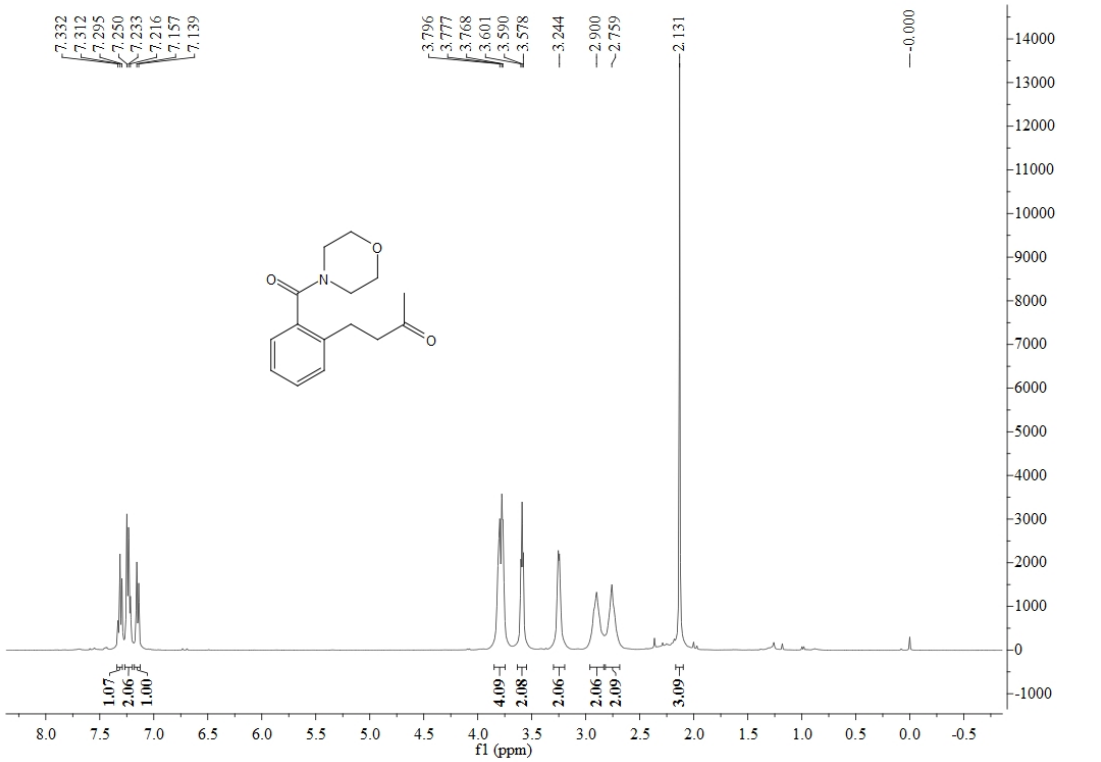

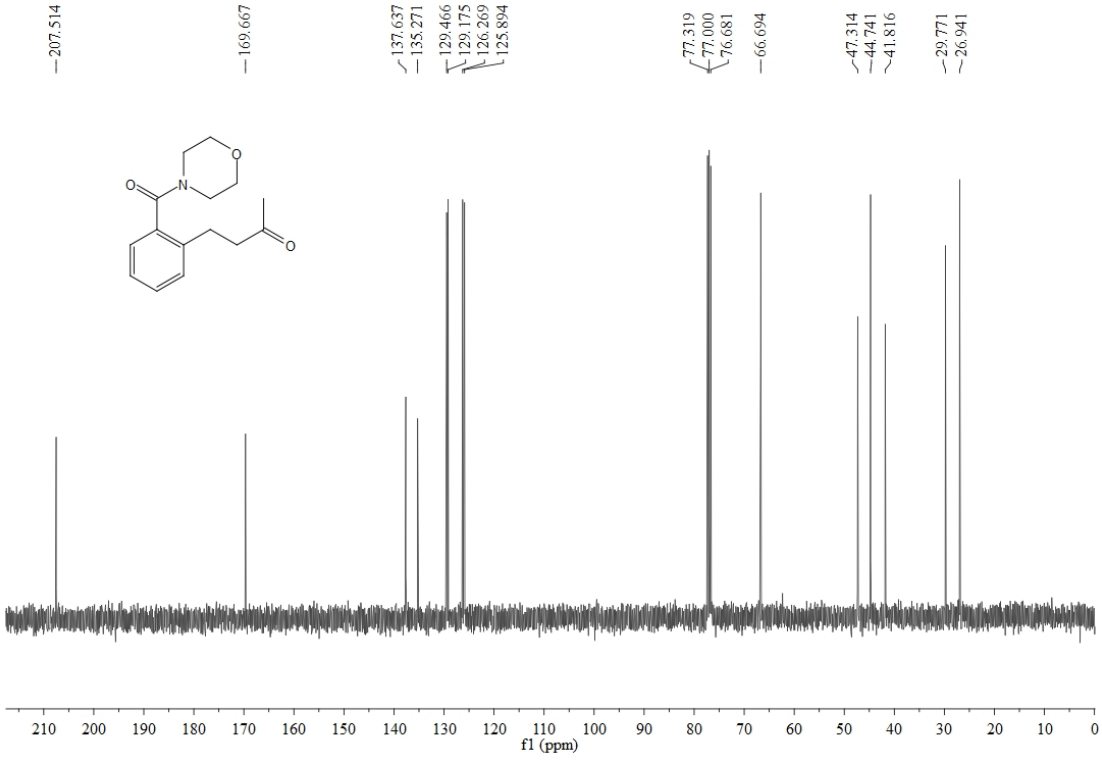

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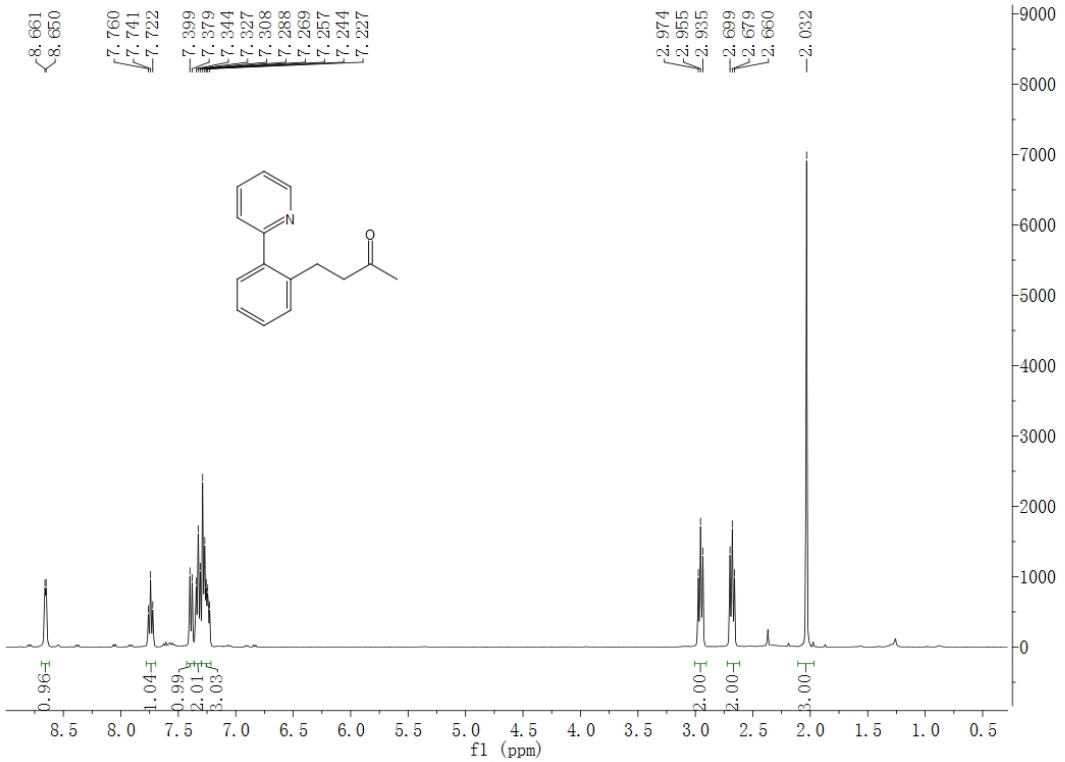

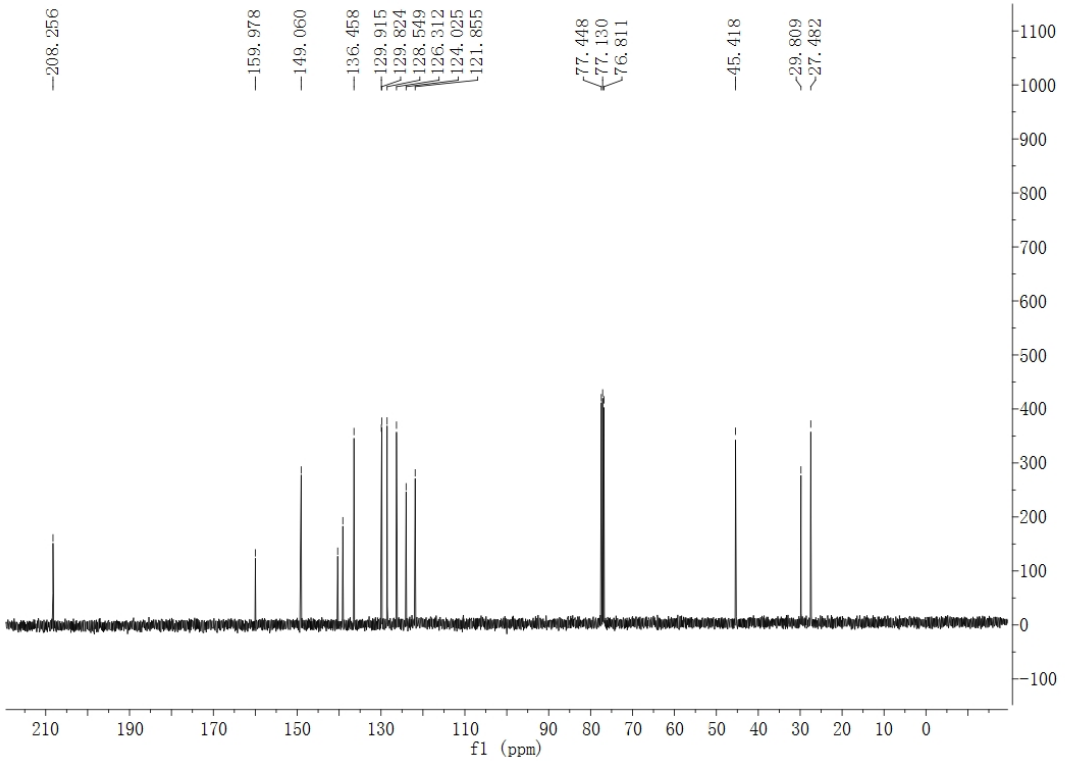

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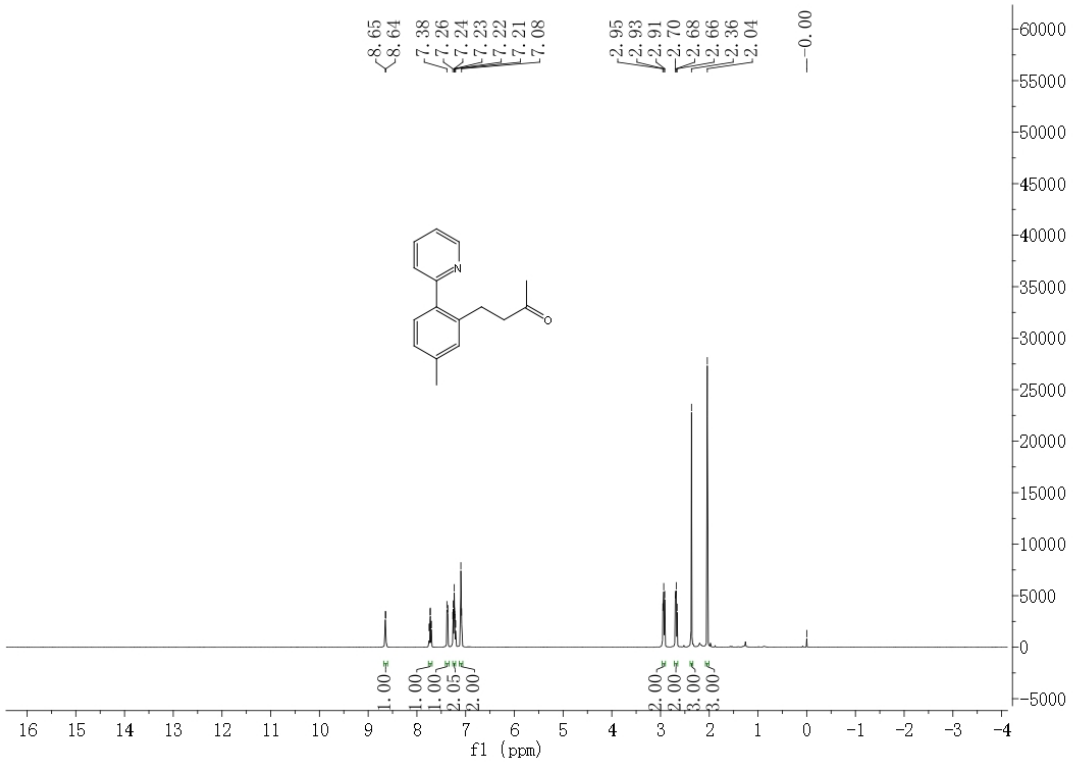

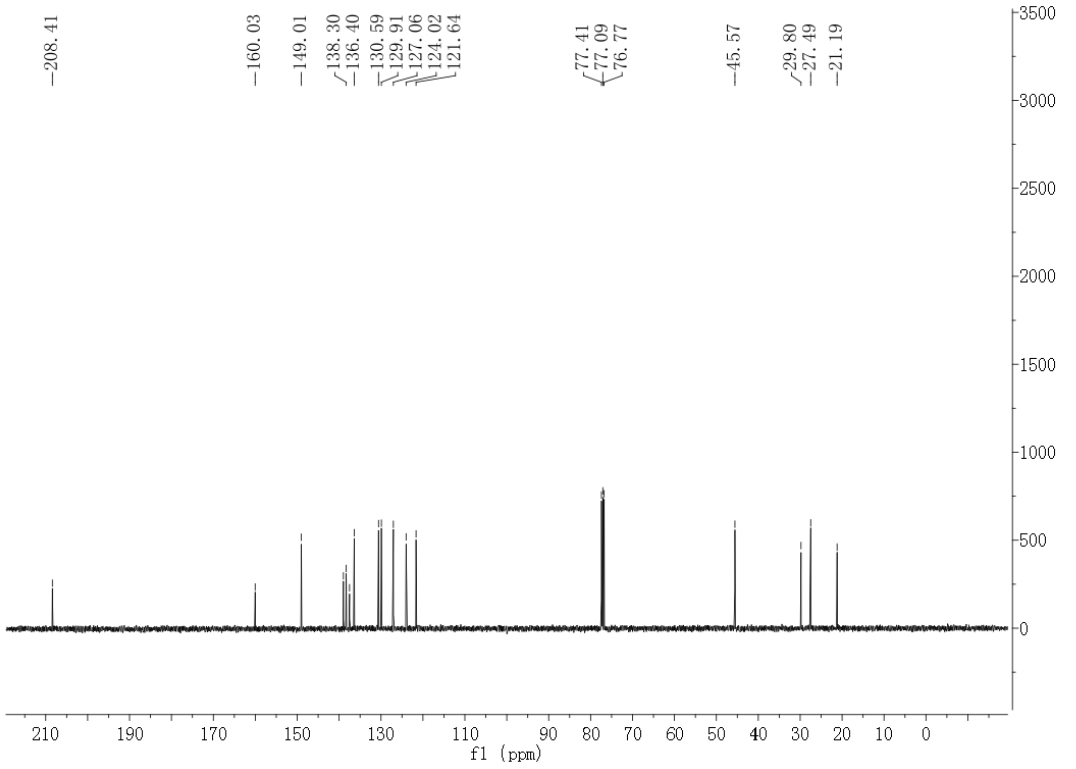

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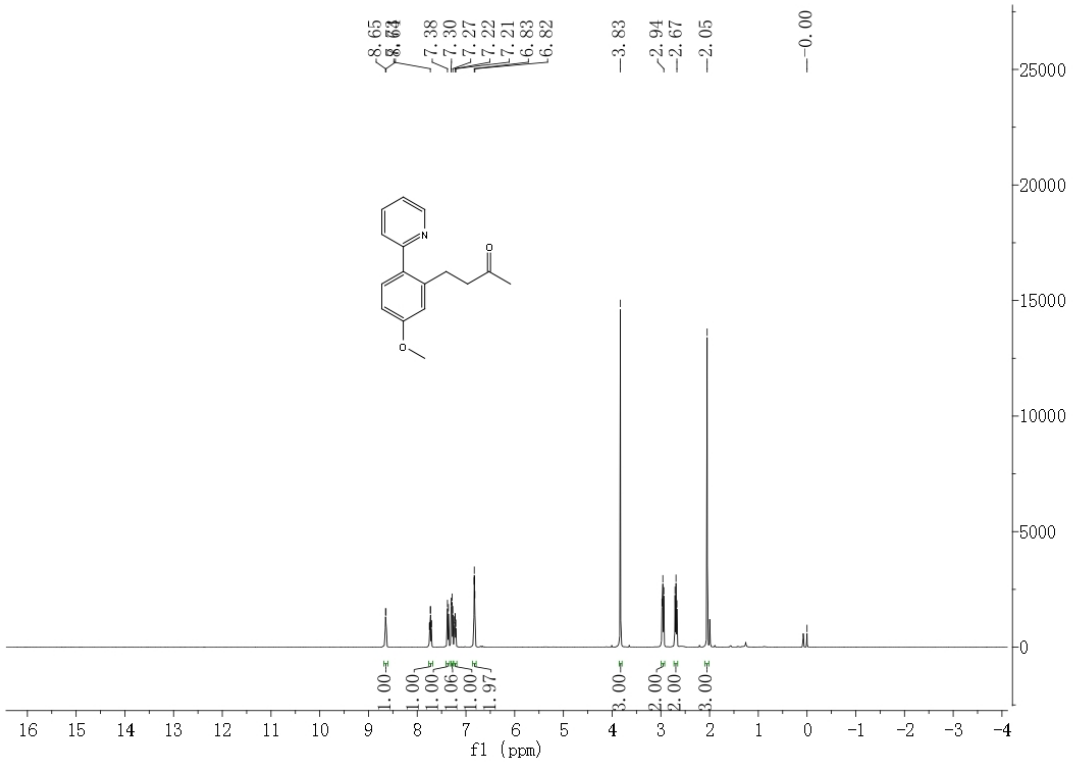

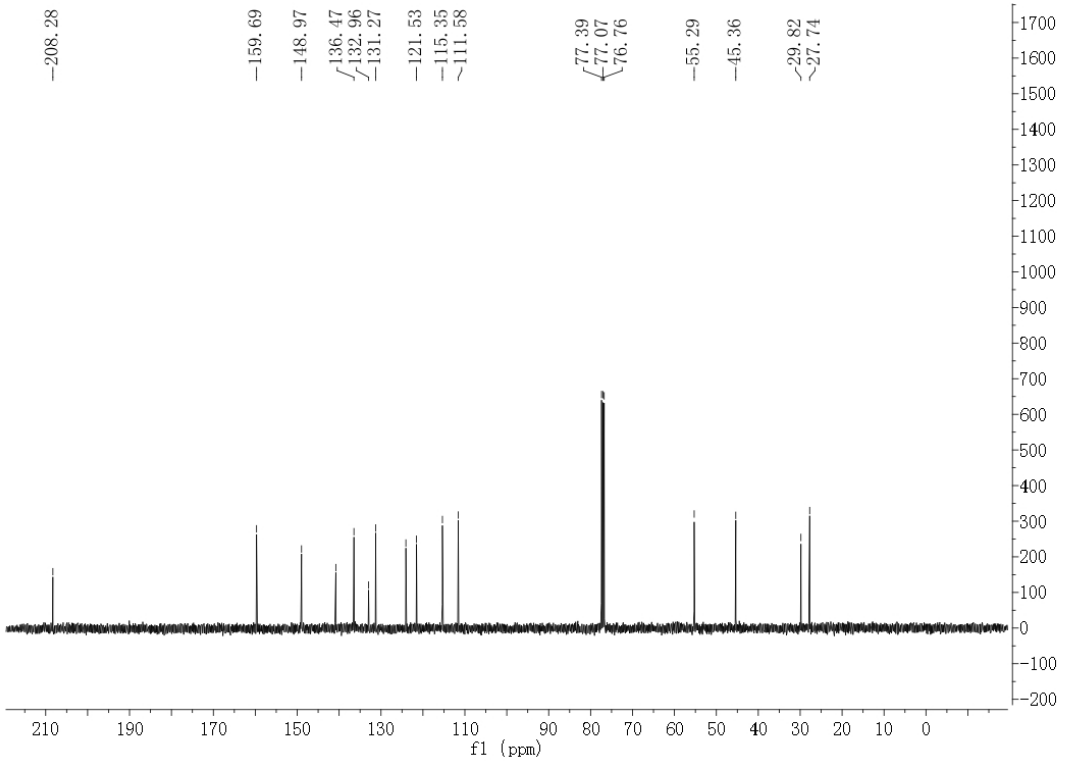

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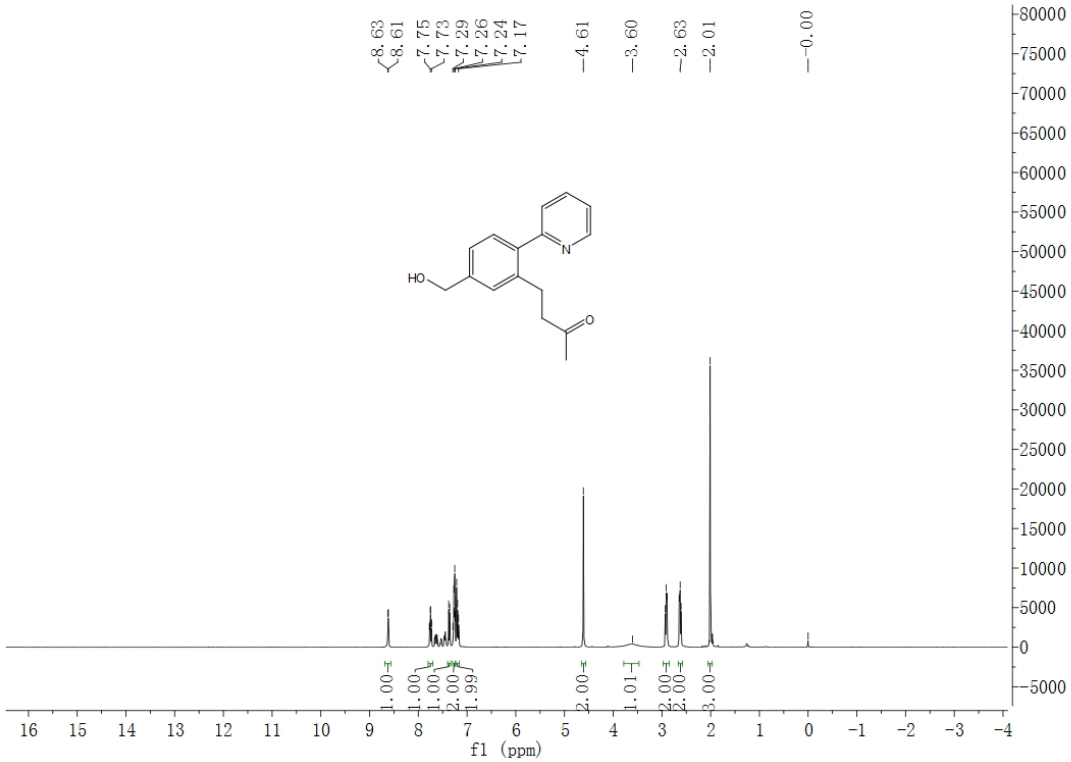

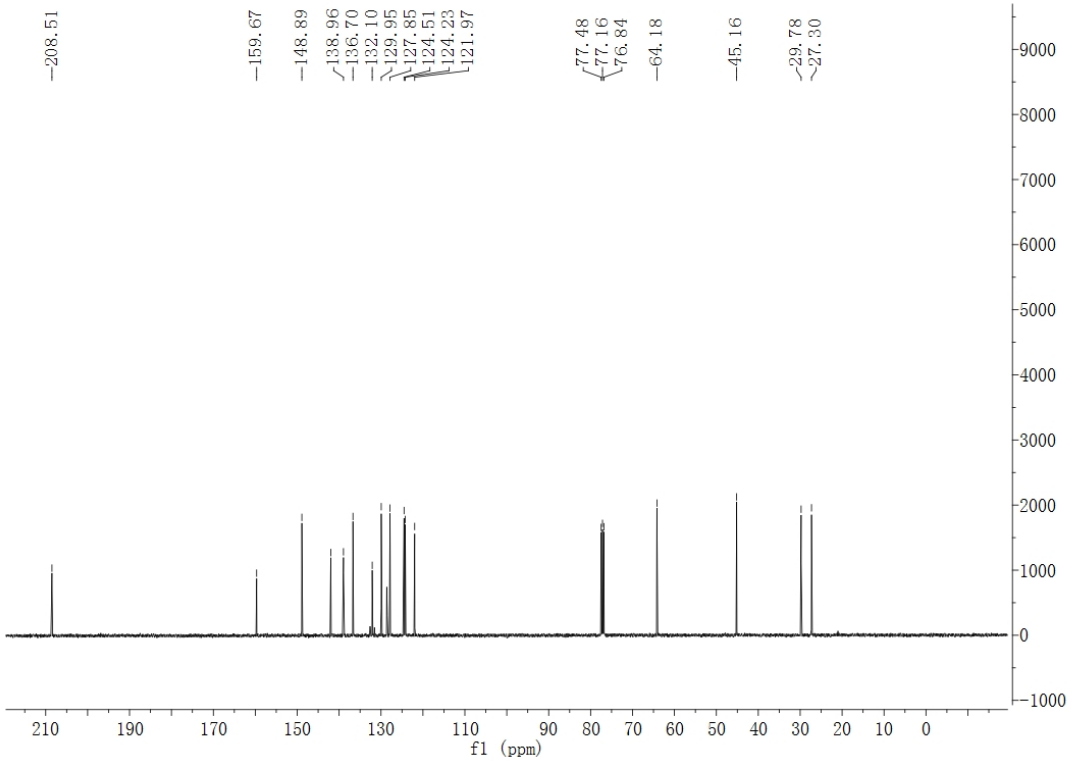

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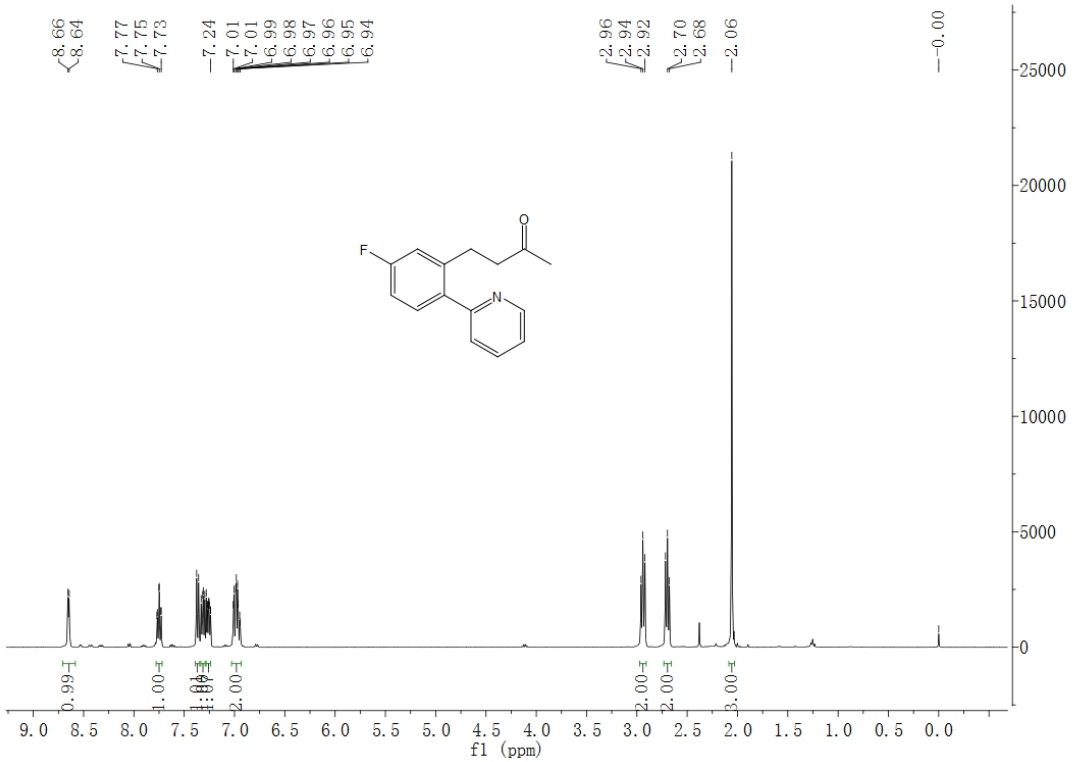

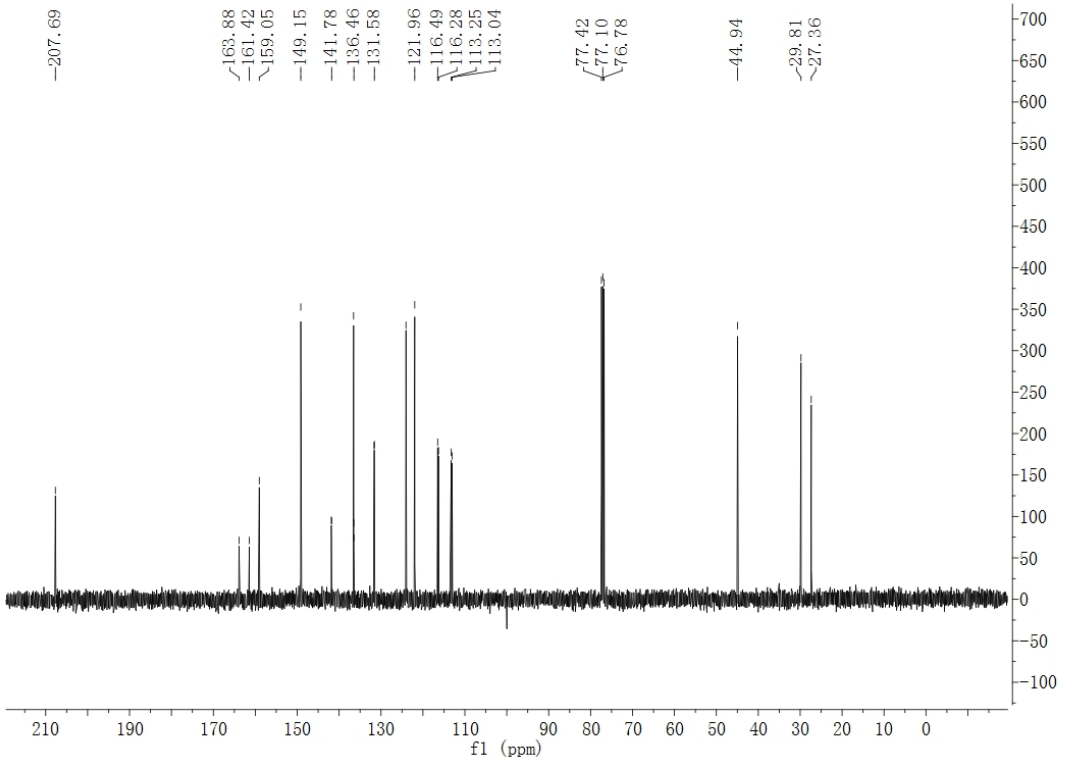

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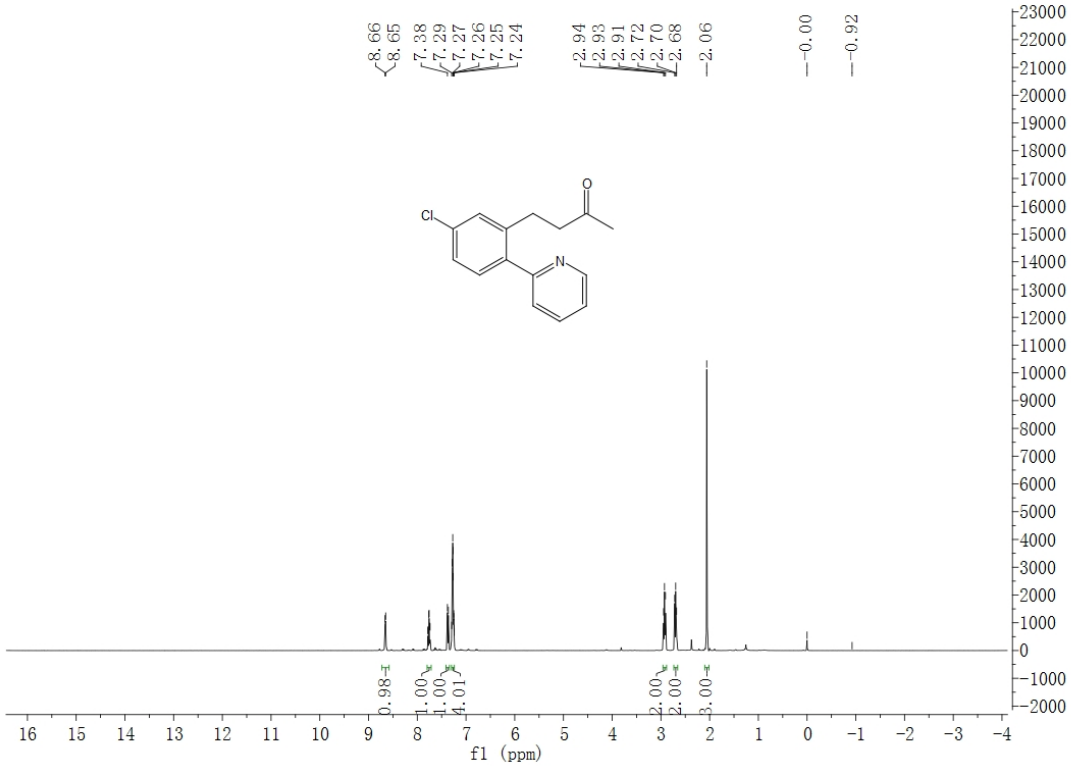

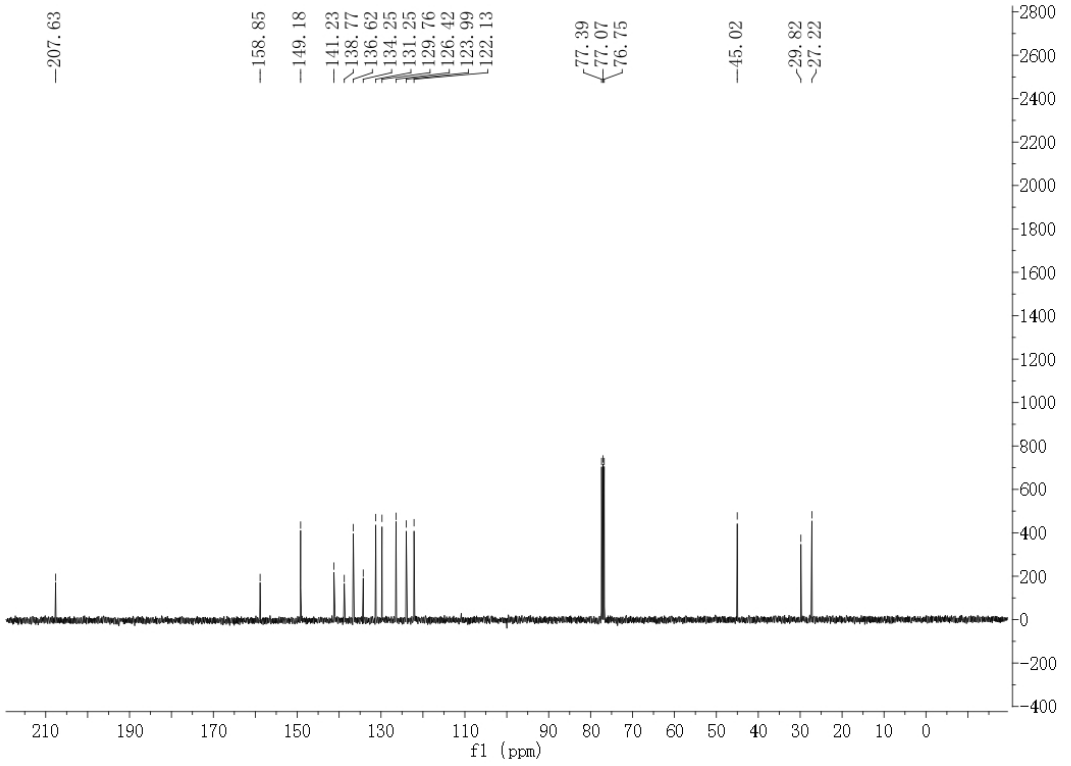

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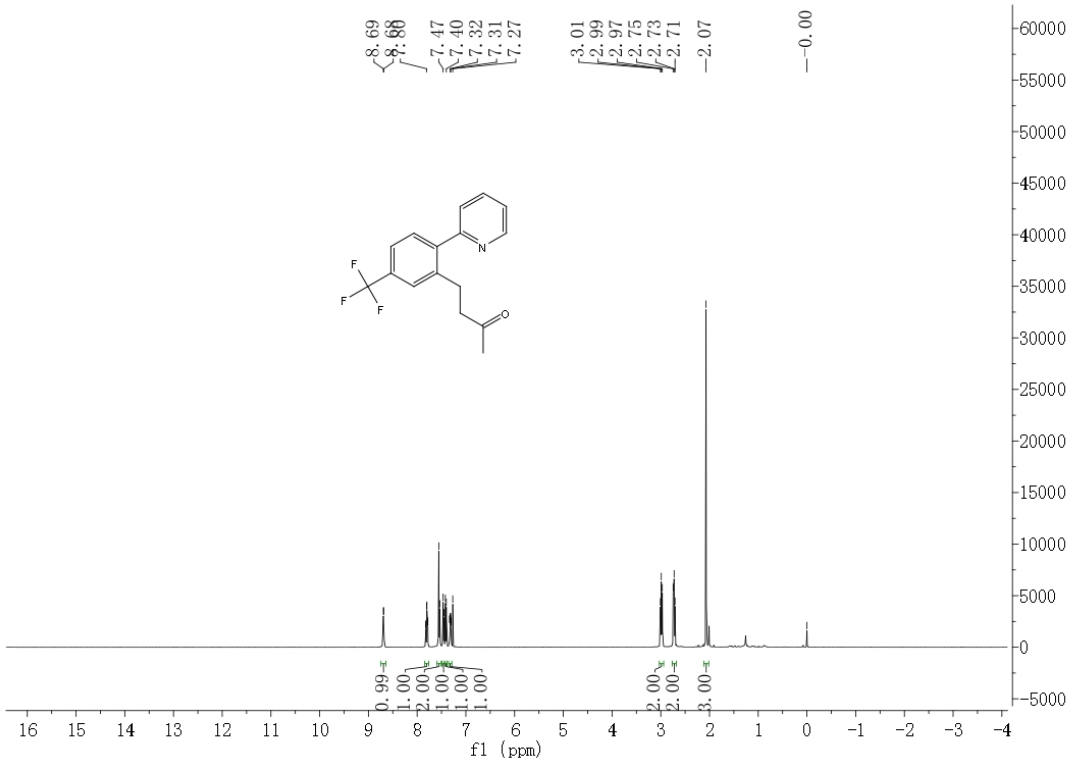

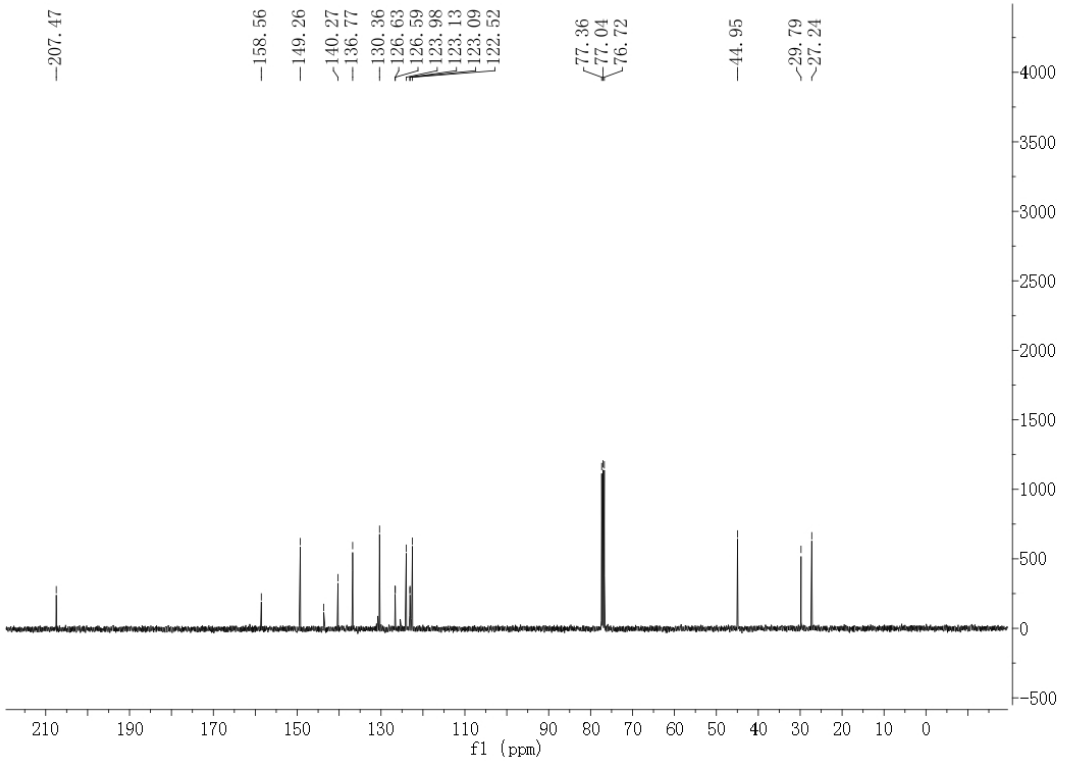

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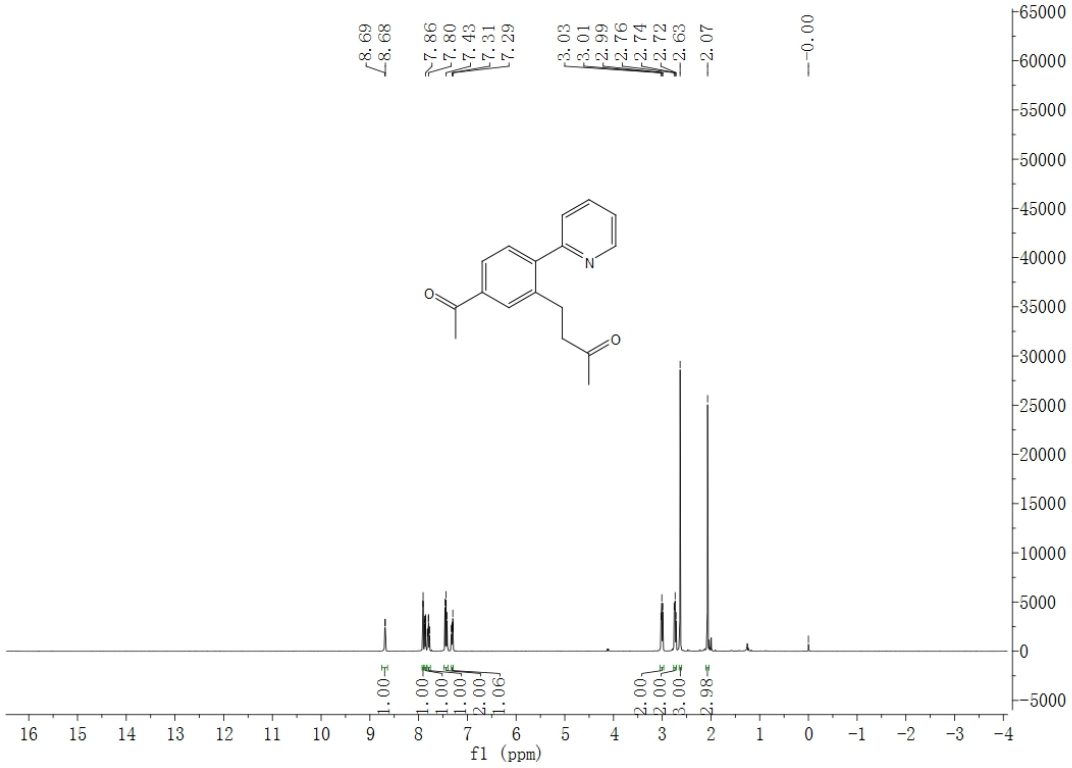

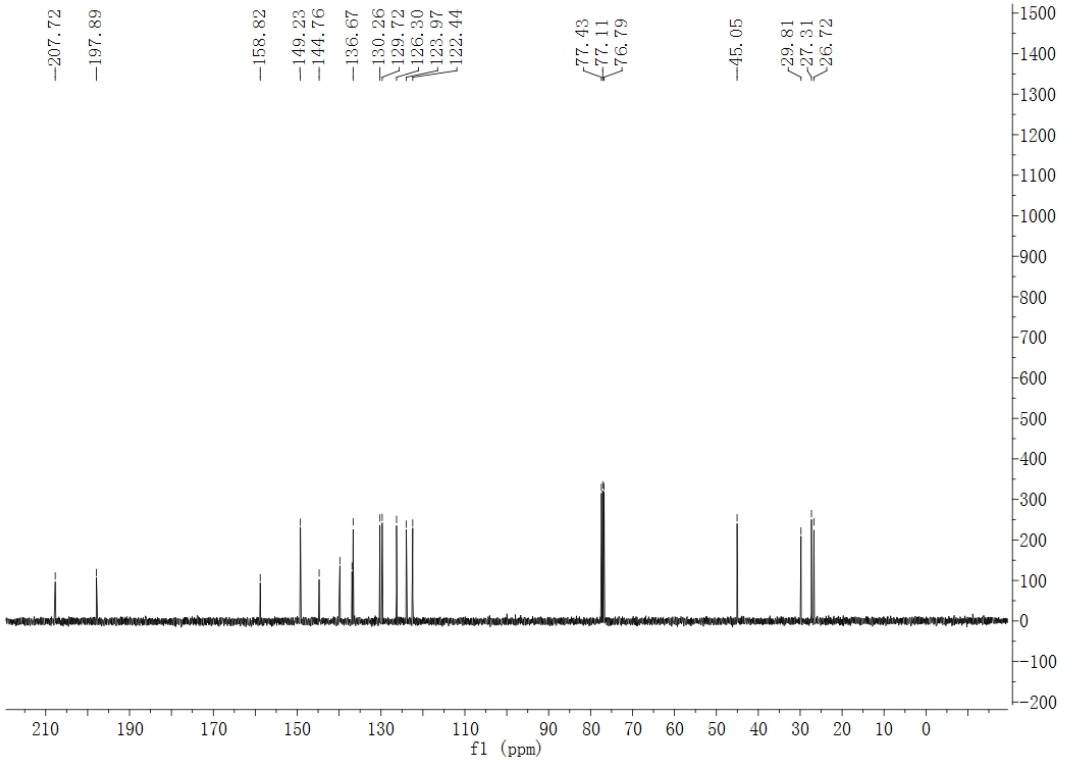

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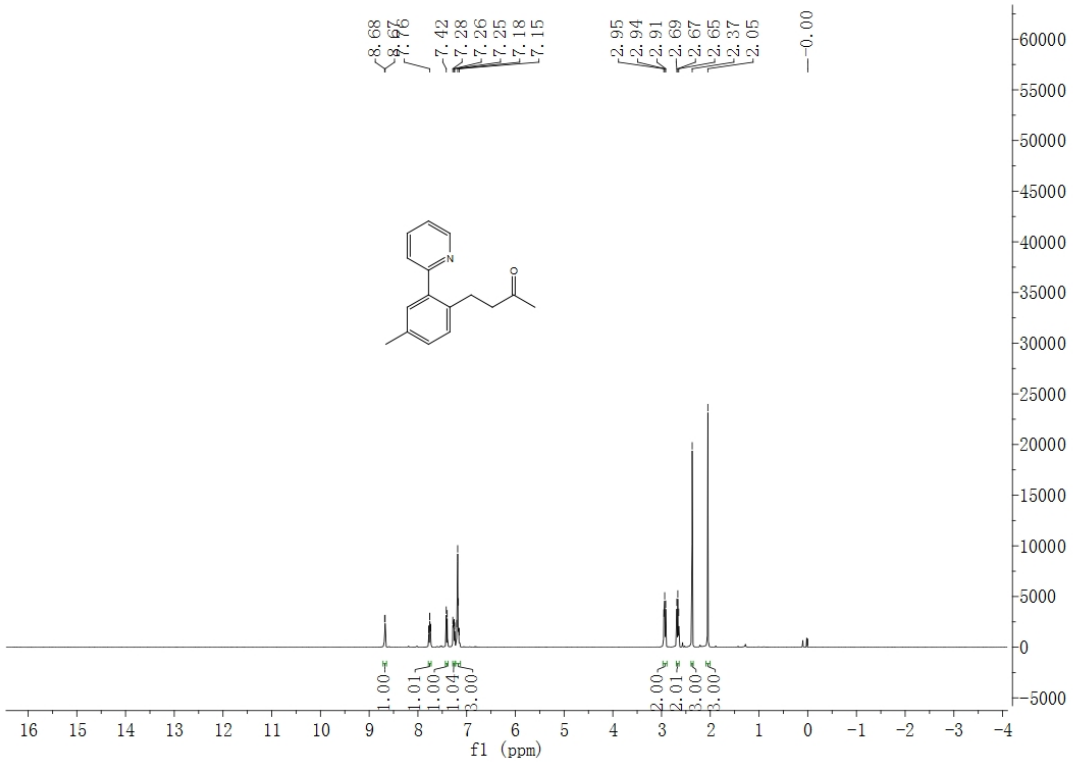

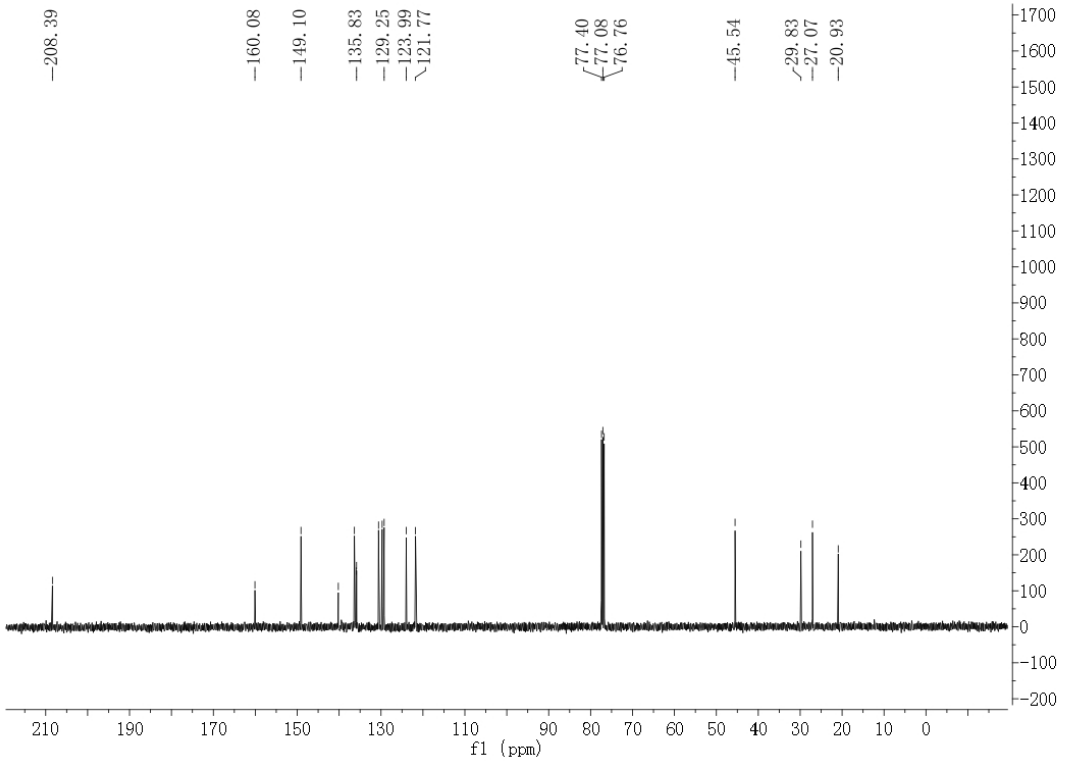

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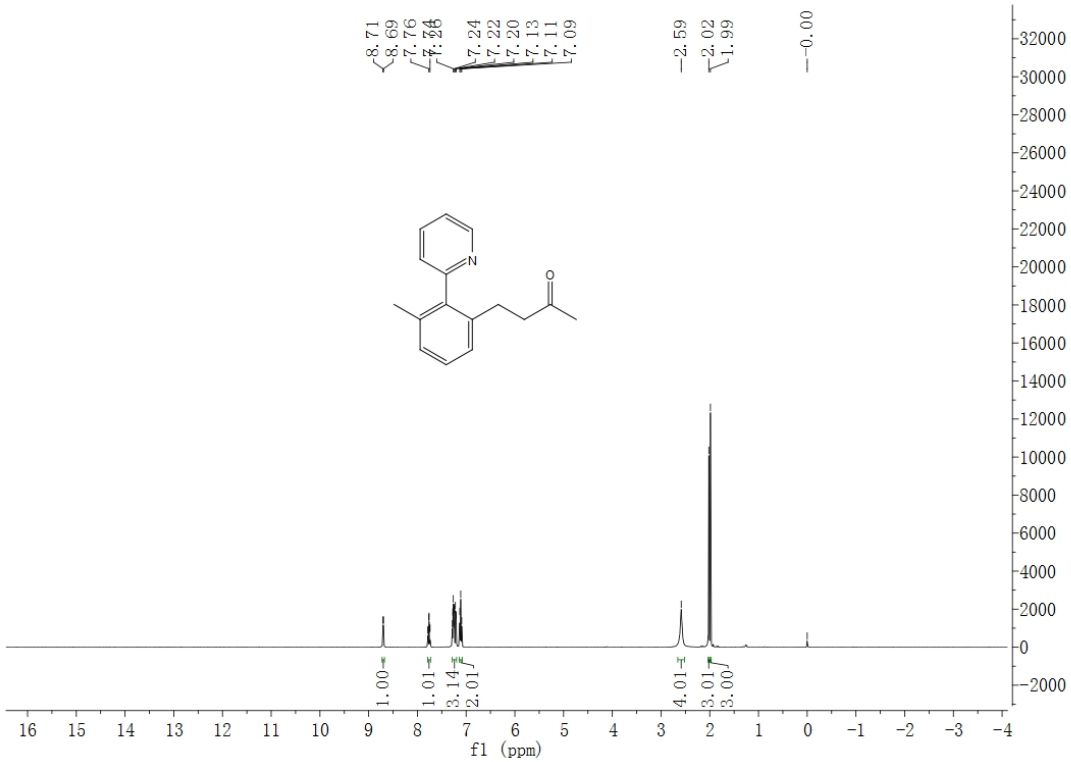

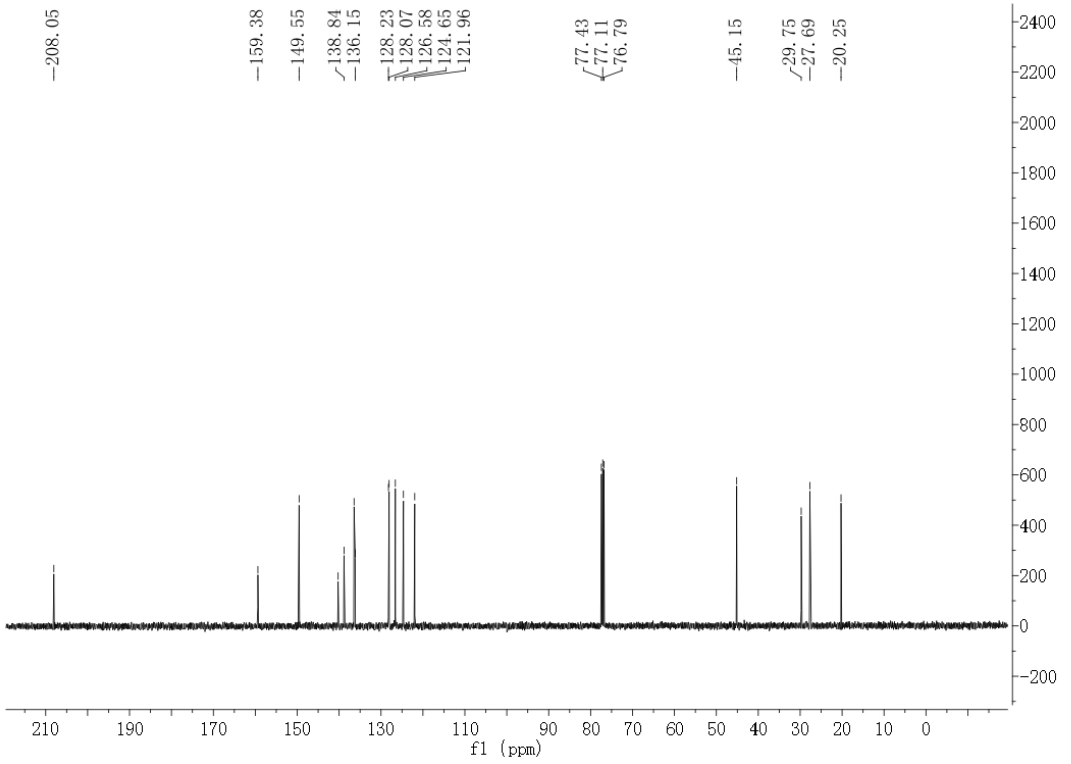

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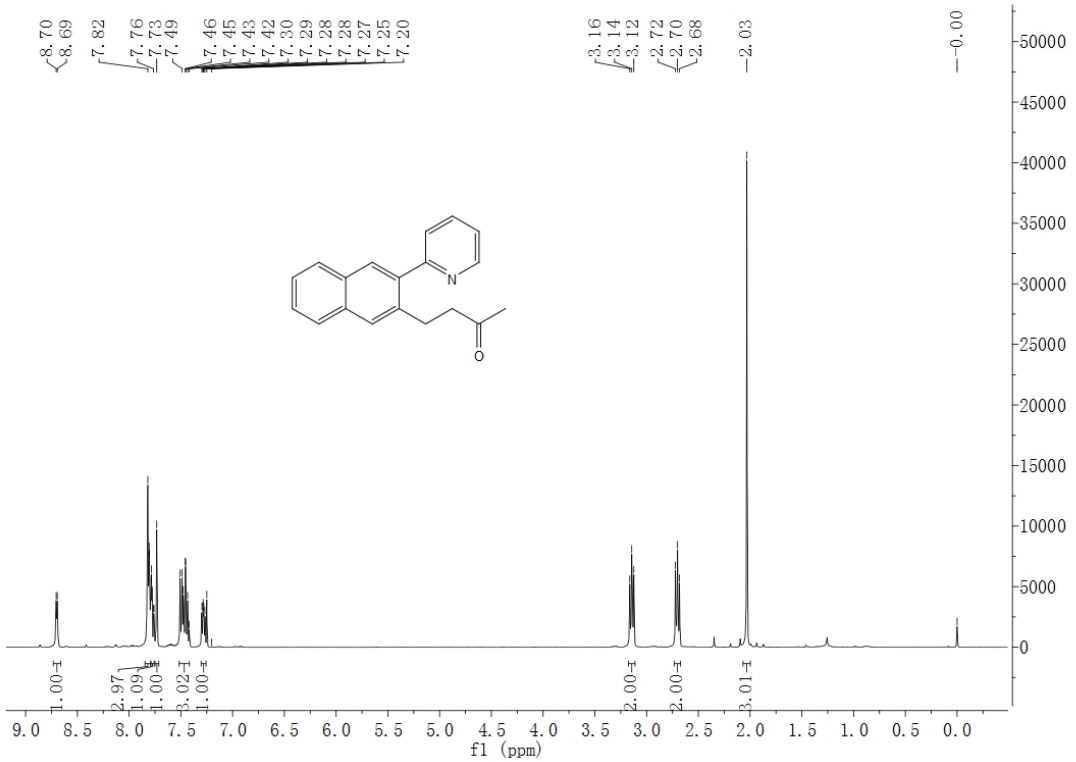

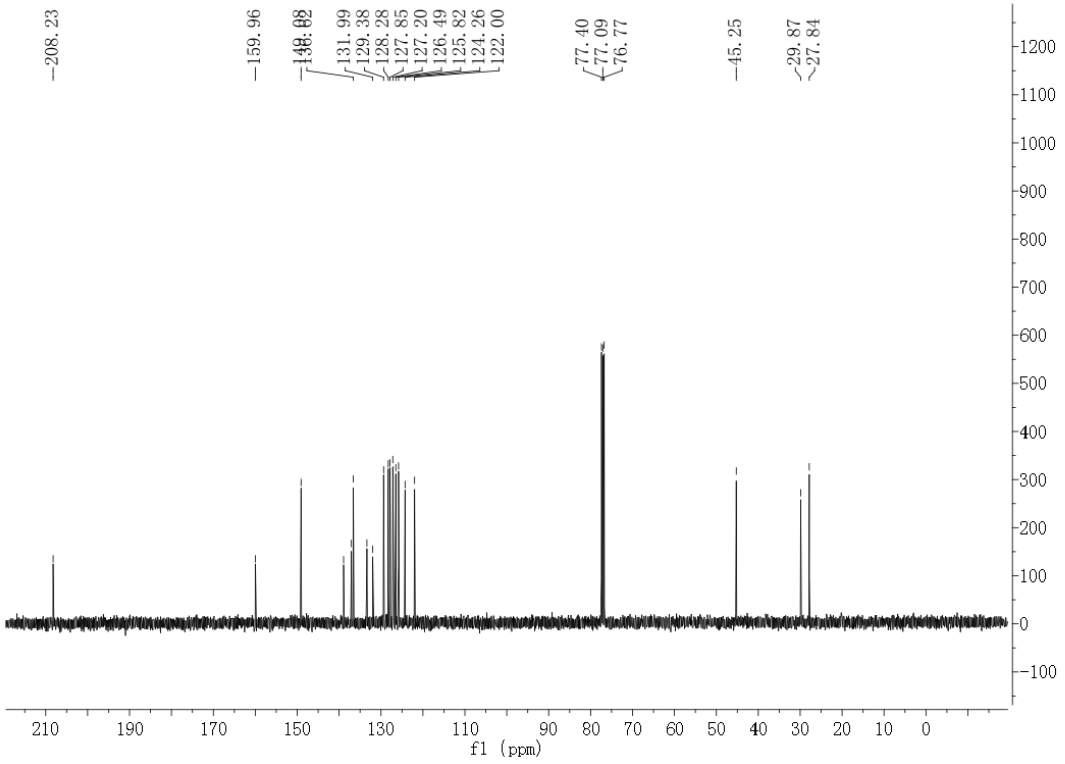

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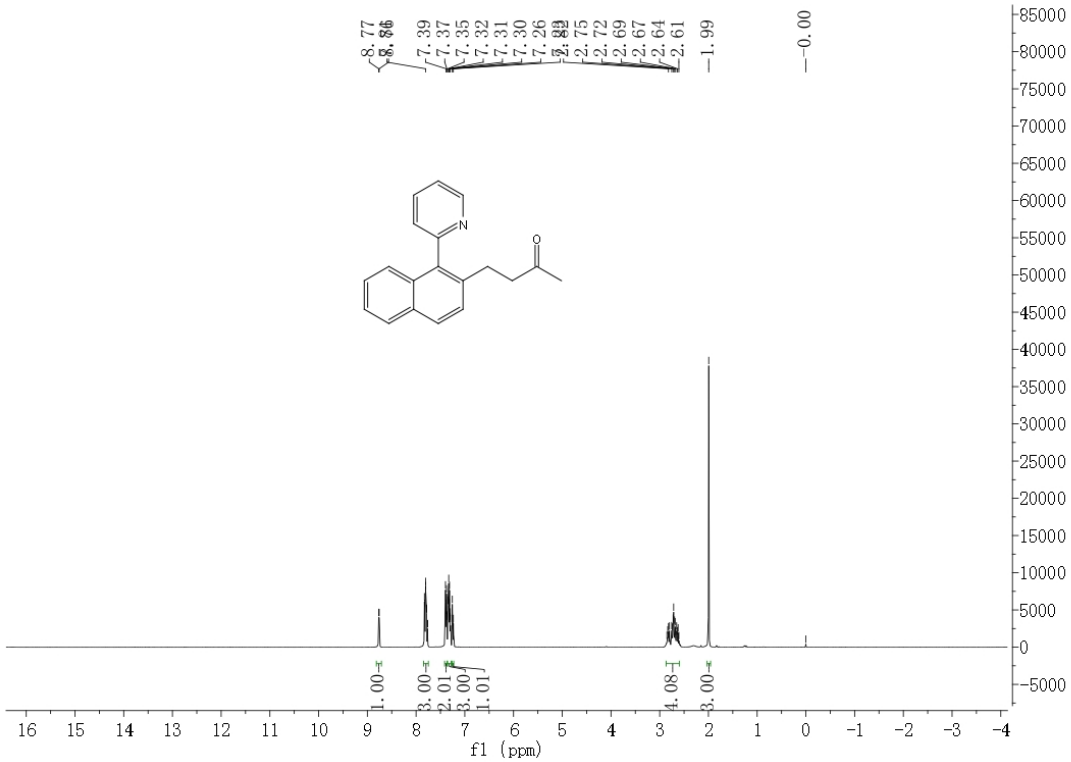

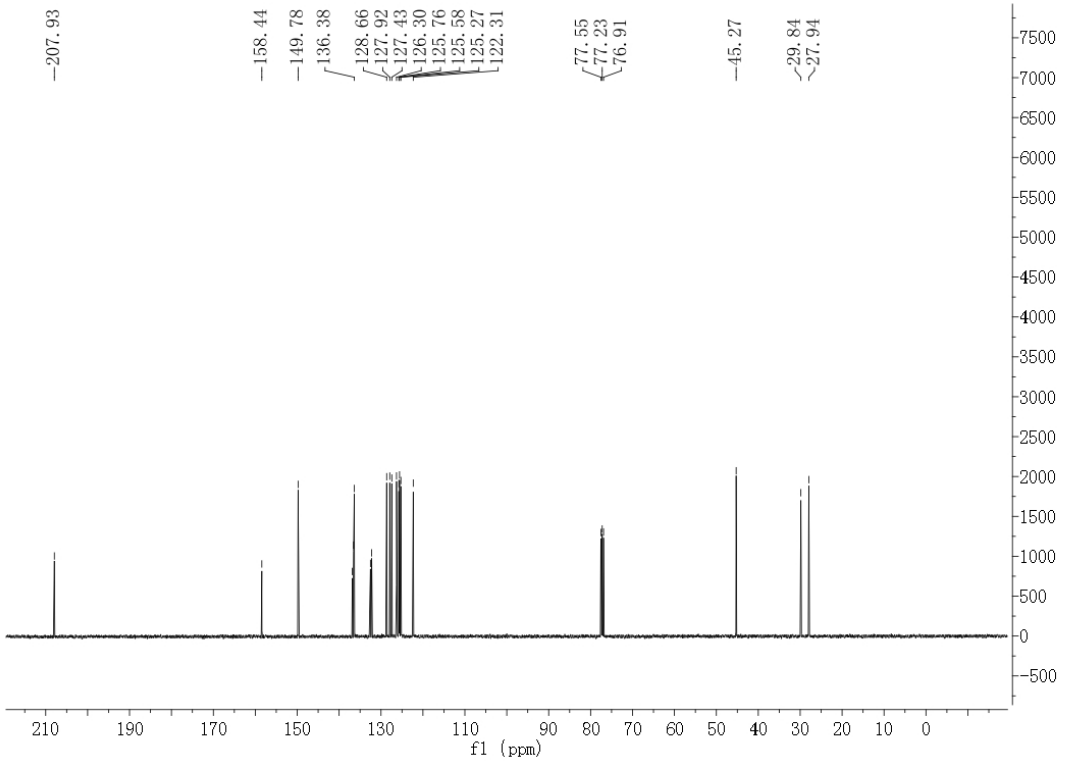

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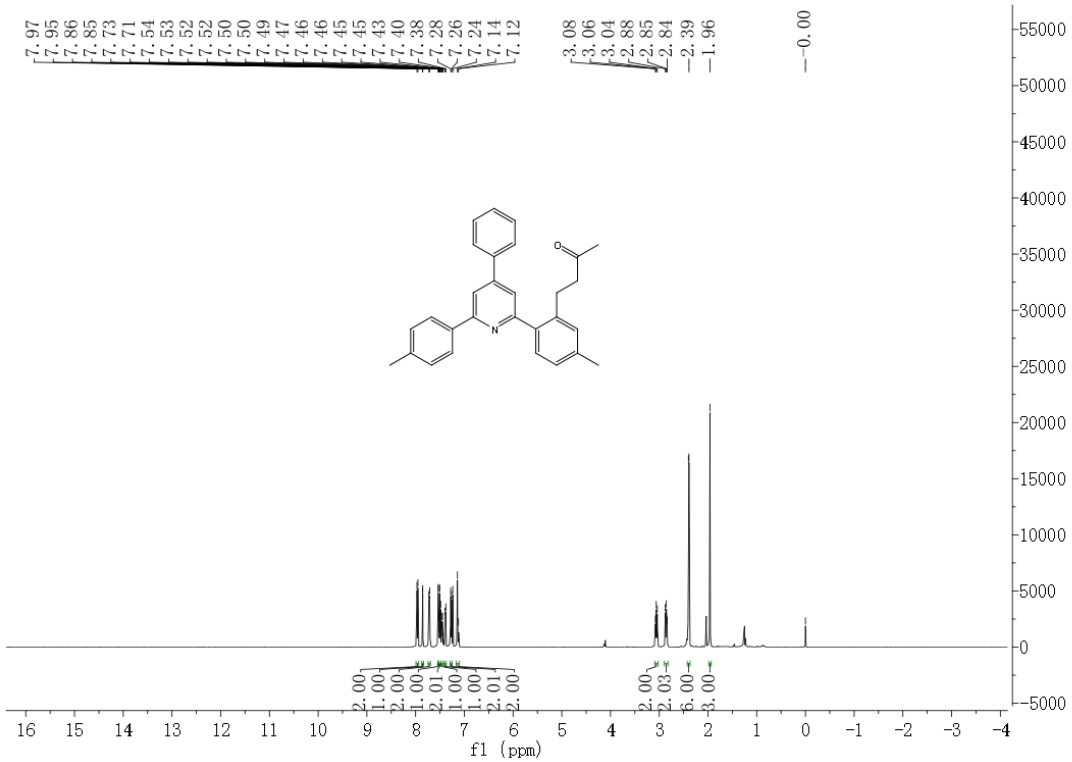

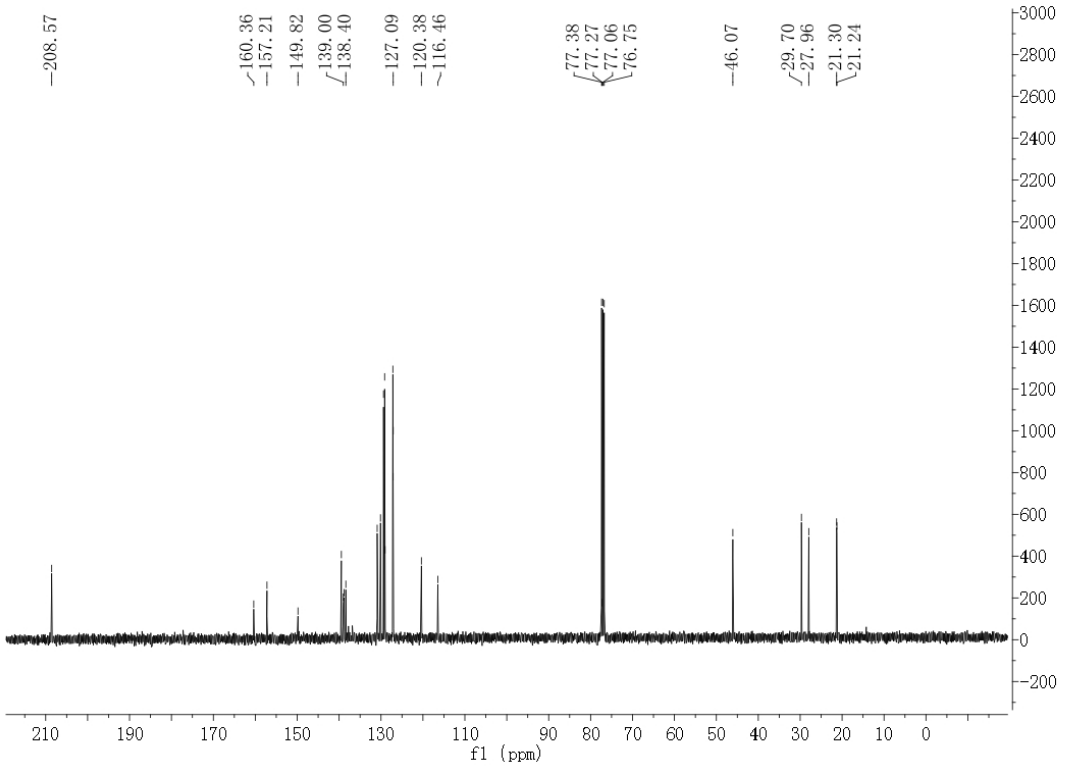

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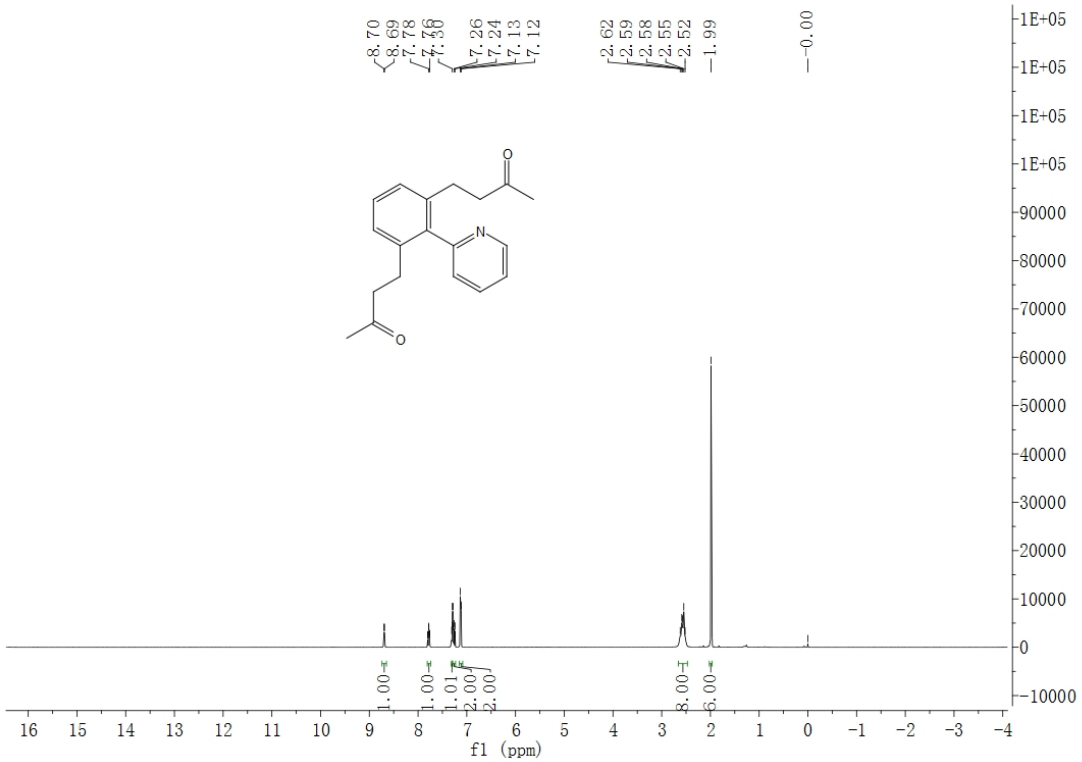

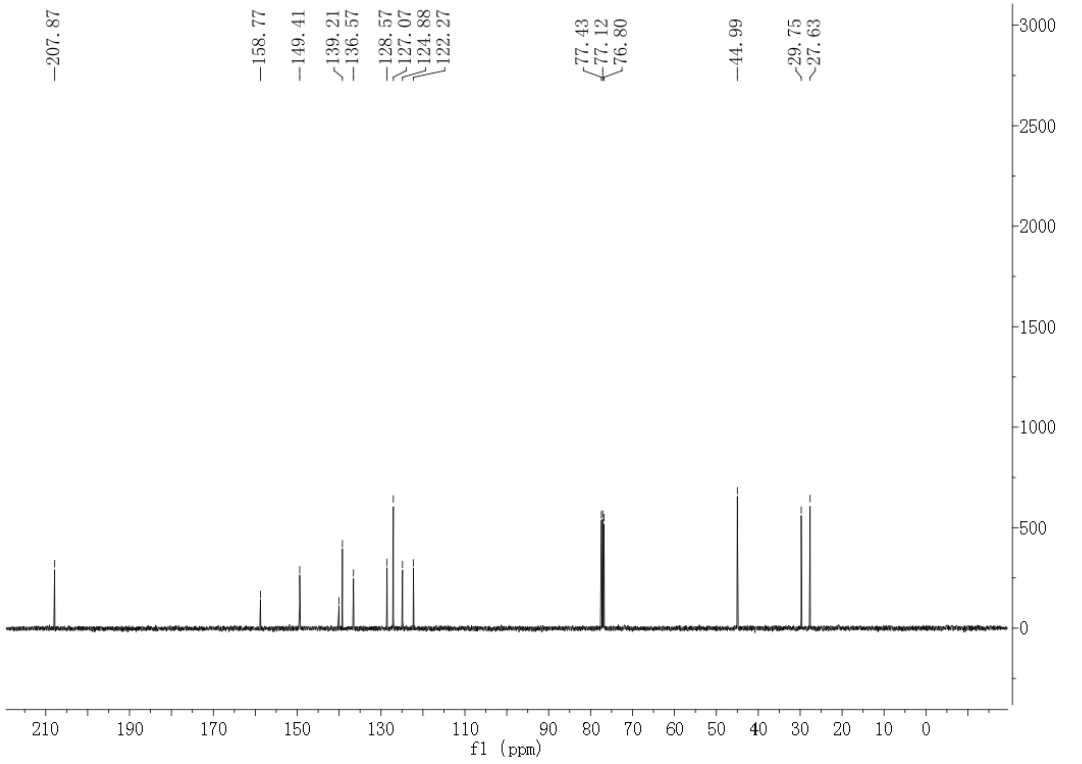

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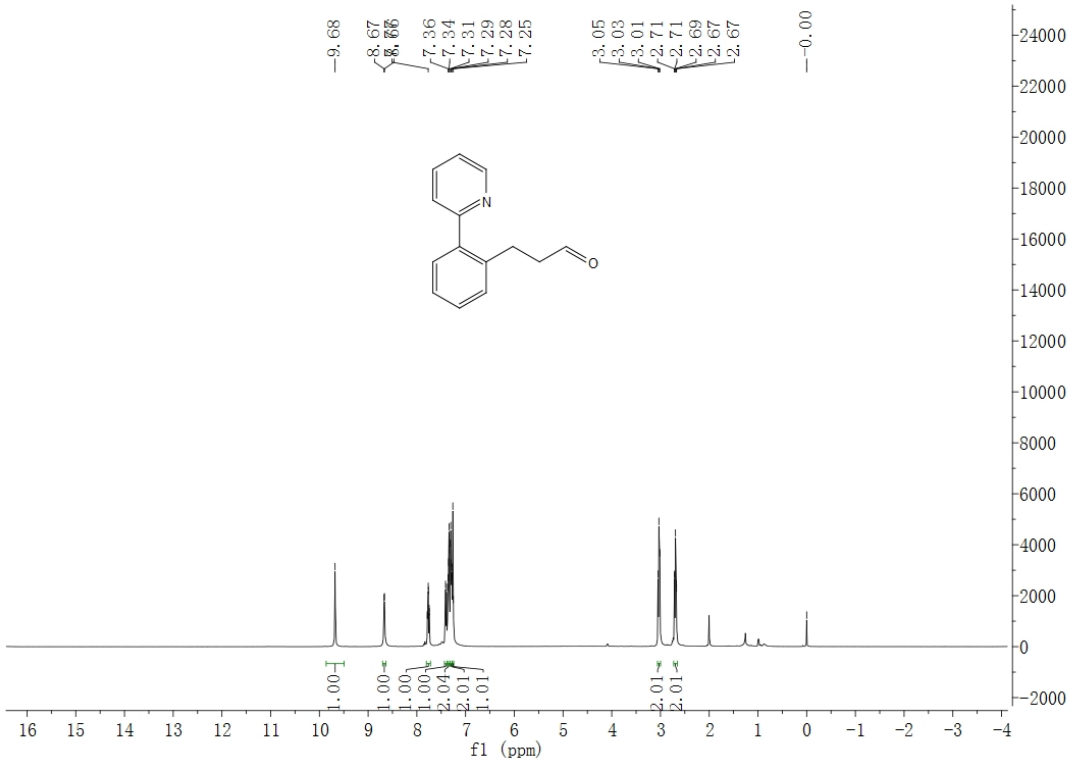

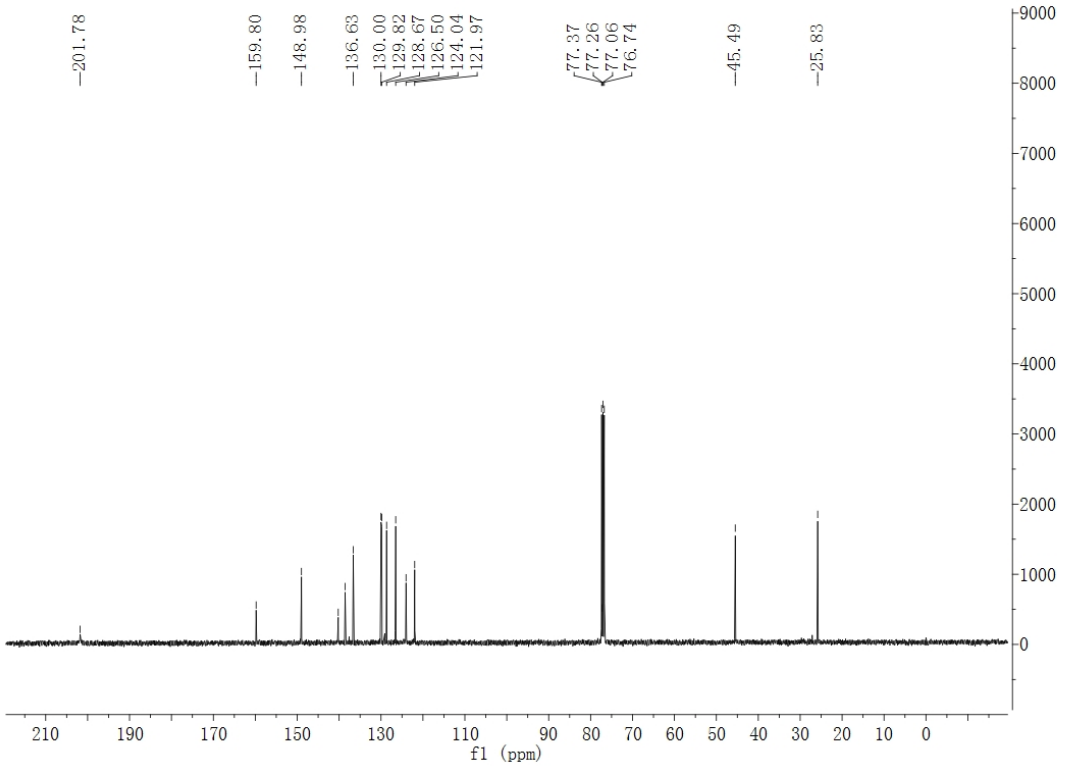

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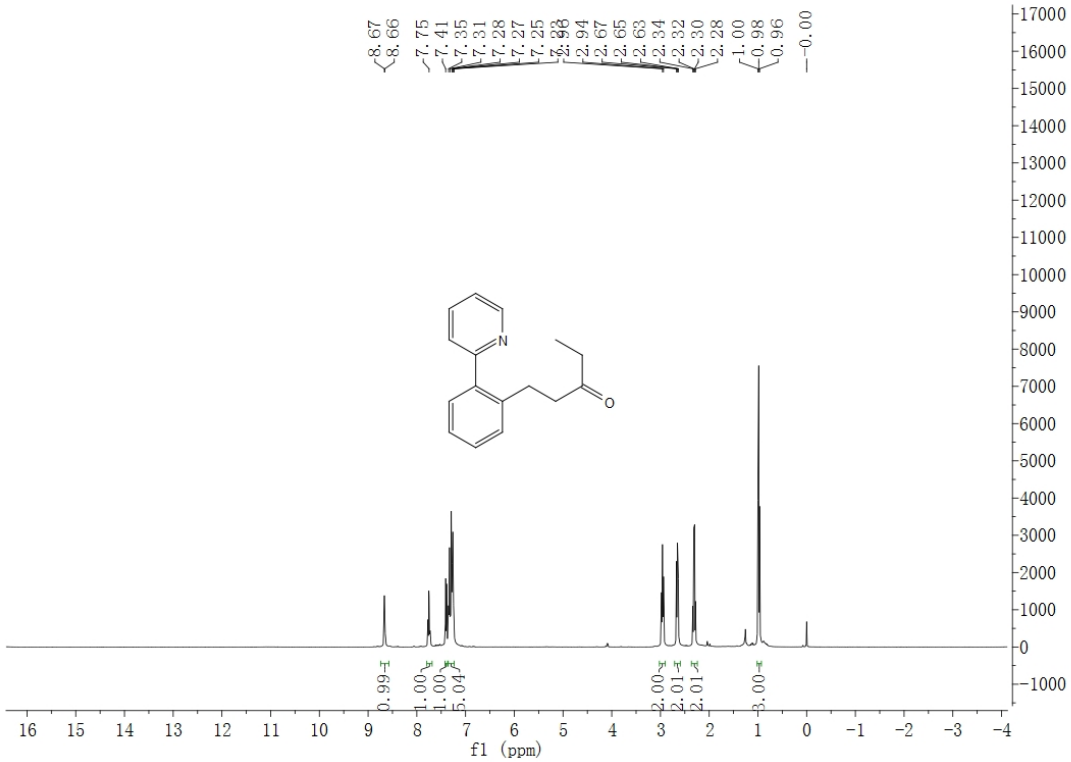

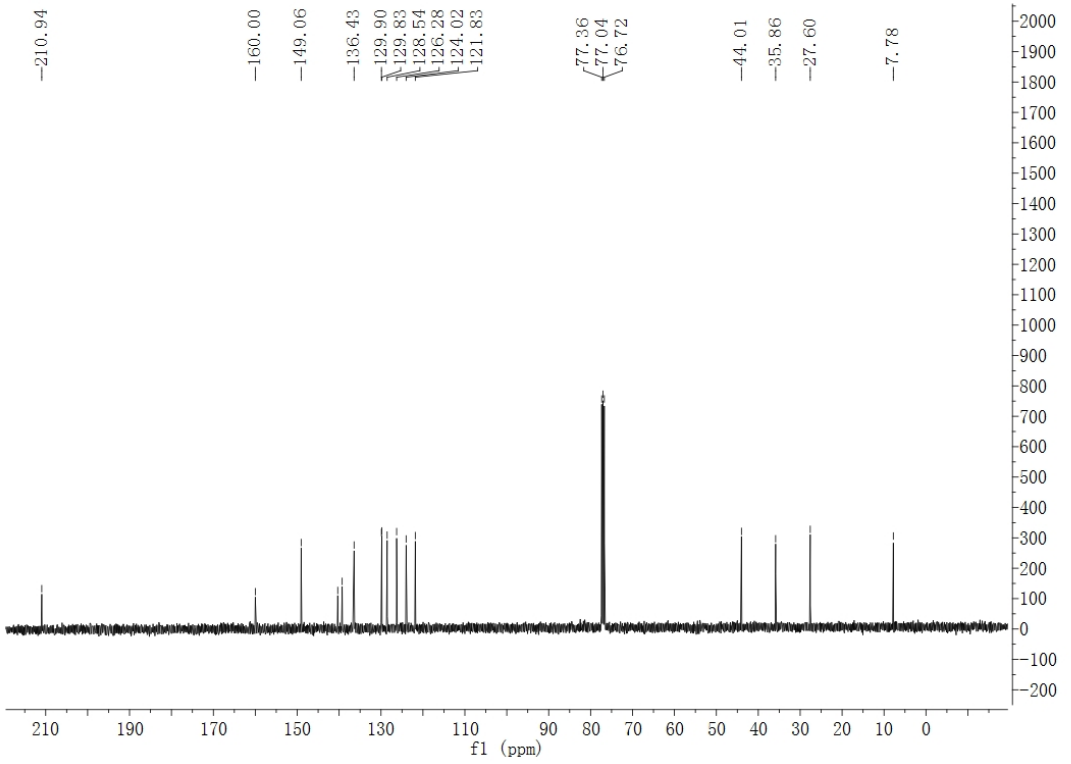

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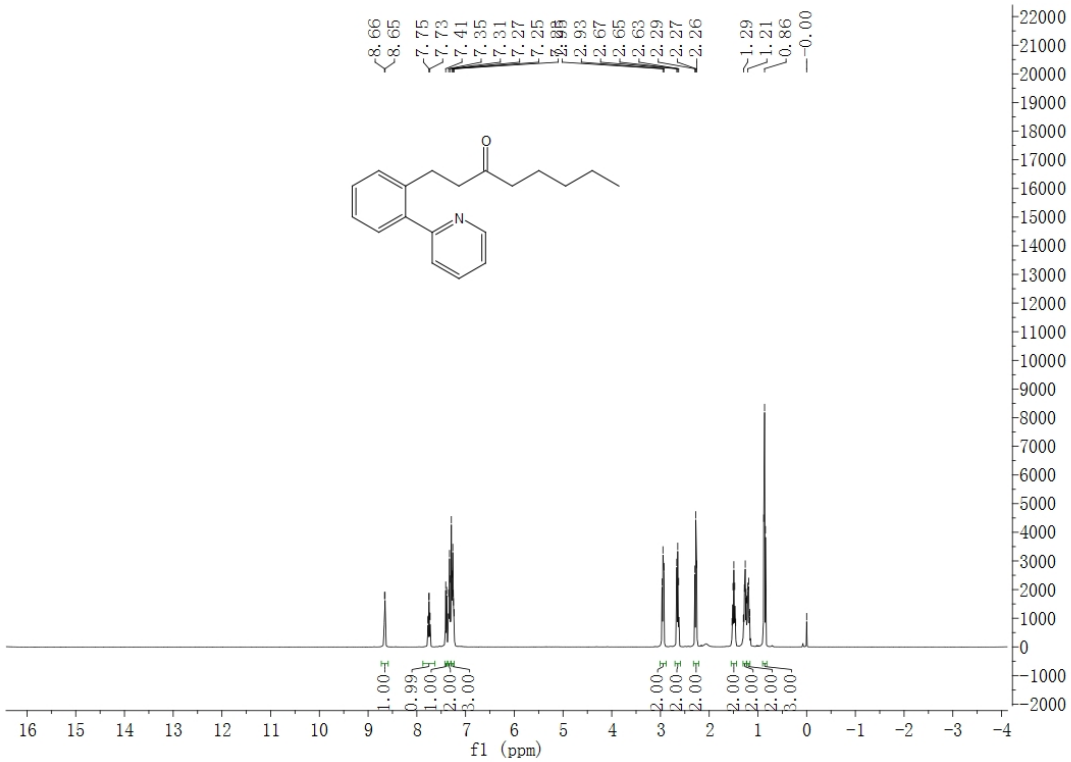

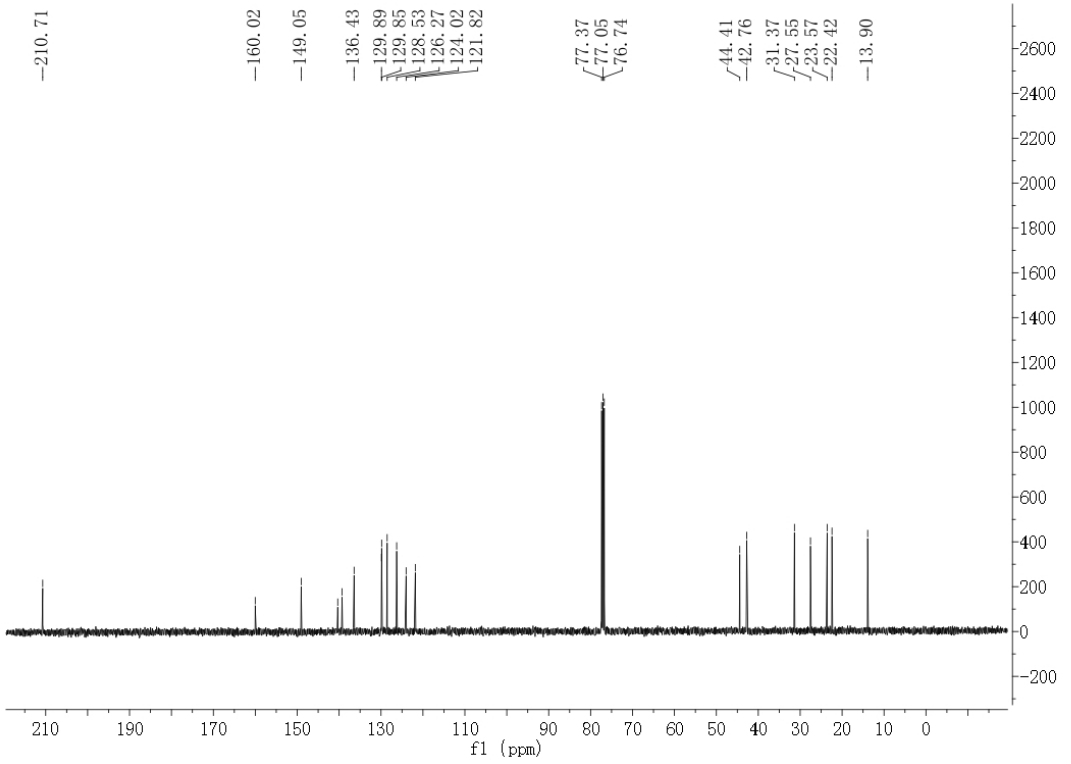

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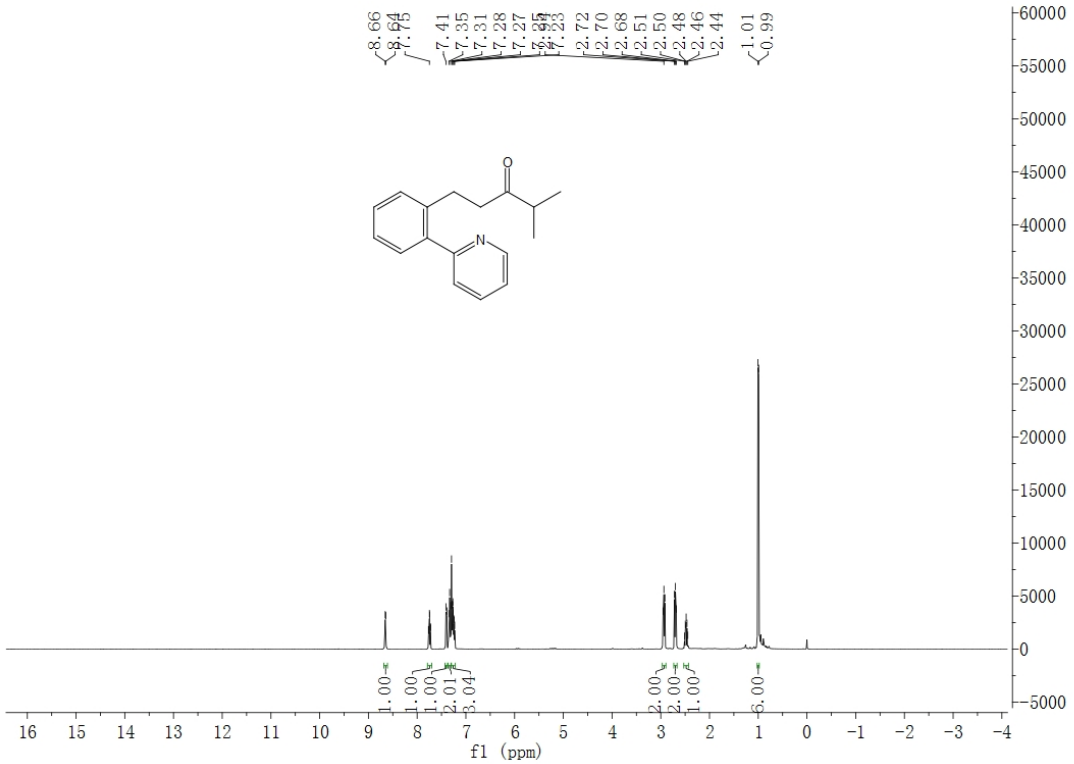

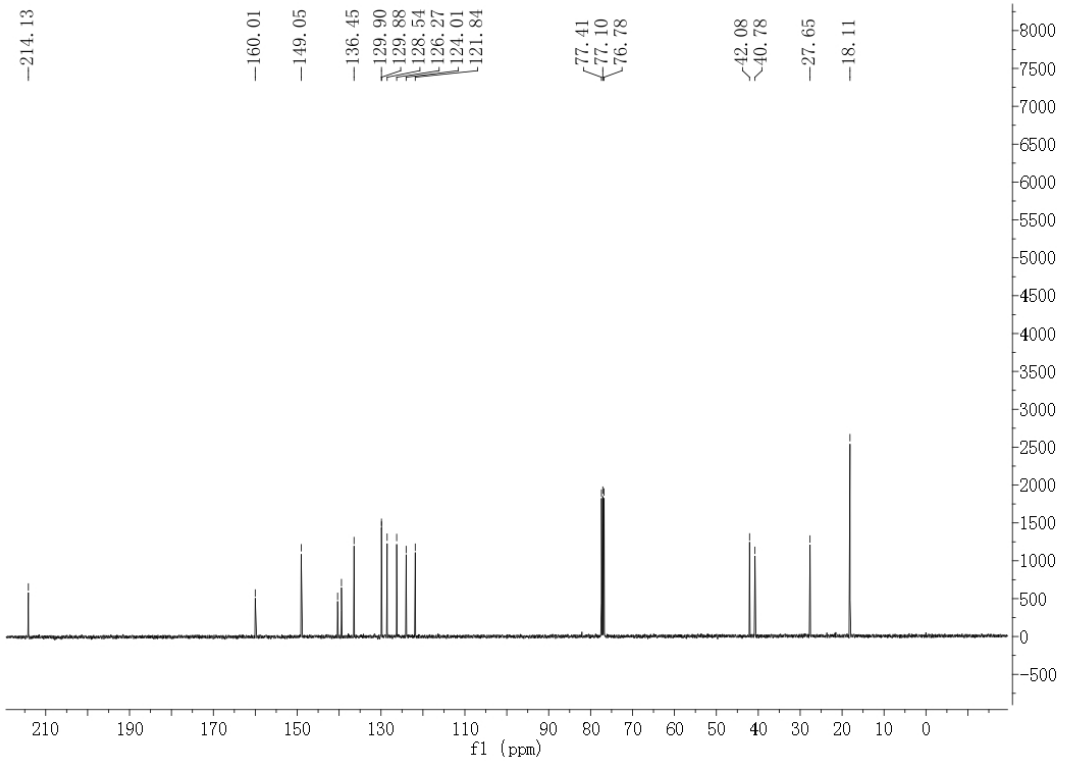

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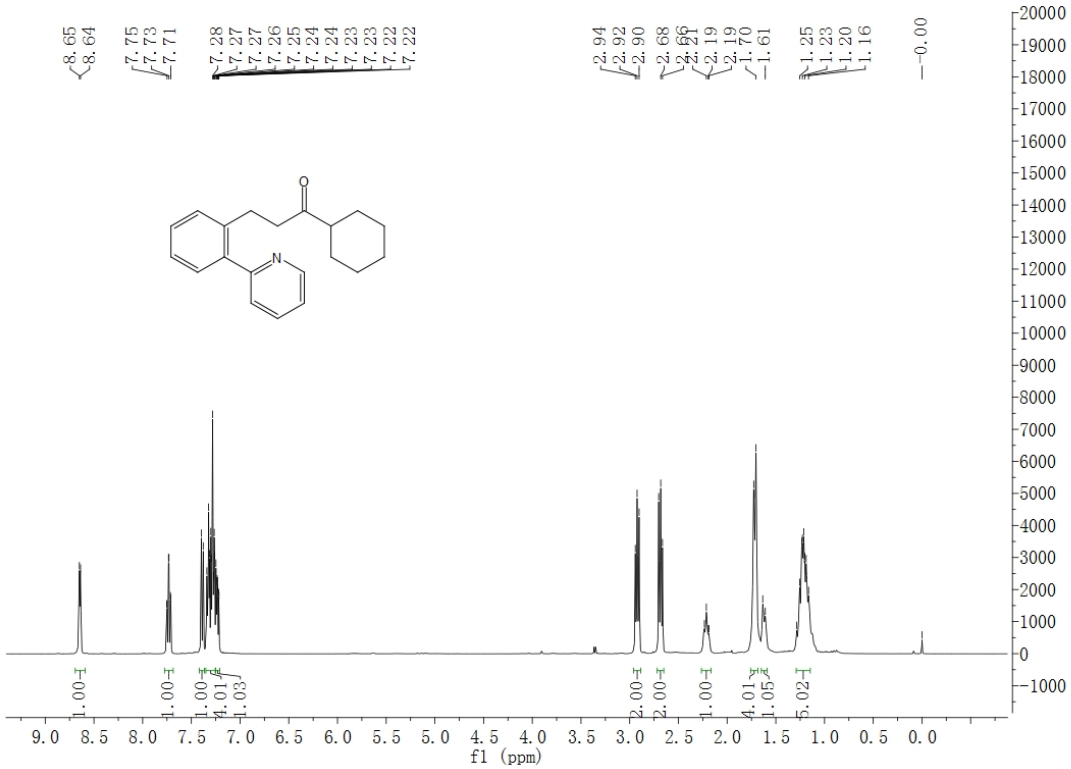

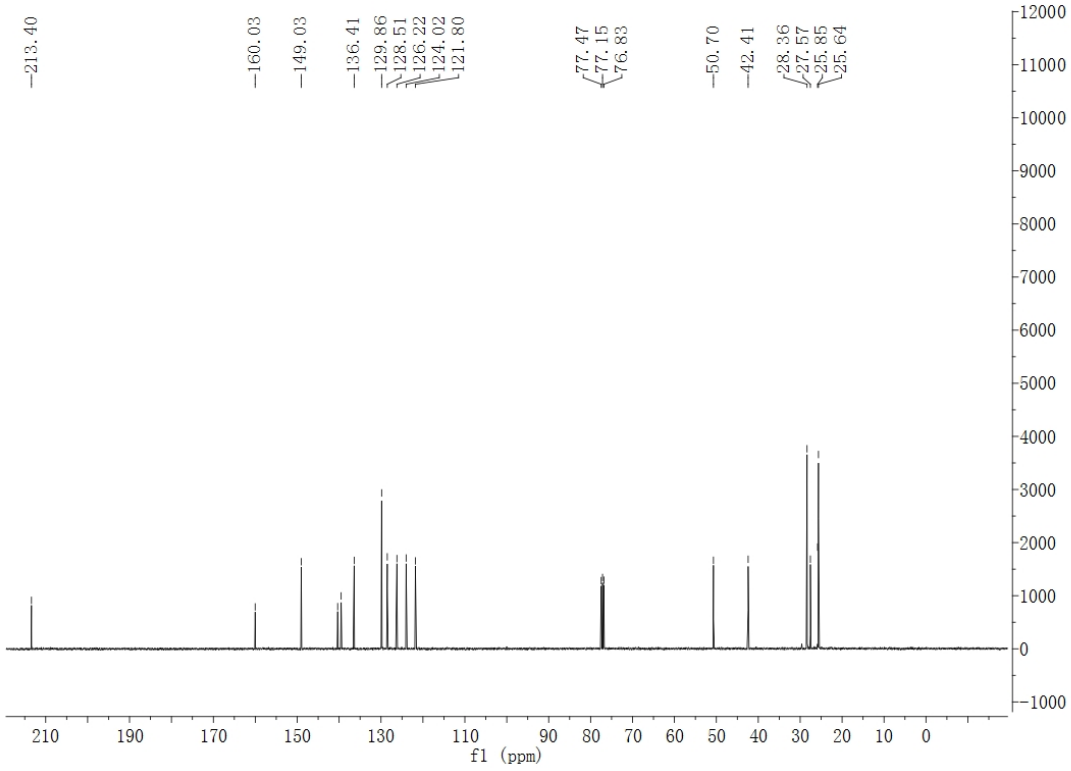

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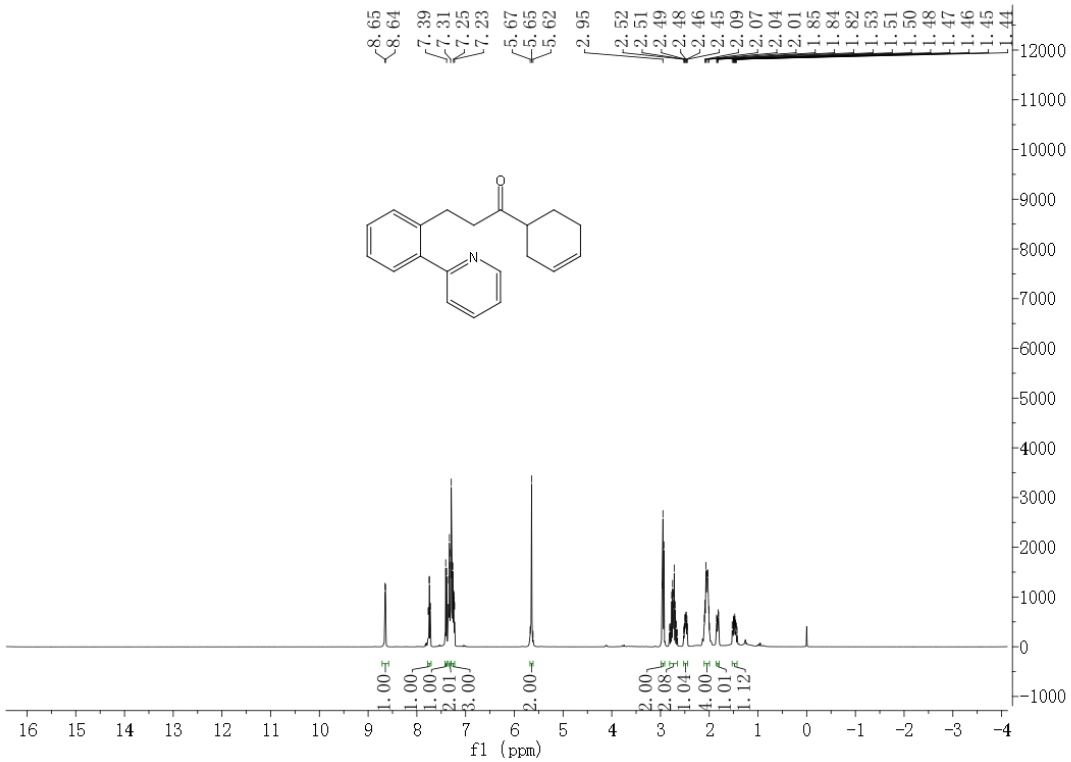

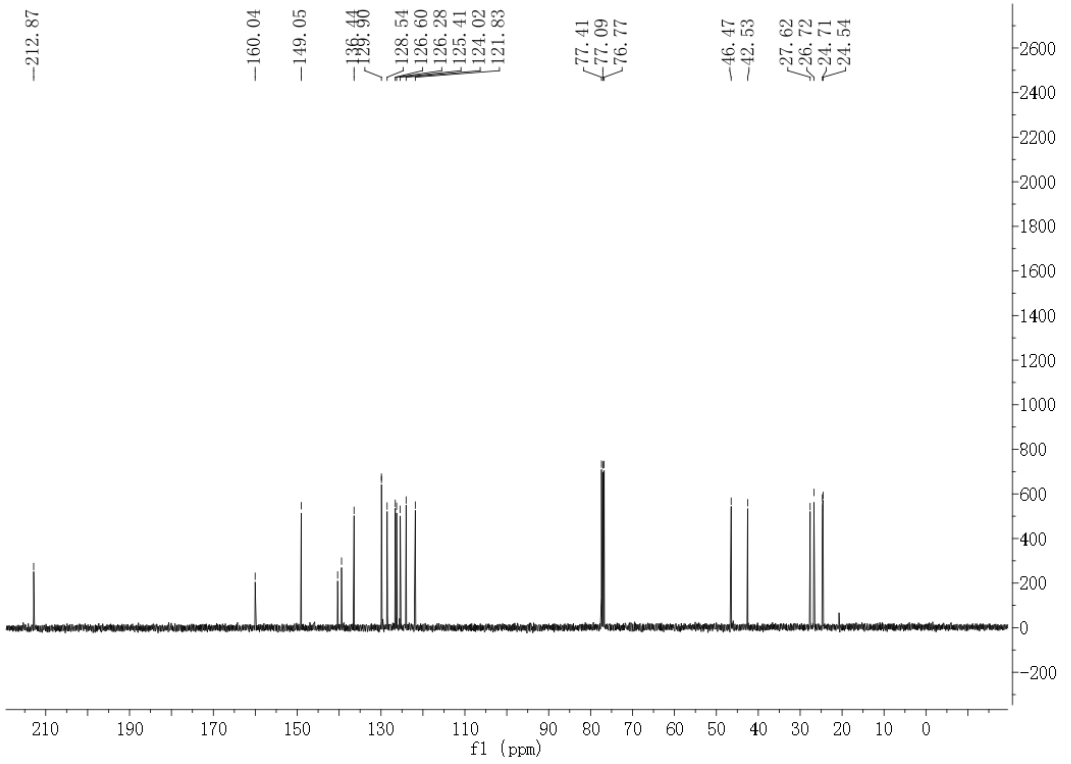

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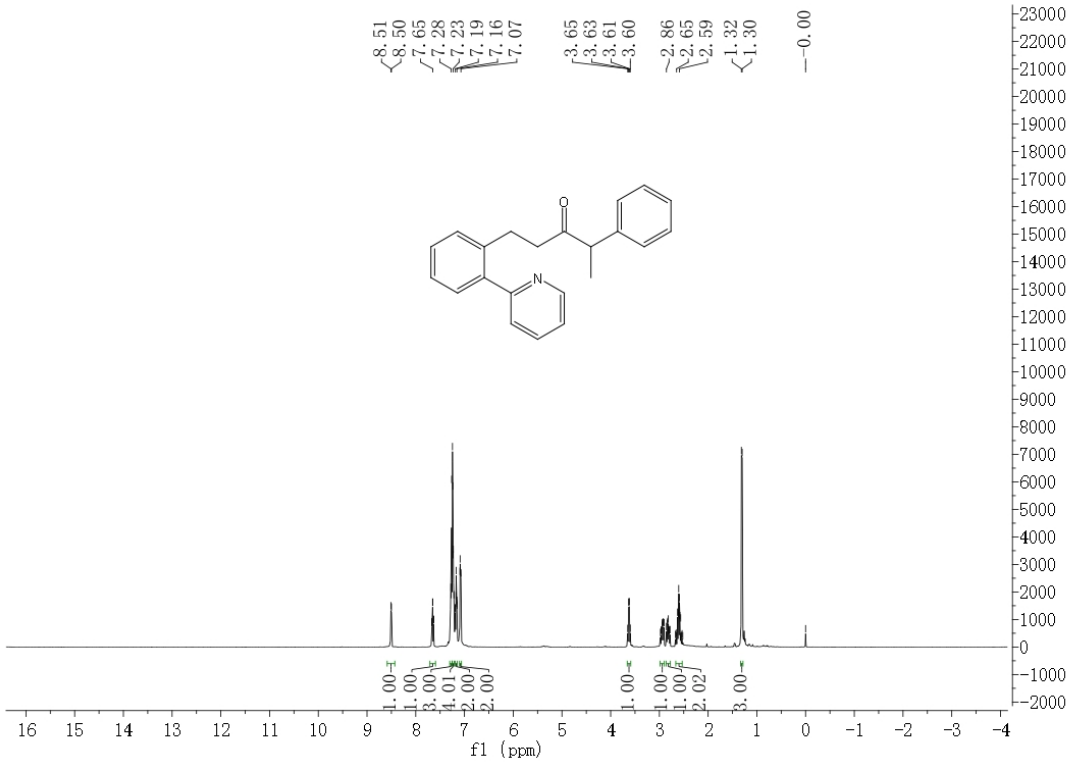

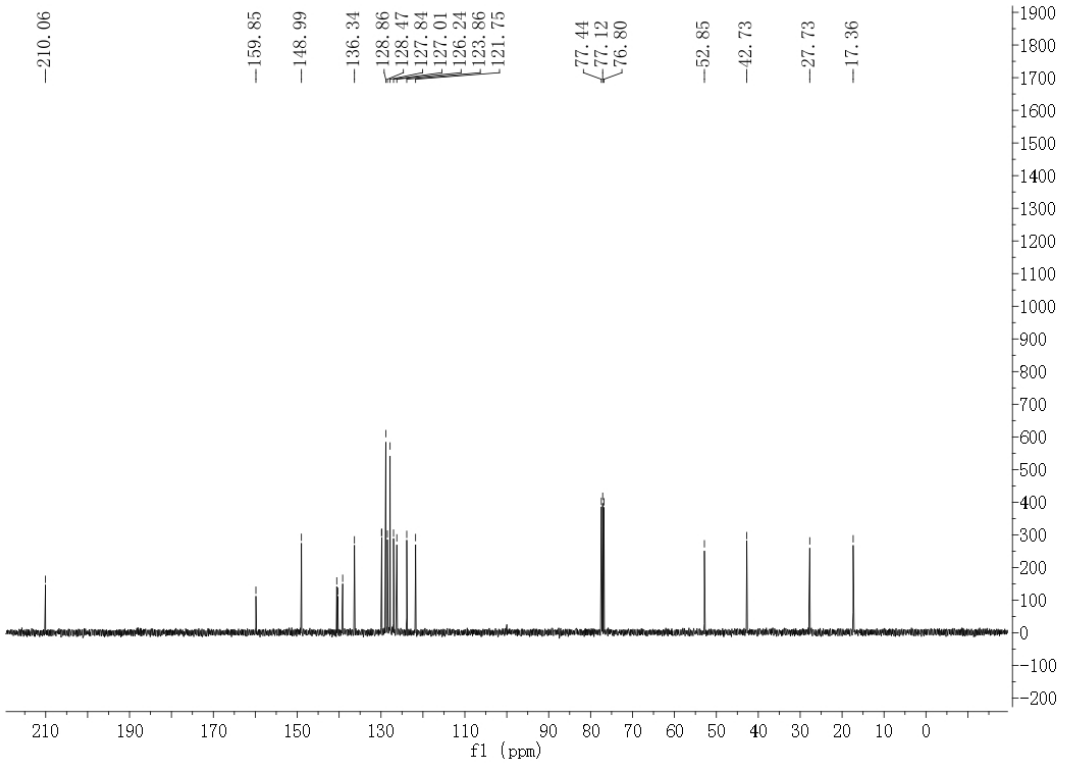

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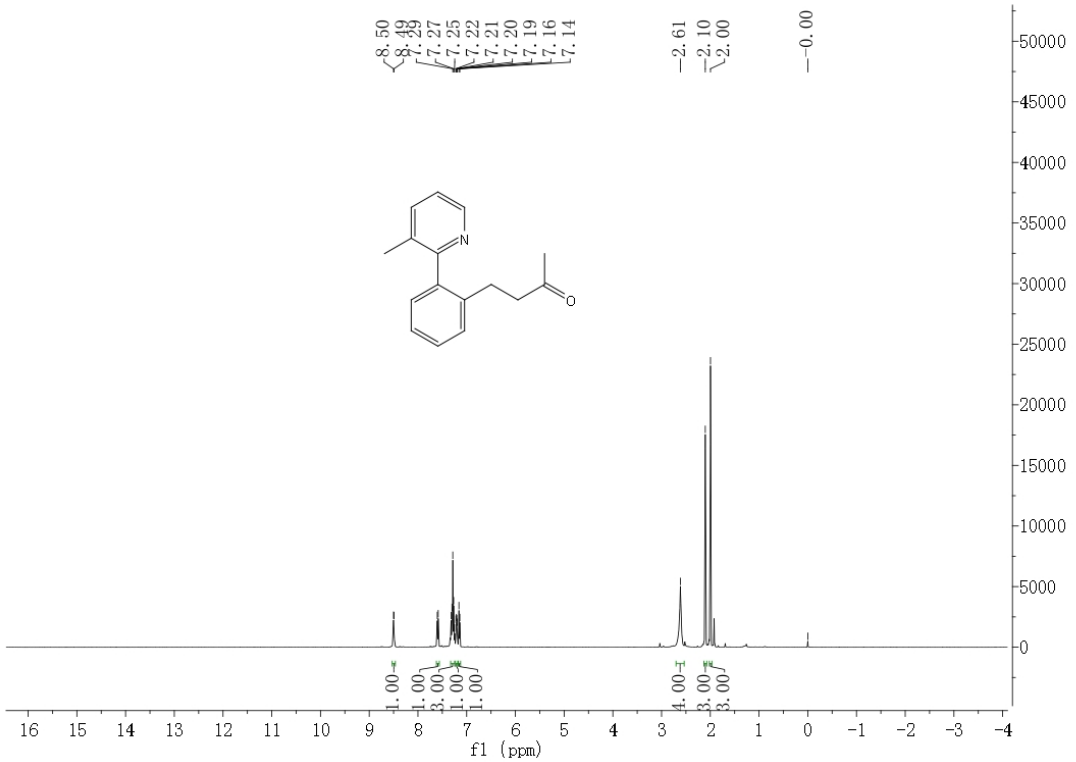

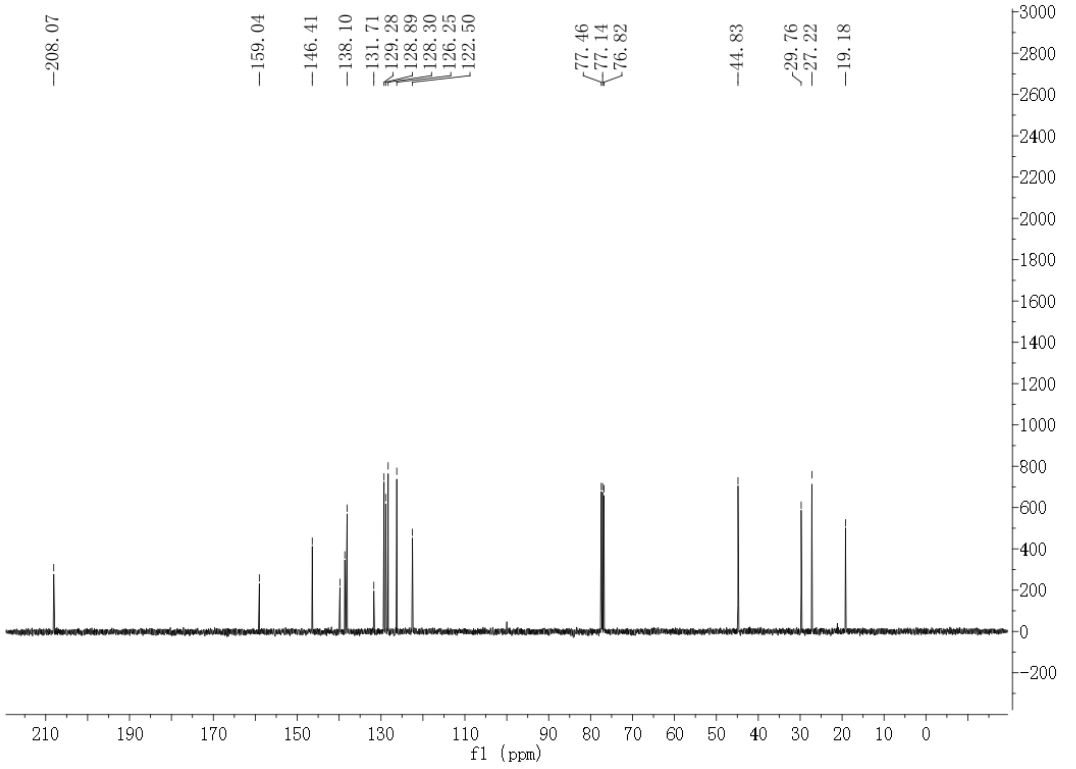

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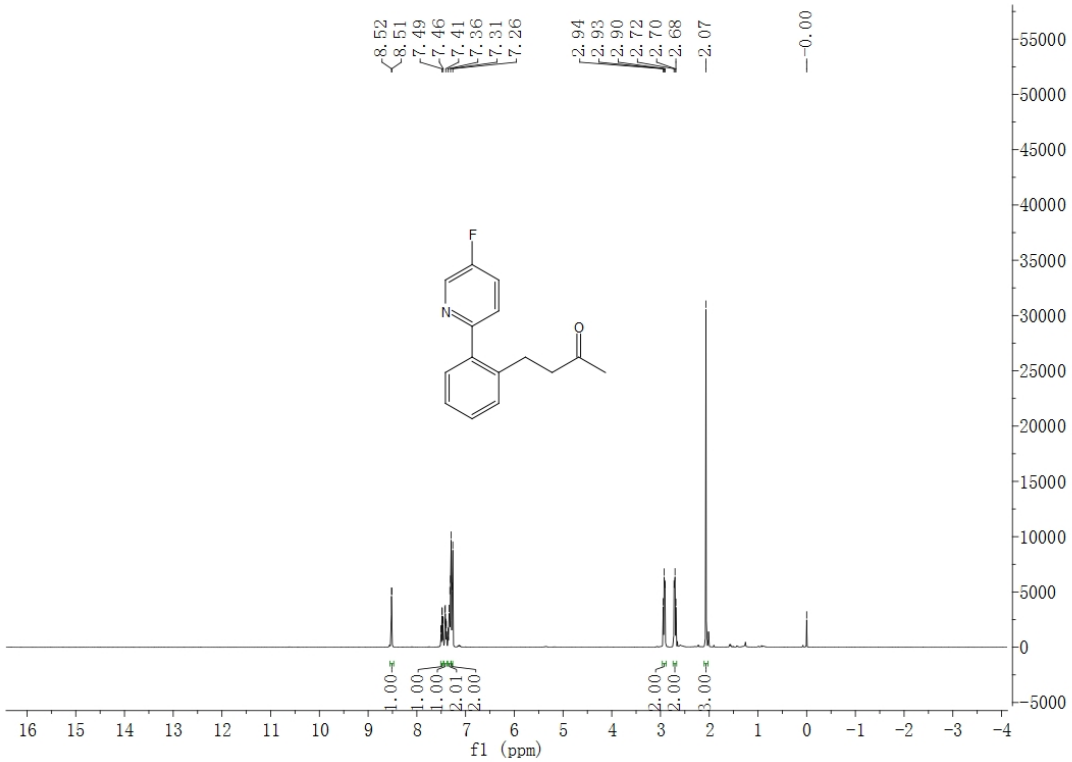

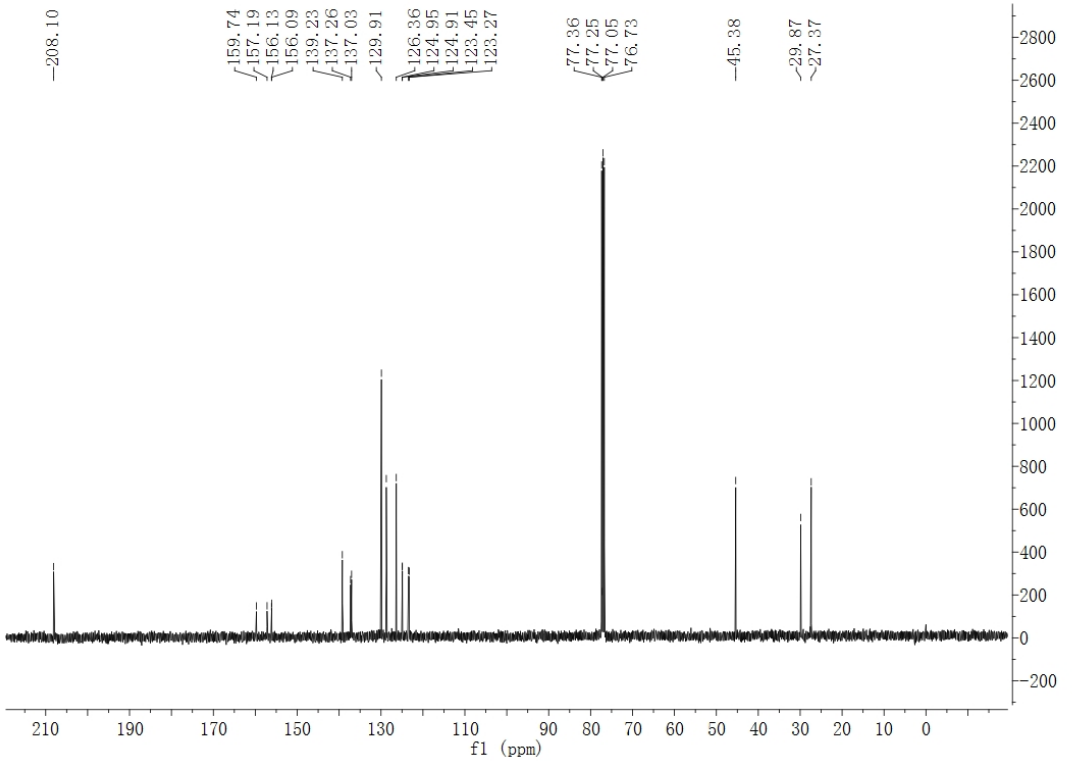

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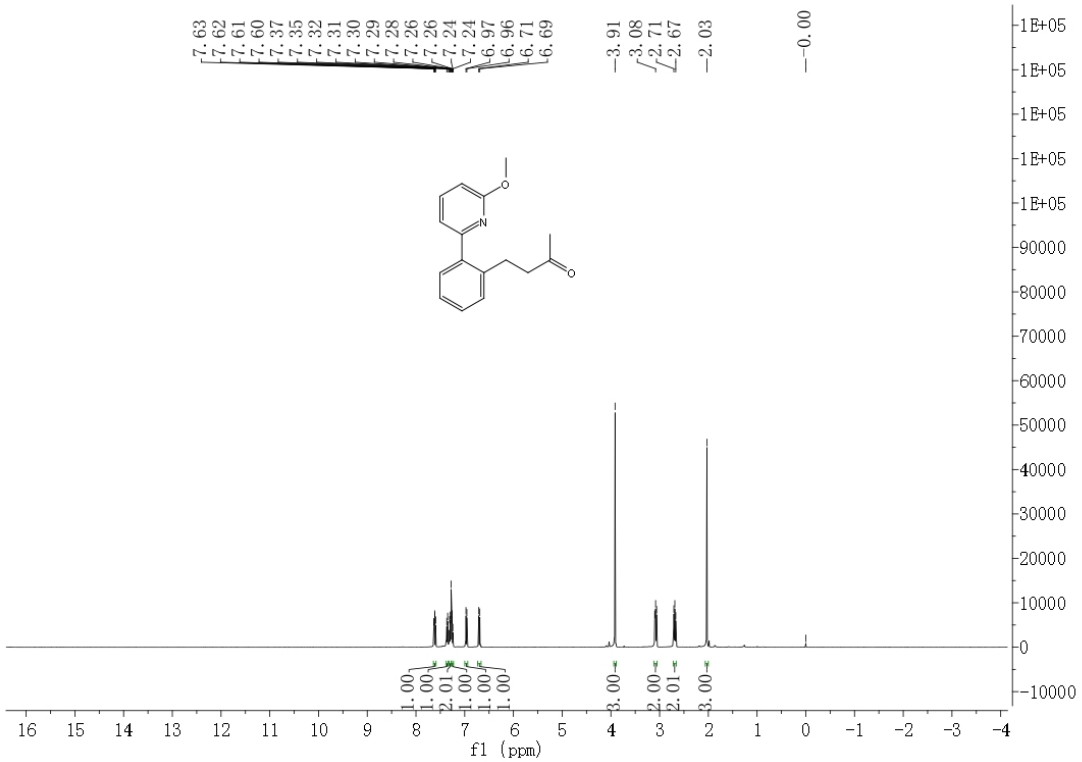

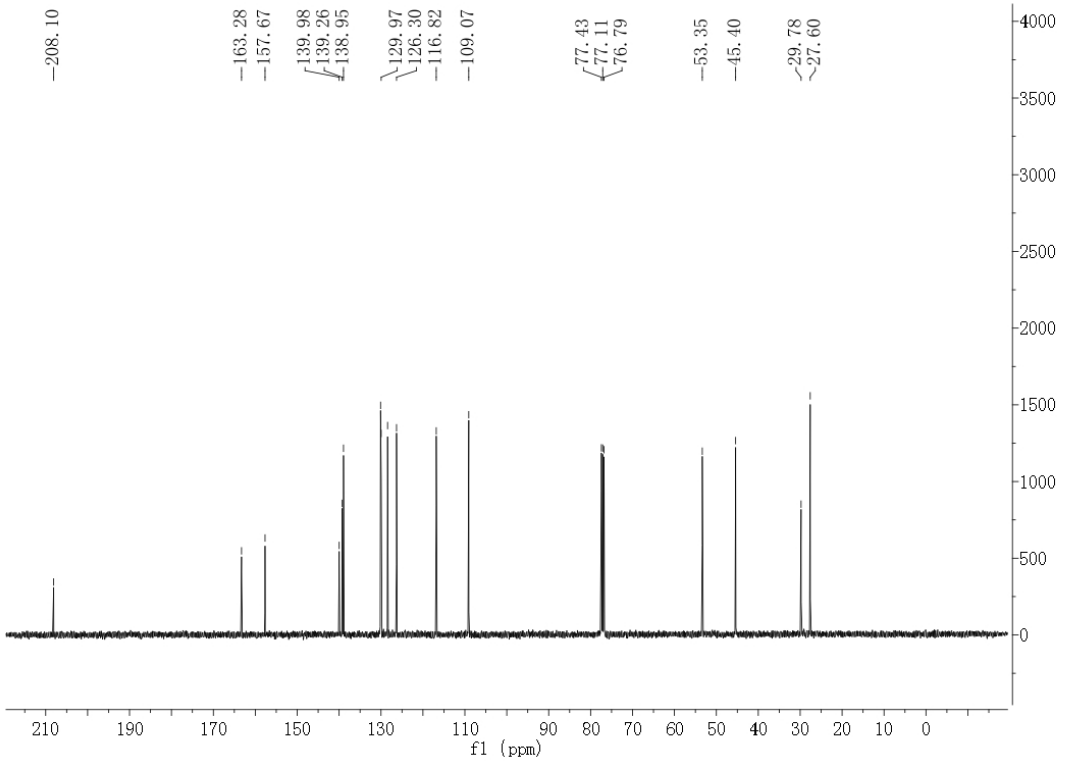

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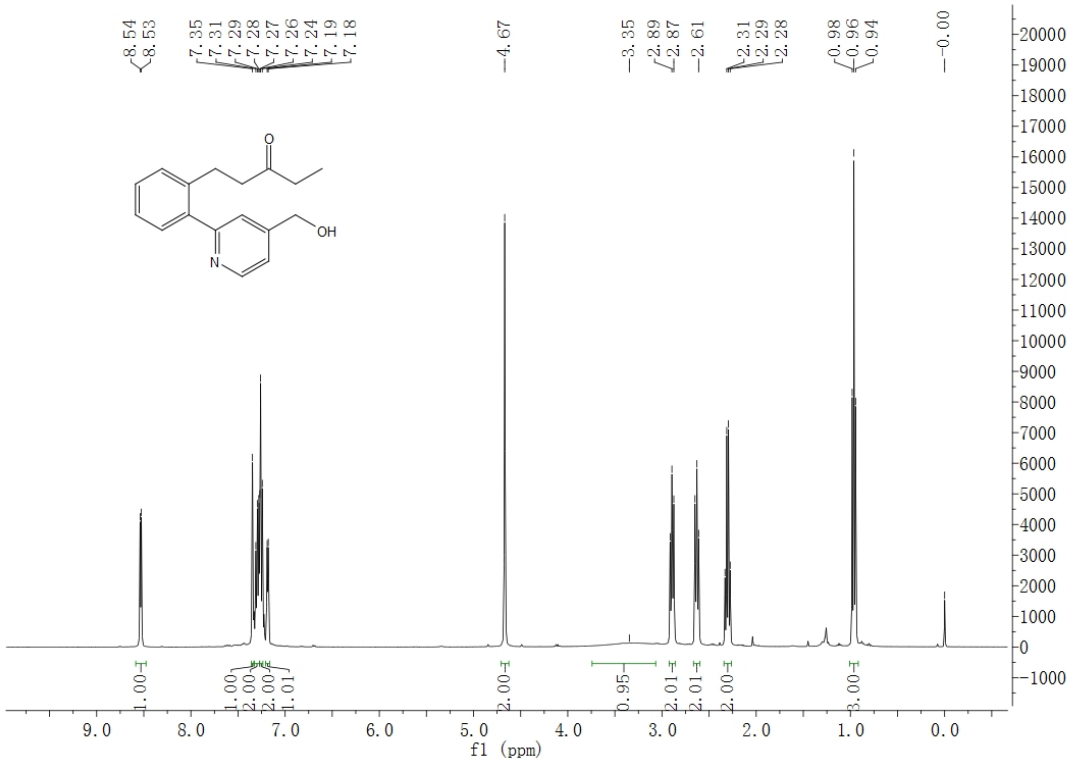

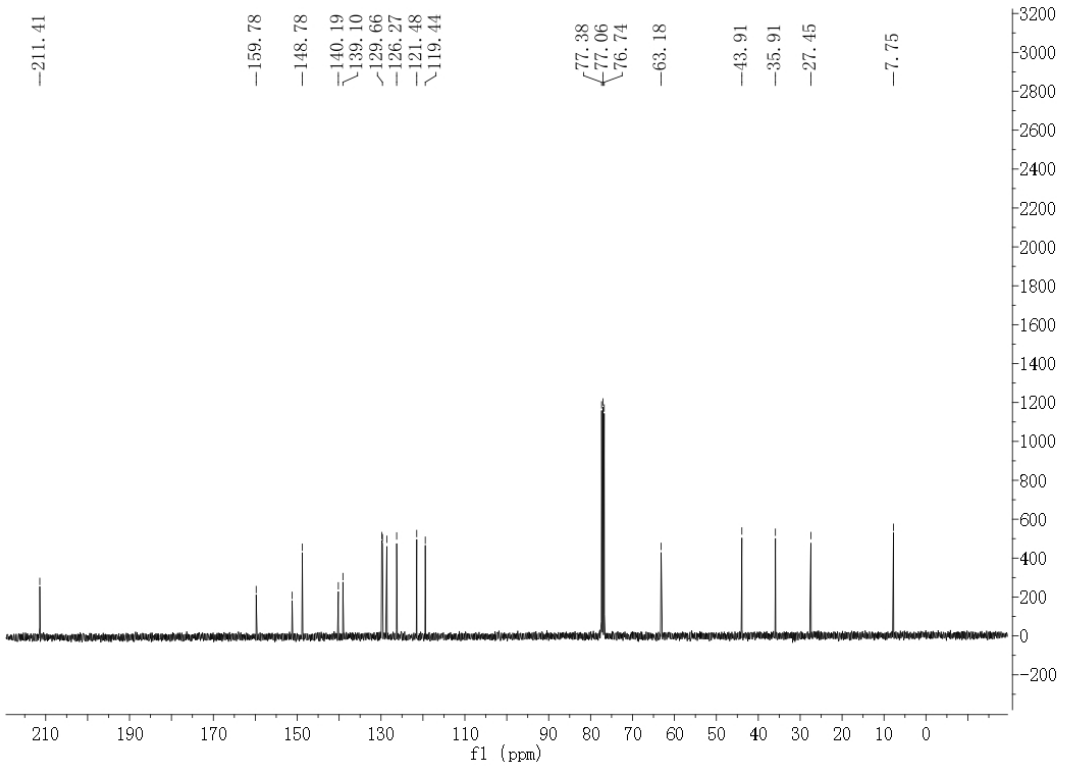

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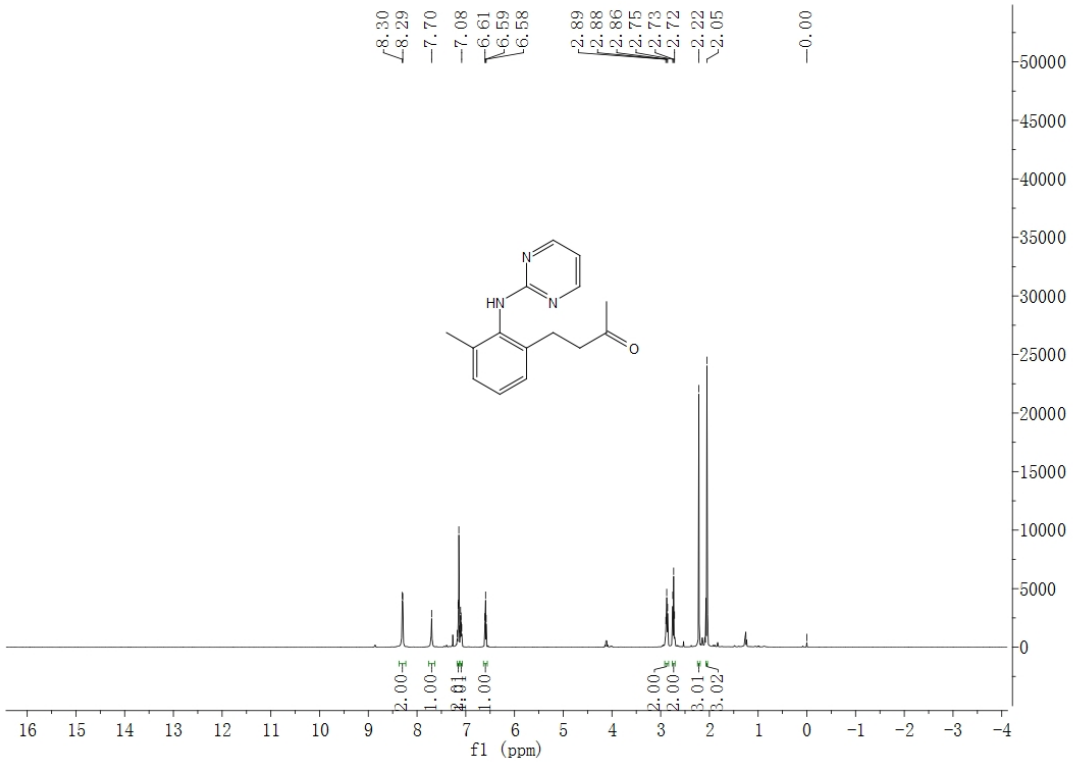

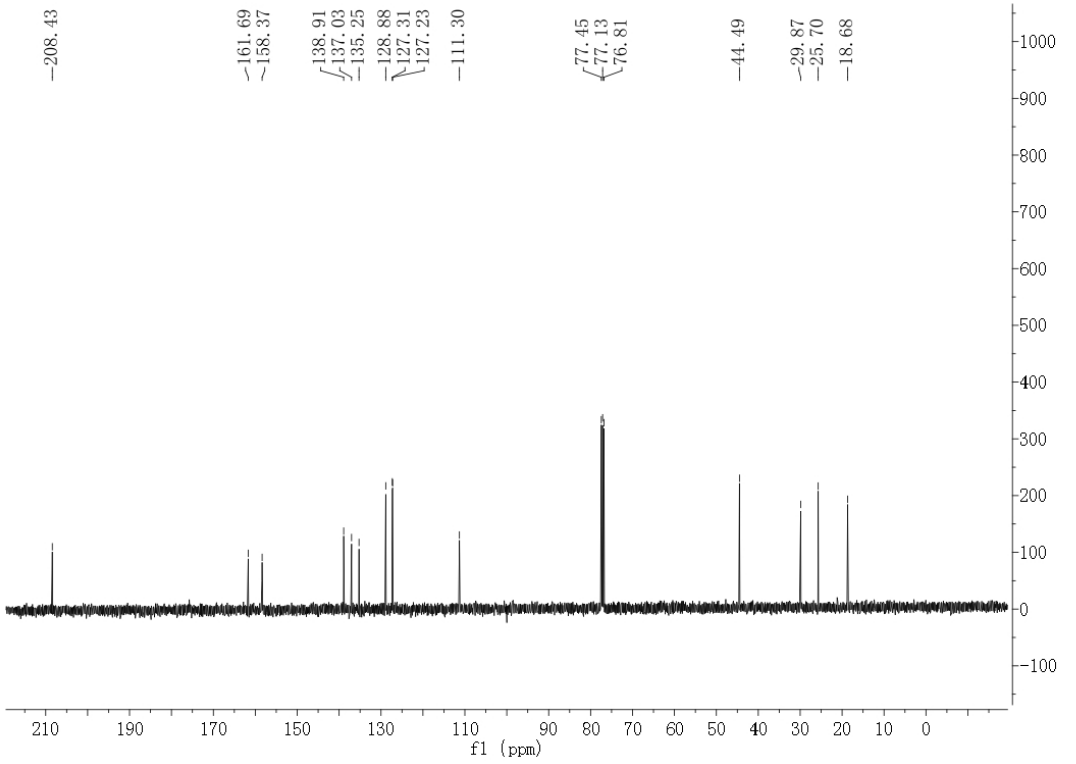

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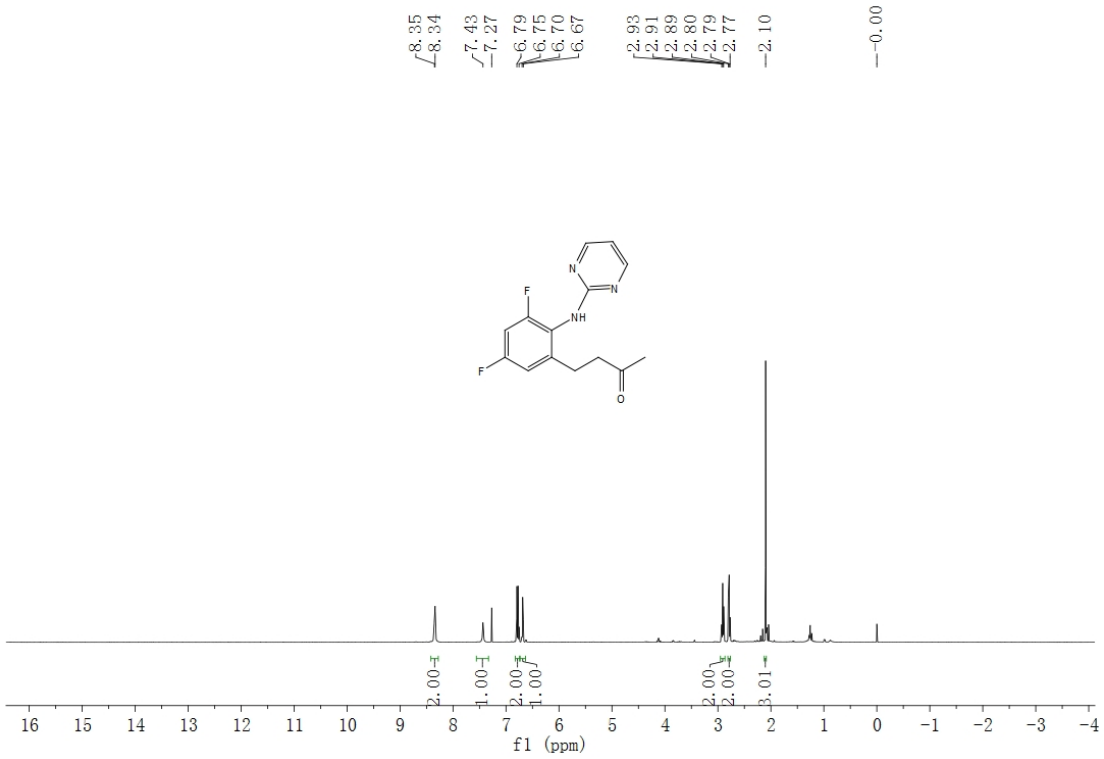

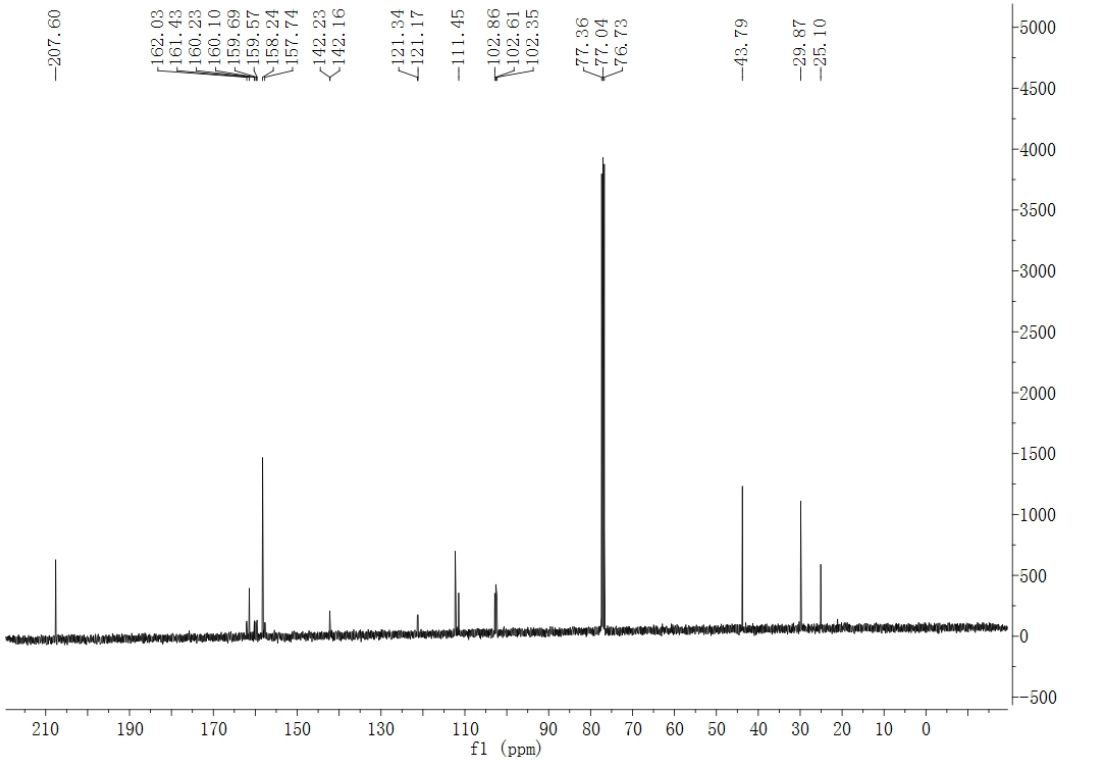

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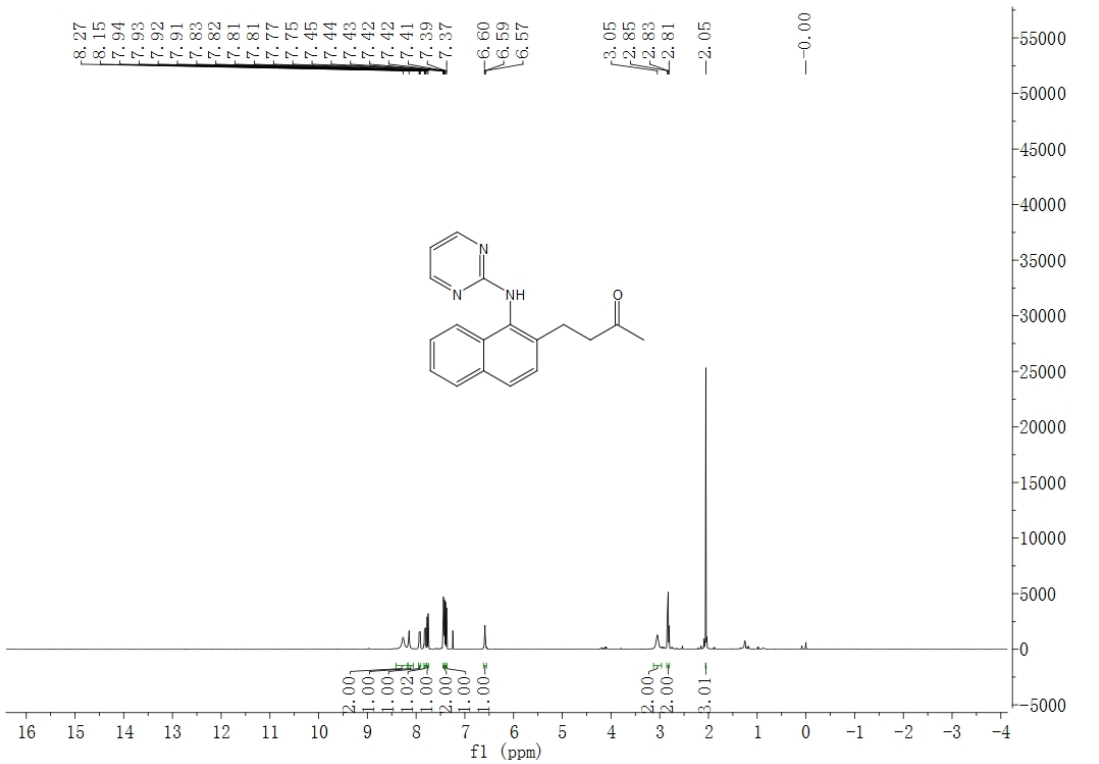

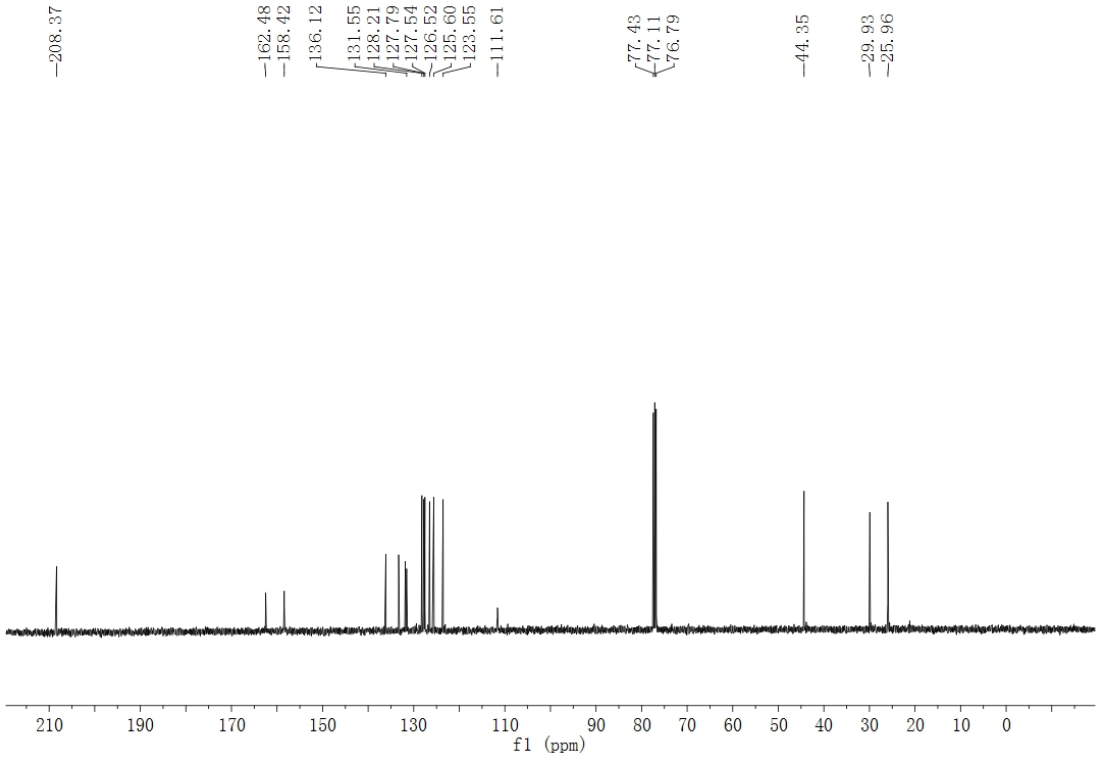

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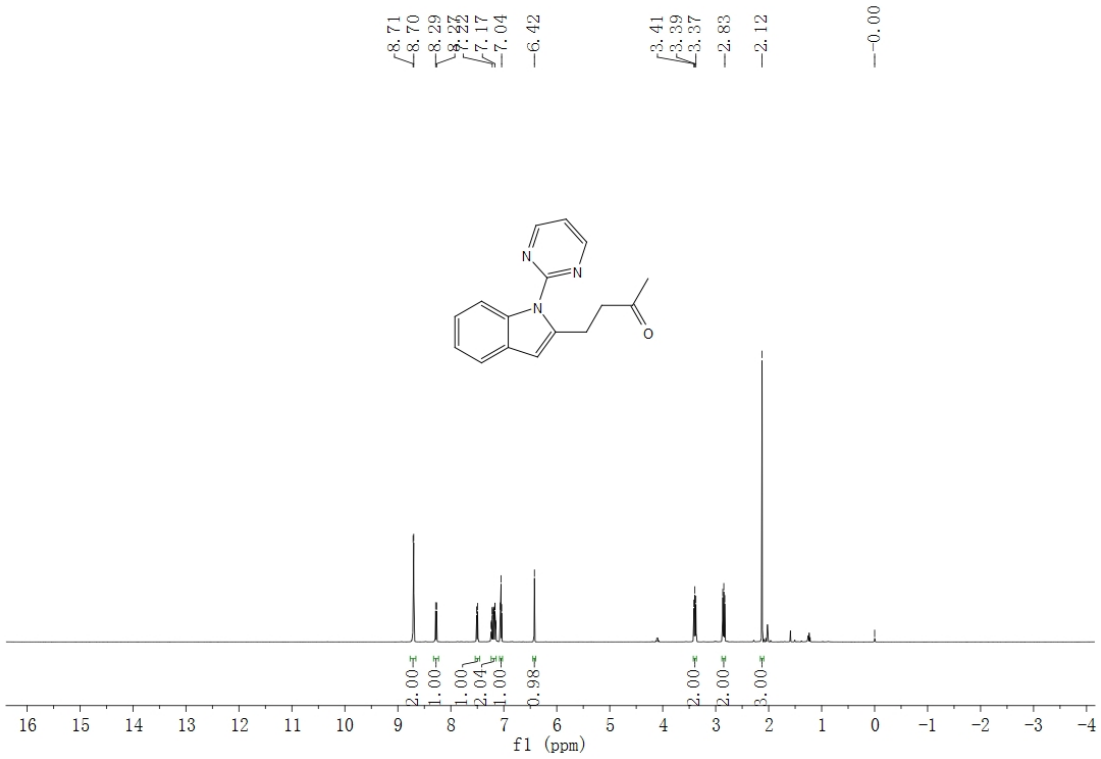

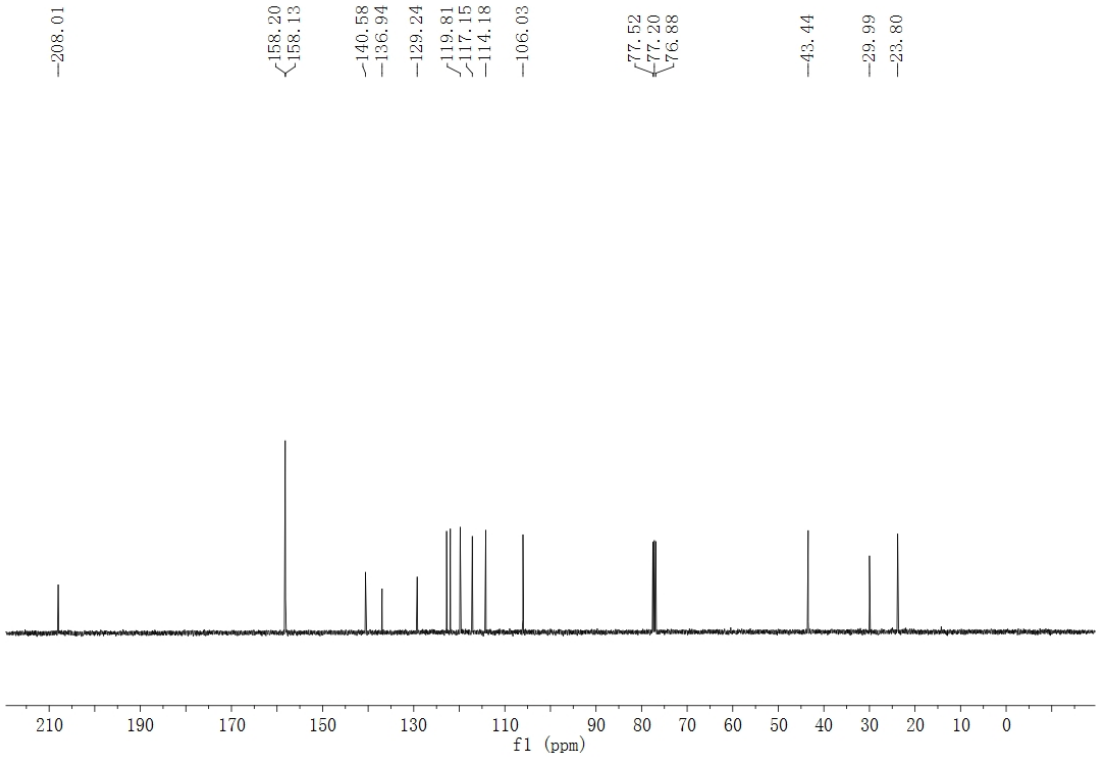

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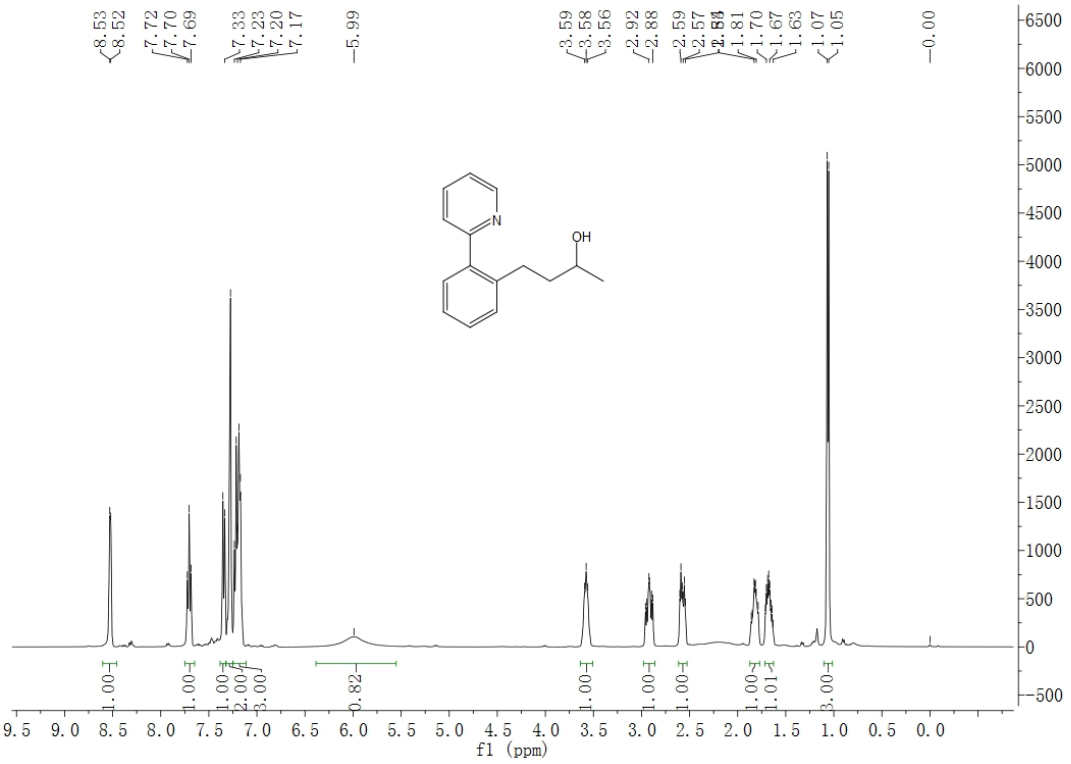

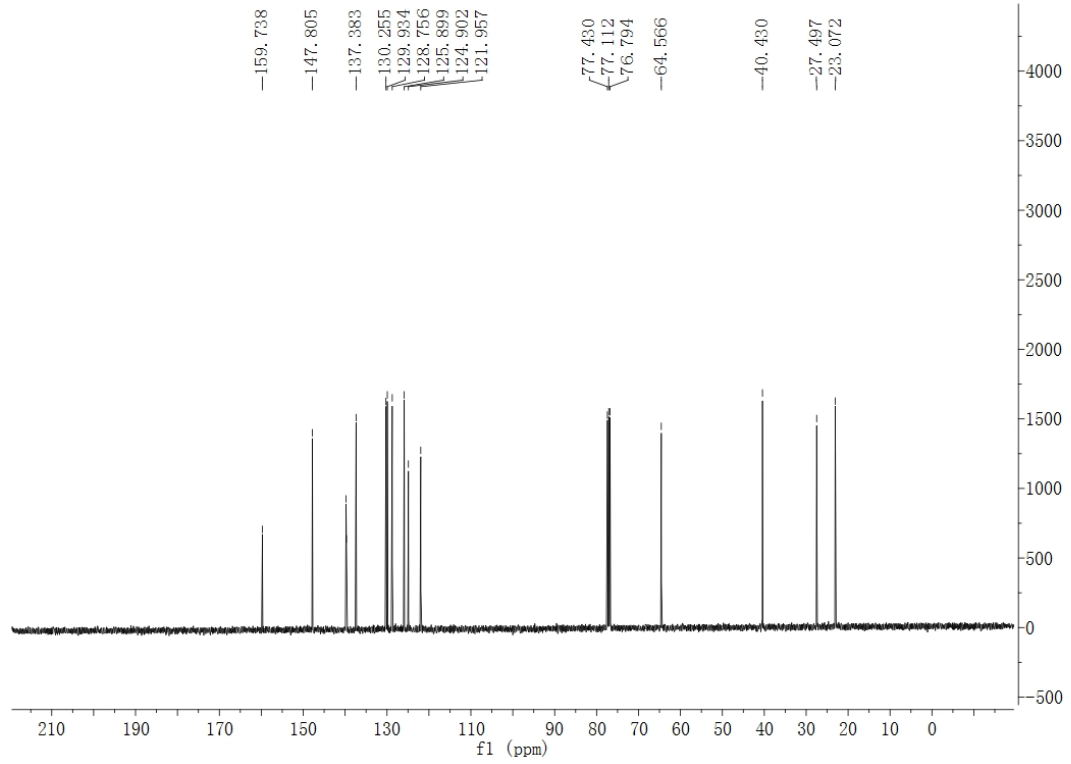

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