Electronic Supporting Information

Cp*Co(III)-Catalyzed Amidation of Olefinic and Aryl C-H Bonds: Highly Selective Synthesis of Enamides and Pyrimidones

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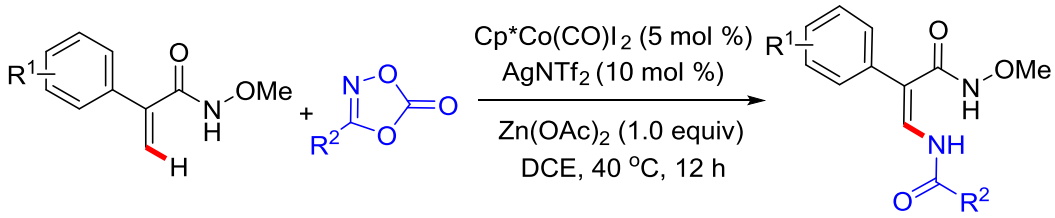
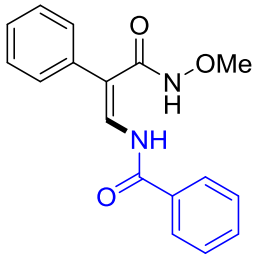
I. General Remarks

All chemicals were obtained from commercial sources and were used as received unless otherwise noted. All reactions were carried out using Schlenk techniques or in a N_2 filled glovebox. NMR Spectra were recorded on a 400 MHz NMR spectrometer in the solvent indicated. The chemical shift is given in dimensionless δ values and is frequency referenced relative to TMS in ^1H and ^{13}C NMR spectroscopy. HRMS data were obtained on a Thermo Scientific LTQ Orbitrap Discovery spectrometer (Bremen, Germany). Column chromatography was performed on silica gel (300-400 mesh) using ethyl acetate/hexanes. *N*-methoxy-acrylamides[1] and dioxazolones[2] were prepared according to literature reports.

II. General procedures for the synthesis of compound 3,4 and 5



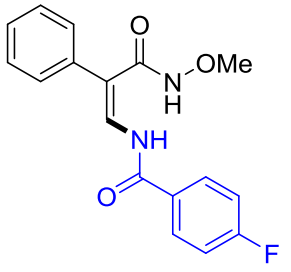
Typical Reaction Conditions for synthesis of **3**: *N*-methoxy-acrylamide (0.2 mmol), dioxazolones (0.24 mmol), Cp*Co(CO)I_2 (5 mol%), $AgNTf_2$ (10 mol%), $Zn(OAc)_2$ (0.2 mmol) and DCE (2 mL) were charged into a pressure tube. The reaction mixture was stirred under N_2 at 40 ℃ for 12 h. After the solvent was removed under reduced pressure, the residue was purified by silica gel chromatography using PE/EA to afford the product **3**.



3aa

(*Z*)-*N*-(3-(methoxyamino)-3-oxo-2-phenylprop-1-en-1-yl)benzamide

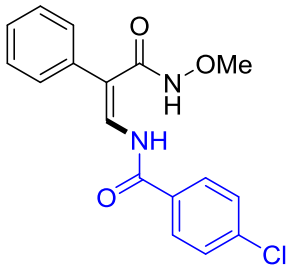
White solid, Yield 93% (55.0 mg). ^1H NMR (400 MHz, $CDCl_3$) δ 12.38 (d, J = 10.0 Hz, 1H), 8.16 (s, 1H), 8.02 (d, J = 7.6 Hz, 2H), 7.64 – 7.57 (m, 2H), 7.52 – 7.48 (m, 2H), 7.45 – 7.38 (m, 3H), 7.35 – 7.33 (m, 2H), 3.81 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.6, 164.7, 136.9, 134.9, 132.8, 132.4, 130.0, 129.2, 128.9, 128.5, 127.8, 110.9, 64.9. HRMS (ESI) Calcd for $[C_{17}H_{16}N_2O_3+H]^+$ 297.1234, Found 297.1233.



3ab

(*Z*)-4-Fluoro-*N*-(3-(methoxyamino)-3-oxo-2-phenylprop-1-en-1-yl)benzamide

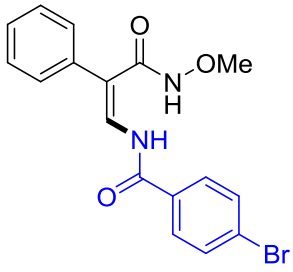
White solid, Yield 80% (50.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.39 (d, J = 10.4 Hz, 1H), 8.34 (s, 1H), 8.05 – 7.99 (m, 2H), 7.56 (d, J = 10.4 Hz, 1H), 7.43 – 7.35 (m, 3H), 7.35 – 7.30 (m, 2H), 7.20 – 7.14 (m, 2H), 3.81 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.5, 165.5 (d, $J_{C\text{-}F}$ = 253.0 Hz), 163.6, 136.7, 134.8, 130.3 (d, $J_{C\text{-}F}$ = 9.0 Hz), 129.9, 129.2, 128.6 (d, $J_{C\text{-}F}$ = 3.0 Hz) 128.5, 116.0 (d, $J_{C\text{-}F}$ = 22.0 Hz), 111.2, 64.8. HRMS (ESI) Calcd for $[C_{17}H_{15}FN_2O_3+H]^+$ 315.1139, Found 315.1139.



3ac

(*Z*)-4-Chloro-*N*-(3-(methoxyamino)-3-oxo-2-phenylprop-1-en-1-yl)benzamide

White solid, Yield 88% (58.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.42 (d, J = 10.4 Hz, 1H), 8.18 (s, 1H), 7.97 – 7.95 (m, 2H), 7.60 (d, J = 10.4 Hz, 1H), 7.49 – 7.46 (m, 2H), 7.45 – 7.38 (m, 3H), 7.34 – 7.32 (m, 2H), 3.82 (s, 3H). ^{13}C NMR (100MHz, $CDCl_3$) δ 167.5, 163.6, 139.2, 136.6, 134.7, 130.8, 129.9, 129.20, 129.19, 129.15, 128.5, 111.4, 64.8. HRMS (ESI) Calcd for $[C_{17}H_{15}ClN_2O_3+H]^+$ 331.0844, Found 331.0844.

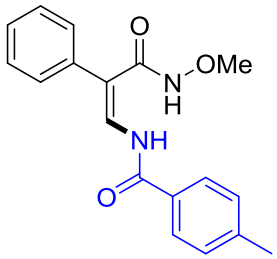


3ad

(*Z*)-4-Bromo-*N*-(3-(methoxyamino)-3-oxo-2-phenylprop-1-en-1-yl)benzamide

White solid, Yield 77% (57.9 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.42 (d, J = 9.6 Hz, 1H), 8.20 (s, 1H), 7.88 (d, J = 8.0 Hz, 2H), 7.64 (d, J = 8.0 Hz, 2H), 7.59 (d, J = 10.4 Hz, 1H), 7.43 – 7.41 (m, 3H), 7.34 – 7.32 (m, 2H), 3.81 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.5, 163.7, 136.5, 134.7, 132.1,

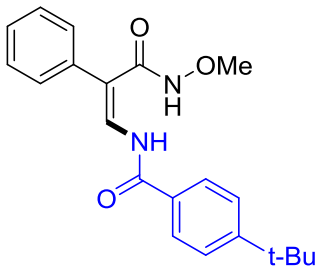
131.2, 129.9, 129.3, 129.2, 128.6, 127.8, 111.4, 64.8. HRMS (ESI) Calcd for $[C_{17}H_{15}BrN_2O_3+H]^+$ 375.0339, Found 375.0338.



3ae

(*Z*)-*N*-(3-(methoxyamino)-3-oxo-2-phenylprop-1-en-1-yl)-4-methylbenzamide

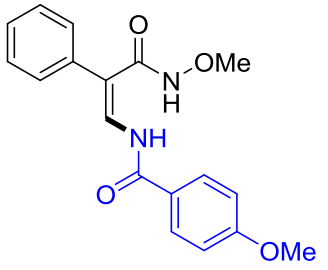
White solid, Yield 91% (56.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.33 (d, J = 10.8 Hz, 1H), 8.18 (s, 1H), 7.92 (d, J = 8.0 Hz, 2H), 7.62 (d, J = 10.8 Hz, 1H), 7.44 – 7.38 (m, 3H), 7.36 – 7.32 (m, 2H), 7.30 (d, J = 8.0 Hz, 2H), 3.81 (s, 3H), 2.43 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.6, 164.6, 143.6, 136.9, 135.0, 129.9, 129.54, 129.51, 129.1, 128.4, 127.8, 110.7, 64.8, 21.6. HRMS (ESI) Calcd for $[C_{18}H_{18}N_2O_3+H]^+$ 311.1390, Found 311.1392.



3af

(*Z*)-4-(Tert-butyl)-*N*-(3-(methoxyamino)-3-oxo-2-phenylprop-1-en-1-yl)benzamide

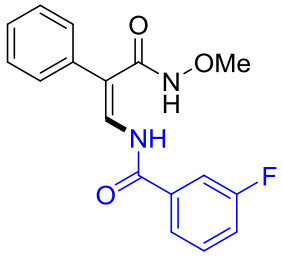
Colorless liquid, Yield 83% (58.5 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.33 (d, J = 10.8 Hz, 1H), 8.16 (s, 1H), 7.95 (m, 2H), 7.63 (d, J = 8.0 Hz, 1H), 7.51 (m, 2H), 7.45 – 7.37 (m, 3H), 7.35 – 7.33 (m, 2H), 3.81 (s, 3H), 1.36 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.6, 164.7, 156.5, 137.1, 135.0, 130.0, 129.6, 129.2, 128.4, 127.7, 125.8, 110.6, 64.8, 35.1, 31.1. HRMS (ESI) Calcd for $[C_{21}H_{24}N_2O_3+H]^+$ 353.1860, Found 353.1862.



3ag

(*Z*)-4-Methoxy-*N*-(3-(methoxyamino)-3-oxo-2-phenylprop-1-en-1-yl)benzamide

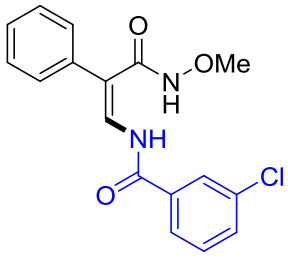
White solid, Yield 83% (54.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.31 (d, J = 10.8 Hz, 1H), 8.14 (s, 1H),8.02 – 7.97 (m, 2H), 7.63 (d, J = 10.8 Hz, 1H), 7.46 – 7.37 (m, 3H), 7.35 – 7.32 (m, 2H), 7.00 – 6.97 (m, 2H), 3.88 (s, 3H), 3.82 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.7, 164.2, 163.3, 137.2, 135.1, 130.0, 129.9, 129.2, 128.4, 124.7, 114.1, 110.3, 64.9, 55.5. HRMS (ESI) Calcd for $[C_{18}H_{18}N_2O_4+H]^+$ 327.1339, Found 327.1339.



3ah

(*Z*)-3-Fluoro-*N*-(3-(methoxyamino)-3-oxo-2-phenylprop-1-en-1-yl)benzamide

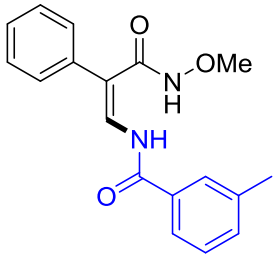
White solid, Yield 89% (56.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.39 (d, J = 10.4 Hz, 1H), 8.38 (s, 1H), 7.77 – 7.75 (m, 1H), 7.73 – 7.69 (m, 1H), 7.55 (d, J = 10.4 Hz, 1H), 7.52 – 7.45 (m, 1H), 7.43 – 7.36 (m, 3H), 7.34 – 7.25 (m, 3H), 3.81 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.4, 163.5 (d, $J_{C\text{-}F}$ = 3.0 Hz), 162.9 (d, $J_{C\text{-}F}$ = 247.0 Hz), 136.4, 134.74, 134.68, 130.5 (d, $J_{C\text{-}F}$ = 8.0 Hz), 129.9, 129.2, 128.6, 123.1 (d, $J_{C\text{-}F}$ = 3.0 Hz), 119.8 (d, $J_{C\text{-}F}$ = 22.0 Hz), 115.2 (d, $J_{C\text{-}F}$ = 23.0 Hz), 111.6, 64.8. HRMS (ESI) Calcd for $[C_{17}H_{15}FN_2O_3+H]^+$ 315.1139, Found 315.1140.



3ai

(*Z*)-3-Chloro-*N*-(3-(methoxyamino)-3-oxo-2-phenylprop-1-en-1-yl)benzamide

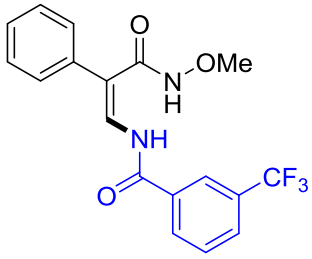
Colorless liquid, Yield 88% (58.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.37 (d, J = 10.4 Hz, 1H), 8.25 (s, 1H), 8.00 (t, J = 1.6 Hz, 1H), 7.87 – 7.85 (m, 1H), 7.59 – 7.54 (m, 2H), 7.46 – 7.38 (m, 4H), 7.34 – 7.32 (m, 2H), 3.81 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.4, 163.4, 136.4, 135.2, 134.7, 134.2, 132.8, 130.1, 129.9, 129.2, 128.6, 128.2, 125.6, 111.7, 64.8. HRMS (ESI) Calcd for $[C_{17}H_{15}ClN_2O_3+H]^+$ 331.0844, Found 331.0846.



3aj

(*Z*)-*N*-(3-(methoxyamino)-3-oxo-2-phenylprop-1-en-1-yl)-3-methylbenzamide

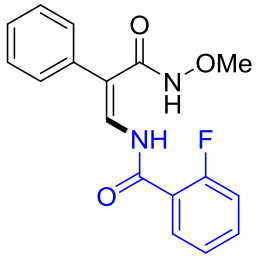
Colorless liquid, Yield 92% (57.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.28 (d, J = 10.4 Hz, 1H), 8.26 (s, 1H), 7.81 – 7.79 (m, 2H), 7.60 (d, J = 10.4 Hz, 1H), 7.43 – 7.36 (m, 5H), 7.35 – 7.32 (m, 2H), 3.81 (s, 3H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.5, 164.9, 138.8, 136.8, 135.0, 133.6, 132.3, 129.9, 129.1, 128.7, 128.40, 128.39, 124.8, 110.9, 64.8, 21.4. HRMS (ESI) Calcd for $[C_{18}H_{18}N_2O_3+H]^+$ 311.1390, Found 311.1392.



3ak

(*Z*)-*N*-(3-(methoxyamino)-3-oxo-2-phenylprop-1-en-1-yl)-3-(trifluoromethyl)benzamide

White solid, Yield 98% (71.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.47 (d, J = 10.4 Hz, 1H), 8.37 (s, 1H), 8.30 (s, 1H), 8.14 (d, J = 7.6 Hz, 1H), 7.85 (d, J = 7.6 Hz, 1H), 7.65 (t, J = 7.8 Hz, 1H), 7.57 (d, J = 10.4 Hz, 1H), 7.43 – 7.37 (m, 3H), 7.36 – 7.31 (m, 2H), 3.81 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.3, 163.3, 136.3, 134.6, 133.4, 131.6 (q, $J_{C\text{-}F}$ = 32.0 Hz), 130.4, 129.9, 129.5, 129.3, 129.2, 128.6, 125.3 (q, $J_{C\text{-}F}$ = 3.0 Hz), 123.6 (q, $J_{C\text{-}F}$ = 271.0 Hz), 112.0, 64.8. HRMS (ESI) Calcd for $[C_{18}H_{15}F_3N_2O_3+H]^+$ 365.1108, Found 365.1110.

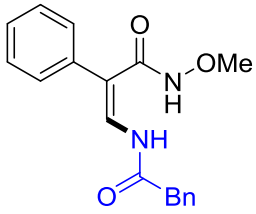


3al

(*Z*)-2-Fluoro-*N*-(3-(methoxyamino)-3-oxo-2-phenylprop-1-en-1-yl)benzamide

White solid, Yield 87% (54.9 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.30 (t, J = 10.4 Hz, 1H), 8.33 (s, 1H), 8.10 (td, J_1 = 7.2 Hz, J_2 = 1.6 Hz, 1H), 7.62 – 7.52 (m, 2H), 7.42 – 7.34 (m, 3H), 7.34 – 7.28 (m,

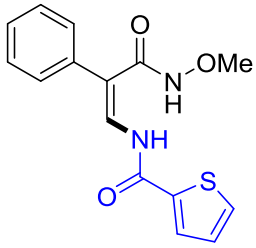
3H), 7.23 – 7.18 (m, 1H), 3.79 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.7, 161.7 (d, $J_{C\text{-}F}$ = 3.0 Hz), 161.1 (d, $J_{C\text{-}F}$ =251.0 Hz), 135.6, 135.1, 134.5 (d, $J_{C\text{-}F}$ = 9.0 Hz), 132.1 (d, $J_{C\text{-}F}$ = 1.0 Hz), 129.9, 129.1, 128.4, 124.8 (d, $J_{C\text{-}F}$ = 3.0 Hz), 120.1 (d, $J_{C\text{-}F}$ = 11.0 Hz), 116.6 (d, $J_{C\text{-}F}$ = 24.0 Hz), 112.1, 64.7. HRMS (ESI) Calcd for $[C_{17}H_{15}FN_2O_3+H]^+$ 315.1139, Found 315.1140.



3am

(*Z*)-*N*-methoxy-2-phenyl-3-(2-phenylacetamido)acrylamide

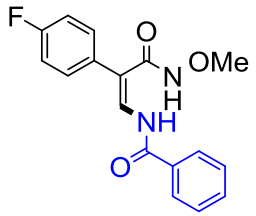
Colorless liquid, Yield 80% (49.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.25 (d, J = 10.8 Hz, 1H), 8.16 (s, 1H), 7.40 – 7.28 (m, 9H), 7.23 – 7.21 (m, 2H), 3.71 (s, 3H), 3.68 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.5, 166.9, 135.8, 134.9, 133.7, 129.8, 129.3, 129.10, 129.05, 128.4, 127.5, 110.9, 64.7, 44.2. HRMS (ESI) Calcd for $[C_{18}H_{18}N_2O_3+H]^+$ 311.1390, Found 311.1389.



3an

(*Z*)-*N*-(3-(methoxyamino)-3-oxo-2-phenylprop-1-en-1-yl)thiophene-2-carboxamide

Yellow solid, Yield 52% (33.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.24 (d, J = 10.6 Hz, 1H), 8.24 (s, 1H), 7.78 – 7.77 (dd, J_1 = 3.6 Hz, J_2 = 0.8 Hz, 1H), 7.62 (dd, J_1 =4.8 Hz, J_2 = 0.8 Hz, 1H), 7.52 (d, J = 10.6 Hz, 1H), 7.43 – 7.36 (m, 3H), 7.33 – 7.31 (m, 2H), 7.16 – 7.14 (m, 1H), 3.81 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.4, 159.5, 137.7, 136.4, 134.8, 132.4, 129.94, 129.93, 129.2, 128.5, 128.1, 110.7, 64.8. HRMS (ESI) Calcd for $[C_{15}H_{14}N_2O_3S+H]^+$ 303.0798, Found 303.0798.

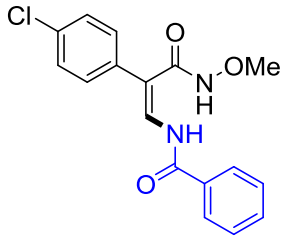


3ba

(*Z*)-*N*-(2-(4-fluorophenyl)-3-(methoxyamino)-3-oxoprop-1-en-1-yl)benzamide

White solid, Yield 91% (57.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.35 (d, J = 10.8 Hz, 1H), 8.22 (s, 1H), 8.02 – 7.98 (m, 2H), 7.61 – 7.56 (m, 2H), 7.52 – 7.49 (m, 2H), 7.33 – 7.28 (m, 2H), 7.13 – 7.07

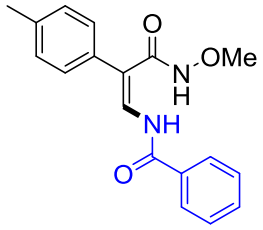
(m, 2H), 3.81 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.5, 164.7, 162.8 (d, $J_{C\text{-}F}$ = 247.0 Hz), 137.0, 132.9, 132.2, 131.8 (d, $J_{C\text{-}F}$ = 8.0 Hz), 130.8 (d, $J_{C\text{-}F}$ = 4.0 Hz), 128.9, 127.8, 116.2 (d, $J_{C\text{-}F}$ = 22.0 Hz), 109.8, 64.8. HRMS (ESI) Calcd for $[C_{17}H_{15}FN_2O_3+H]^+$ 315.1139, Found 315.1139.



3ca

(*Z*)-*N*-(2-(4-chlorophenyl)-3-(methoxyamino)-3-oxoprop-1-en-1-yl)benzamide

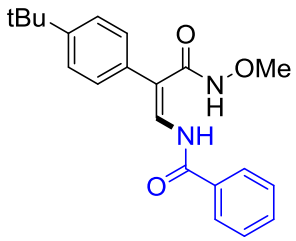
White solid, Yield 78% (51.5 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.35 (d, J = 10.8 Hz, 1H), 8.25 (s, 1H), 8.02 – 7.97 (m, 2H), 7.62 – 7.56 (m, 2H), 7.52 – 7.49 (m, 2H), 7.40 – 7.35 (m, 2H), 7.29 – 7.25 (m, 2H), 3.81 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.3, 164.7, 137.1, 134.6, 133.3, 132.9, 132.2, 131.3, 129.4, 128.9, 127.8, 109.8, 64.9. HRMS (ESI) Calcd for $[C_{17}H_{15}ClN_2O_3+H]^+$ 331.0844, Found 331.0841.



3da

(*Z*)-*N*-(3-(methoxyamino)-3-oxo-2-(p-tolyl)prop-1-en-1-yl)benzamide

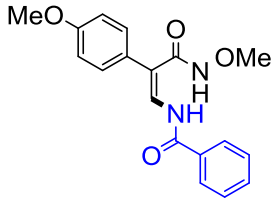
White solid, Yield 77% (47.7 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.37 (d, J = 10.8 Hz, 1H), 8.26 (s, 1H), 8.03 – 7.99 (m, 2H), 7.61 – 7.56 (m, 2H), 7.52 – 7.48 (m, 2H), 7.23 – 7.19 (m, 4H), 3.80 (s, 3H), 2.38 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.7, 164.7, 138.4, 136.5, 132.7, 132.4, 131.8, 129.9, 129.8, 128.9, 127.8, 110.9, 64.8, 21.2. HRMS (ESI) Calcd for $[C_{18}H_{18}N_2O_3+H]^+$ 311.1390, Found 311.1389.



3ea

(*Z*)-*N*-(2-(4-(tert-butyl)phenyl)-3-(methoxyamino)-3-oxoprop-1-en-1-yl)benzamide

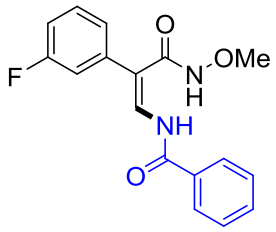
White solid, Yield 54% (37.8 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.38 (d, J = 10.8 Hz, 1H), 8.25 (s, 1H), 8.04 – 8.00 (m, 2H), 7.61 (d, J = 10.8 Hz, 1H), 7.58 – 7.56 (m, 1H), 7.52 – 7.48 (m, 2H), 7.44 – 7.42 (m, 2H), 7.27 – 7.25 (m, 2H), 3.82 (s, 3H), 1.35 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.7, 164.7, 151.6, 136.6, 132.7, 132.5, 131.8, 129.6, 128.9, 127.8, 126.1, 110.9, 64.8, 34.7, 31.3. HRMS (ESI) Calcd for $[C_{21}H_{24}N_2O_3+H]^+$ 353.1860, Found 353.1861.



3fa

(*Z*)-*N*-(3-(methoxyamino)-2-(4-methoxyphenyl)-3-oxoprop-1-en-1-yl)benzamide

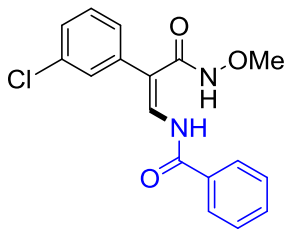
White solid, Yield 77% (50.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.35 (d, J = 10.4 Hz, 1H), 8.33 (s, 1H), 8.03 – 7.98 (m, 2H), 7.61 – 7.53 (m, 2H), 7.51 – 7.48 (m, 2H), 7.26 – 7.21 (m, 2H), 6.94 – 6.89 (m, 2H), 3.81 (s, 3 H), 3.80 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.8, 164.6, 159.7, 136.3, 132.7, 132.4, 131.2, 128.8, 127.8, 126.8, 114.5, 110.6, 64.8, 55.3. HRMS (ESI) Calcd for $[C_{18}H_{18}N_2O_4+H]^+$ 327.1339, Found 327.1340.



3ga

(*Z*)-*N*-(2-(3-fluorophenyl)-3-(methoxyamino)-3-oxoprop-1-en-1-yl)benzamide

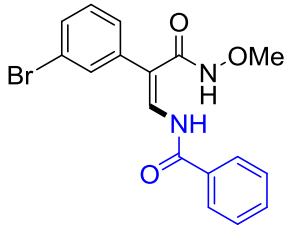
White solid, Yield 98% (64.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.36 (d, J = 10.4 Hz, 1H), 8.32 (s, 1H), 8.01 – 7.99 (m, 2H), 7.64 – 7.56 (m, 2H), 7.53 – 7.49 (m, 2H), 7.41 – 7.34 (m, 1H), 7.14 – 7.03 (m, 3H), 3.82 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.1, 164.7, 162.9 (d, $J_{C\text{-}F}$ = 247.0 Hz), 137.3, 137.1 (d, $J_{C\text{-}F}$ = 8.0 Hz), 132.9, 132.2, 130.8 (d, $J_{C\text{-}F}$ = 9.0 Hz), 128.9, 127.8, 125.6 (d, $J_{C\text{-}F}$ = 3.0 Hz), 117.0 (d, $J_{C\text{-}F}$ = 22.0 Hz), 115.5 (d, $J_{C\text{-}F}$ = 21.0 Hz), 109.8 (d, $J_{C\text{-}F}$ = 1.0 Hz), 64.9. HRMS (ESI) Calcd for $[C_{17}H_{15}FN_2O_3+H]^+$ 315.1139, Found 315.1142.



3ha

(*Z*)-*N*-(2-(3-chlorophenyl)-3-(methoxyamino)-3-oxoprop-1-en-1-yl)benzamide

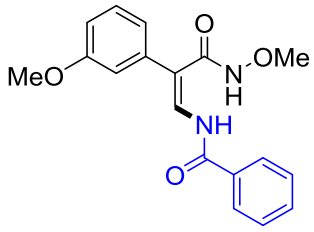
White solid, Yield 73% (48.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.35 (d, J = 10.4 Hz, 1H), 8.29 (s, 1H), 8.03 – 7.97 (m, 2H), 7.62 – 7.58 (m, 2H), 7.53 – 7.49 (m, 2H), 7.38 – 7.31 (m, 3H), 7.24 – 7.20 (m, 1H), 3.82 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.1, 164.7, 137.4, 136.8, 135.0, 132.9, 132.2, 130.4, 130.0, 128.9, 128.6, 128.1, 127.8, 109.7, 64.9. HRMS (ESI) Calcd for $[C_{17}H_{15}ClN_2O_3+H]^+$ 331.0844, Found 331.0846.



3ia

(*Z*)-*N*-(2-(3-bromophenyl)-3-(methoxyamino)-3-oxoprop-1-en-1-yl)benzamide

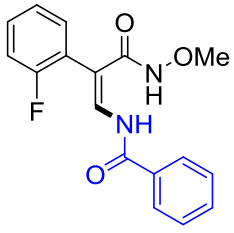
White solid, Yield 82% (61.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.35 (d, J = 10.4 Hz, 1H), 8.26 (s, 1H), 8.02 – 7.98 (m, 2H), 7.62 – 7.58 (m, 2H), 7.53 – 7.48 (m, 4H), 7.28 – 7.27 (m, 2H), 3.82 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.1, 164.7, 137.5, 137.0, 132.94, 132.88, 132.2, 131.6, 130.6, 128.9, 128.5, 127.8, 123.2, 109.6, 64.9. HRMS (ESI) Calcd for $[C_{17}H_{15}BrN_2O_3+H]^+$ 375.0339, Found 375.0338.



3ja

(*Z*)-*N*-(3-(methoxyamino)-2-(3-methoxyphenyl)-3-oxoprop-1-en-1-yl)benzamide

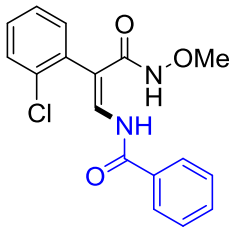
White solid, Yield 90% (58.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.39 (d, J = 10.6 Hz, 1H), 8.35 (s, 1H), 8.02 – 8.00 (m, 2H), 7.65 – 7.56 (m, 2H), 7.52 – 7.48 (m, 2H), 7.31 (t, J = 8.0 Hz, 1H), 6.92 – 6.90 (m, 2H), 6.87 – 6.84 (m, 1H), 3.82 (s, 3H), 3.81 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.4, 164.7, 160.0, 136.7, 136.2, 132.8, 132.4, 130.2, 128.9, 127.8, 122.1, 115.5, 114.0, 110.9, 64.8, 55.4. HRMS (ESI) Calcd for $[C_{18}H_{18}N_2O_4+H]^+$ 327.1339, Found 327.1337.



3ka

(*Z*)-*N*-(2-(2-fluorophenyl)-3-(methoxyamino)-3-oxoprop-1-en-1-yl)benzamide

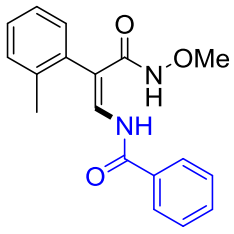
White solid, Yield 80% (49.5 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.42 (d, J = 10.4 Hz, 1H), 8.24 (s, 1H), 8.03 – 7.98 (m, 2H), 7.62 – 7.57 (m, 2H), 7.52 – 7.49 (m, 2H), 7.41 – 7.34 (m, 1H), 7.31 – 7.27 (m, 1H), 7.21 – 7.17 (m, 1H), 7.15 – 7.11 (m, 1H), 3.80 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.9, 164.7, 160.5 (d, $J_{C\text{-}F}$ = 246.0 Hz), 138.1, 132.9, 132.6 (d, $J_{C\text{-}F}$ = 2.0 Hz), 132.2, 130.9 (d, $J_{C\text{-}F}$ = 8.0 Hz), 128.9, 127.8, 124.9 (d, $J_{C\text{-}F}$ = 3.0 Hz), 122.3 (d, $J_{C\text{-}F}$ = 16.0 Hz), 116.3 (d, $J_{C\text{-}F}$ = 22.0 Hz), 104.4, 64.8. HRMS (ESI) Calcd for $[C_{17}H_{15}FN_2O_3+H]^+$ 315.1139, Found 315.1139.



3la

(*Z*)-*N*-(2-(2-chlorophenyl)-3-(methoxyamino)-3-oxoprop-1-en-1-yl)benzamide

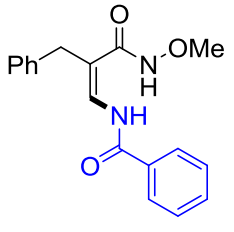
White solid, Yield 78% (51.6 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.38 (d, J = 10.4 Hz, 1H), 8.07 (s, 1H), 8.02 – 8.01 (m, 2H), 7.62 – 7.53 (m, 2H), 7.52 – 7.49 (m, 2H), 7.47 – 7.45 (m, 1H), 7.37 – 7.31 (m, 3H), 3.80 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 164.7, 137.7, 135.4, 133.3, 132.88, 132.86, 132.2, 130.4, 130.2, 128.9, 127.9, 127.6, 108.5, 64.7. HRMS (ESI) Calcd for $[C_{17}H_{15}ClN_2O_3+H]^+$ 331.0844, Found 331.0845.



3ma

(*Z*)-*N*-(3-(methoxyamino)-3-oxo-2-(o-tolyl)prop-1-en-1-yl)benzamide

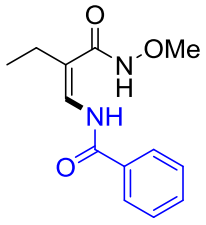
White solid, Yield 78% (47.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.39 (d, J = 10.4 Hz, 1H), 8.03 – 8.02 (m, 2H), 7.95 (s, 1H), 7.61 – 7.57 (m, 1H), 7.55 – 7.47 (m, 3H), 7.33 – 7.18 (m, 4H), 3.77 (s, 3H), 2.29 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.4, 164.7, 138.2, 136.7, 133.5, 132.8, 132.4, 131.4, 130.7, 129.1, 128.9, 127.8, 126.7, 109.8, 64.7, 19.9. HRMS (ESI) Calcd for $[C_{18}H_{18}N_2O_3+H]^+$ 311.1390, Found 311.1392.



3na

(*Z*)-*N*-(2-benzyl-3-(methoxyamino)-3-oxoprop-1-en-1-yl)benzamide

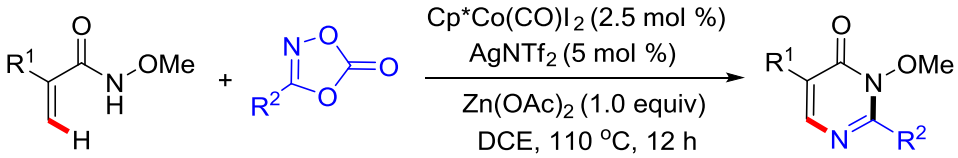
Colorless liquid, Yield 89% (55.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.36 (d, J = 10.4 Hz, 1H), 8.06 (s, 1H), 8.01 (d, J = 7.6 Hz, 2H), 7.69 (d, J = 10.4 Hz, 1H), 7.59 – 7.55 (m, 1H), 7.51 – 7.47 (m, 2H), 7.37 – 7.33 (m, 2H), 7.30 – 7.25 (m, 3H), 3.66 (s, 3H), 3.58 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.7, 164.7, 137.8, 137.2, 132.7, 132.4, 129.3, 128.9, 128.0, 127.8, 127.5, 106.2, 64.6, 36.4. HRMS (ESI) Calcd for $[C_{18}H_{18}N_2O_3+H]^+$ 311.1390, Found 311.1397.



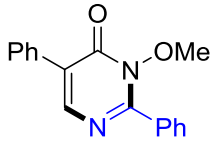
3oa

(*Z*)-*N*-(2-(methoxycarbamoyl)but-1-en-1-yl)benzamide

White solid, Yield 76% (37.7 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.28 (d, J = 10.3 Hz, 1H), 8.52 (s, 1H), 8.03 – 7.95 (m, 2H), 7.61 – 7.50 (m, 2H), 7.53 – 7.43 (m, 2H), 3.86 (s, 3H), 2.23 (q, J = 7.4 Hz, 2H), 1.19 (t, J = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.4, 164.7, 134.5, 132.58, 132.57, 128.8, 127.7, 109.2, 64.8, 22.7, 13.7. HRMS (ESI) Calcd for $[C_{13}H_{16}N_2O_3+Na]^+$ 271.1053, Found 271.1059.



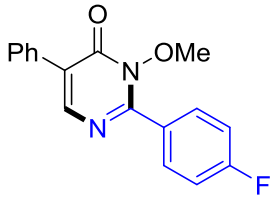
Typical Reaction Conditions for synthesis of **4**: *N*-methoxy-acrylamide (0.2 mmol), dioxazolone (0.21 mmol), Cp*Co(CO)I_2 (2.5 mol%), $AgNTf_2$ (5 mol%), $Zn(OAc)_2$ (0.2 mmol) and DCE (2 mL) were charged into a pressure tube. The reaction mixture was stirred under N_2 at 110 ℃ for 12 h. After the solvent was removed under reduced pressure, the residue was purified by silica gel chromatography using PE/EA to afford the product **4**.



4aa

3-Methoxy-2,5-diphenylpyrimidin-4(3*H*)-one

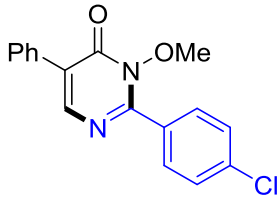
Yellow solid, Yield 90% (50.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.95 – 7.91 (m, 2H), 7.77 – 7.73 (m, 2H), 7.57 – 7.43 (m, 5H), 7.41 – 7.37 (m, 1H), 3.82 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.5, 156.6, 149.0, 132.7, 131.4, 131.3, 129.6, 128.64, 128.56, 128.44, 128.42, 127.4, 64.1. HRMS (ESI) Calcd for $[C_{17}H_{14}N_2O_2+H]^+$ 279.1128, Found 279.1128.



4ab

2-(4-Fluorophenyl)-3-methoxy-5-phenylpyrimidin-4(3*H*)-one

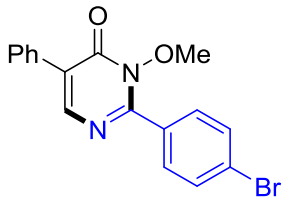
Yellow solid, Yield 81% (48.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (s, 1H), 8.00 – 7.97 (m, 2H), 7.75 – 7.73 (m, 2H), 7.48 – 7.44 (m, 2H), 7.41 – 7.38 (m, 1H), 7.23 – 7.18 (m, 2H), 3.83 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.6 (d, $J_{C\text{-}F}$ = 252.0 Hz), 157.4, 155.4, 148.8, 132.6, 132.1 (d, $J_{C\text{-}F}$ = 9.0 Hz), 128.7, 128.6, 128.4, 127.5, 127.3 (d, $J_{C\text{-}F}$ = 3.0 Hz), 115.7 (d, $J_{C\text{-}F}$ = 22.0 Hz), 64.0. HRMS (ESI) Calcd for $[C_{17}H_{13}FN_2O_2+H]^+$ 297.1034, Found 297.1036.



4ac

2-(4-Chlorophenyl)-3-methoxy-5-phenylpyrimidin-4(3*H*)-one

Yellow solid, Yield 78% (48.8 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (s, 1H), 7.94 – 7.89 (m, 2H), 7.75 – 7.71 (m, 2H), 7.52 – 7.42 (m, 4H), 7.42 – 7.36 (m, 1H), 3.83 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.3, 155.4, 148.8, 137.8, 132.6, 131.1, 129.6, 128.8, 128.7, 128.6, 128.4, 127.7, 64.1. HRMS (ESI) Calcd for $[C_{17}H_{13}ClN_2O_2+H]^+$ 313.0738, Found 313.0738.

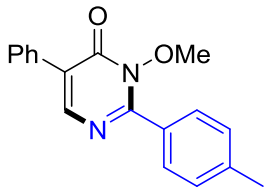


4ad

2-(4-Bromophenyl)-3-methoxy-5-phenylpyrimidin-4(3*H*)-one

Yellow solid, Yield 80% (57.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (s, 1H), 7.85 – 7.83 (m, 2H), 7.74 – 7.72 (m, 2H), 7.67 – 7.65 (m, 2H), 7.47 – 7.44 (m, 2H), 7.42 – 7.38 (m, 1H), 3.84 (s, 3H). ^{13}C

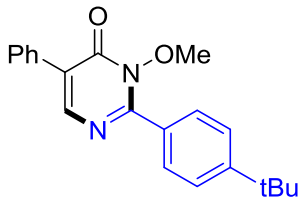
NMR (100 MHz, $CDCl_3$) δ 157.3, 155.4, 148.8, 132.6, 131.8, 131.2, 130.1, 128.8, 128.6, 128.4, 127.7, 126.3, 64.2. HRMS (ESI) Calcd for $[C_{17}H_{13}BrN_2O_2+H]^+$ 357.0233, Found 357.0231.



4ae

3-Methoxy-5-phenyl-2-(p-tolyl)pyrimidin-4(3*H*)-one

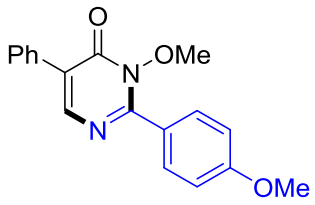
Yellow solid, Yield 74% (43.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (s, 1H), 7.87 – 7.83 (m, 2H), 7.75 – 7.73 (m, 2H), 7.48 – 7.42 (m, 2H), 7.41 – 7.36 (m, 1H), 7.32 – 7.30 (m, 2H), 3.82 (s, 3H), 2.45 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.6, 156.6, 149.0, 142.0, 132.8, 129.6, 129.165, 129.162, 128.6, 128.5, 128.4, 127.0, 63.9, 21.6. One signal is missing due to overlap. HRMS (ESI) Calcd for $[C_{18}H_{16}N_2O_2+H]^+$ 293.1285, Found 293.1287.



4af

2-(4-(Tert-butyl)phenyl)-3-methoxy-5-phenylpyrimidin-4(3*H*)-one

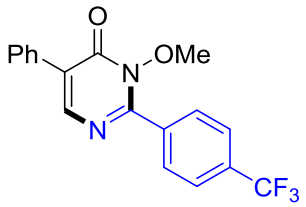
Yellow solid, Yield 70% (46.6 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.83 – 7.81 (m, 2H), 7.69 – 7.63 (m, 2H), 7.45 – 7.43 (m, 2H), 7.39 – 7.35 (m, 2H), 7.32 – 7.28 (m, 1H), 3.76 (s, 3H), 1.29 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.6, 156.5, 155.0, 149.1, 132.9, 129.4, 128.5, 128.39, 128.35, 127.0, 125.5, 64.0, 35.0, 31.2. One signal is missing due to overlap. HRMS (ESI) Calcd for $[C_{21}H_{22}N_2O_2+H]^+$ 335.1754, Found 335.1757.



4ag

2-Methoxy-2-(4-methoxyphenyl)-5-phenylpyrimidin-4(3*H*)-one

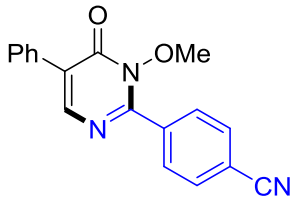
Yellow solid, Yield 60% (36.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (s, 1H), 8.00 – 7.95 (m, 2H), 7.75 – 7.73 (m, 2H), 7.47 – 7.42 (m, 2H), 7.40 – 7.37 (m, 1H), 7.03 – 6.99 (m, 2H), 3.89 (s, 3H), 3.83 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.2, 157.6, 156.1, 149.1, 132.9, 131.6, 128.53, 128.47, 128.4, 126.5, 123.4, 113.9, 63.8, 55.5. HRMS (ESI) Calcd for $[C_{18}H_{16}N_2O_3+H]^+$ 309.1234, Found 309.1235.



4ah

3-Methoxy-5-phenyl-2-(4-(trifluoromethyl)phenyl)pyrimidin-4(3*H*)-one

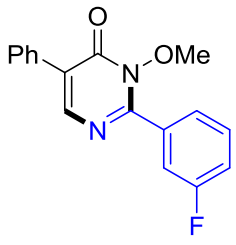
Yellow solid, Yield 70% (48.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (s, 1H), 8.07 (d, J = 8.0 Hz, 2H), 7.79 (d, J = 8.4 Hz, 2H), 7.77 – 7.72 (m, 2H), 7.50 – 7.44 (m, 2H), 7.44 – 7.39 (m, 1H), 3.85 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.2, 155.1, 148.7, 134.6, 133.0 (q, $J_{C\text{-}F}$ = 33.0 Hz), 132.4, 130.1, 128.9, 128.6, 128.4, 128.3, 125.4 (q, $J_{C\text{-}F}$ = 11.0 Hz), 123.7 (q, $J_{C\text{-}F}$ = 270.0 Hz), 64.3. HRMS (ESI) Calcd for $[C_{18}H_{13}F_3N_2O_2+H]^+$ 347.1002, Found 347.1004.



4ai

4-(1-Methoxy-6-oxo-5-phenyl-1,6-dihydropyrimidin-2-yl)benzonitrile

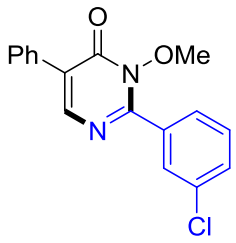
Yellow solid, Yield 68% (41.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (s, 1H), 8.08 – 8.06 (m, 2H), 7.83 – 7.81 (m, 2H), 7.75 – 7.73 (m, 2H), 7.49 – 7.40 (m, 3H), 3.86 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.0, 154.5, 148.6, 135.3, 132.3, 132.2, 130.3, 129.0, 128.7, 128.6, 128.4, 118.0, 115.0, 64.4. HRMS (ESI) Calcd for $[C_{18}H_{13}N_3O_2+H]^+$ 304.1081, Found 304.1081.



4aj

2-(3-Fluorophenyl)-3-methoxy-5-phenylpyrimidin-4(3*H*)-one

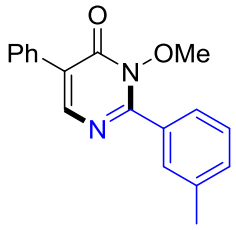
Yellow liquid, Yield 92% (54.7 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (s, 1H), 7.77 – 7.71 (m, 3H), 7.70 – 7.65 (m, 1H), 7.53 – 7.43 (m, 3H), 7.42 – 7.37 (m, 1H), 7.30 – 7.24 (m, 1H), 3.85 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.3 (d, $J_{C\text{-}F}$ = 246.0 Hz), 157.3, 155.1 (d, $J_{C\text{-}F}$ = 2.0 Hz), 148.8, 133.1 (d, $J_{C\text{-}F}$ = 8.0 Hz), 132.5, 130.2 (d, $J_{C\text{-}F}$ = 8.0 Hz), 128.8, 128.6, 128.4, 127.9, 125.4 (d, $J_{C\text{-}F}$ = 3.0 Hz), 118.5 (d, $J_{C\text{-}F}$ = 21.0 Hz), 116.8 (d, $J_{C\text{-}F}$ = 24.0 Hz), 64.2. HRMS (ESI) Calcd for $[C_{17}H_{13}FN_2O_2+H]^+$ 297.1034, Found 297.1034.



4ak

2-(3-Chlorophenyl)-3-methoxy-5-phenylpyrimidin-4(3*H*)-one

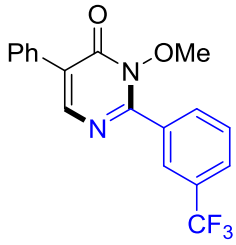
Yellow solid, Yield 82% (50.7 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (s, 1H), 7.95 – 7.93 (m, 1H), 7.86 – 7.82 (m, 1H), 7.75 – 7.73 (m, 2H), 7.55 – 7.52 (m, 1H), 7.49 – 7.43 (m, 3H), 7.42 – 7.37 (m, 1H), 3.85 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.2, 155.1, 148.7, 134.5, 132.8, 132.5, 131.5, 129.74, 129.69, 128.8, 128.6, 128.4, 128.0, 127.7, 64.3. HRMS (ESI) Calcd for $[C_{17}H_{13}ClN_2O_2+H]^+$ 313.0738, Found 313.0739.



4al

2-Methoxy-5-phenyl-2-(m-tolyl)pyrimidin-4(3*H*)-one

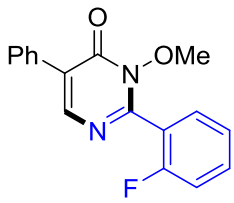
Yellow solid, Yield 95% (55.8 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (s, 1H), 7.77 – 7.71 (m, 4H), 7.48 – 7.44 (m, 2H), 7.42 – 7.36 (m, 3H), 3.82 (s, 3H), 2.45 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.5, 156.8, 149.0, 138.3, 132.8, 132.1, 131.2, 130.0, 128.61, 128.56, 128.4, 128.3, 127.3, 126.6, 64.1, 21.5. HRMS (ESI) Calcd for $[C_{18}H_{16}N_2O_2+H]^+$ 293.1285, Found 293.1287.



4am

3-Methoxy-5-phenyl-2-(3-(trifluoromethyl)phenyl)pyrimidin-4(3*H*)-one

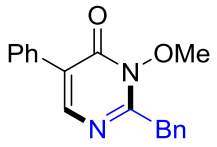
Yellow solid, Yield 75% (52.6 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (s, 1H), 8.17 – 8.15 (m, 2H), 7.84 – 7.82 (m, 1H), 7.77 – 7.72 (m, 2H), 7.66 (t, J = 7.9 Hz, 1H), 7.49 – 7.44 (m, 2H), 7.44 – 7.38 (m, 1H), 3.86 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.2, 154.9, 148.7, 132.8, 132.4, 132.0, 131.1 (q, J_{C-F} = 32.0 Hz), 129.1, 128.9, 128.6, 128.4, 128.2, 128.0 (q, J_{C-F} = 3.0 Hz), 126.7 (q, J_{C-F} = 4.0 Hz), 123.7 (q, J_{C-F} = 271.0 Hz), 64.3. HRMS (ESI) Calcd for $[C_{18}H_{13}F_3N_2O_2+H]^+$ 347.1002, Found 347.1001.



4an

2-(2-Fluorophenyl)-3-methoxy-5-phenylpyrimidin-4(3*H*)-one

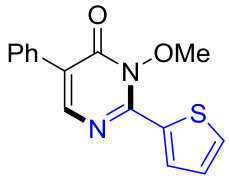
Yellow solid, Yield 60% (35.8 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (s, 1H), 7.77 – 7.72 (m, 2H), 7.61 – 7.52 (m, 2H), 7.49 – 7.38 (m, 3H), 7.33 – 7.29 (m, 1H), 7.25 – 7.21 (m, 1H), 3.87 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9 (d, $J_{C\text{-}F}$ = 251.0 Hz), 157.1, 153.4, 148.7, 132.8 (d, $J_{C\text{-}F}$ = 9.0 Hz), 132.5, 130.5 (d, $J_{C\text{-}F}$ = 2.0 Hz), 128.8, 128.7, 128.6, 128.5, 124.3 (d, $J_{C\text{-}F}$ = 4.0 Hz), 120.2 (d, $J_{C\text{-}F}$ = 15.0 Hz), 116.1 (d, $J_{C\text{-}F}$ = 21.0 Hz), 64.5 (d, $J_{C\text{-}F}$ = 1.0 Hz). HRMS (ESI) Calcd for $[C_{17}H_{13}FN_2O_2+H]^+$ 297.1034, Found 297.1034.



4ao

2-Benzyl-3-methoxy-5-phenylpyrimidin-4(3*H*)-one

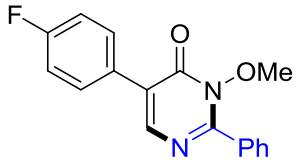
Yellow liquid, Yield 60% (35.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (s, 1H), 7.68 – 7.63 (m, 2H), 7.45 – 7.39 (m, 2H), 7.39 – 7.33 (m, 5H), 7.32 – 7.26 (m, 1H), 4.20 (s, 2H), 3.86 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.8, 157.6, 148.7, 134.9, 132.7, 129.2, 128.9, 128.52, 128.51, 128.4, 127.6, 127.5, 64.3, 39.5. HRMS (ESI) Calcd for $[C_{18}H_{16}N_2O_2+H]^+$ 293.1285, Found 293.1285.



4ap

3-Methoxy-5-phenyl-2-(thiophen-2-yl)pyrimidin-4(3*H*)-one

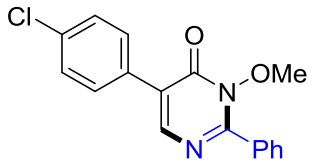
Yellow solid, Yield 55% (31.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 – 8.18 (m, 1H), 8.08 (s, 1H), 7.75 – 7.71 (m, 2H), 7.67 – 7.66 (m, 1H), 7.48 – 7.42 (m, 2H), 7.39 – 7.36 (m, 1H), 7.22 – 7.20 (m, 1H), 4.16 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.4, 150.5, 149.3, 133.4, 133.2, 133.0, 132.9, 128.6, 128.5, 128.4, 128.3, 125.8, 64.0. HRMS (ESI) Calcd for $[C_{15}H_{12}N_2O_2S+H]^+$ 285.0692, Found 285.0691.



4ba

5-(4-Fluorophenyl)-3-methoxy-2-phenylpyrimidin-4(3*H*)-one

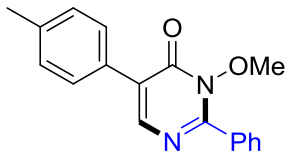
Yellow solid, Yield 70% (41.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (s, 1H), 7.95 – 7.90 (m, 2H), 7.76 – 7.72 (m, 2H), 7.60 – 7.49 (m, 3H), 7.17 – 7.12 (m, 2H), 3.82 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.0 (d, $J_{C\text{-}F}$ = 247.0 Hz), 157.4, 156.6, 148.7, 131.4, 131.2, 130.2 (d, $J_{C\text{-}F}$ = 8.0 Hz), 129.5, 128.7 (d, $J_{C\text{-}F}$ = 3.0 Hz), 128.5, 126.5, 115.6 (d, $J_{C\text{-}F}$ = 21.0 Hz), 64.1. HRMS (ESI) Calcd for $[C_{17}H_{13}FN_2O_2+H]^+$ 297.1034, Found 297.1035.



4ca

5-(4-Chlorophenyl)-3-methoxy-2-phenylpyrimidin-4(3*H*)-one

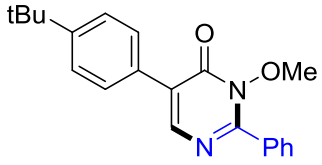
Yellow solid, Yield 70% (43.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (s, 1H), 7.95 – 7.90 (m, 2H), 7.73 – 7.68 (m, 2H), 7.60 – 7.49 (m, 3H), 7.45 – 7.40 (m, 2H), 3.82 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.3, 156.8, 148.9, 134.7, 131.5, 131.2, 131.1, 129.7, 129.6, 128.8, 128.5, 126.2, 64.1. HRMS (ESI) Calcd for $[C_{17}H_{13}ClN_2O_2+H]^+$ 313.0738, Found 313.0737.



4da

3-Methoxy-2-phenyl-5-(p-tolyl)pyrimidin-4(3*H*)-one

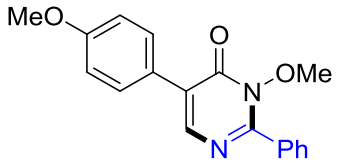
Yellow solid, Yield 51% (29.5 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (s, 1H), 7.95 – 7.90 (m, 2H), 7.66 – 7.64 (m, 2H), 7.59 – 7.48 (m, 3H), 7.28 – 7.26 (m, 2H), 3.81 (s, 3H), 2.40 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.5, 156.2, 148.5, 138.7, 131.34, 131.29, 129.8, 129.5, 129.3, 128.4, 128.3, 127.4, 64.0, 21.3. HRMS (ESI) Calcd for $[C_{18}H_{16}N_2O_2+H]^+$ 293.1285, Found 293.1284.



4ea

5-(4-(Tert-butyl)phenyl)-3-methoxy-2-phenylpyrimidin-4(3*H*)-one

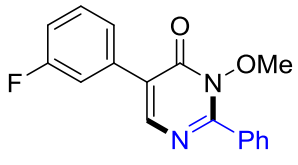
Yellow liquid, Yield 40% (24.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.96 – 7.90 (m, 2H), 7.72 – 7.66 (m, 2H), 7.58 – 7.47 (m, 5H), 3.82 (s, 3H), 1.36 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.6, 156.3, 151.8, 148.6, 131.33, 131.30, 129.8, 129.5, 128.4, 128.1, 127.4, 125.6, 64.0, 34.7, 31.3. HRMS (ESI) Calcd for $[C_{21}H_{22}N_2O_2+H]^+$ 335.1754, Found 335.1755.



4fa

3-Methoxy-5-(4-methoxyphenyl)-2-phenylpyrimidin-4(3*H*)-one

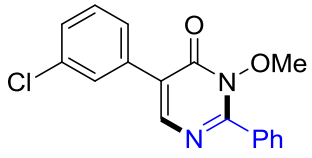
Yellow solid, Yield 60% (37.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (s, 1H), 7.94 – 7.89 (m, 2H), 7.75 – 7.69 (m, 2H), 7.58 – 7.49 (m, 3H), 7.02 – 6.96 (m, 2H), 3.85 (s, 3H), 3.81 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 157.6, 155.9, 148.0, 131.4, 131.3, 129.7, 129.5, 128.4, 127.1, 125.1, 114.0, 64.0, 55.4. HRMS (ESI) Calcd for $[C_{18}H_{16}N_2O_3+H]^+$ 309.1234, Found 309.1236.



4ga

5-(3-Fluorophenyl)-3-methoxy-2-phenylpyrimidin-4(3*H*)-one

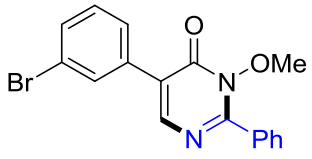
Yellow solid, Yield 88% (52.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (s, 1H), 7.96 – 7.91 (m, 2H), 7.60 – 7.49 (m, 5H), 7.44 – 7.39 (m, 1H), 7.12 – 7.06 (m, 1H), 3.82 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.8 (d, $J_{C\text{-}F}$ = 244.0 Hz), 157.2, 157.0, 149.3, 134.8 (d, $J_{C\text{-}F}$ = 8.0 Hz), 131.5, 131.1, 130.0 (d, $J_{C\text{-}F}$ = 9.0 Hz), 129.6, 128.5, 126.1 (d, $J_{C\text{-}F}$ = 2.0 Hz), 123.9 (d, $J_{C\text{-}F}$ = 3.0 Hz), 115.6 (d, $J_{C\text{-}F}$ = 3.0 Hz), 115.4 (d, $J_{C\text{-}F}$ = 5.0 Hz), 64.1. HRMS (ESI) Calcd for $[C_{17}H_{13}FN_2O_2+H]^+$ 297.1034, Found 297.1035.



4ha

5-(3-Chlorophenyl)-3-methoxy-2-phenylpyrimidin-4(3*H*)-one

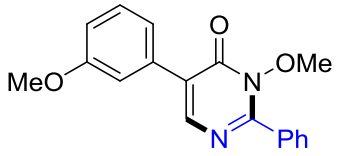
Yellow solid, Yield 71% (44.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.96 – 7.91 (m, 2H), 7.78 – 7.76 (m, 1H), 7.65 – 7.62 (m, 1H), 7.60 – 7.49 (m, 3H), 7.42 – 7.35 (m, 2H), 3.82 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.2, 157.1, 149.3, 134.47, 134.46, 131.6, 131.1, 129.8, 129.6, 128.7, 128.5, 128.4, 126.5, 126.0, 64.1. HRMS (ESI) Calcd for $[C_{17}H_{13}ClN_2O_2+H]^+$ 313.0738, Found 313.0740.



4ia

5-(3-Bromophenyl)-3-methoxy-2-phenylpyrimidin-4(3*H*)-one

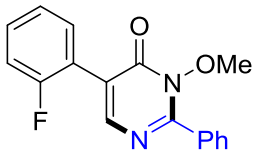
Yellow solid, Yield 66% (47.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (s, 1H), 7.94 – 7.92 (m, 3H), 7.70 – 7.67 (m, 1H), 7.61 – 7.49 (m, 4H), 7.32 (t, J = 7.9 Hz, 1H), 3.82 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.2, 157.1, 149.3, 134.7, 131.58, 131.56, 131.3, 131.1, 130.0, 129.6, 128.5, 127.0, 125.9, 122.6, 64.1. HRMS (ESI) Calcd for $[C_{17}H_{13}BrN_2O_2+H]^+$ 357.0233, Found 357.0233.



4ja

3-Methoxy-5-(3-methoxyphenyl)-2-phenylpyrimidin-4(3*H*)-one

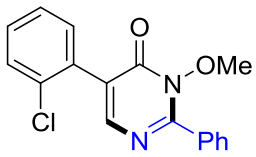
Yellow liquid, Yield 77% (47.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (s, 1H), 7.96 – 7.90 (m, 2H), 7.57 – 7.50 (m, 3H), 7.39 – 7.34 (m, 2H), 7.31 – 7.29 (m, 1H), 6.97 – 6.94 (m, 1H), 3.86 (s, 3H), 3.82 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.6, 157.4, 156.6, 149.1, 134.0, 131.4, 131.2, 129.56, 129.55, 128.5, 127.2, 120.7, 114.6, 113.9, 64.1, 55.4. HRMS (ESI) Calcd for $[C_{18}H_{16}N_2O_3+H]^+$ 309.1234, Found 309.1233.



4ka

5-(2-Fluorophenyl)-3-methoxy-2-phenylpyrimidin-4(3*H*)-one

Yellow liquid, Yield 77% (45.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, J = 1.6 Hz, 1H), 7.95 – 7.93 (m, 2H), 7.65 – 7.49 (m, 4H), 7.41 – 7.36 (m, 1H), 7.26 – 7.15 (m, 2H), 3.83 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.1 (d, $J_{C\text{-}F}$ = 248.0 Hz), 157.3, 157.0, 151.2 (d, $J_{C\text{-}F}$ = 5.0 Hz), 131.49, 131.45, 131.2, 130.4 (d, $J_{C\text{-}F}$ = 9.0 Hz), 129.6, 128.5, 124.2 (d, $J_{C\text{-}F}$ = 4.0 Hz), 122.8 (d, $J_{C\text{-}F}$ = 2.0 Hz), 120.4 (d, $J_{C\text{-}F}$ = 14.0 Hz), 116.0 (d, $J_{C\text{-}F}$ = 22.0 Hz), 64.1. HRMS (ESI) Calcd for $[C_{17}H_{13}FN_2O_2+H]^+$ 297.1034, Found 297.1032.

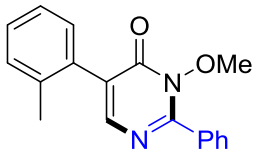


4la

5-(2-Chlorophenyl)-3-methoxy-2-phenylpyrimidin-4(3*H*)-one

Yellow solid, Yield 83% (51.7 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.98 – 7.93 (m, 2H), 7.60 – 7.48 (m, 4H), 7.45 – 7.41 (m, 1H), 7.37 – 7.32 (m, 2H), 3.83 (s, 3H). ^{13}C NMR (100 MHz,

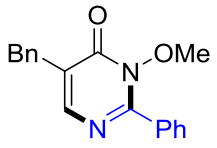
$CDCl_3$) δ 157.6, 156.8, 151.2, 134.0, 131.72, 131.68, 131.5, 131.2, 130.0, 129.7, 128.4, 126.9, 126.6, 64.1. One signal is missing due to overlap. HRMS (ESI) Calcd for $[C_{17}H_{13}ClN_2O_2+H]^+$ 313.0738, Found 313.0735.



4ma

3-Methoxy-2-phenyl-5-(o-tolyl)pyrimidin-4(3*H*)-one

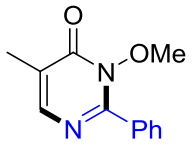
Yellow liquid, Yield 85% (49.3 mg). ^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.86 – 7.82 (m, 2H), 7.81 (s, 1H), 7.51 – 7.41 (m, 3H), 7.26 – 7.19 (m, 2H), 7.17 – 7.14 (m, 2H), 3.69 (s, 3H), 2.21 (s, 3H). ^{13}C NMR (100 MHz, CD_2Cl_2) δ 157.1, 156.9, 150.4, 137.7, 132.9, 131.5, 131.2, 130.2, 130.1, 129.6, 129.1, 128.7, 128.3, 125.7, 63.9, 19.7. HRMS (ESI) Calcd for $[C_{18}H_{16}N_2O_2+H]^+$ 293.1285, Found 293.1288.



4na

5-Benzyl-3-methoxy-2-phenylpyrimidin-4(3*H*)-one

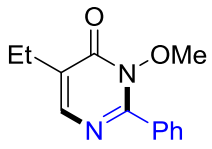
Yellow liquid, Yield 82% (48.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 – 7.82 (m, 2H), 7.72 (s, 1H), 7.55 – 7.44 (m, 3H), 7.36 – 7.29 (m, 4H), 7.26 – 7.21 (m, 1H), 3.87 (s, 2H), 3.75 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.4, 156.0, 148.9, 138.3, 131.4, 131.1, 129.4, 129.1, 128.7, 128.6, 128.4, 126.6, 64.0, 33.8. HRMS (ESI) Calcd for $[C_{18}H_{16}N_2O_2+H]^+$ 293.1285, Found 293.1284.



4oa

3-Methoxy-5-methyl-2-phenylpyrimidin-4(3*H*)-one

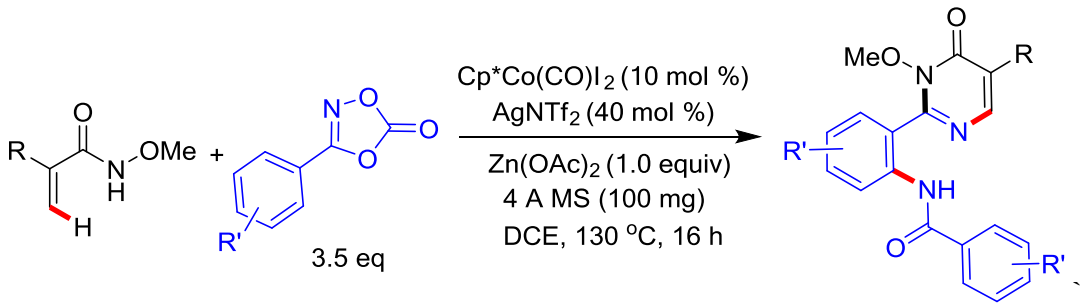
White solid, Yield 64% (29.8 mg). ^{1}H NMR (400 MHz, CD_3OD) δ 7.90 – 7.89 (m, 1H), 7.83 – 7.79 (m, 2H), 7.61 – 7.50 (m, 3H), 3.71 (s, 3H), 2.12 (d, J = 0.9 Hz, 3H). ^{13}C NMR (100 MHz, CD_3OD) δ 159.4, 156.3, 148.6, 131.2, 130.9, 129.1, 128.0, 125.2, 63.2, 11.9. HRMS (ESI) Calcd for $[C_{12}H_{12}N_2O_2+H]^+$ 217.0972, Found 217.0974.



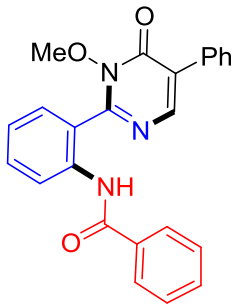
4pa

3-Methoxy-5-ethyl -2-phenylpyrimidin-4(3*H*)-one

White solid, Yield 67% (30.6 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 – 7.82 (m, 2H), 7.80 (s, 1H), 7.56 – 7.45 (m, 3H), 3.76 (s, 3H), 2.59 (q, J = 8.0 Hz, 2H), 1.26 (t, J = 8.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.5, 155.6, 147.5, 131.5, 131.0, 130.7, 129.3, 128.3, 63.9, 21.1, 12.6. HRMS (ESI) Calcd for $[C_{13}H_{14}N_2O_2+H]^+$ 231.1128, Found 231.1126.



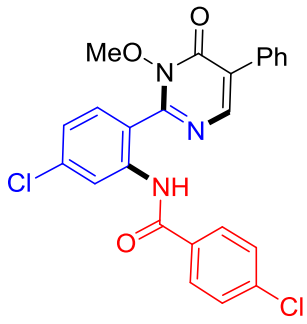
Typical Reaction Conditions for synthesis of **5**: *N*-methoxy-acrylamide (0.2 mmol), dioxazolone (0.71 mmol), Cp*Co(CO)I_2 (10 mol%), $AgNTf_2$ (40 mol%), $Zn(OAc)_2$ (0.2 mmol), 4 Å M.S. (100 mg) and DCE (2 mL) were charged into a pressure tube. The reaction mixture was stirred under N_2 at 130 ℃ for 16 h. After the solvent was removed under reduced pressure, the residue was purified by silica gel chromatography using PE/EA to afford the product **5**.



5aa

N-(2-(1-methoxy-6-oxo-5-phenyl-1,6-dihydropyrimidin-2-yl)phenyl)benzamide

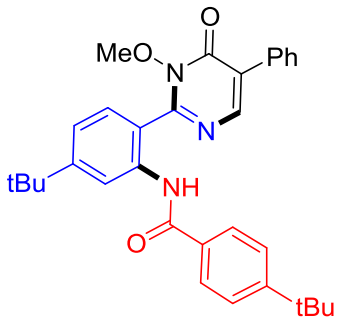
Yellow solid, Yield 81% (64.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.77 (s, 1H), 8.50 (d, J = 8.0 Hz, 1H), 8.14 (s, 1H), 7.92 (d, J = 7.2 Hz, 2H), 7.87 (d, J = 8.0 Hz, 1H), 7.73 (d, J = 7.2 Hz, 2H), 7.60 – 7.42 (m, 7H), 7.28 – 7.25 (m, 1H), 3.81 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.2, 157.2, 155.4, 146.9, 137.4, 134.7, 132.4, 132.2, 132.1, 130.9, 129.0, 128.9, 128.7, 128.4, 128.2, 127.2, 123.6, 123.2, 119.5, 64.6. HRMS (ESI) Calcd for $[C_{24}H_{19}N_3O_3+H]^+$ 398.1499, Found 398.1497.



5ab

4-Chloro-*N*-(5-chloro-2-(1-methoxy-6-oxo-5-phenyl-1,6-dihydropyrimidin-2-yl)phenyl)benzamide

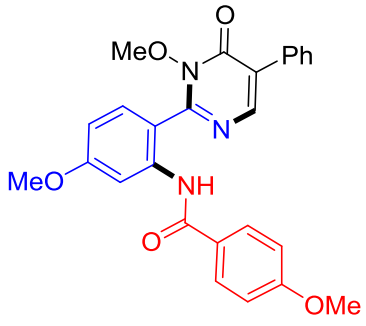
Yellow solid, Yield 75% (70.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.17 (s, 1H), 8.65 (d, J = 1.6 Hz, 1H), 8.11 (s, 1H), 7.89 – 7.84 (m, 3H), 7.74 – 7.72 (m, 2H), 7.51 – 7.42 (m, 5H), 7.26 – 7.23 (m, 1H), 3.82 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.2, 157.0, 154.6, 146.4, 138.8, 138.74, 138.70, 132.8, 132.1, 132.0, 129.3, 129.2, 128.7, 128.6, 128.5, 128.4, 123.8, 122.7, 116.6, 64.6. HRMS (ESI) Calcd for $[C_{24}H_{17}Cl_2N_3O_3+H]^+$ 466.0720, Found 466.0717.



5ac

4-(Tert-butyl)-*N*-(5-(tert-butyl)-2-(1-methoxy-6-oxo-5-phenyl-1,6-dihydropyrimidin-2-yl)phenyl) benzamide

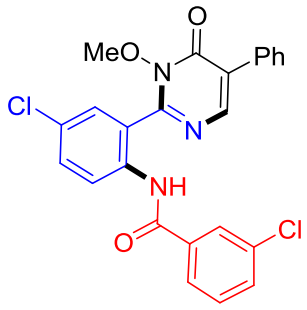
Yellow solid, Yield 80% (80.9 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.93 (s, 1H), 8.63 (s, 1H), 8.18 (s, 1H), 7.90 (d, J = 8.0 Hz, 2H), 7.86 (d, J = 8.4 Hz, 1H), 7.78 (d, J = 8.0 Hz, 2H), 7.56 – 7.44 (m, 5H), 7.32 – 7.28 (m, 1H), 3.84 (s, 3H), 1.44 (s, 9H), 1.38 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.2, 157.4, 156.3, 155.7, 155.6, 147.1, 137.5, 132.4, 131.9, 130.6, 128.9, 128.6, 128.5, 127.7, 127.0, 125.9, 120.7, 120.2, 116.4, 64.5, 35.4, 35.1, 31.2, 31.1. HRMS (ESI) Calcd for $[C_{32}H_{35}N_3O_3+H]^+$ 510.2751, Found 510.2753.



5ad

4-Methoxy-*N*-(5-methoxy-2-(1-methoxy-6-oxo-5-phenyl-1,6-dihydropyrimidin-2-yl)phenyl)benzamide

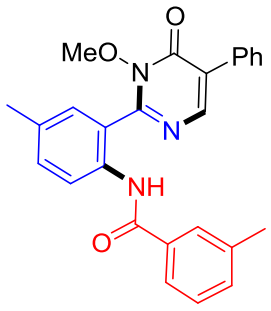
Yellow solid, Yield 75% (69.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.41 (s, 1H), 8.28 (d, J = 2.4 Hz, 1H), 8.14 (s, 1H), 7.96 – 7.89 (m, 3H), 7.76 (d, J = 7.2 Hz, 2H), 7.51 – 7.44 (m, 3H), 7.02 (d, J = 8.8 Hz, 2H), 6.80 – 6.78 (dd, J_1 = 8.8 Hz, J_2 = 2.4 Hz, 1H), 3.96 (s, 3H), 3.90 (s, 3H), 3.83 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.0, 162.7, 157.4, 155.5, 146.9, 140.3, 132.5, 132.4, 129.1, 128.8, 128.6, 128.4, 127.2, 127.1, 114.1, 110.4, 110.3, 106.4, 64.2, 55.6, 55.5. One signal is missing due to overlap. HRMS (ESI) Calcd for $[C_{26}H_{23}N_3O_5+H]^+$ 458.1710, Found 458.1708.



5ae

3-Chloro-*N*-(4-chloro-2-(1-methoxy-6-oxo-5-phenyl-1,6-dihydropyrimidin-2-yl)phenyl)benzamide

Yellow solid, Yield 62% (58.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.84 (s, 1H), 8.40 (d, J = 9.0 Hz, 1H), 8.07 (s, 1H), 7.85 – 7.80 (m, 2H), 7.71 – 7.65 (m, 3H), 7.48 – 7.44 (m, 2H), 7.41 – 7.34 (m, 4H), 3.77 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.8, 157.0, 153.9, 146.6, 136.1, 135.9, 135.1, 132.4, 132.2, 131.9, 130.7, 130.3, 129.2, 129.1, 128.9, 128.7, 128.4, 127.6, 125.3, 124.2, 120.3, 64.8. HRMS (ESI) Calcd for $[C_{24}H_{17}Cl_2N_3O_3+H]^+$ 466.0720, Found 466.0721.

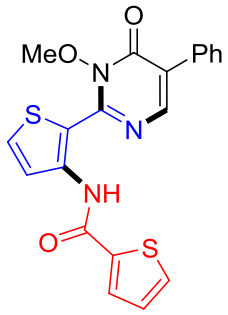


5af

N-(2-(1-methoxy-6-oxo-5-phenyl-1,6-dihydropyrimidin-2-yl)-4-methylphenyl)-3-methylbenzamide

Yellow solid, Yield 75% (63.7 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.41 (s, 1H), 8.33 (d, J = 8.4 Hz, 1H), 8.15 (s, 1H), 7.76 – 7.74 (m, 3H), 7.69 – 7.68 (m, 2H), 7.50 – 7.38 (m, 6H), 3.84 (s, 3H), 2.45 (s, 3H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.4, 157.3, 155.6, 147.2, 138.7, 134.72, 134.68, 133.4, 133.1, 132.8, 132.3, 131.0, 128.9, 128.7, 128.6, 128.4, 128.064, 128.063, 123.9, 123.3, 120.0,

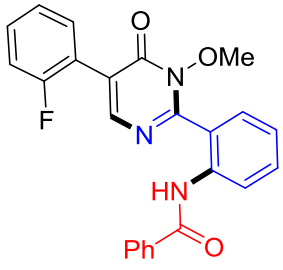
64.6, 21.5, 21.0. One signal is missing due to overlap. HRMS (ESI) Calcd for $[C_{26}H_{23}N_3O_3+H]^+$ 426.1812, Found 426.1813.



5ag

N-(2-(1-methoxy-6-oxo-5-phenyl-1,6-dihydropyrimidin-2-yl)thiophen-3-yl)thiophene-2-carboxamide

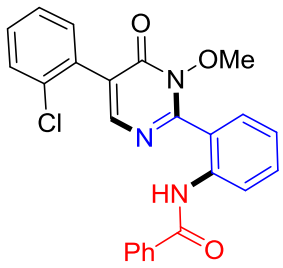
Yellow solid, Yield 57% (46.7 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.37 (s, 1H), 8.43 (d, J = 5.6 Hz, 1H), 8.15 (s, 1H), 7.78 – 7.74 (m, 3H), 7.66 (d, J = 5.6 Hz, 1H), 7.59 (d, J = 4.8 Hz, 1H), 7.49 – 7.45 (m, 2H), 7.42 – 7.38 (m, 1H), 7.20 – 7.16 (m, 1H), 4.21 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2, 157.1, 152.6, 147.1, 145.5, 139.4, 133.5, 132.5, 131.3, 129.5, 128.6, 128.3, 128.1, 124.6, 122.4, 107.1, 64.6. One signal is missing due to overlap. HRMS (ESI) Calcd for $[C_{20}H_{15}N_3O_3S_2+H]^+$ 410.0628, Found 410.0627.



5ba

N-(2-(5-(2-fluorophenyl) -1-methoxy-6-oxo-1,6-dihydropyrimidin-2-yl)phenyl)benzamide

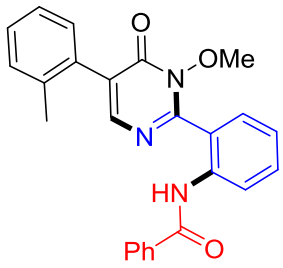
Yellow solid, Yield 65% (53.5 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.78 (s, 1H), 8.52 (d, J = 8.4 Hz, 1H), 8.16 (s, 1H), 7.92 – 7.88 (m, 3H), 7.67 – 7.48 (m, 5H), 7.43 – 7.38 (m, 1H), 7.29 – 7.17 (m, 3H), 3.80 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.2, 160.0 (d, $J_{C\text{-}F}$ = 248.0 Hz), 156.8, 156.1, 149.4 (d, $J_{C\text{-}F}$ = 5.0 Hz), 137.5, 134.6, 132.5, 132.1, 131.5 (d, $J_{C\text{-}F}$ = 3.0 Hz), 130.9, 130.8 (d, $J_{C\text{-}F}$ = 8.0 Hz), 128.9, 127.2, 124.2 (d, $J_{C\text{-}F}$ = 4.0 Hz), 123.6, 123.3 (d, $J_{C\text{-}F}$ = 2.0 Hz), 123.1, 119.9 (d, $J_{C\text{-}F}$ = 14.0 Hz), 119.3, 116.1 (d, $J_{C\text{-}F}$ = 22.0 Hz), 64.6. HRMS (ESI) Calcd for $[C_{24}H_{18}FN_3O_3+H]^+$ 416.1405, Found 416.1406.



5ca

N-(2-(5-(2-chlorophenyl)-1-methoxy-6-oxo-1,6-dihydropyrimidin-2-yl)phenyl)benzamide

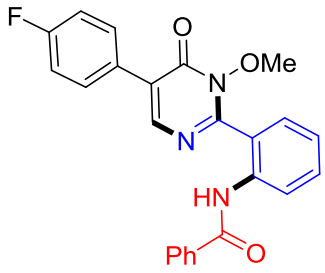
Yellow solid, Yield 61% (52.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.74 (s, 1H), 8.52 (d, J = 8.4 Hz, 1H), 8.07 (s, 1H), 7.93 – 7.89 (m, 3H), 7.63 – 7.59 (m, 1H), 7.56 – 7.45 (m, 5H), 7.37 – 7.35 (m, 2H), 7.30 – 7.26 (m, 1H), 3.81 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.2, 156.7, 156.4, 149.6, 137.5, 134.6, 133.8, 132.5, 132.2, 131.7, 131.1, 130.9, 130.3, 130.1, 128.9, 127.2, 127.0, 126.9, 123.6, 123.2, 119.5, 64.6. HRMS (ESI) Calcd for $[C_{24}H_{18}ClN_3O_3+H]^+$ 432.1109, Found 432.1111.



5da

N-(2-(1-methoxy-6-oxo-5-(o-tolyl)-1,6-dihydropyrimidin-2-yl)phenyl)benzamide

Yellow solid, Yield 62% (50.8 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.79 (s, 1H), 8.51 (d, J = 8.4 Hz, 1H), 7.96 (s, 1H), 7.94 – 7.89 (m, 3H), 7.62 – 7.48 (m, 4H), 7.34 – 7.26 (m, 5H), 3.80 (s, 3H), 2.32 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.2, 156.9, 155.9, 148.7, 137.5, 137.4, 134.6, 132.4, 132.2, 131.9, 130.9, 130.5, 130.1, 129.9, 129.1, 128.9, 127.1, 125.9, 123.6, 123.2, 119.5, 64.5, 20.1. HRMS (ESI) Calcd for $[C_{25}H_{21}N_3O_3+H]^+$ 412.1656, Found 412.1658.

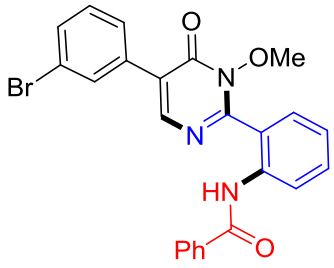


5ea

N-(2-(5-(4-fluorophenyl)-1-methoxy-6-oxo-1,6-dihydropyrimidin-2-yl)phenyl)benzamide

Yellow solid, Yield 77% (63.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.72 (s, 1H), 8.49 (d, J = 8.0 Hz, 1H), 8.11 (s, 1H), 7.91 (d, J = 7.6 Hz, 2H), 7.87 (d, J = 8.0 Hz, 1H), 7.76 – 7.70 (m, 2H), 7.61 – 7.49 (m, 4H), 7.28 – 7.25 (m, 1H), 7.17 – 7.13 (m, 2H), 3.80 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.2,

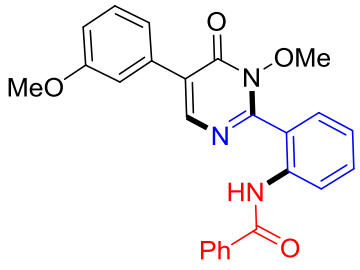
163.1 (d, $J_{C\text{-}F}$ = 247.0 Hz), 157.2, 155.4, 146.8, 137.4, 134.7, 132.4, 132.2, 130.9, 130.3 (d, $J_{C\text{-}F}$ = 8.0 Hz), 128.9, 128.2 (d, $J_{C\text{-}F}$ = 3.0 Hz), 127.2, 127.1, 123.6, 123.2, 119.5, 115.7 (d, $J_{C\text{-}F}$ = 22.0 Hz), 64.6. HRMS (ESI) Calcd for $[C_{24}H_{18}FN_3O_3+H]^+$ 416.1405, Found 416.1403.



5fa

N-(2-(5-(3-bromophenyl)-1-methoxy-6-oxo-1,6-dihydropyrimidin-2-yl)phenyl)benzamide

Yellow solid, Yield 58% (54.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.68 (s, 1H), 8.48 (d, J = 8.0 Hz, 1H), 8.12 (s, 1H), 7.92 – 7.86 (m, 4H), 7.68 (d, J = 7.6 Hz, 1H), 7.61 – 7.50 (m, 5H), 7.33 (t, J = 8.0 Hz, 1H), 7.29 – 7.25 (m, 1H), 3.80 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.3, 157.0, 155.9, 147.4, 137.4, 134.6, 134.2, 132.6, 132.2, 131.9, 131.2, 130.9, 130.1, 129.0, 127.1, 127.0, 126.7, 123.7, 123.3, 122.7, 119.4, 64.6. HRMS (ESI) Calcd for $[C_{24}H_{18}BrN_3O_3+H]^+$ 476.0604, Found 476.0602.

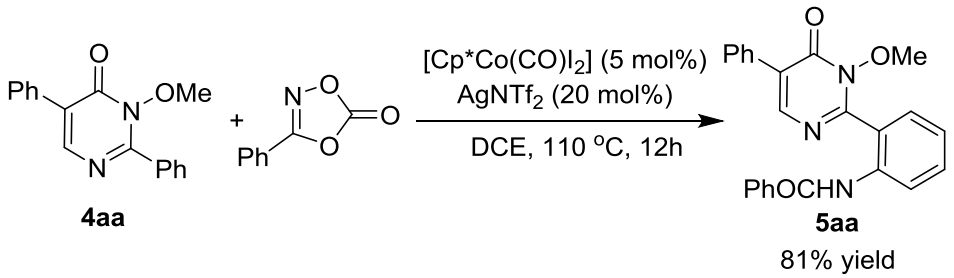


5ga

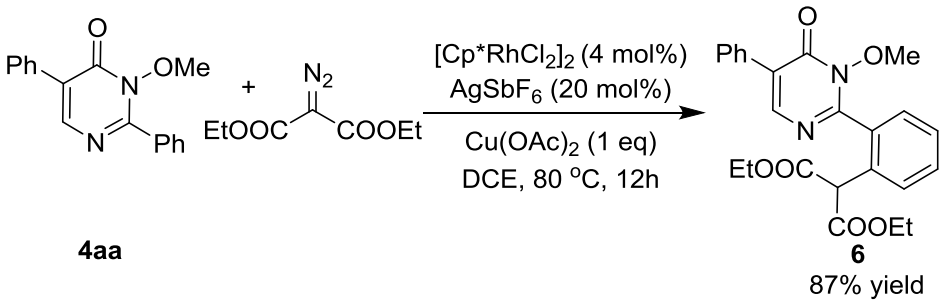
N-(2-(1-methoxy-5-(3-methoxyphenyl)-6-oxo-1,6-dihydropyrimidin-2-yl)phenyl)benzamide

Yellow solid, Yield 72% (61.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.78 (s, 1H), 8.51 (d, J = 8.4 Hz, 1H), 8.15 (s, 1H), 7.92 – 7.90 (m, 2H), 7.88 (d, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.62 – 7.48 (m, 4H), 7.40 – 7.34 (m, 2H), 7.30 – 7.24 (m, 2H), 6.97 (J_1 = 8.0 Hz, J_2 = 2.4 Hz, 1H), 3.86 (s, 3H), 3.80 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.2, 159.7, 157.2, 155.4, 147.1, 137.4, 134.7, 133.6, 132.4, 132.1, 130.9, 129.7, 128.9, 127.9, 127.2, 123.6, 123.1, 120.7, 119.4, 114.8, 114.0, 64.6, 55.4. HRMS (ESI) Calcd for $[C_{25}H_{21}N_3O_4+H]^+$ 428.1605, Found 428.1603.

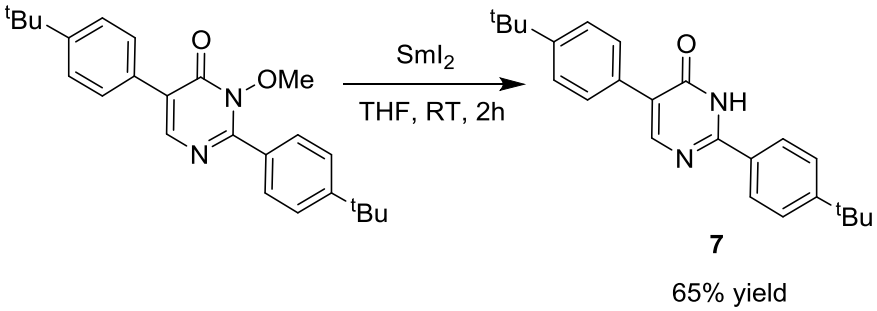
III. Derivatization of amidated products



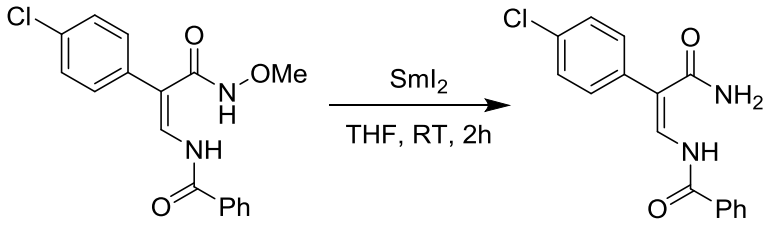
4aa (27.8 mg, 0.1 mmol), 3-phenyl-1,4,2-dioxazol-5-one (24.5 mg, 0.15 mmol), $[Cp^*Co(CO)I]_2$ (2.4 mg, 0.005 mmol), $AgNTf_2$ (7.8 mg, 0.02 mmol) and $Zn(OAc)_2$ (18.3 mg, 0.1 mmol) were dissolved in DCE (1 mL) under N_2 atmosphere. The mixture was stirred at 110°C overnight. After that the solvent was removed under reduced pressure. The residue was purified by silica gel chromatography using PE/EA to afford compound **5aa** as a yellow solid (32.2 mg, 81%).



4aa (27.8 mg, 0.1 mmol), diazo compound (27.9 mg, 0.15 mmol), $[Cp^*RhCl_2]_2$ (2.5 mg, 0.004 mmol), $AgSbF_6$ (6.9 mg, 0.02 mmol) and $Cu(OAc)_2$ (18.2 mg, 0.1 mmol) were dissolved in DCE (1 mL) under N_2 atmosphere. The mixture was stirred at 80°C overnight. After that the solvent was removed under reduced pressure. The residue was purified by silica gel chromatography using PE/EA to afford compound **6** as a yellow solid (38.0 mg, 87%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (s, 1H), 7.79 – 7.74 (m, 2H), 7.73 – 7.68 (m, 1H), 7.63 – 7.56 (m, 2H), 7.51 – 7.44 (m, 3H), 7.41 (m, 1H), 4.85 (s, 1H), 4.22 (q, J = 7.2 Hz, 4H), 3.74 (s, 3H), 1.25 (t, J = 7.2 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.8, 157.1, 156.2, 148.5, 132.5, 132.2, 131.4, 130.8, 130.1, 129.6, 128.8, 128.6, 128.5, 128.3, 127.9, 64.1, 62.0, 54.9, 14.0.

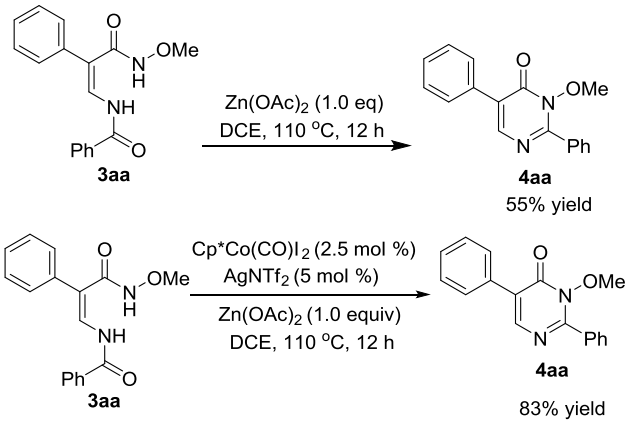


In a Schlenk tube, 2,5-Bis(4-(tert-butyl)phenyl)-3-methoxypyrimidin-4(3*H*)-one (78.0 mg, 0.2 mmol) was dissolved in dry THF (4 mL). SmI_2 solution (0.1 M in THF, 4.0 mL, 0.4 mmol) was added slowly via a syringe. The reaction mixture was stirred at RT about 2 h (The process of the reaction could be monitored by TLC analysis). The solvent was removed under reduced pressure and the residue was purified by flash column chromatography (DCM/MeOH = 95:5) to afford **7** as a white solid (47.1 mg, 65% yield). ^{1}H NMR (400 MHz, CD_2Cl_2) δ 13.05 (s, 1H), 8.28 (s, 1H), 8.20 (d, J = 8.2 Hz, 2H), 7.74 (d, J = 8.4 Hz, 2H), 7.49 (d, J = 8.4 Hz, 2H), 7.45 (d, J = 8.0 Hz, 2H), 1.31 (s, 9H), 1.30 (s, 9H). ^{13}C NMR (100 MHz, CD_2Cl_2) δ 174.3, 155.71, 155.68, 152.8, 151.5, 130.4, 129.0, 128.0, 127.4, 125.9, 125.2, 124.4, 34.9, 34.6, 31.1, 30.9. HRMS (ESI) Calcd for $[C_{24}H_{28}N_2O+H]^+$ 361.2274, Found 361.2279.



3ca **8** 61% yield

Compound **8** was prepared according to the above procedure of preparing **7**.white solid, 61% yield ^{1}H NMR (400 MHz, CDCl3) δ 12.44 (d, J = 10.0 Hz, 1H), 7.97 (d, J = 7.6 Hz, 2H), 7.66 (d, J = 10.0 Hz, 1H), 7.60 – 7.56 (m, 1H), 7.52 – 7.48 (m, 2H), 7.40 – 7.38 (m, 2H), 7.33 – 7.31 (m, 2H), 5.84 (s, 1H), 5.58 (s, 1H). 13C NMR (100 MHz, CDCl3) δ 164.8, 136.8, 135.1, 134.3, 132.8, 132.5, 131.2, 129.3, 128.9, 127.8. HRMS (ESI) Calcd for $[C_{16}H_{13}N_2O_2Cl+H]^+$ 301.0738, Found 301.0734.



3aa **4aa** 55% yield

3aa **4aa** 83% yield

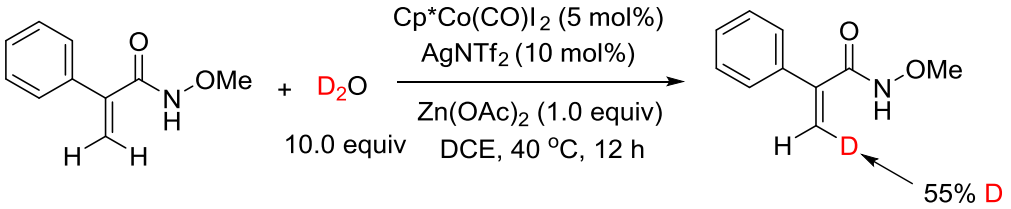
3aa (29.6 mg, 0.10 mmol), $Zn(OAc)_2$ (18.3 mg, 0.1 mmol) were dissolved in DCE (1 mL) under

N_2 atmosphere. The mixture was stirred at 110°C overnight. After that the solvent was removed under reduced pressure. The residue was purified by silica gel chromatography using PE/EA to afford compound **4aa** (15.3mg, 55%).

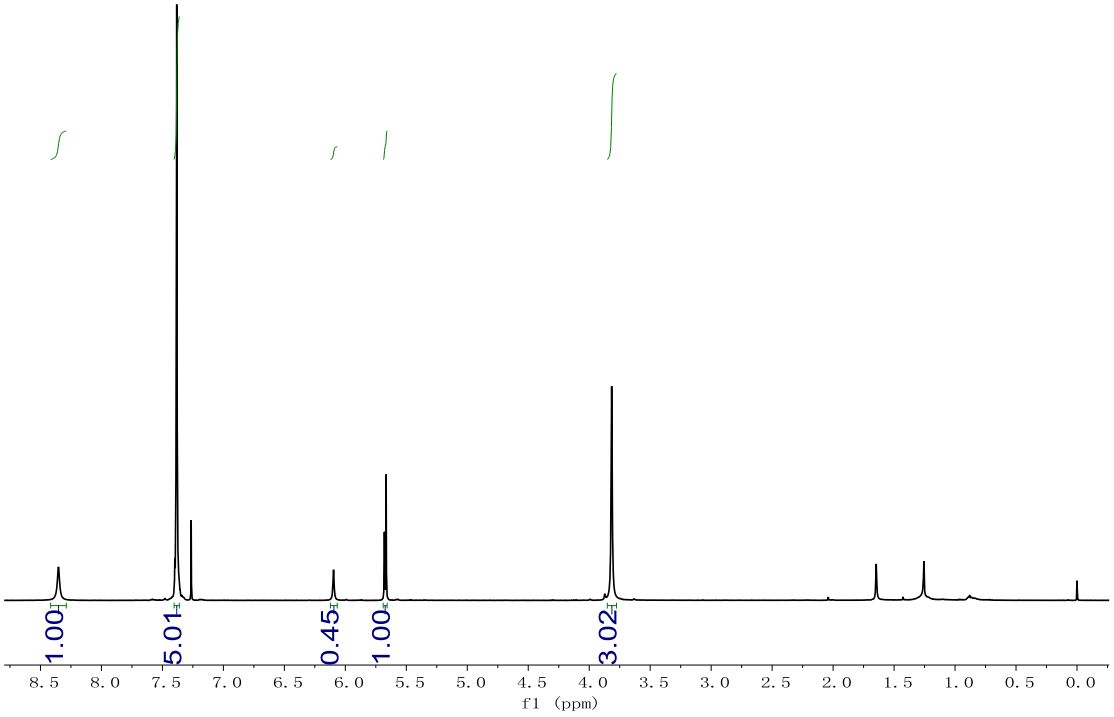
3aa (29.6 mg, 0.1 mmol), $[Cp^*Co(CO)I]_2$ (1.2 mg, 0.0025 mmol), $AgNTf_2$ (1.9 mg, 0.005 mmol) and $Zn(OAc)_2$ (18.3 mg, 0.1 mmol) were dissolved in DCE (1 mL) under N_2 atmosphere. The mixture was stirred at 110°C overnight. After that the solvent was removed under reduced pressure. The residue was purified by silica gel chromatography using PE/EA to afford compound **4aa** (23.1 mg, 83%).

IV. Mechanistic Studies

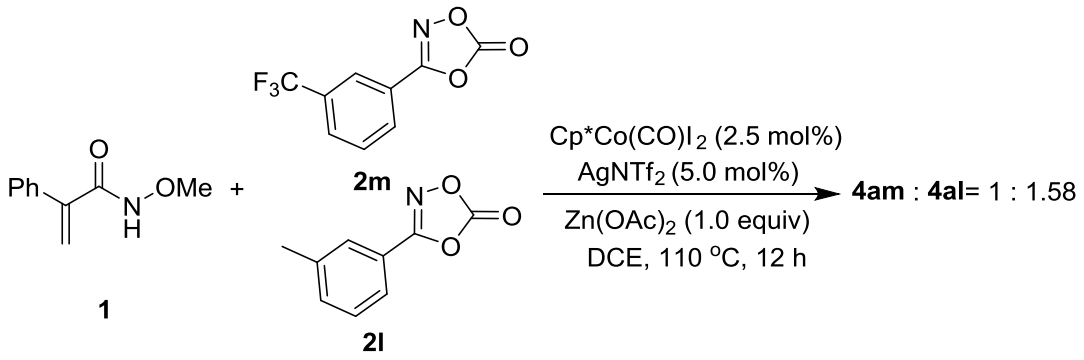
(a) H/D Exchange Experiments



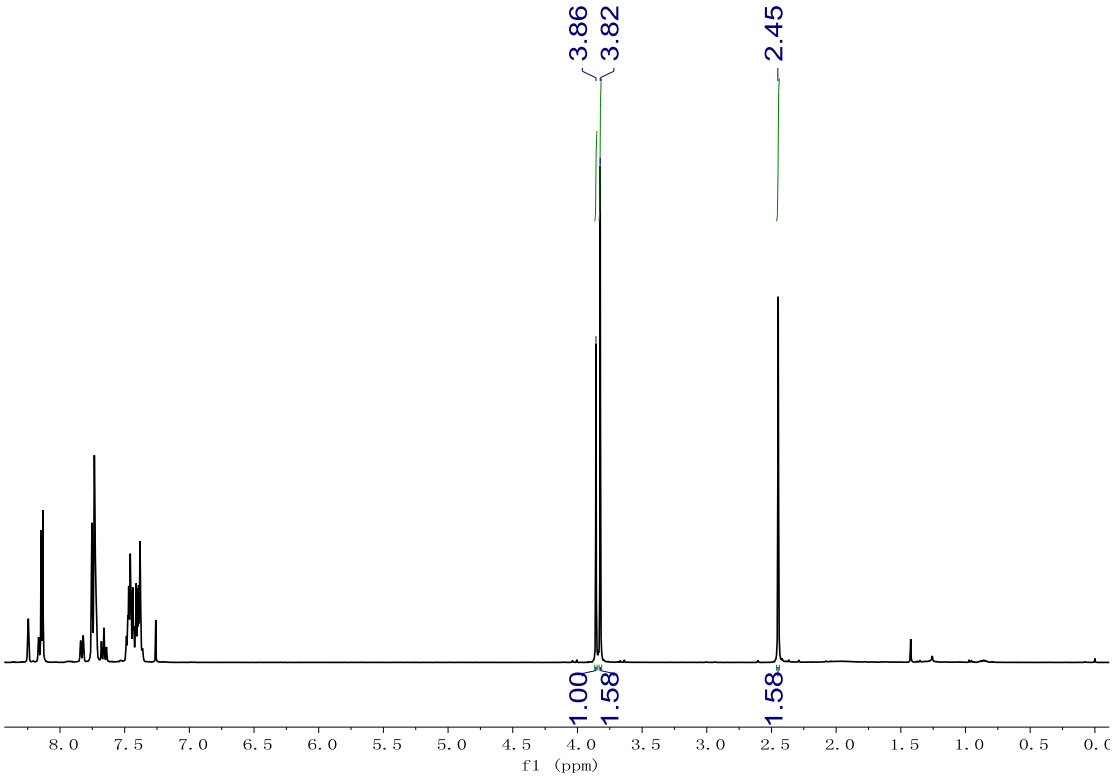
1 (17.7 mg, 0.1 mmol), $Cp^*Co(CO)I_2$ (2.4 mg, 0.005 mmol), $AgNTf_2$ (3.9 mg, 0.01 mmol), $Zn(OAc)_2$ (18.3 mg, 0.1 mmol), and D_2O (20 mg, 1 mmol) were dissolved in DCE (1 mL) under N_2 atmosphere. The reaction mixture was stirred at 40 ℃ for 12 h. After that, the solvent was removed under reduced pressure and the residue was purified by silica gel chromatography using PE/EA to afford an oil, which was characterized by ^1H NMR spectroscopy.



(b) Competition Reaction



A mixture of **1** (35.44 mg, 0.2 mmol), **2m** (46.2 mg, 0.2 mmol), **2l** (35.4 mg, 0.2 mmol), Cp*Co(CO)I_2 (2.1 mg, 0.005 mmol), $AgNTf_2$ (3.9 mg, 0.01 mmol), and $Zn(OAc)_2$ (36.7 mg, 0.2 mmol) were dissolved in DCE (2 mL) under N_2 atmosphere. The reaction mixture was stirred at 110 ℃ for 12 h. After that, the solvent was removed under reduced pressure and the residue was purified by silica gel chromatography using PE/EA to afford **4am** and **4al**, which were characterized by ^{1}H NMR spectroscopy.



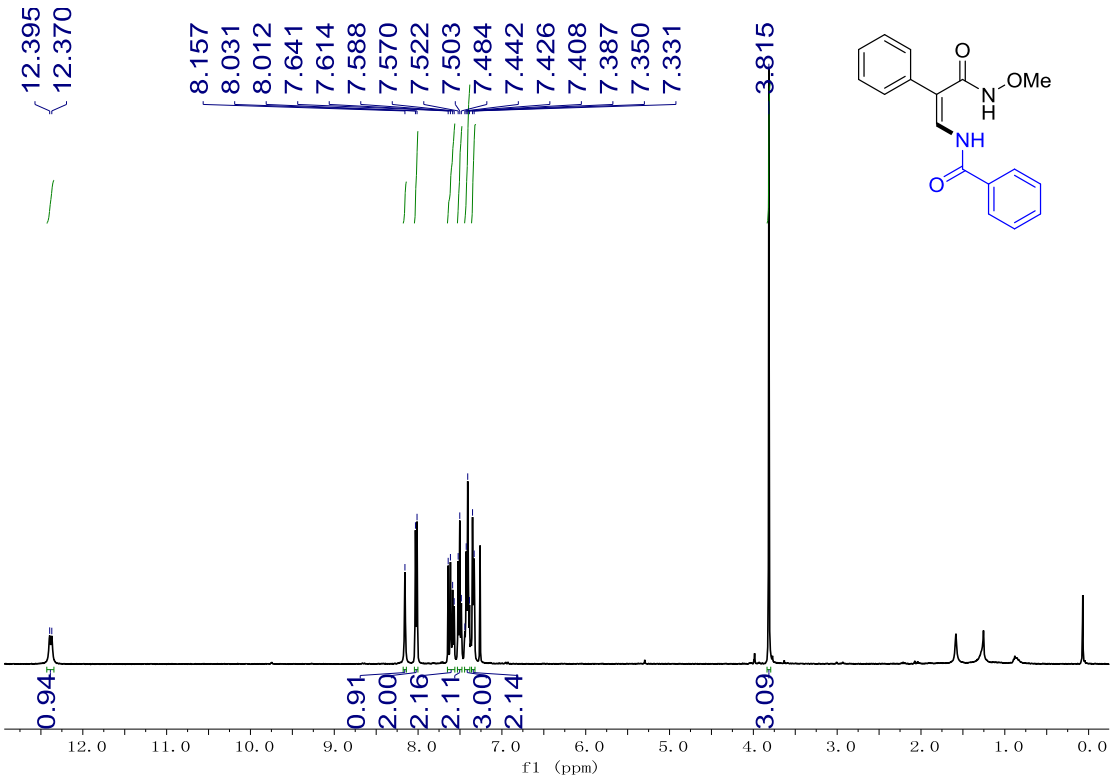
V. References

[1] (a) C. Yu, F. Li, J. Zhang, G. Zhong, *Chem. Commun.* **2017**, *53*, 533. (b) Z. Zhou, G. Liu, X. Lu, Org. Lett. **2016**, *18*, 5668.

[2] (a) M. Chen, N. Sun, H. Chen, Y. Liu, *Chem. Commun.*, **2016**, 52, 6324--6327

VI. NMR Spectra of Products

3aa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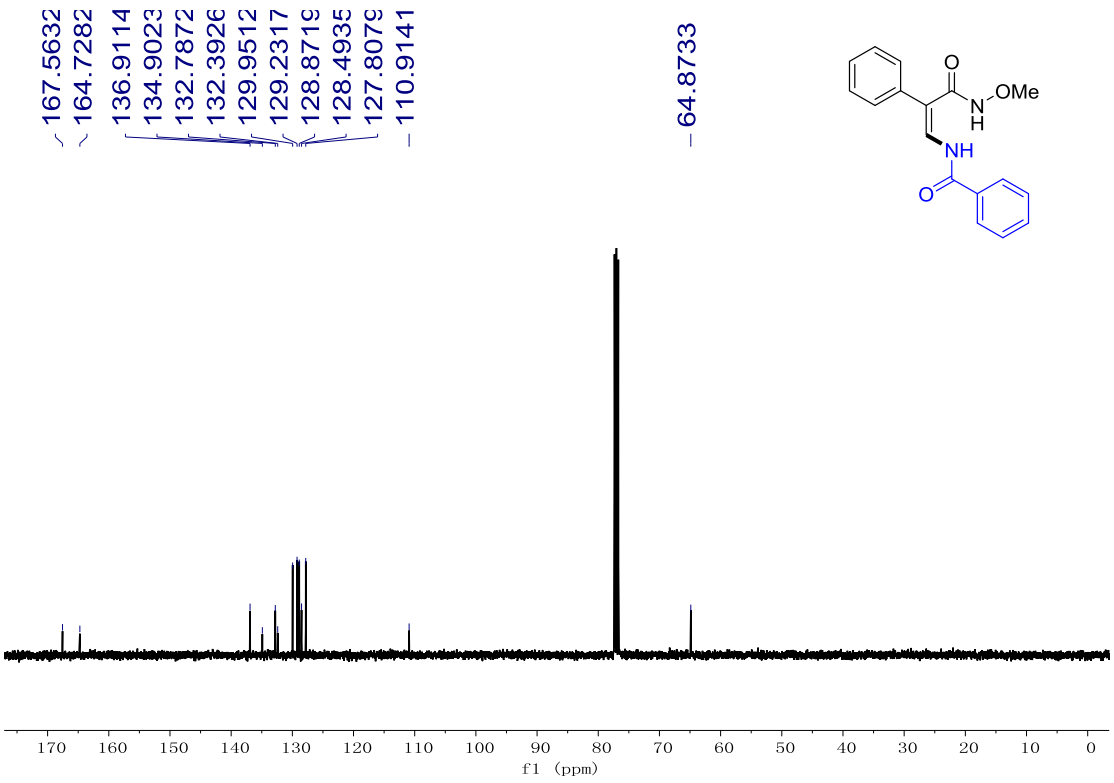
7.442
7.426
7.408
7.387
7.350
7.331
3.815
O
N
OMe
H
NH
O
0.94
0.91
2.00
2.16
2.11
3.00
2.14
3.09
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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132.3926
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128.8719
128.4935
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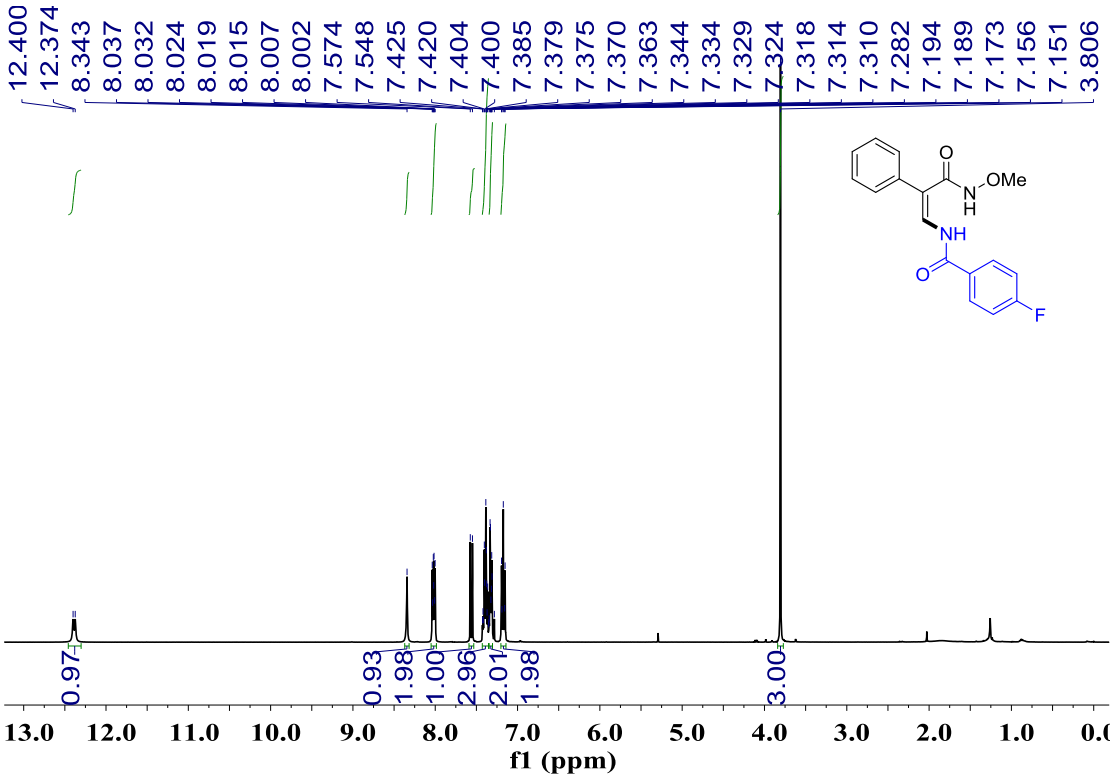
110.9141
64.8733
O
N
OMe
H
NH
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

3ab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7.548
7.425
7.420
7.404
7.400
7.385
7.379
7.375
7.370
7.363
7.344
7.334
7.329
7.324
7.318
7.314
7.310
7.282
7.194
7.189
7.173
7.156
7.151
3.806
0.97
0.93
1.98
1.00
2.96
2.01
1.98
3.00
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)
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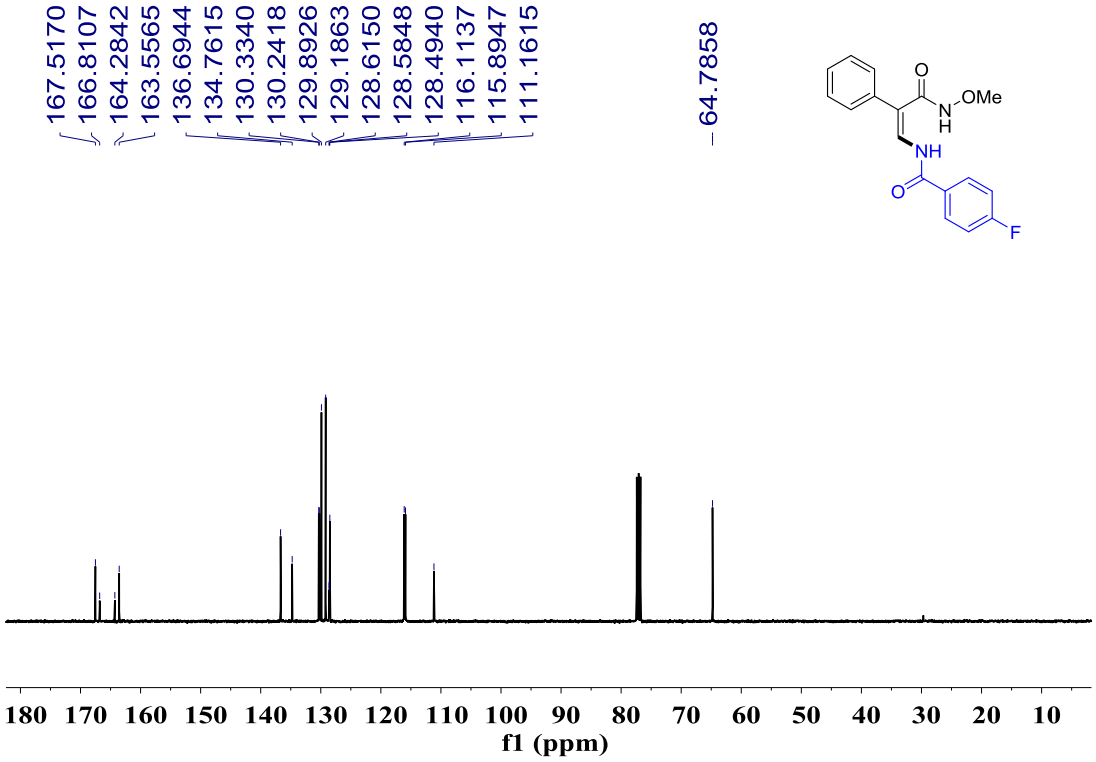
N
OMe
H
NH
O
F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163.5565
136.6944
134.7615
130.3340
130.2418
129.8926
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128.6150
128.5848
128.4940
116.1137
115.8947
111.1615
64.7858
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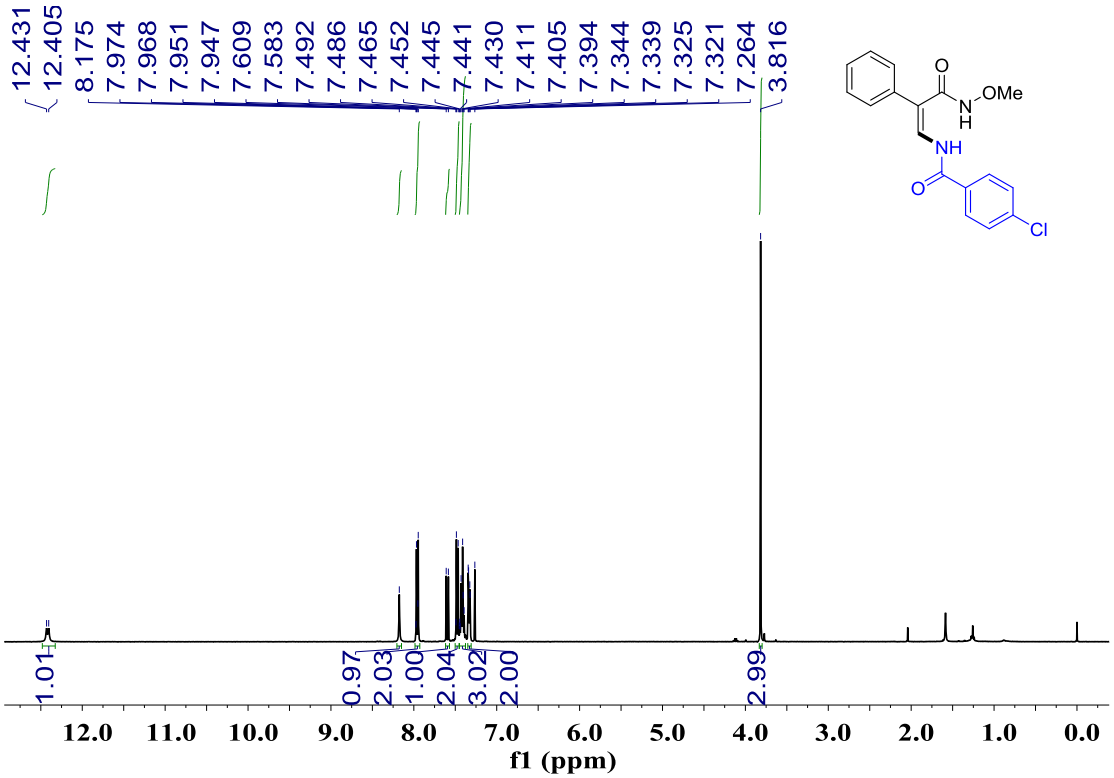
OMe
H
NH
O
F
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

3ac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7.445
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7.394
7.344
7.339
7.325
7.321
7.264
3.816
O
N
OMe
H
NH
O
Cl
1.01
0.97
2.03
1.00
2.04
3.02
2.00
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12.0
11.0
10.0
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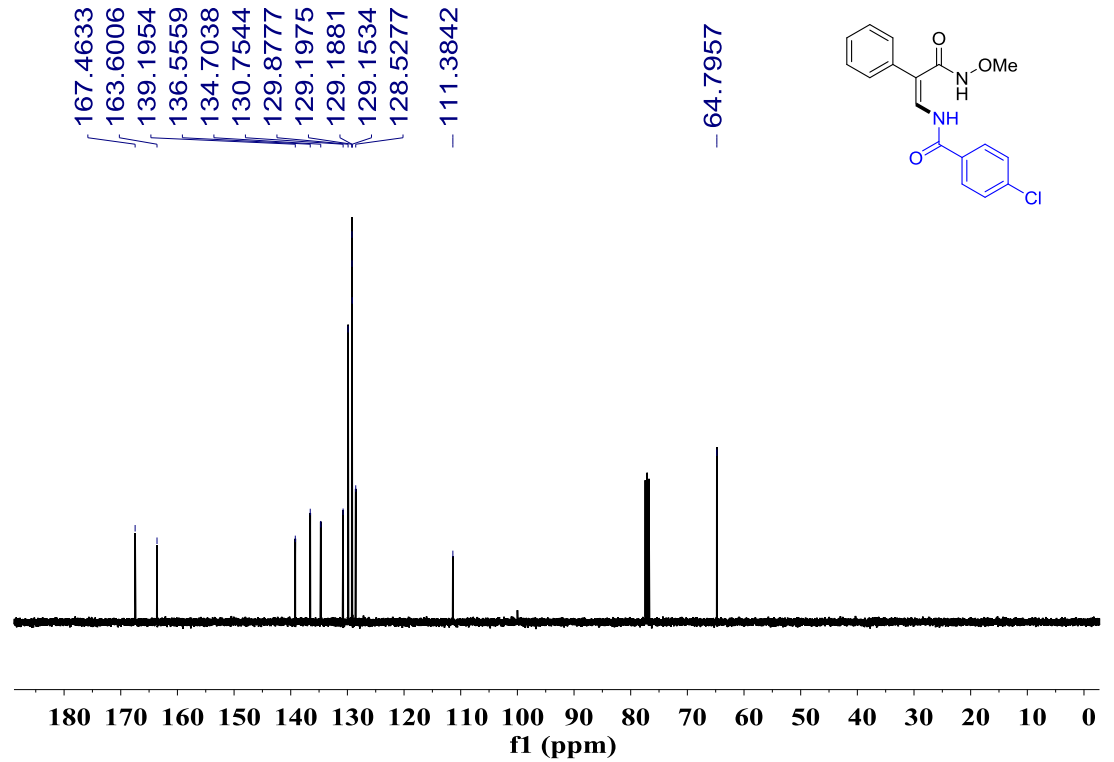
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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136.5559
134.7038
130.7544
129.8777
129.1975
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129.1534
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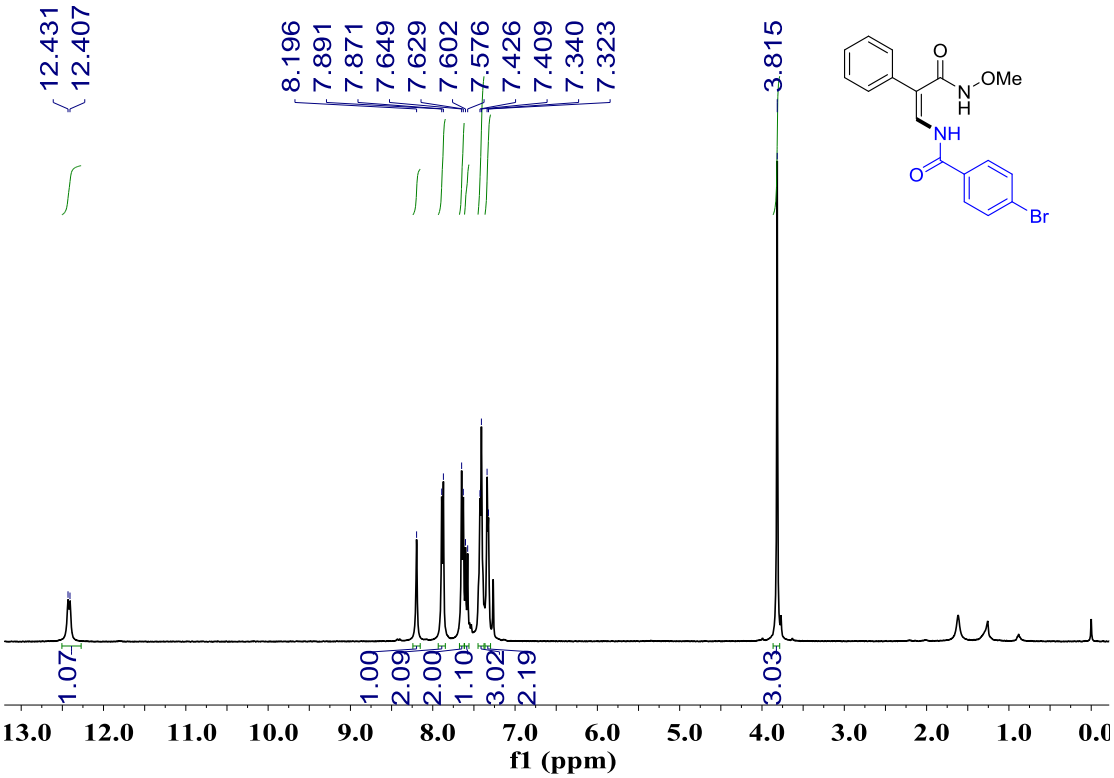
64.7957
O
N
OMe
H
NH
O
Cl
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

3ad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7.602
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7.323
3.815
O
N
OMe
H
NH
O
Br
1.07
1.00
2.09
2.00
1.10
3.02
2.19
3.03
13.0
12.0
11.0
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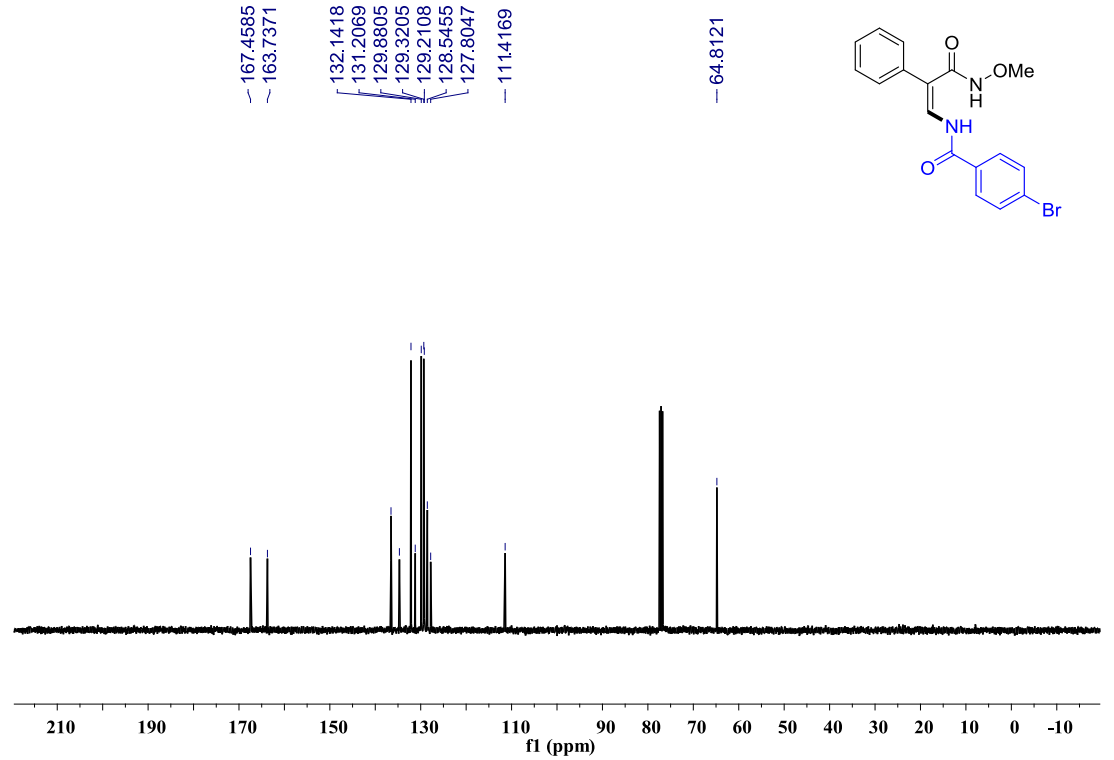
f1 (ppm)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OMe
H
NH
O
Br
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190
170
150
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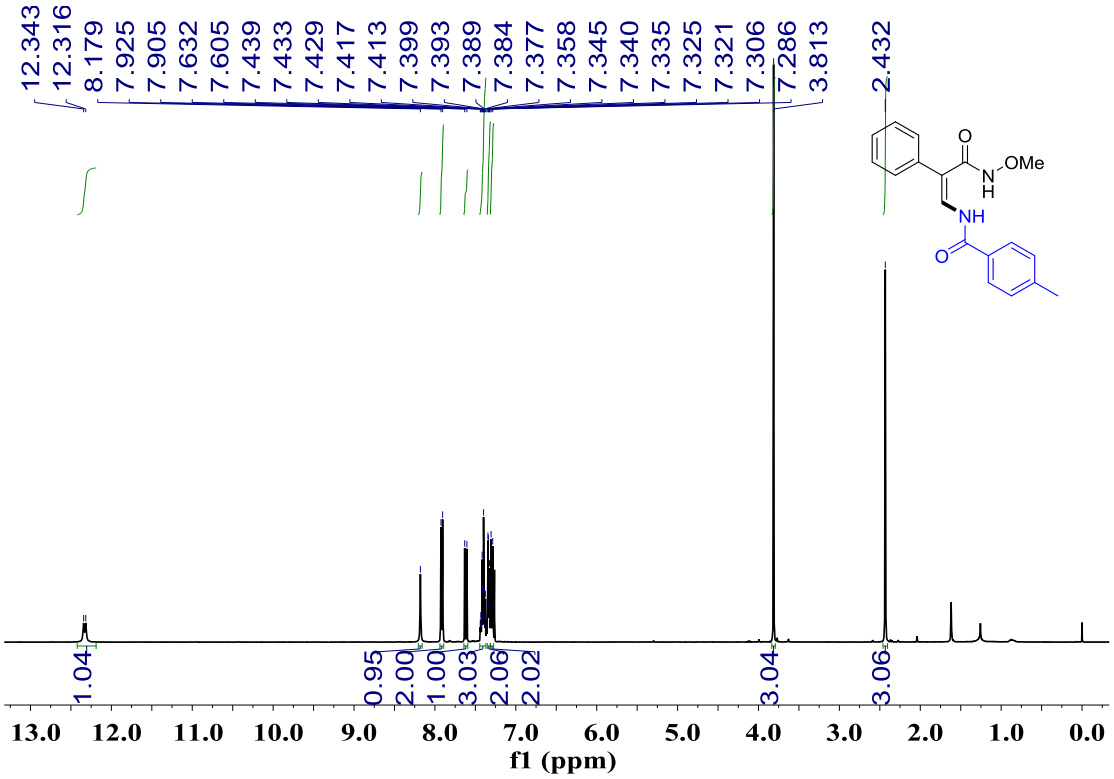
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

3ae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7.429
7.417
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7.399
7.393
7.389
7.384
7.377
7.358
7.345
7.340
7.335
7.325
7.321
7.306
7.286
3.813
2.432
1.04
0.95
2.00
1.00
3.03
2.06
2.02
3.04
3.06
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12.0
11.0
10.0
9.0
8.0
7.0
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5.0
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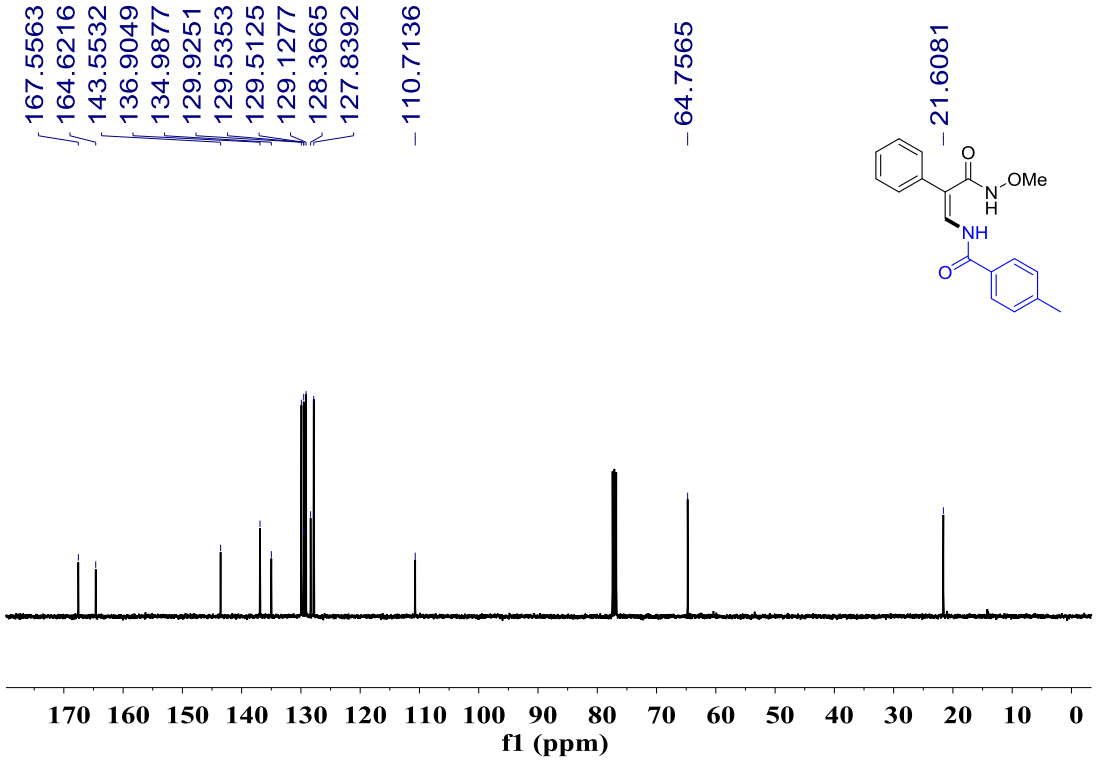
1.0
0.0
f1 (ppm)
O
N
OMe
H
NH
O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O
N
OMe
H
NH
O
170
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150
140
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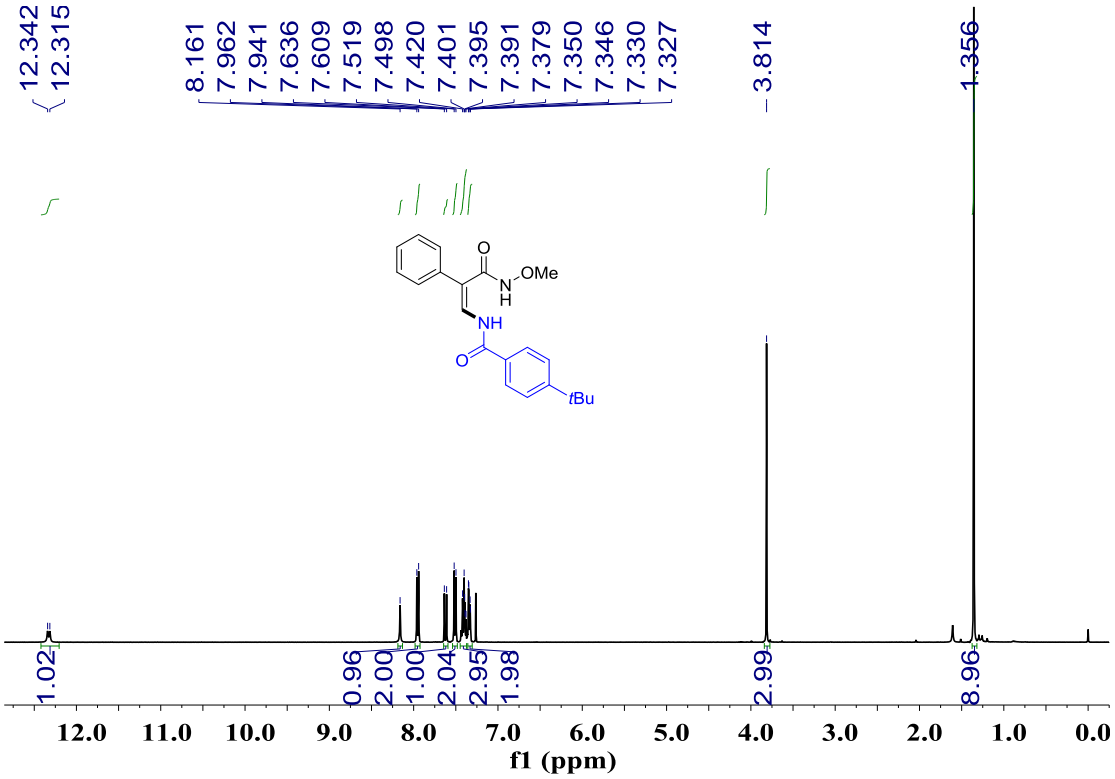
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

3af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7.379
7.350
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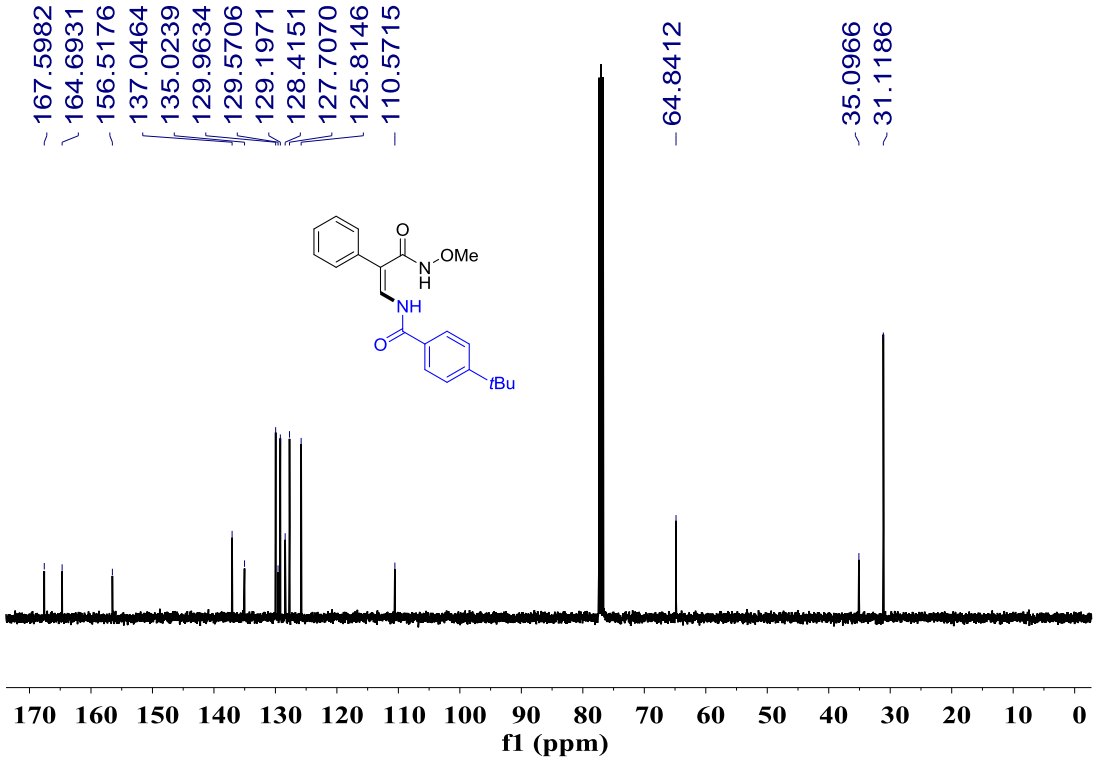
7.330
7.327
3.814
1.356
OMe
N
H
NH
O
tBu
1.02
0.96
2.00
1.00
2.04
2.95
1.98
2.99
8.96
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)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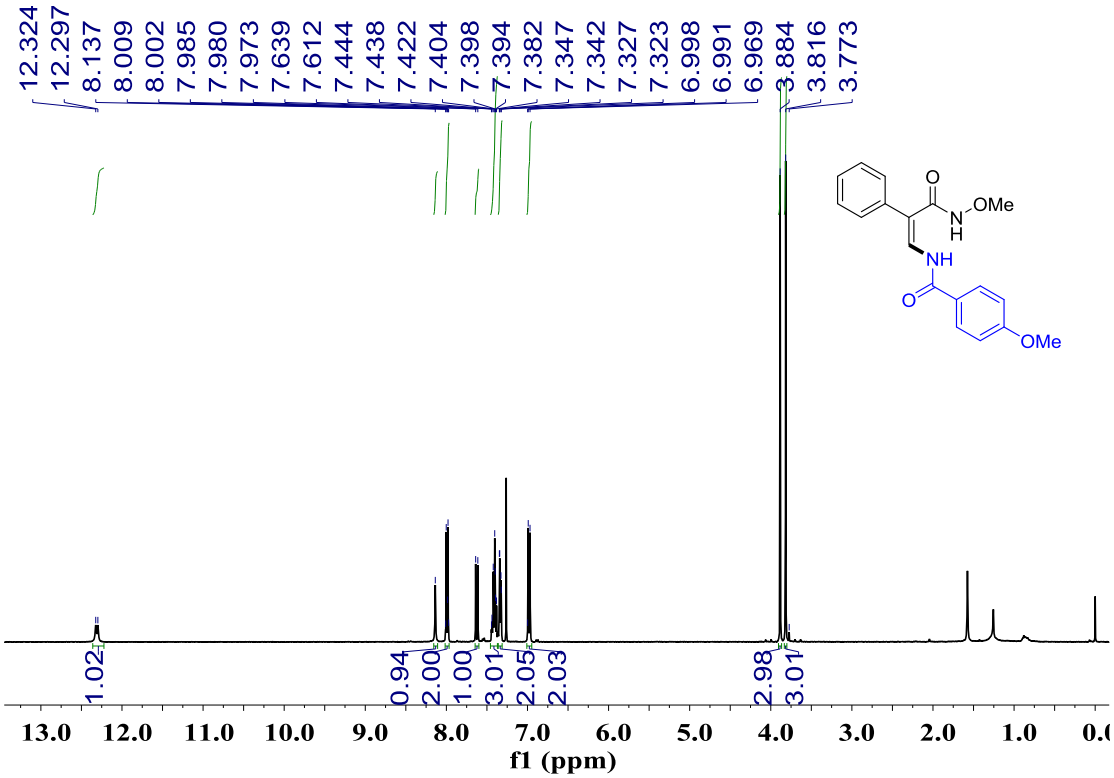
H
NH
O
tBu
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3ag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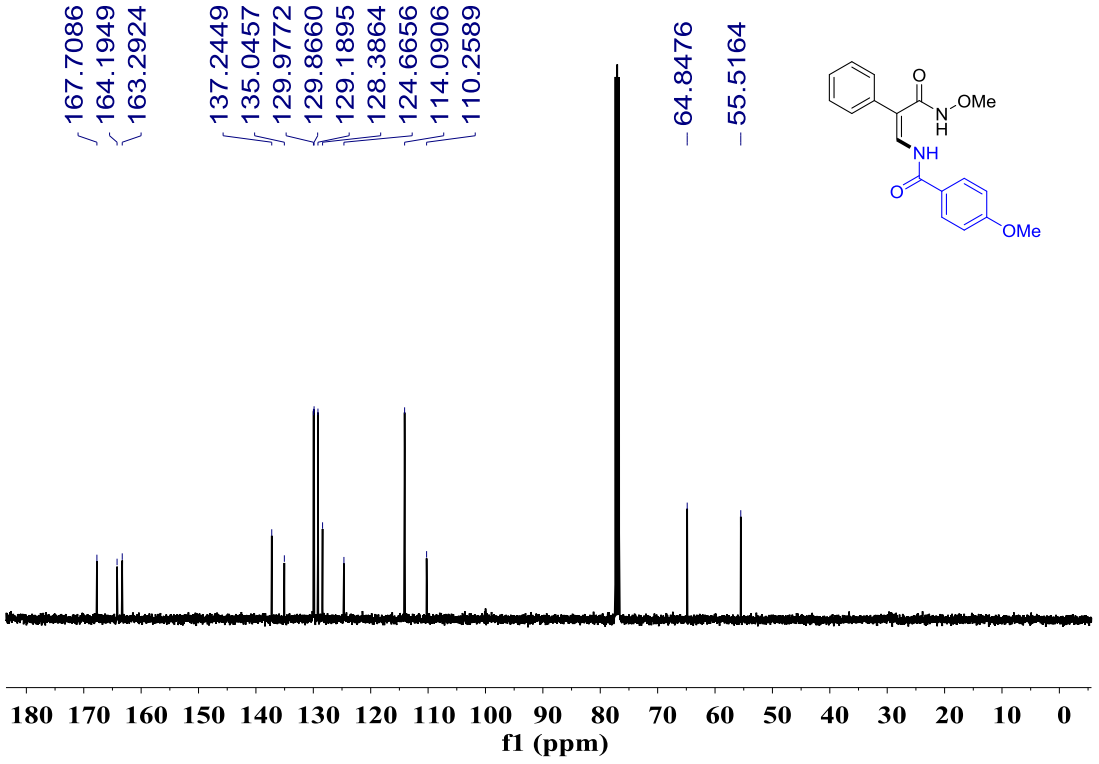
8.009
8.002
7.985
7.980
7.973
7.639
7.612
7.444
7.438
7.422
7.404
7.398
7.394
7.382
7.347
7.342
7.327
7.323
6.998
6.991
6.969
3.884
3.816
3.773
O
N
OMe
H
NH
O
OMe
1.02
0.94
2.00
1.00
3.01
2.05
2.03
2.98
3.01
13.0 12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.(
f1 (ppm)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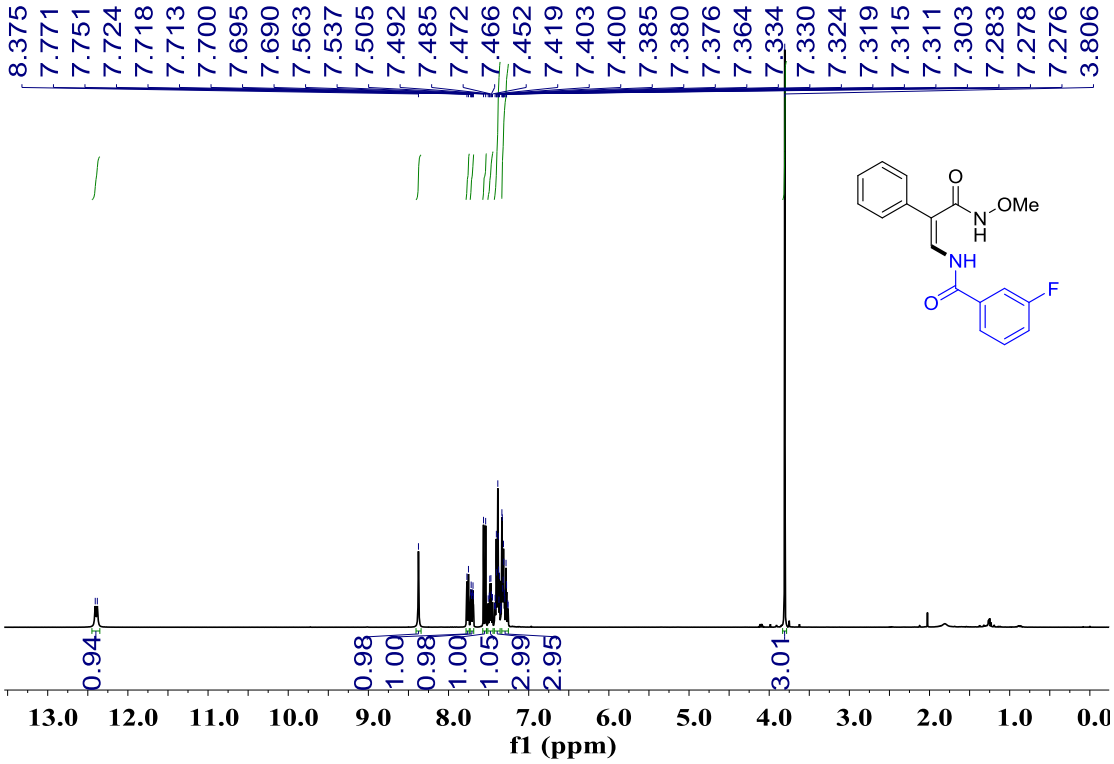
164.1949
163.2924
137.2449
135.0457
129.9772
129.8660
129.1895
128.3864
124.6656
114.0906
110.2589
64.8476
55.5164
O
N
OMe
H
NH
O
OMe
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3ah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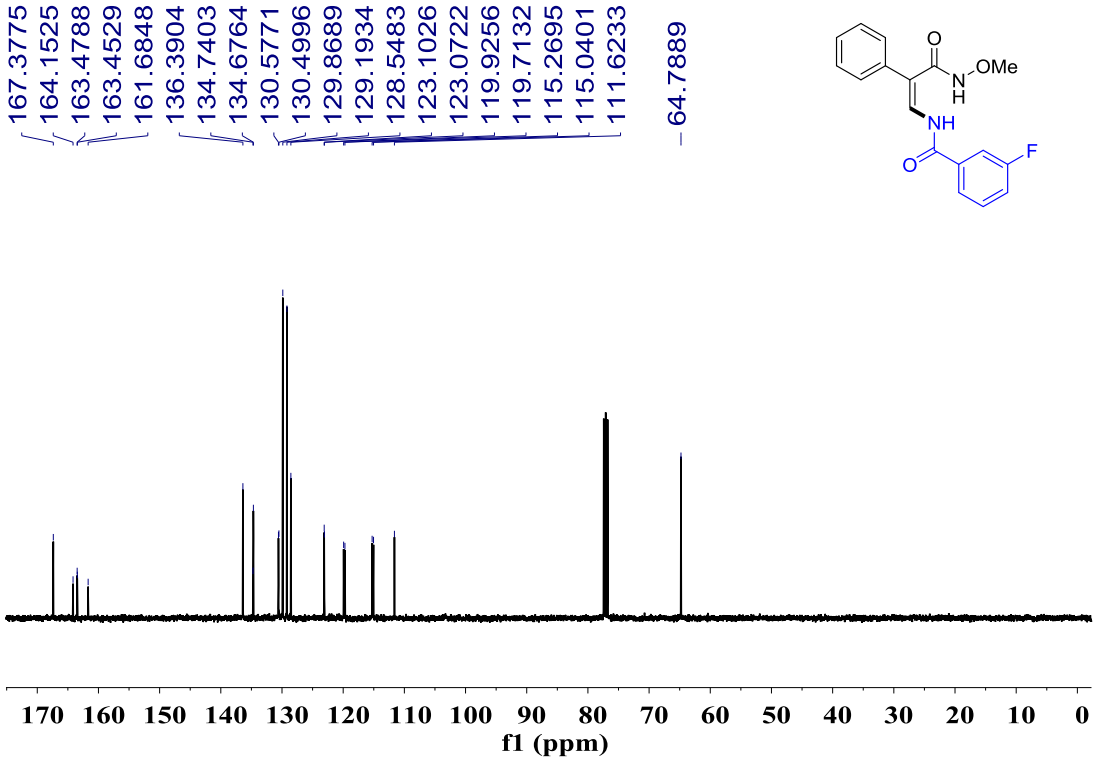
7.771
7.751
7.724
7.718
7.713
7.700
7.695
7.690
7.563
7.537
7.505
7.492
7.485
7.472
7.466
7.452
7.419
7.403
7.400
7.385
7.380
7.376
7.364
7.334
7.330
7.324
7.319
7.315
7.311
7.303
7.283
7.278
7.276
3.806
O
N
H
OMe
NH
O
F
0.94
0.98
1.00
0.98
1.00
1.05
2.99
2.95
3.01
13.0 12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)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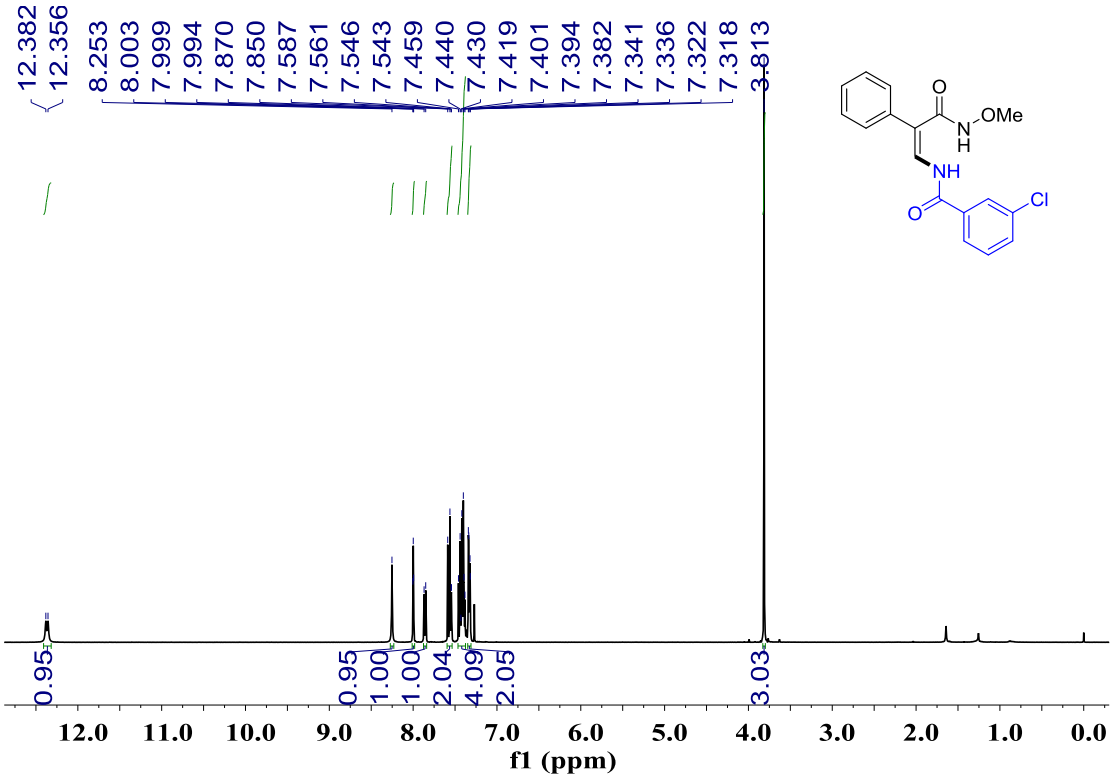
164.1525
163.4788
163.4529
161.6848
136.3904
134.7403
134.6764
130.5771
130.4996
129.8689
129.1934
128.5483
123.1026
123.0722
119.9256
119.7132
115.2695
115.0401
111.6233
64.7889
O
N
H
OMe
NH
O
F
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3ai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12.356
8.253
8.003
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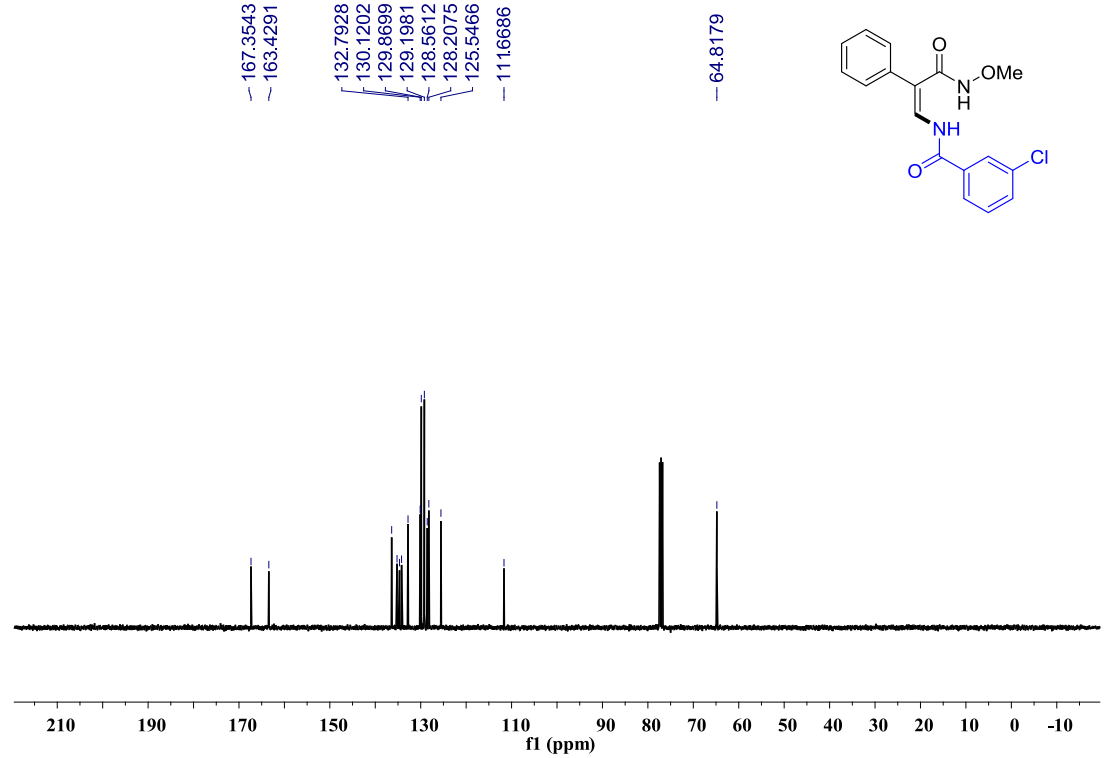
7.994
7.870
7.850
7.587
7.561
7.546
7.543
7.459
7.440
7.430
7.419
7.401
7.394
7.382
7.341
7.336
7.322
7.318
3.813
0.95
0.95
1.00
1.00
2.04
4.09
2.05
3.03
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)
O
N
OMe
H
NH
O
Cl


167.3543
163.4291
132.7928
130.1202
129.8699
129.1981
128.5612
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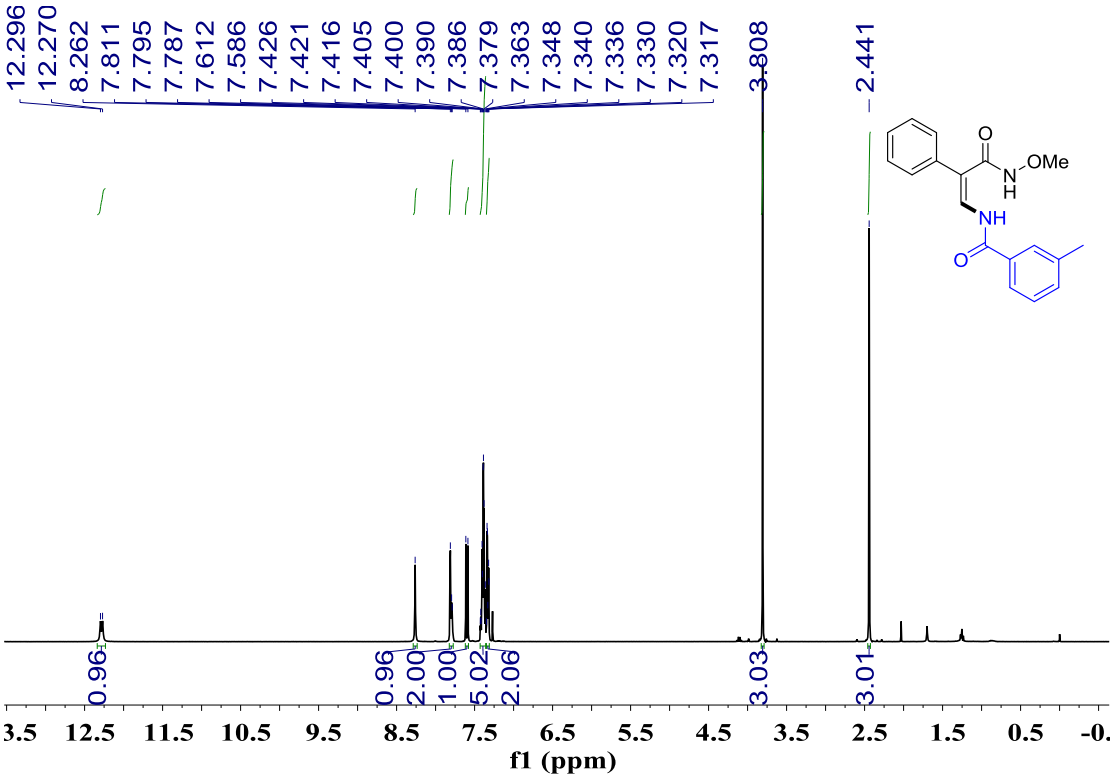
125.5466
111.6686
64.8179
O
N
OMe
H
NH
O
Cl
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

3aj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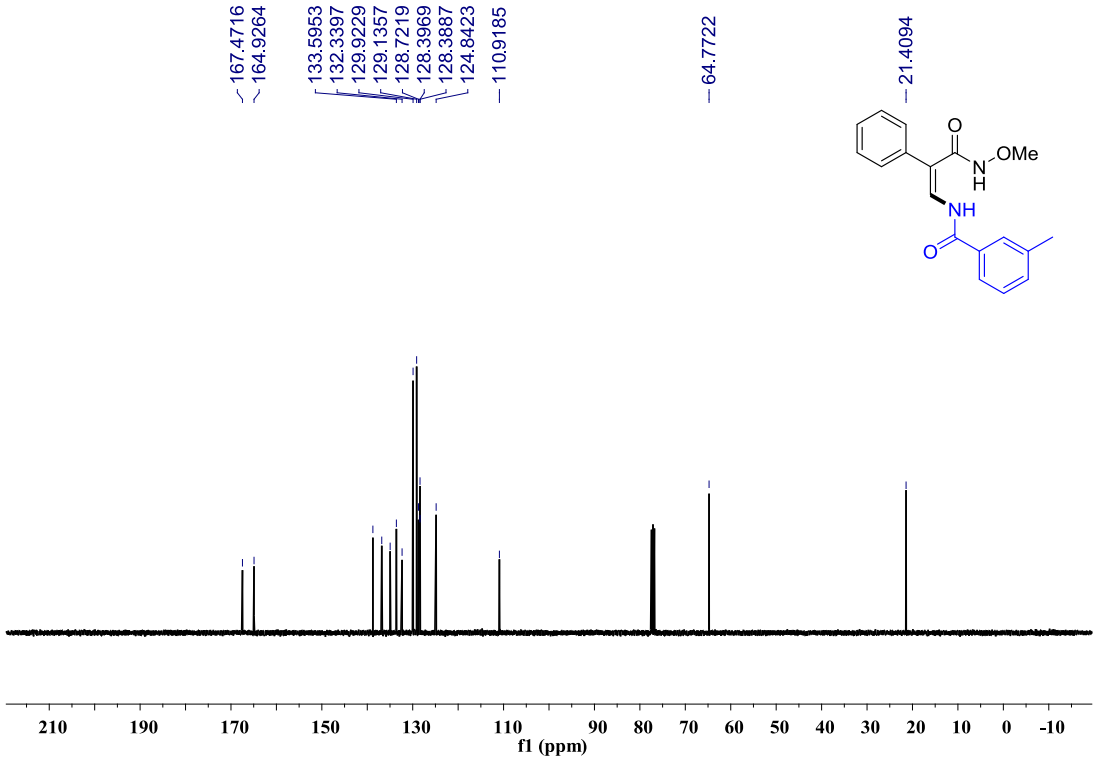
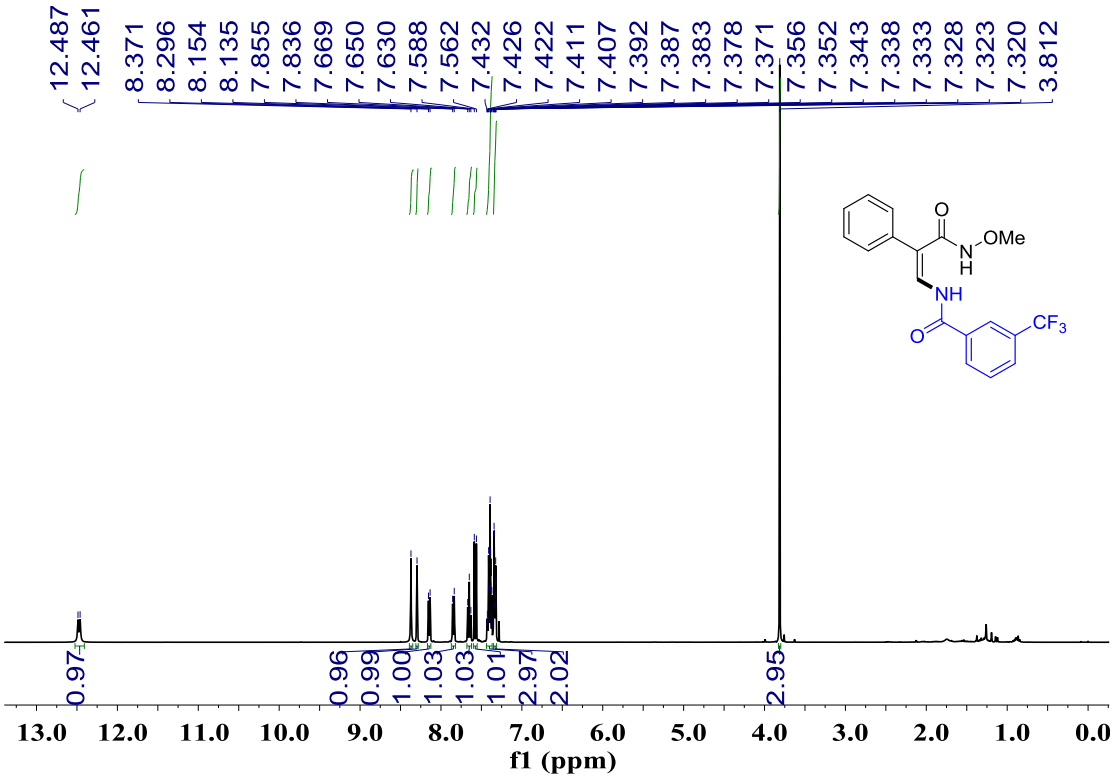
12.270
8.262
7.811
7.795
7.787
7.612
7.586
7.426
7.421
7.416
7.405
7.400
7.390
7.386
7.379
7.363
7.348
7.340
7.336
7.330
7.320
7.317
3.808
2.441
0.96
0.96
2.00
1.00
5.02
2.06
3.03
3.01
f1 (ppm)


167.4716
164.9264
133.5953
132.3397
129.9229
129.1357
128.7219
128.3969
128.3887
124.8423
110.9185
64.7722
21.4094
f1 (ppm)

3ak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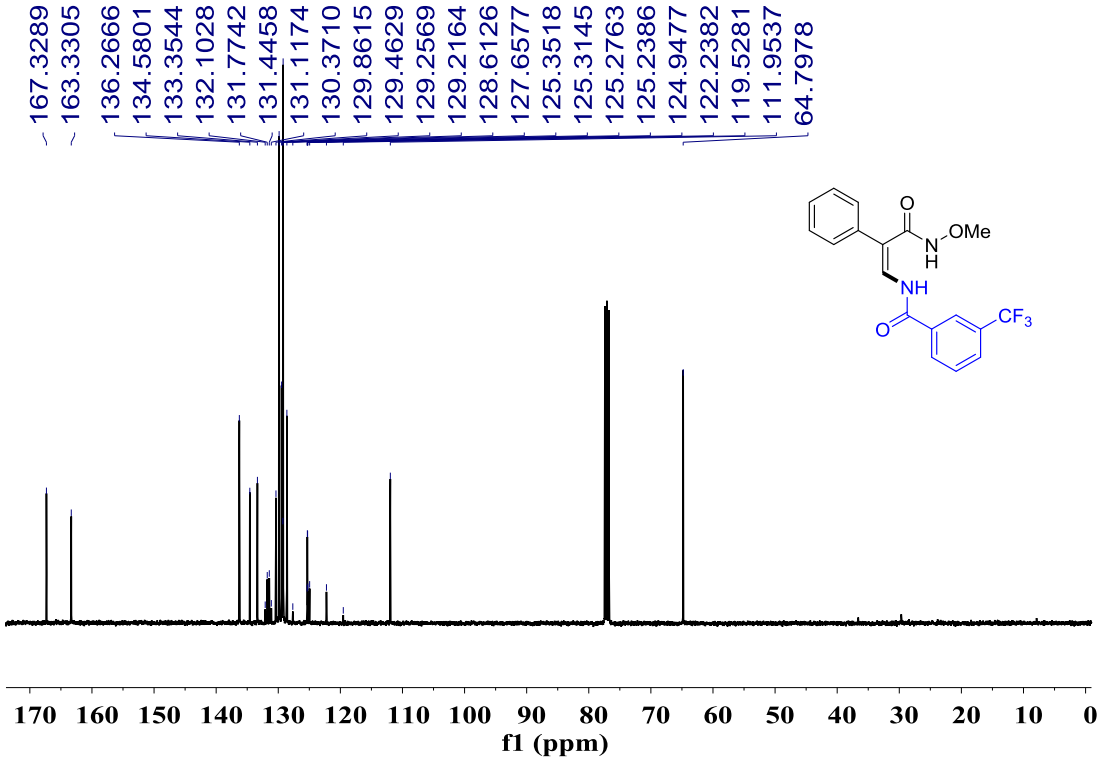
12.461
8.371
8.296
8.154
8.135
7.855
7.836
7.669
7.650
7.630
7.588
7.562
7.432
7.426
7.422
7.411
7.407
7.392
7.387
7.383
7.378
7.371
7.356
7.352
7.343
7.338
7.333
7.328
7.323
7.320
3.812
O
N
H
OMe
NH
O
CF3
0.97
0.96
0.99
1.00
1.03
1.03
1.01
2.97
2.02
2.95
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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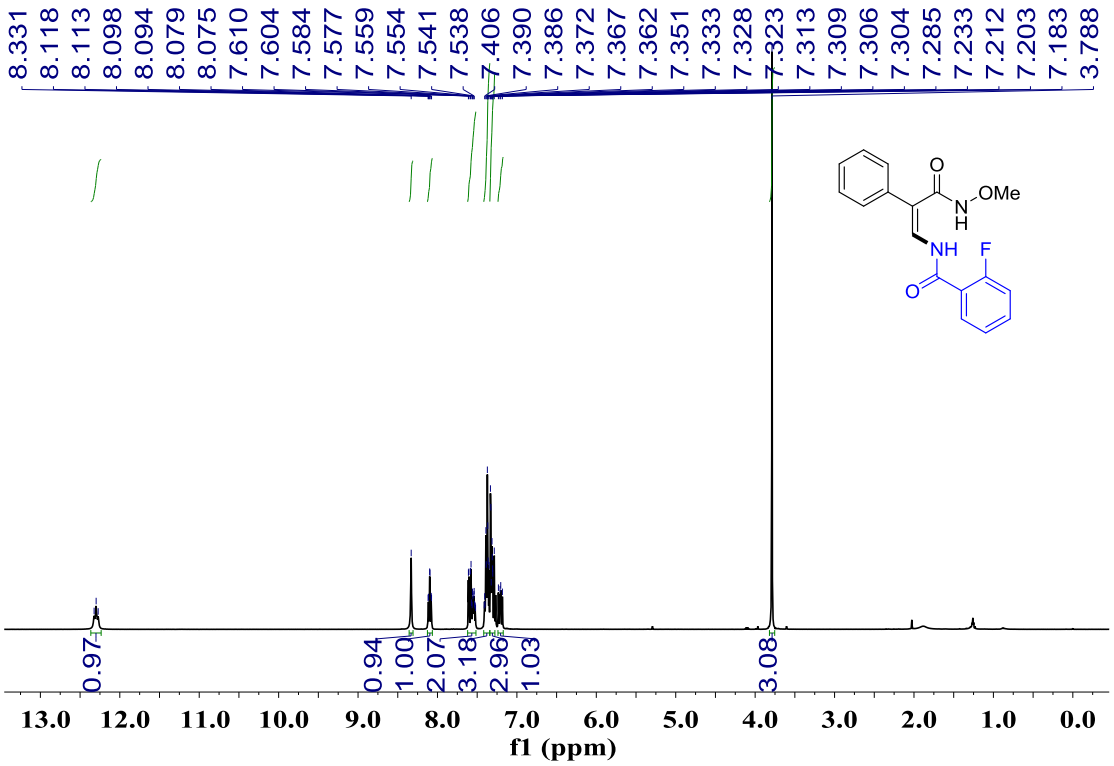
163.3305
136.2666
134.5801
133.3544
132.1028
131.7742
131.4458
131.1174
130.3710
129.8615
129.4629
129.2569
129.2164
128.6126
127.6577
125.3518
125.3145
125.2763
125.2386
124.9477
122.2382
119.5281
111.9537
64.7978
O
N
H
OMe
NH
O
CF3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

3al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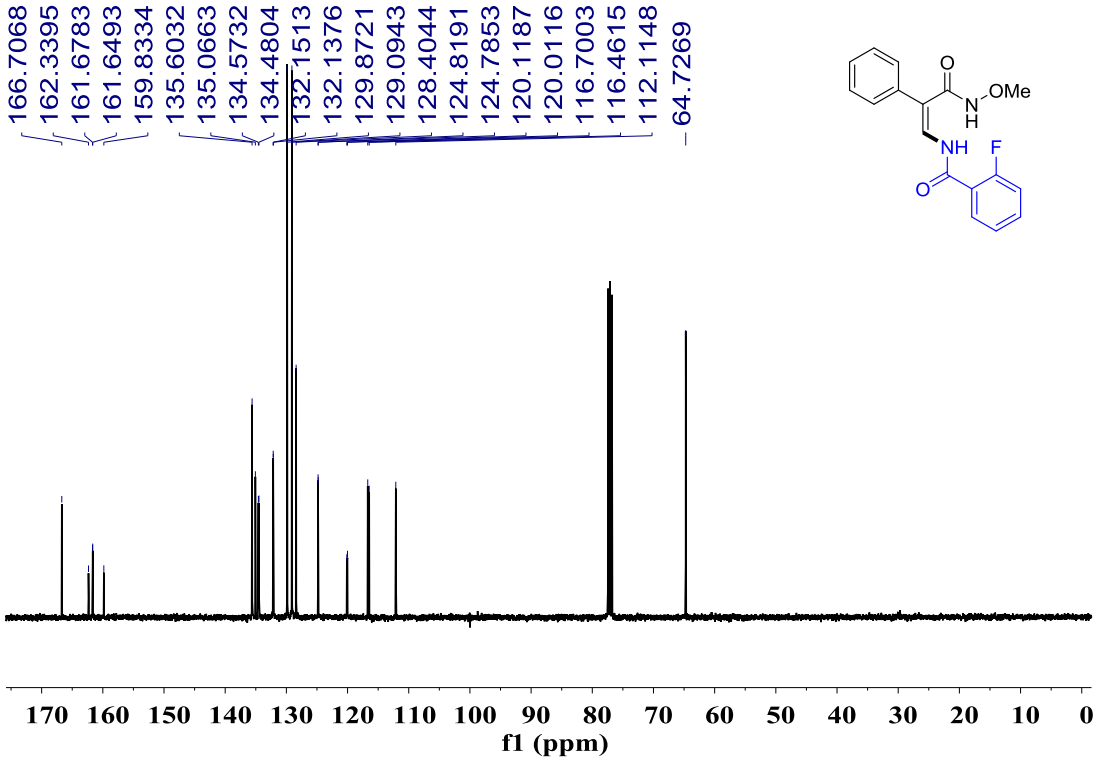
8.118
8.113
8.098
8.094
8.079
8.075
7.610
7.604
7.584
7.577
7.559
7.554
7.541
7.538
7.406
7.390
7.386
7.372
7.367
7.362
7.351
7.333
7.328
7.323
7.313
7.309
7.306
7.304
7.285
7.233
7.212
7.203
7.183
3.788
O
N
OMe
H
NH
F
O
0.97
0.94
1.00
2.07
3.18
2.96
1.03
3.08
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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162.3395
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161.6493
159.8334
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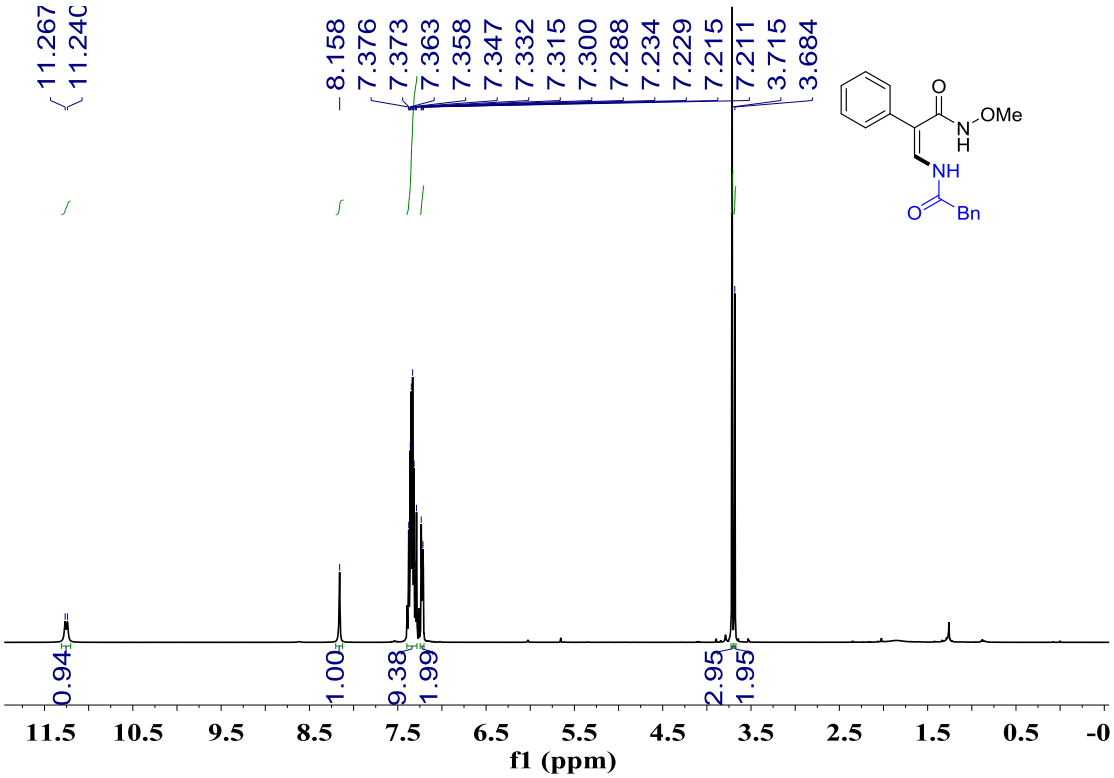
135.0663
134.5732
134.4804
132.1513
132.1376
129.8721
129.0943
128.4044
124.8191
124.7853
120.1187
120.0116
116.7003
116.4615
112.1148
64.7269
O
N
OMe
H
NH
F
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

3am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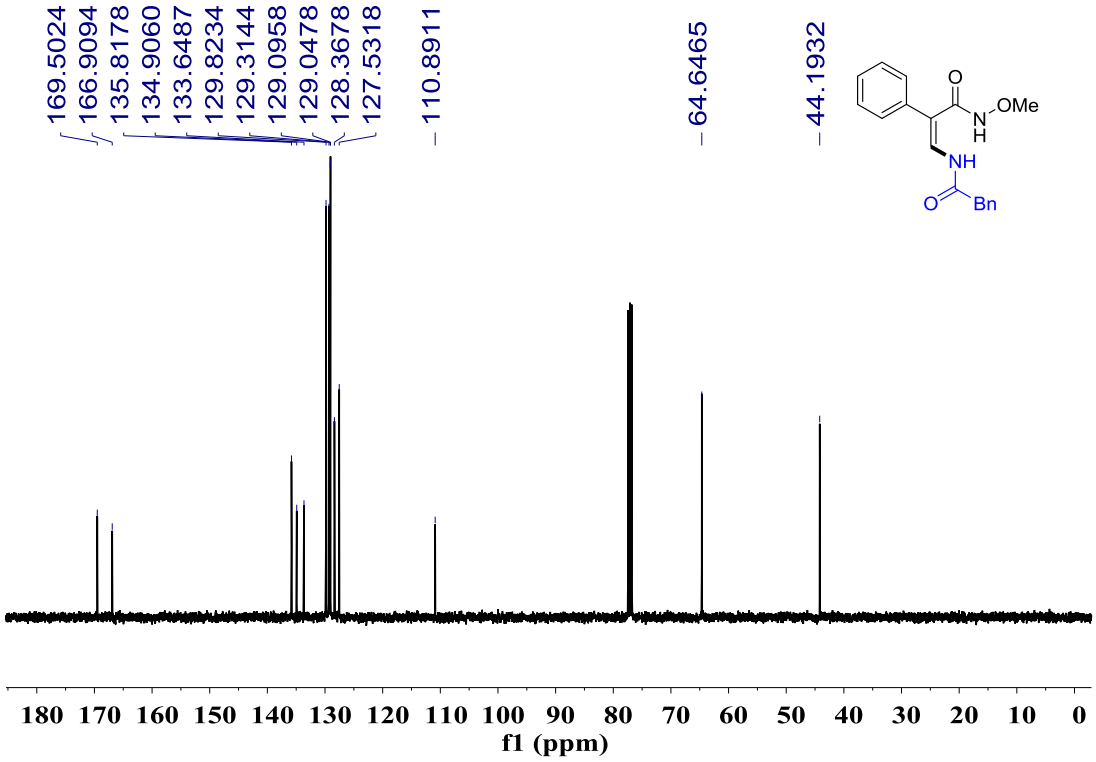
11.240
8.158
7.376
7.373
7.363
7.358
7.347
7.332
7.315
7.300
7.288
7.234
7.229
7.215
7.211
3.715
3.684
0.94
1.00
9.38
1.99
2.95
1.95
11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0
f1 (ppm)
OMe
NH
Bn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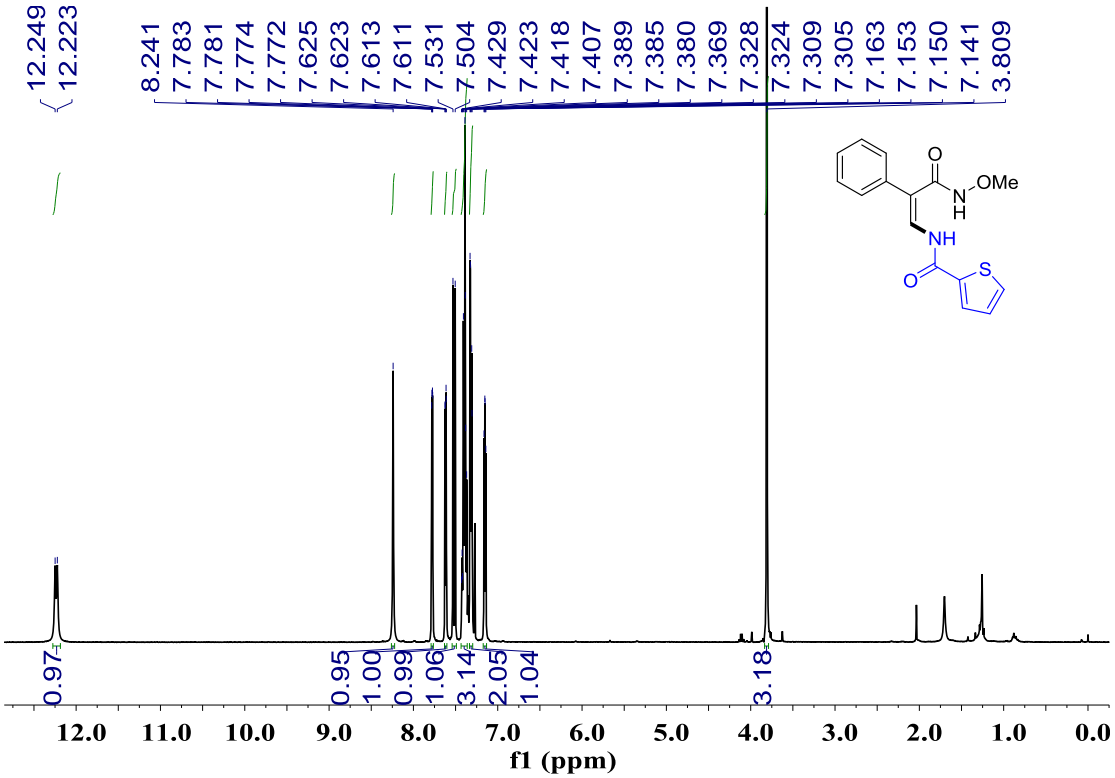
166.9094
135.8178
134.9060
133.6487
129.8234
129.3144
129.0958
129.0478
128.3678
127.5318
110.8911
64.6465
44.1932
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
OMe
NH
Bn

3an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8.241
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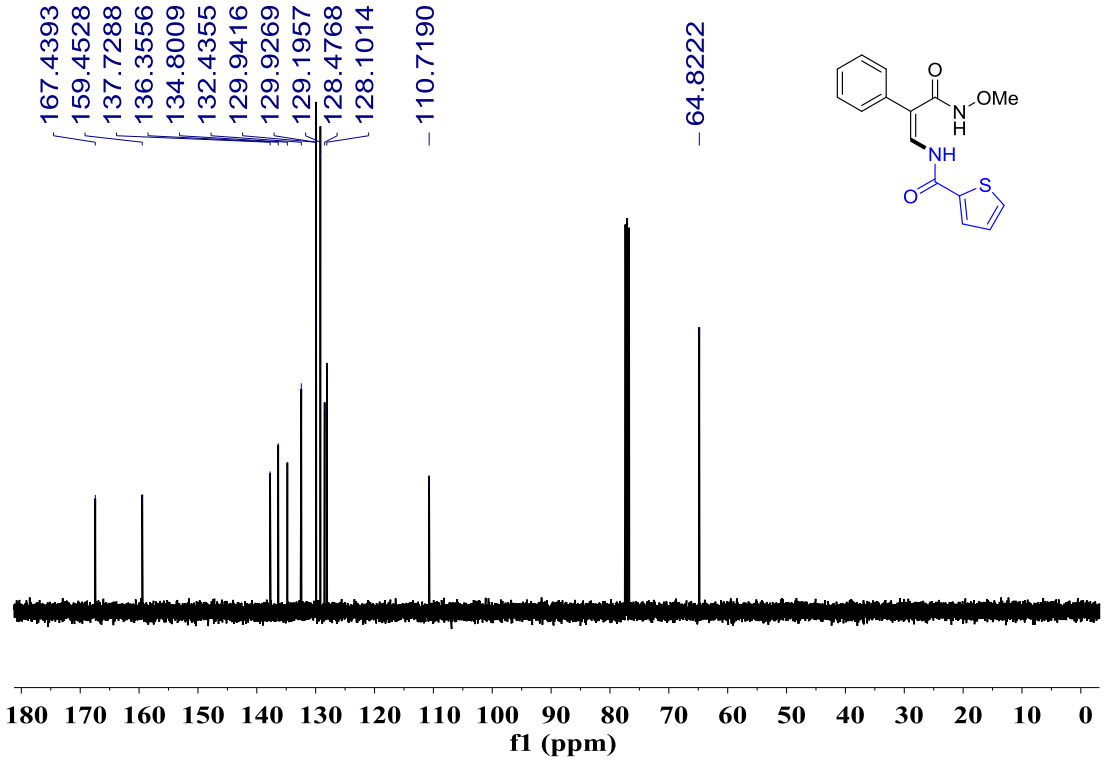
7.781
7.774
7.772
7.625
7.623
7.613
7.611
7.531
7.504
7.429
7.423
7.418
7.407
7.389
7.385
7.380
7.369
7.328
7.324
7.309
7.305
7.163
7.153
7.150
7.141
3.809
0.97
0.95
1.00
0.99
1.06
3.14
2.05
1.04
3.18
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)
O
N
H
OMe
NH
O
S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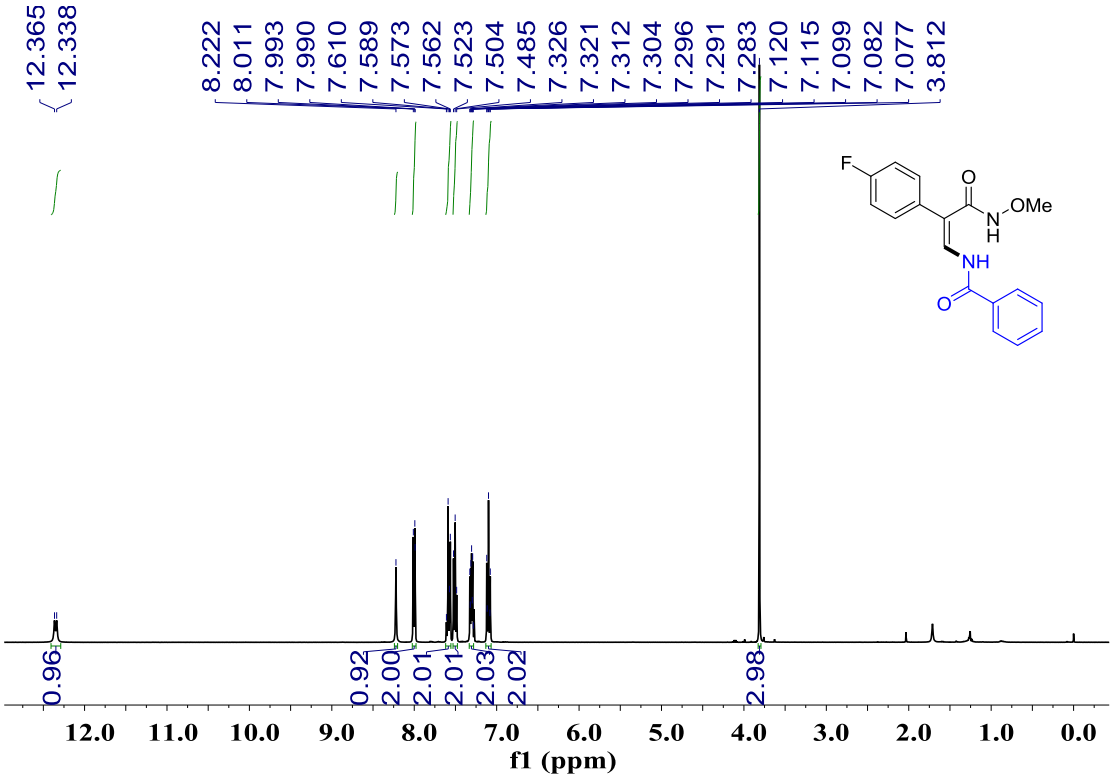
159.4528
137.7288
136.3556
134.8009
132.4355
129.9416
129.9269
129.1957
128.4768
128.1014
110.7190
64.8222
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
O
N
H
OMe
NH
O
S

3ba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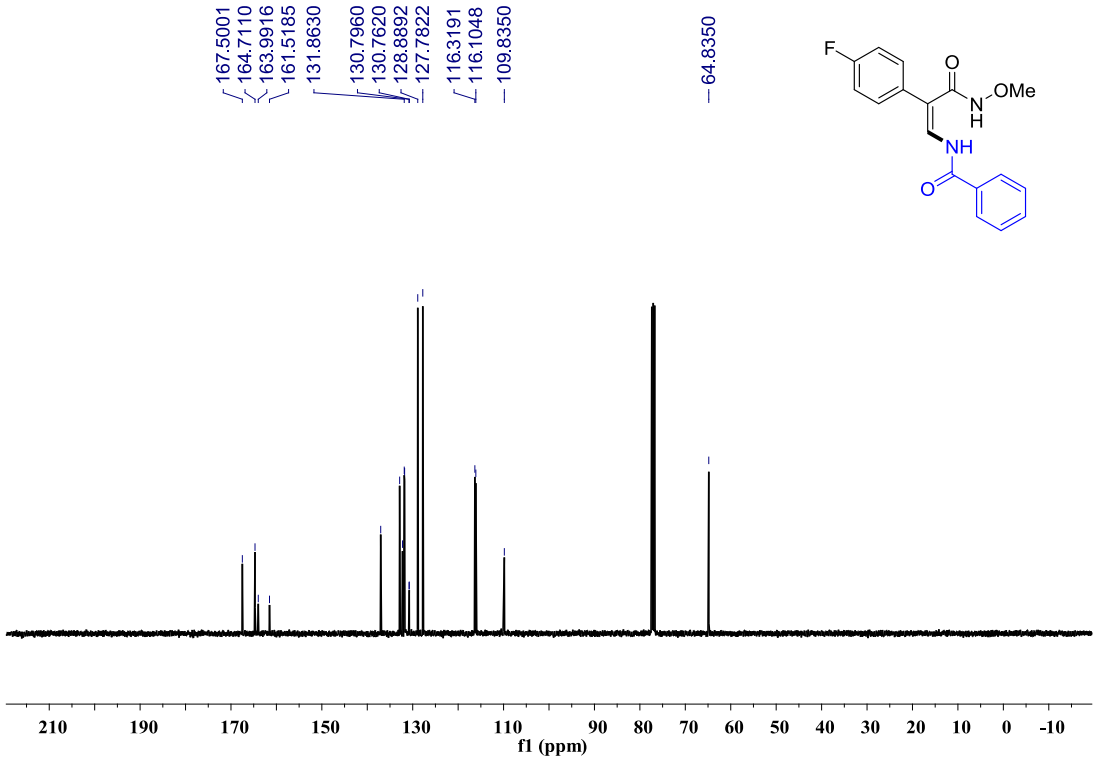
8.011
7.993
7.990
7.610
7.589
7.573
7.562
7.523
7.504
7.485
7.326
7.321
7.312
7.304
7.296
7.291
7.283
7.120
7.115
7.099
7.082
7.077
3.812
F
O
N
OMe
H
NH
O
0.96
0.92
2.00
2.01
2.01
2.03
2.02
2.98
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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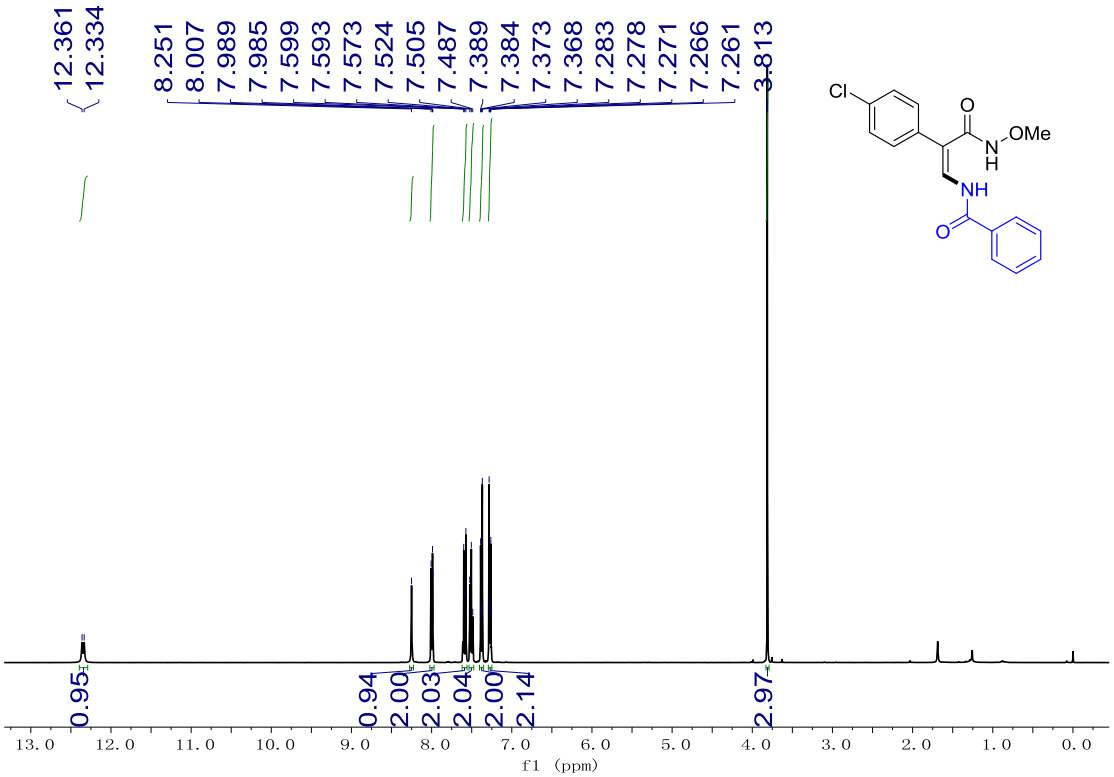
163.9916
161.5185
131.8630
130.7960
130.7620
128.8892
127.7822
116.3191
116.1048
109.8350
64.8350
F
O
N
OMe
H
NH
O
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

3ca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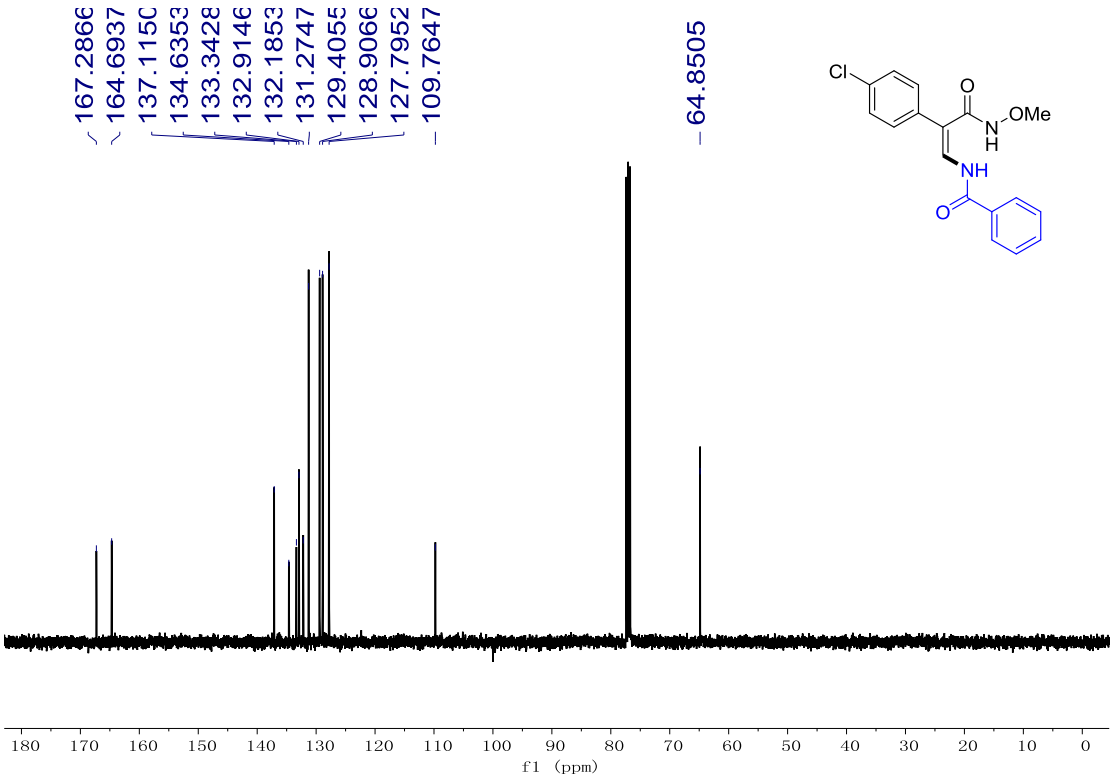
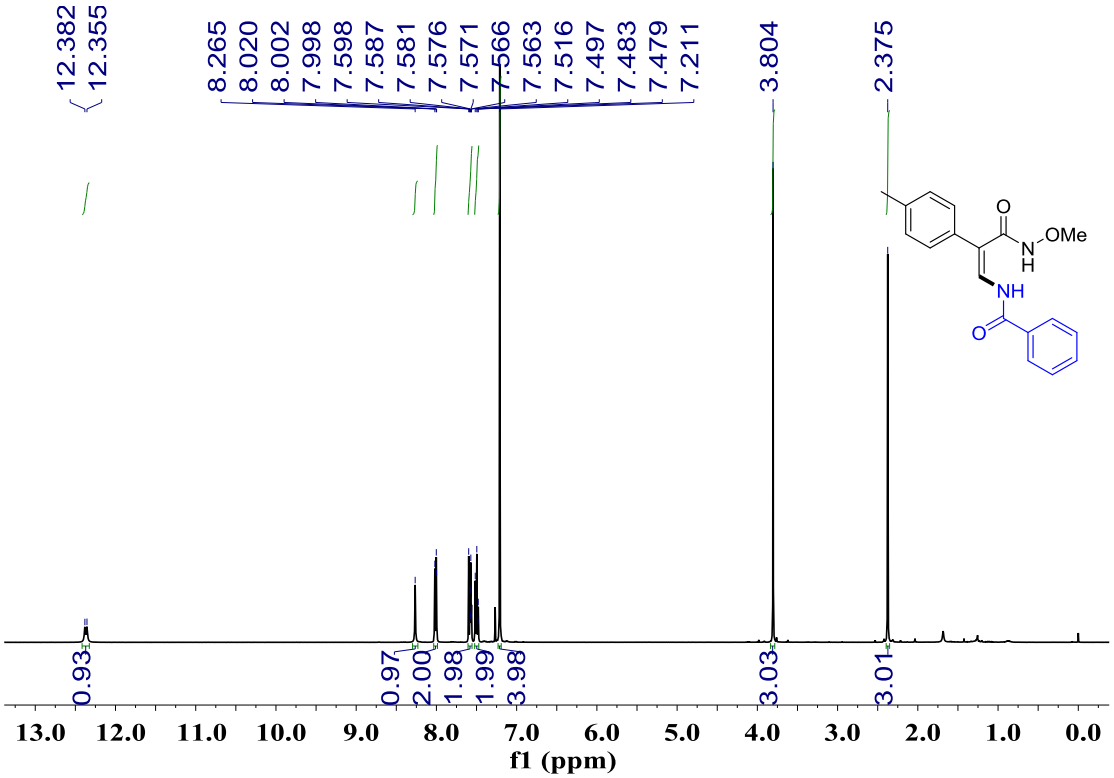
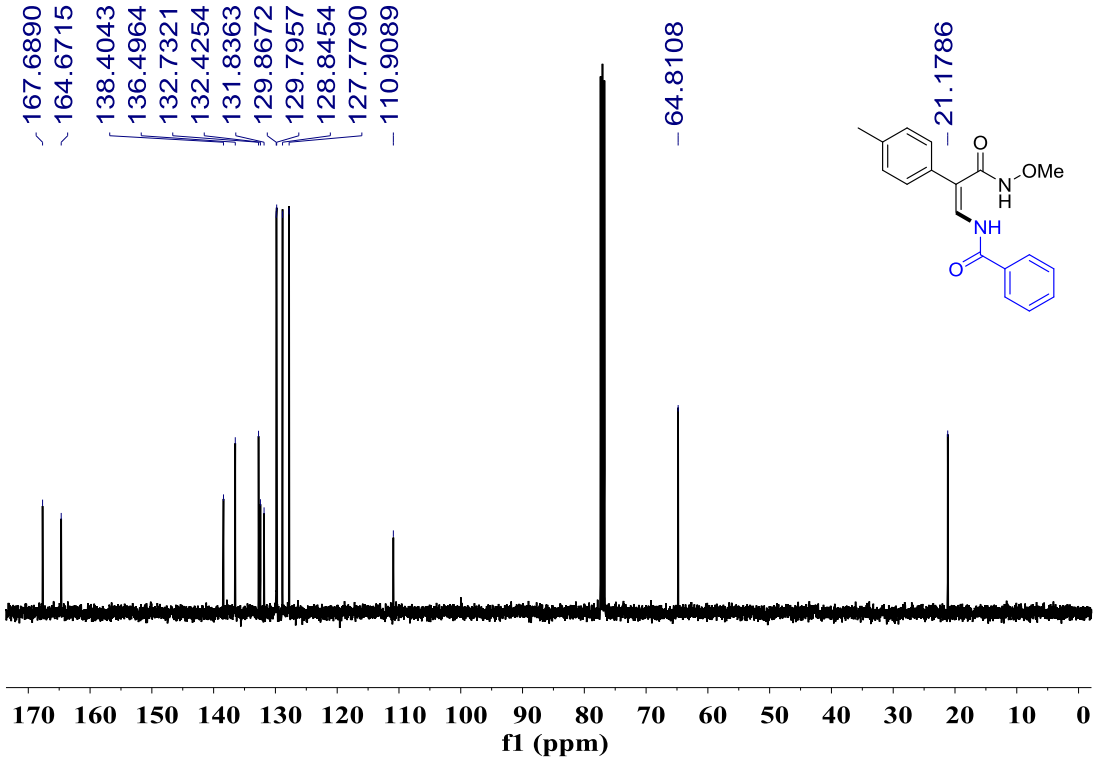
7.985
7.599
7.593
7.573
7.524
7.505
7.487
7.389
7.384
7.373
7.368
7.283
7.278
7.271
7.266
7.261
3.813
Cl
O
N
OMe
H
NH
O
0.95
0.94
2.00
2.03
2.04
2.00
2.14
2.97
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


167.2866
164.6937
137.1150
134.6353
133.3428
132.9146
132.1853
131.2747
129.4055
128.9066
127.7952
109.7647
64.8505
Cl
O
N
OMe
H
NH
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

3da


12.382
12.355
8.265
8.020
8.002
7.998
7.598
7.587
7.581
7.576
7.571
7.566
7.563
7.516
7.497
7.483
7.479
7.211
3.804
2.375
0.93
0.97
2.00
1.98
1.99
3.98
3.03
3.01
13.0 12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)
O
N
OMe
H
NH
O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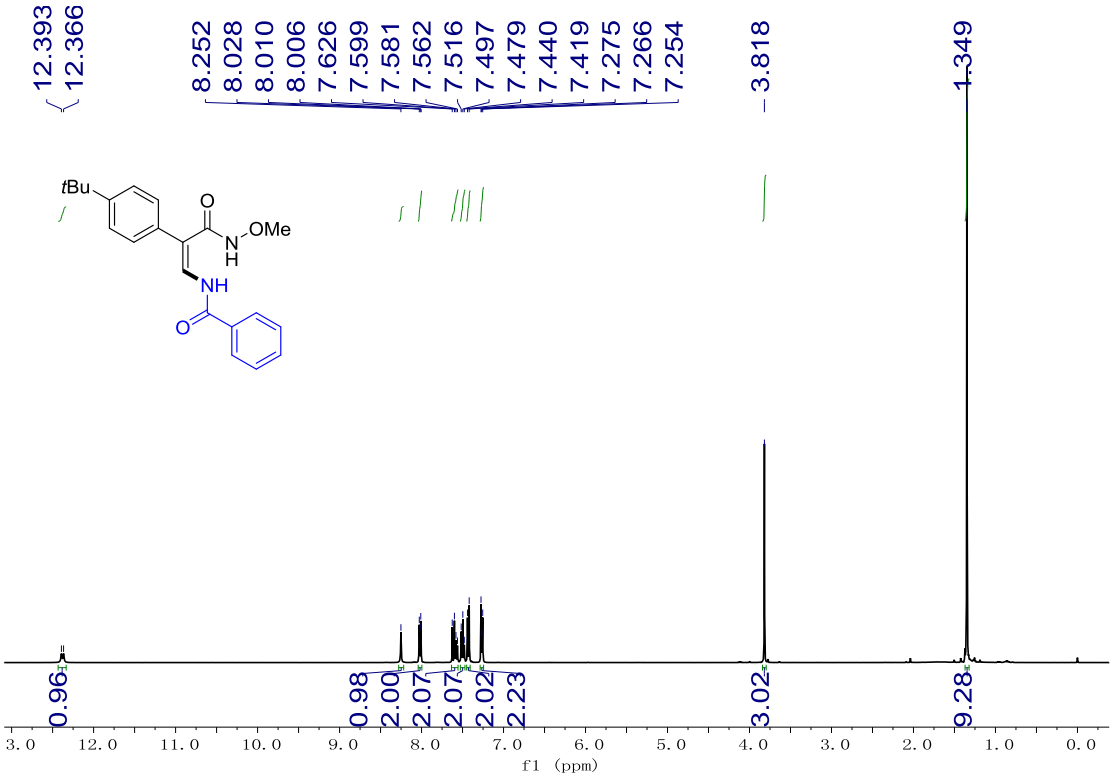
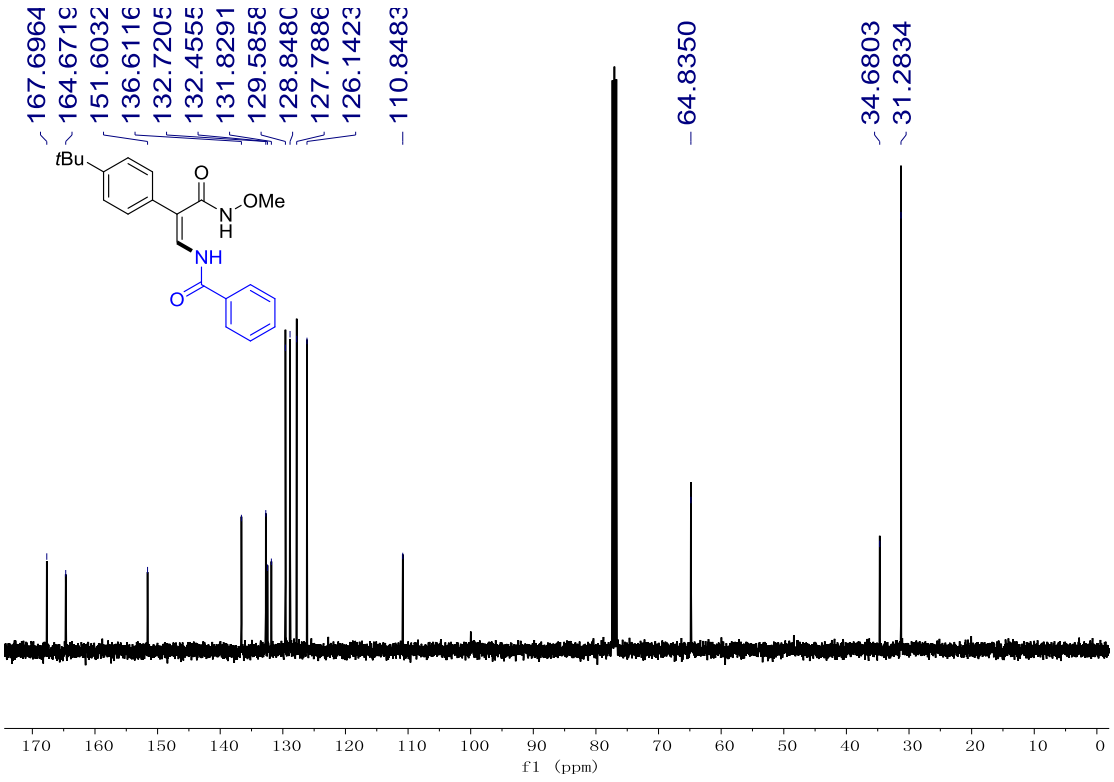
138.4043
136.4964
132.7321
132.4254
131.8363
129.8672
129.7957
128.8454
127.7790
110.9089
64.8108
21.1786
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
O
N
OMe
H
NH
O

3ea


12.393
12.366
8.252
8.028
8.010
8.006
7.626
7.599
7.581
7.562
7.516
7.497
7.479
7.440
7.419
7.275
7.266
7.254
3.818
1.349
tBu
O
N
OMe
H
NH
O
0.96
0.98
2.00
2.07
2.07
2.02
2.23
3.02
9.28
f1 (ppm)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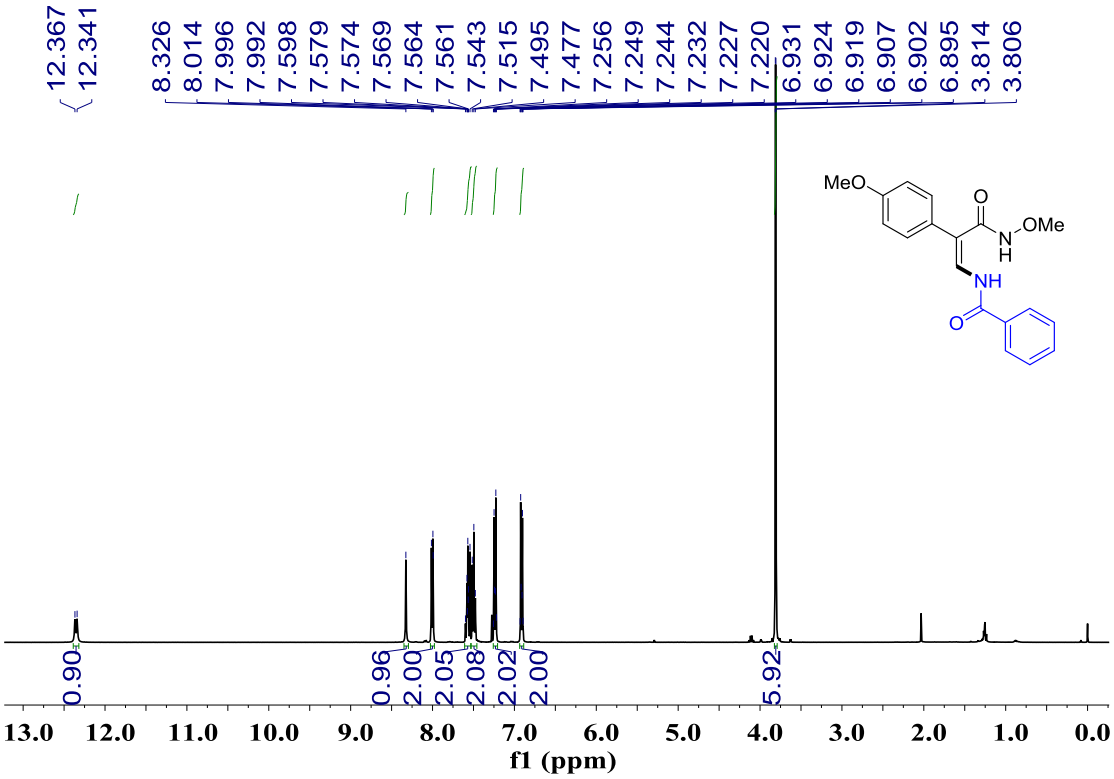
164.6719
151.6032
136.6116
132.7205
132.4555
131.8291
129.5858
128.8480
127.7886
126.1423
110.8483
64.8350
34.6803
31.2834
tBu
O
N
OMe
H
NH
O
f1 (ppm)

3fa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12.341
8.326
8.014
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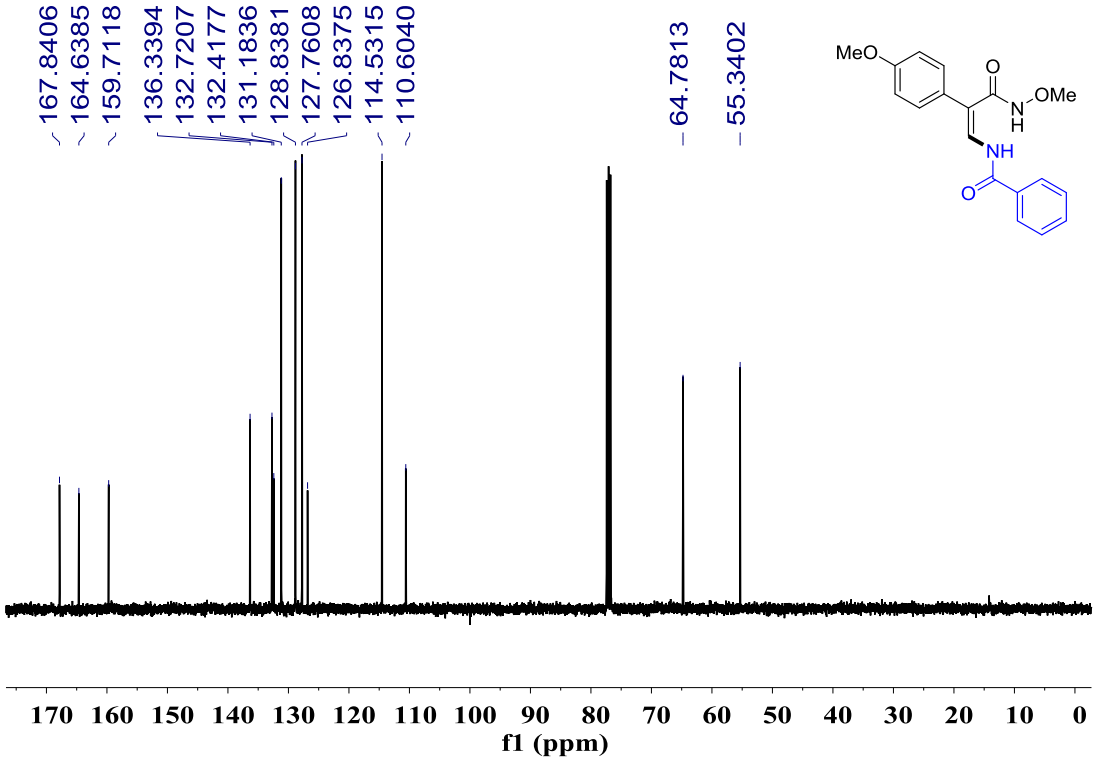
7.992
7.598
7.579
7.574
7.569
7.564
7.561
7.543
7.515
7.495
7.477
7.256
7.249
7.244
7.232
7.227
7.220
6.931
6.924
6.919
6.907
6.902
6.895
3.814
3.806
MeO
O
N
OMe
H
NH
O
0.90
0.96
2.00
2.05
2.08
2.02
2.00
5.92
13.0 12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)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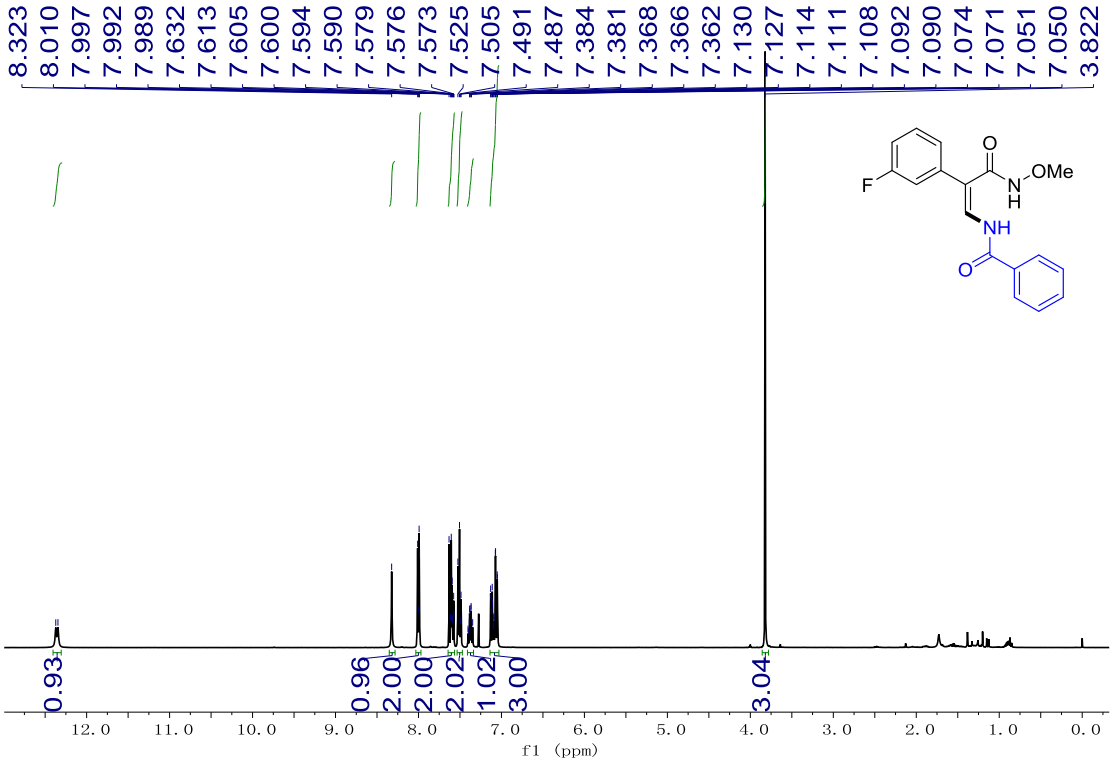
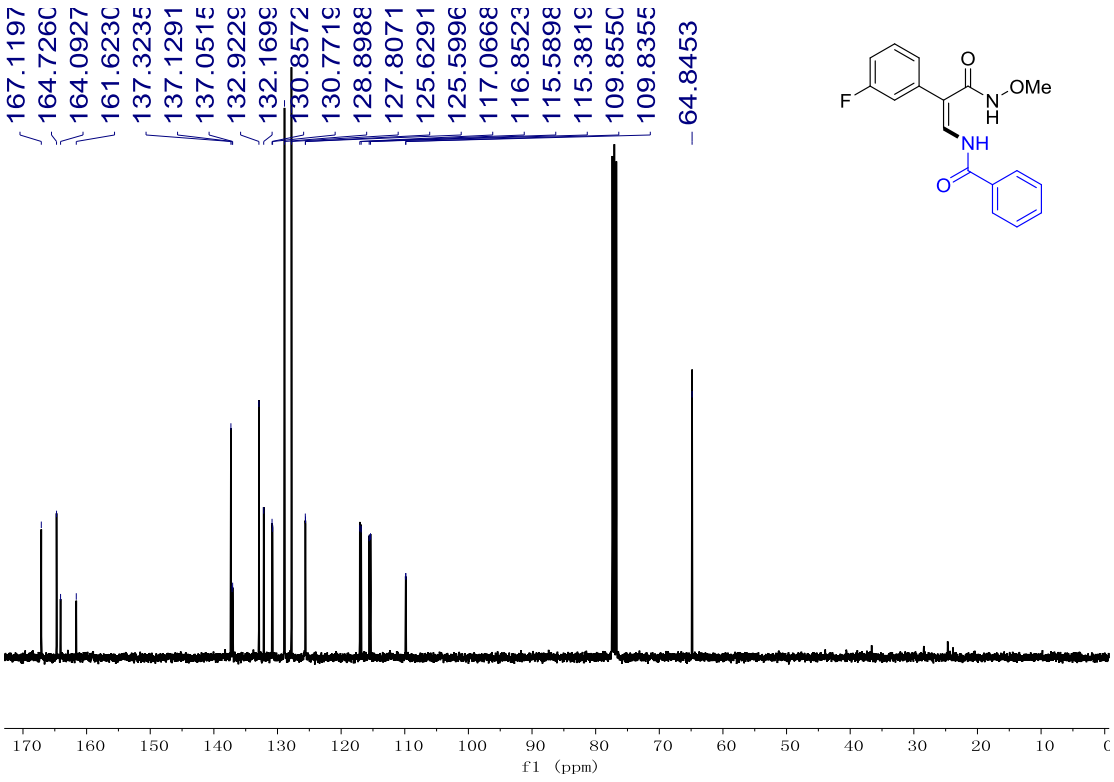
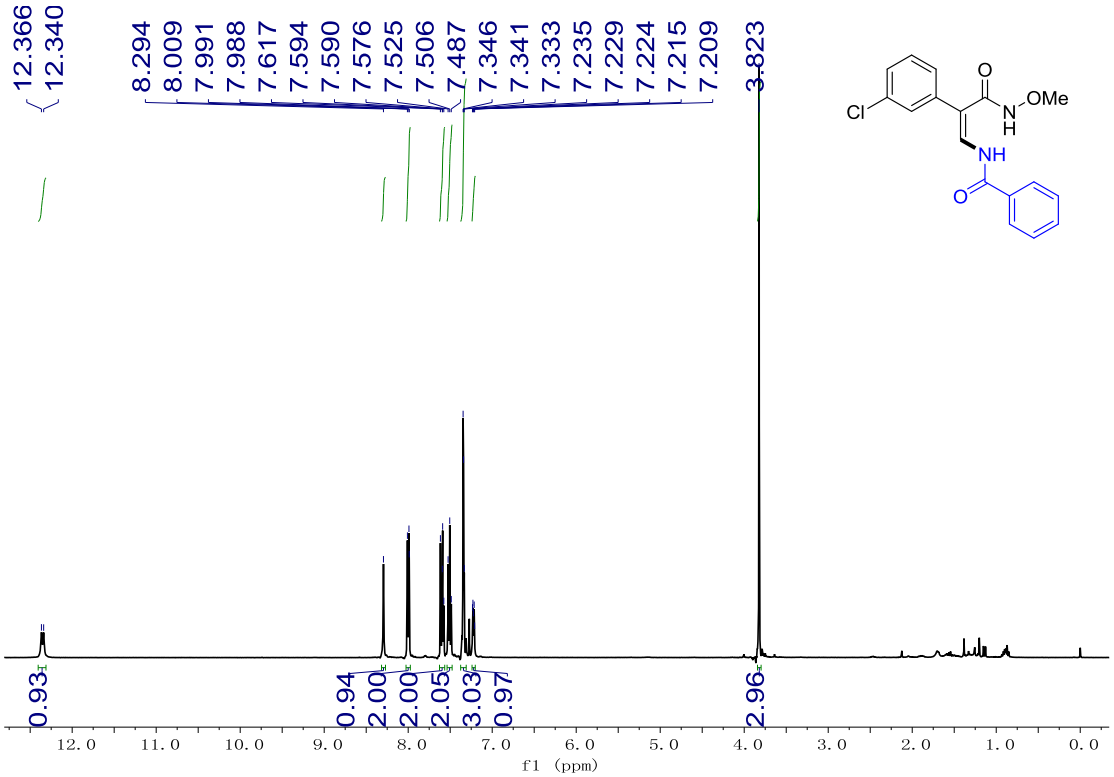
164.6385
159.7118
136.3394
132.7207
132.4177
131.1836
128.8381
127.7608
126.8375
114.5315
110.6040
64.7813
55.3402
MeO
O
N
OMe
H
NH
O
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3ga


8.323
8.010
7.997
7.992
7.989
7.632
7.613
7.605
7.600
7.594
7.590
7.579
7.576
7.573
7.525
7.505
7.491
7.487
7.384
7.381
7.368
7.366
7.362
7.130
7.127
7.114
7.111
7.108
7.092
7.090
7.074
7.071
7.051
7.050
3.822
0.93
0.96
2.00
2.00
2.02
1.02
3.00
3.04
F
O
N
OMe
H
NH
O
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


167.1197
164.7266
164.0927
161.6230
137.3235
137.1291
137.0515
132.9229
132.1699
130.8572
130.7719
128.8988
127.8071
125.6291
125.5996
117.0668
116.8523
115.5898
115.3819
109.8550
109.8355
64.8453
F
O
N
OMe
H
NH
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

3ha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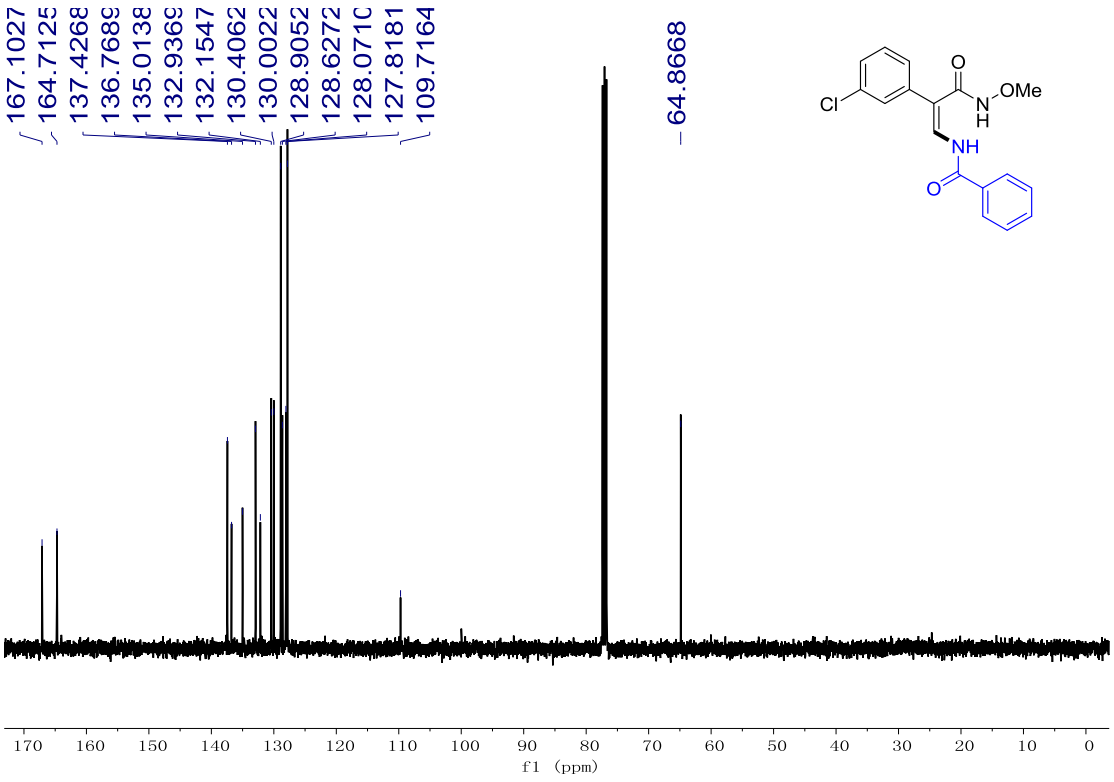
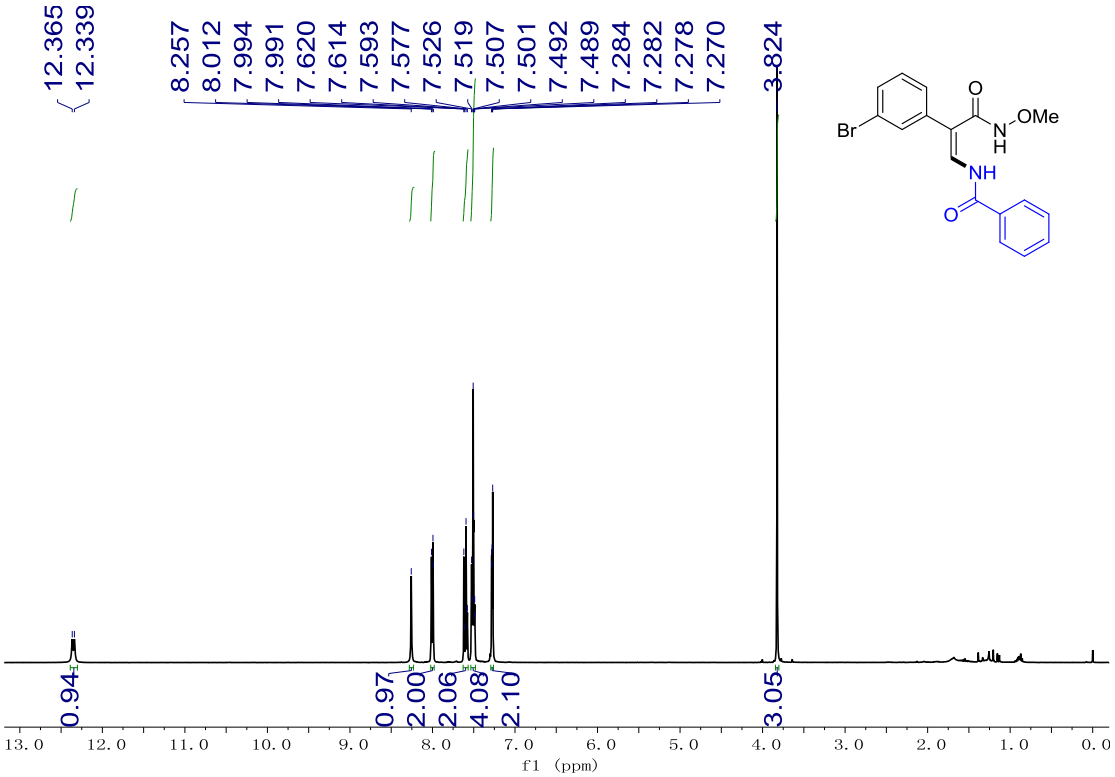
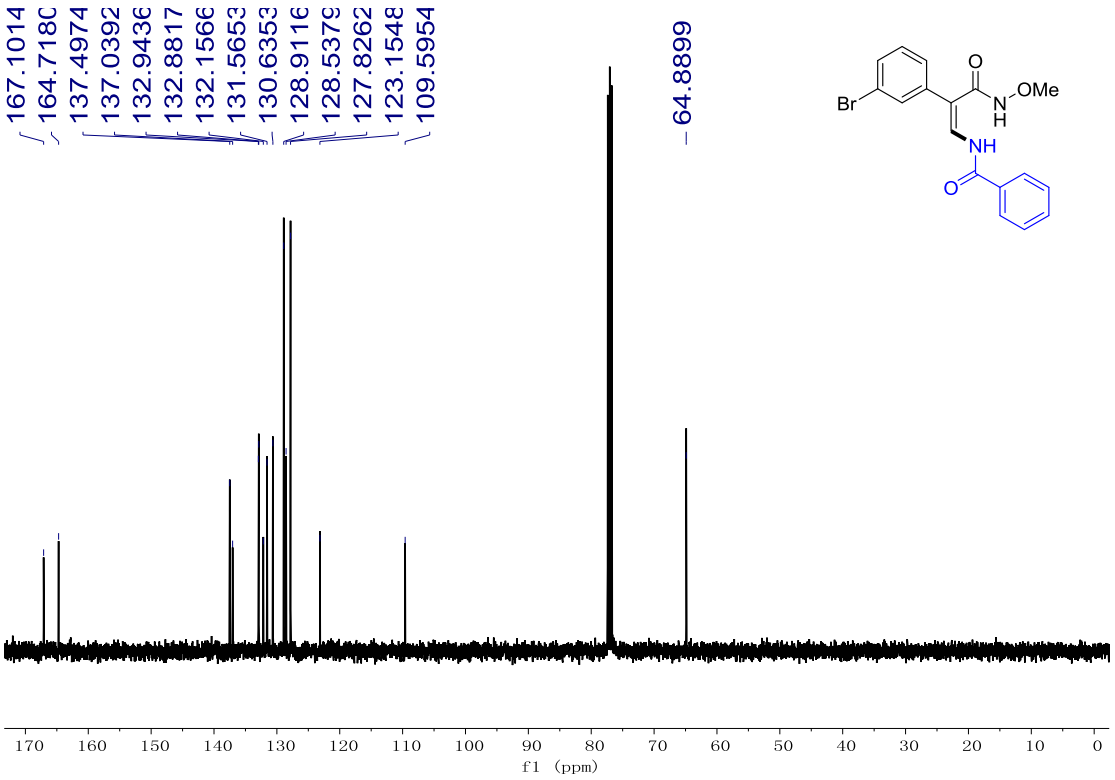
12.340
8.294
8.009
7.991
7.988
7.617
7.594
7.590
7.576
7.525
7.506
7.487
7.346
7.341
7.333
7.235
7.229
7.224
7.215
7.209
3.823
0.93
0.94
2.00
2.00
2.05
3.03
0.97
2.96
Cl
O
N
OMe
H
NH
O
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

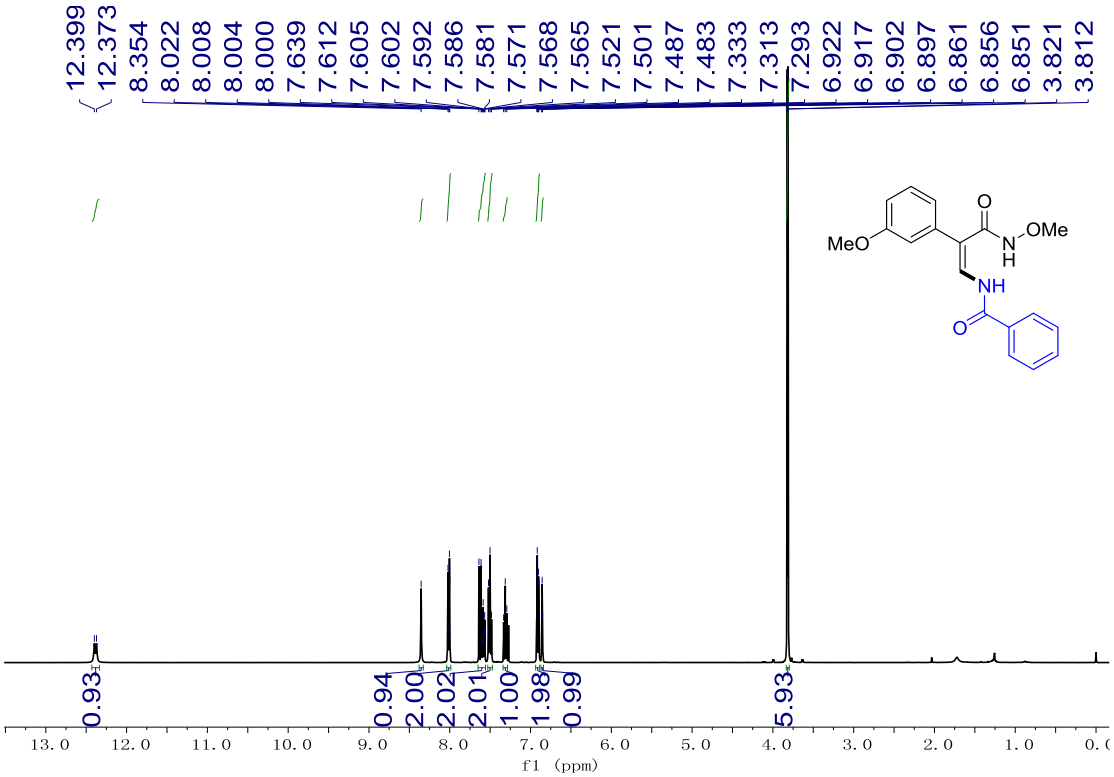

167.1027
164.7125
137.4268
136.7689
135.0138
132.9369
132.1547
130.4062
130.0022
128.9052
128.6272
128.0710
127.8181
109.7164
64.8668
Cl
O
N
OMe
H
NH
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

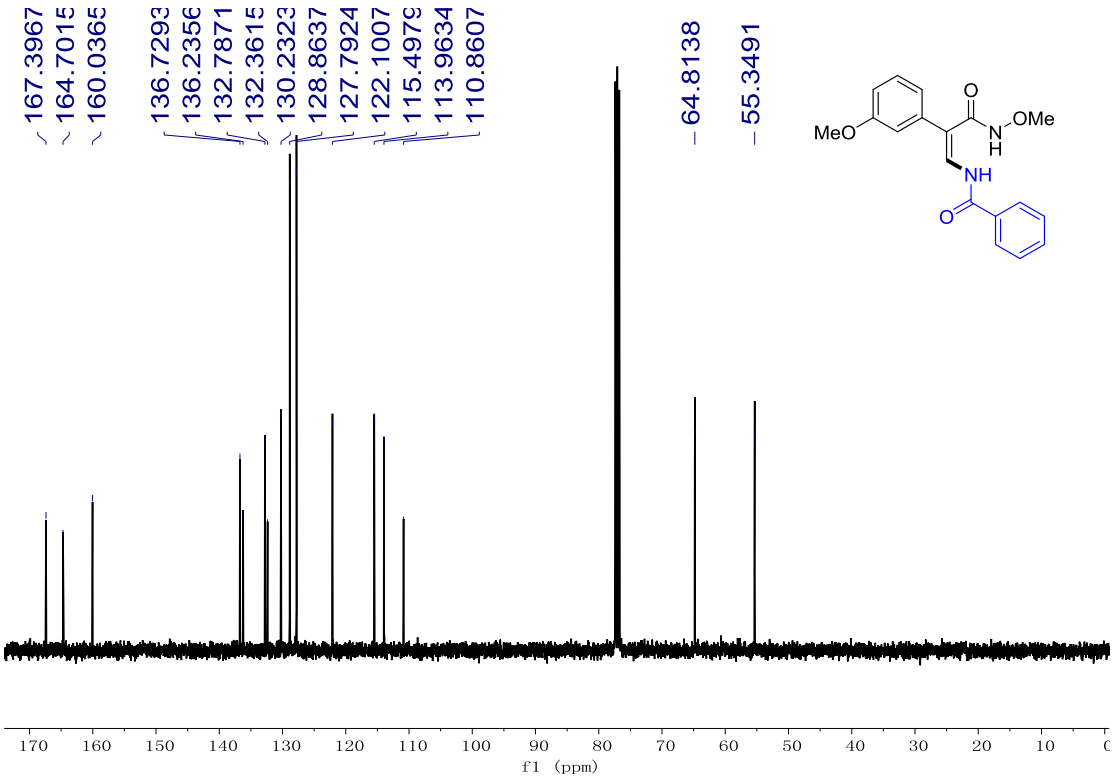
3ia


12.365
12.339
8.257
8.012
7.994
7.991
7.620
7.614
7.593
7.577
7.526
7.519
7.507
7.501
7.492
7.489
7.284
7.282
7.278
7.270
3.824
Br
O
N
OMe
H
NH
O
0.94
0.97
2.00
2.06
4.08
2.10
3.05
f1 (ppm)


167.1014
164.7180
137.4974
137.0392
132.9436
132.8817
132.1566
131.5653
130.6353
128.9116
128.5379
127.8262
123.1548
109.5954
64.8899
Br
O
N
OMe
H
NH
O
f1 (ppm)

3ja


12.399
12.373
8.354
8.022
8.008
8.004
8.000
7.639
7.612
7.605
7.602
7.592
7.586
7.581
7.571
7.568
7.565
7.521
7.501
7.487
7.483
7.333
7.313
7.293
6.922
6.917
6.902
6.897
6.861
6.856
6.851
3.821
3.812
MeO
O
N
OMe
H
NH
O
0.93
0.94
2.00
2.02
2.01
1.00
1.98
0.99
5.93
f1 (ppm)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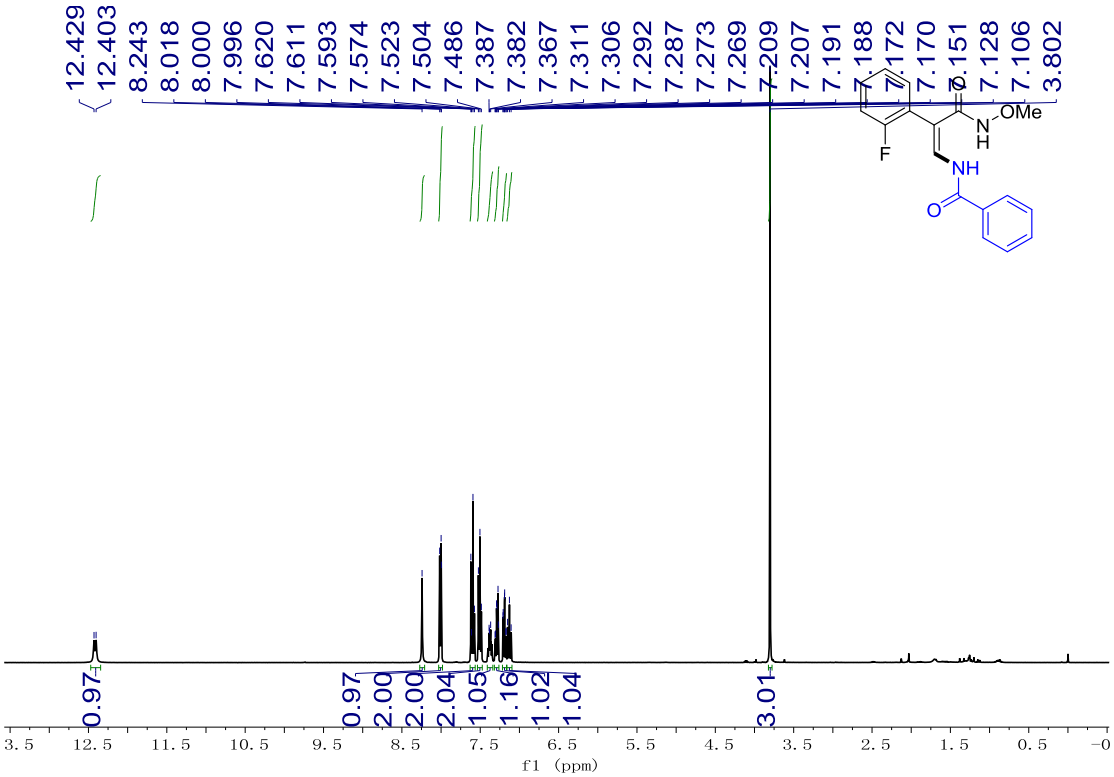
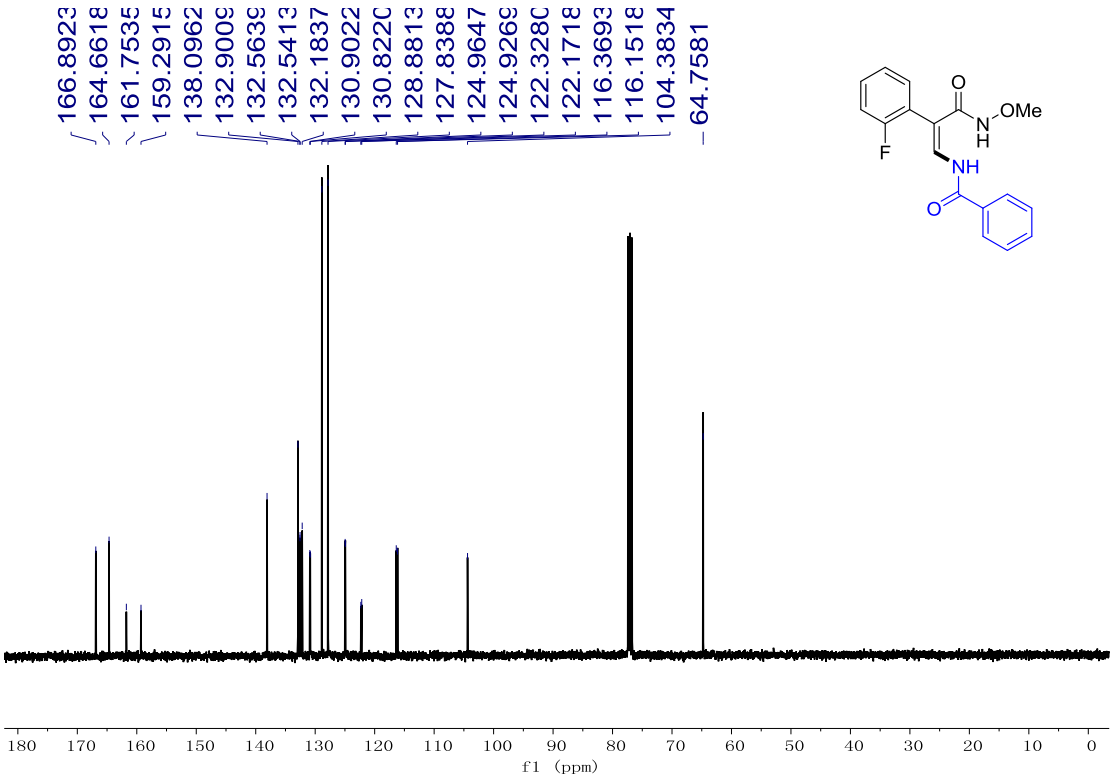
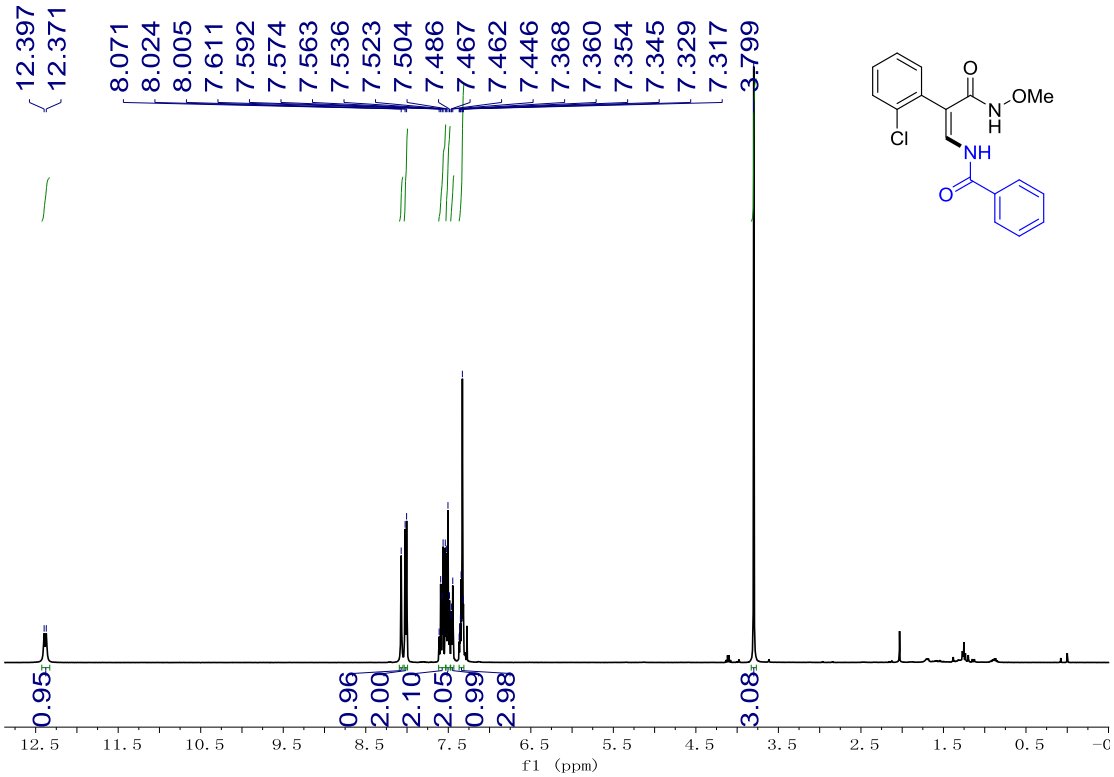
164.7015
160.0365
136.7293
136.2356
132.7871
132.3615
130.2323
128.8637
127.7924
122.1007
115.4979
113.9634
110.8607
64.8138
55.3491
MeO
O
N
OMe
H
NH
O
f1 (ppm)

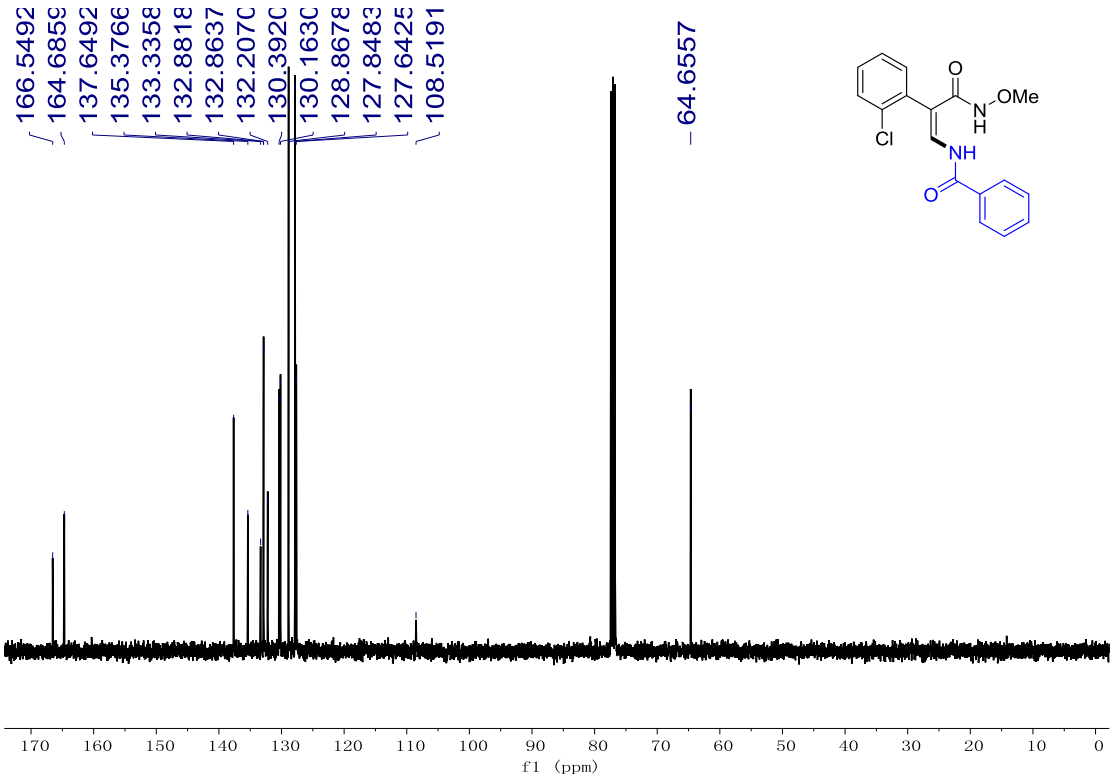
3ka


12.429
12.403
8.243
8.018
8.000
7.996
7.620
7.611
7.593
7.574
7.523
7.504
7.486
7.387
7.382
7.367
7.311
7.306
7.292
7.287
7.273
7.269
7.209
7.207
7.191
7.188
7.172
7.170
7.151
7.128
7.106
3.802
OMe
N
H
F
NH
O
0.97
2.00
2.00
2.04
1.05
1.16
1.02
1.04
3.01
f1 (ppm)


166.8923
164.6618
161.7535
159.2915
138.0962
132.9009
132.5639
132.5413
132.1837
130.9022
130.8220
128.8813
127.8388
124.9647
124.9269
122.3280
122.1718
116.3693
116.1518
104.3834
64.7581
OMe
N
H
F
NH
O
f1 (ppm)

3la


12.397
12.371
8.071
8.024
8.005
7.611
7.592
7.574
7.563
7.536
7.523
7.504
7.486
7.467
7.462
7.446
7.368
7.360
7.354
7.345
7.329
7.317
3.799
0.95
0.96
2.00
2.10
2.05
0.99
2.98
3.08
f1 (ppm)
Cl
NH
O
N
H
OMe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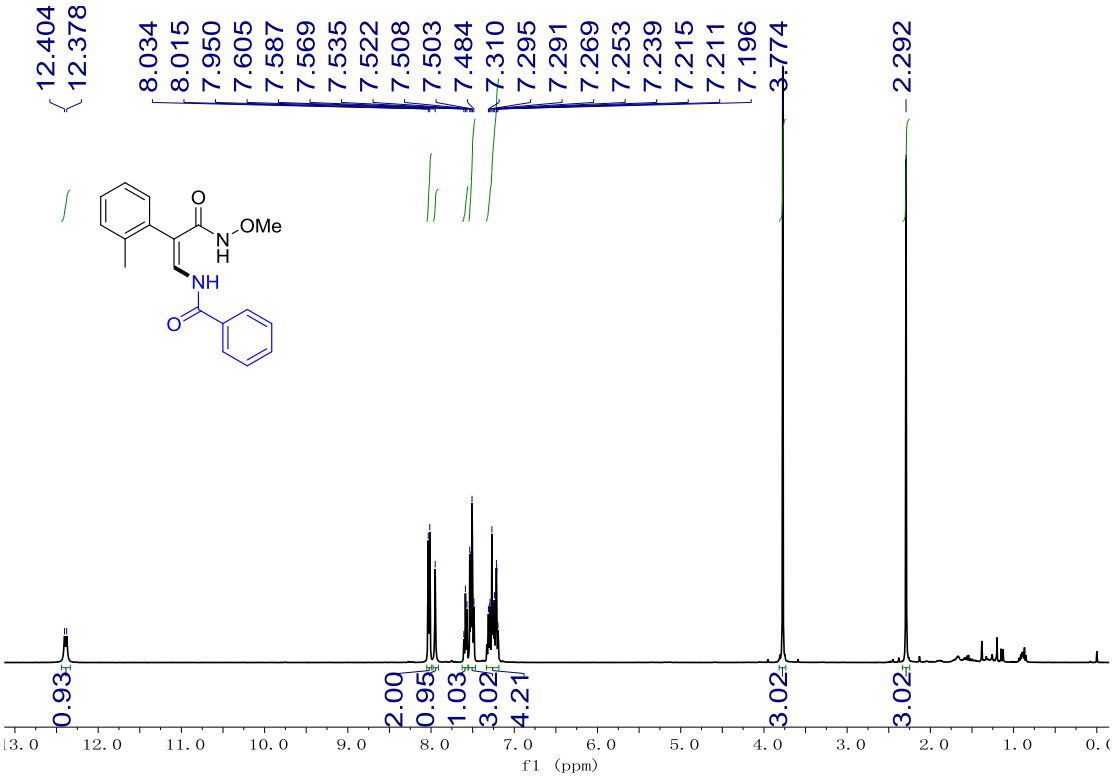
164.6859
137.6492
135.3766
133.3358
132.8818
132.8637
132.2070
130.3920
130.1630
128.8678
127.8483
127.6425
108.5191
64.6557
f1 (ppm)
Cl
NH
O
N
H
OMe

3ma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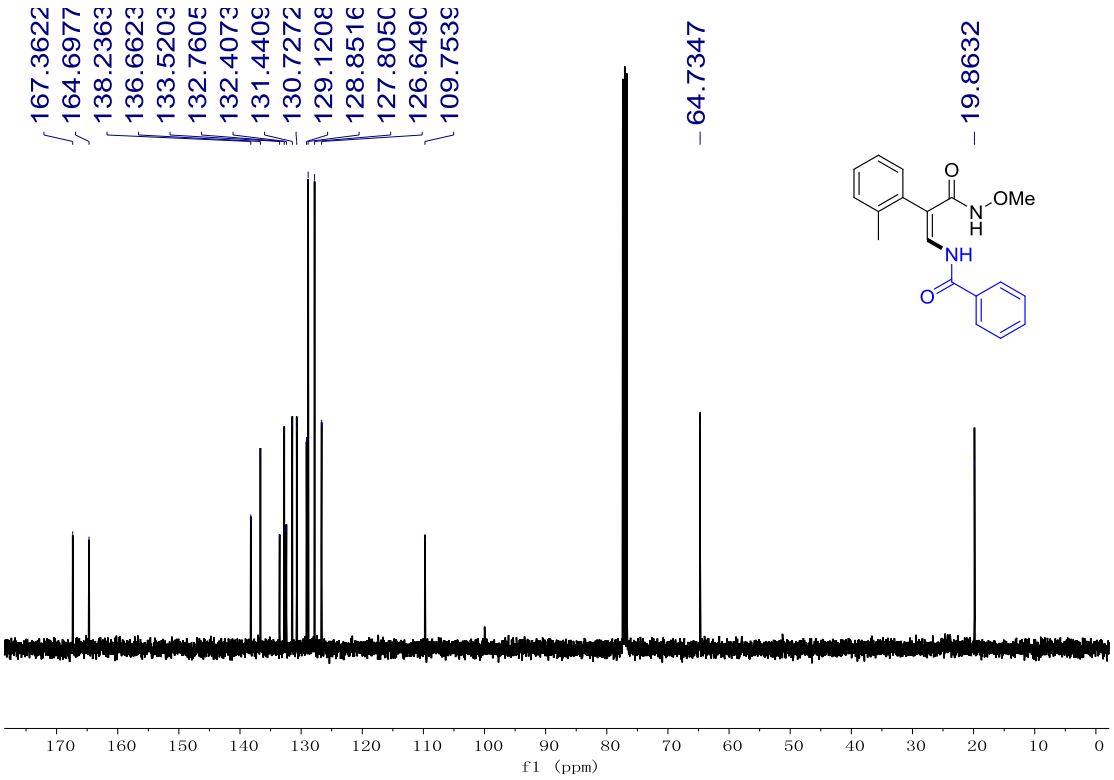
12.378
8.034
8.015
7.950
7.605
7.587
7.569
7.535
7.522
7.508
7.503
7.484
7.310
7.295
7.291
7.269
7.253
7.239
7.215
7.211
7.196
3.774
2.292
O
N
H
OMe
NH
O
0.93
2.00
0.95
1.03
3.02
4.21
3.02
3.02
f1 (ppm)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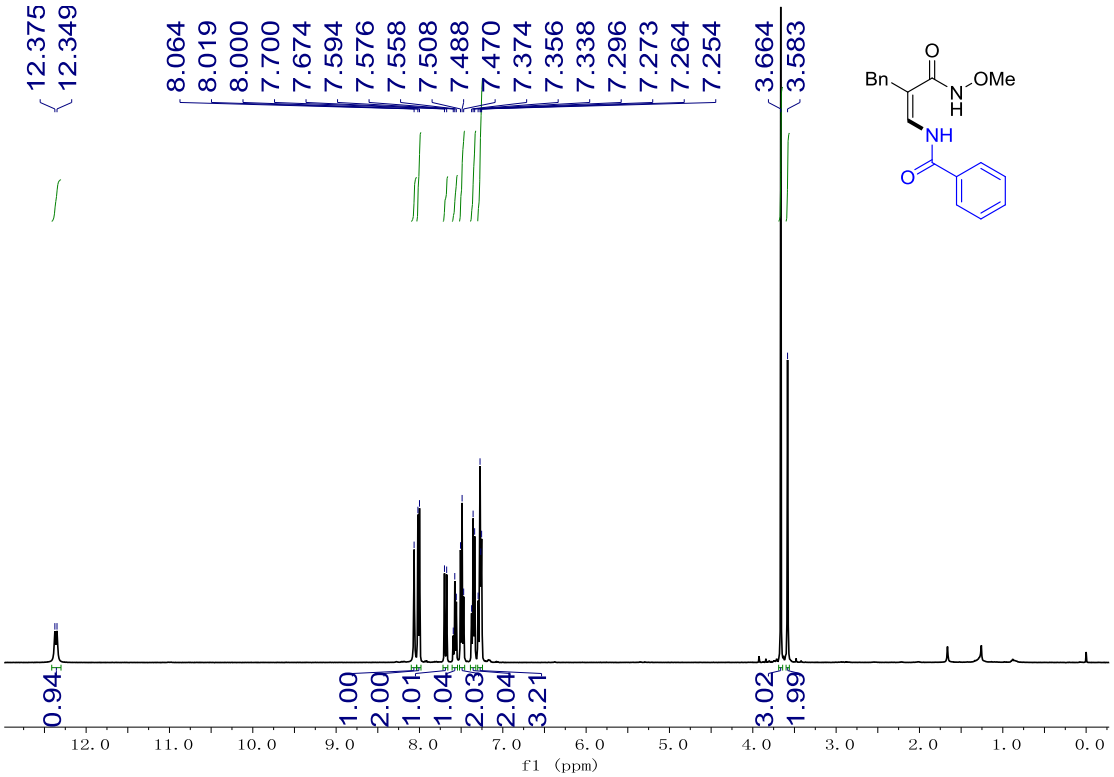
164.6977
138.2363
136.6623
133.5203
132.7605
132.4073
131.4409
130.7272
129.1208
128.8516
127.8050
126.6490
109.7539
64.7347
19.8632
O
N
H
OMe
NH
O
f1 (ppm)

3na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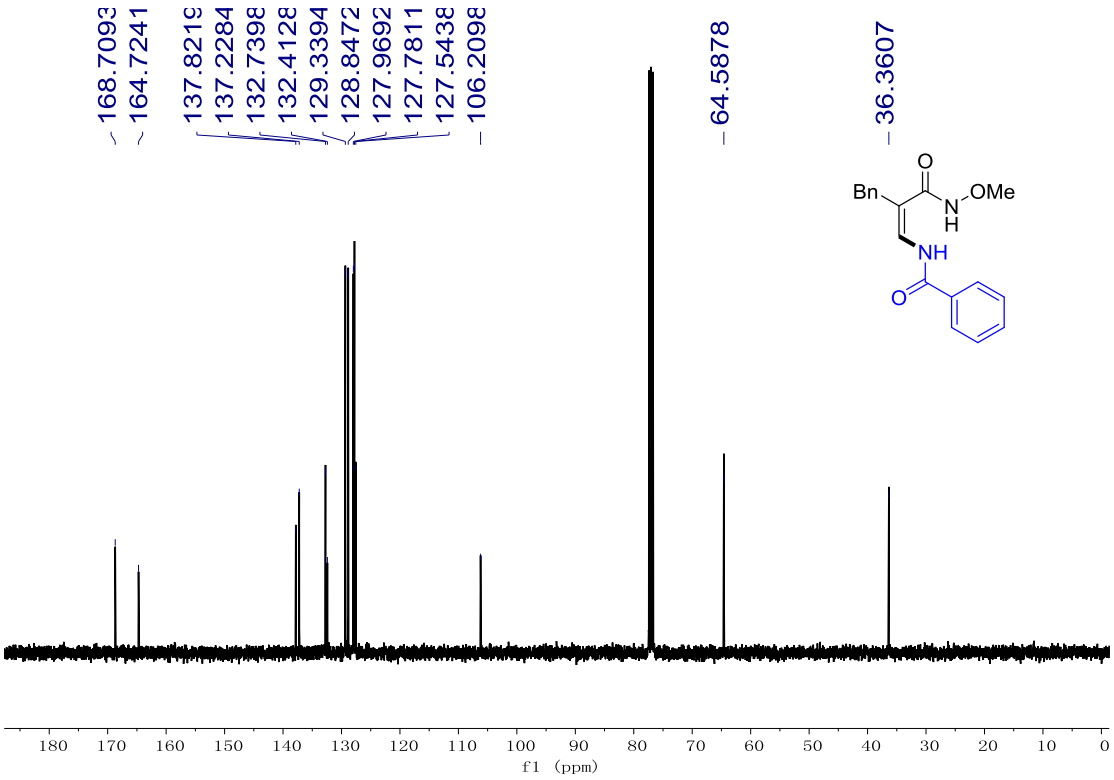
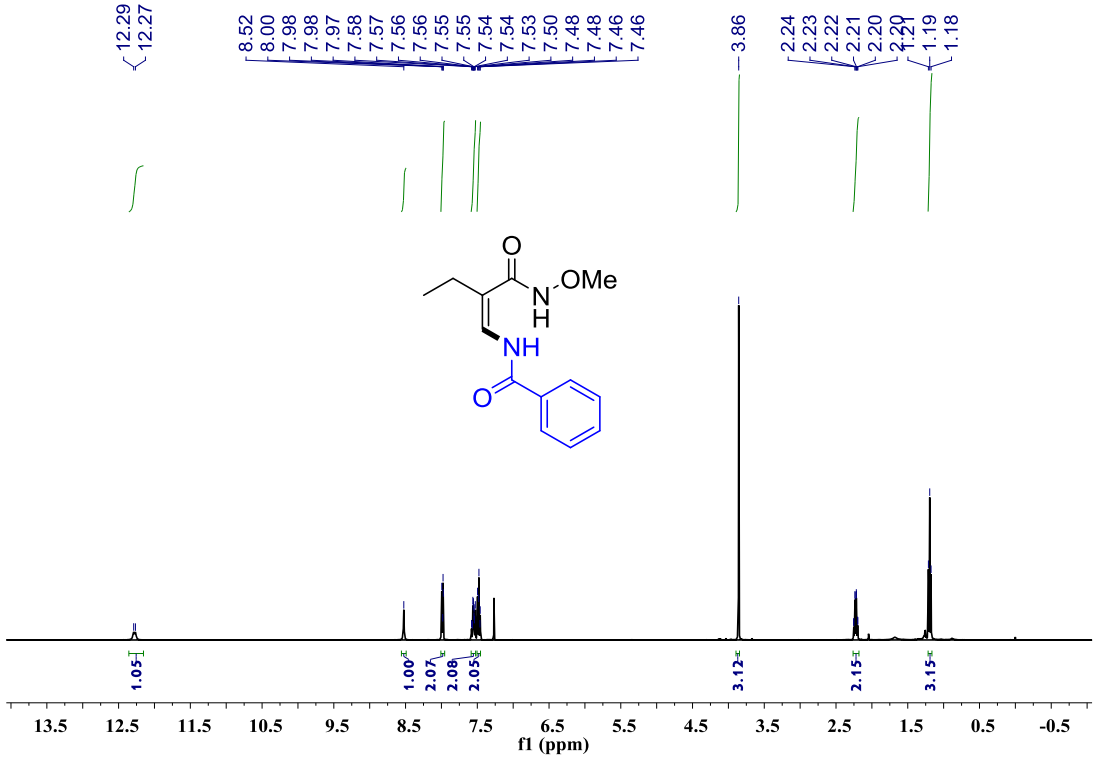
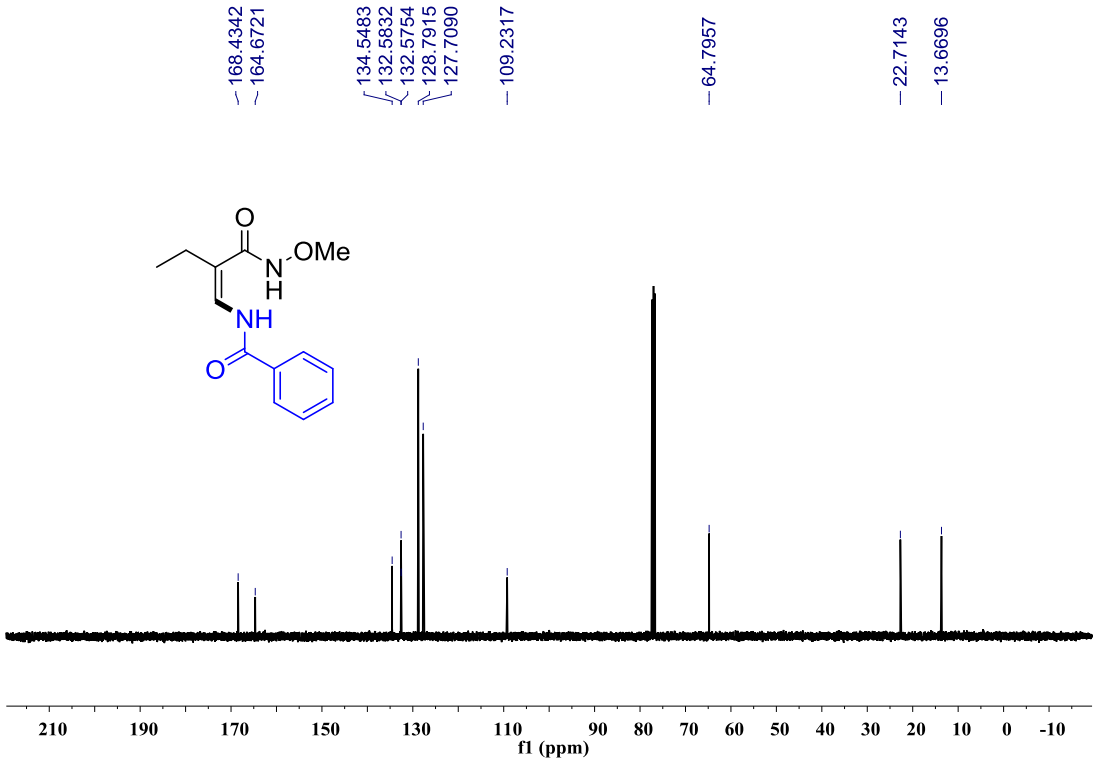
8.000
7.700
7.674
7.594
7.576
7.558
7.508
7.488
7.470
7.374
7.356
7.338
7.296
7.273
7.264
7.254
3.664
3.583
0.94
1.00
2.00
1.01
1.04
2.03
2.04
3.21
3.02
1.99
f1 (ppm)
Bn
OMe
NH
O


168.7093
164.7241
137.8219
137.2284
132.7398
132.4128
129.3394
128.8472
127.9692
127.7811
127.5438
106.2098
64.5878
36.3607
f1 (ppm)
Bn
OMe
NH
O

3oa


12.29
12.27
8.52
8.00
7.98
7.98
7.97
7.58
7.57
7.56
7.56
7.55
7.55
7.54
7.54
7.53
7.50
7.48
7.48
7.46
7.46
3.86
2.24
2.23
2.22
2.21
2.20
1.21
1.19
1.18
O
N
H
OMe
NH
O
1.05
1.00
2.07
2.08
2.05
3.12
2.15
3.15
13.5
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)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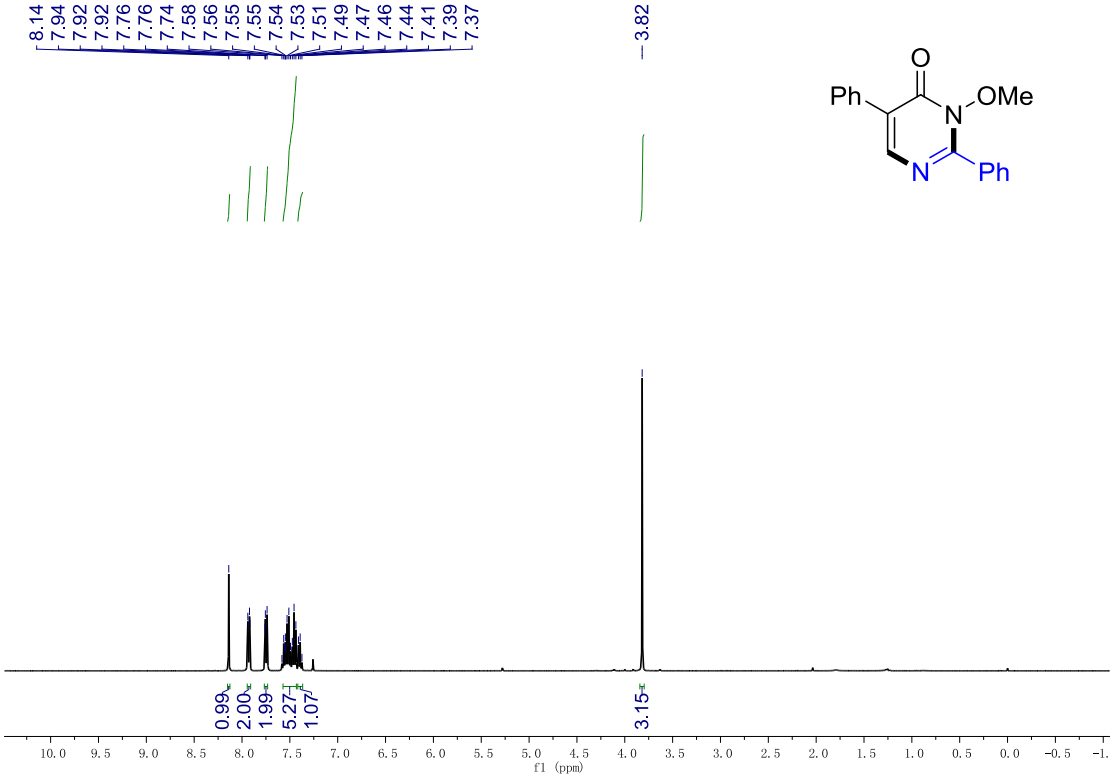
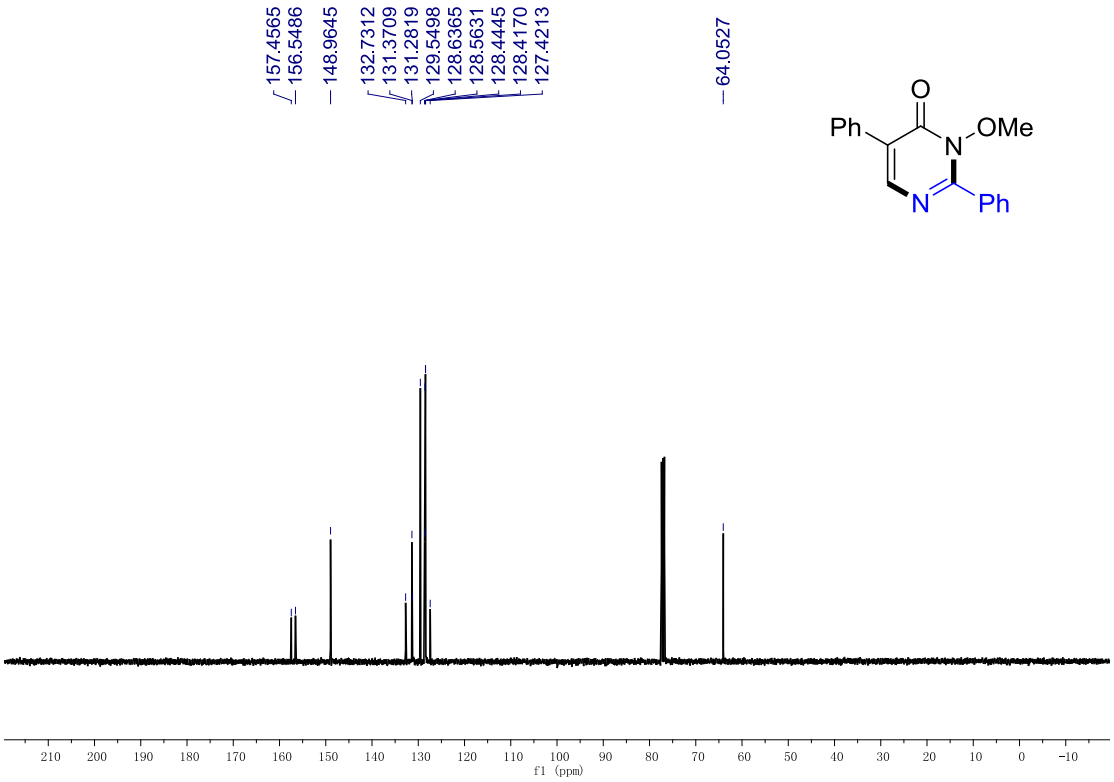
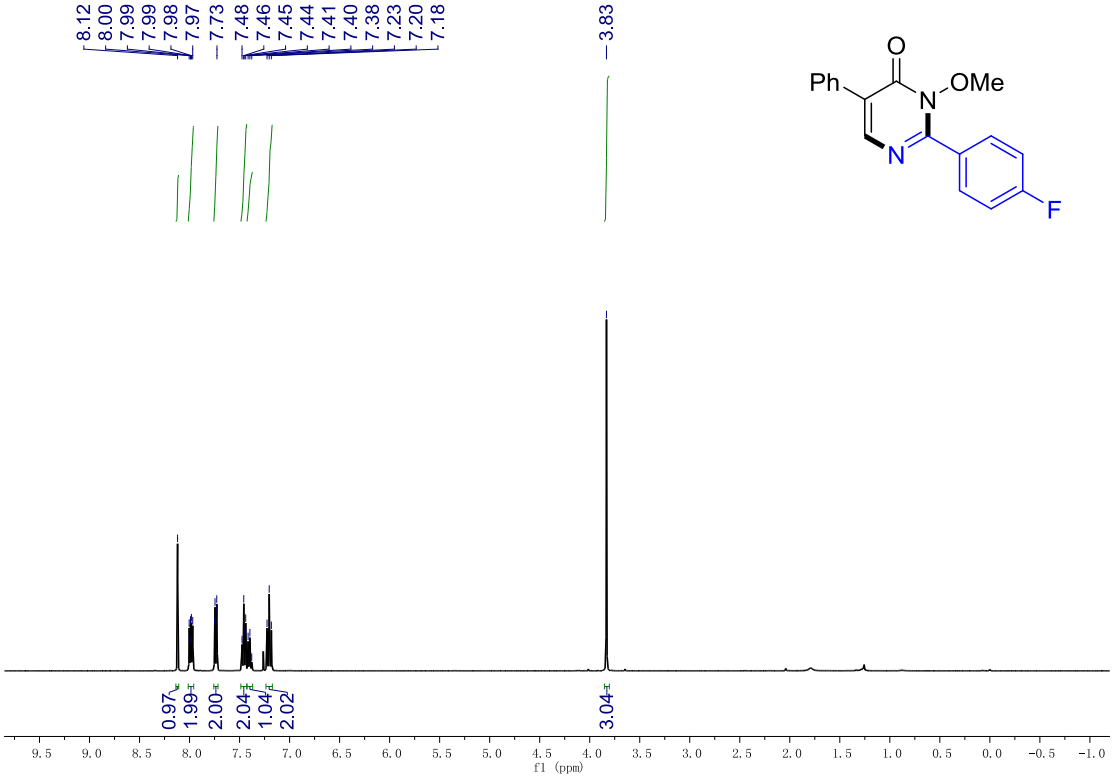
134.5483
132.5832
132.5754
128.7915
127.7090
109.2317
64.7957
22.7143
13.6696
O
N
H
OMe
NH
O
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

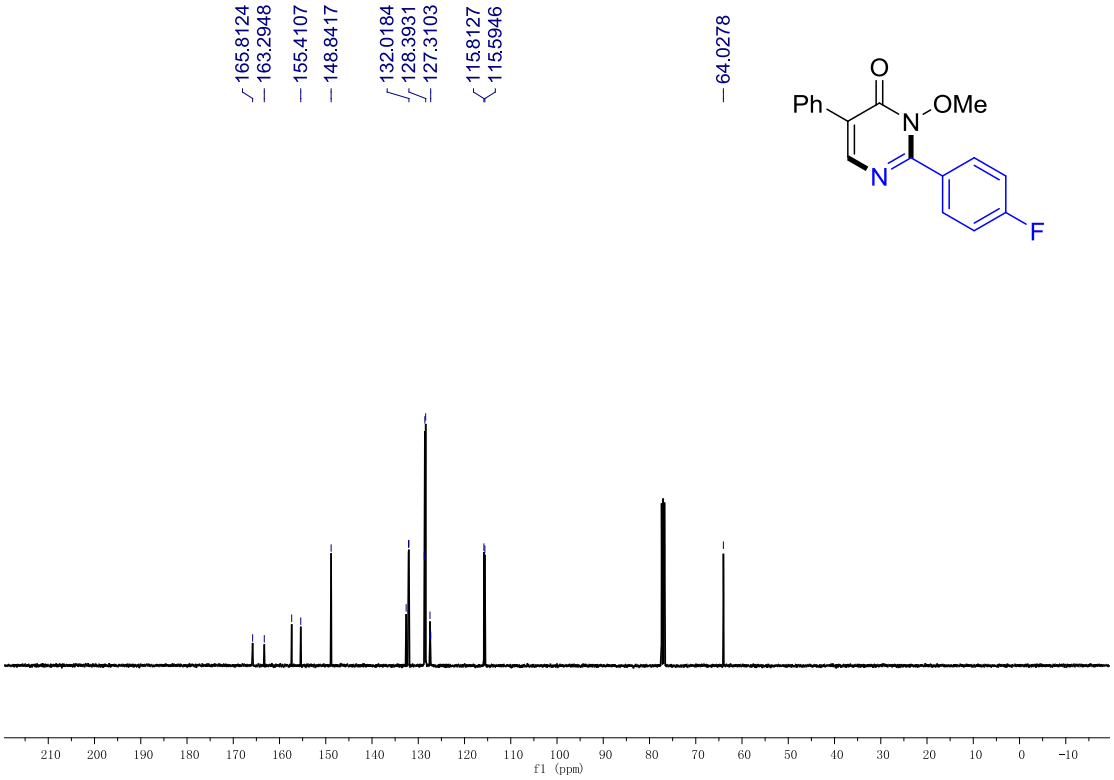
4aa


8.14
7.94
7.92
7.92
7.76
7.76
7.74
7.58
7.56
7.55
7.55
7.54
7.53
7.51
7.49
7.47
7.46
7.44
7.41
7.39
7.37
3.82
Ph
O
N
OMe
N
Ph
0.99
2.00
1.99
5.27
1.07
3.15
f1 (ppm)

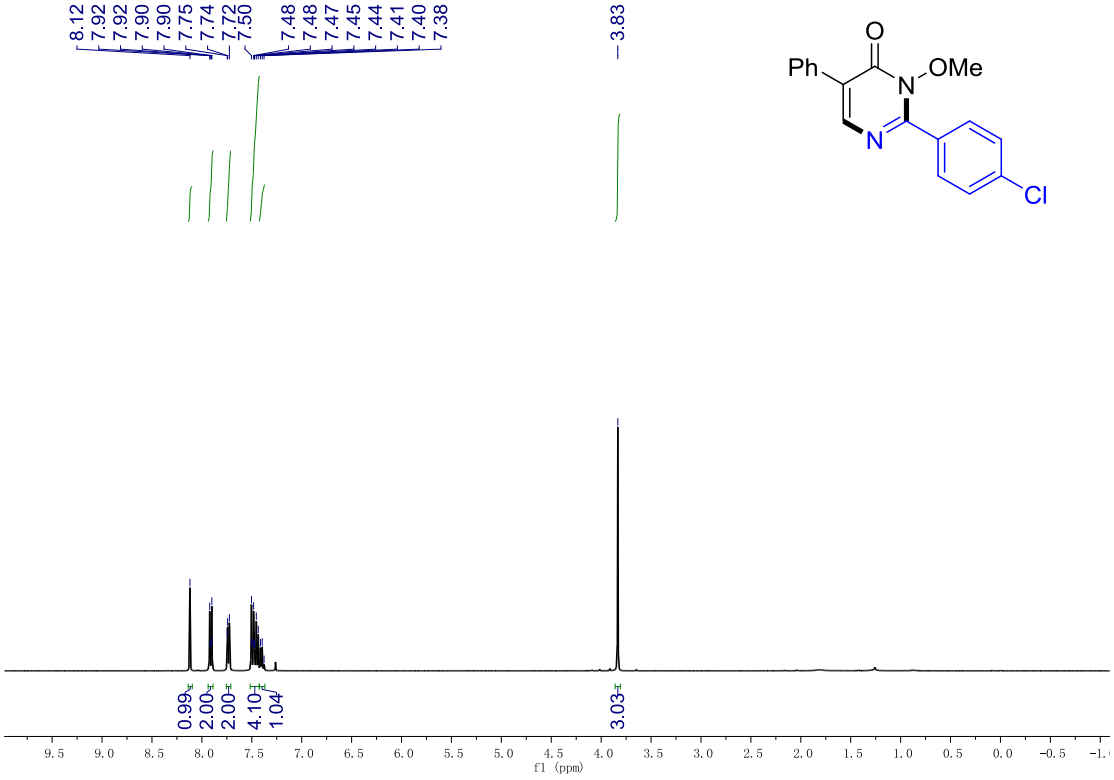

157.4565
156.5486
148.9645
132.7312
131.3709
131.2819
129.5498
128.6365
128.5631
128.4445
128.4170
127.4213
64.0527
Ph
O
N
OMe
N
Ph
f1 (ppm)

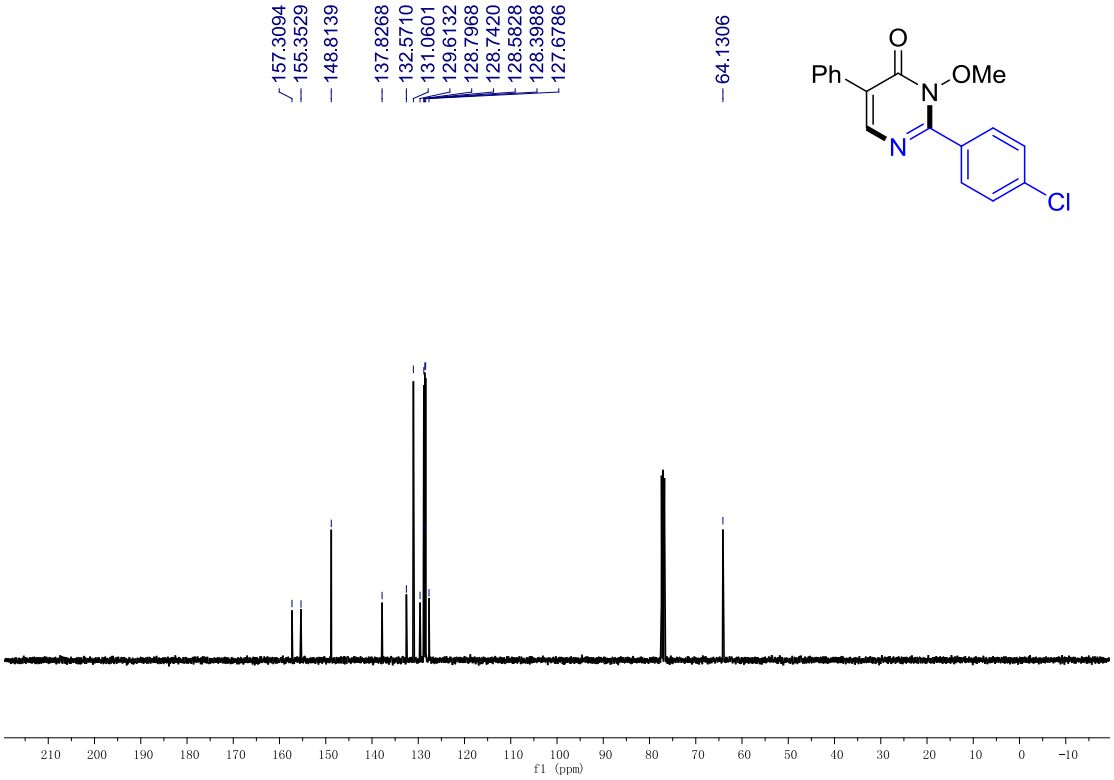
4ab


8.12
8.00
7.99
7.99
7.98
7.97
7.73
7.48
7.46
7.45
7.44
7.41
7.40
7.38
7.23
7.20
7.18
3.83
Ph
O
N
OMe
N
F
0.97
1.99
2.00
2.04
1.04
2.02
3.04
f1 (ppm)


165.8124
163.2948
155.4107
148.8417
132.0184
128.3931
127.3103
115.8127
115.5946
64.0278
Ph
O
N
OMe
N
F
f1 (ppm)

4ac


8.12
7.92
7.92
7.90
7.90
7.75
7.74
7.72
7.50
7.48
7.48
7.47
7.45
7.44
7.41
7.40
7.38
3.83
Ph
O
N
OMe
N
Cl
0.99
2.00
2.00
4.10
1.04
3.03
f1 (ppm)


157.3094
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132.5710
131.0601
129.6132
128.7968
128.7420
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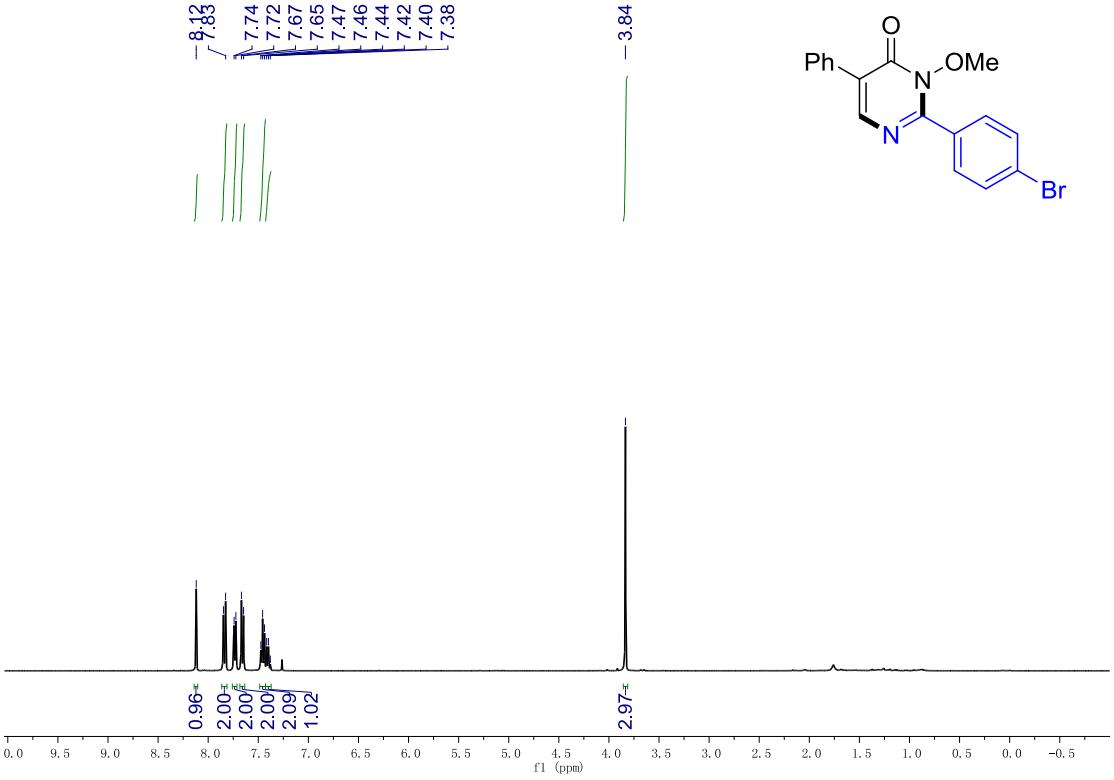
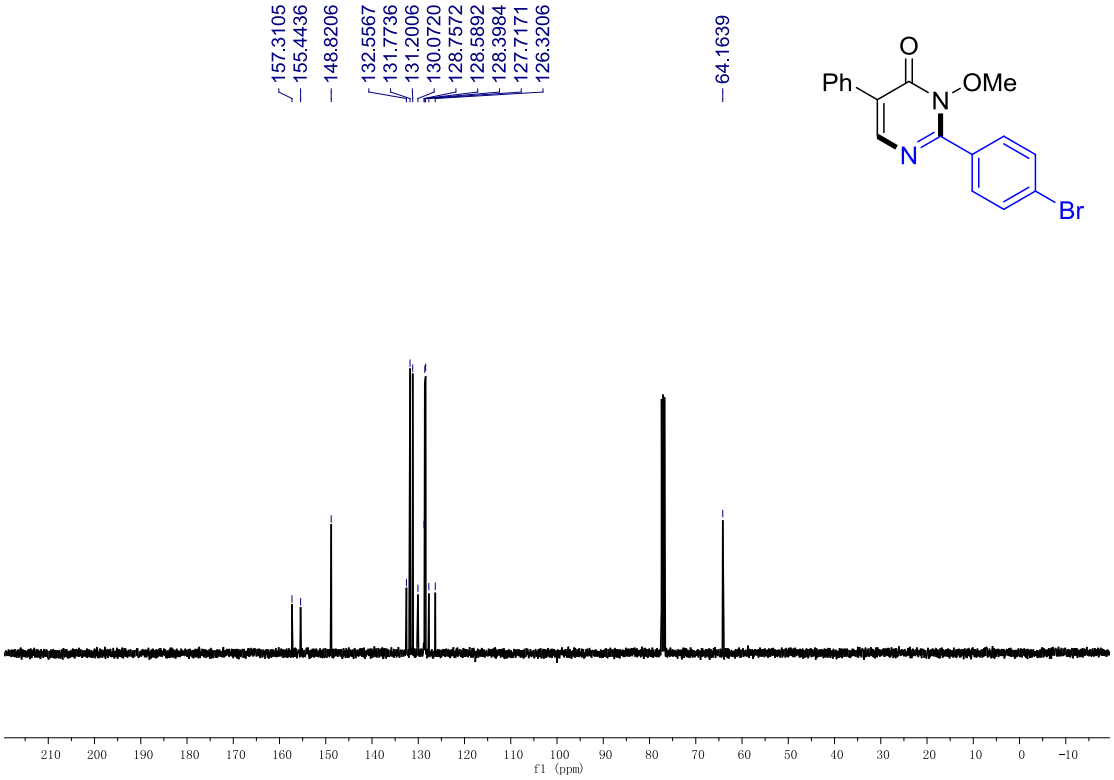
128.3988
127.6786
64.1306
Ph
O
N
OMe
N
Cl
f1 (ppm)

4ad


8.12
7.83
7.74
7.72
7.67
7.65
7.47
7.46
7.44
7.42
7.40
7.38
3.84
Ph
O
N
OMe
N
Br
0.96
2.00
2.00
2.00
2.09
1.02
2.97
f1 (ppm)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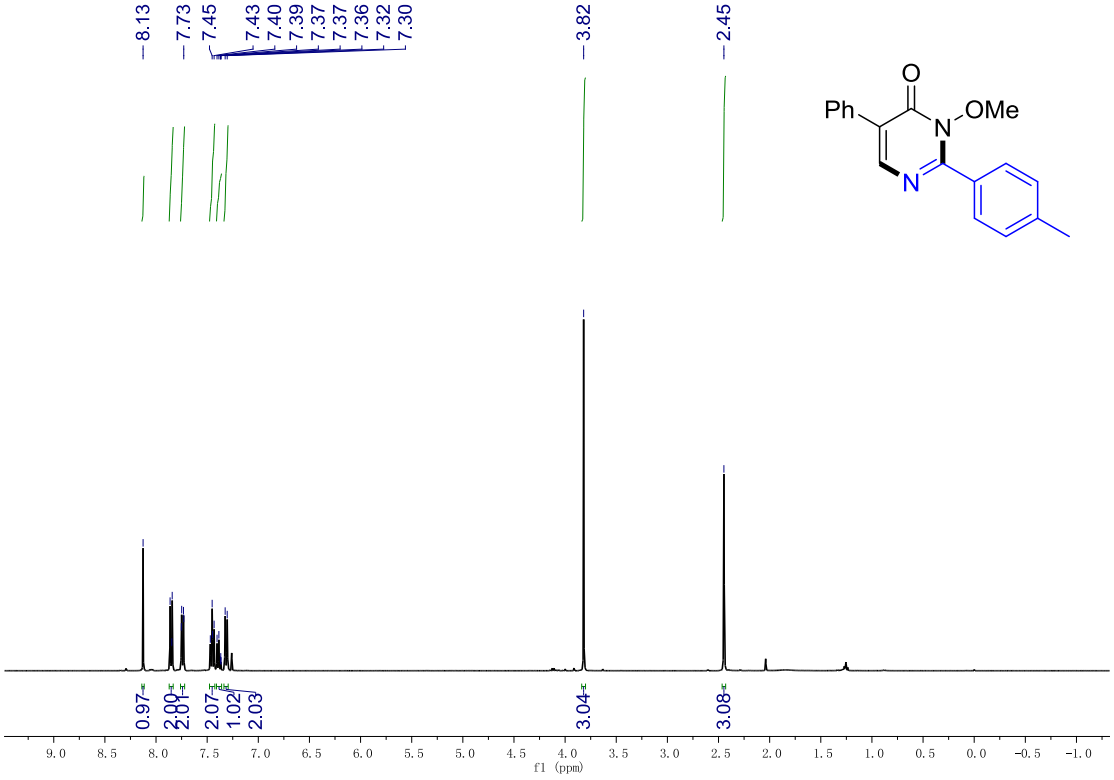
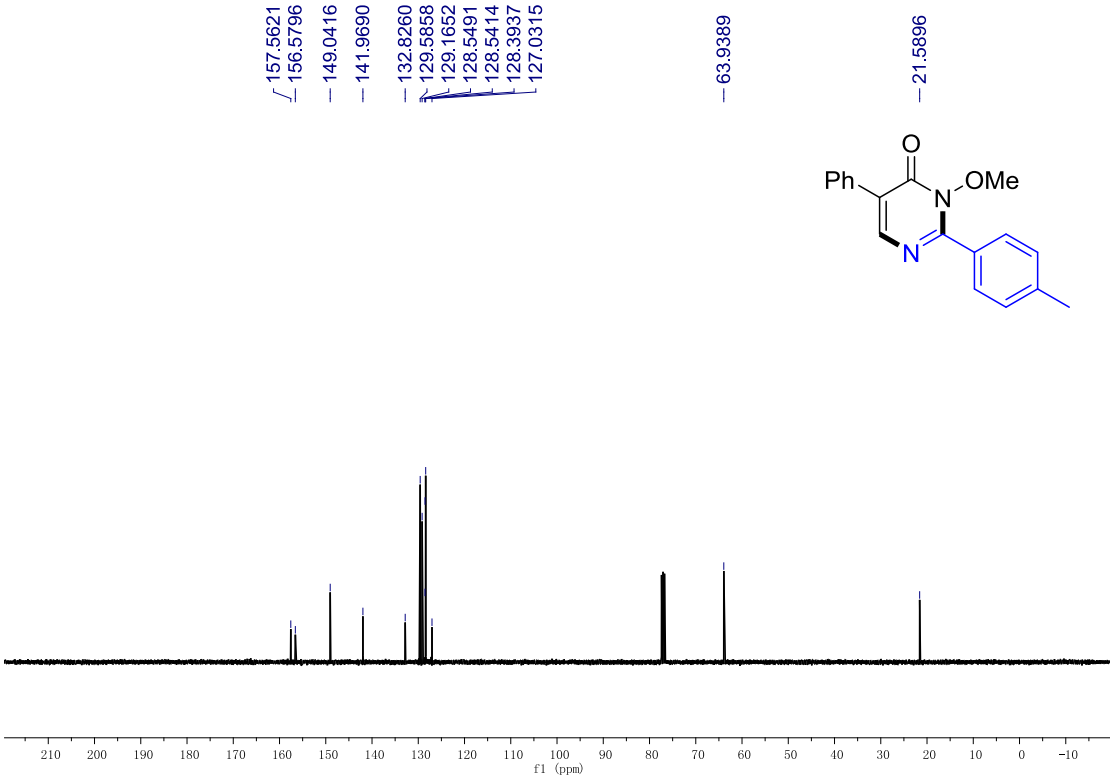
155.4436
148.8206
132.5567
131.7736
131.2006
130.0720
128.7572
128.5892
128.3984
127.7171
126.3206
64.1639
Ph
O
N
OMe
N
Br
f1 (ppm)

4ae


8.13
7.73
7.45
7.43
7.40
7.39
7.37
7.37
7.36
7.32
7.30
3.82
2.45
Ph
O
N
OMe
N
0.97
2.00
2.01
2.07
1.02
2.03
3.04
3.08
f1 (ppm)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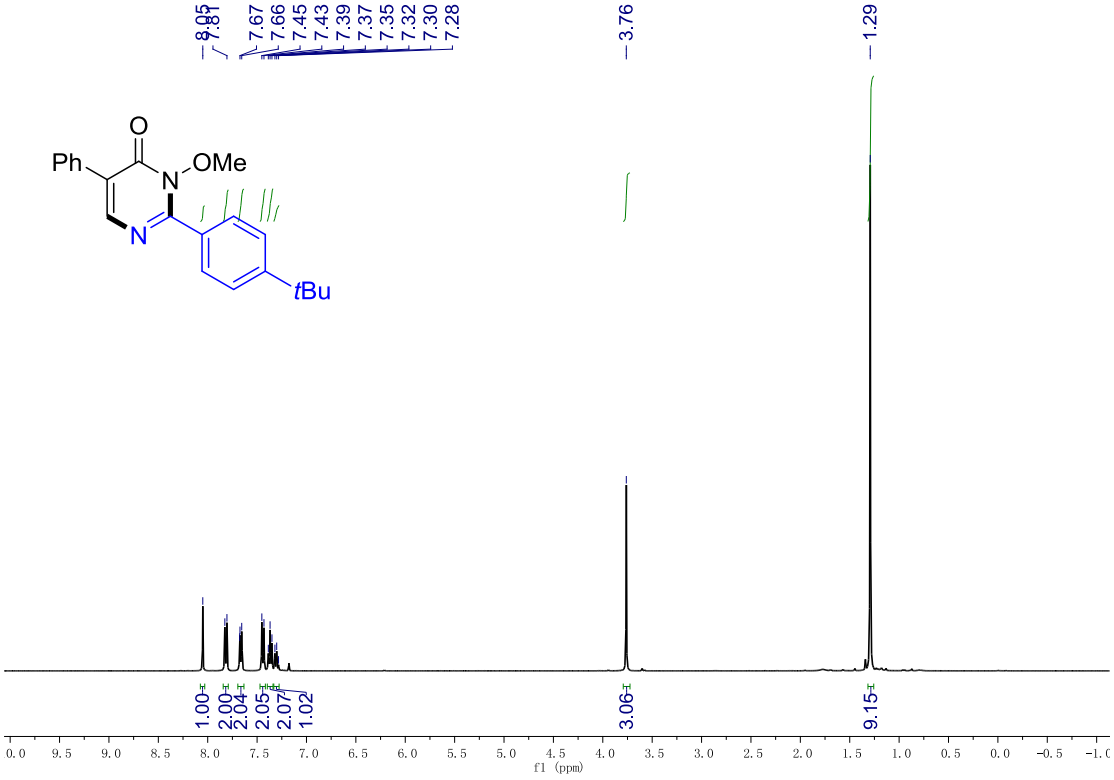
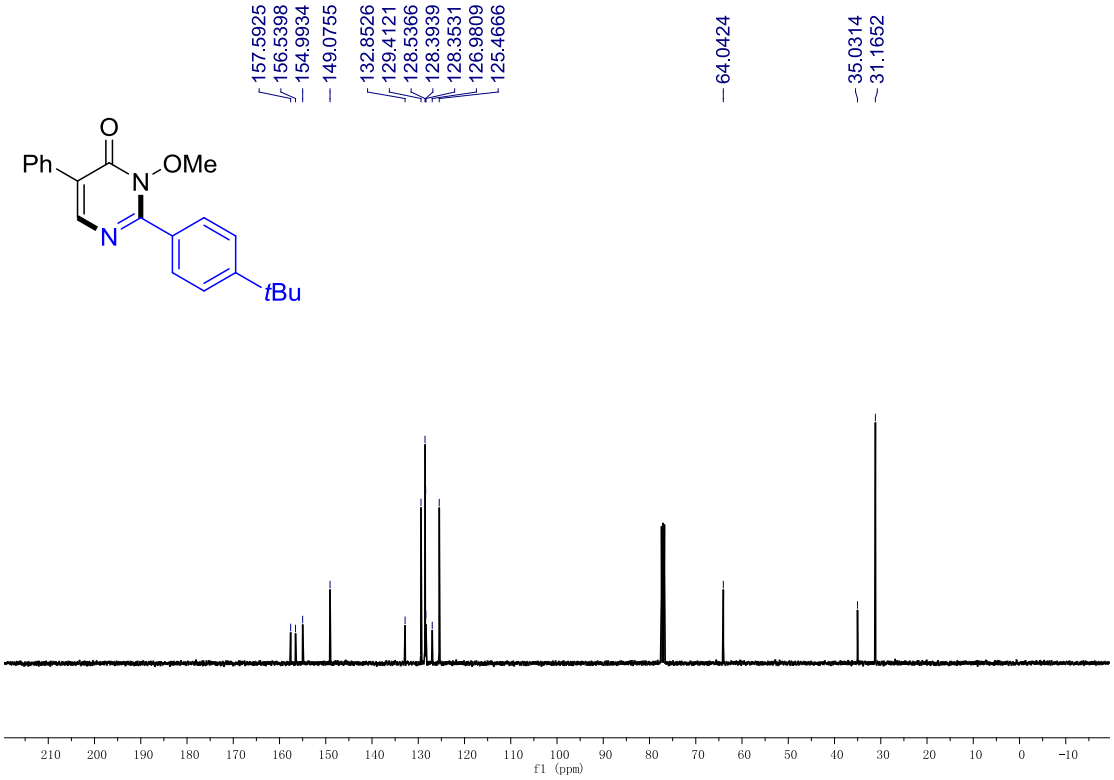
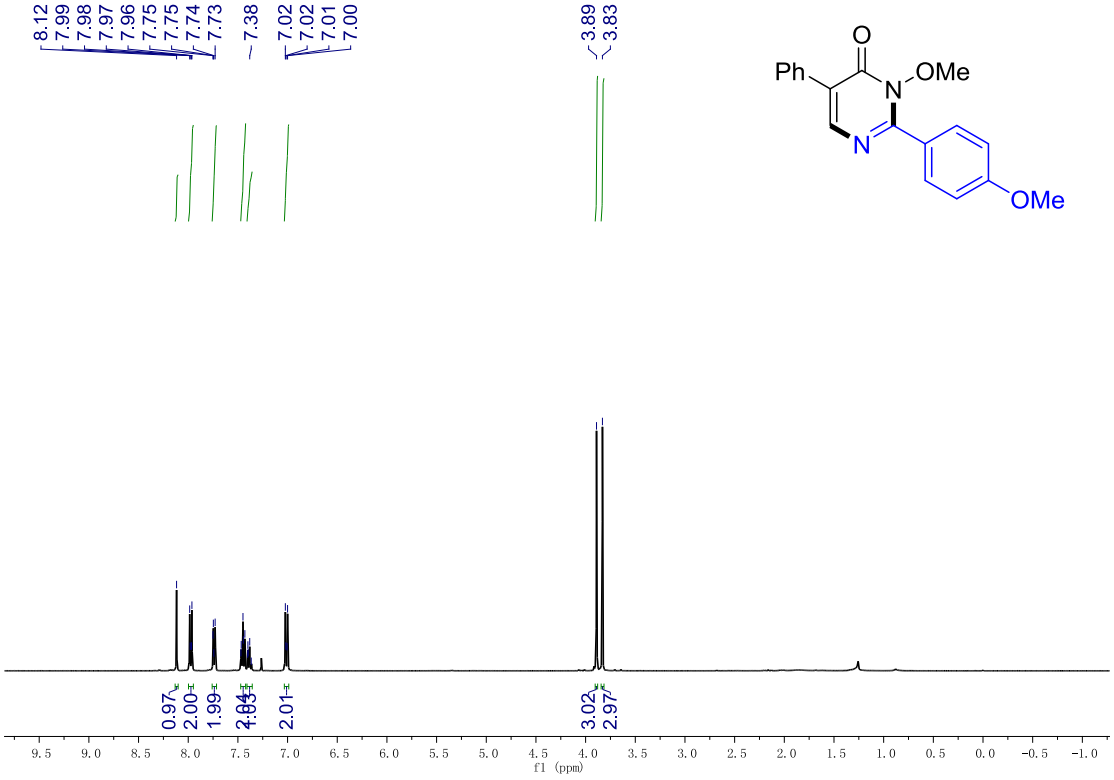
156.5796
149.0416
141.9690
132.8260
129.5858
129.1652
128.5491
128.5414
128.3937
127.0315
63.9389
21.5896
Ph
O
N
OMe
N
f1 (ppm)

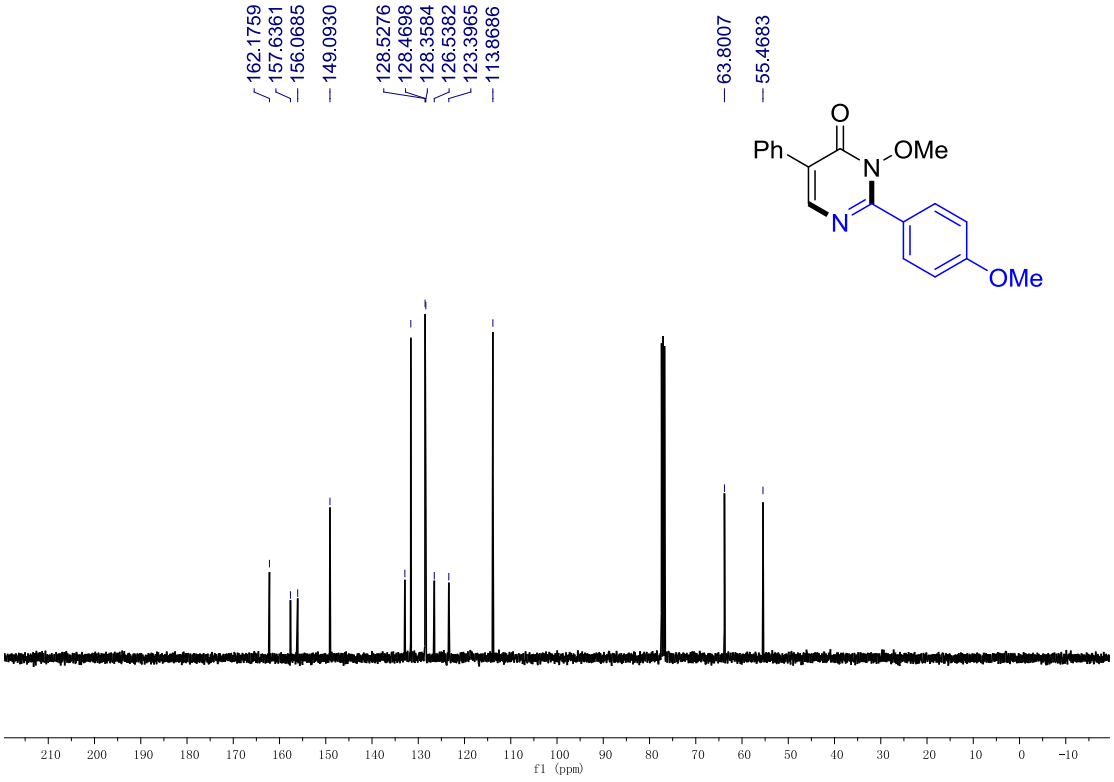
4af


8.05
7.81
7.67
7.66
7.45
7.43
7.39
7.37
7.35
7.32
7.30
7.28
3.76
1.29
Ph
O
N
OMe
N
tBu
1.00
2.00
2.04
2.05
2.07
1.02
3.06
9.15
f1 (ppm)


157.5925
156.5398
154.9934
149.0755
132.8526
129.4121
128.5366
128.3939
128.3531
126.9809
125.4666
64.0424
35.0314
31.1652
Ph
O
N
OMe
N
tBu
f1 (ppm)

4ag


8.12
7.99
7.98
7.97
7.96
7.75
7.75
7.74
7.73
7.38
7.02
7.02
7.01
7.00
3.89
3.83
Ph
O
N
OMe
N
OMe
0.97
2.00
1.99
2.04
2.03
2.01
3.02
2.97
f1 (ppm)


162.1759
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156.0685
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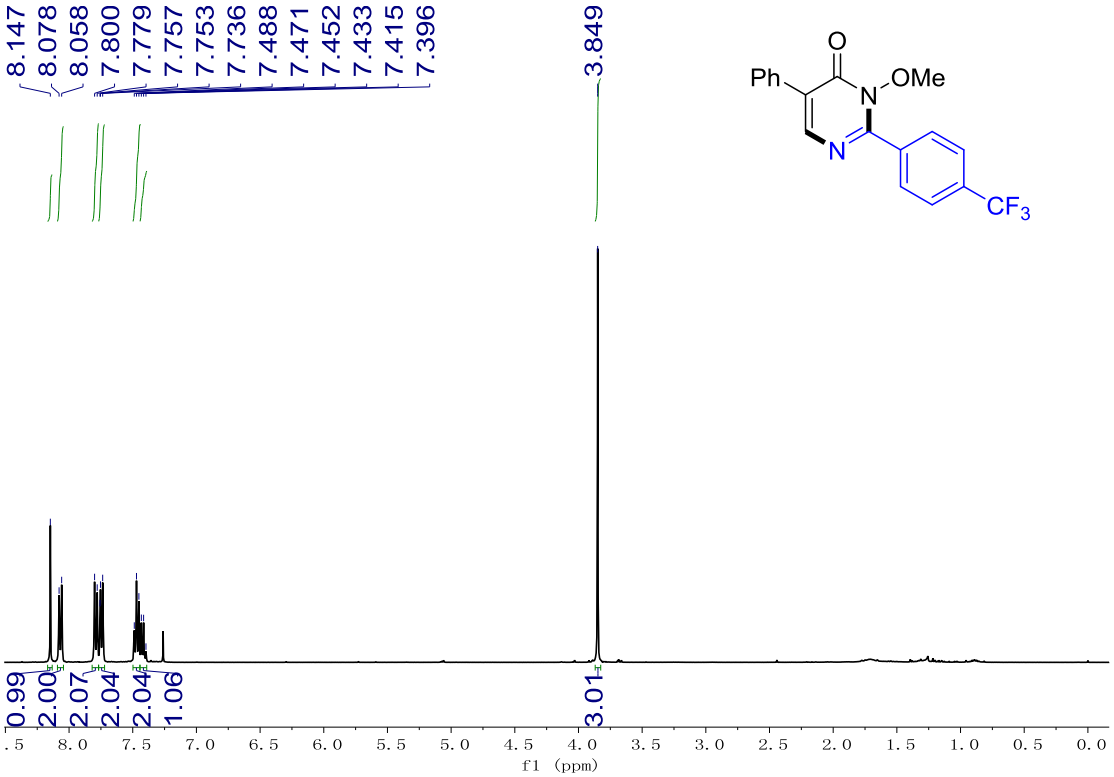
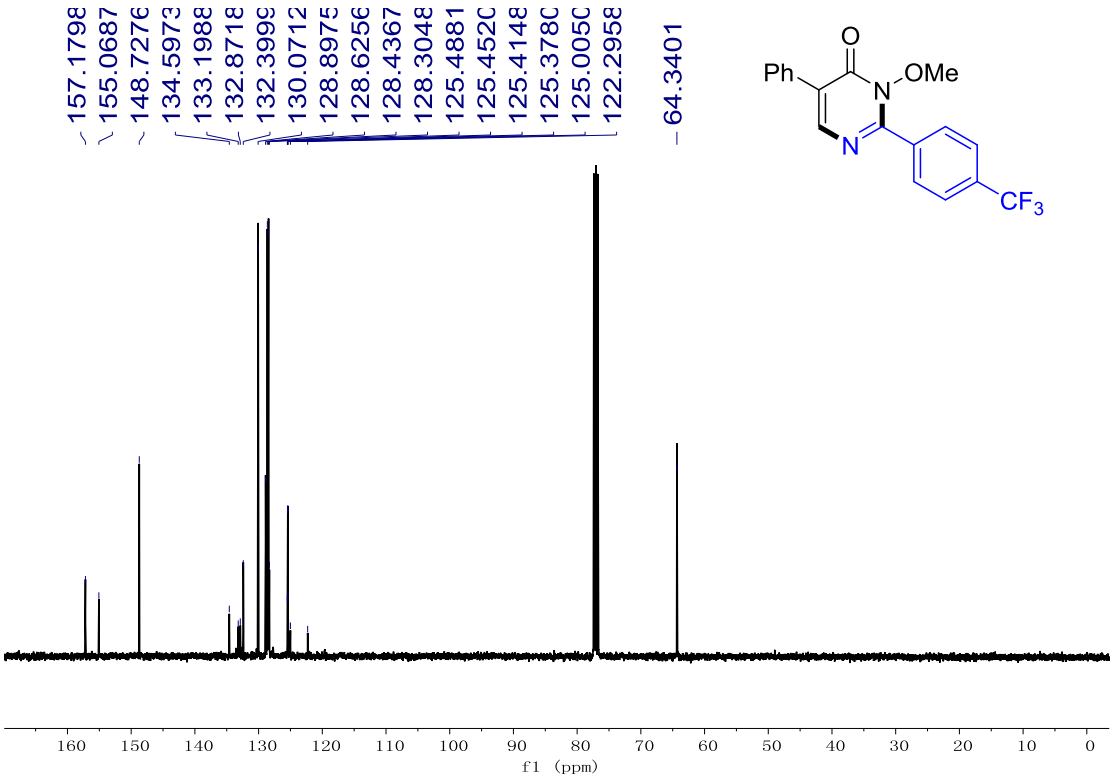
128.5276
128.4698
128.3584
126.5382
123.3965
113.8686
63.8007
55.4683
Ph
O
N
OMe
N
OMe
f1 (ppm)

4ah


8.147
8.078
8.058
7.800
7.779
7.757
7.753
7.736
7.488
7.471
7.452
7.433
7.415
7.396
3.849
Ph
O
N
OMe
N
CF3
0.99
2.00
2.07
2.04
2.04
1.06
3.01
f1 (ppm)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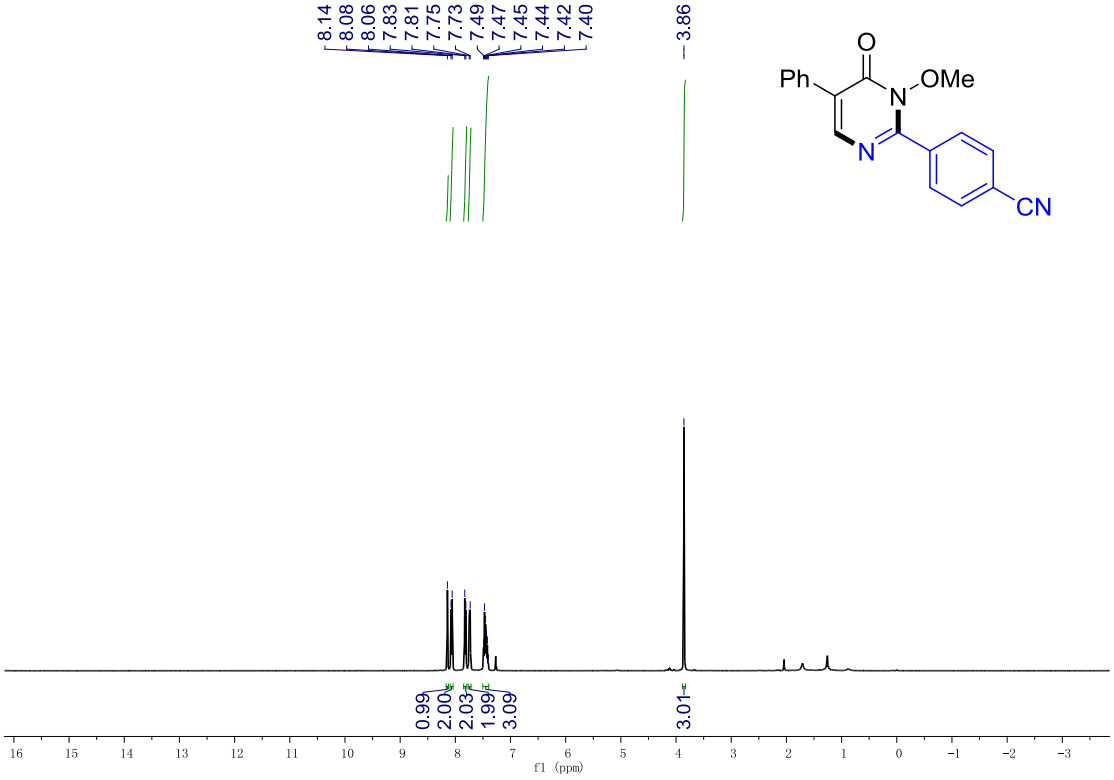
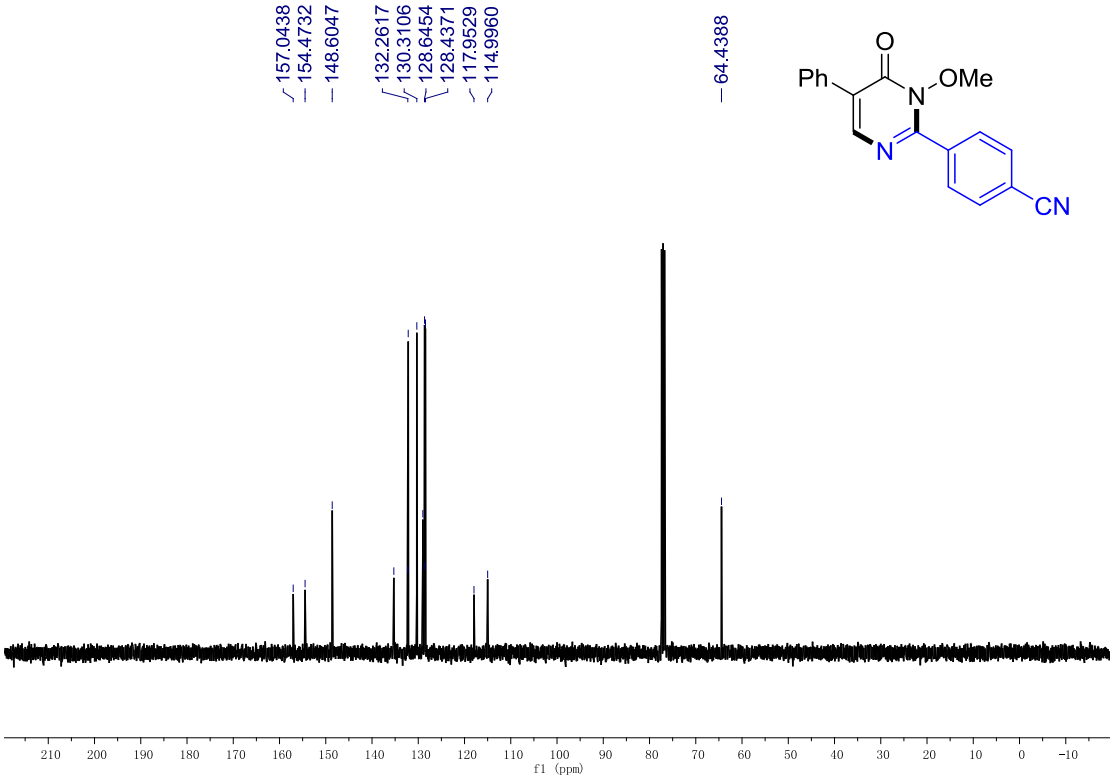
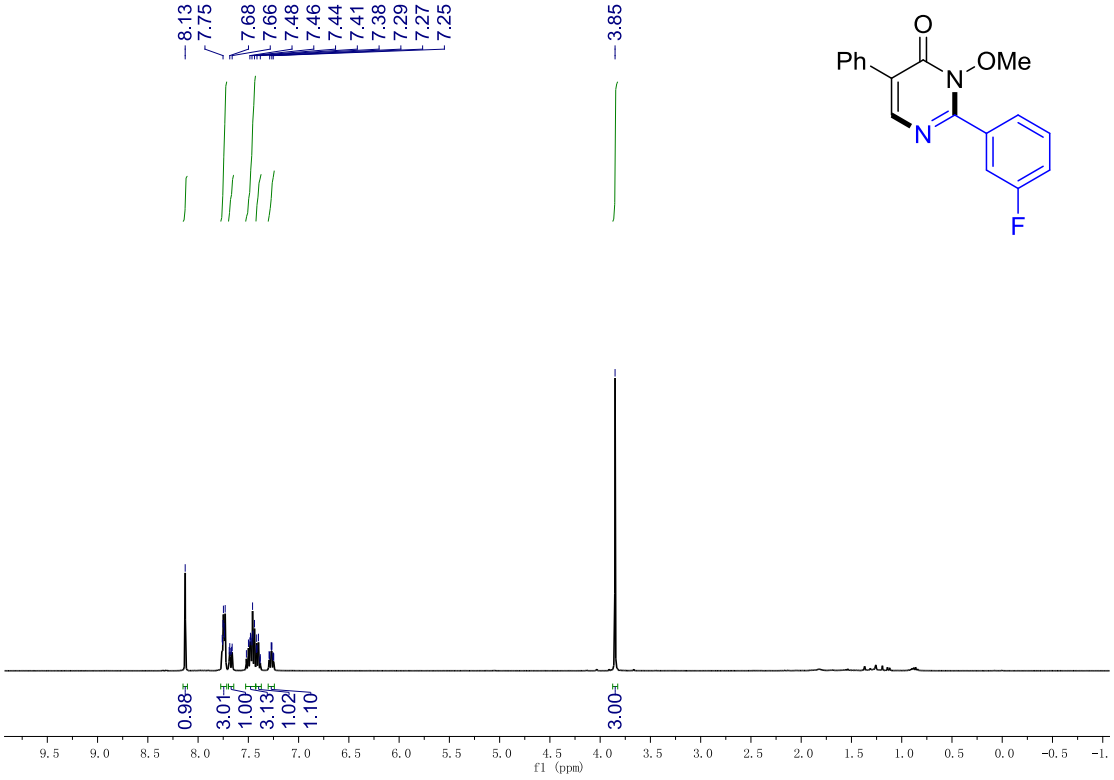
148.7276
134.5973
133.1988
132.8718
132.3999
130.0712
128.8975
128.6256
128.4367
128.3048
125.4881
125.4520
125.4148
125.3780
125.0050
122.2958
64.3401
Ph
O
N
OMe
N
CF3
f1 (ppm)

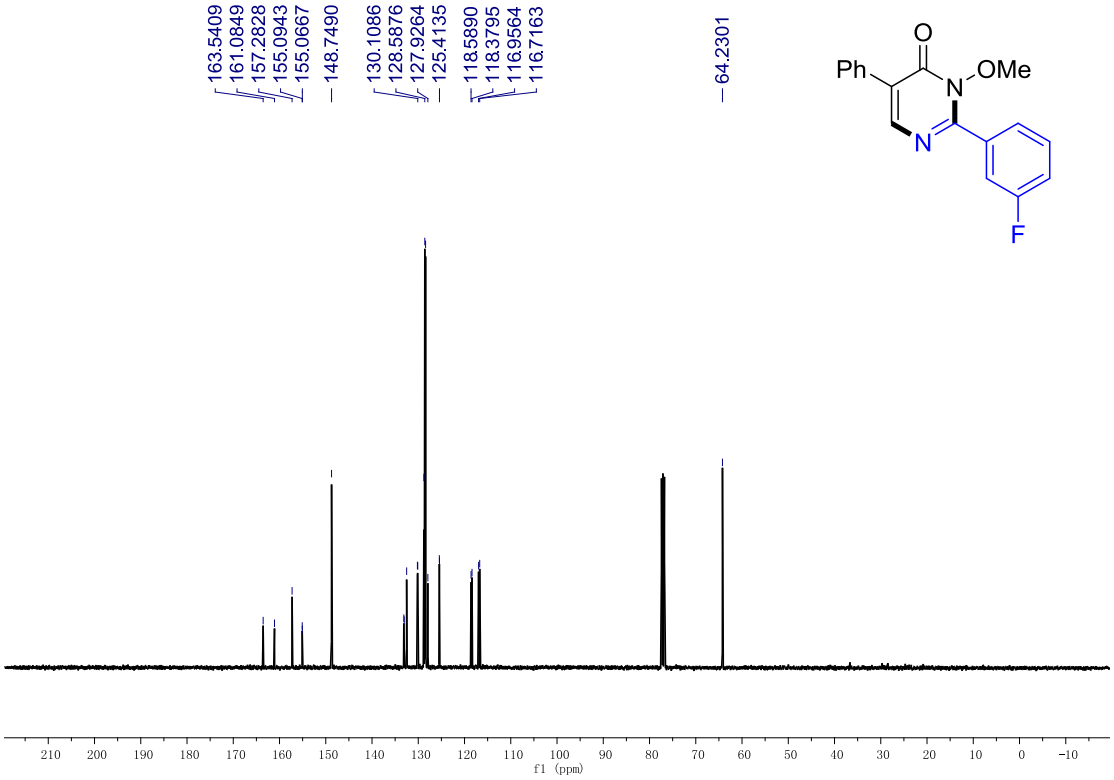
4ai


8.14
8.08
8.06
7.83
7.81
7.75
7.73
7.49
7.47
7.45
7.44
7.42
7.40
3.86
Ph
O
N
OMe
N
CN
0.99
2.00
2.03
1.99
3.09
3.01
f1 (ppm)

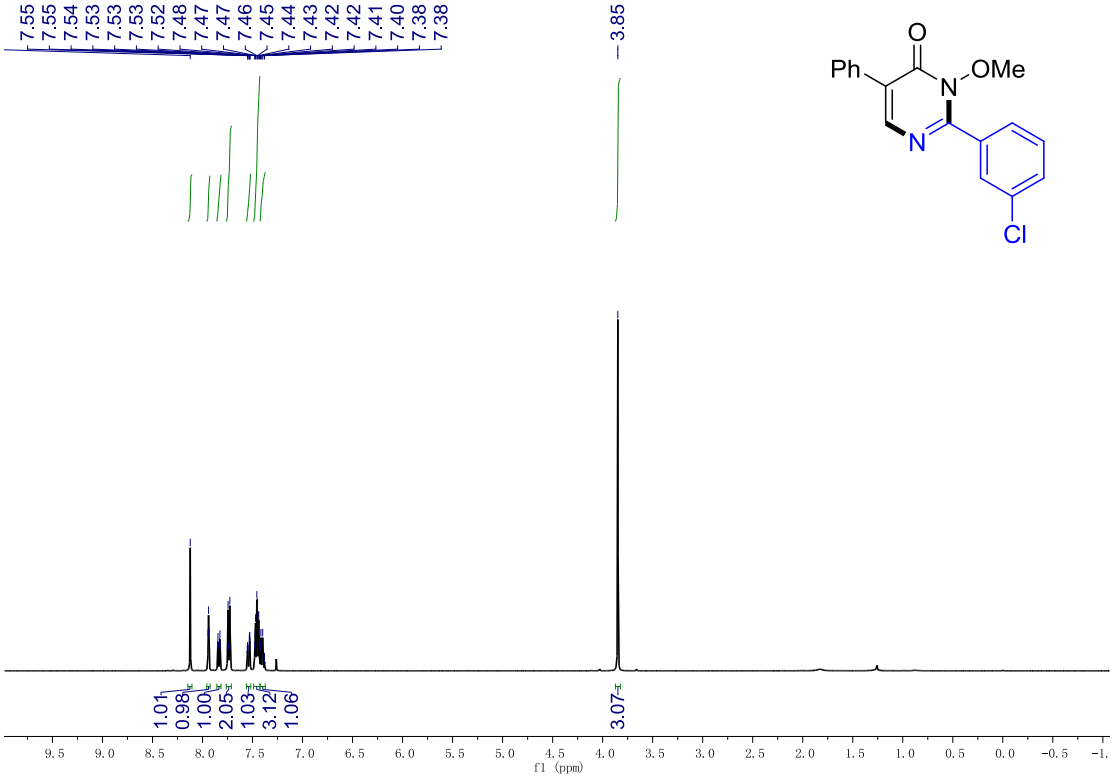

157.0438
154.4732
148.6047
132.2617
130.3106
128.6454
128.4371
117.9529
114.9960
64.4388
Ph
O
N
OMe
N
CN
f1 (ppm)

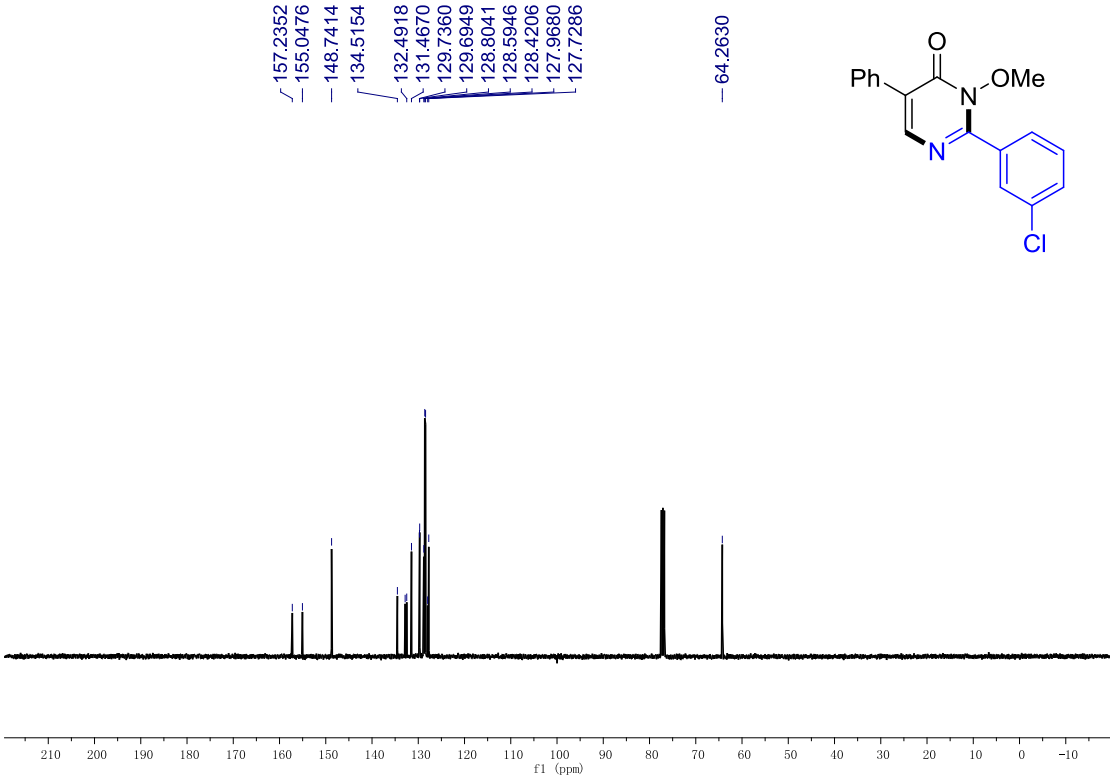
4aj


8.13
7.75
7.68
7.66
7.48
7.46
7.44
7.41
7.38
7.29
7.27
7.25
3.85
O
Ph
N
OMe
N
F
0.98
3.01
1.00
3.13
1.02
1.10
3.00
f1 (ppm)


163.5409
161.0849
157.2828
155.0943
155.0667
148.7490
130.1086
128.5876
127.9264
125.4135
118.5890
118.3795
116.9564
116.7163
64.2301
O
Ph
N
OMe
N
F
f1 (ppm)

4ak


7.55
7.55
7.54
7.53
7.53
7.53
7.52
7.48
7.47
7.47
7.46
7.45
7.44
7.43
7.42
7.42
7.41
7.40
7.38
7.38
3.85
Ph
O
N
OMe
N
Cl
1.01
0.98
1.00
2.05
1.03
3.12
1.06
3.07
f1 (ppm)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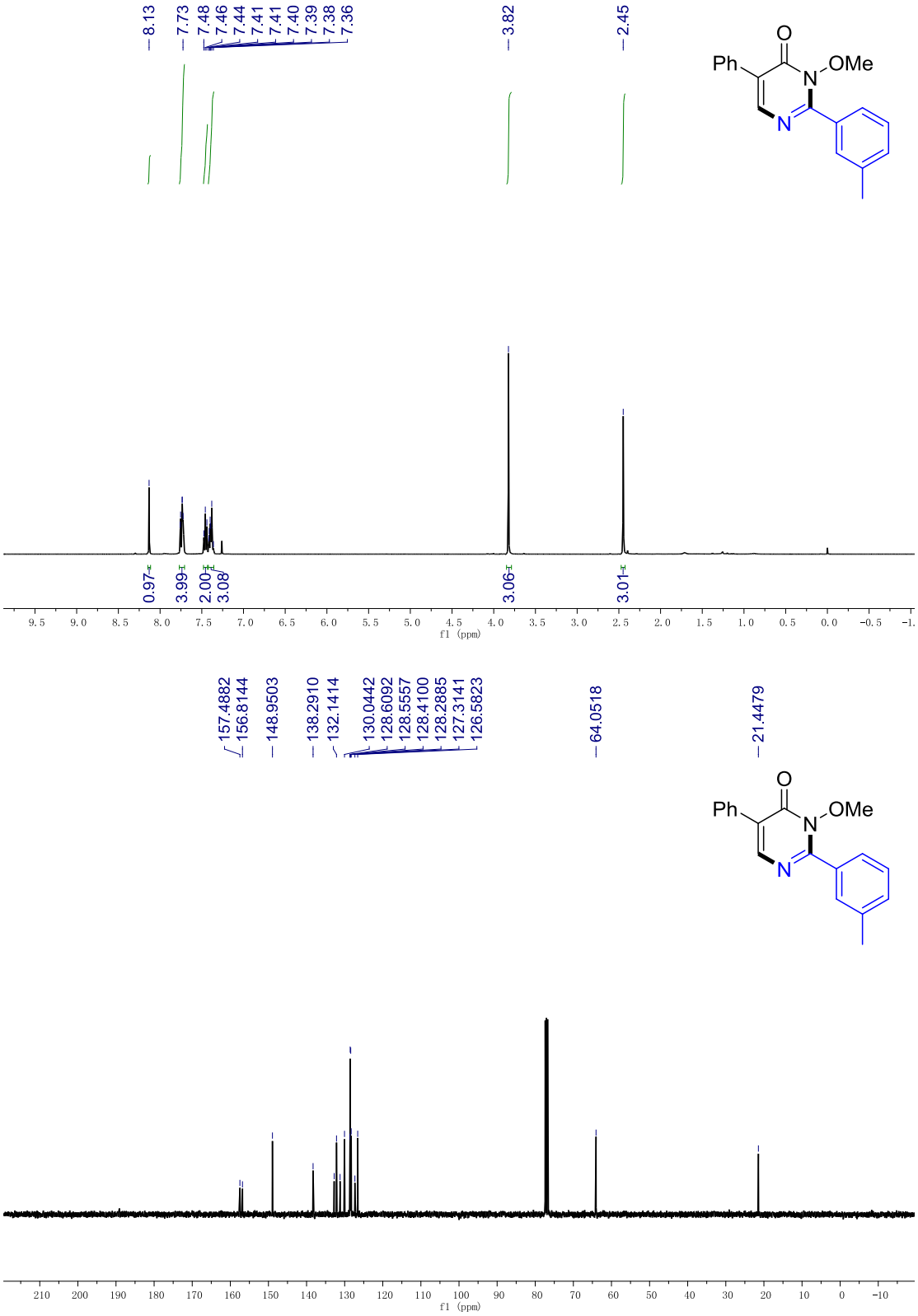
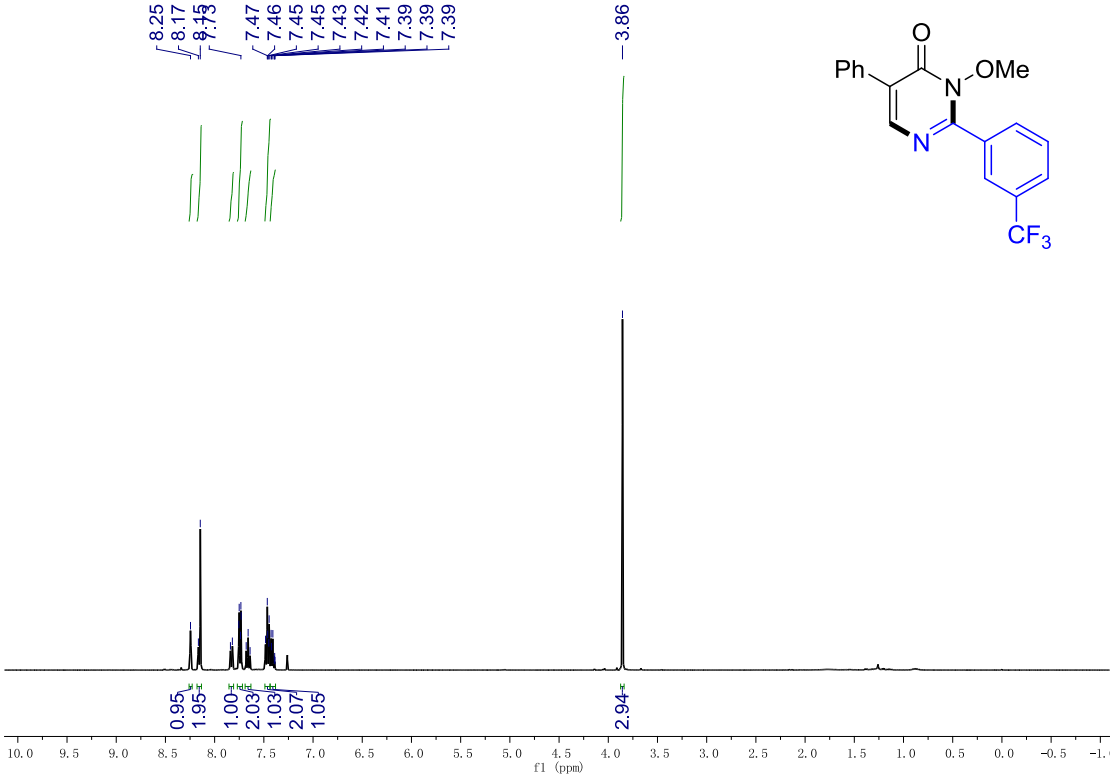
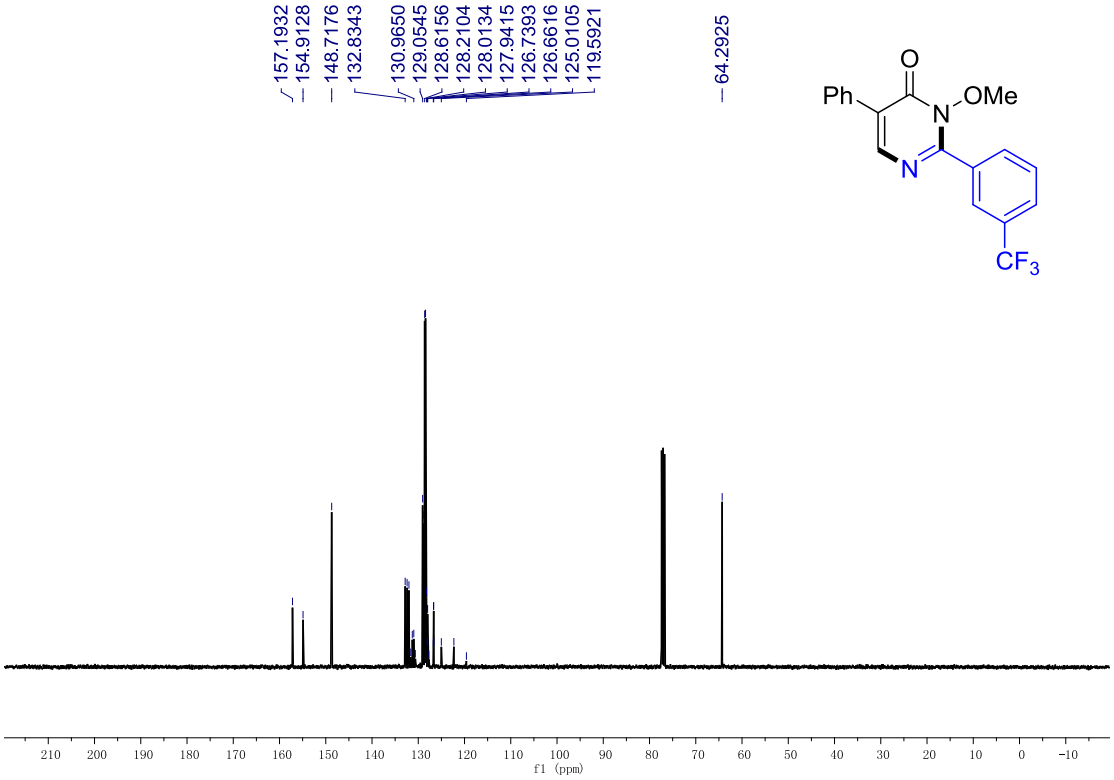
148.7414
134.5154
132.4918
131.4670
129.7360
129.6949
128.8041
128.5946
128.4206
127.9680
127.7286
64.2630
Ph
O
N
OMe
N
Cl
f1 (ppm)

4al


8.13
7.73
7.48
7.46
7.44
7.41
7.41
7.40
7.39
7.38
7.36
3.82
2.45
Ph
O
N
OMe
N
0.97
3.99
2.00
3.08
3.06
3.01
f1 (ppm)
157.4882
156.8144
148.9503
138.2910
132.1414
130.0442
128.6092
128.5557
128.4100
128.2885
127.3141
126.5823
64.0518
21.4479
Ph
O
N
OMe
N
f1 (ppm)

4am


8.25
8.17
8.15
7.73
7.47
7.46
7.45
7.45
7.43
7.42
7.41
7.39
7.39
7.39
3.86
Ph
O
N
OMe
N
CF3
0.95
1.95
1.00
2.03
1.03
2.07
1.05
2.94
f1 (ppm)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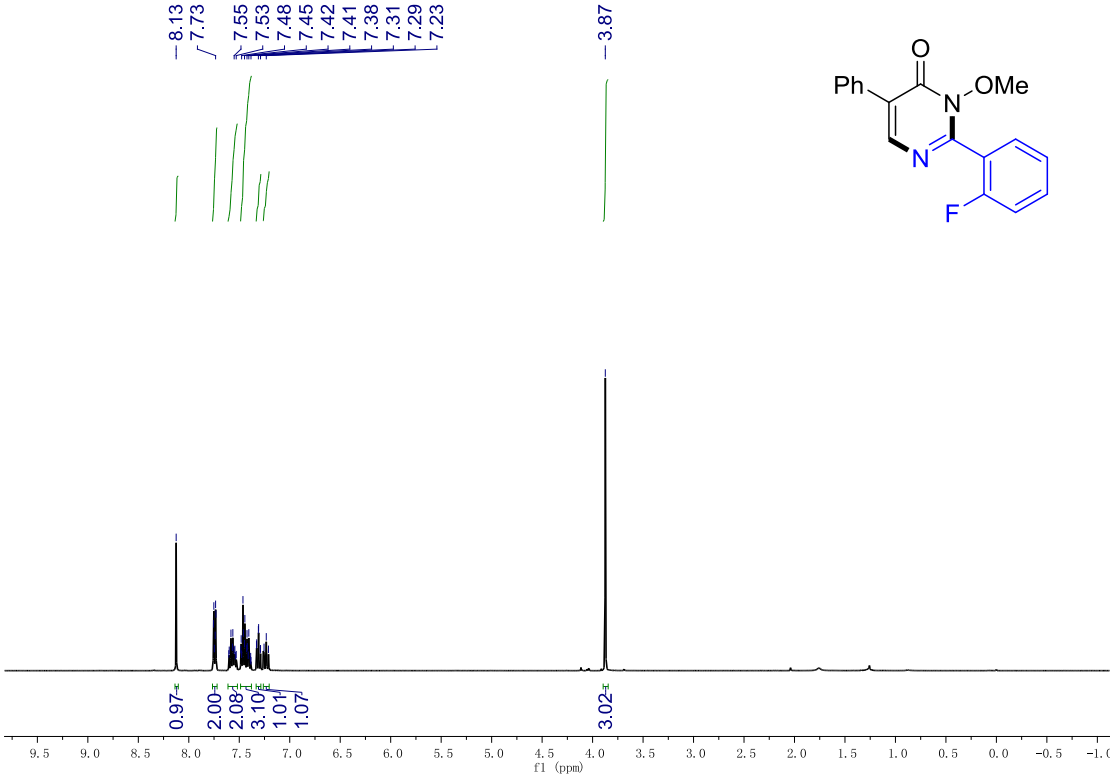
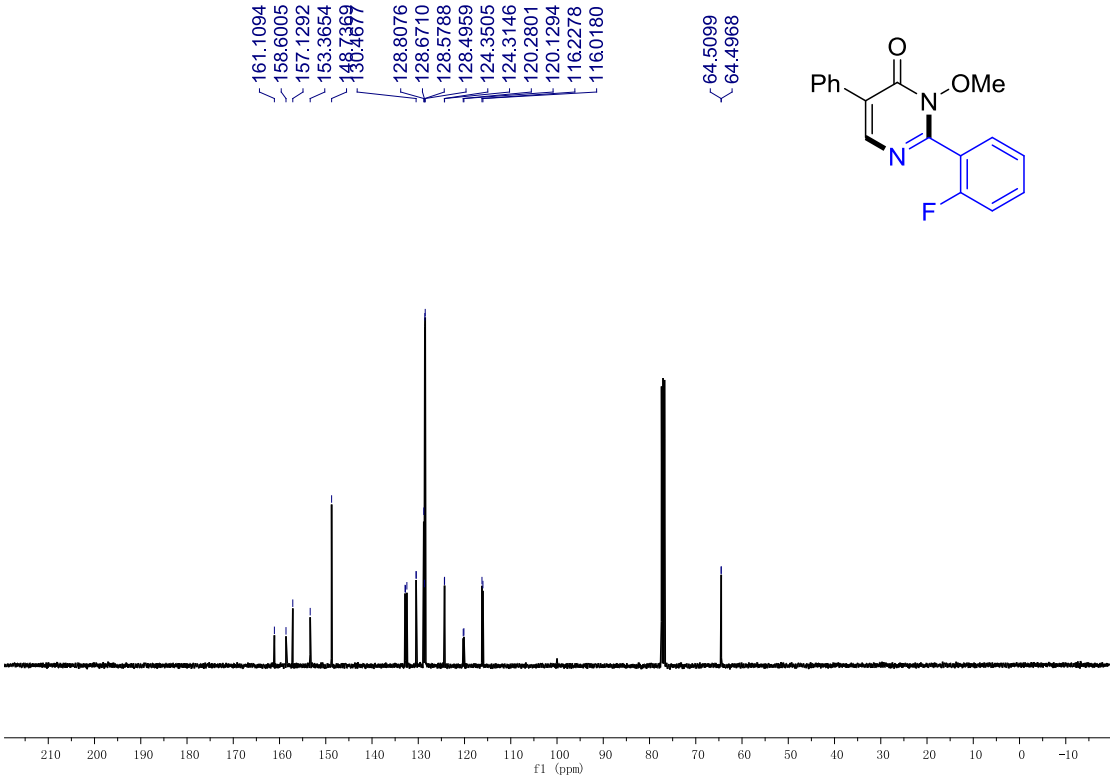
148.7176
132.8343
130.9650
129.0545
128.6156
128.2104
128.0134
127.9415
126.7393
126.6616
125.0105
119.5921
64.2925
Ph
O
N
OMe
N
CF3
f1 (ppm)

4an


8.13
7.73
7.55
7.53
7.48
7.45
7.42
7.41
7.38
7.31
7.29
7.23
3.87
O
Ph
N
OMe
N
F
0.97
2.00
2.08
3.10
1.01
1.07
3.02
f1 (ppm)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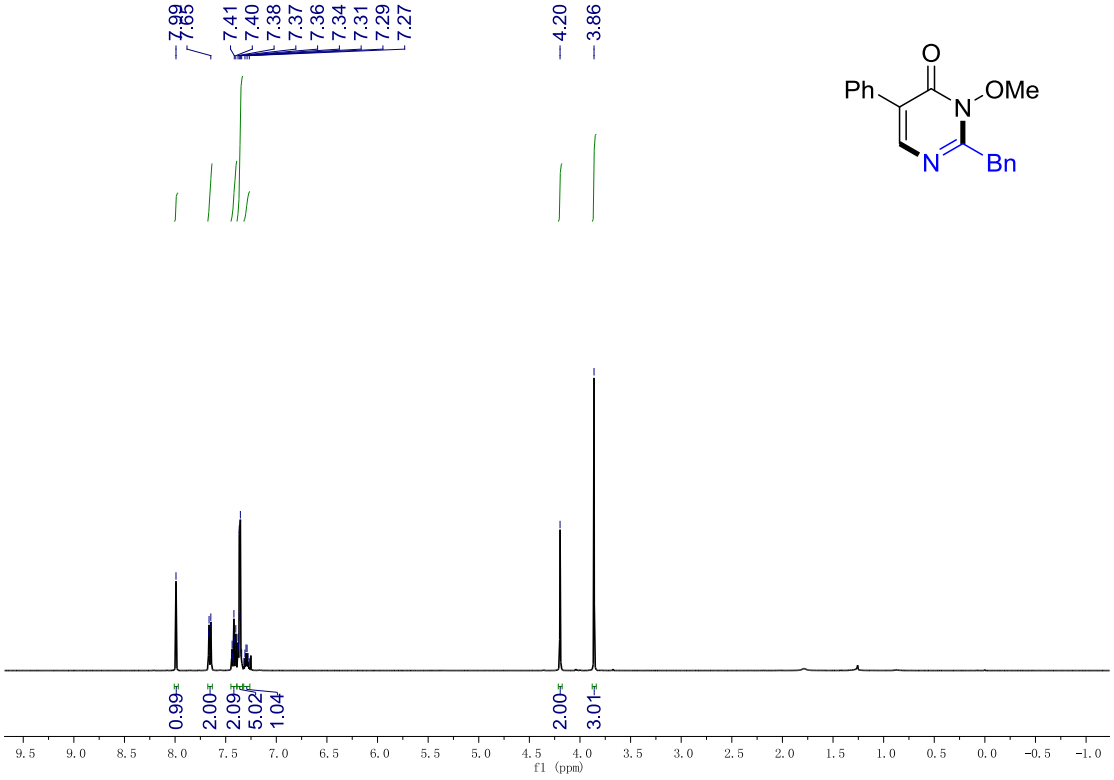
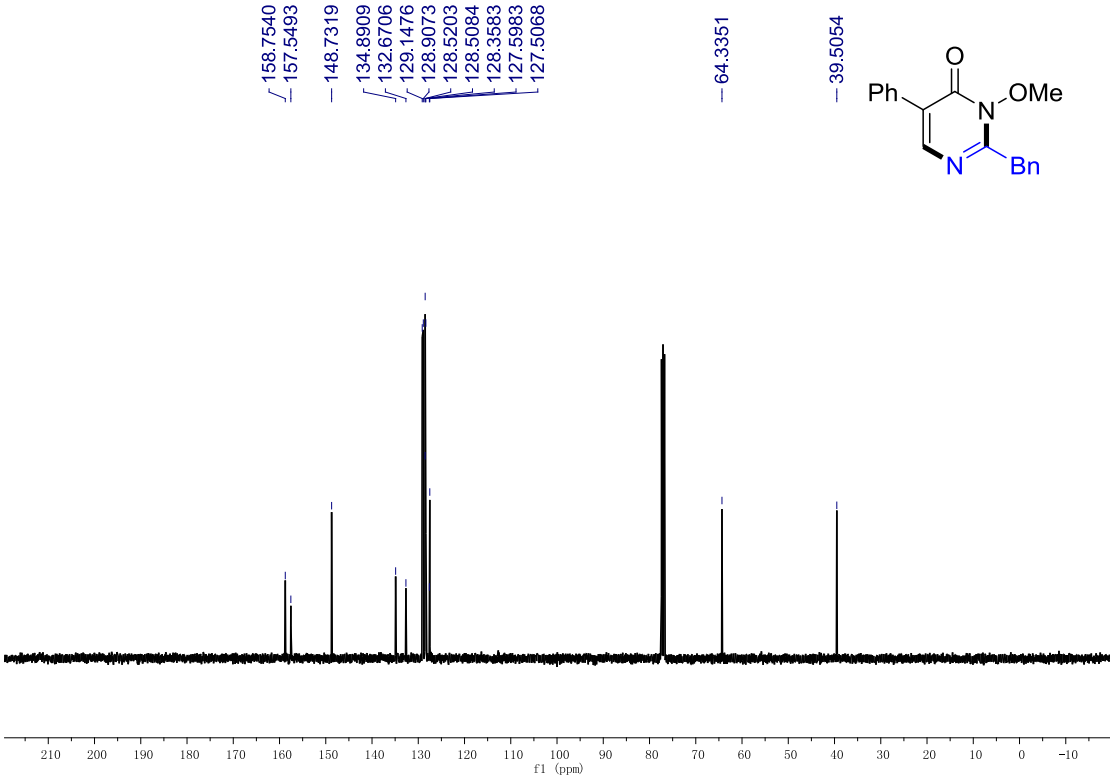
157.1292
153.3654
128.8076
128.6710
128.5788
128.4959
124.3505
124.3146
120.2801
120.1294
116.2278
116.0180
64.5099
64.4968
O
Ph
N
OMe
N
F
f1 (ppm)

4ao


7.99
7.65
7.41
7.40
7.38
7.37
7.36
7.34
7.31
7.29
7.27
4.20
3.86
Ph
O
N
OMe
N
Bn
0.99
2.00
2.09
5.02
1.04
2.00
3.01
f1 (ppm)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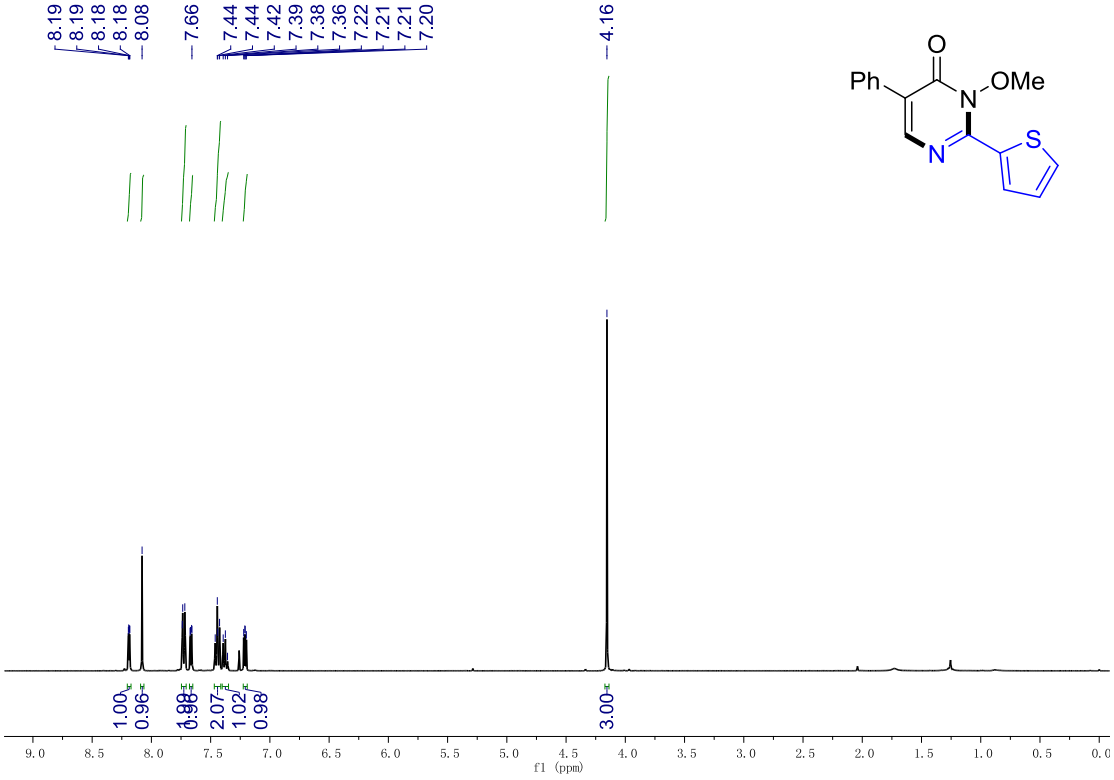
132.6706
129.1476
128.9073
128.5203
128.5084
128.3583
127.5983
127.5068
64.3351
39.5054
Ph
O
N
OMe
N
Bn
f1 (ppm)

4ap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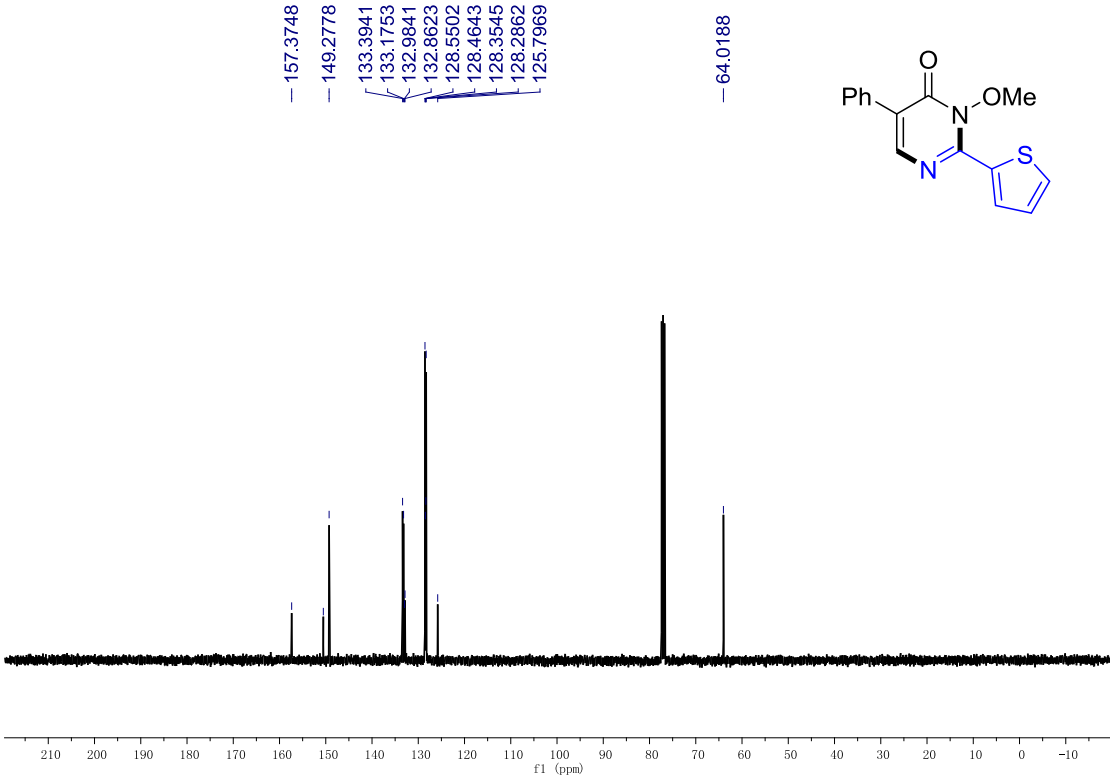
8.19
8.18
8.18
8.08
7.66
7.44
7.44
7.42
7.39
7.38
7.36
7.22
7.21
7.21
7.20
4.16
Ph
O
N
OMe
N
S
1.00
0.96
2.07
1.02
0.98
3.00
f1 (ppm)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132.9841
132.8623
128.5502
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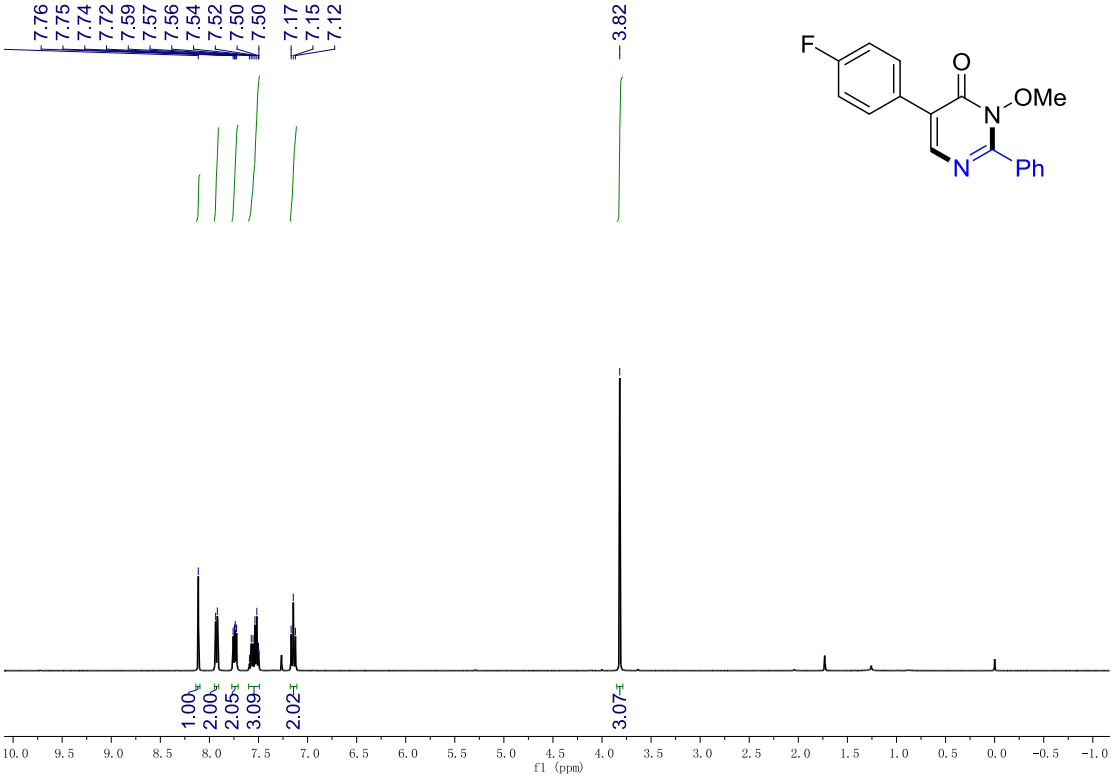
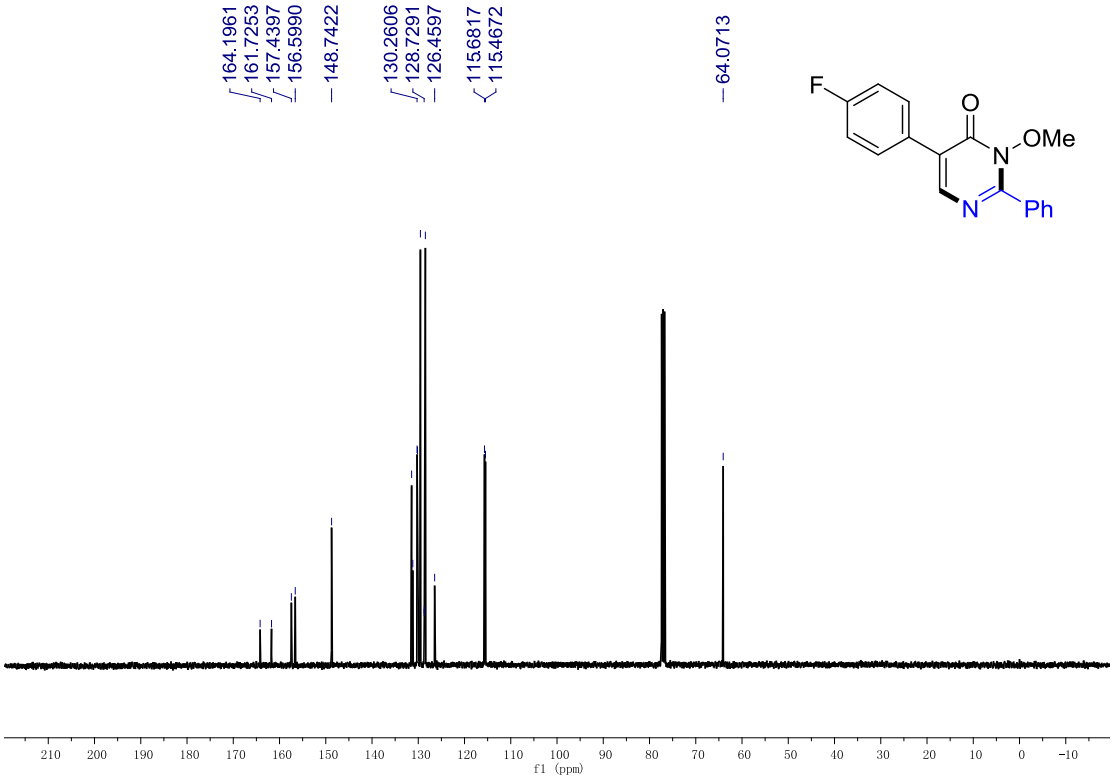
128.2862
125.7969
64.0188
Ph
O
N
OMe
N
S
f1 (ppm)

4ba


7.76
7.75
7.74
7.72
7.59
7.57
7.56
7.54
7.52
7.50
7.50
7.17
7.15
7.12
3.82
F
O
N
OMe
N
Ph
1.00
2.00
2.05
3.09
2.02
3.07
f1 (ppm)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157.4397
156.5990
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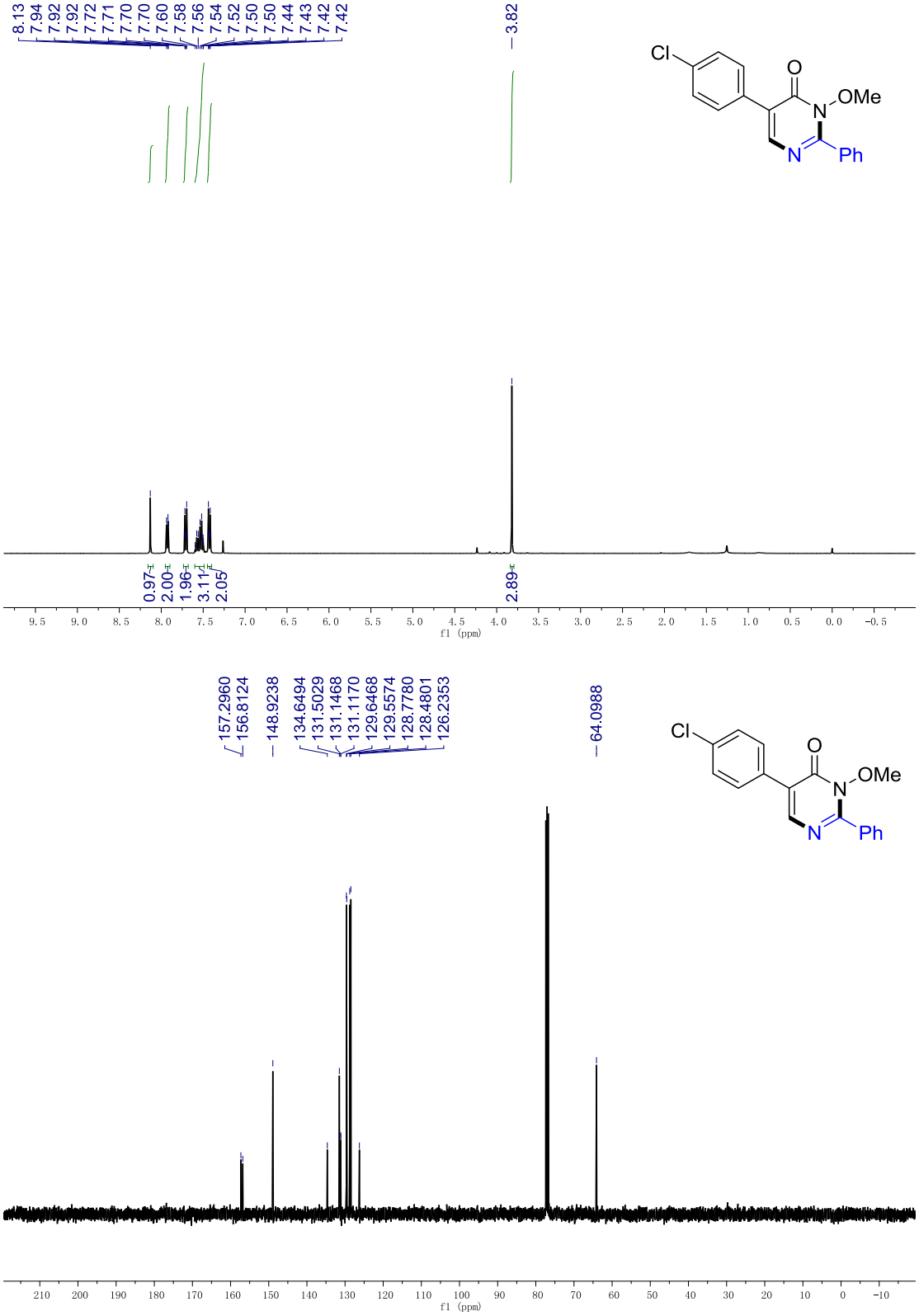
115.6817
115.4672
64.0713
F
O
N
OMe
N
Ph
f1 (ppm)

4ca


8.13
7.94
7.92
7.92
7.72
7.71
7.70
7.70
7.60
7.58
7.56
7.54
7.52
7.50
7.50
7.44
7.43
7.42
7.42
3.82
Cl
O
N
OMe
N
Ph
0.97
2.00
1.96
3.11
2.05
2.89
f1 (ppm)
157.2960
156.8124
148.9238
134.6494
131.5029
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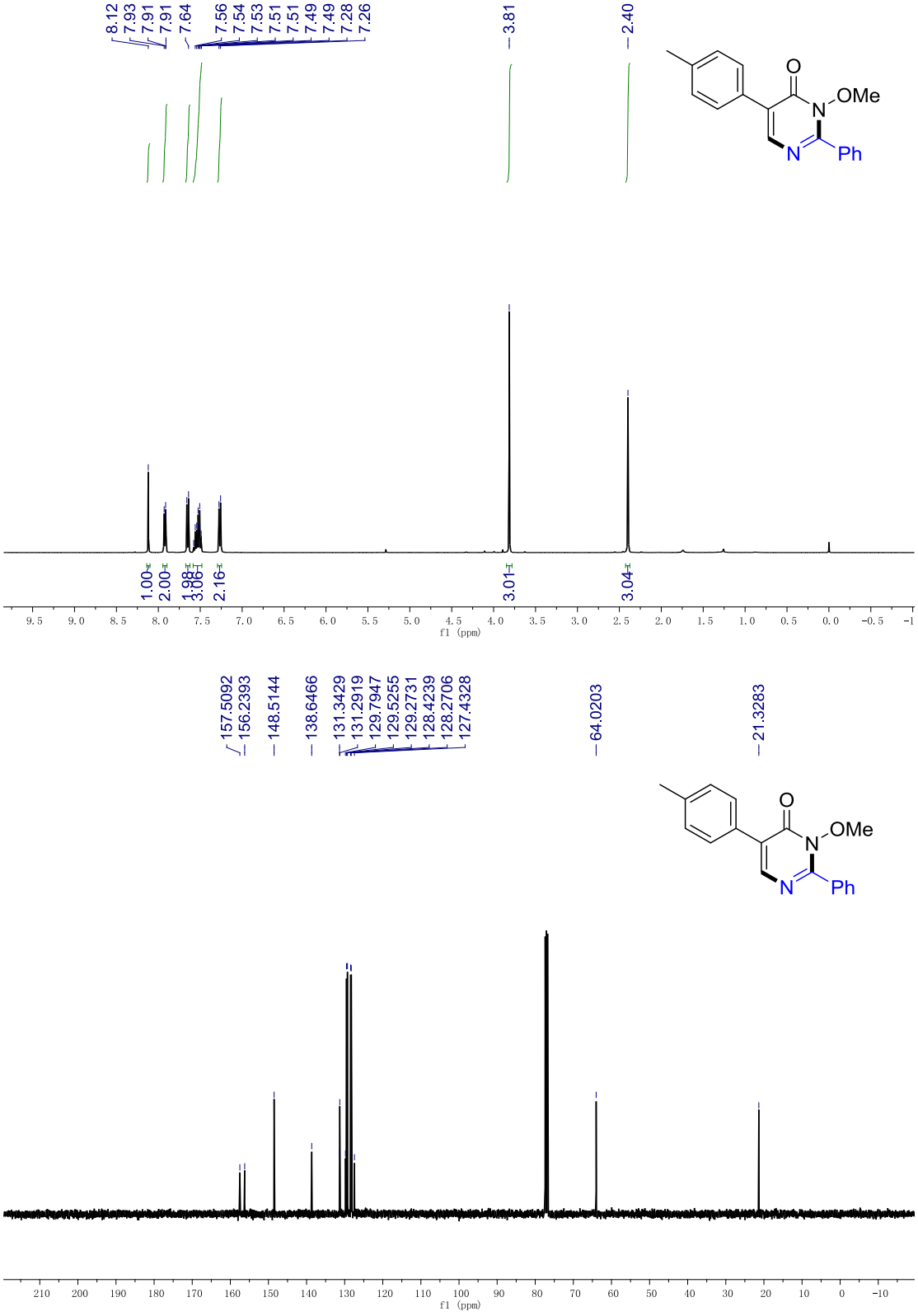
129.6468
129.5574
128.7780
128.4801
126.2353
64.0988
f1 (ppm)

4da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7.91
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7.56
7.54
7.53
7.51
7.51
7.49
7.49
7.28
7.26
3.81
2.40
O
N
OMe
N
Ph
1.00
2.00
1.98
3.06
2.16
3.01
3.04
f1 (ppm)
157.5092
156.2393
148.5144
138.6466
131.3429
131.2919
129.7947
129.5255
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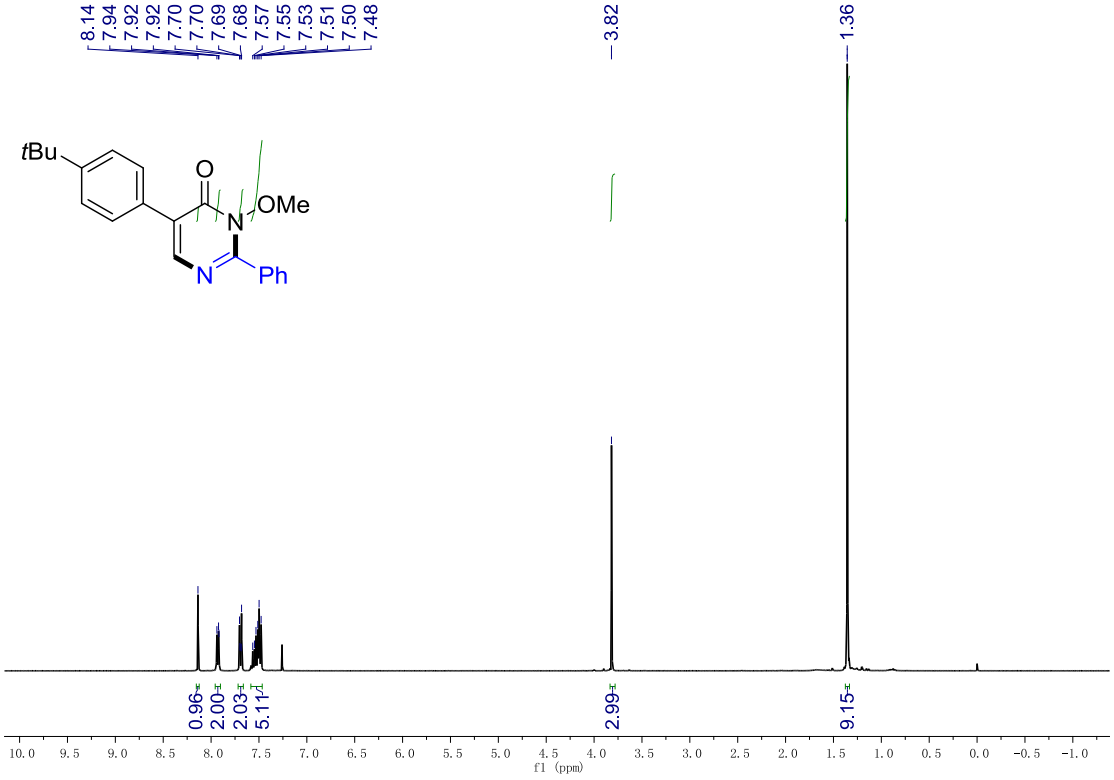
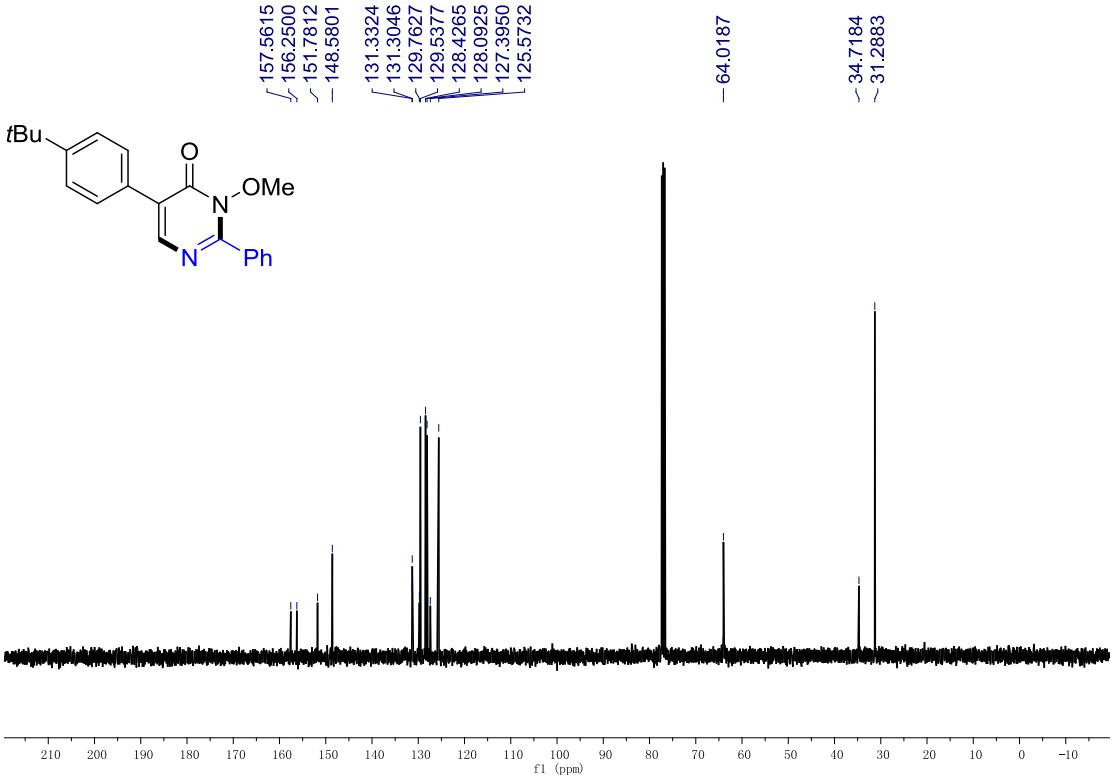
N
OMe
N
Ph
f1 (ppm)

4ea


8.14
7.94
7.92
7.92
7.70
7.70
7.69
7.68
7.57
7.55
7.53
7.51
7.50
7.48
3.82
1.36
tBu
O
N
OMe
N
Ph
0.96
2.00
2.03
5.11
2.99
9.15
f1 (ppm)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131.3046
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128.0925
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64.0187
34.7184
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tBu
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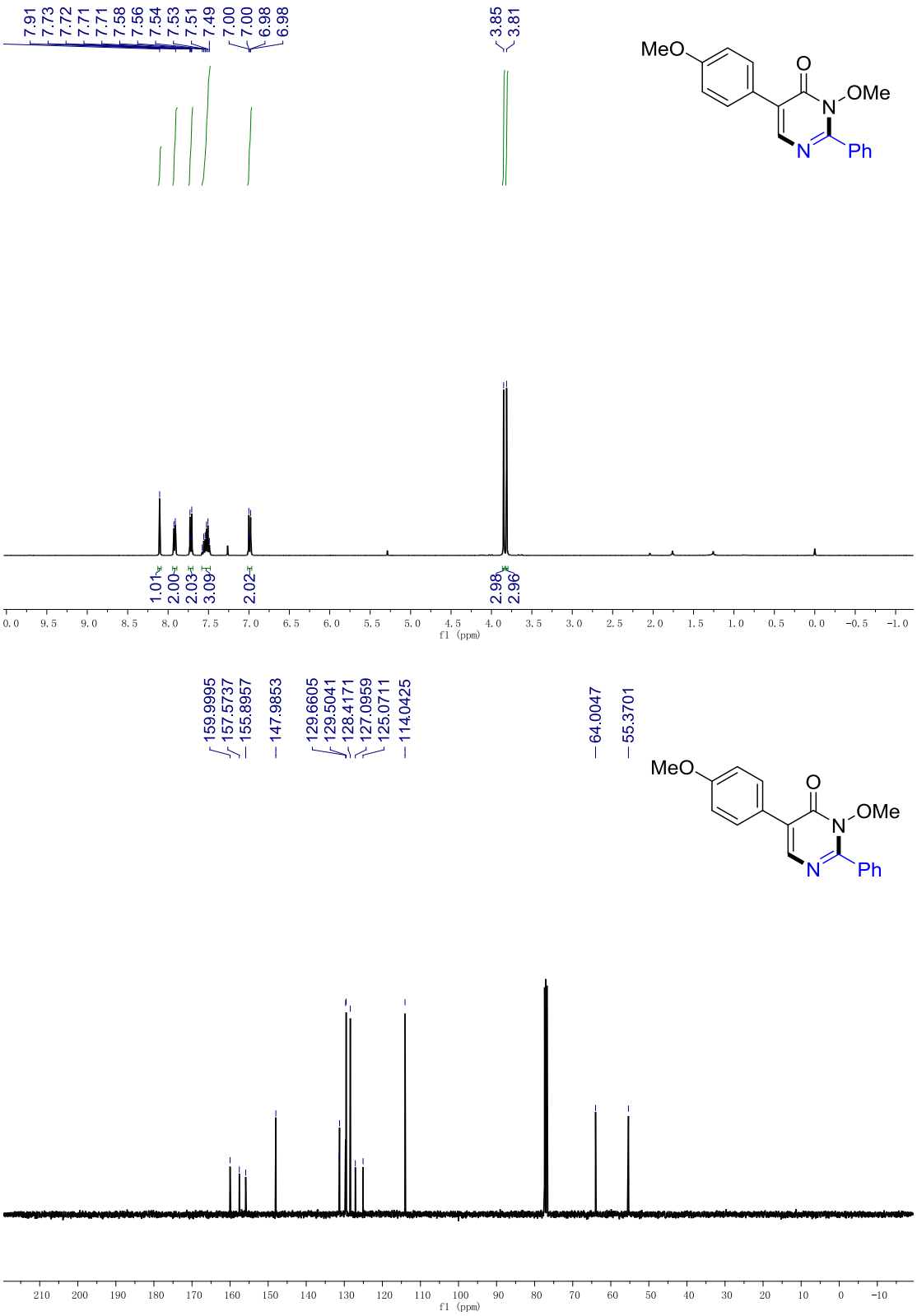
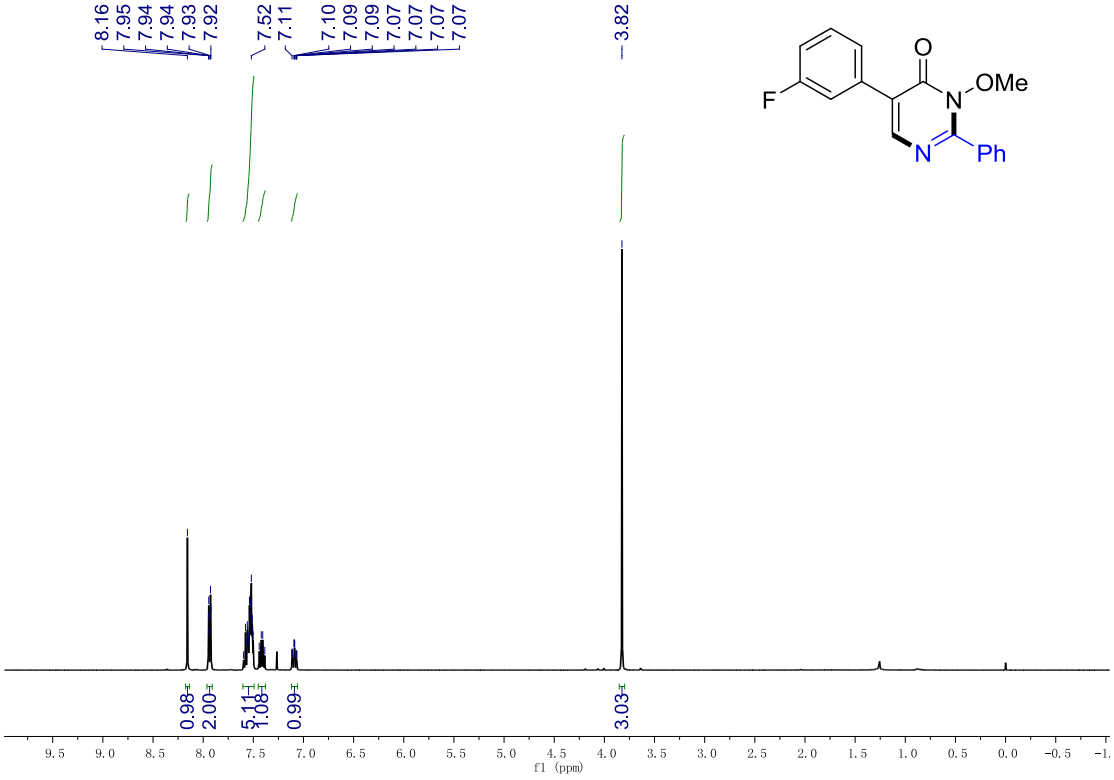
N
OMe
N
Ph
f1 (ppm)

4fa


7.91
7.73
7.72
7.71
7.71
7.58
7.56
7.54
7.53
7.51
7.49
7.00
7.00
6.98
6.98
3.85
3.81
MeO
O
N
OMe
N
Ph
1.01
2.00
2.03
3.09
2.02
2.98
2.96
f1 (ppm)
159.9995
157.5737
155.8957
147.9853
129.6605
129.5041
128.4171
127.0959
125.0711
114.0425
64.0047
55.3701
MeO
O
N
OMe
N
Ph
f1 (ppm)

4ga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7.95
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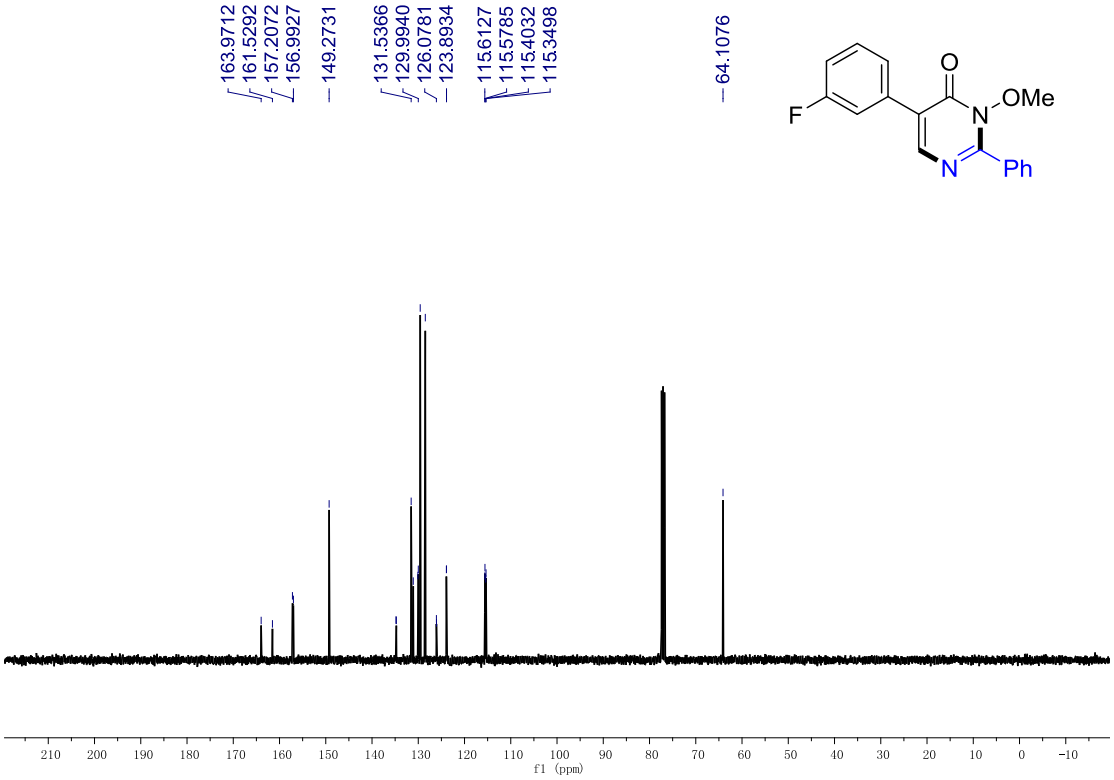
7.94
7.93
7.92
7.52
7.11
7.10
7.09
7.09
7.07
7.07
7.07
7.07
3.82
0.98
2.00
5.11
1.08
0.99
3.03
f1 (ppm)
F
O
N
OMe
N
Ph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161.5292
157.2072
156.9927
149.2731
131.5366
129.9940
126.0781
123.8934
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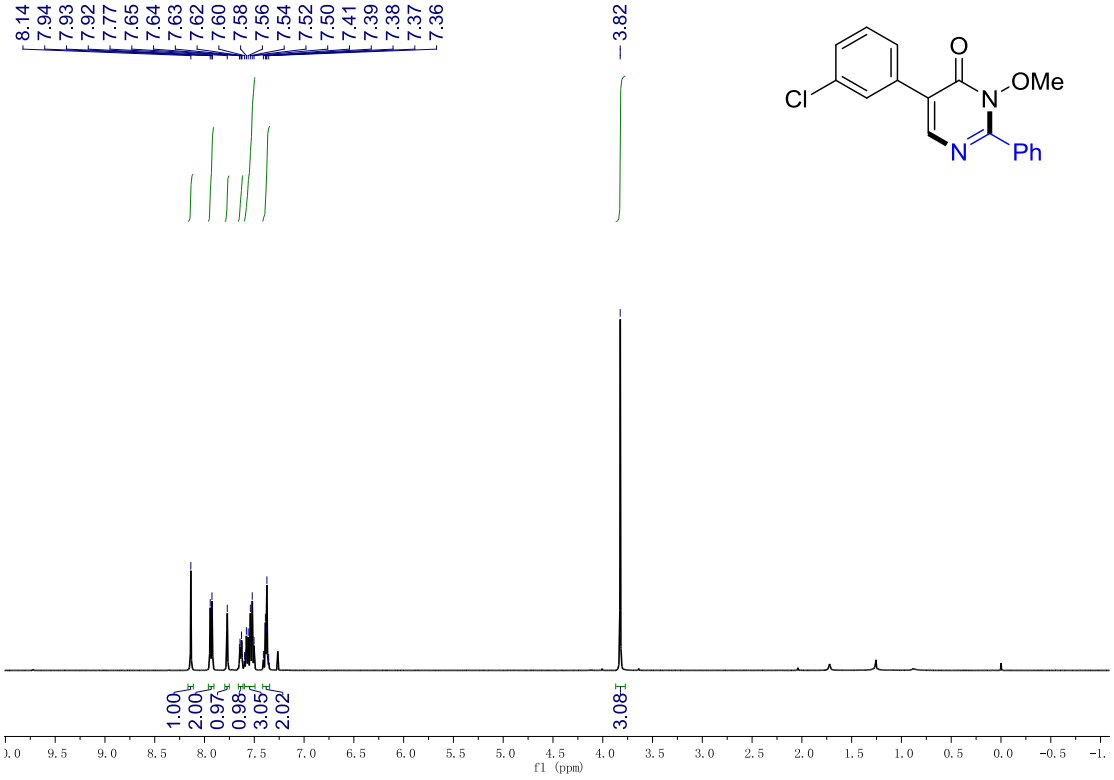
115.5785
115.4032
115.3498
64.1076
f1 (ppm)
F
O
N
OMe
N
Ph

4ha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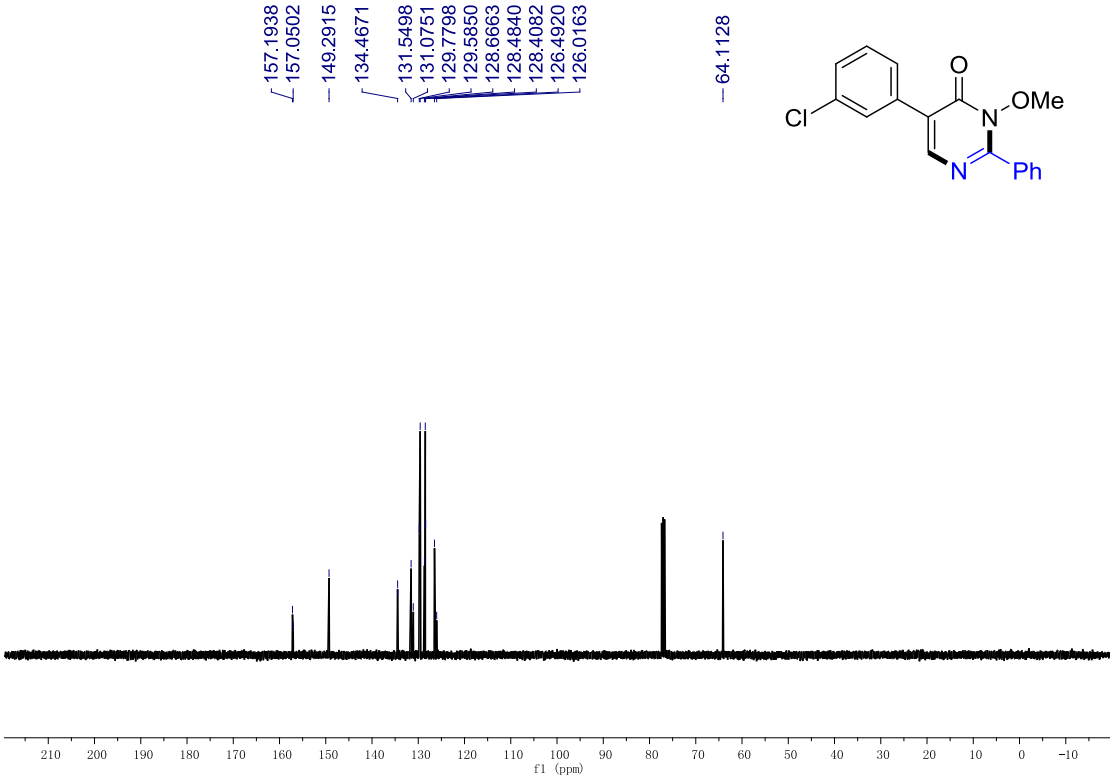
7.94
7.93
7.92
7.77
7.65
7.64
7.63
7.62
7.60
7.58
7.56
7.54
7.52
7.50
7.41
7.39
7.38
7.37
7.36
3.82
Cl
O
N
OMe
N
Ph
1.00
2.00
0.97
0.98
3.05
2.02
3.08
f1 (ppm)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149.2915
134.4671
131.5498
131.0751
129.7798
129.5850
128.6663
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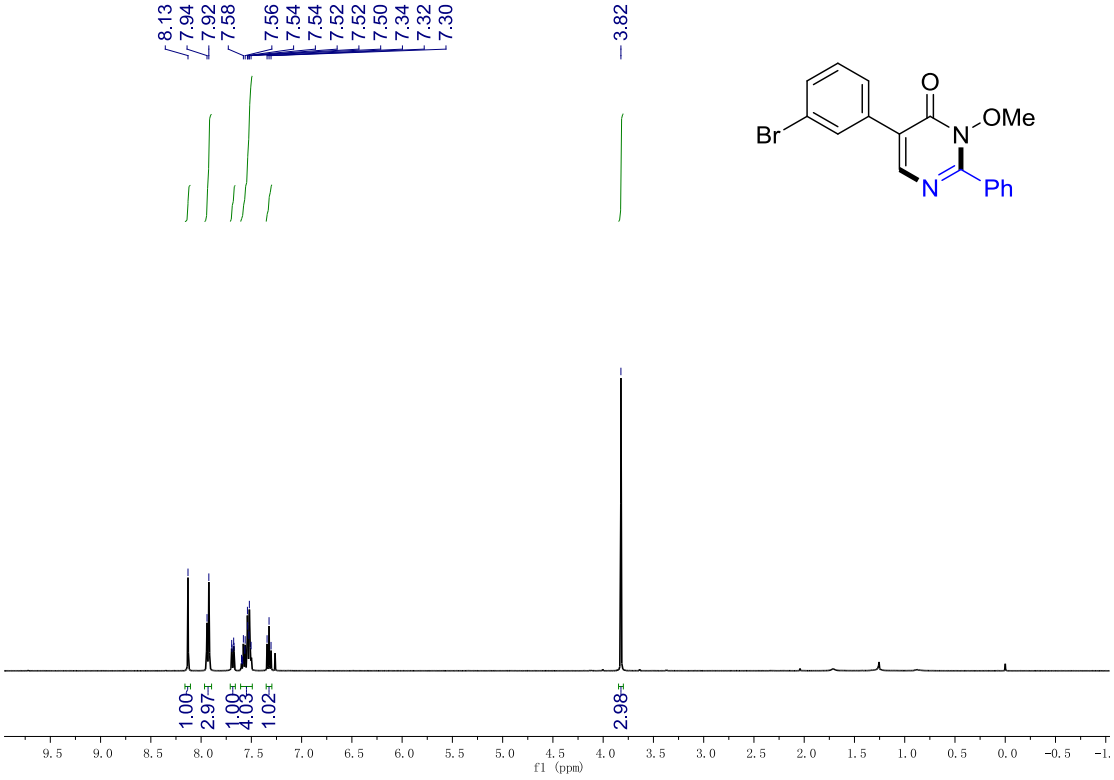
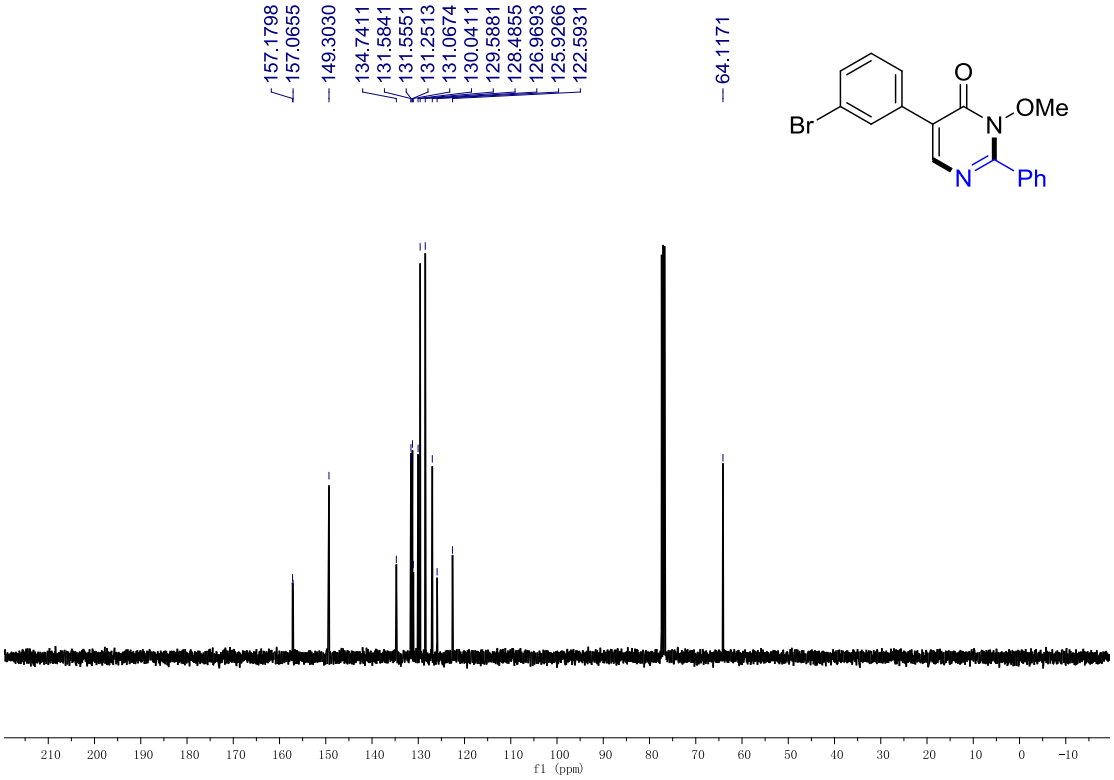
126.4920
126.0163
64.1128
Cl
O
N
OMe
N
Ph
f1 (ppm)

4ia


8.13
7.94
7.92
7.58
7.56
7.54
7.54
7.52
7.52
7.50
7.34
7.32
7.30
3.82
Br
O
N
OMe
N
Ph
1.00
2.97
1.00
4.03
1.02
2.98
f1 (ppm)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157.0655
149.3030
134.7411
131.5841
131.5551
131.2513
131.0674
130.0411
129.5881
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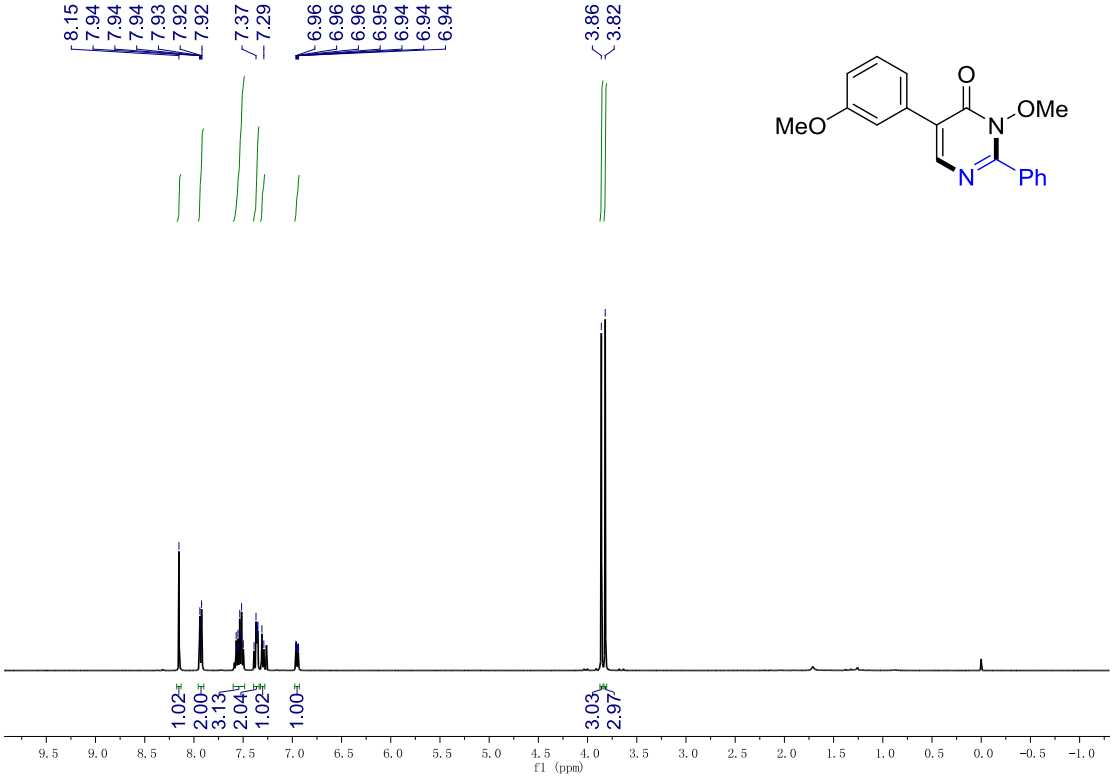
126.9693
125.9266
122.5931
64.1171
Br
O
N
OMe
N
Ph
f1 (ppm)

4ja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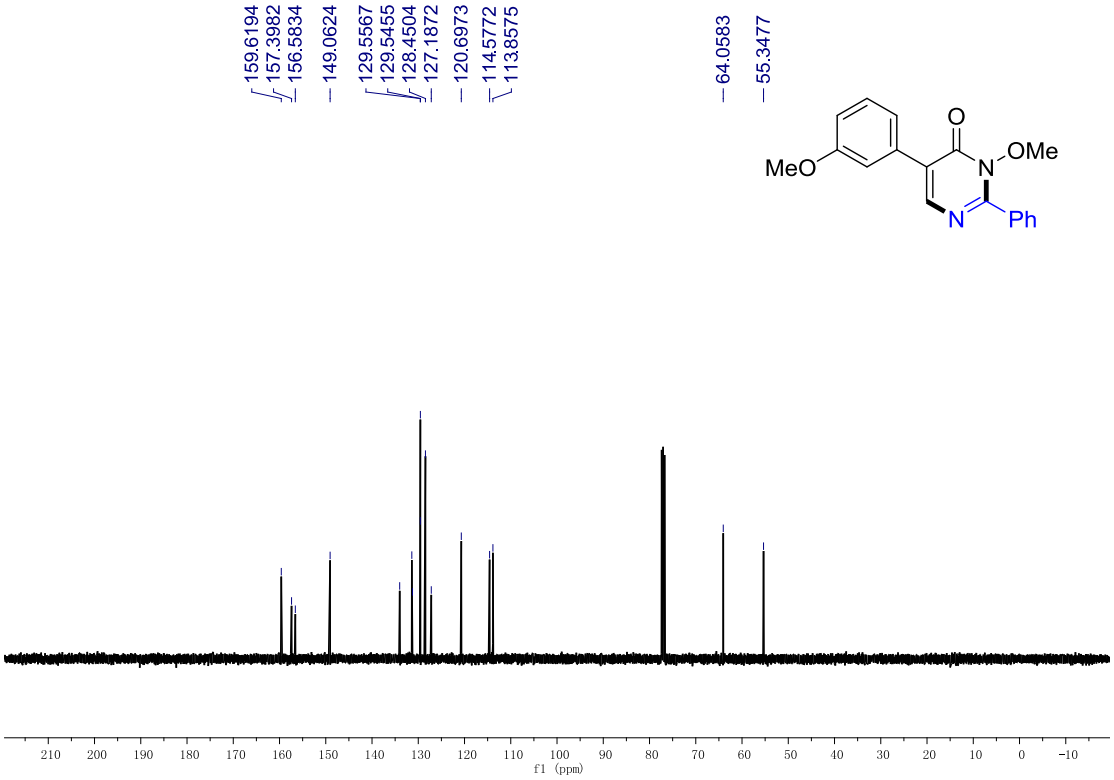
7.94
7.94
7.94
7.93
7.92
7.92
7.37
7.29
6.96
6.96
6.96
6.95
6.94
6.94
6.94
3.86
3.82
MeO
O
N
OMe
N
Ph
1.02
2.00
3.13
2.04
1.02
1.00
3.03
2.97
f1 (ppm)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157.3982
156.5834
149.0624
129.5567
129.5455
128.4504
127.1872
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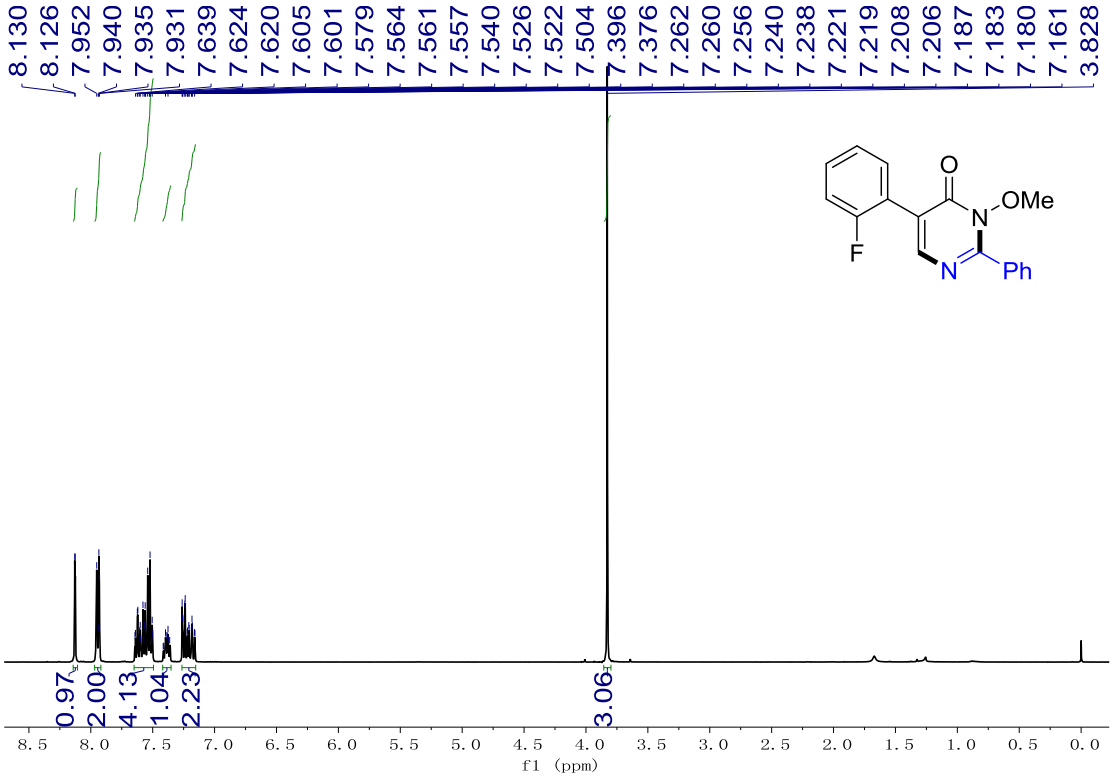
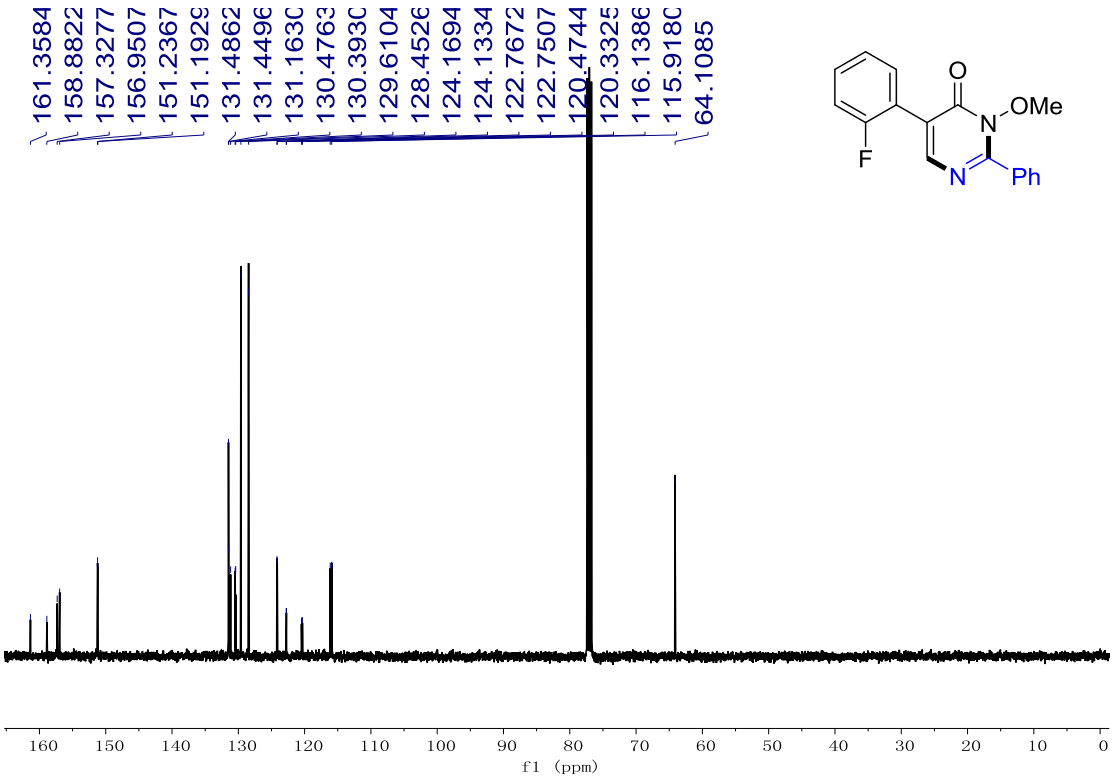
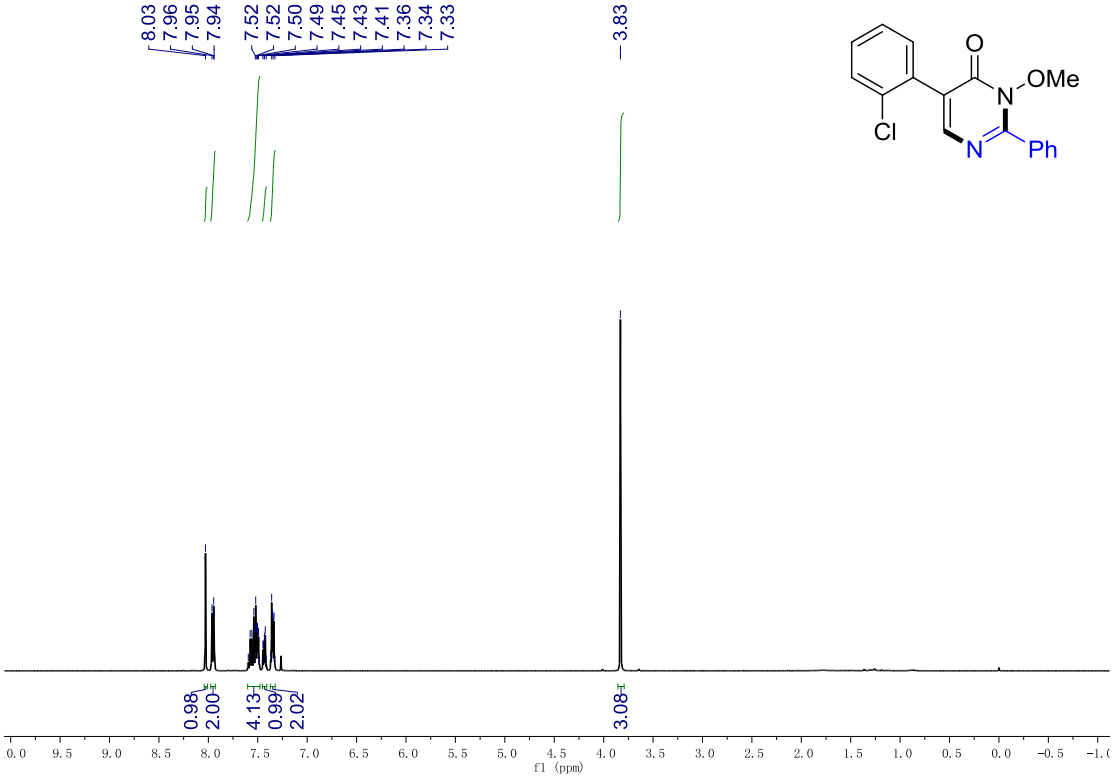
113.8575
64.0583
55.3477
MeO
O
N
OMe
N
Ph
f1 (ppm)

4ka


8.130
8.126
7.952
7.940
7.935
7.931
7.639
7.624
7.620
7.605
7.601
7.579
7.564
7.561
7.557
7.540
7.526
7.522
7.504
7.396
7.376
7.262
7.260
7.256
7.240
7.238
7.221
7.219
7.208
7.206
7.187
7.183
7.180
7.161
3.828
0.97
2.00
4.13
1.04
2.23
3.06
O
OMe
N
F
N
Ph
f1 (ppm)


161.3584
158.8822
157.3277
156.9507
151.2367
151.1929
131.4862
131.4496
131.1630
130.4763
130.3930
129.6104
128.4526
124.1694
124.1334
122.7672
122.7507
120.4744
120.3325
116.1386
115.9180
64.1085
O
OMe
N
F
N
Ph
f1 (ppm)

4la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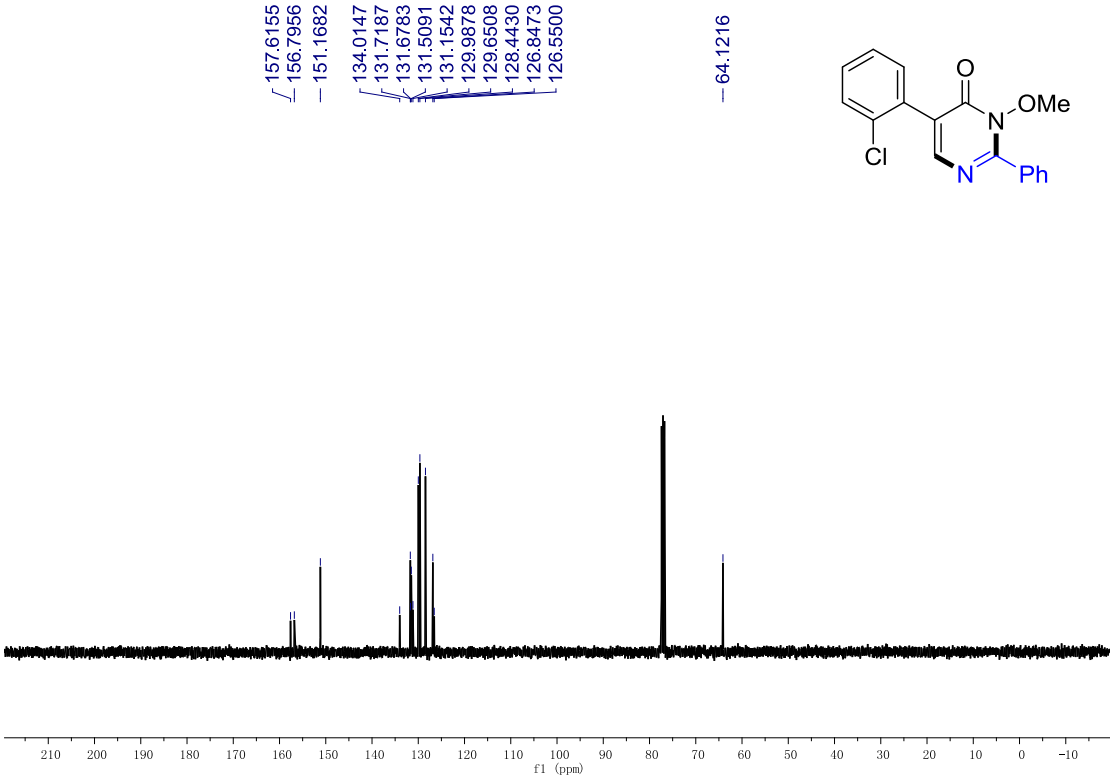
7.96
7.95
7.94
7.52
7.52
7.50
7.49
7.45
7.43
7.41
7.36
7.34
7.33
3.83
O
N
OMe
Cl
N
Ph
0.98
2.00
4.13
0.99
2.02
3.08
f1 (ppm)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156.7956
151.1682
134.0147
131.7187
131.6783
131.5091
131.1542
129.9878
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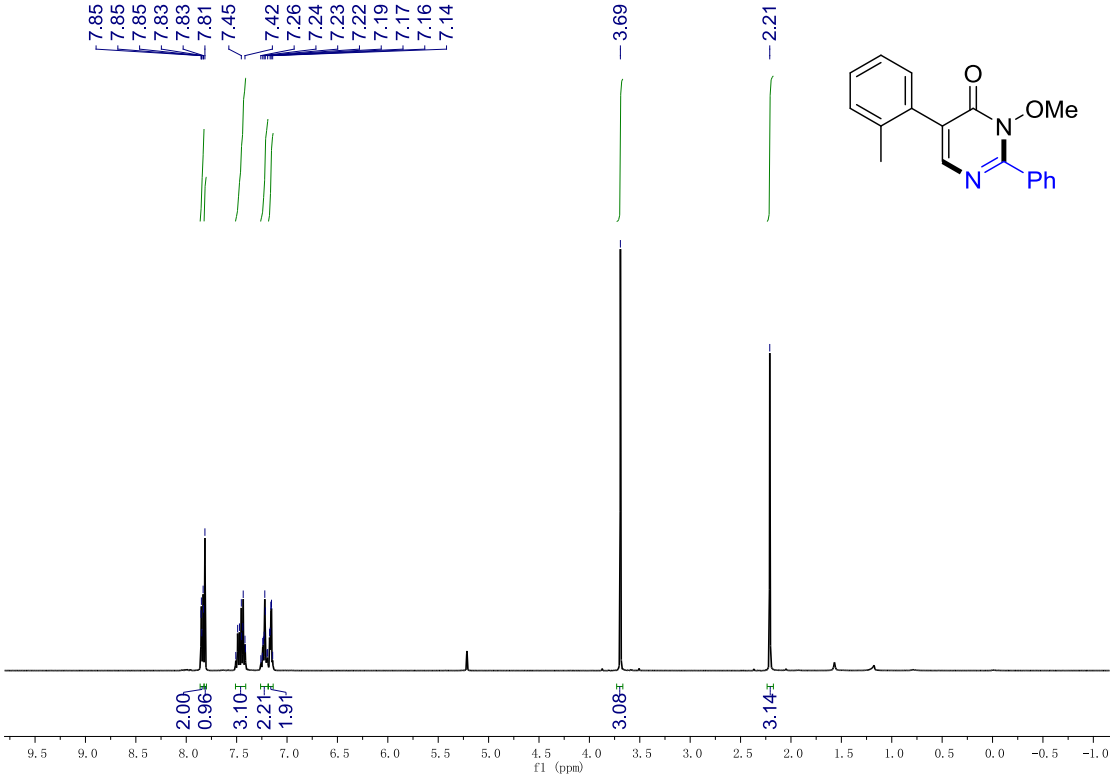
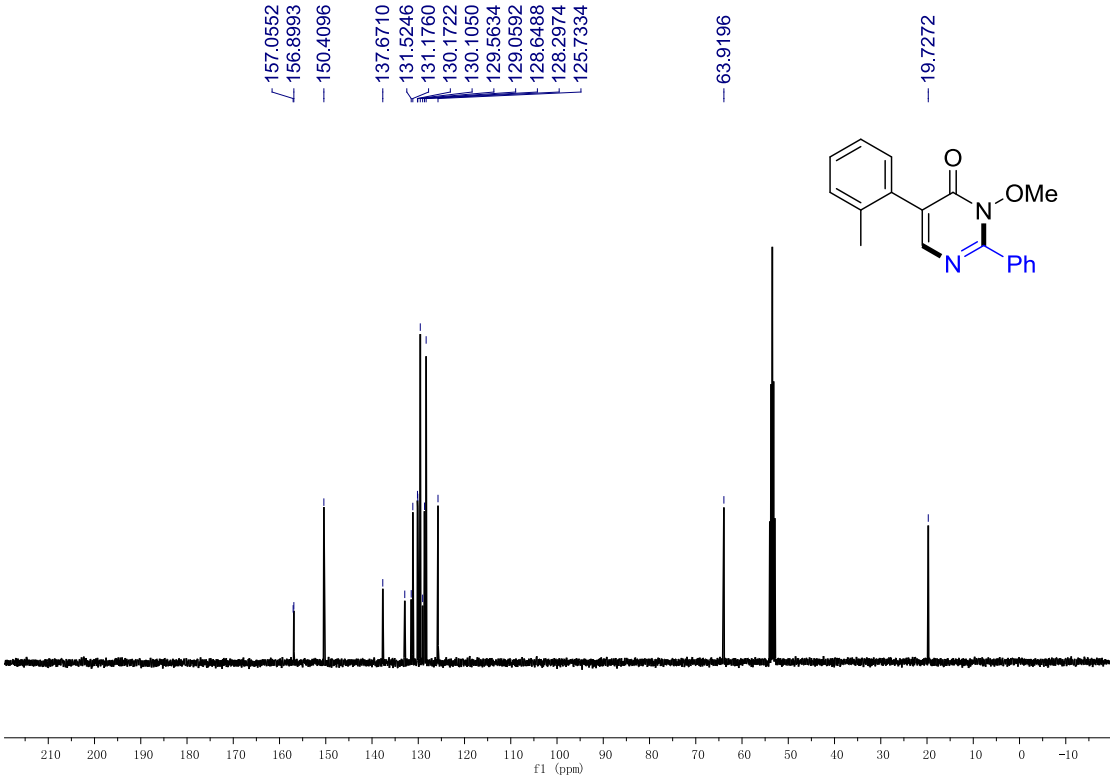
128.4430
126.8473
126.5500
64.1216
O
N
OMe
Cl
N
Ph
f1 (ppm)

4ma


7.85
7.85
7.85
7.83
7.83
7.81
7.45
7.42
7.26
7.24
7.23
7.22
7.19
7.17
7.16
7.14
3.69
2.21
O
N
OMe
N
Ph
2.00
0.96
3.10
2.21
1.91
3.08
3.14
f1 (ppm)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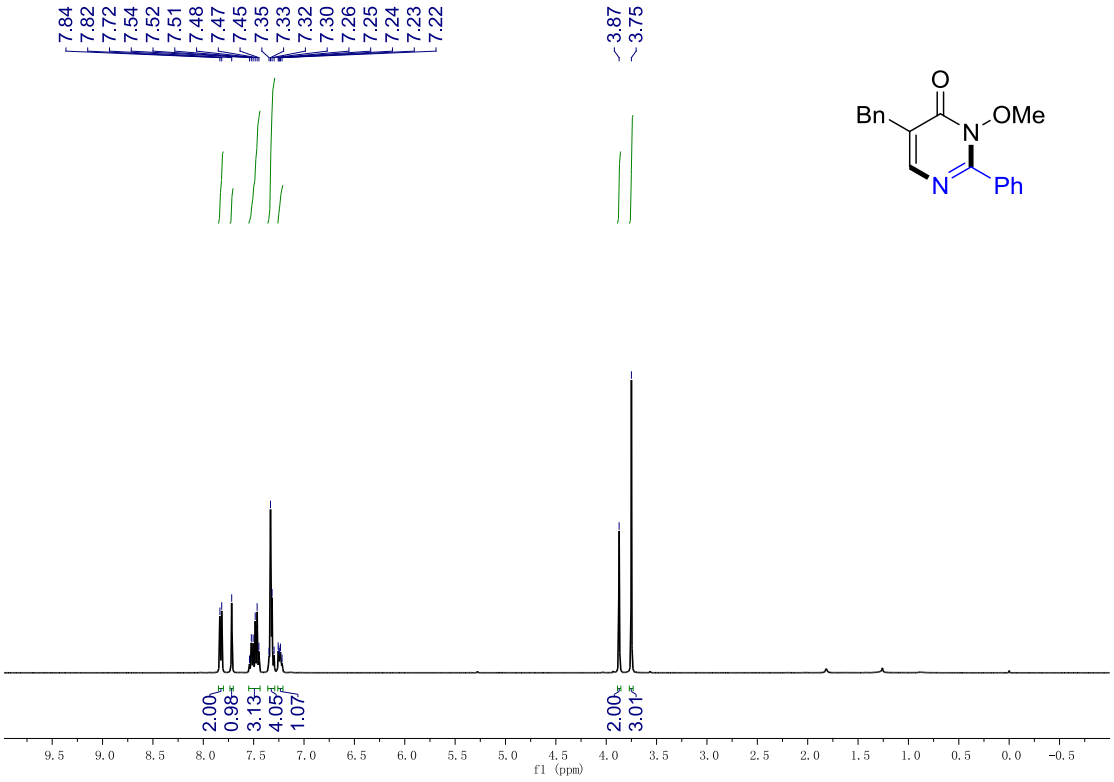
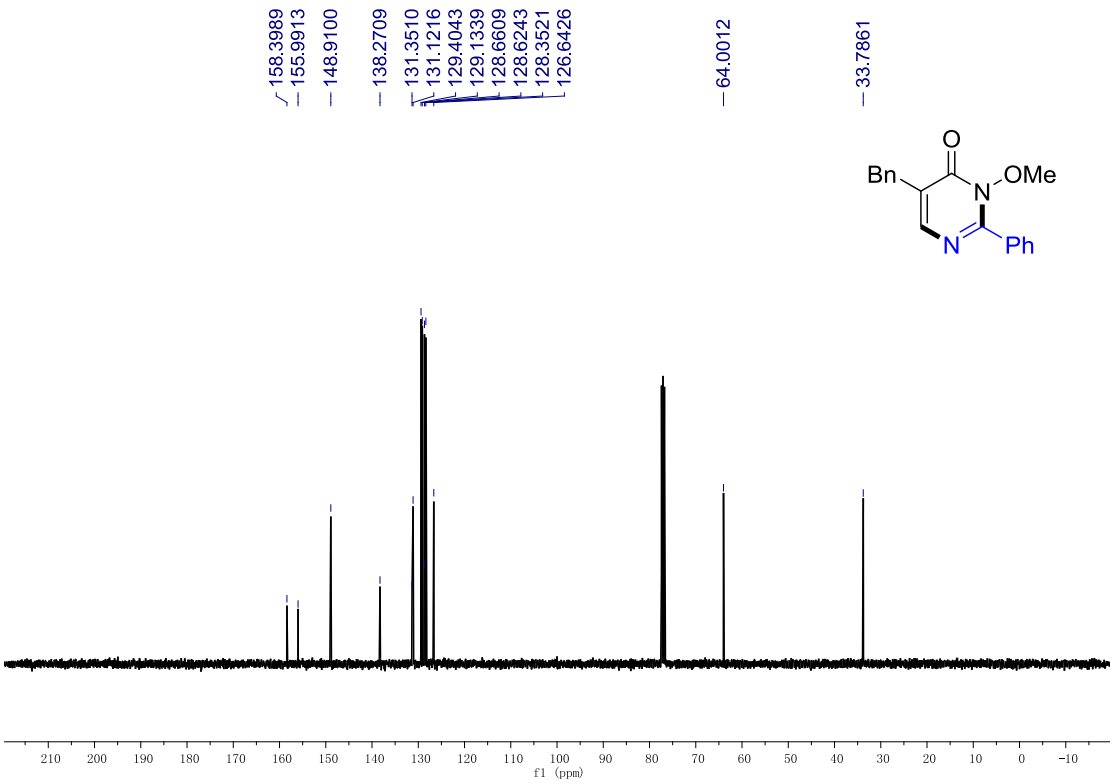
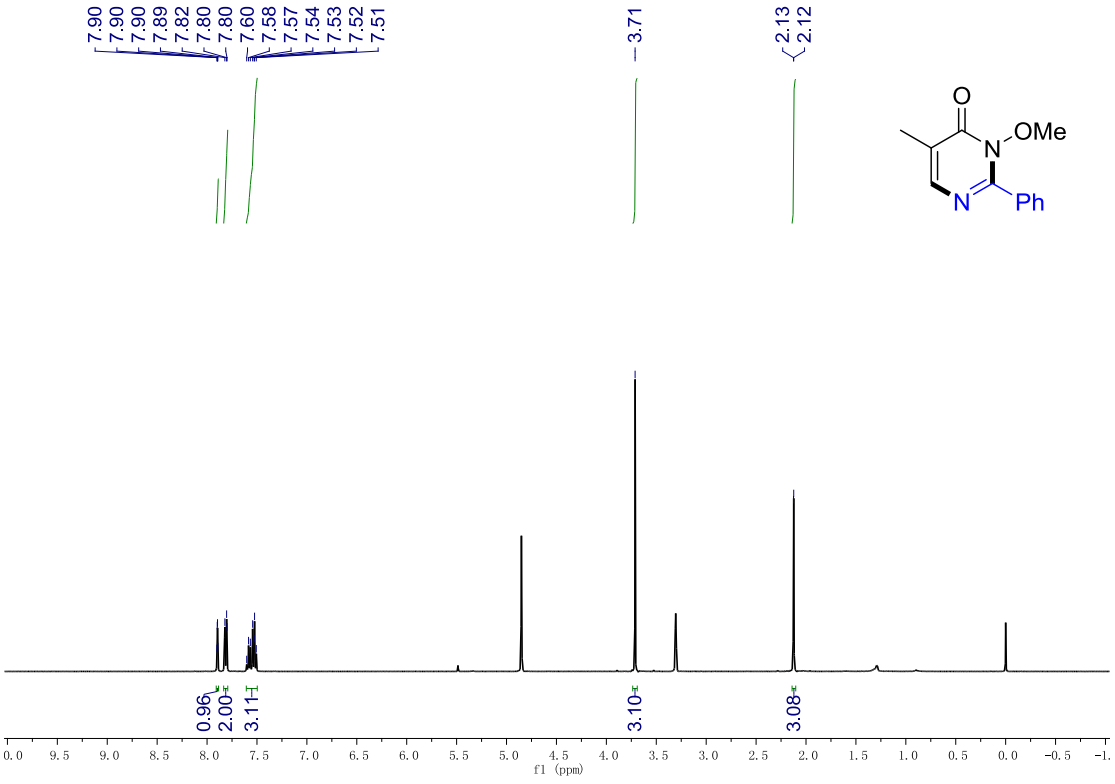
156.8993
150.4096
137.6710
131.5246
131.1760
130.1722
130.1050
129.5634
129.0592
128.6488
128.2974
125.7334
63.9196
19.7272
O
N
OMe
N
Ph
f1 (ppm)

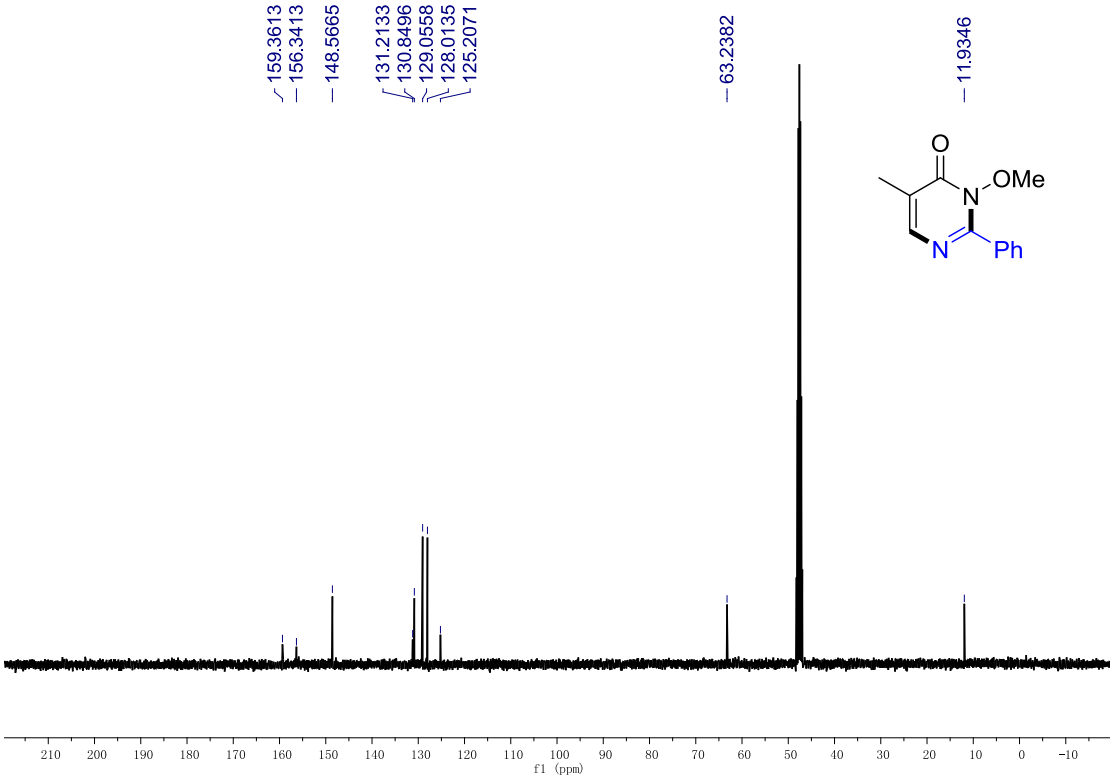
4na


7.84
7.82
7.72
7.54
7.52
7.51
7.48
7.47
7.45
7.35
7.33
7.32
7.30
7.26
7.25
7.24
7.23
7.22
3.87
3.75
Bn
O
N
OMe
N
Ph
2.00
0.98
3.13
4.05
1.07
2.00
3.01
f1 (ppm)


158.3989
155.9913
148.9100
138.2709
131.3510
131.1216
129.4043
129.1339
128.6609
128.6243
128.3521
126.6426
64.0012
33.7861
Bn
O
N
OMe
N
Ph
f1 (ppm)

4oa


7.90
7.90
7.90
7.89
7.82
7.80
7.80
7.60
7.58
7.57
7.54
7.53
7.52
7.51
3.71
2.13
2.12
O
N
OMe
N
Ph
0.96
2.00
3.11
3.10
3.08
f1 (ppm)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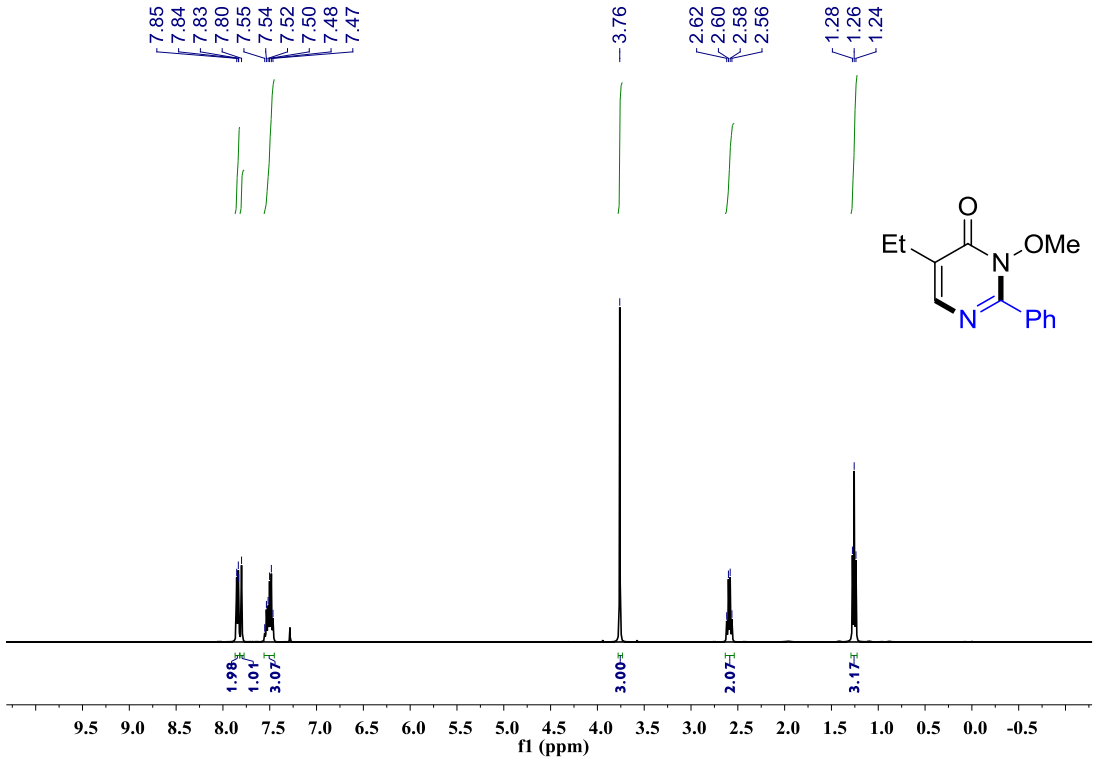
156.3413
148.5665
131.2133
130.8496
129.0558
128.0135
125.2071
63.2382
11.9346
O
N
OMe
N
Ph
f1 (ppm)

4pa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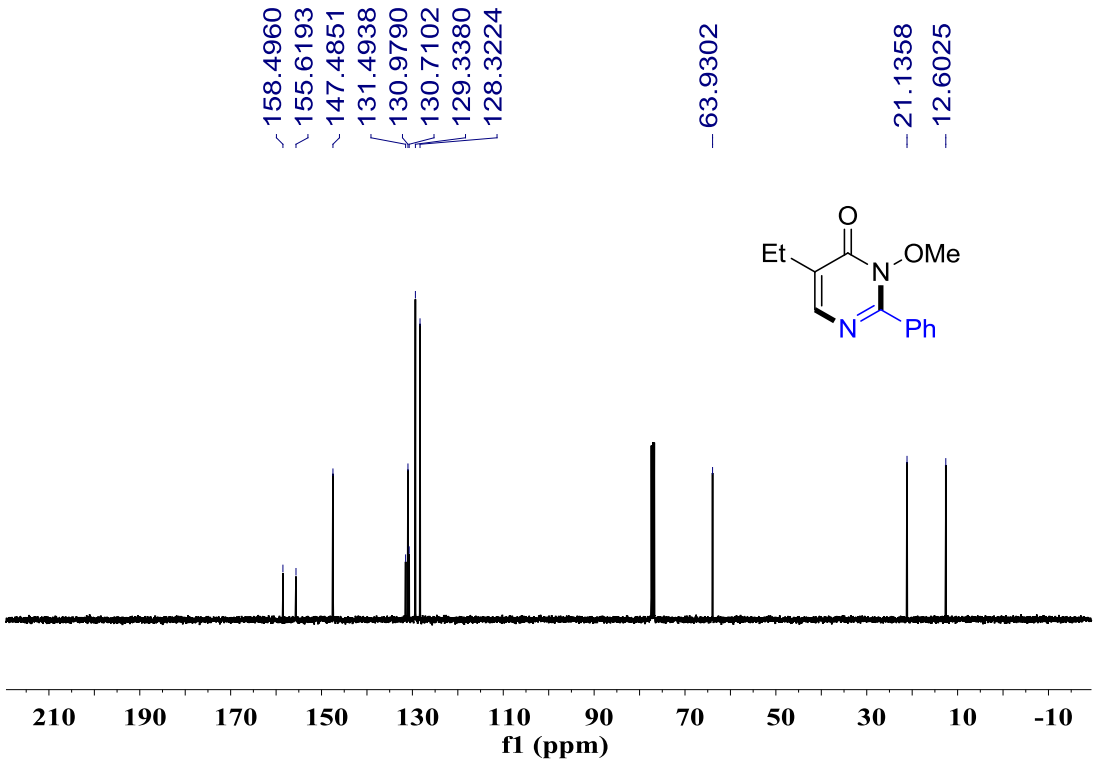
7.84
7.83
7.80
7.55
7.54
7.52
7.50
7.48
7.47
3.76
2.62
2.60
2.58
2.56
1.28
1.26
1.24
O
Et
N
OMe
N
Ph
1.98
1.01
3.07
3.00
2.07
3.17
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


158.4960
155.6193
147.4851
131.4938
130.9790
130.7102
129.3380
128.3224
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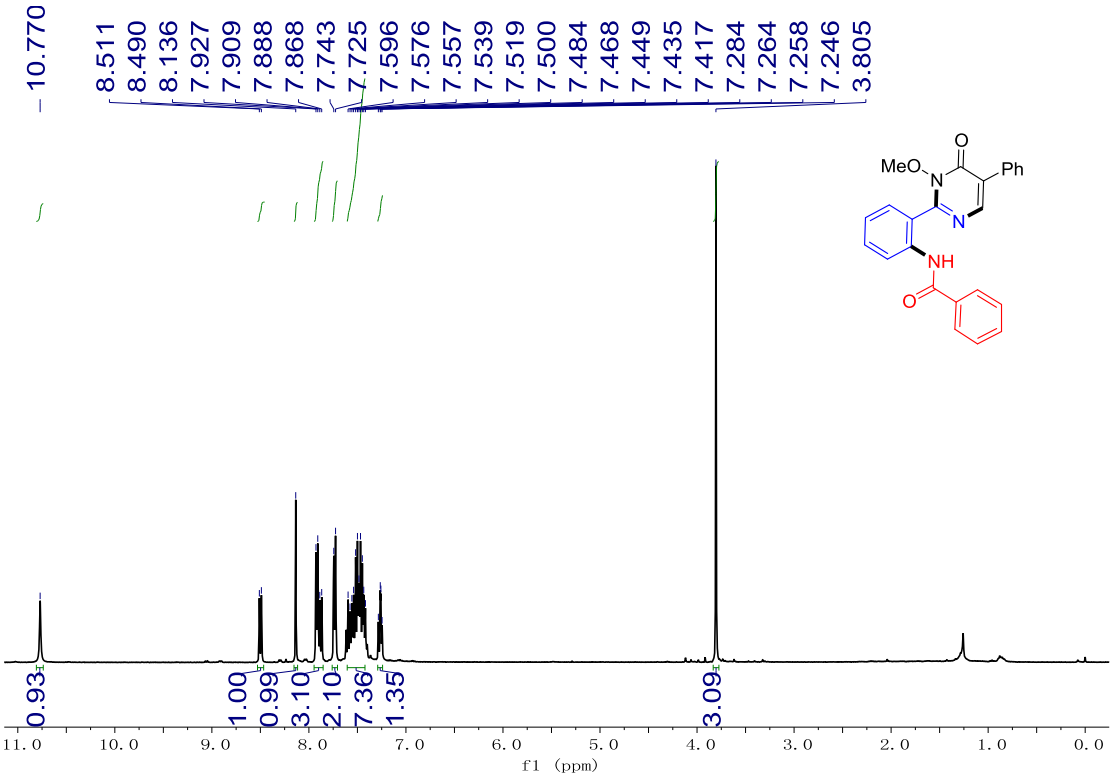
21.1358
12.6025
O
Et
N
OMe
N
Ph
210 190 170 150 130 110 90 70 50 30 10 -10
f1 (ppm)

5aa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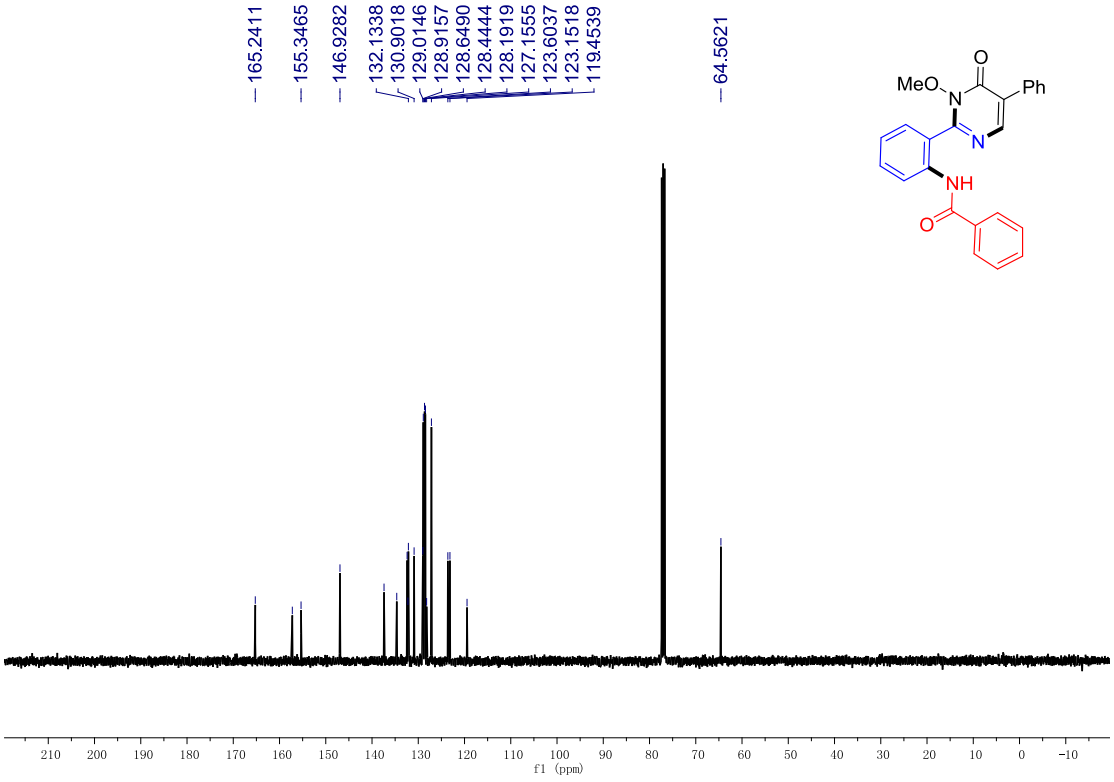
8.490
8.136
7.927
7.909
7.888
7.868
7.743
7.725
7.596
7.576
7.557
7.539
7.519
7.500
7.484
7.468
7.449
7.435
7.417
7.284
7.264
7.258
7.246
3.805
MeO
N
O
Ph
N
NH
O
0.93
1.00
0.99
3.10
2.10
7.36
1.35
3.09
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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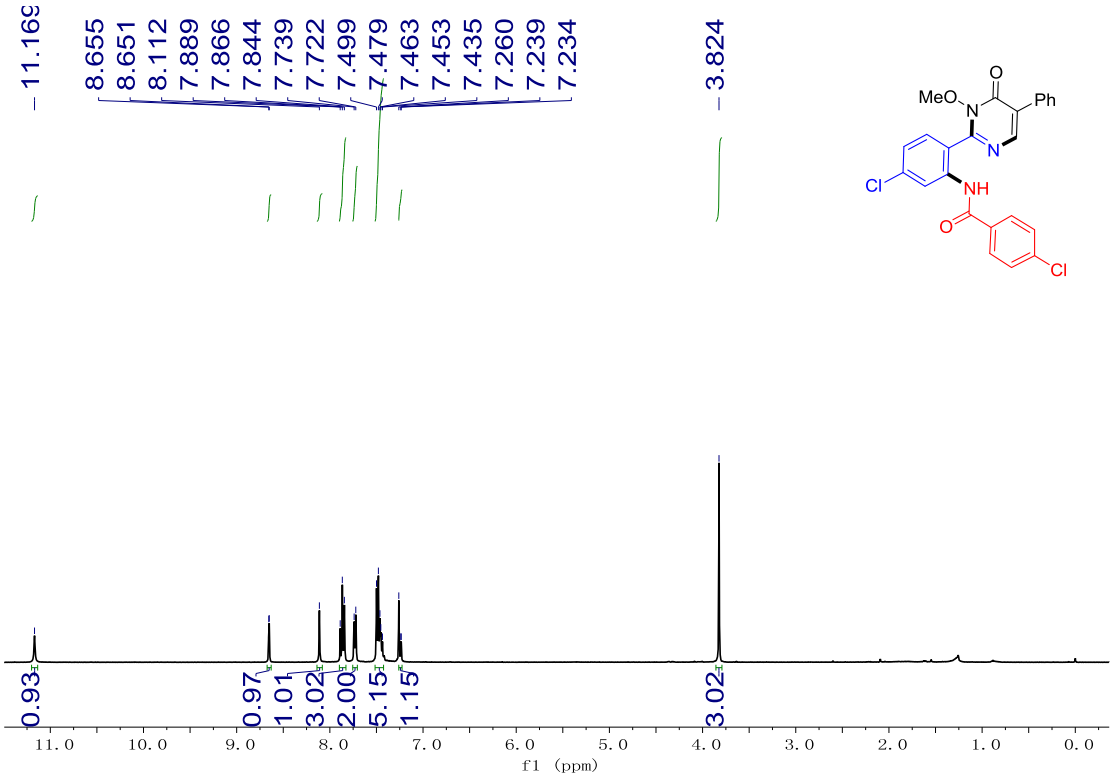
146.9282
132.1338
130.9018
129.0146
128.9157
128.6490
128.4444
128.1919
127.1555
123.6037
123.1518
119.4539
64.5621
MeO
N
O
Ph
N
NH
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

5ab


11.16
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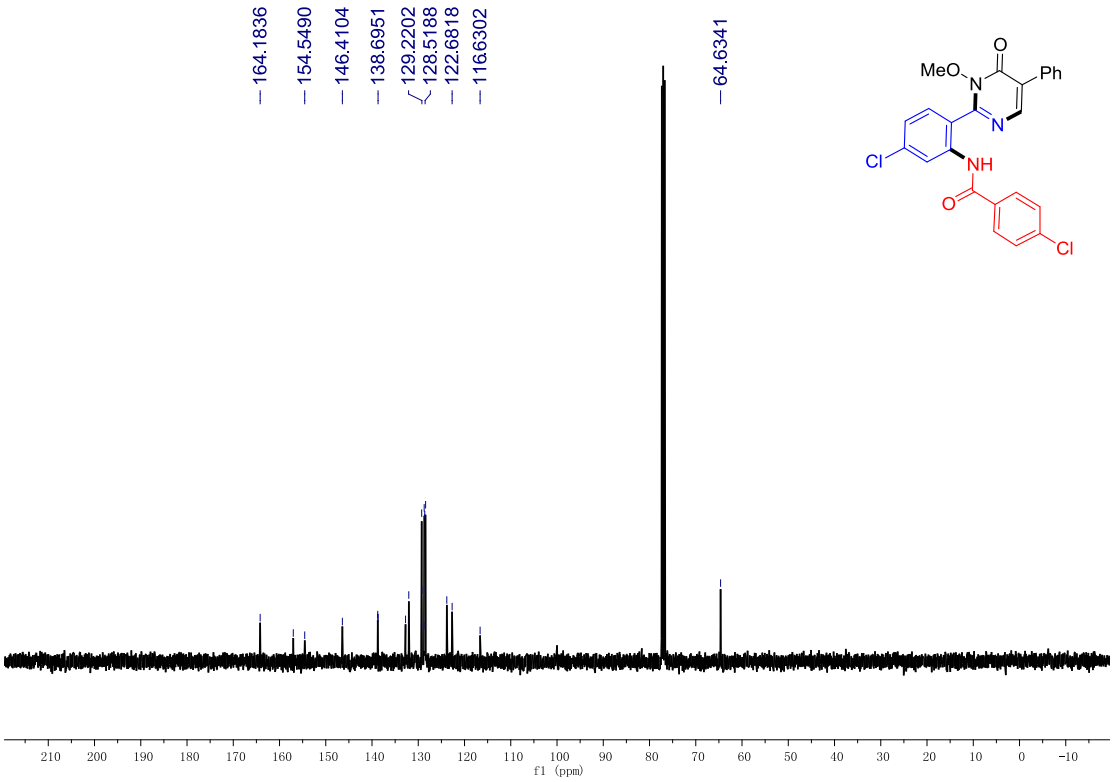
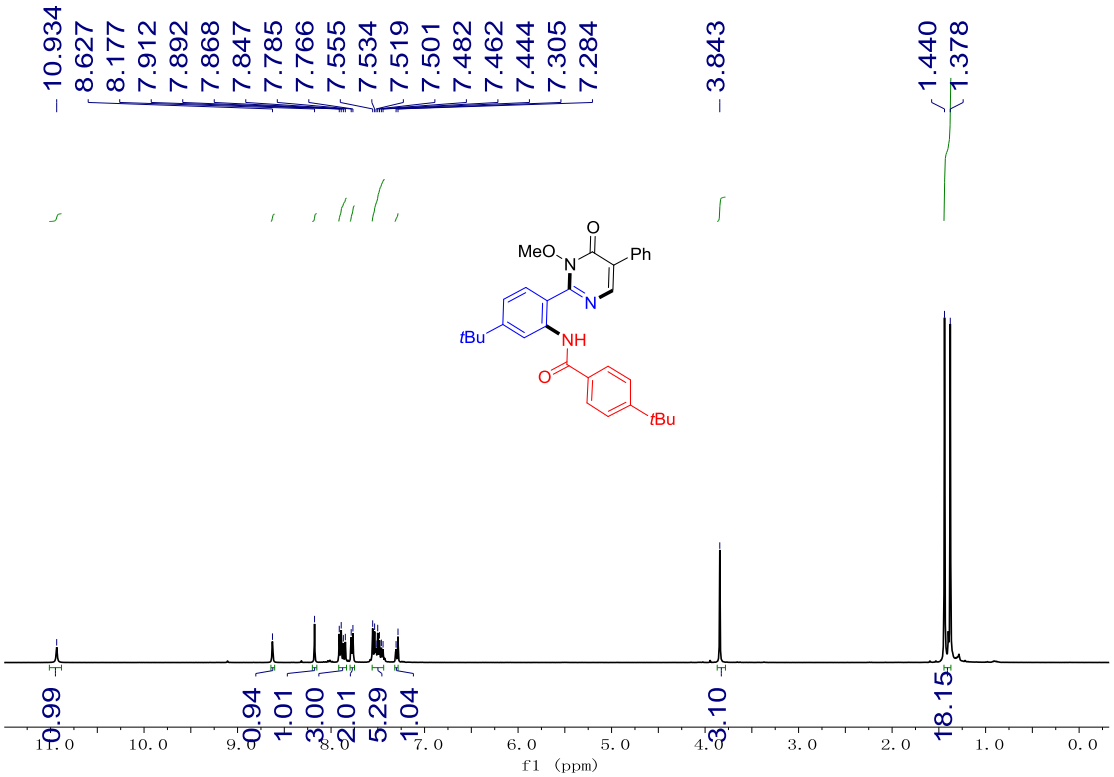
8.651
8.112
7.889
7.866
7.844
7.739
7.722
7.499
7.479
7.463
7.453
7.435
7.260
7.239
7.234
3.824
MeO
N
O
Ph
N
Cl
NH
O
Cl
0.93
0.97
1.01
3.02
2.00
5.15
1.15
3.02
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


164.1836
154.5490
146.4104
138.6951
129.2202
128.5188
122.6818
116.6302
64.6341
MeO
N
O
Ph
N
Cl
NH
O
Cl
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)

5ac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8.177
7.912
7.892
7.868
7.847
7.785
7.766
7.555
7.534
7.519
7.501
7.482
7.462
7.444
7.305
7.284
3.843
1.440
1.378
MeO
N
O
Ph
N
tBu
NH
O
tBu
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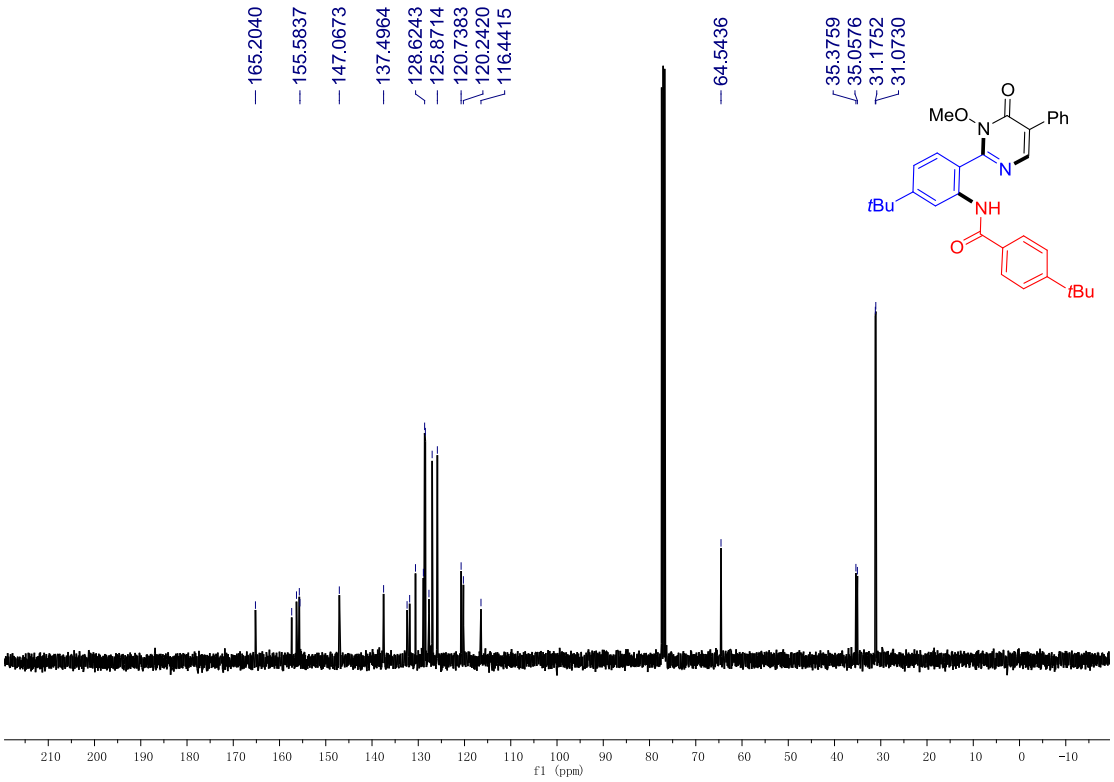
1.01
3.00
2.01
5.29
1.04
3.10
18.15
f1 (ppm)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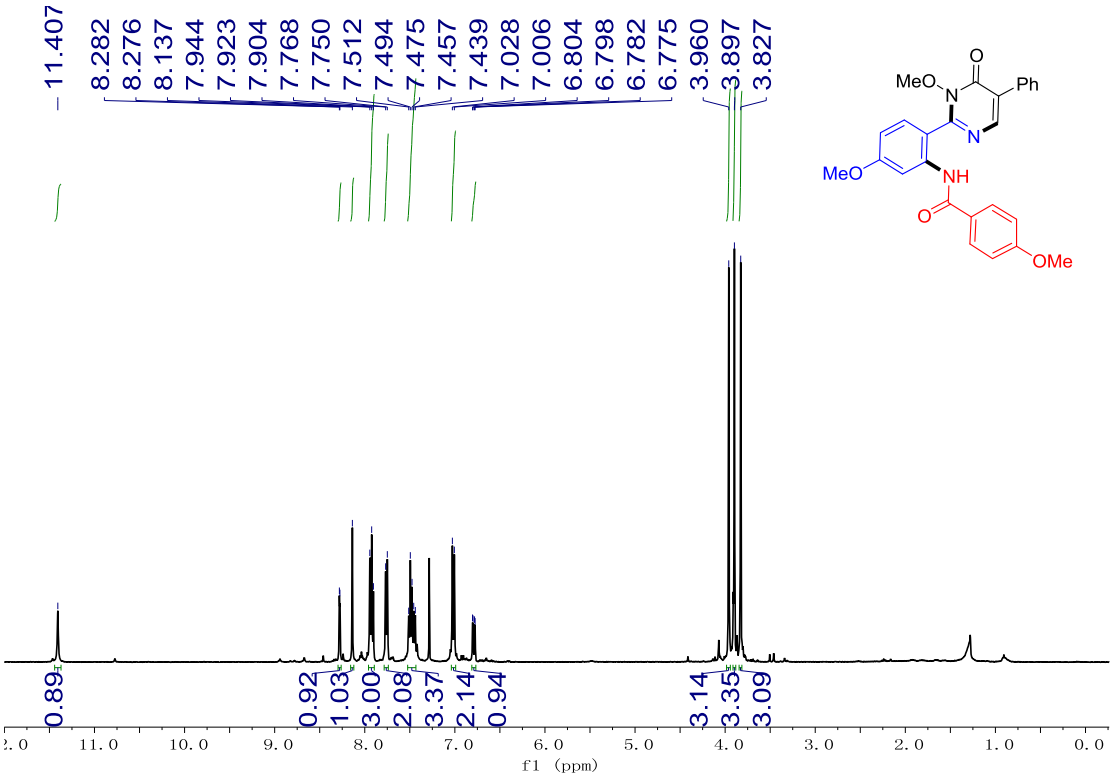
137.4964
128.6243
125.8714
120.7383
120.2420
116.4415
64.5436
35.3759
35.0576
31.1752
31.0730
MeO
N
O
Ph
N
tBu
NH
O
tBu
f1 (ppm)

5ad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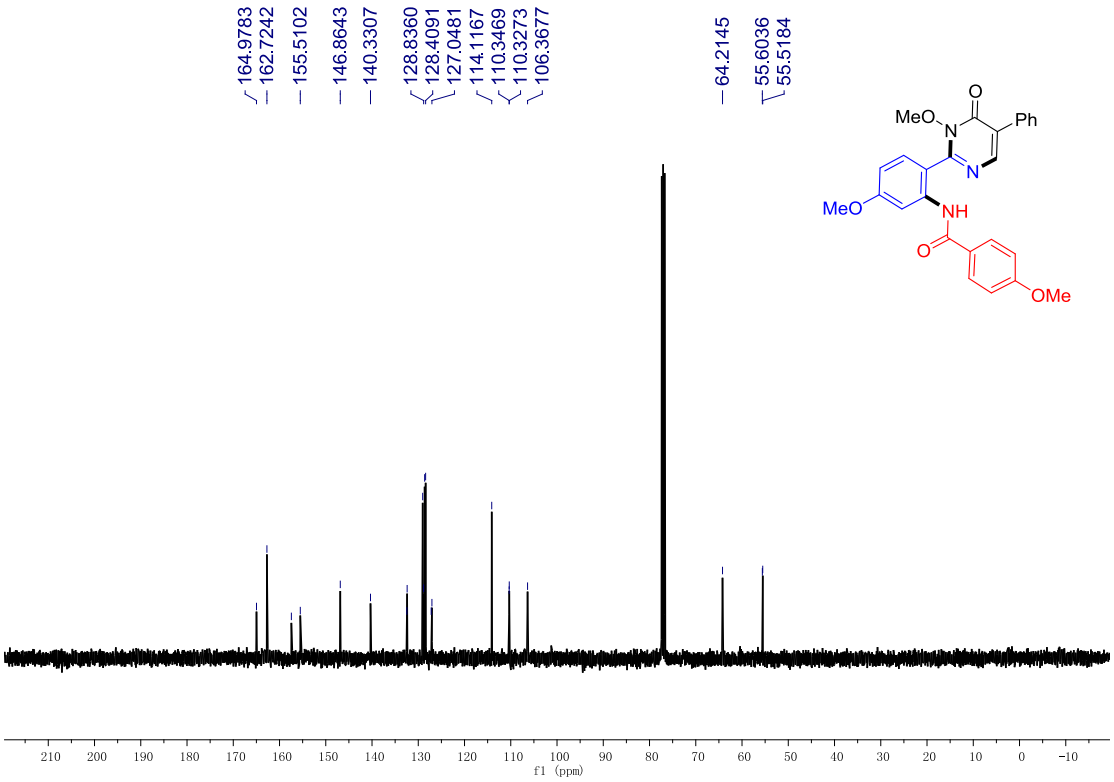
8.137
7.944
7.923
7.904
7.768
7.750
7.512
7.494
7.475
7.457
7.439
7.028
7.006
6.804
6.798
6.782
6.775
3.960
3.897
3.827
MeO
N
O
Ph
N
MeO
NH
O
OMe
0.89
0.92
1.03
3.00
2.08
3.37
2.14
0.94
3.14
3.35
3.09
f1 (ppm)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114.1167
110.3469
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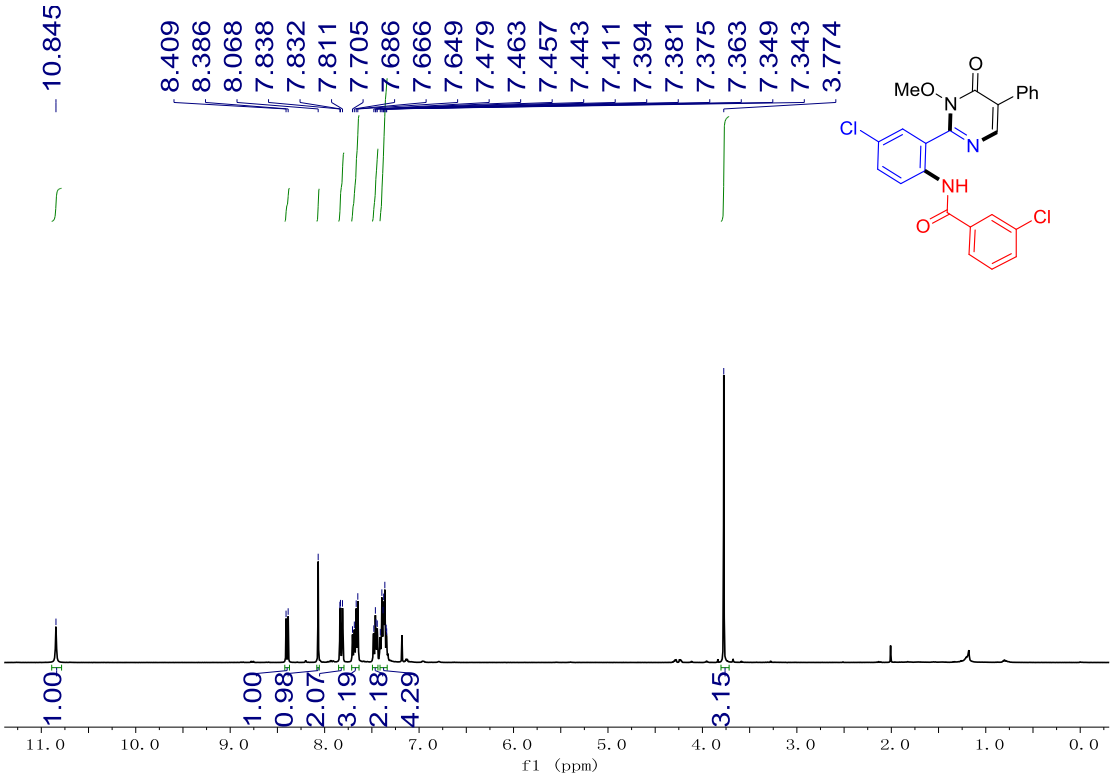
106.3677
64.2145
55.6036
55.5184
MeO
N
O
Ph
N
MeO
NH
O
OMe
f1 (ppm)

5ae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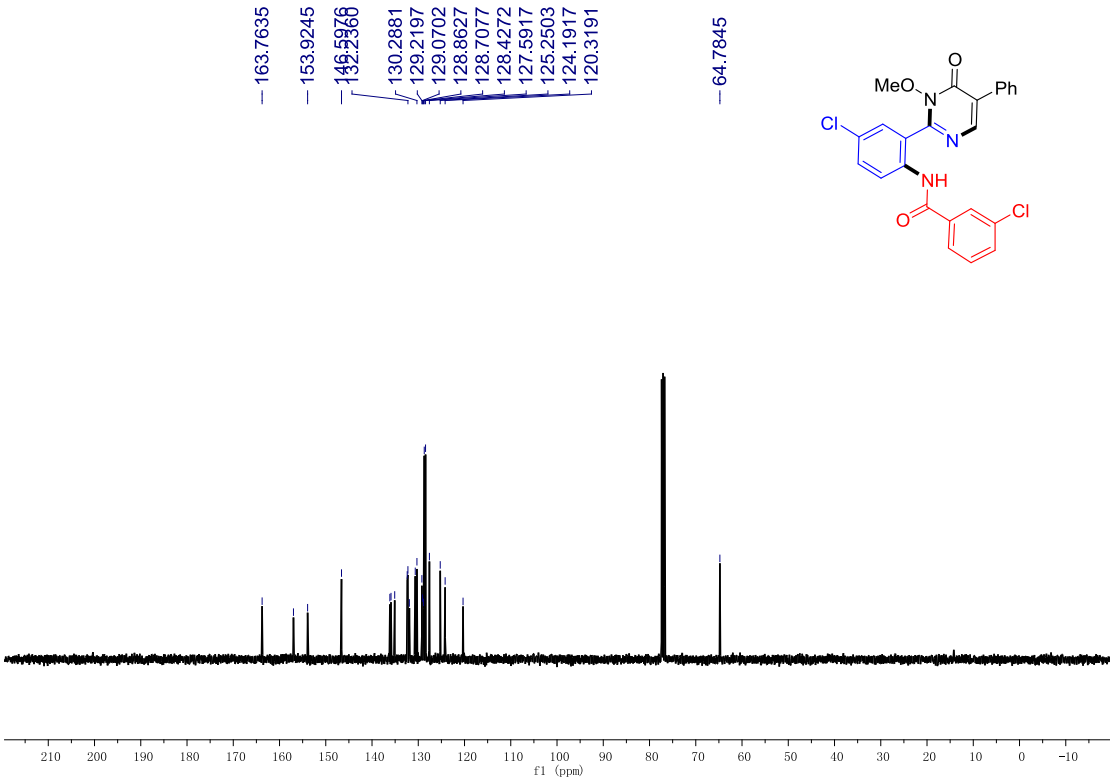
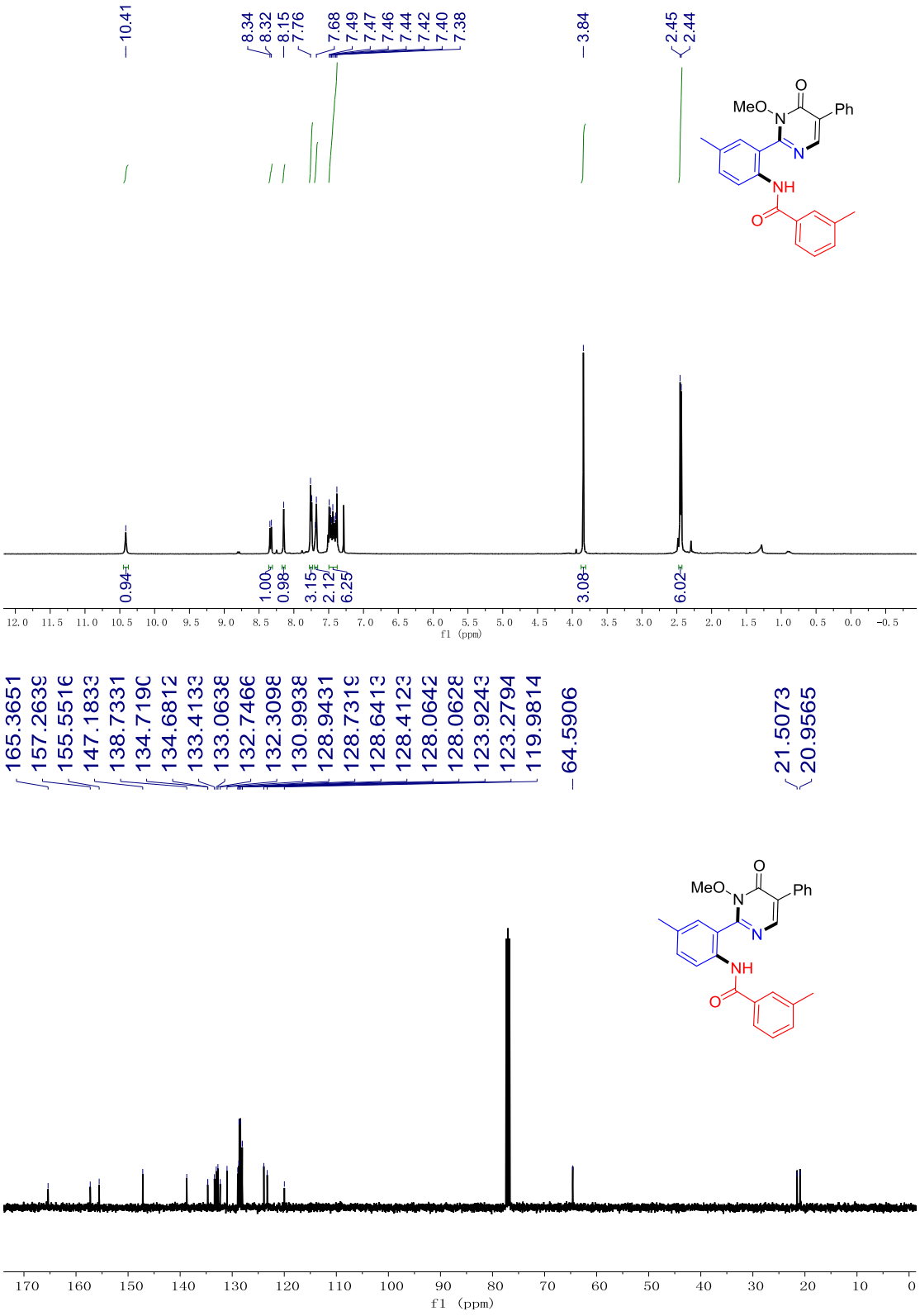
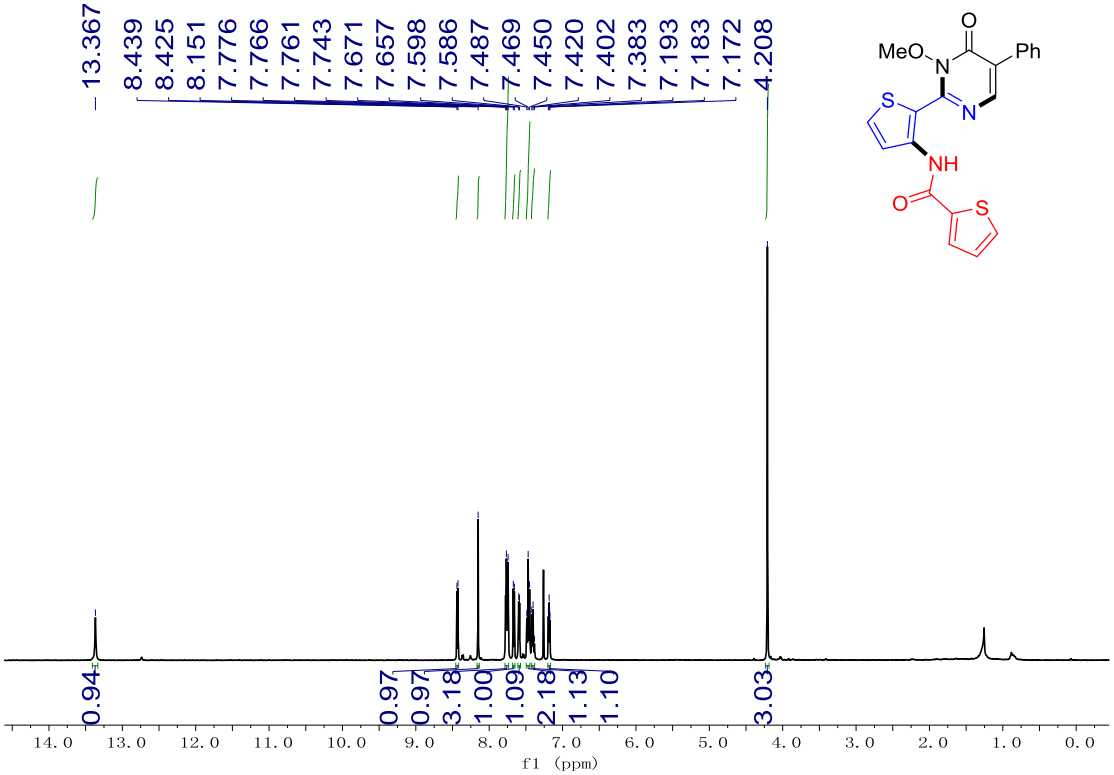
8.409
8.386
8.068
7.838
7.832
7.811
7.705
7.686
7.666
7.649
7.479
7.463
7.457
7.443
7.411
7.394
7.381
7.375
7.363
7.349
7.343
3.774
MeO
N
O
Ph
Cl
N
NH
O
Cl
1.00
1.00
0.98
2.07
3.19
2.18
4.29
3.15
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

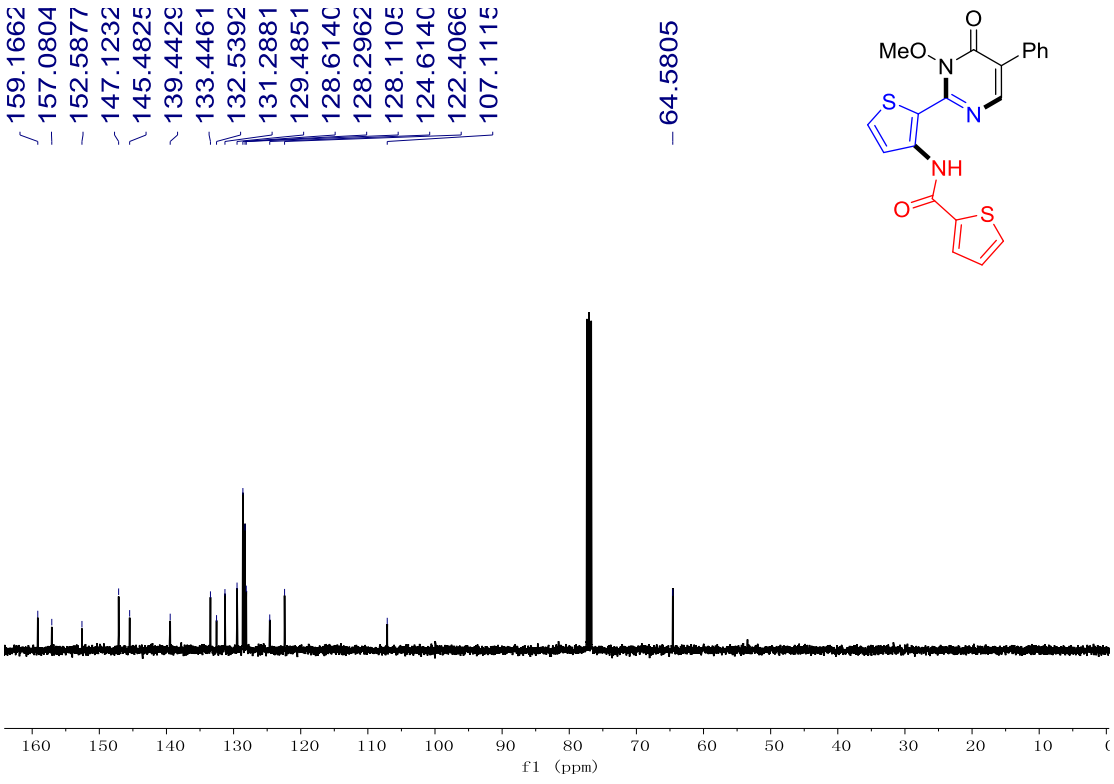

163.7635
153.9245
146.5976
132.2360
130.2881
129.2197
129.0702
128.8627
128.7077
128.4272
127.5917
125.2503
124.1917
120.3191
64.7845
MeO
N
O
Ph
Cl
N
NH
O
Cl
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

5af

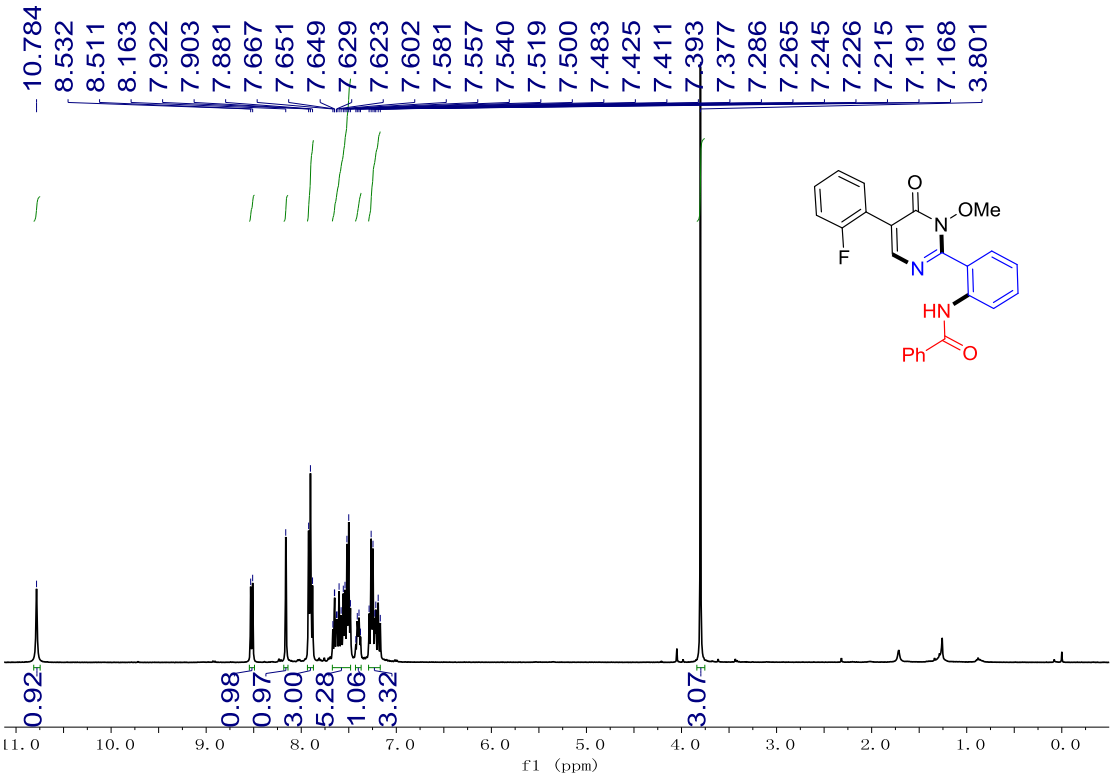

10.41
8.34
8.32
8.15
7.76
7.68
7.49
7.47
7.46
7.44
7.42
7.40
7.38
3.84
2.45
2.44
MeO
N
O
Ph
N
NH
O
0.94
1.00
0.98
3.15
2.12
2.25
3.08
6.02
f1 (ppm)
165.3651
157.2639
155.5516
147.1833
138.7331
134.7190
134.6812
133.4133
133.0638
132.7466
132.3098
130.9938
128.9431
128.7319
128.6413
128.4123
128.0642
128.0628
123.9243
123.2794
119.9814
64.5906
21.5073
20.9565
f1 (ppm)

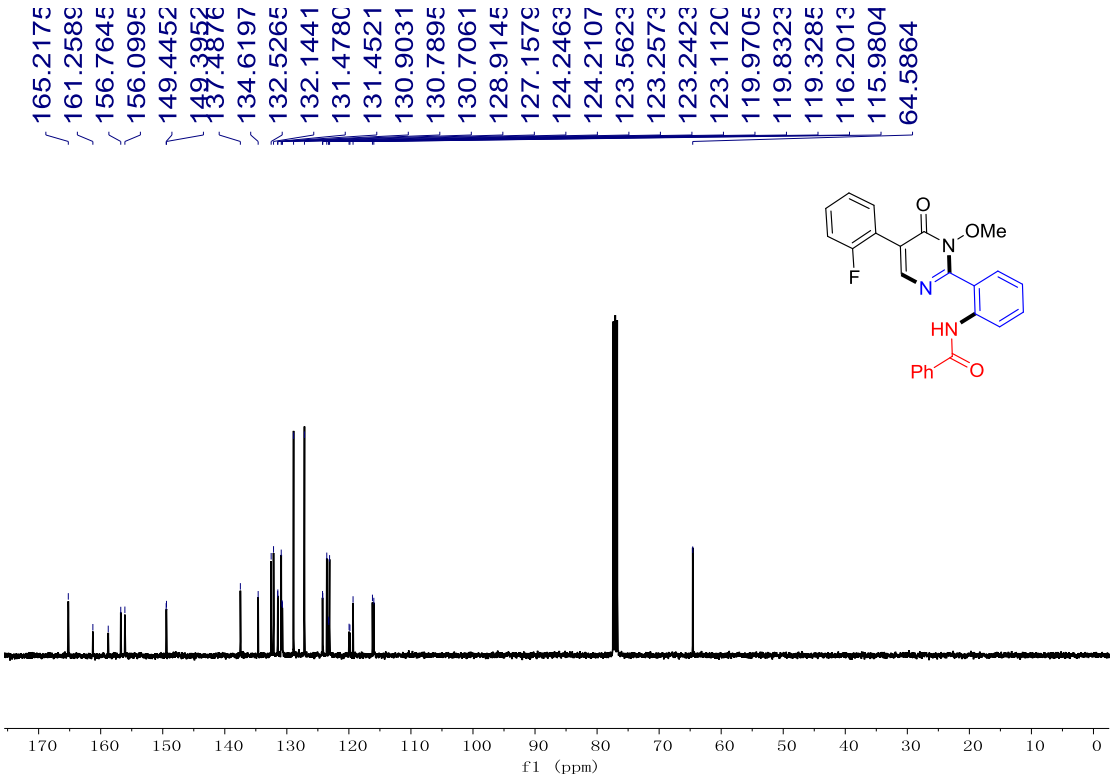
5ag


13.367
8.439
8.425
8.151
7.776
7.766
7.761
7.743
7.671
7.657
7.598
7.586
7.487
7.469
7.450
7.420
7.402
7.383
7.193
7.183
7.172
4.208
0.94
0.97
0.97
3.18
1.00
1.09
2.18
1.13
1.10
3.03
MeO
N
O
Ph
S
N
NH
O
S
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

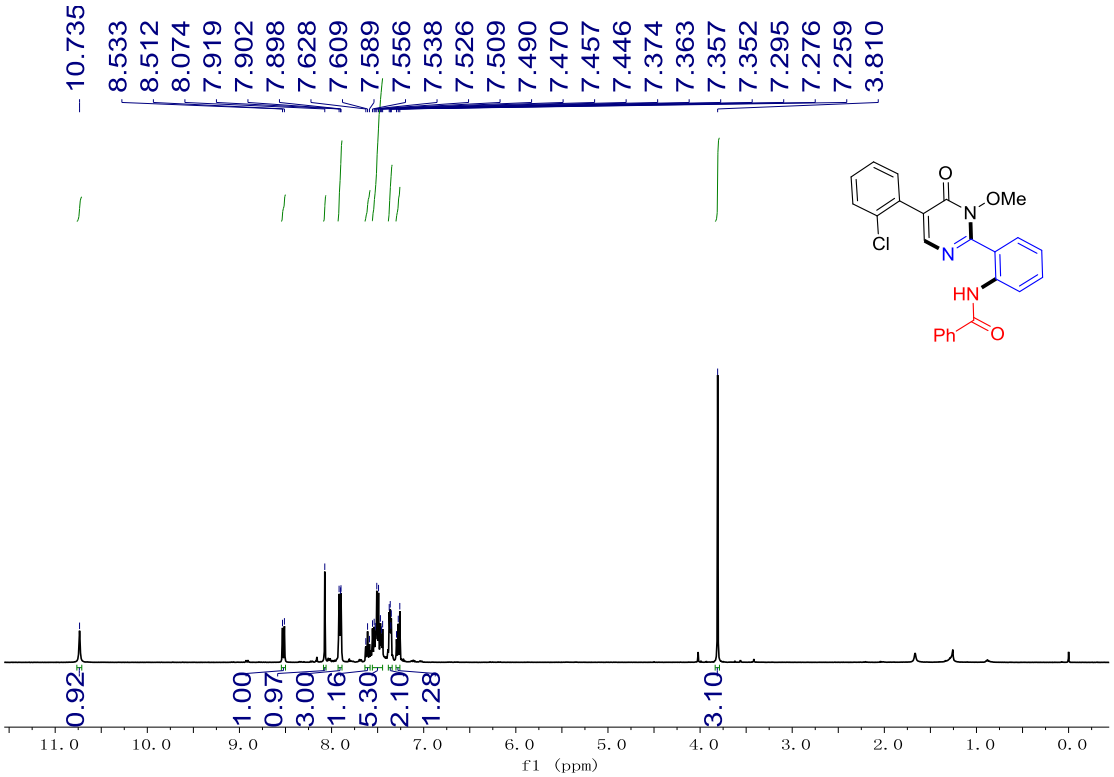

159.1662
157.0804
152.5877
147.1232
145.4825
139.4429
133.4461
132.5392
131.2881
129.4851
128.6140
128.2962
128.1105
124.6140
122.4066
107.1115
64.5805
MeO
N
O
Ph
S
N
NH
O
S
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

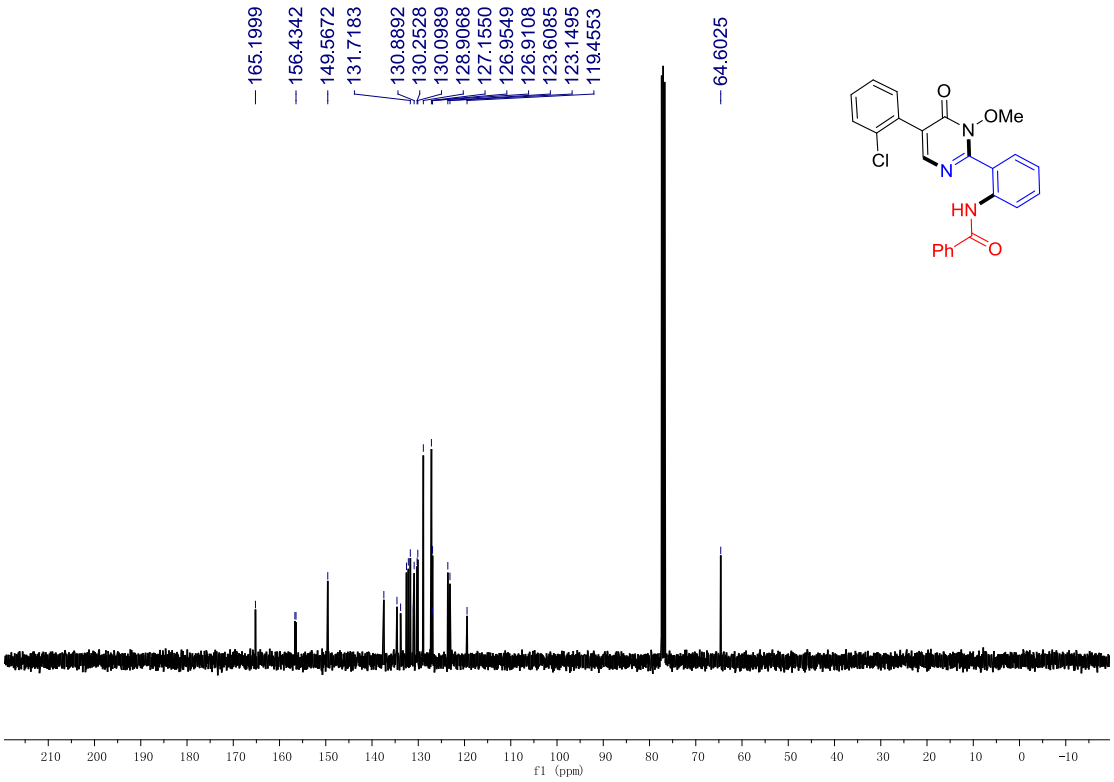
5ba


10.784
8.532
8.511
8.163
7.922
7.903
7.881
7.667
7.651
7.649
7.629
7.623
7.602
7.581
7.557
7.540
7.519
7.500
7.483
7.425
7.411
7.393
7.377
7.286
7.265
7.245
7.226
7.215
7.191
7.168
3.801
0.92
0.98
0.97
3.00
5.28
1.06
3.32
3.07
f1 (ppm)
OMe
F
HN
Ph
O

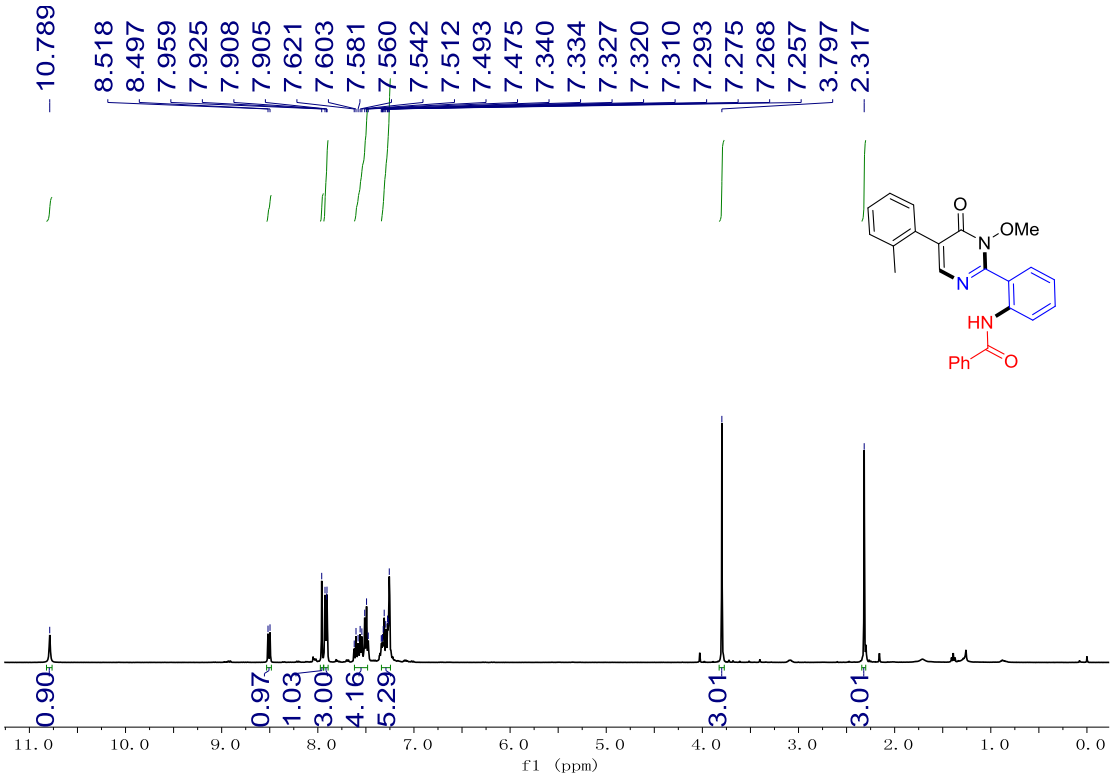

165.2175
161.2589
156.7645
156.0995
149.4452
134.6197
132.5265
132.1441
131.4780
131.4521
130.9031
130.7895
130.7061
128.9145
127.1579
124.2463
124.2107
123.5623
123.2573
123.2423
123.1120
119.9705
119.8323
119.3285
116.2013
115.9804
64.5864
f1 (ppm)
OMe
F
HN
Ph
O

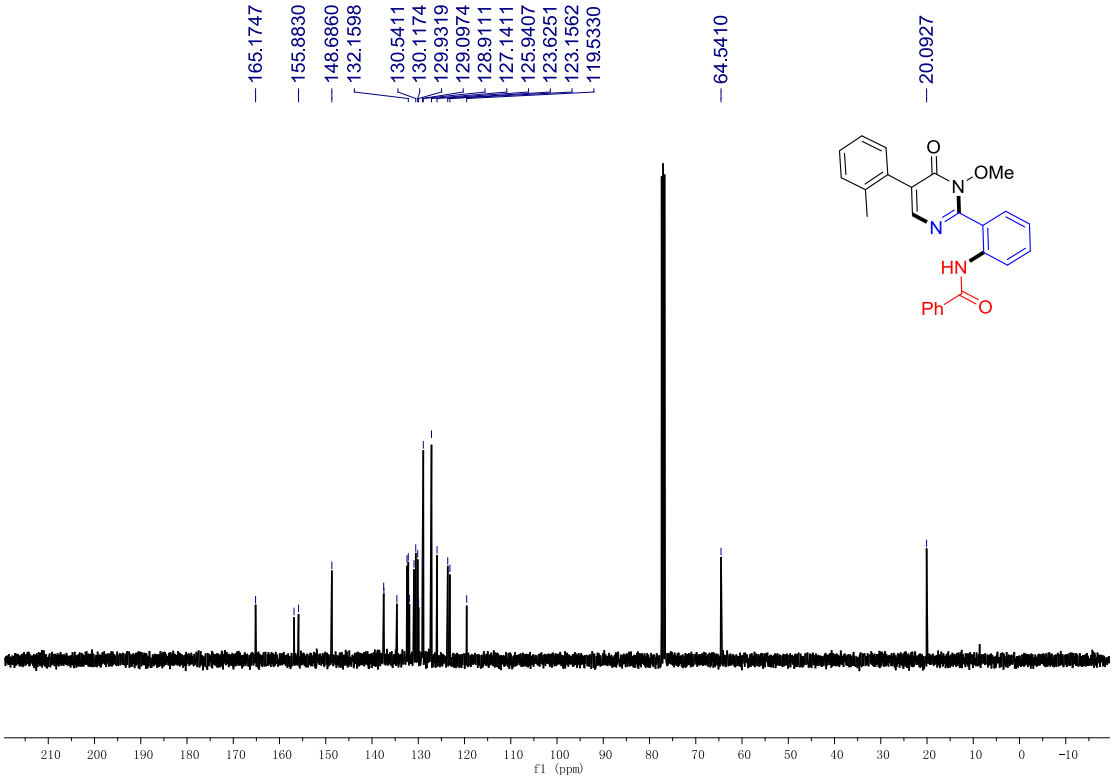
5ca


10.735
8.533
8.512
8.074
7.919
7.902
7.898
7.628
7.609
7.589
7.556
7.538
7.526
7.509
7.490
7.470
7.457
7.446
7.374
7.363
7.357
7.352
7.295
7.276
7.259
3.810
O
N
OMe
Cl
N
HN
Ph
O
0.92
1.00
0.97
3.00
1.16
5.30
2.10
1.28
3.10
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

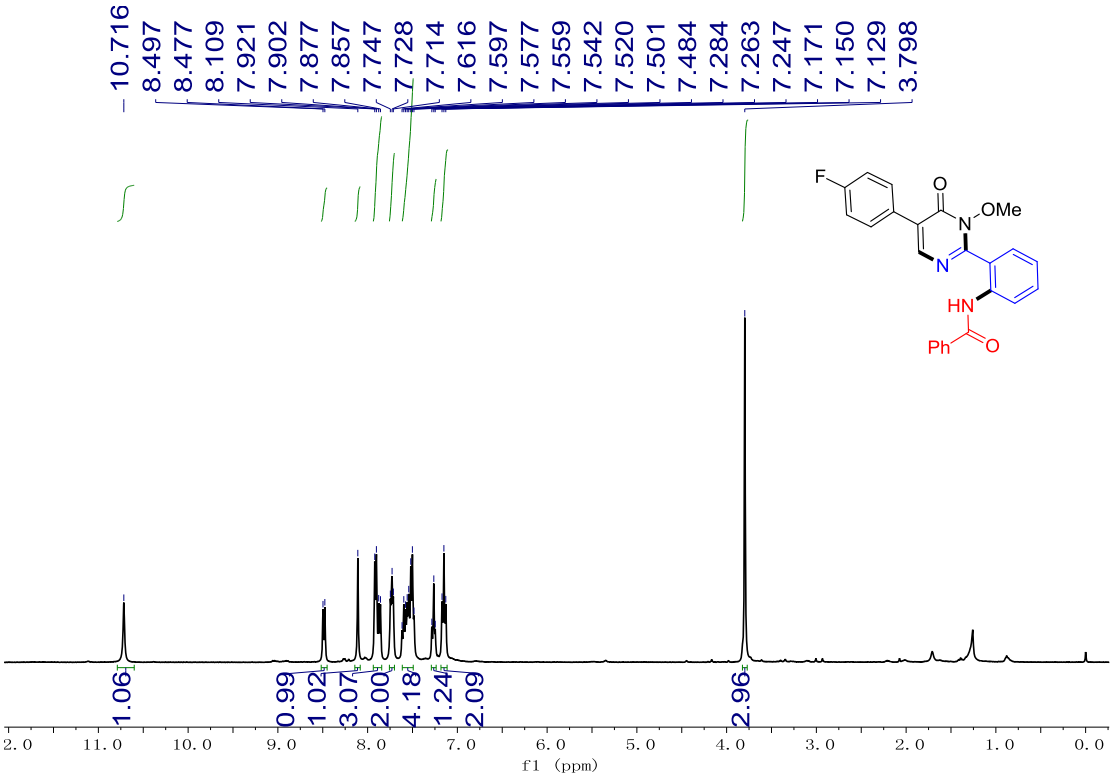

165.1999
156.4342
149.5672
131.7183
130.8892
130.2528
130.0989
128.9068
127.1550
126.9549
126.9108
123.6085
123.1495
119.4553
64.6025
O
N
OMe
Cl
N
HN
Ph
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

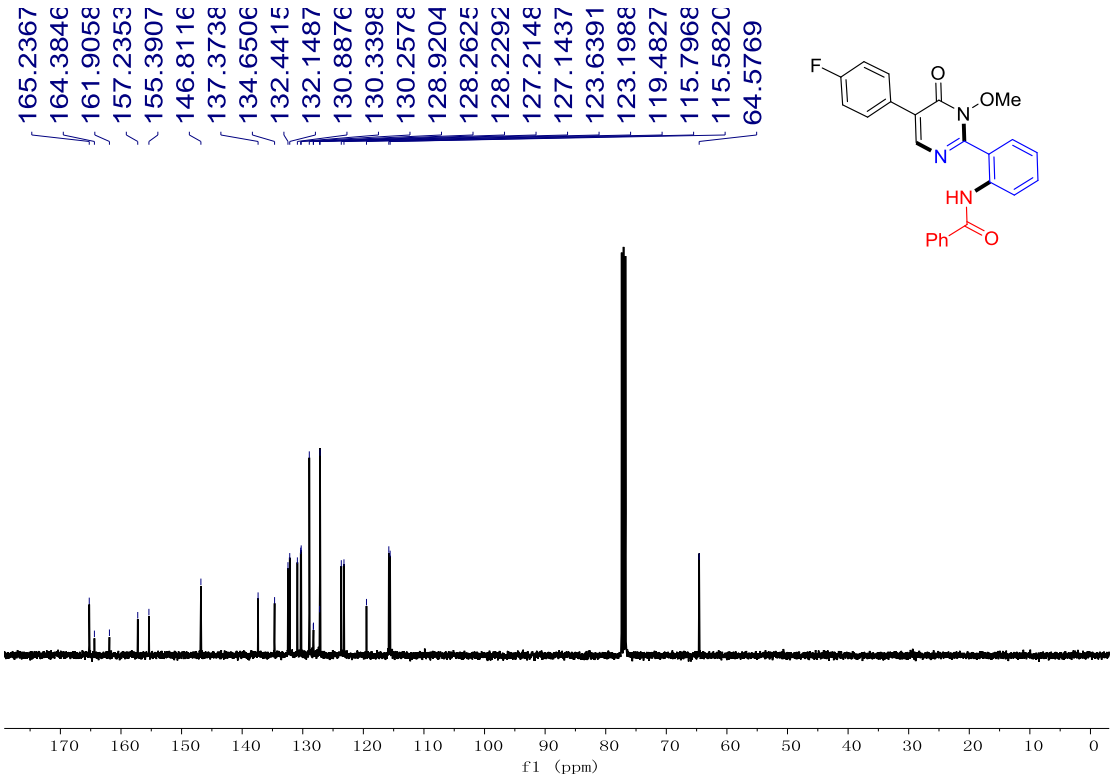
5da


10.789
8.518
8.497
7.959
7.925
7.908
7.905
7.621
7.603
7.581
7.560
7.542
7.512
7.493
7.475
7.340
7.334
7.327
7.320
7.310
7.293
7.275
7.268
7.257
3.797
2.317
O
N
OMe
N
HN
Ph
O
0.90
0.97
1.03
3.00
4.16
5.29
3.01
3.01
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

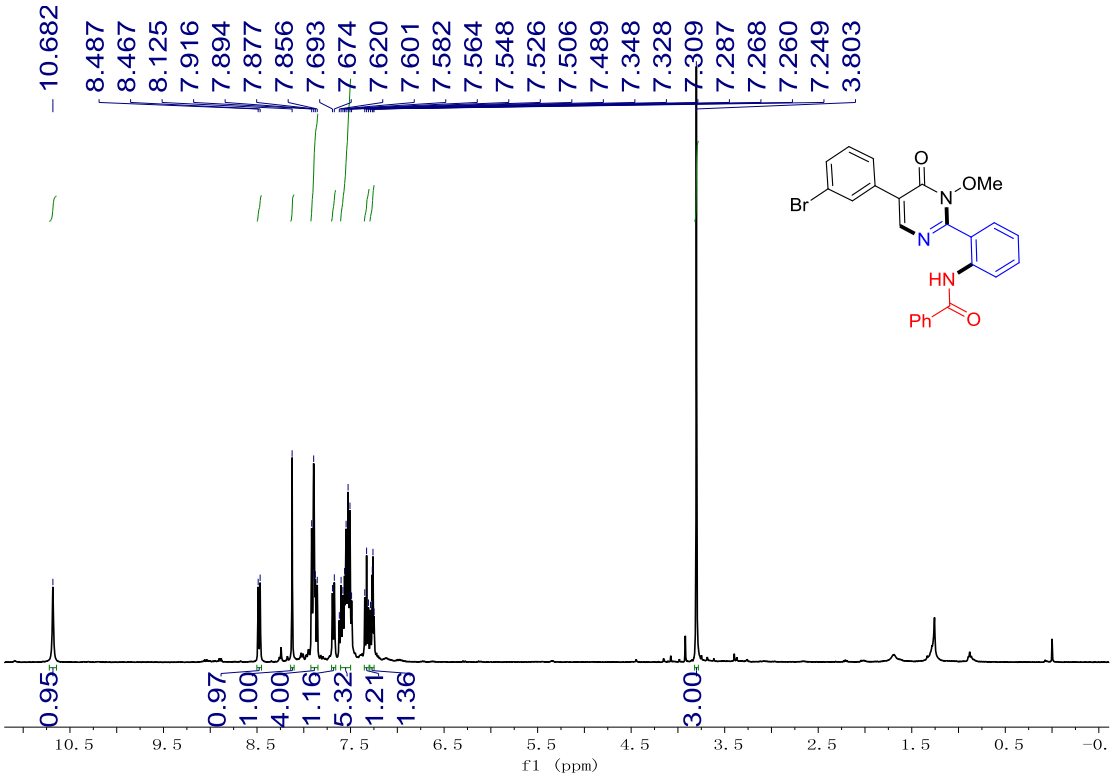

165.1747
155.8830
148.6860
132.1598
130.5411
130.1174
129.9319
129.0974
128.9111
127.1411
125.9407
123.6251
123.1562
119.5330
64.5410
20.0927
O
N
OMe
N
HN
Ph
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

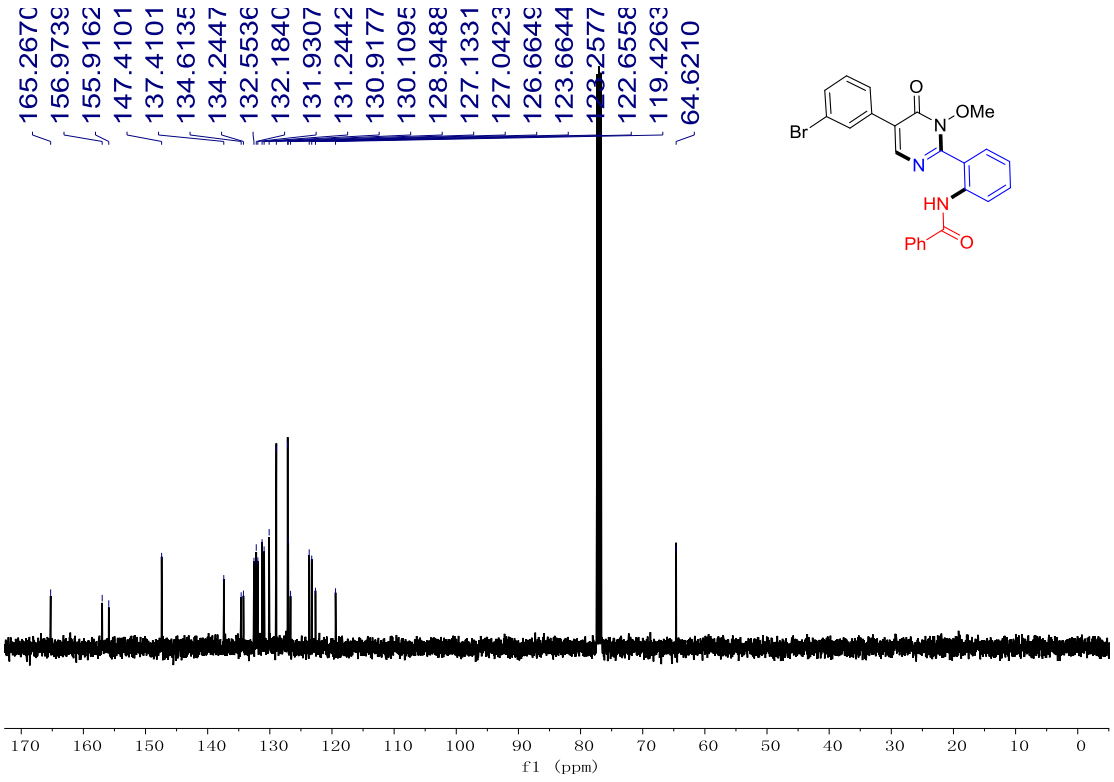
5ea


10.716
8.497
8.477
8.109
7.921
7.902
7.877
7.857
7.747
7.728
7.714
7.616
7.597
7.577
7.559
7.542
7.520
7.501
7.484
7.284
7.263
7.247
7.171
7.150
7.129
3.798
1.06
0.99
1.02
3.07
2.00
4.18
1.24
2.09
2.96
F
O
N
OMe
N
HN
Ph
O
f1 (ppm)

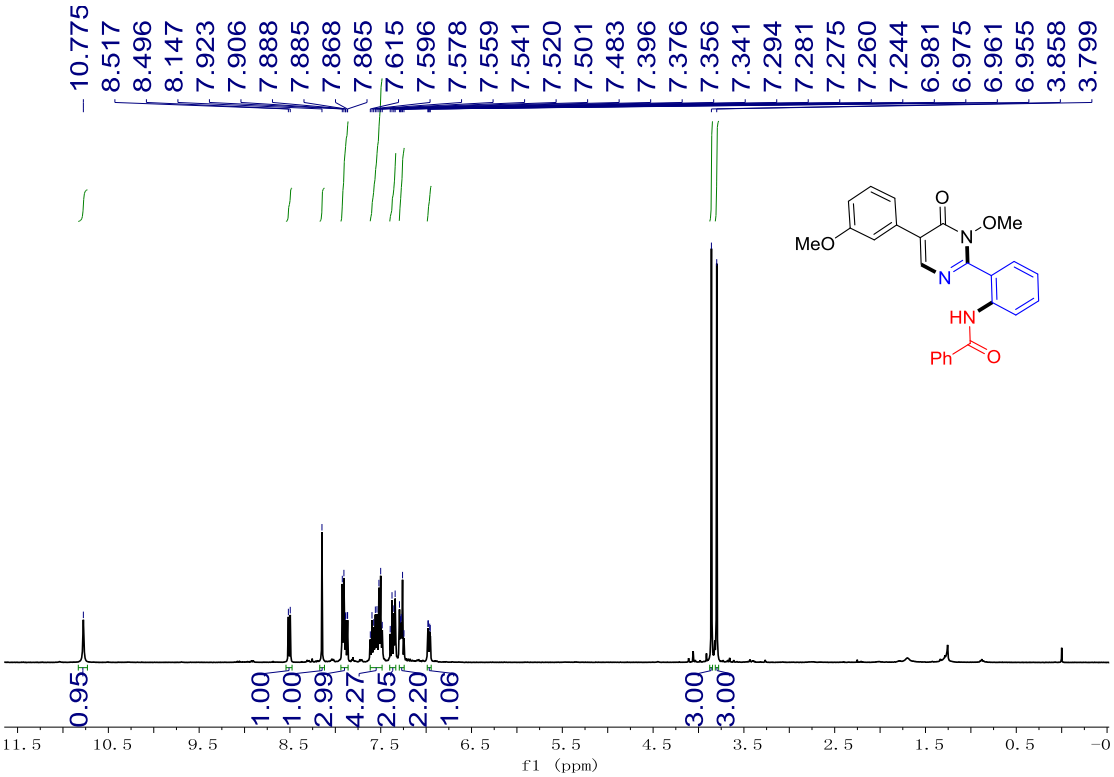

165.2367
164.3846
161.9058
157.2353
155.3907
146.8116
137.3738
134.6506
132.4415
132.1487
130.8876
130.3398
130.2578
128.9204
128.2625
128.2292
127.2148
127.1437
123.6391
123.1988
119.4827
115.7968
115.5820
64.5769
F
O
N
OMe
N
HN
Ph
O
f1 (ppm)

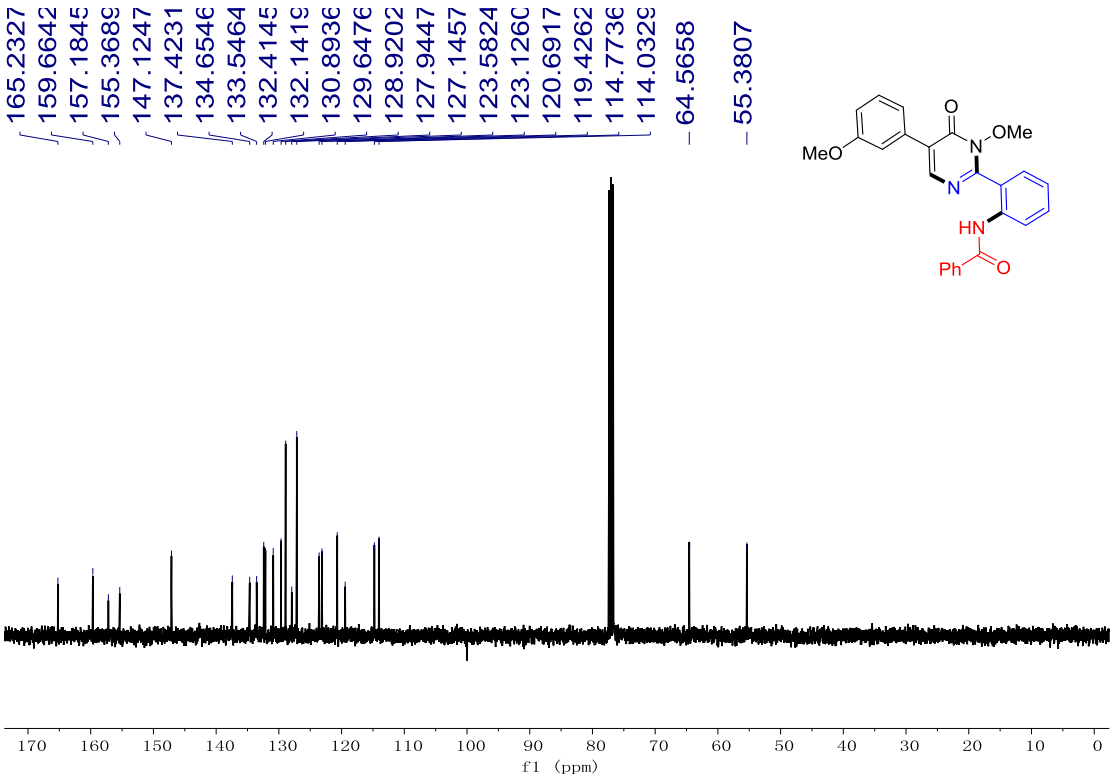
5fa


10.682
8.487
8.467
8.125
7.916
7.894
7.877
7.856
7.693
7.674
7.620
7.601
7.582
7.564
7.548
7.526
7.506
7.489
7.348
7.328
7.309
7.287
7.268
7.260
7.249
3.803
0.95
0.97
1.00
4.00
1.16
5.32
1.21
1.36
3.00
Br
O
N
OMe
N
HN
Ph
O
f1 (ppm)

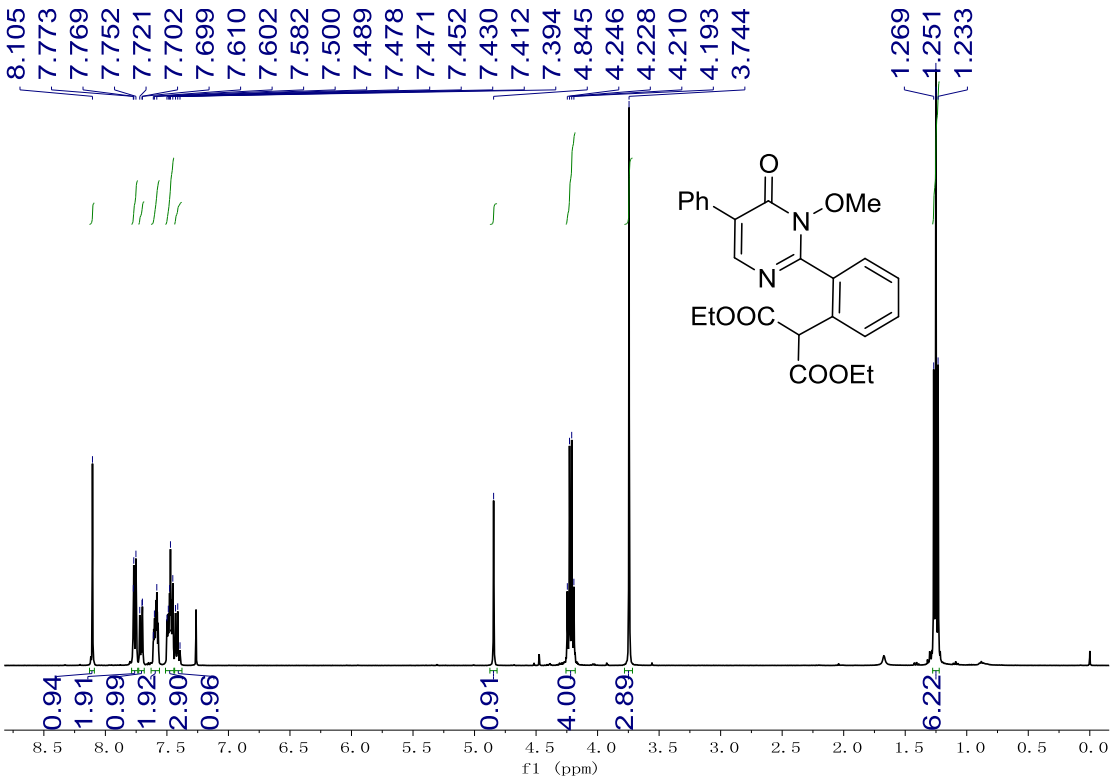

165.2670
156.9739
155.9162
147.4101
137.4101
134.6135
134.2447
132.5536
132.1840
131.9307
131.2442
130.9177
130.1095
128.9488
127.1331
127.0423
126.6649
123.6644
122.2577
122.6558
119.4263
64.6210
Br
O
N
OMe
N
HN
Ph
O
f1 (ppm)

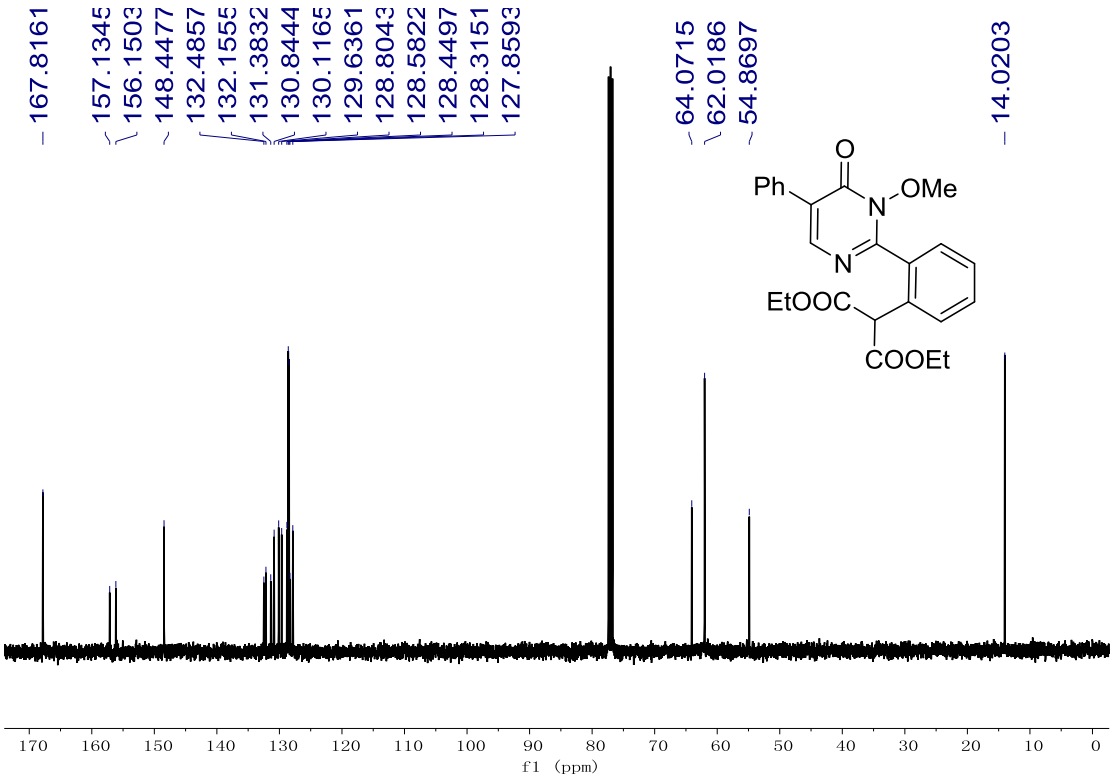
5ga


10.775
8.517
8.496
8.147
7.923
7.906
7.888
7.885
7.868
7.865
7.615
7.596
7.578
7.559
7.541
7.520
7.501
7.483
7.396
7.376
7.356
7.341
7.294
7.281
7.275
7.260
7.244
6.981
6.975
6.961
6.955
3.858
3.799
MeO
N
OMe
O
HN
Ph
O
0.95
1.00
1.00
2.99
4.27
2.05
2.20
1.06
3.00
3.00
f1 (ppm)

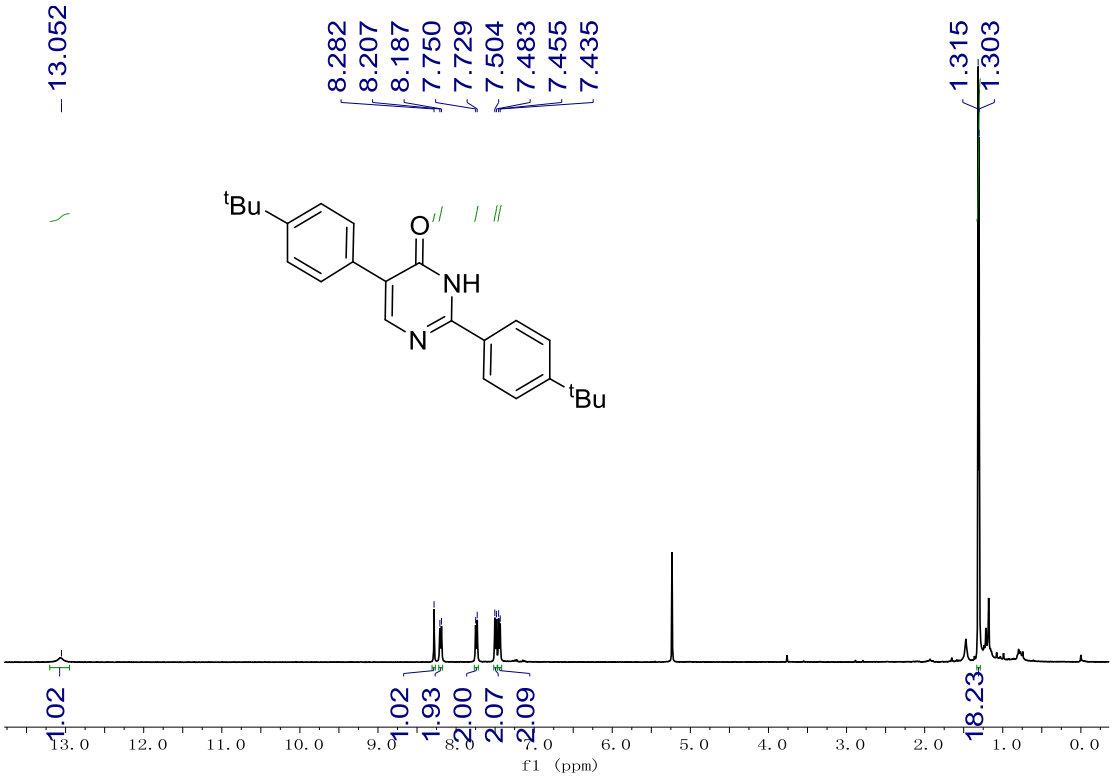

165.2327
159.6642
157.1845
155.3689
147.1247
137.4231
134.6546
133.5464
132.4145
132.1419
130.8936
129.6476
128.9202
127.9447
127.1457
123.5824
123.1260
120.6917
119.4262
114.7736
114.0329
64.5658
55.3807
MeO
N
OMe
O
HN
Ph
O
f1 (ppm)

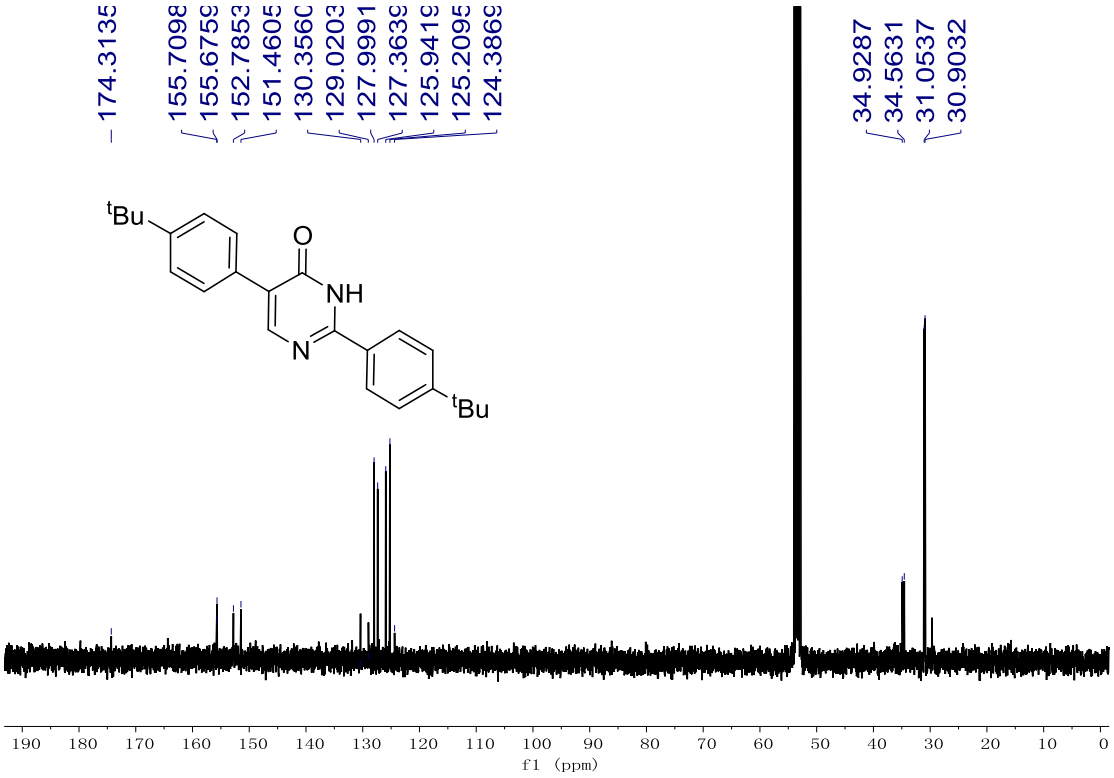
6


8.105
7.773
7.769
7.752
7.721
7.702
7.699
7.610
7.602
7.582
7.500
7.489
7.478
7.471
7.452
7.430
7.412
7.394
4.845
4.246
4.228
4.210
4.193
3.744
1.269
1.251
1.233
Ph
O
N
OMe
N
EtOOC
COOEt
0.94
1.91
0.99
1.92
2.90
0.96
0.91
4.00
2.89
6.22
f1 (ppm)

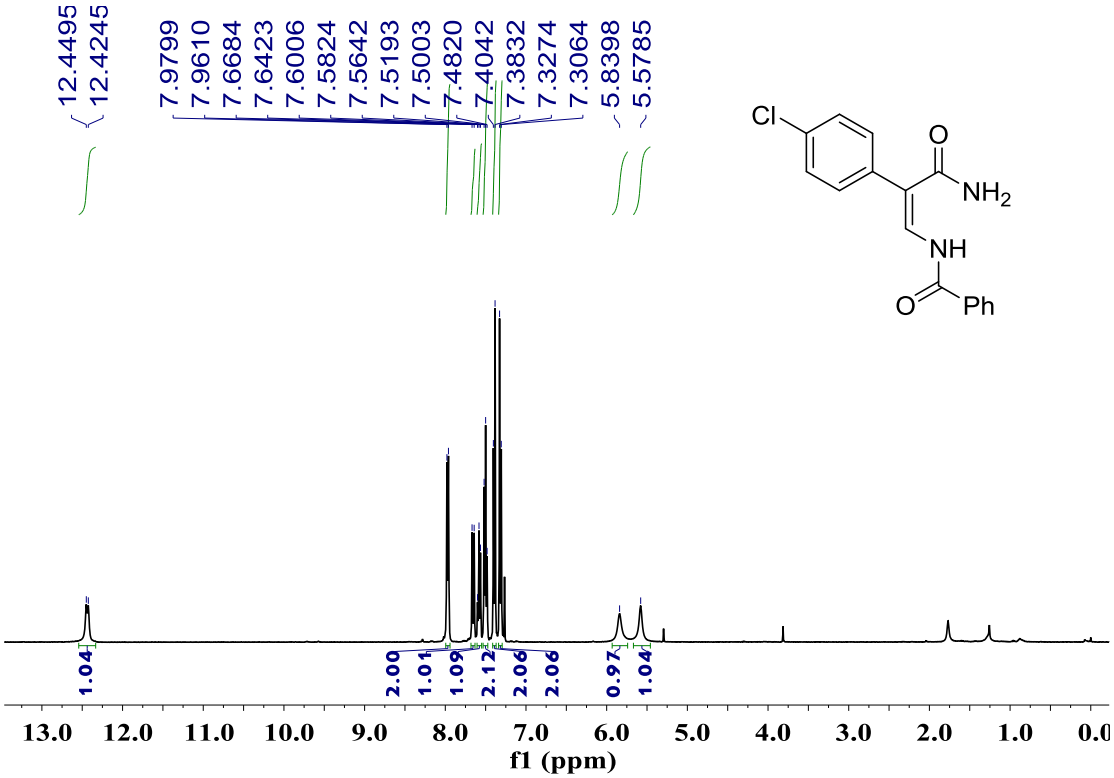

167.8161
157.1345
156.1503
148.4477
132.4857
132.1555
131.3832
130.8444
130.1165
129.6361
128.8043
128.5822
128.4497
128.3151
127.8593
64.0715
62.0186
54.8697
14.0203
Ph
O
N
OMe
N
EtOOC
COOEt
f1 (ppm)

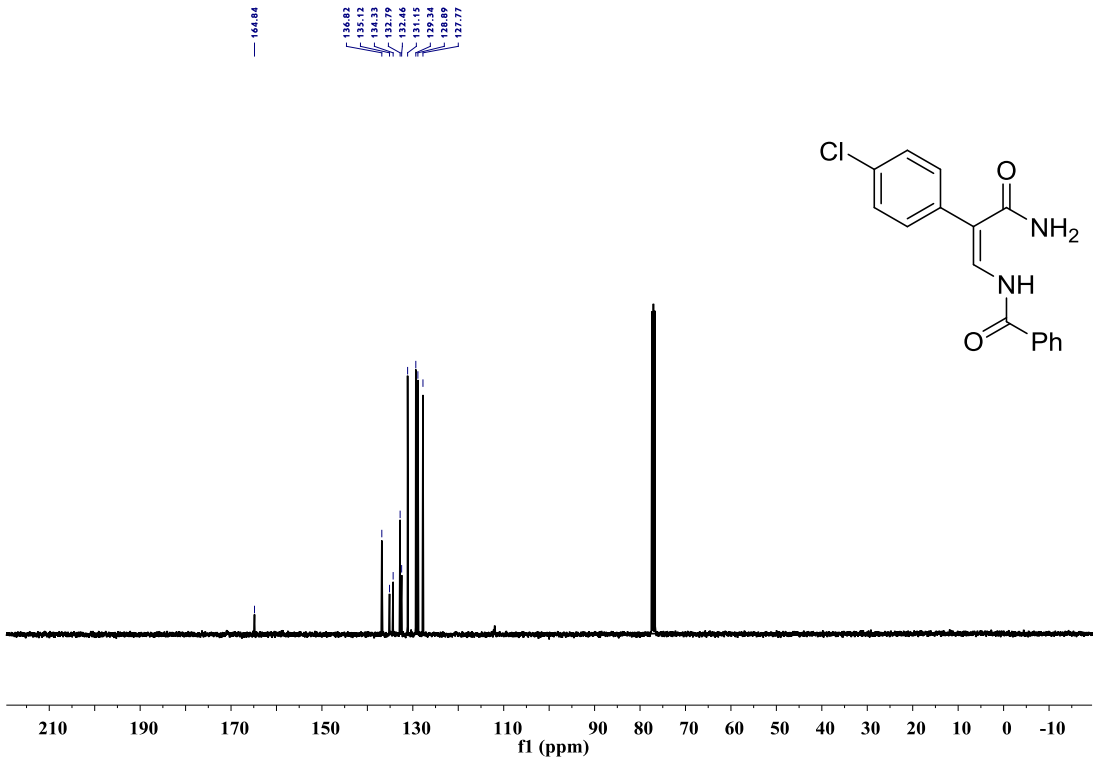
7


13.052
8.282
8.207
8.187
7.750
7.729
7.504
7.483
7.455
7.435
1.315
1.303
tBu
O
NH
N
tBu
1.02
1.02
1.93
2.00
2.07
2.09
18.23
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


174.3135
155.7098
155.6759
152.7853
151.4605
130.3560
129.0203
127.9991
127.3639
125.9419
125.2095
124.3869
34.9287
34.5631
31.0537
30.9032
tBu
O
NH
N
tBu
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

8


12.4495
12.4245
7.9799
7.9610
7.6684
7.6423
7.6006
7.5824
7.5642
7.5193
7.5003
7.4820
7.4042
7.3832
7.3274
7.3064
5.8398
5.5785
Cl
O
NH2
NH
O
Ph
1.04
2.00
1.01
1.09
2.12
2.06
2.06
0.97
1.04
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


164.84
136.82
135.12
134.33
132.79
132.46
131.15
129.34
128.89
127.77
Cl
O
NH2
NH
O
Ph
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)