Supporting Information

Visible-Light-Promoted Oxidative Desulphurisation: A Strategy for the Preparation of Unsymmetrical Ureas from Isothiocyanates and Amines Using Molecular Oxygen

Ziyu Gan,[†,‡] Guoqing Li,[‡] Qiuli Yan,[†] Weiseng Deng,[§] Yuan-Ye Jiang,*[,‡] and Daoshan Yang*[,†,‡]

[†] Key Laboratory of Optic-electric Sensing and Analytical Chemistry for Life Science, MOE, State Key Laboratory Base of Eco-Chemical Engineering, College of Chemistry and Molecular Engineering, Qingdao University of Science and Technology, Qingdao, 266042, P. R. China.

[‡] School of Chemistry and Chemical Engineering, Qufu Normal University, Qufu 273165, Shandong, P. R. China.

[§] Hunan Provincial Key Laboratory of Materials Protection for Electric Power and Transportation, Changsha University of Science and Technology, Changsha, Wanjiali Road No. 960, 410114, China.

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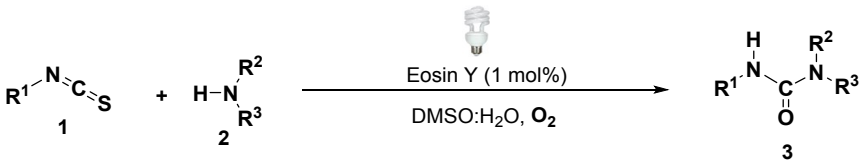
General considerations

All reagents and solvents were obtained from commercial suppliers and used without further purification. Organic dyes were purchased from Sigma Aldrich. Flash chromatography was performed on silica gel (200 ~ 300 mesh). ^{1}H and ^{13}C NMR data were recorded at 500 and 125 MHz on a BRUKER 500 spectrometer. Chemical shifts (δ) are expressed in parts per million (ppm), coupling constants (J) are in Hz. Proton and carbon magnetic resonance spectra (^{1}H NMR and ^{13}C NMR) were recorded using tetramethylsilane (TMS) as the internal standard in DMSO-d_6 or in $CDCl_3$. Mass analyses and HRMS were obtained by ESI on a TOF mass analyzer. All diffraction data were obtained on a Bruker Smart Apex CCD diffractometer equipped with graphite-monochromated Mo Kα radiation. UV-visible spectroscopy of reaction solution was recorded on a SHIMADZU UV 3600 UV-visible spectrophotometer. The fluorescenceemission intensity of reaction solution was recorded on a F-4600 spectrofluorimeter. The reactor was 3.0 cm from 12W Blue LED.

General procedure for the synthesis of unsymmetrical ureas



A 25 ml Schlenk tube equipped with a magnetic stirring bar was charged with **1** (0.2 mmol), **2** (0.3 mmol), and Eosin Y (1 mol%). The tube was evacuated twice and backfilled with oxygen, and 2 mL of DMSO/H_2O (v_1/v_2 = 99:1) was added to the tube under oxygen atmosphere. The tube was sealed with an oxygen balloon and then the mixture was allowed to stir at room temperature with the irradiation of a 12 W blue

LED for 8h. After completion of the reaction, the solvent was removed with the aid of a rotary evaporator. The residue was purified by column chromatography on silica gel using petroleum ether/ethyl acetate as eluent to provide the desired products **3**.

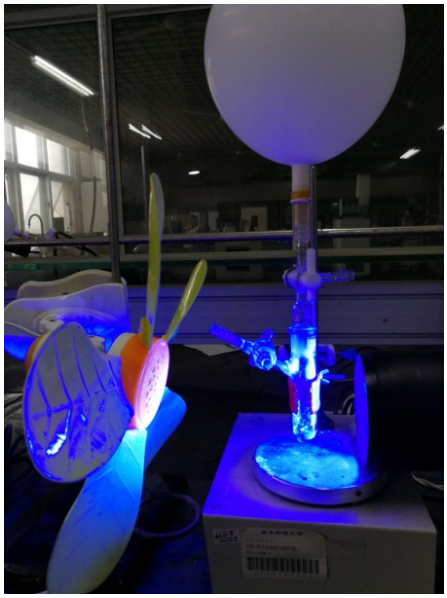
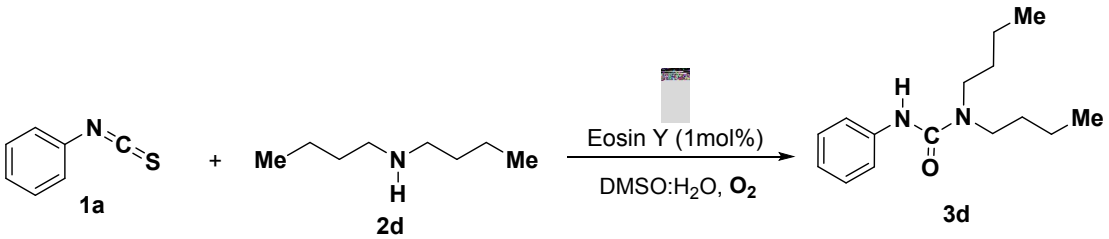


Figure S1. Photograph of the reaction setup

Synthesis of 3d on a gram scale

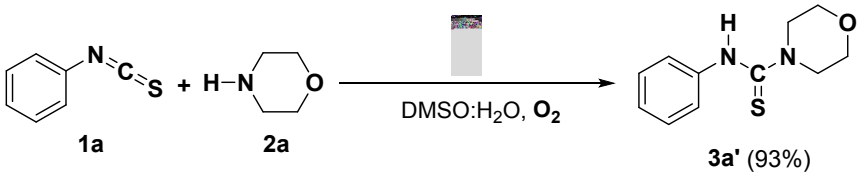


6 mmol, 0.81g 9 mmol, 1.16g 1.03 g, 69% isolated yield

A 50 ml oven-dried Schlenk bottle equipped with a magnetic stirring bar was charged with isothiocyanatobenzene **1a** (6 mmol, 0.81 g), dibutylamine **2d** (9 mmol, 1.16 g), Eosin Y (1 mol%, 0.039 g). The tube was evacuated and backfilled with oxygen (three times), 15 mL of DMSO/H_2O (v_1/v_2 = 99:1) was added by syringe under a oxygen atmosphere. The solution was stirred at room temperature with the irradiation

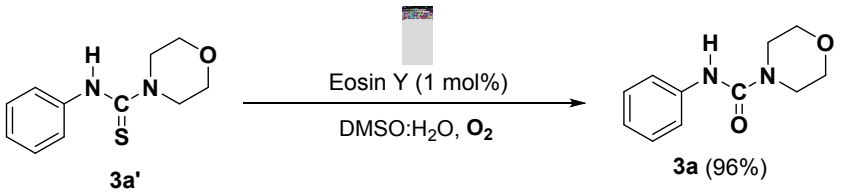
of three 12 W blue LED lights for 12 h. After completion of the reaction (TLC), the solvent was removed with the aid of a rotary evaporator. The residue was purified by column chromatography on silica gel using petroleum ether/ethyl acetate (3:1) as eluent to give the corresponding product **4a** in 69% yield, 1.03g.

Experiments of investigations on the mechanism



1a **2a** **3a'** (93%)

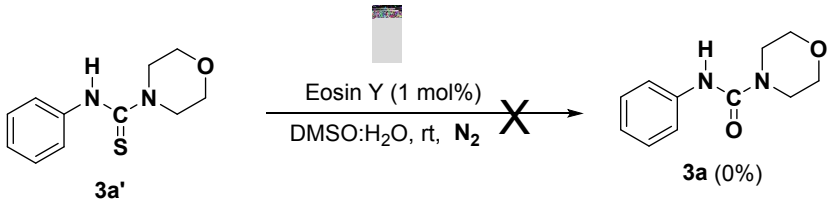
A 25 ml Schlenk tube equipped with a magnetic stirring bar was charged with isothiocyanatobenzene **1a** (0.2 mmol), morpholine **2a** (0.3 mmol). The tube was evacuated twice and backfilled with oxygen, and 2 mL of DMSO/H_2O (v_1/v_2 = 99:1) was added to the tube under oxygen atmosphere. The tube was sealed with an oxygen balloon and then the mixture was allowed to stir at room temperature with the irradiation of a 12 W blue LED for 8 h. Upon completion of the reaction, the mixture was removed under vacuo. The residue was purified by column chromatography on silica gel using petroleum ether/ethyl acetate (1:1) as eluent to give *N*-phenylmorpholine-4-carbothioamide **3a'** in 93% yield (41 mg).



3a' **3a** (96%)

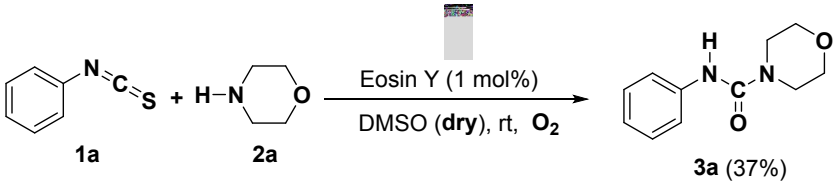
A 25 ml Schlenk tube equipped with a magnetic stirring bar was charged with *N*-phenylmorpholine-4-carbothioamide **3a'** (0.2 mmol), Eosin Y (1 mol%, 0.039 g). The tube was evacuated twice and backfilled with oxygen, and 2 mL of DMSO/H_2O (v_1/v_2

= 99:1) was added to the tube under oxygen atmosphere. The tube was sealed with an oxygen balloon and then the mixture was allowed to stir at room temperature with the irradiation of a 12 W blue LED for 8 h. Upon completion of the reaction, the mixture was removed under vacuo. The residue was purified by column chromatography on silica gel using petroleum ether/ethyl acetate (1:1) as eluent to give the corresponding product **3a** in 96% yield (39.5 mg).



3a' **3a** (0%)

A 25 ml Schlenk tube equipped with a magnetic stirring bar was charged with *N*-phenylmorpholine-4-carbothioamide **3a'** (0.2 mmol), Eosin Y (1 mol%, 0.039 g). The tube was evacuated twice and backfilled with nitrogen, and 2 mL of DMSO/H_2O (v_1/v_2 = 99:1) was added to the tube under nitrogen atmosphere. The tube was sealed with an nitrogen balloon and then the mixture was allowed to stir at room temperature with the irradiation of a 12 W blue LED for 8 h. There was no conversion detected by TLC.

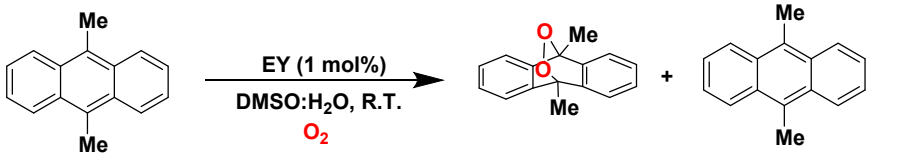


1a **2a** **3a** (37%)

A 25 ml Schlenk tube equipped with a magnetic stirring bar was charged with isothiocyanatobenzene **1a** (0.2 mmol), morpholine **2a** (0.3 mmol). The tube was evacuated twice and backfilled with oxygen, and 2 mL anhydrous DMSO was added to the tube under oxygen atmosphere. The tube was sealed with an oxygen balloon

and then the mixture was allowed to stir at room temperature with the irradiation of a 12 W blue LED for 8 h. Upon completion of the reaction, the mixture was removed under vacuo. The residue was purified by column chromatography on silica gel using petroleum ether/ethyl acetate (1:1) as eluent to give **3a** in 37% yield (22.8 mg).

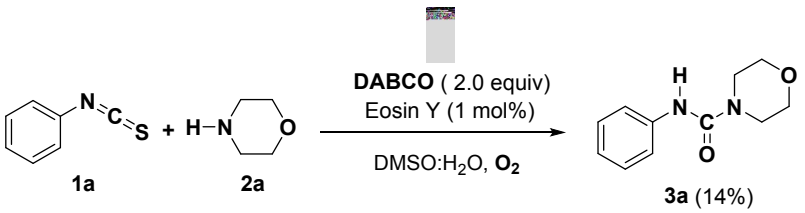
The trapping experiments of $^1O_2$



	5	4
dark	trace	98% recovered
hv	81%	trace

It is well known that singlet oxygen is usually generated by the energy transfer from photosensitizer to molecular oxygen under light, and accompanied by the change of O_2 electron configuration. We know that visible light and oxygen are necessary for this transformation. However, we wondered about the key enabling factor featuring this process. One possibility is that singlet oxygen is produced and is responsible for the oxidative procedure coupling process under our standard conditions. Trapping experiments using 9,10-dimethylanthracene **4** under the standard conditions afforded **5** formed through [4+2] cycloaddition involving $^1O_2$, while the corresponding **5** were not detected in the dark.

The quenching experiments of $^1O_2$ by DABCO



A 25 ml Schlenk tube equipped with a magnetic stirring bar was charged with isothiocyanatobenzene **1a** (0.2 mmol), morpholine **2a** (0.3 mmol), DABCO (0.4 mmol), and Eosin Y (1 mol%). The tube was evacuated twice and backfilled with oxygen, and 2 mL of DMSO/H_2O (v_1/v_2 = 99:1) was added to the tube under oxygen atmosphere. The tube was sealed with an oxygen balloon and then the mixture was allowed to stir at room temperature with the irradiation of a 12 W blue LED lamp for 8 h. Upon completion of the reaction, the solvent was removed under vacuum and the residue was purified by column chromatography on silica gel using petroleum ether/ethyl acetate (1:1) as eluent to give the corresponding product **3a** in 14% yield (6 mg).

Fluorescence quenching experiments

The fluorescence emission intensities were recorded on a F-4600 spectrofluorimeter. The excitation wavelength was fixed at 510 nm, and the emission wavelength was measured at 565 nm (emission maximum). The samples were prepared by mixing Eosin Y (10^{-6} mol/L) and different amount of **3a'** in DMSO/H_2O (v_1/v_2 = 99:1) in a light path quartz fluorescence cuvette. The concentrationof **3a'** stock solution is 10^{-5} mol/L in DMSO/H_2O (v_1/v_2 = 99:1). For each quenching experiment, 0.3 mL of **3a'** stock solution was titrated to a mixed solution of Eosin Y (0.3mL, in a total volume = 3.0 mL). Then the emission intensity was collected and the results were presented in Figure S2. There is no fluorescence quenching phenomenon of Eosin Y under various concentrations of **3a'** was demonstrated in a curve of [I_0/I] vs C[**3a'**], as shown in Figure S2.

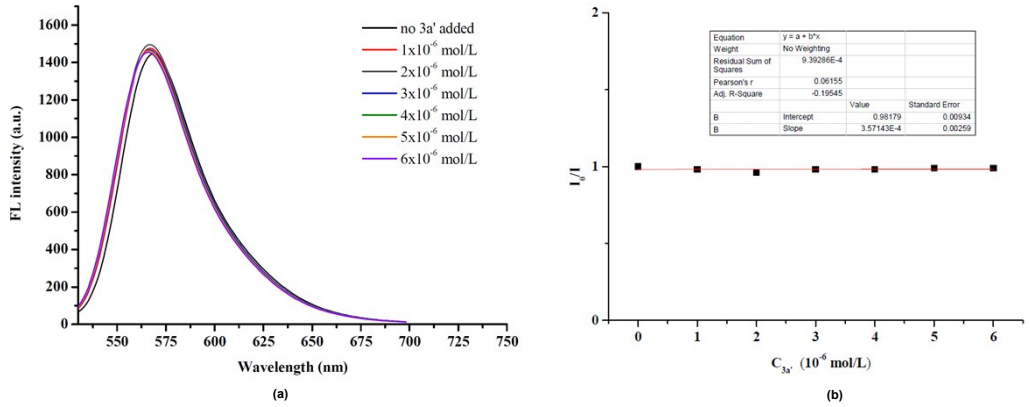


Figure S2. Quenching of the Eosin Y fluorescence emission in the presence of TBHP (a). Stern–Volmer plots (b).

Effect of Visible Light Irradiation

The reaction between isothiocyanatobenzene **1a** and morpholine **2a** was conducted under the standard conditions on a 0.2 mmol scale. The mixture was subjected to sequential periods of stirring under visible light irradiation (12 W blue LED) followed by stirring in the absence of light. At each time point, one reaction system was suspended, which was then purified with chromatography column on silica gel (gradient eluent of EtOAc:petroleum ether: 1:1) to give the corresponding products **3a**. The yield of **3a** was measured by weight of the product.

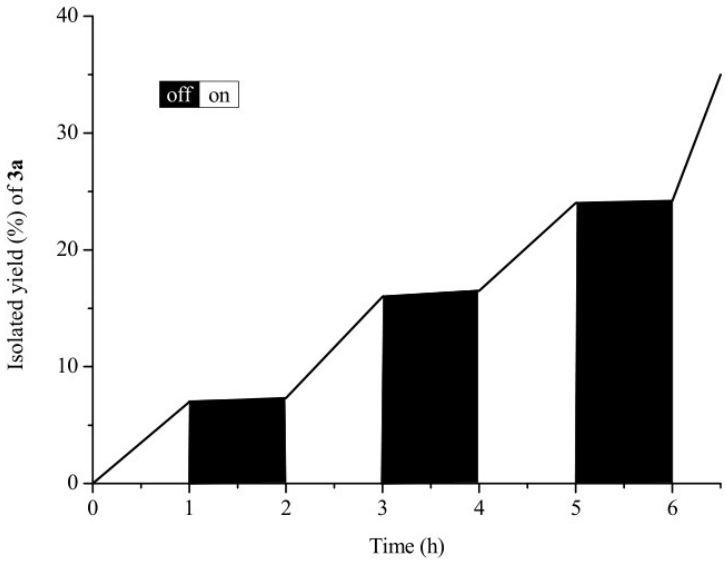
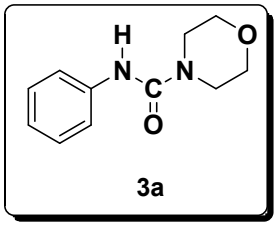
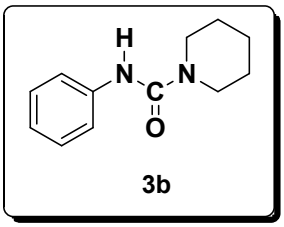


Figure S3. Visible Light Irradiation on/off experiment

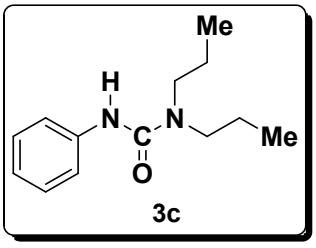
Characterization data of compounds 3a-3ah and 5



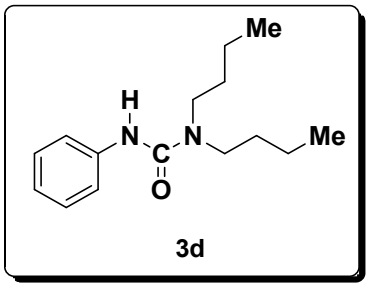
***N*-Phenylmorpholine-4-carboxamide (3a).**[1] Eluent petroleum ether/ethyl acetate (1:1). White solid, 33 mg, 81% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.30 (d, 2H, J = 7.9 Hz), 7.22 (t, 2H, J = 7.7 Hz), 7.16 (br, s, 1H), 7.01 (t, 1H, J = 7.2 Hz), 3.56 (t, 4H, J = 4.3 Hz), 3.36 (d, 4H, J = 4.4 Hz). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 155.4, 138.8, 128.6, 123.2, 120.5, 66.3, 44.1. HRMS calcd for $C_{11}H_{14}N_2NaO_2$ $[M+Na]^+$: 229.0947; found 229.0948.



***N*-Phenylpiperidine-1-carboxamide (3b).**[1] Eluent petroleum ether/ethyl acetate (1:1). Yellow solid, 31 mg, 75% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.27 (t, 2H, J = 4.1 Hz), 7.17 (t, 2H, J = 7.5 Hz), 6.92 (t, 1H, J = 7.4 Hz), 6.51 (br, s, 1H), 3.36-3.34 (m, 4H), 1.50-1.49 (m, 6H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 155.1, 139.3, 128.7, 122.7, 120.0, 45.1, 25.6, 24.3. HRMS calcd for $C_{12}H_{16}N_2NaO$ $[M+Na]^+$: 227.1155; found 227.1151.

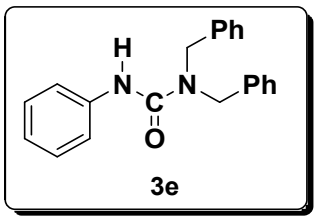


3-Phenyl-1,1-dipropylurea (3c).[1] Eluent petroleum ether/ethyl acetate (3:1). Yellow oil, 34 mg, 78% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.38 (d, 2H, J = 7.6 Hz), 7.27-7.24 (m, 2H), 7.00 (t, 1H, J = 7.4 Hz), 6.37 (br, s, 1H), 3.25 (t, 4H, J = 7.7 Hz), 1.66-1.61 (m, 4H), 0.95-0.92 (m, 6H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 155.0, 139.3, 128.7, 122.6, 119.8, 49.3, 21.8, 11.3. HRMS calcd for $C_{13}H_{20}N_2NaO$ $[M+Na]^+$: 243.1468; found 243.1466.



3d

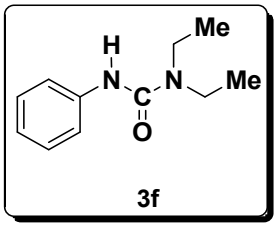
1,1-Dibutyl-3-phenylurea (3d).[1] Eluent petroleum ether/ethyl acetate (2:1). White solid, 38 mg, 76% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.30 (d, 2H, J = 7.9 Hz), 7.17 (t, 2H, J = 7.7 Hz), 6.91 (t, 1H, J = 7.3 Hz), 6.33 (br, s, 1H), 3.19 (t, 4H, J = 7.6 Hz), 1.50 (t, 4H, J = 7.5 Hz), 1.29-1.25 (m, 4H), 0.87 (t, 6H, J = 7.4 Hz). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 154.9, 139.3, 128.6, 122.5, 119.7, 47.2, 30.7, 20.1, 13.8. HRMS calcd for $C_{15}H_{24}N_2NaO$ $[M+Na]^+$: 271.1781; found 271.1778.



3e

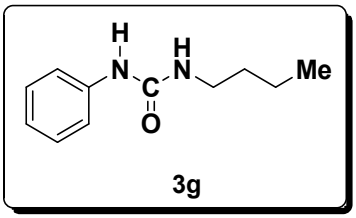
1,1-Dibenzyl-3-phenylurea (3e).[2] Eluent petroleum ether/ethyl acetate (3:1). White solid, 52 mg, 83% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.40-7.37 (m, 4H), 7.34-7.31 (m, 6H), 7.24-7.23 (m, 4H), 7.02-6.99 (m, 1H), 6.41 (br, s, 1H), 4.62 (s, 4H). ^{13}C

NMR ($CDCl_3$, 125 MHz, ppm) δ 155.8, 138.9, 137.1, 128.9, 128.7, 127.7, 127.3, 123.0, 119.8, 50.6. HRMS calcd for $C_{21}H_{20}N_2NaO$ $[M+Na]^+$: 339.1468; found 339.1466.



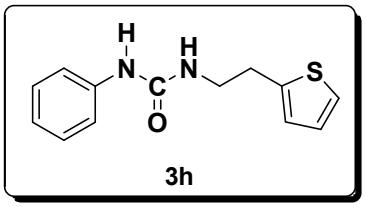
3f

1,1-Diethyl-3-phenylurea (3f).[1] Eluent petroleum ether/ethyl acetate (2:1). White solid, 30 mg, 77% yield. ^1H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.38 (d, 2H, J = 8.0 Hz), 7.26 (t, 2H, J = 7.5 Hz), 7.00 (t, 1H, J = 7.3 Hz), 6.40 (br, s, 1H), 3.37-3.33 (q, 4H, J = 7.1 Hz), 1.20 (t, 6H, J = 7.1 Hz). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 154.6, 139.2, 128.7, 122.7, 119.8, 41.5, 13.9. HRMS calcd for $C_{11}H_{16}N_2NaO$ $[M+Na]^+$: 215.1155; found 215.1157.



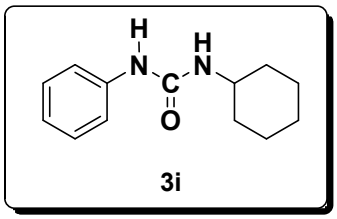
3g

1-Butyl-3-phenylurea (3g).[3] Eluent petroleum ether/ethyl acetate (1:1). White solid, 32 mg, 83% yield. ^1H NMR (DMSO-d_6, 500 MHz, ppm) δ 8.38 (br, s, 1H), 7.39 (d, 2H, J = 7.8 Hz), 7.20 (t, 2H, J = 7.9 Hz), 6.87 (t, 1H, J = 7.4 Hz), 6.12 (t, 1H, J = 5.5 Hz), 3.10-3.06 (m, 2H), 1.44-1.38 (m, 2H), 1.34-1.27 (m, 2H), 0.89 (t, 3H, J = 7.3 Hz). ^{13}C NMR (DMSO-d_6, 125 MHz, ppm) δ 155.7, 141.1, 129.1, 121.4, 118.1, 39.2, 32.4, 20.0, 14.2. HRMS calcd for $C_{11}H_{16}N_2NaO$ $[M+Na]^+$: 215.1155; found 215.1151.



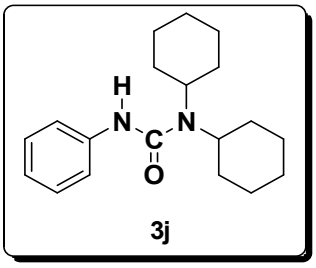
3h

1-Phenyl-3-(2-(thiophen-2-yl)ethyl)urea (3h). Eluent petroleum ether/ethyl acetate (1:1). White solid, 42 mg, 86% yield. ^{1}H NMR (DMSO-d_6, 500 MHz, ppm) δ 8.53 (br, s, 1H), 7.40 (d, 2H, J = 7.7 Hz), 7.34 (d, 1H, J = 6.2 Hz), 7.21 (t, 2H, J = 7.9 Hz), 6.98-6.96 (m, 1H), 6.92-6.87 (m, 2H), 6.21 (t, 1H, J = 5.7 Hz), 3.38-3.36 (m, 2H), 2.97 (t, 2H, J = 7.0 Hz) ^{13}C NMR (DMSO-d_6, 125 MHz, ppm) δ 155.6, 142.2, 141.0, 129.1, 127.5, 125.7, 124.5, 121.5, 118.1, 41.3, 30.6. HRMS calcd for $C_{13}H_{14}N_2NaOS$ $[M+Na]^+$: 269.0719; found 269.0716.



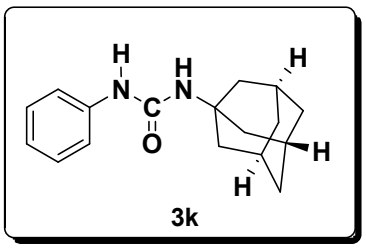
3i

1-Cyclohexyl-3-phenylurea (3i).[4] Eluent petroleum ether/ethyl acetate (3:1). White solid, 39 mg, 89% yield. ^{1}H NMR (DMSO-d_6, 500 MHz, ppm) δ 8.29 (br, s, 1H), 7.38 (d, 2H, J = 8.1 Hz), 7.20 (t, 2H, J = 7.6 Hz), 6.87 (t, 1H, J = 7.2 Hz), 6.06 (d, 1H, J = 7.7 Hz), 3.48-3.43 (m, 1H), 1.80 (d, 2H, J = 9.4 Hz), 1.66-1.63 (m, 2H), 1.53-1.51 (m, 1H), 1.33-1.25 (m, 2H), 1.20-1.12 (m, 3H). ^{13}C NMR (DMSO-d_6, 125 MHz, ppm) δ 155.0, 141.1, 129.1, 121.4, 118.0, 48.1, 33.5, 25.8, 24.9. HRMS calcd for $C_{13}H_{18}N_2NaO$ $[M+Na]^+$: 241.1311; found 241.1313.



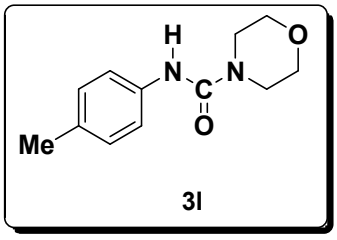
3j

1,1-Dicyclohexyl-3-phenylurea (3j).[1] Eluent petroleum ether/ethyl acetate (1:1). White solid, 55 mg, 91% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.34-7.32 (m, 2H), 7.24-7.22 (m, 2H), 6.97 (t, 1H, J = 7.3 Hz), 6.24 (br, s, 1H), 3.49-3.43 (m, 2H), 1.83-1.64 (m, 15H), 1.35-1.31 (m, 3H), 1.17-1.10 (m, 2H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 154.9, 139.4, 128.8, 122.5, 119.6, 55.4, 31.9, 26.4, 25.5. HRMS calcd for $C_{19}H_{28}N_2NaO$ [M+Na]$^+$: 323.2094; found 323.2093.



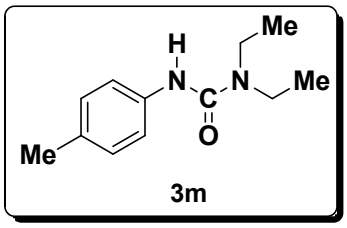
3k

1-((3s,5s,7s)-Adamantan-1-yl)-3-phenylurea (3k). Eluent petroleum ether/ethyl acetate (3:1). White solid, 50 mg, 93% yield. ^{1}H NMR (DMSO-d_6, 500 MHz, ppm) δ 8.22 (br, s, 1H), 7.33 (d, 2H, J = 7.7 Hz), 7.18 (t, 2H, J = 7.9 Hz), 6.85 (t, 1H, J = 7.3 Hz), 5.85 (br, s, 1H), 2.03-2.01 (m, 3H), 1.93-1.92 (m, 6H), 1.63-1.62 (m, 6H). ^{13}C NMR (DMSO-d_6, 125 MHz, ppm) δ 154.5, 141.2, 129.1, 121.2, 117.8, 50.3, 42.2, 36.6, 29.4. HRMS calcd for $C_{17}H_{22}N_2NaO$ [M+Na]$^+$: 293.1624; found 293.1620.



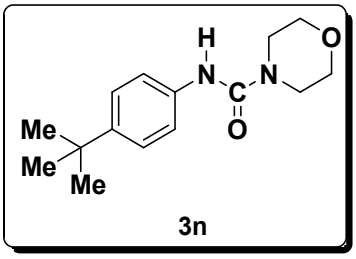
3l

***N*-(*p*-Tolyl)morpholine-4-carboxamide (3l).**[5] Eluent petroleum ether/ethyl acetate (3:1). White solid, 35 mg, 80% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.20 (d, 2H, J = 8.3 Hz), 7.07 (d, 2H, J = 8.2 Hz), 6.58 (br, s, 1H), 3.66 (t, 4H, J = 4.8 Hz), 3.41 (t, 4H, J = 4.8 Hz), 2.28 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 155.5, 136.1, 132.9, 129.3, 120.6, 66.4, 44.2, 20.7. HRMS calcd for $C_{12}H_{16}N_2NaO_2$ $[M+Na]^+$: 243.1104; found 243.1103.



3m

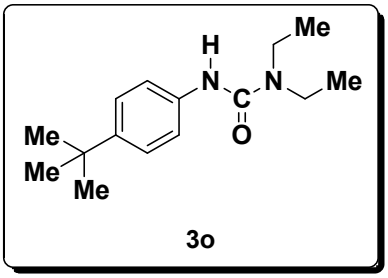
1,1-Diethyl-3-(*p*-tolyl)urea (3m).[6] Eluent petroleum ether/ethyl acetate (1:1). Yellow solid, 35 mg, 86% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.26 (d, 2H, J = 8.2 Hz), 7.08 (d, 2H, J = 8.2 Hz), 6.26 (br, s, 1H), 3.39-3.34 (m, 4H), 2.29 (s, 3H), 1.22 (t, 6H, J = 7.2 Hz). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 154.7, 136.6, 132.2, 129.2, 120.0, 41.5, 20.7, 13.9. HRMS calcd for $C_{12}H_{18}N_2NaO$ $[M+Na]^+$: 229.1311; found 229.1312.



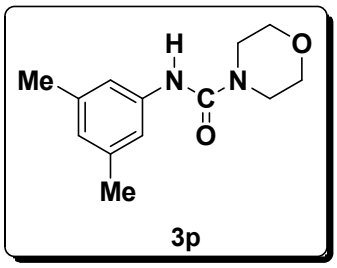
3n

***N*-(4-(*tert*-Butyl)phenyl)morpholine-4-carboxamide (3n).** Eluent petroleum ether/ethyl acetate (1:1). White solid, 43 mg, 82% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.31 (d, 2H, J = 8.8 Hz), 7.25 (d, 2H, J = 8.8 Hz), 6.34 (br, s, 1H), 3.73 (t, 4H, J = 4.9 Hz), 3.46 (t, 4H, J = 4.9 Hz), 1.29 (s, 9H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 155.3, 146.4, 136.0, 125.8, 120.0, 66.5, 44.3, 31.4. HRMS calcd for $C_{15}H_{22}N_2NaO_2$

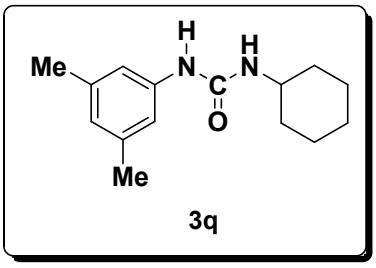
[M+Na]$^+$: 285.1573; found 285.1569.



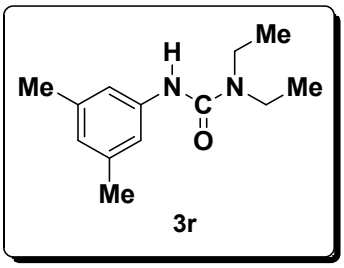
3-(4-(*tert*-Butyl)phenyl)-1,1-diethylurea (3o). Eluent petroleum ether/ethyl acetate (3:1). White solid, 45 mg, 90% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.29 (s, 4H), 6.22 (br, s, 1H), 3.39-3.34 (m, 4H), 1.29 (s, 9H), 1.22 (t, 6H, J = 7.2 Hz). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 154.7, 145.7, 136.5, 125.6, 119.7, 41.6, 34.2, 31.4, 13.9. HRMS calcd for $C_{15}H_{24}N_2NaO$ [M+Na]$^+$: 271.1781; found 271.1780.



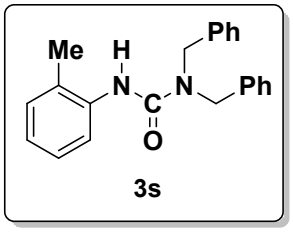
***N*-(3,5-Dimethylphenyl)morpholine-4-carboxamide (3p).** Eluent petroleum ether/ethyl acetate (1:1). Yellow solid, 38 mg, 82% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 6.96 (s, 2H), 6.68 (s, 1H), 6.52 (br, s, 1H), 3.67 (t, 4H, J = 4.8 Hz), 3.43 (t, 4H, J = 4.8 Hz), 2.25 (s, 6H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 155.3, 138.5, 138.4, 125.1, 118.0, 66.4, 44.2, 21.3. HRMS calcd for $C_{13}H_{18}N_2NaO_2$ [M+Na]$^+$: 257.1260; found 257.1263



1-Cyclohexyl-3-(3,5-dimethylphenyl)urea (3q). Eluent petroleum ether/ethyl acetate (1:1). White solid, 46 mg, 94% yield. ^{1}H NMR (DMSO-d_6, 500 MHz, ppm) δ 8.11 (s, 1H), 6.98 (s, 2H), 6.51 (s, 1H), 6.01 (d, 1H, J = 7.8 Hz), 3.44 (t, 1H, J = 3.9 Hz), 2.48 (s, 6H), 1.81-1.77 (m, 2H), 1.67-1.63 (m, 2H), 1.54-1.52 (m, 1H), 1.31-1.13 (m, 5H),. ^{13}C NMR (DMSO-d_6, 125 MHz, ppm) δ 154.9, 140.9, 138.0, 123.0, 115.8, 48.1, 33.5, 25.7, 24.9, 21.6. HRMS calcd for $C_{15}H_{22}N_2NaO$ [M+Na]$^+$: 269.1624; found 269.1622.

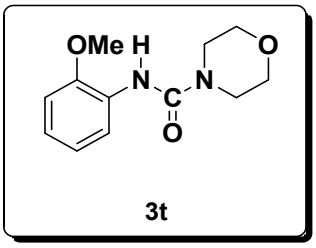


3-(3,5-Dimethylphenyl)-1,1-diethylurea (3r). Eluent petroleum ether/ethyl acetate (2:1). Yellow solid, 40 mg, 90% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.03 (s, 2H), 6.67 (s, 1H), 6.18 (br, s, 1H), 3.39-3.34 (m, 4H), 2.28 (s, 6H), 1.22 (t, 6H, J = 7.1 Hz). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 154.7, 139.0, 138.4, 124.5, 117.5, 41.6, 21.3, 13.9. HRMS calcd for $C_{13}H_{20}N_2NaO$ [M+Na]$^+$: 243.1468; found 243.1470.

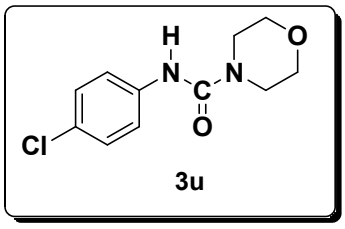


1,1-dibenzyl-3-(*o*-tolyl)urea (3s). Eluent petroleum ether/ethyl acetate (1:1). Yellow

solid, 59 mg, 89% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.78 (d, 1H, J = 8.1 Hz), 7.40-7.32 (m, 10H), 7.17 (t, 1H, J = 7.6 Hz), 7.04 (d, 1H, J = 7.4 Hz), 6.95 (t, 1H, J = 7.4 Hz), 6.12 (br, s, 1H), 4.67 (s, 4H), 1.71 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 156.0, 137.3, 137.1, 130.1, 129.0, 127.8, 127.7, 127.3, 126.6, 123.5, 122.1, 51.2, 17.0. HRMS calcd for $C_{22}H_{22}N_2NaO$ $[M+Na]^+$: 353.1624; found 353.1625.

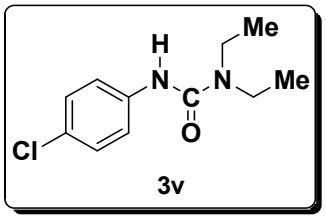


***N*-(2-Methoxyphenyl)morpholine-4-carboxamide (3t).** Eluent petroleum ether/ethyl acetate (2:1). White solid, 41 mg, 86% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 8.15-8.12 (m, 1H), 7.09 (br, s, 1H), 6.97-6.94 (m, 2H), 6.86-6.84 (m, 1H), 3.87 (s, 3H), 3.75-3.73 (m, 4H), 3.49-3.47 (m, 4H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 154.7, 147.5, 128.4, 122.1, 121.1, 118.9, 109.6, 66.4, 55.6, 44.0. HRMS calcd for $C_{12}H_{16}N_2NaO_3$ $[M+Na]^+$: 259.1053; found 259.1051.



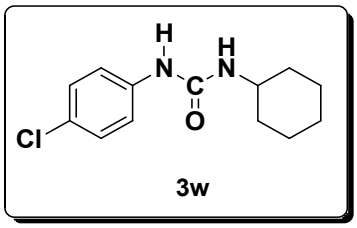
***N*-(4-Chlorophenyl)morpholine-4-carboxamide (3u).**[5] Eluent petroleum ether/ethyl acetate (3:1). White solid, 43 mg, 90% yield. ^{1}H NMR (DMSO-d_6, 500 MHz, ppm) δ 8.65 (br, s, 1H), 7.50 (d, 2H, J = 8.8 Hz), 7.27 (d, 2H, J = 8.8 Hz), 3.63-3.60 (m, 4H), 3.42-3.40 (m, 4H). ^{13}C NMR (DMSO-d_6, 125 MHz, ppm) δ 155.4, 139.9, 128.7, 125.8, 121.5, 66.5, 44.6. HRMS calcd for $C_{11}H_{13}ClN_2NaO_2$ $[M+Na]^+$: 263.0558;

found 263.0554.



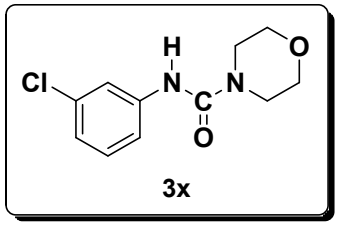
3v

3-(4-Chlorophenyl)-1,1-diethylurea (3v).[7] Eluent petroleum ether/ethyl acetate (1:1). Yellow oil, 40 mg, 88% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.33 (d, 2H, J = 8.7 Hz), 7.21 (d, 2H, J = 8.7 Hz), 6.35 (br, s, 1H), 3.37-3.33 (m, 4H), 1.20 (t, 6H, J = 7.1 Hz). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 154.4, 137.9, 128.7, 127.6, 121.0, 41.6, 13.9. HRMS calcd for $C_{11}H_{15}ClN_2NaO$ $[M+Na]^+$: 249.0765; found 249.0766.



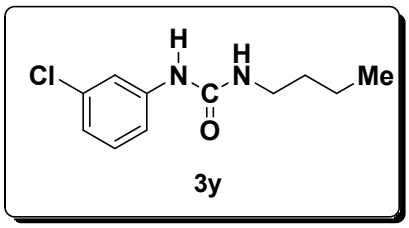
3w

1-(4-Chlorophenyl)-3-cyclohexylurea (3w).[8] Eluent petroleum ether/ethyl acetate (3:1). Yellow solid, 42 mg, 84% yield. ^{1}H NMR (DMSO-d_6, 500 MHz, ppm) δ 8.43 (br, s, 1H), 7.38 (d, 2H, J = 8.9 Hz), 7.24 (d, 2H, J = 8.9 Hz), 6.09 (br, d, 1H, J = 7.8 Hz), 3.45-3.42 (m, 1H), 1.80-1.77 (m, 2H), 1.66-1.63 (m, 2H), 1.54-1.51 (m, 1H), 1.30-1.14 (m, 5H). ^{13}C NMR (DMSO-d_6, 125 MHz, ppm) δ 154.8, 140.1, 129.0, 124.9, 119.5, 48.1, 33.4, 25.7, 24.9. HRMS calcd for $C_{13}H_{17}ClN_2NaO$ $[M+Na]^+$: 275.0922; found 275.0924.



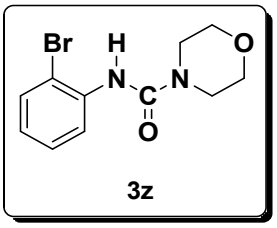
3x

***N*-(3-Chlorophenyl)morpholine-4-carboxamide (3x)**.[9] Eluent petroleum ether/ethyl acetate (5:1). Brown solid, 36 mg, 76% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.43 (br, s, 1H), 7.18 (d, 2H, J = 6.3 Hz), 7.02-7.00 (m, 1H), 6.60 (br, s, 1H), 3.70 (t, 4H, J = 4.9 Hz), 3.46 (t, 4H, J = 4.8 Hz). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 154.8, 140.0, 134.4, 129.8, 123.3, 120.1, 118.0, 66.4, 44.2. HRMS calcd for $C_{11}H_{13}ClN_2NaO_2$ $[M+Na]^+$: 263.0558; found 263.0560.



3y

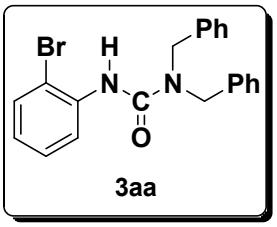
1-Butyl-3-(3-chlorophenyl)urea (3y). Eluent petroleum ether/ethyl acetate (7:1). White solid, 40 mg, 89% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.29 (br, s, 1H), 7.34 (s, 1H), 7.11-7.10 (m, 2H), 6.94-6.92 (m, 1H), 5.79 (br, s, 1H), 3.18-3.14 (m, 2H), 1.42-1.40 (m, 2H), 1.30-1.26 (m, 2H), 0.86 (t, 3H, J = 5.1 Hz). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 156.4, 140.3, 134.5, 129.9, 122.7, 119.7, 117.7, 40.0, 32.1, 20.0,13.7. HRMS calcd for $C_{11}H_{15}ClN_2NaO$ $[M+Na]^+$: 249.0765; found 249.0764.



3z

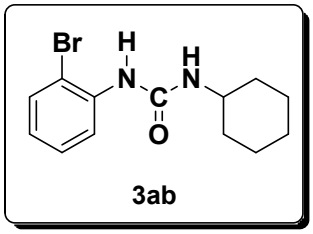
***N*-(2-Bromophenyl)morpholine-4-carboxamide (3z).** Eluent petroleum ether/ethyl acetate (2:1). Yellow solid, 45 mg, 80% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 8.18 (d, 1H, J = 8.3 Hz), 7.49 (d, 1H, J = 8.0 Hz), 7.28 (t, 1H, J = 7.8 Hz), 7.01 (br, s, 1H), 6.90 (t, 1H, J = 7.2 Hz), 3.76 (t, 4H, J = 4.9 Hz), 3.52 (t, 4H, J = 4.9 Hz). ^{13}C

NMR ($CDCl_3$, 125 MHz, ppm) δ 154.2, 136.5, 131.9, 128.4, 123.8, 121.1, 113.2, 66.4, 44.1. HRMS calcd for $C_{11}H_{13}BrN_2NaO_2$ $[M+Na]^+$: 307.0053; found 307.0050.



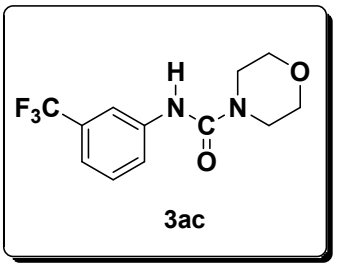
3aa

1,1-Dibenzyl-3-(2-bromophenyl)urea (3aa).[10] Eluent petroleum ether/ethyl acetate (3:1). Red solid, 69 mg, 88% yield. ^1H NMR ($CDCl_3$, 500 MHz, ppm) δ 8.22 (d, 1H, J = 9.8 Hz), 7.39-7.27 (m, 12H), 6.96 (s, 1H), 6.84 (t, 1H, J = 8.4 Hz), 4.65 (s, 4H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 155.4, 137.1, 136.8, 131.9, 129.0, 128.1, 127.8, 127.3, 123.6, 121.4, 113.0, 50.8. HRMS calcd for $C_{21}H_{19}BrN_2NaO$ $[M+Na]^+$: 417.0573; found 417.0569.



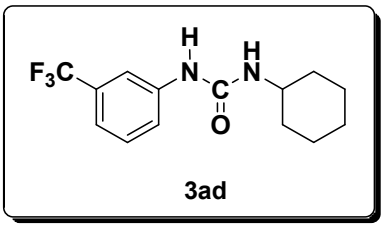
3ab

1-(2-Bromophenyl)-3-cyclohexylurea (3ab). Eluent petroleum ether/ethyl acetate (10:1). Colorless oil, 54 mg, 92% yield. ^1H NMR (DMSO-d_6, 500 MHz, ppm) δ 8.09 (d, 1H, J = 9.7 Hz), 7.74 (br, s, 1H), 7.53 (d, 1H, J = 9.4 Hz), 7.25 (t, 1H, J = 8.5 Hz), 7.05 (d, 1H, J = 7.6 Hz), 6.86 (t, 1H, J = 8.4 Hz), 3.47-3.46 (m, 1H), 1.83-1.80 (m, 2H), 1.69-1.65 (m, 2H), 1.54-1.52 (m, 1H), 1.32-1.15 (m, 5H). ^{13}C NMR (DMSO-d_6, 125 MHz, ppm) δ 154.4, 138.4, 132.8, 128.4, 123.3, 121.7, 112.3, 48.2, 33.3, 25.7, 24.8. HRMS calcd for $C_{13}H_{17}BrN_2NaO$ $[M+Na]^+$: 319.0416; found 319.0412.



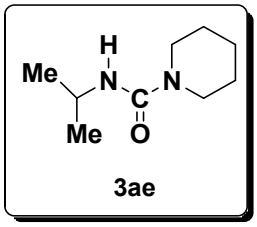
3ac

***N*-(3-(Trifluoromethyl)phenyl)morpholine-4-carboxamide (3ac).** Eluent petroleum ether/ethyl acetate (1:1). Yellow oil, 50 mg, 91% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.52 (s, 1H), 7.45 (d, 1H, J = 8.1 Hz), 7.28 (d, 1H, J = 7.8 Hz), 7.19 (d, 1H, J = 7.1 Hz), 6.88 (br, s, 1H), 3.61 (t, 4H, J = 4.8 Hz), 3.39 (t, 4H, J = 4.7 Hz). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 154.9, 139.4, 131.2 (q, J = 32.1), 124.9, 122.3, 123.6 (q, J = 270.7), 119.7 (q, J = 3.6), 119.7 (q, J = 3.9), 66.4, 44.2. HRMS calcd for $C_{12}H_{13}F_3N_2NaO_2$ $[M+Na]^+$: 297.0821; found 297.0822.



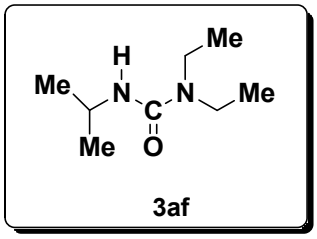
3ad

1-Cyclohexyl-3-(3-(trifluoromethyl)phenyl)urea (3ad).[11] Eluent petroleum ether/ethyl acetate (2:1). White solid, 48 mg, 84% yield. ^{1}H NMR (DMSO-d_6, 500 MHz, ppm) δ 8.66 (s, 1H), 7.97 (s, 1H), 7.43-7.40 (m, 2H), 7.20 (d, 1H, J = 6.5 Hz), 6.19 (d, 1H, J = 7.8 Hz), 3.50-3.44 (m, 1H), 1.82-1.79 (m, 2H), 1.67-1.64 (m, 2H), 1.54-1.52 (m, 1H), 1.31-1.16 (m, 5H). ^{13}C NMR (DMSO-d_6, 125 MHz, ppm) δ 154.7, 141.9, 130.2, 129.9 (q, J = 30.9), 125.8, 124.8 (q, J = 270.5), 117.5 (q, J = 3.8), 113.8 (q, J = 4.0), 48.2, 33.3, 25.7, 24.8. HRMS calcd for $C_{14}H_{17}F_3N_2NaO$ $[M+Na]^+$:309.1185; found 309.1181.



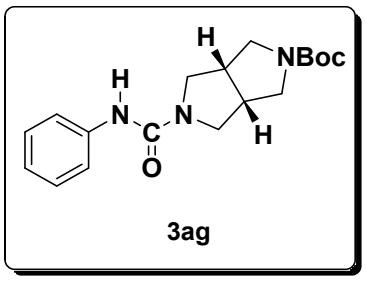
3ae

***N*-Isopropylpiperidine-1-carboxamide (3ae).**[12] Eluent petroleum ether/ethyl acetate (3:1). White solid, 29 mg, 85% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 4.32 (br, d, 1H, J = 4.7 Hz), 3.90-3.87 (m, 1H), 3.23-3.21 (m, 4H), 1.50-1.46 (m, 6H), 1.07 (d, 6H, J = 8.3 Hz). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 157.0, 42.2, 25.4, 24.2, 23.3. HRMS calcd for $C_9H_{18}N_2NaO$ $[M+Na]^+$:193.1311; found 193.1311.



3af

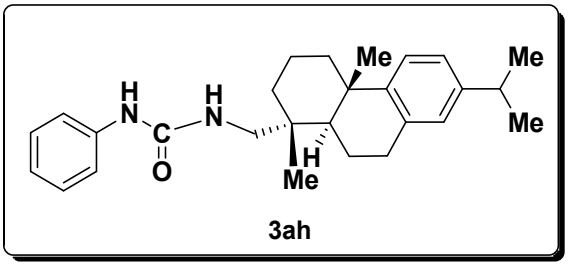
1,1-Diethyl-3-isopropylurea (3af).[13] Eluent petroleum ether/ethyl acetate (2:1). white solid, 29 mg, 91% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 4.09 (br, s, 1H), 3.90 (s, 1H), 3.19-3.14 (m, 4H), 1.08-1.03 (m, 12H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 156.5, 42.1, 40.8, 23.4, 13.6. HRMS calcd for $C_8H_{18}N_2NaO$ $[M+Na]^+$: 181.1311; found 181.1318.



3ag

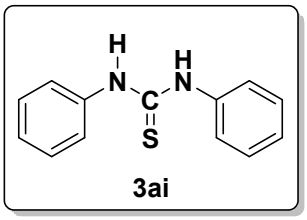
***tert*-Butyl (3aR,6aS)-5-(phenylcarbamoyl)hexahydropyrrolo[3,4-*c*]pyrrole-2(1*H*)-carboxylate (3ag).** Eluent petroleum ether/ethyl acetate (1:2). Yellow oil, 50 mg, 76% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.31 (d, 2H, J = 7.8 Hz), 7.23 (t, 2H, J =

7.8 Hz), 6.98 (t, 1H, *J* = 7.3 Hz), 6.55 (br, s, 1H), 3.64-3.53 (m, 4H), 3.34-3.17 (m, 4H), 2.86 (s, 2H), 1.43 (s, 9H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 154.3, 154.0, 139.0, 128.6, 122.8, 119.8, 79.5, 49.7, 49.5, 49.4, 28.3. HRMS calcd for $C_{18}H_{25}N_3NaO_3$ $[M+Na]^+$: 354.1788; found 354.1786.



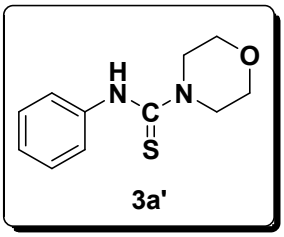
3ah

1-(((1R,4aS,10aR)-7-Isopropyl-1,4a-dimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthren-1-yl)methyl)-3-phenylurea (3ah). Eluent petroleum ether/ethyl acetate (5:1). Yellow solid, 73 mg, 90% yield. ^{1}H NMR (DMSO-d_6, 500 MHz, ppm) δ 8.36 (br, s, 1H), 7.36 (d, 2H, *J* = 7.7 Hz), 7.19 (t, 2H, *J* = 7.9 Hz), 7.15 (d, 1H, *J* = 8.2 Hz), 6.94 (d, 1H, *J* = 9.5 Hz), 6.87-6.84 (m, 2H), 6.12 (t, 1H, *J* = 6.2 Hz), 3.17-3.13 (m, 1H), 2.89-2.73 (m, 4H), 2.27 (d, 1H, *J* = 12.8 Hz), 1.88-1.85 (m, 1H), 1.73 (d, 1H, *J* = 12.4 Hz), 1.62-1.56 (m, 2H), 1.40 (d, 1H, *J* = 12.1 Hz), 1.32 (t, 2H, *J* = 7.7 Hz), 1.22 (t, 1H, *J* = 6.3 Hz), 1.16-1.14 (m, 9H), 0.87 (s, 3H). ^{13}C NMR (DMSO-d_6, 125 MHz, ppm) δ 155.7, 147.6, 145.4, 141.1, 135.0, 129.1, 126.9, 124.6, 124.0, 121.3, 117.8, 60.2, 49.5, 44.5, 38.6, 37.6, 37.4, 35.9, 33.4, 30.2, 25.6, 24.4, 24.3, 19.3, 18.8, 18.7. HRMS calcd for $C_{27}H_{36}N_2NaO$ $[M+Na]^+$: 427.2720; found 427.2716.



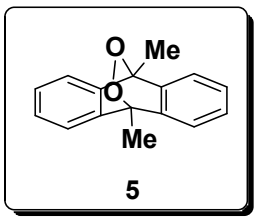
3ai

1,3-diphenylthiourea (3ag).[14] Eluent petroleum ether/ethyl acetate (2:1). White solid, 43.8 mg, 96% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 8.11 (s, br, 2H), 7.41-7.37 (m, 8H), 7.28-7.25 (m, 2H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 179.9, 137.2, 129.6, 127.0, 125.3.



3a'

***N*-Phenylmorpholine-4-carbothioamide (3a').**[15] Eluent petroleum ether/ethyl acetate (1:1). White solid, 41 mg, 93% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.66 (br, s, 1H), 7.21 (t, 2H, J = 7.0 Hz), 7.08-7.03 (m, 3H), 3.65 (d, 4H, J = 3.8 Hz), 3.56 (d, 4H, J = 3.2 Hz). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 182.7, 139.6, 128.7, 125.2, 123.7, 65.8, 49.1. HRMS calcd for $C_{11}H_{14}N_2NaOS$ $[M+Na]^+$: 245.0719; found 245.0718.



5

9,10-Dimethyl-9,10-epidioxyanthracene (5).[16] Eluent petroleum ether/ethyl acetate (15:1). White solid, 39 mg, 81% yield. ^{1}H NMR (DMSO-d_6, 500 MHz, ppm) δ 7.49-7.45 (m, 4H), 7.34-7.30 (m, 4H), 2.07 (s, 6H). ^{13}C NMR (DMSO-d_6, 125 MHz, ppm) δ 141.2, 127.8, 121.2, 79.6, 13.9.

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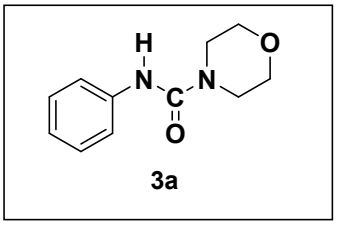
X-ray Crystallography Data of 3a and 3h.

Crystal preparation of compound 3a.

Compound **3a** (25 mg) was dissolved in 5 mL of THF/ *n*-hexane (v_1/v_2 = 5:1), and it was crystallized to give crystal as colorless prisms after the solvent was slowly volatilized in 7 days at room temperature (~ 25 °C).

All diffraction data were obtained on a Bruker Smart Apex CCD diffractometer equipped with graphite-monochromated Mo Kα radiation. X-ray crystallographic data for **3a** is available as Figure S3. X-ray crystallographic data in CIF format are available from the Cambridge Crystallographic Data Centre (http://www.ccdc.cam.ac.uk/).



3a

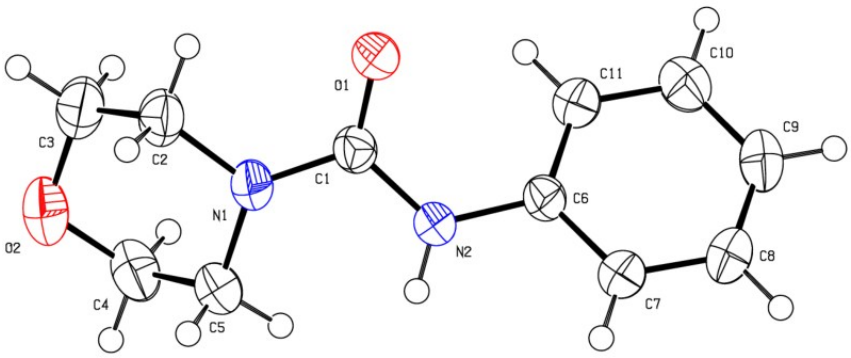


Figure S3 X-ray crystallography of 3a.

Table S1. Crystal data and structure refinement for 3a.

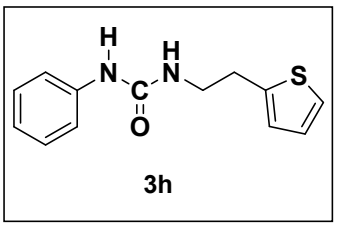
CCDC number	1966547
Empirical formula	C11 H14 N2 O2
Formula weight	206.24
Temperature	298(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 8.1026(7) A alpha = 90 deg.
	b = 15.7929(13) A beta = 104.183(3) deg.
	c = 8.4783(8) A gamma = 90 deg.
Volume	1051.84(16) A^3
Z, Calculated density	4, 1.302 Mg/m^3
Absorption coefficient	0.091 mm^-1
F(000)	440
Crystal size	0.47 x 0.40 x 0.38 mm
Theta range for data collection	2.58 to 25.02 deg.
Limiting indices	-9<=h<=9, -15<=k<=18, -9<=l<=10
Reflections collected / unique	5082 / 1854 [R(int) = 0.0329]
Completeness to theta = 25.02	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9662 and 0.9585
Refinement method	Full-matrix least-squares on F^2

Data / restraints / parameters	1854 / 0 / 137
Goodness-of-fit on F^2	1.039
Final R indices [I>2sigma(I)]	R1 = 0.0371, wR2 = 0.0929
R indices (all data)	R1 = 0.0504, wR2 = 0.1027
Extinction coefficient	0.083(6)
Largest diff. peak and hole	0.139 and -0.170 e.A^-3

Crystal preparation of compound 3h.

Compound **3h** (25 mg) was dissolved in 5 mL of THF/ *n*-hexane (v_1/v_2 = 3:1), and it was crystallized to give crystal as colorless prisms after the solvent was slowly volatilized in 5 days at room temperature (~ 25 °C).

All diffraction data were obtained on a Bruker Smart Apex CCD diffractometer equipped with graphite-monochromated Mo Kα radiation. X-ray crystallographic data for **3h** is available as Figure S4. X-ray crystallographic data in CIF format are available from the Cambridge Crystallographic Data Centre (http://www.ccdc.cam.ac.uk/).



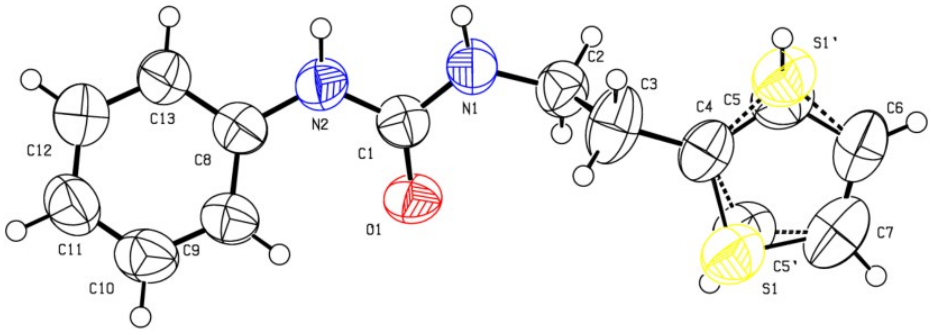
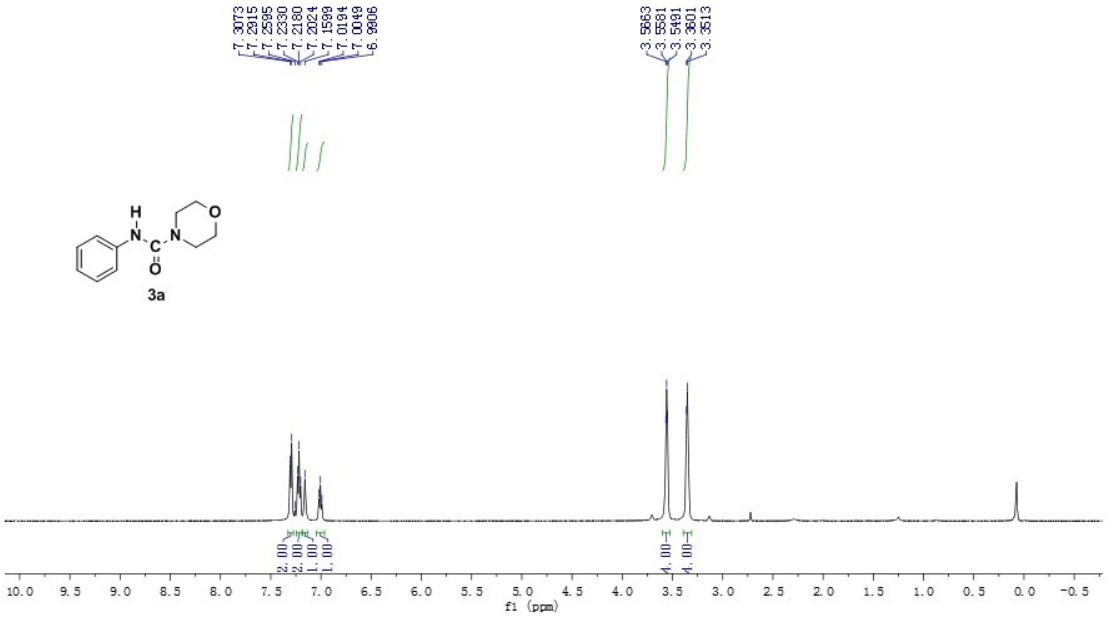


Figure S4 X-ray crystallography of 3h.

Table S2. Crystal data and structure refinement for 3h.

CCDC number	1966544
Empirical formula	C13 H14 N2 O S
Formula weight	246.32
Temperature	298(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 6.7032(6) A alpha = 90 deg.
	b = 8.5139(9) A beta = 90 deg.
	c = 22.447(2) A gamma = 90 deg.
Volume	1281.0(2) A^3
Z, Calculated density	4, 1.277 Mg/m^3
Absorption coefficient	0.238 mm^-1
F(000)	520
Crystal size	0.45 x 0.37 x 0.24 mm
Theta range for data collection	2.56 to 25.01 deg.
Limiting indices	-6<=h<=7, -10<=k<=10, -26<=l<=26
Reflections collected / unique	6334 / 2228 [R(int) = 0.0394]
Completeness to theta = 25.01	99.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9451 and 0.9005
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2228 / 12 / 156
Goodness-of-fit on F^2	1.125
Final R indices [I>2sigma(I)]	R1 = 0.0537, wR2 = 0.0972
R indices (all data)	R1 = 0.1043, wR2 = 0.1177
Absolute structure parameter	0.7(3)
Extinction coefficient	0.0022(11)
Largest diff. peak and hole	0.211 and -0.184 e.A^-3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7.0049
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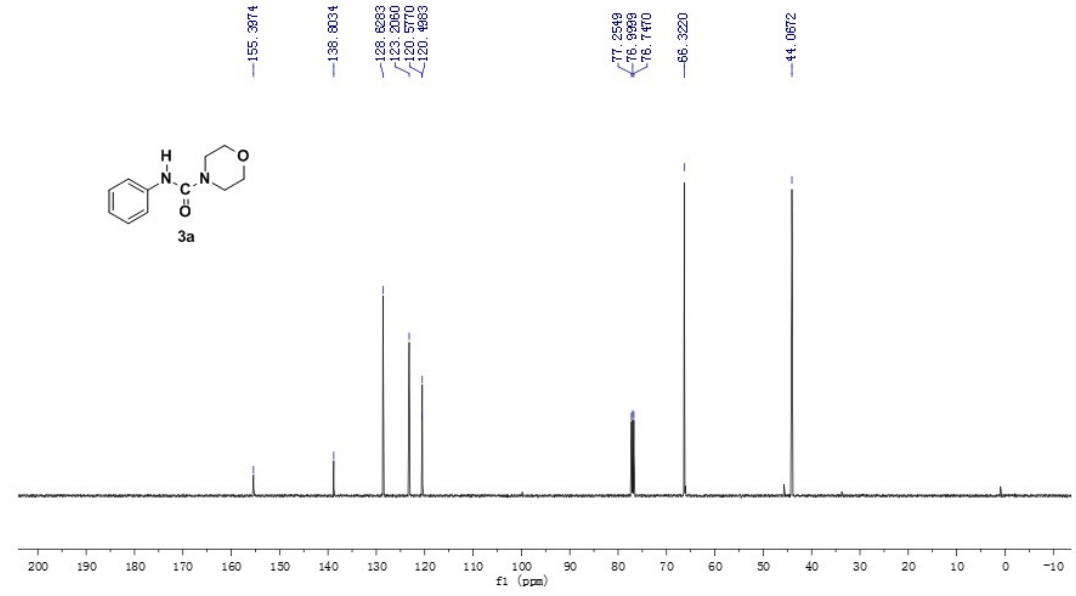
3.5663
3.5581
3.5491
3.3601
3.3513
3a
2.00
2.00
2.00
2.12
1.00
1.00
4.00
4.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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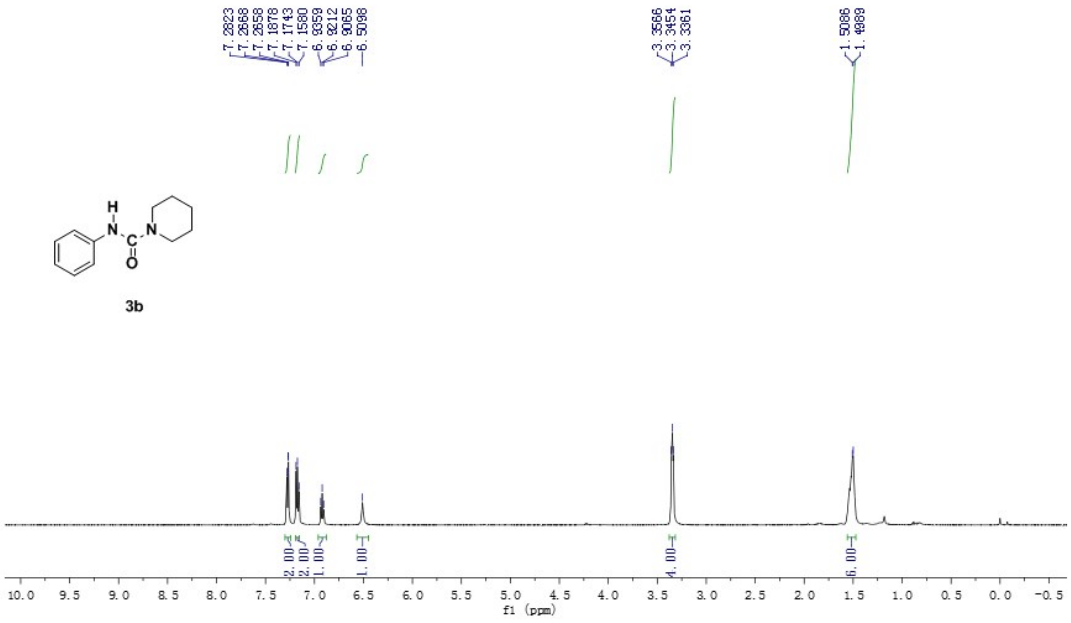
f1 (ppm)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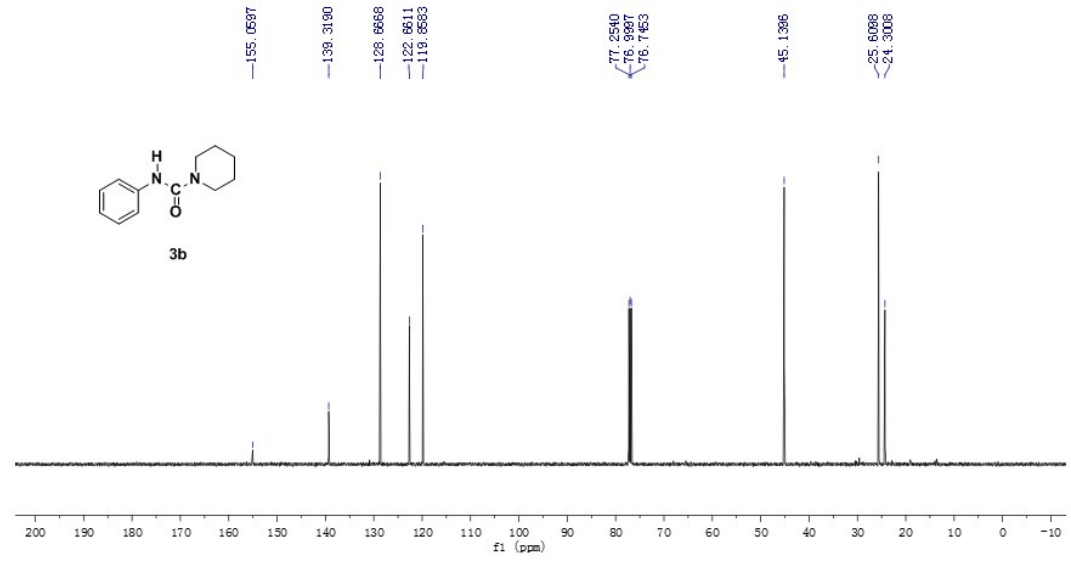
1.00
1.00
4.00
6.00
f1 (ppm)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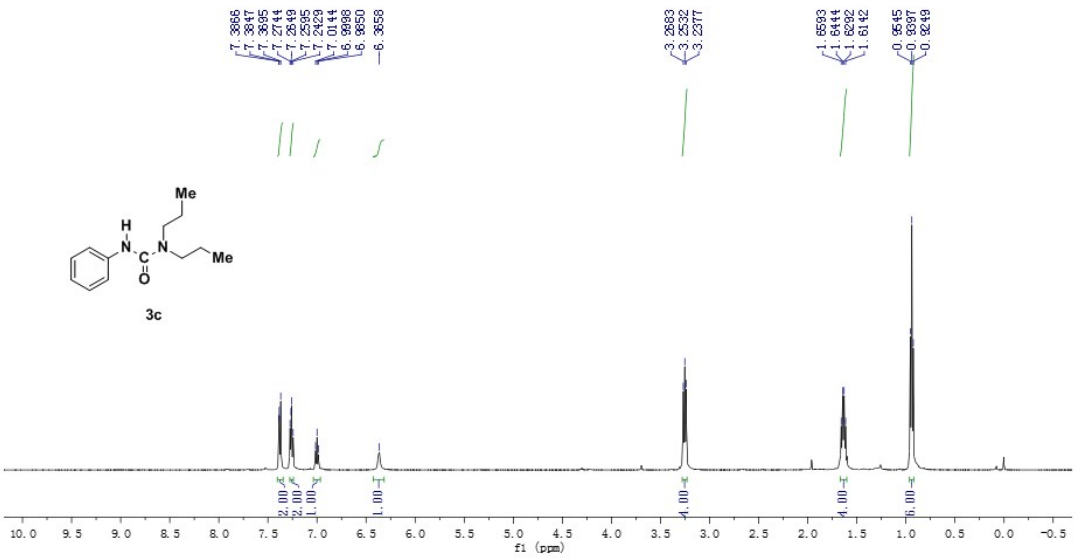
f1 (ppm)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4.00
6.00
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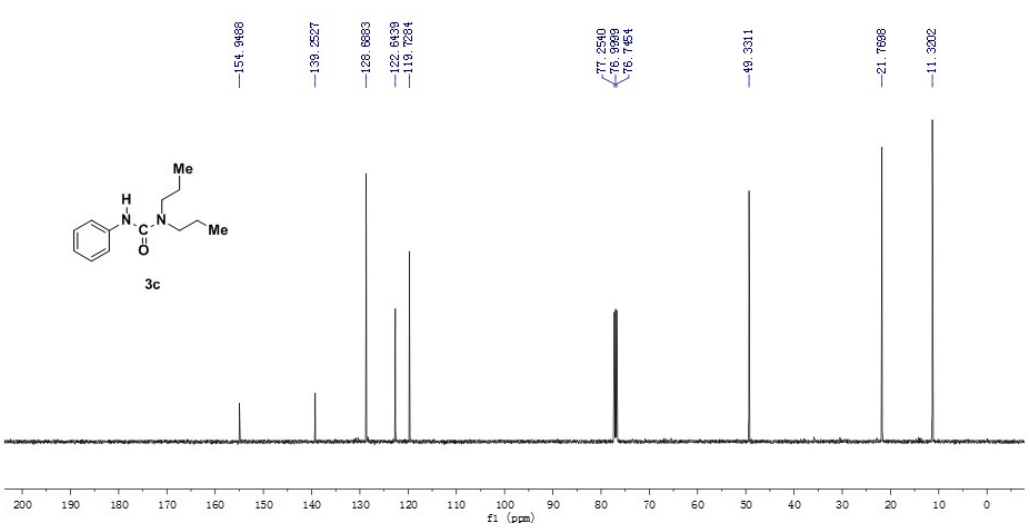
f1 (ppm)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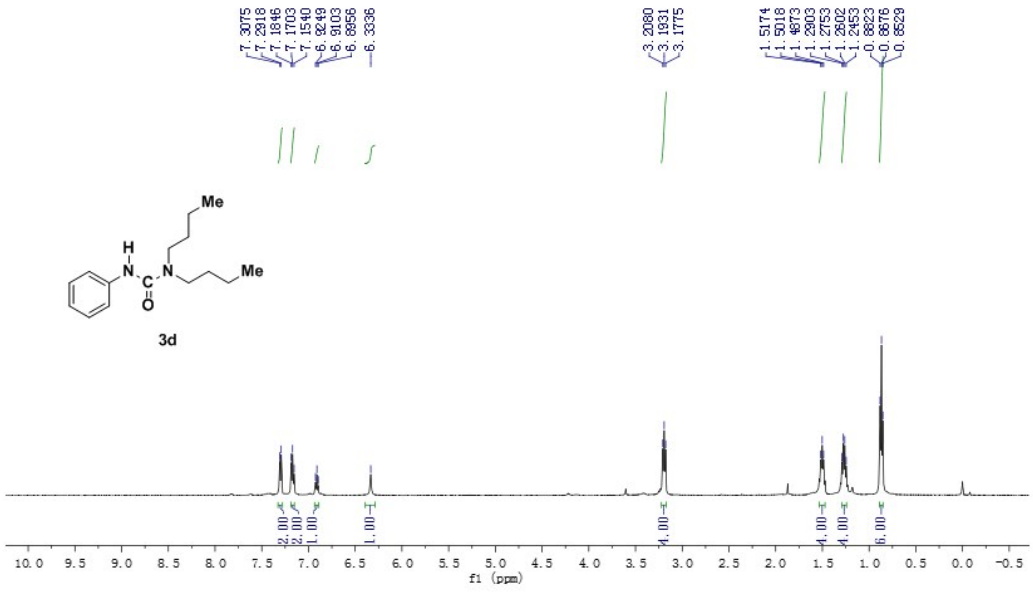
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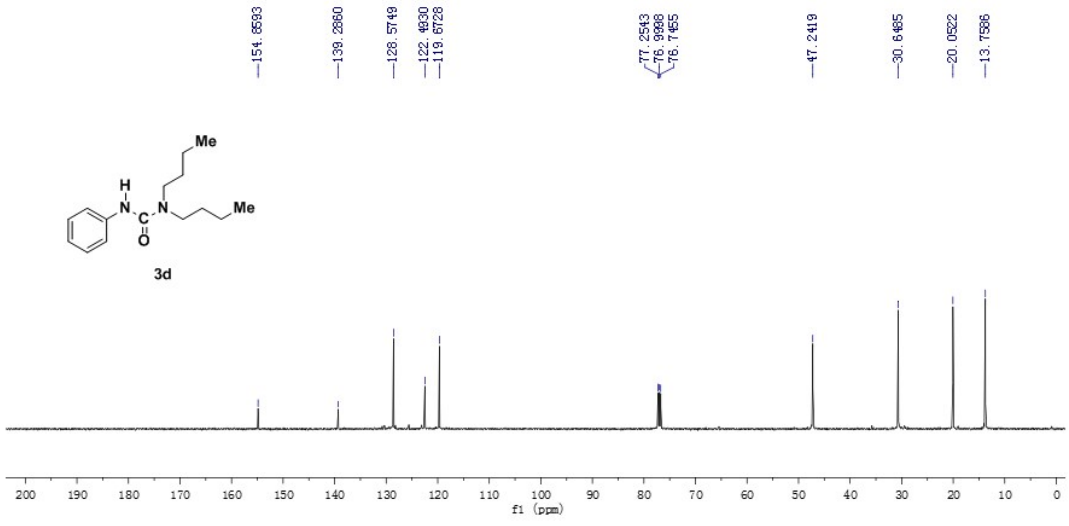
f1 (ppm)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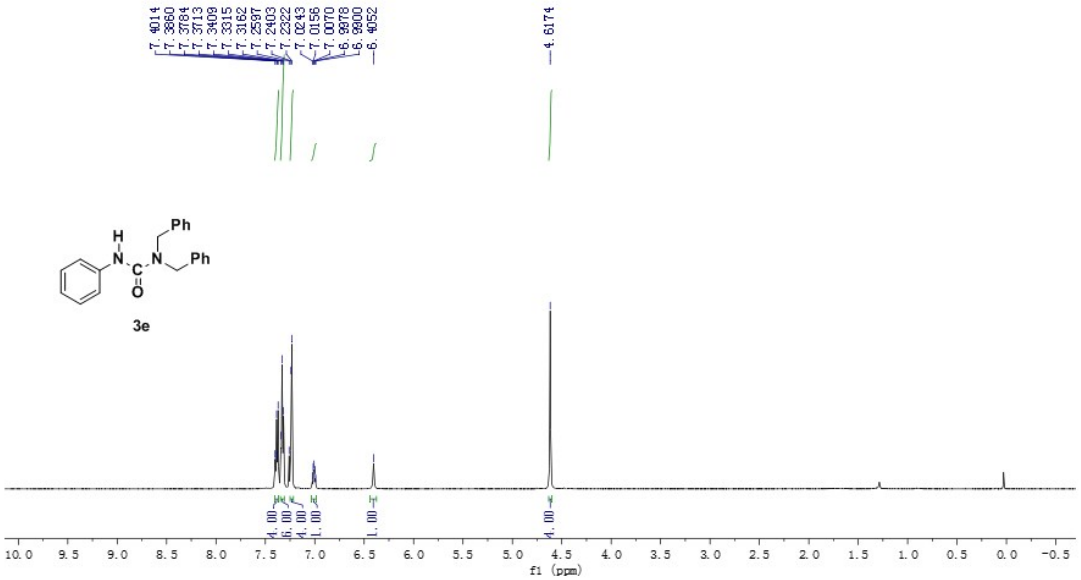
f1 (ppm)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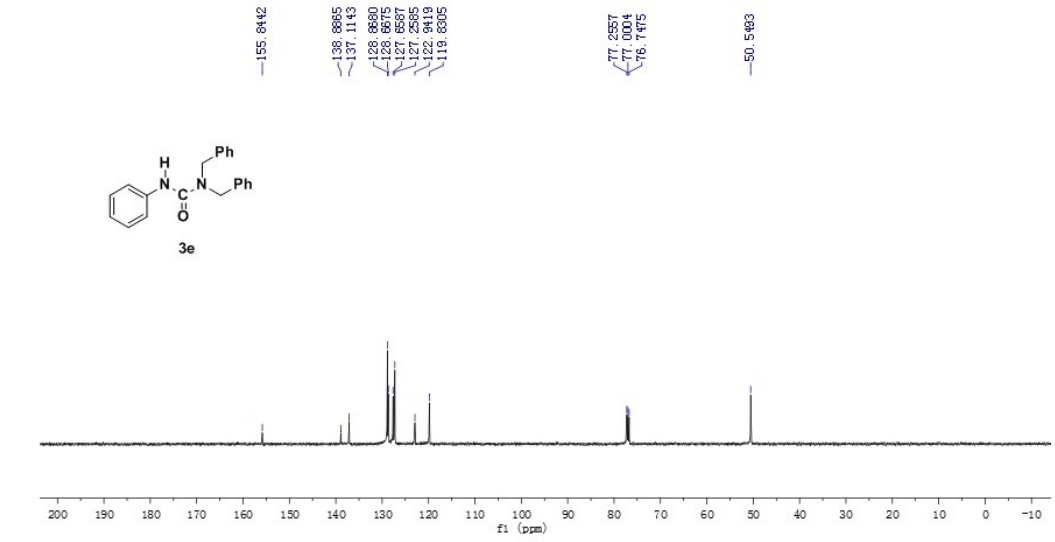
1.00
4.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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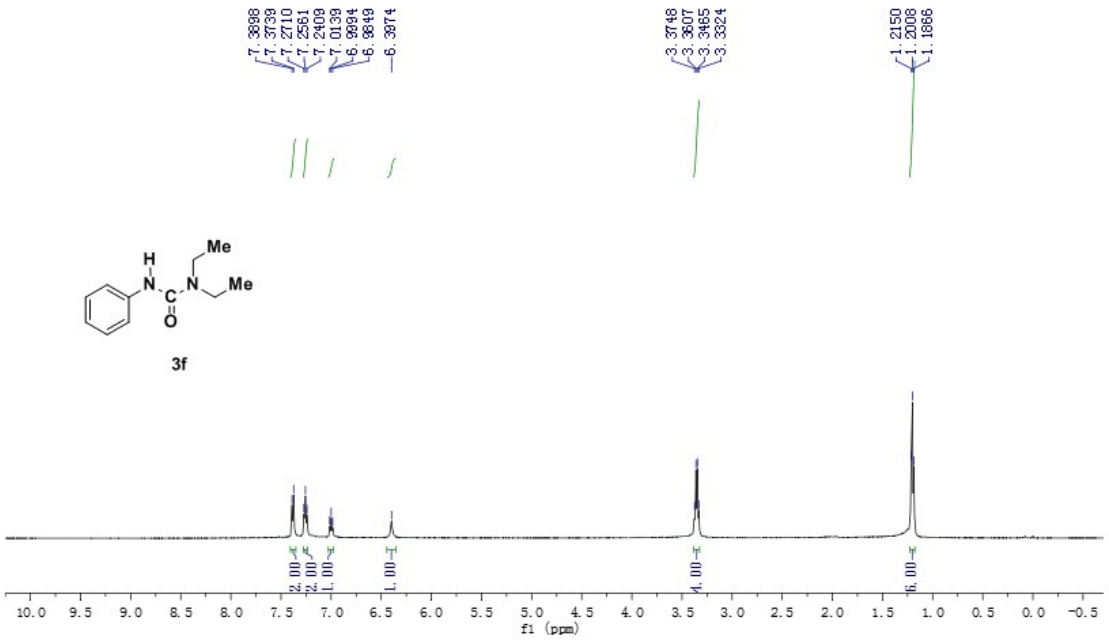
127.6587
127.2585
122.9419
119.8305
77.2557
77.0001
76.7475
50.5493
Ph
H
N
C
O
N
Ph
3e
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.2409
7.0139
6.9994
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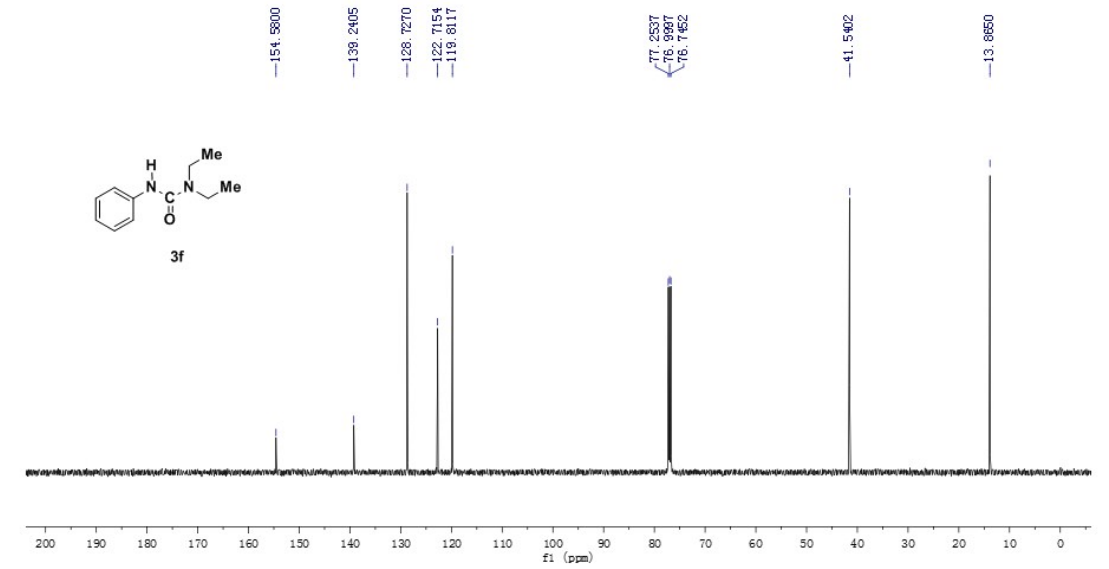
6.3874
3.3748
3.3607
3.3465
3.3324
1.2150
1.2008
1.1866
Me
Me
H
N
C
O
N
3f
2.00
2.00
2.00
1.00
1.00
4.00
6.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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Me
H
N
C
O
N
3f
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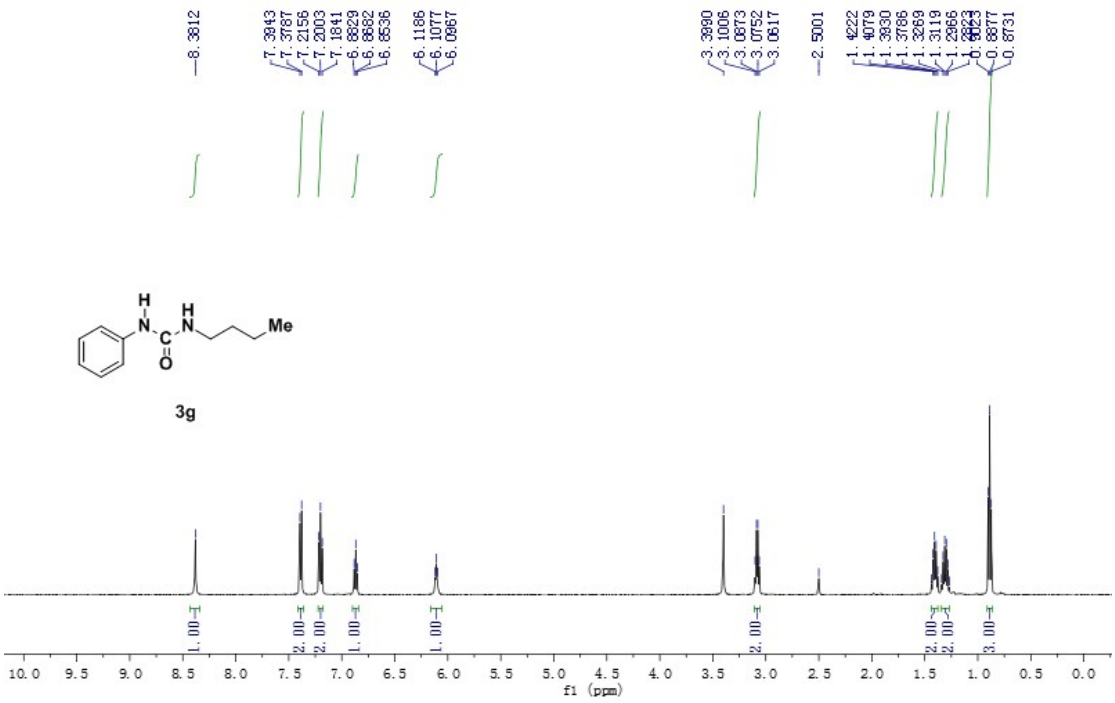
f1 (ppm)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7.1841
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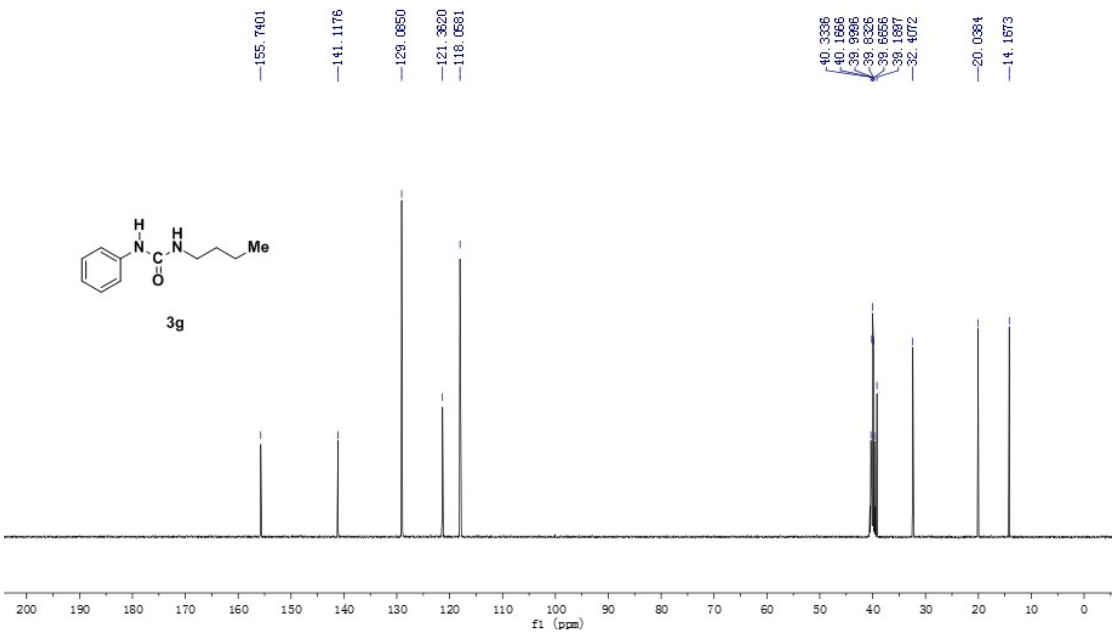
6.1077
6.0967
3.3990
3.1006
3.0873
3.0752
3.0617
2.5001
1.4222
1.4079
1.3930
1.3786
1.3269
1.3119
1.2966
0.8877
0.8731
H
N
H
N
C
O
Me
3g
1.00
2.00
2.00
1.00
1.00
2.00
2.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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39.1897
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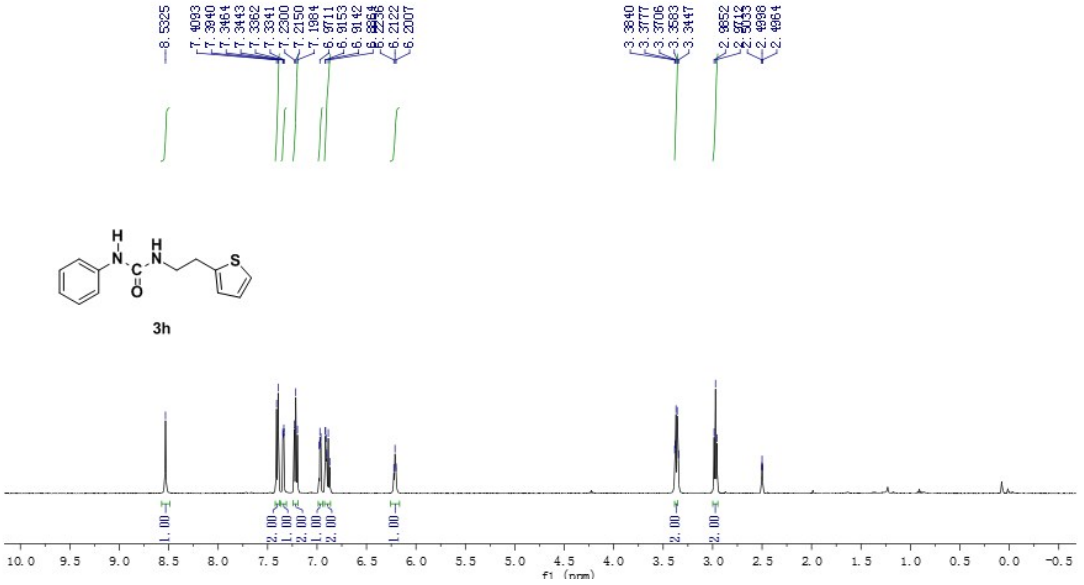
N
H
N
C
O
Me
3g
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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6.9711
6.9153
6.9142
6.2122
6.2007
3.3840
3.3777
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3.3447
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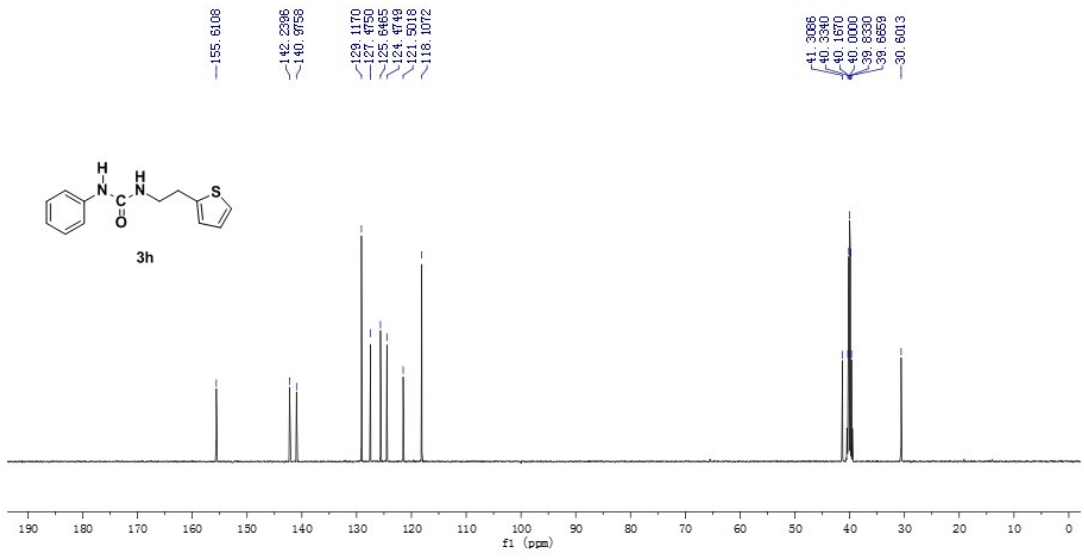
2.9713
2.9573
2.4988
2.4964
3h
f1 (ppm)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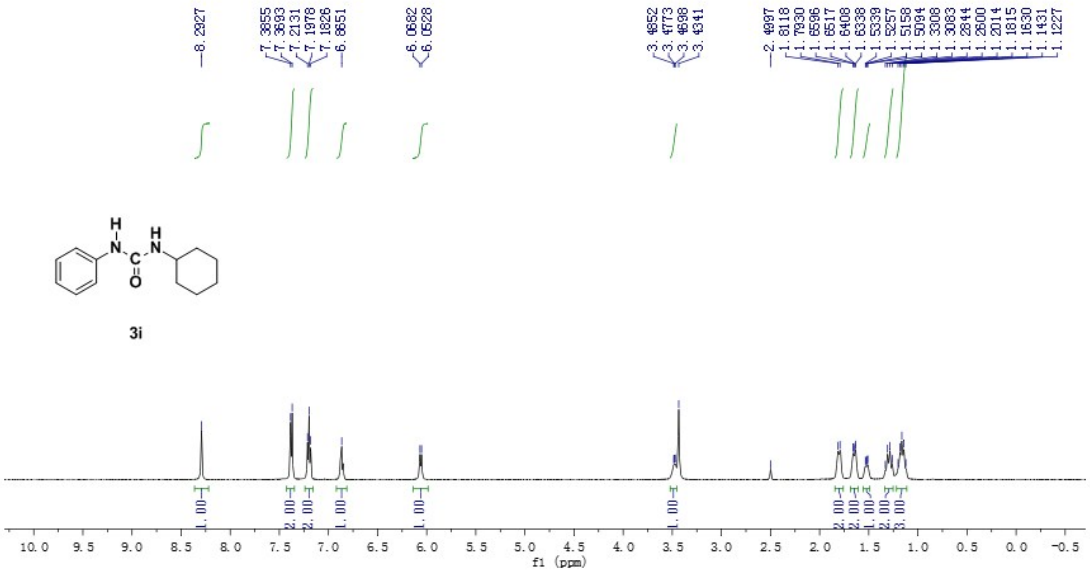
39.6659
30.6013
3h
f1 (ppm)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3.4773
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3.4341
2.4997
1.8118
1.7930
1.6596
1.6517
1.6408
1.6338
1.5339
1.5257
1.5158
1.3094
1.3008
1.3063
1.2844
1.2500
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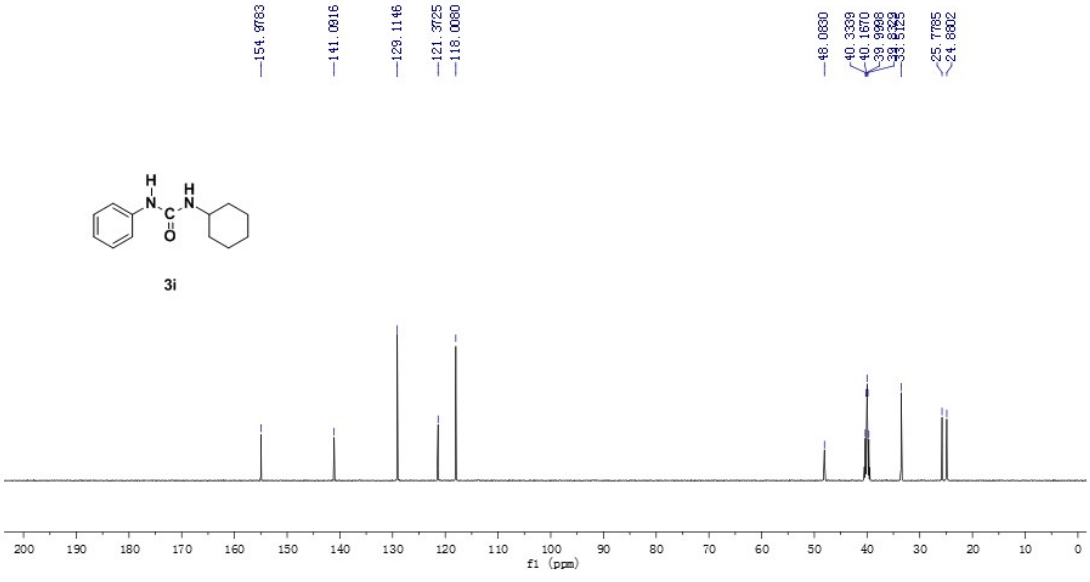
1.1630
1.1431
1.1227
3i
f1 (ppm)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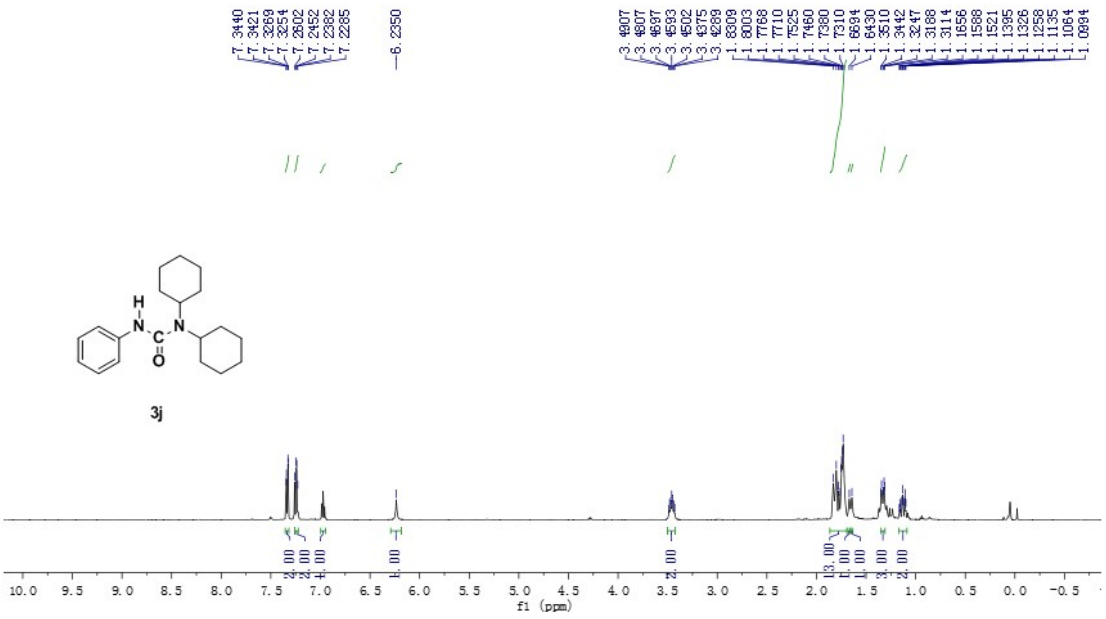
25.7785
24.8802
3i
f1 (ppm)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7.2602
7.2452
7.2382
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6.2350
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3.4697
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3.4502
3.4375
3.4299
1.8309
1.8003
1.7768
1.7710
1.7525
1.7460
1.7380
1.7310
1.6994
1.6430
1.3510
1.3442
1.3247
1.3188
1.3114
1.1656
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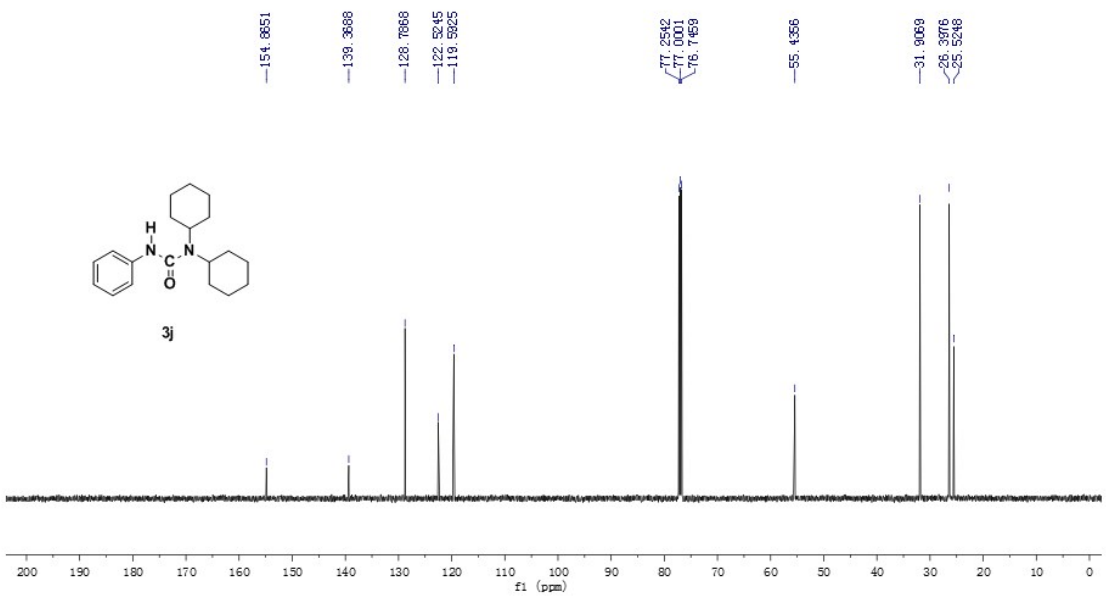
1.1135
1.1064
1.0894
3j
f1 (ppm)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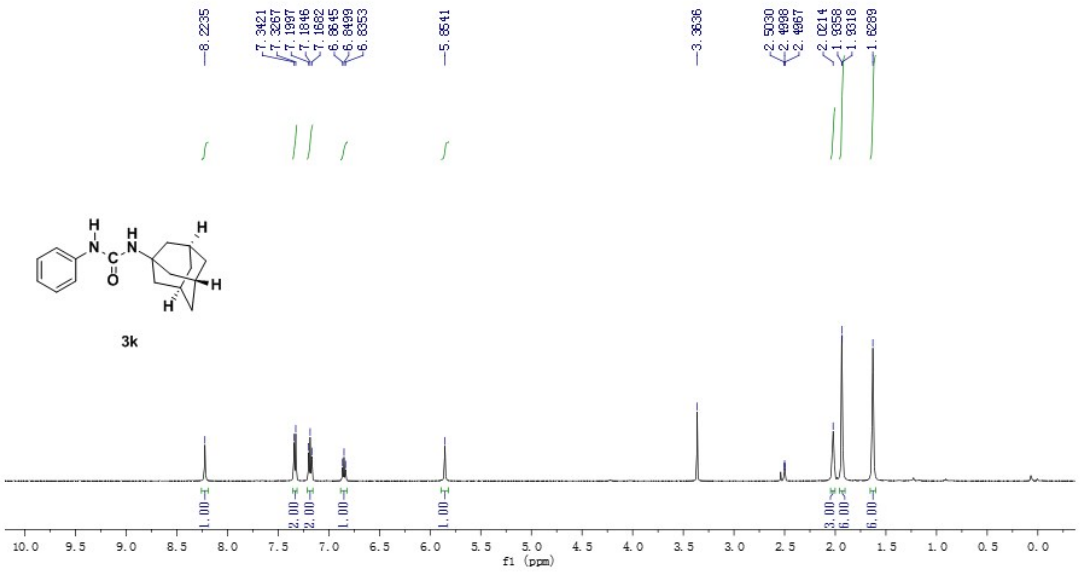
26.3976
25.5248
3j
f1 (ppm)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7.1682
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2.5030
2.4898
2.4767
2.0214
1.9358
1.9318
1.6289
3k
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2.00
2.00
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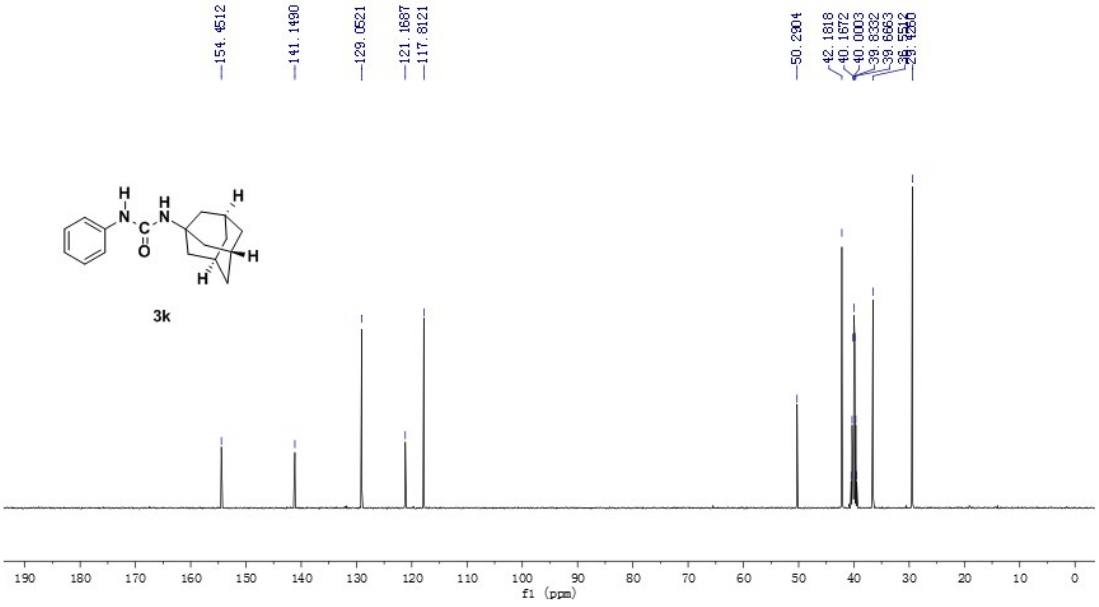
1.00
3.00
6.00
6.00
f1 (ppm)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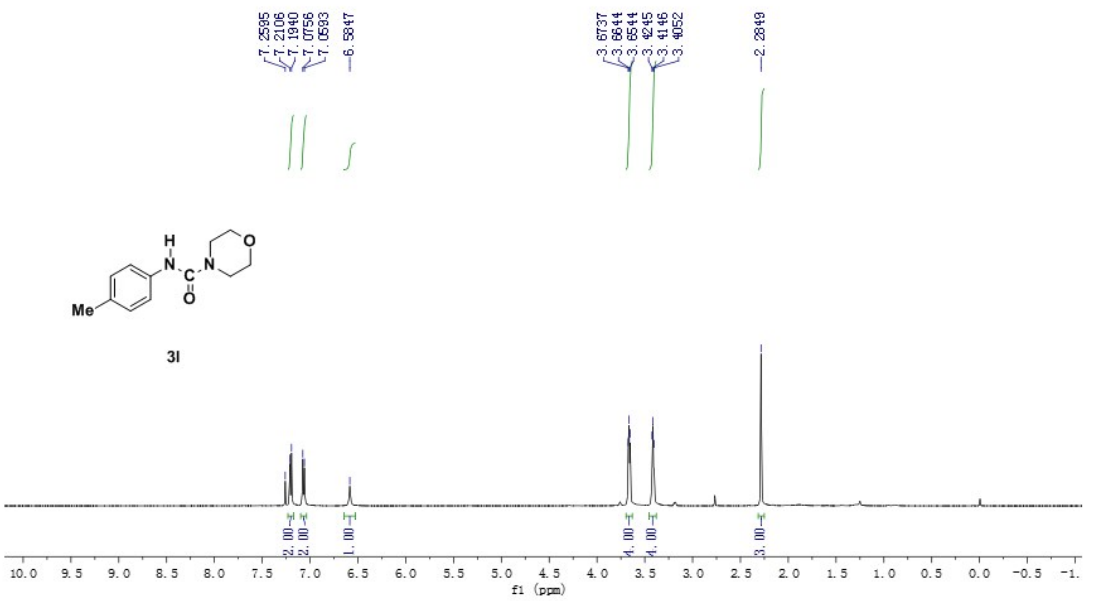
3k
f1 (ppm)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7.1940
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7.0593
6.5847
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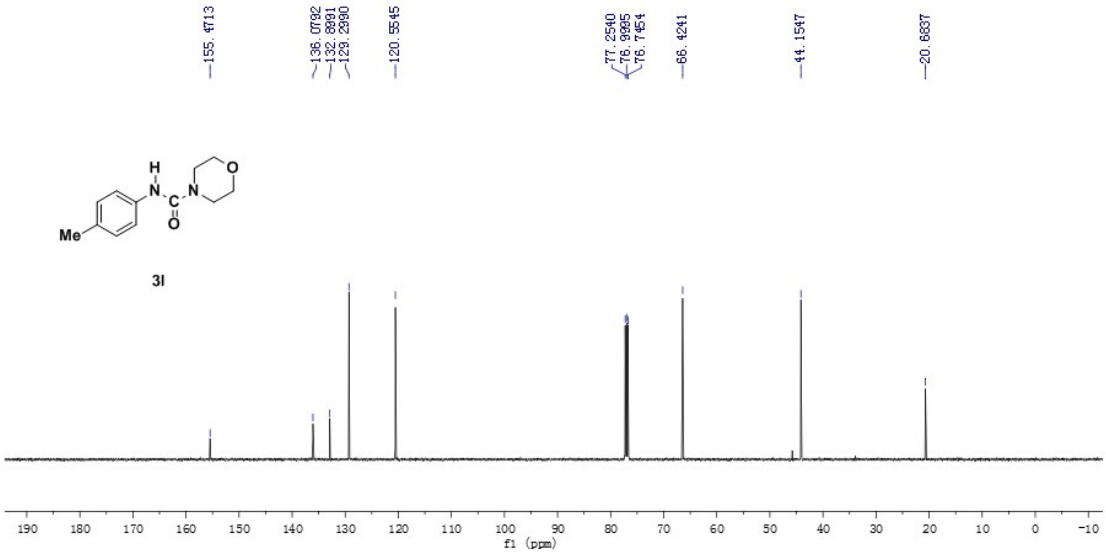
2.2849
Me
3l
2.00
2.22
1.00
4.00
4.00
3.00
f1 (ppm)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77.2540
76.9985
76.7454
66.4241
44.1547
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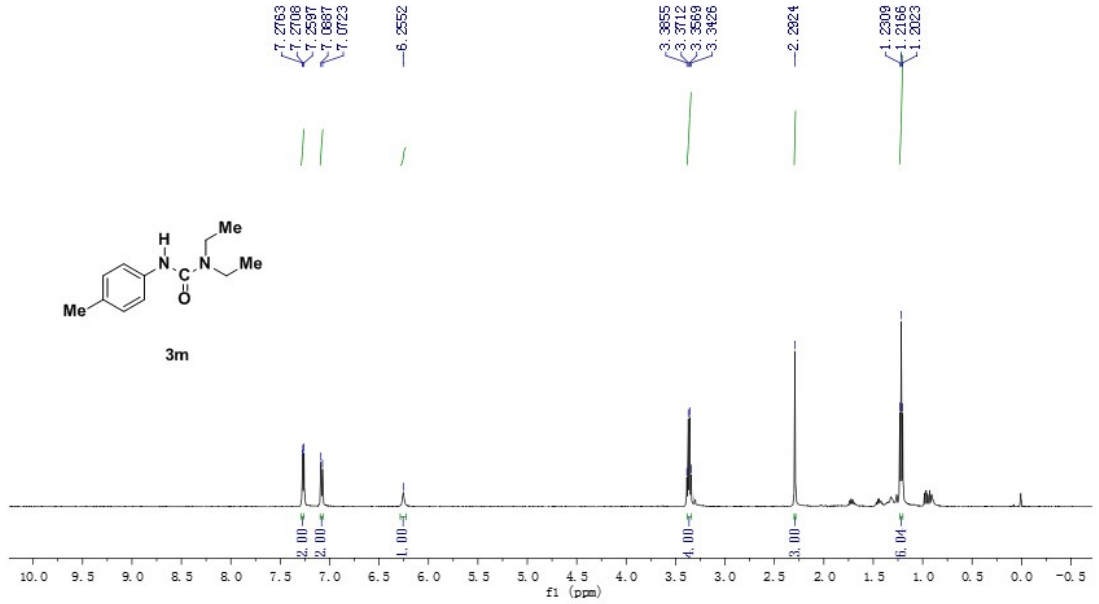
Me
3l
f1 (ppm)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6.2552
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3.3569
3.3426
2.2924
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1.2023
3m
2.00
2.00
1.00
4.00
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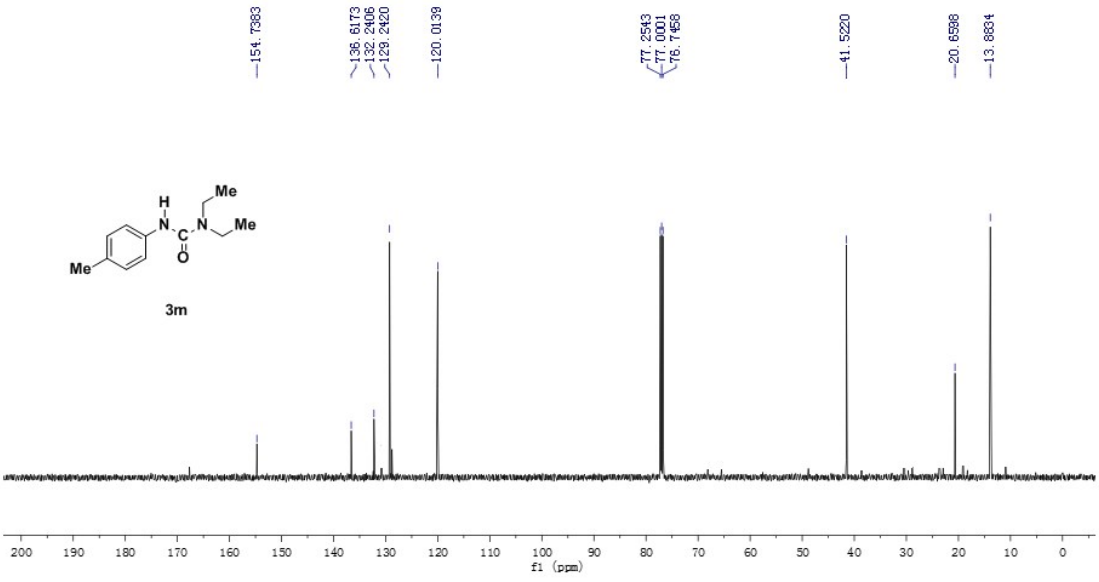
6.04
f1 (ppm)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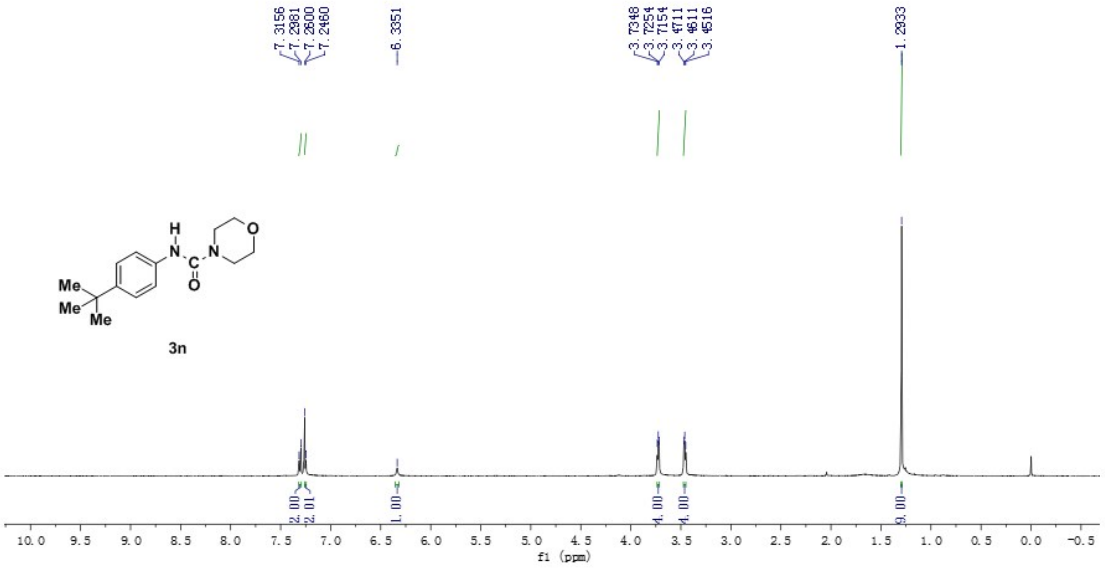
3m
f1 (ppm)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3.7254
3.7154
3.4711
3.4611
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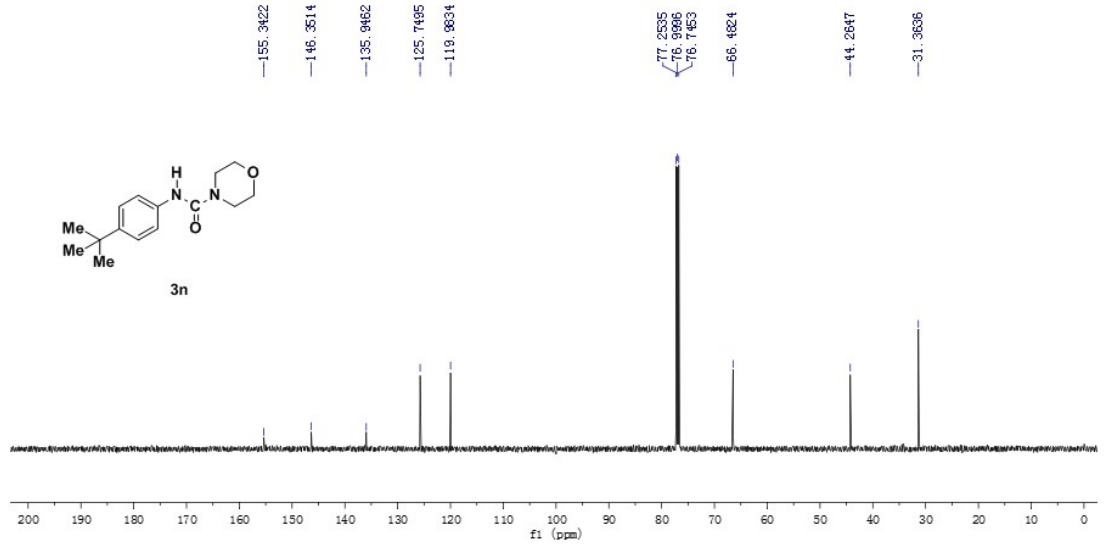
Me
Me
Me
3n
2.00
2.01
1.00
4.00
4.00
9.00
f1 (ppm)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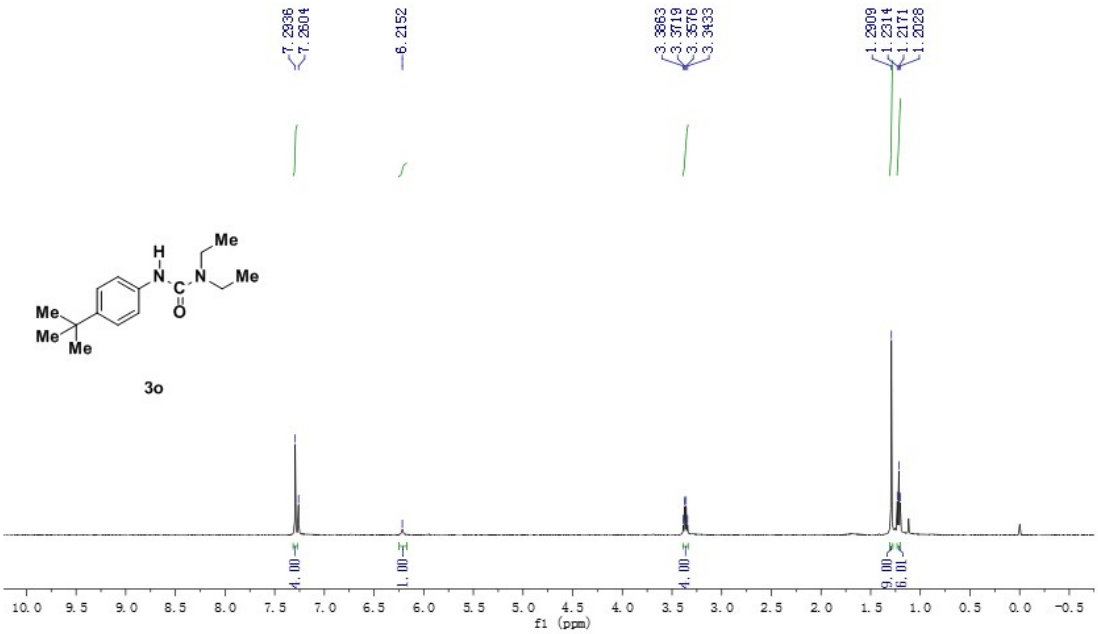
31.3636
Me
Me
Me
3n
f1 (ppm)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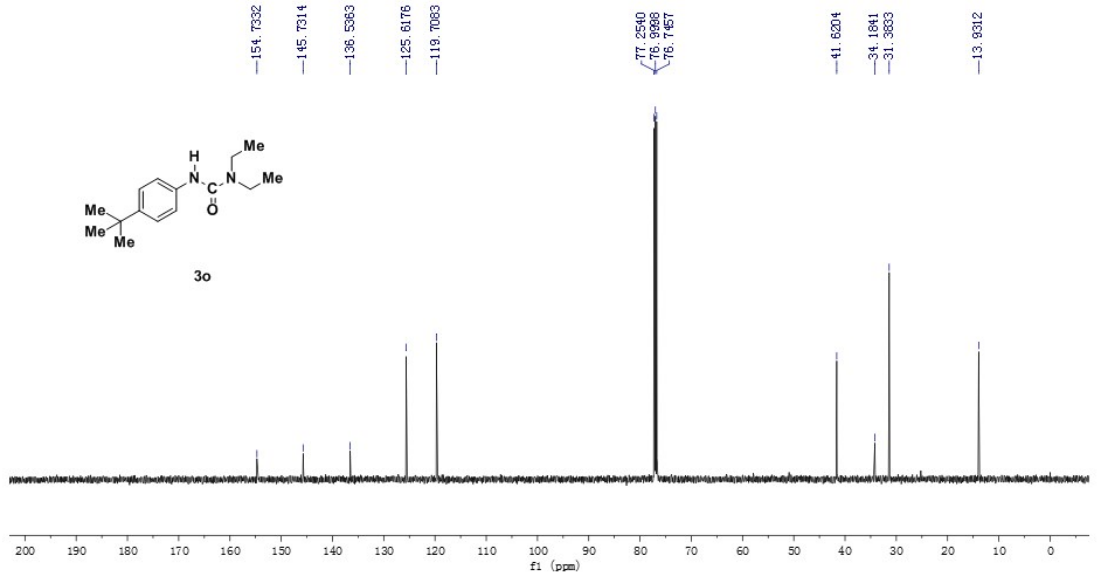
6.01
f1 (ppm)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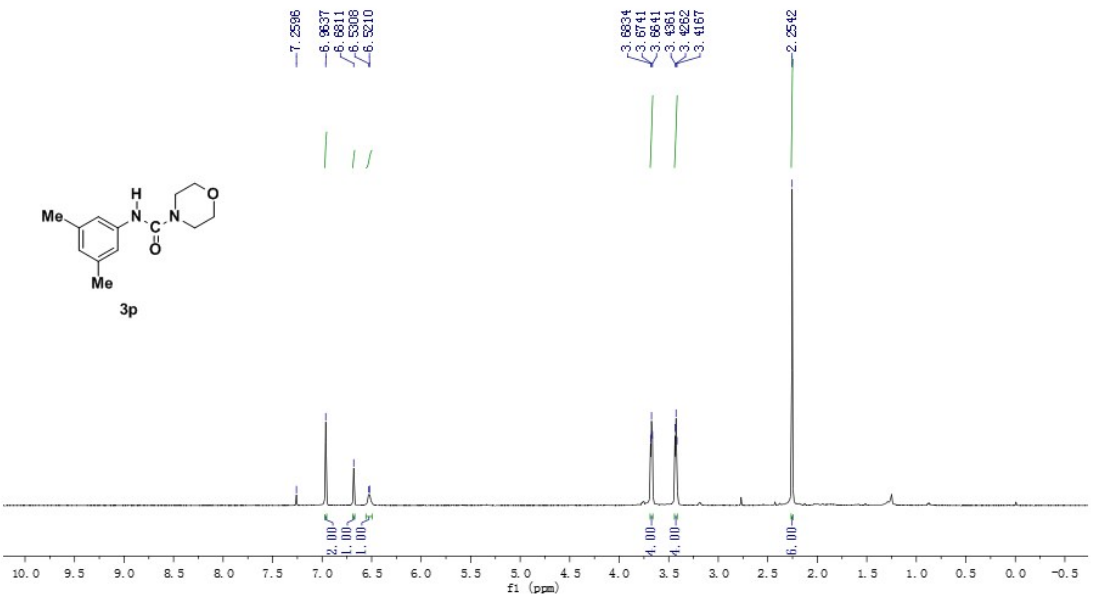
3o
f1 (ppm)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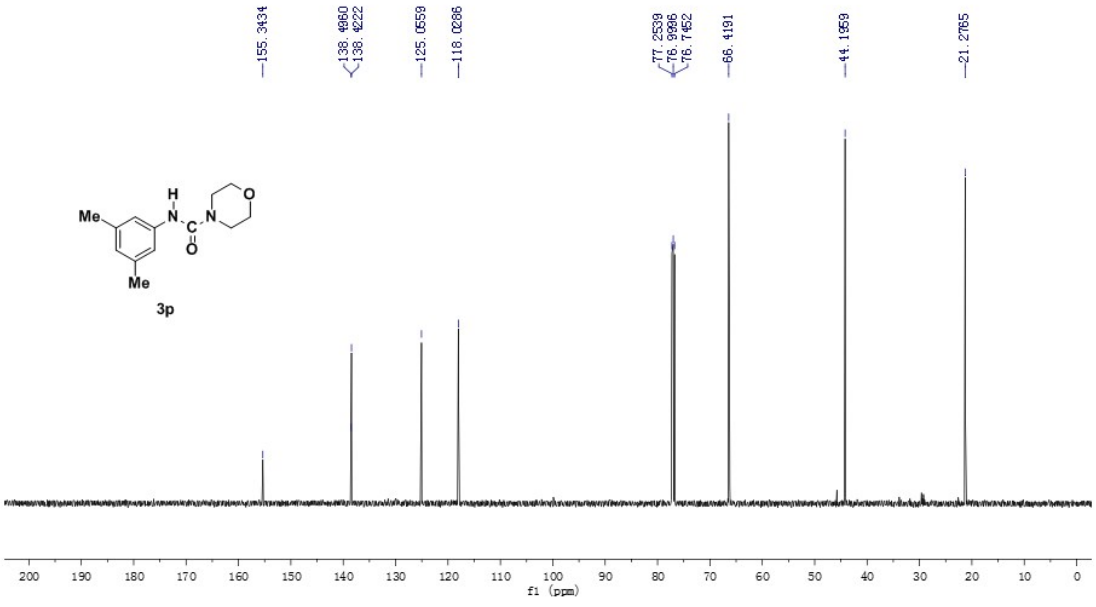
Me
Me
3p
2.00
1.00
1.00
4.00
4.00
6.00
f1 (ppm)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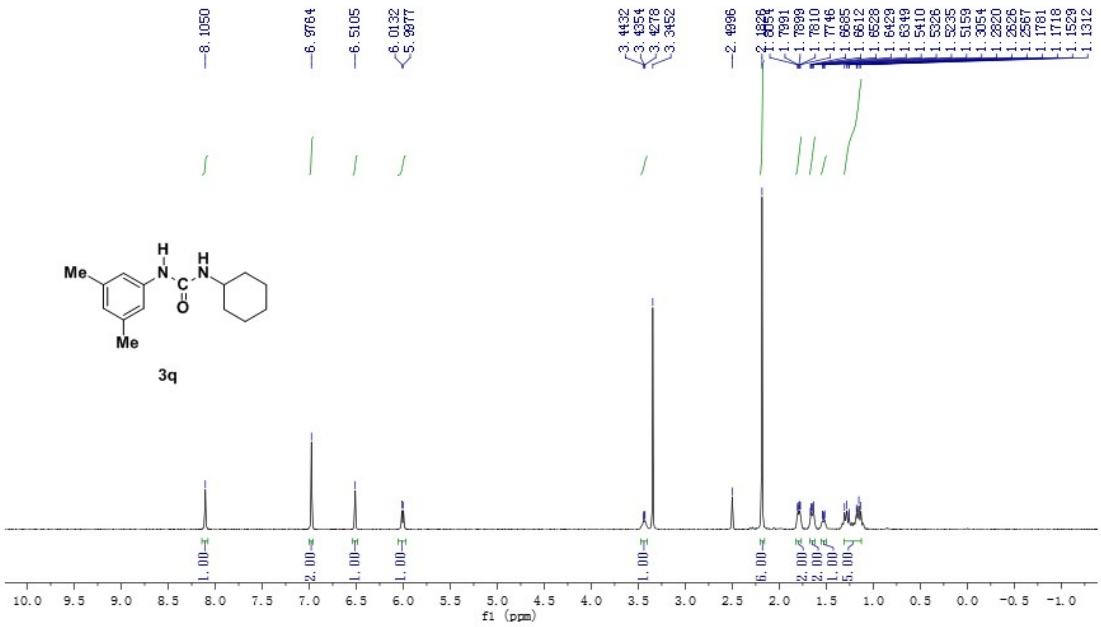
f1 (ppm)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1.5410
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1.00
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5.00
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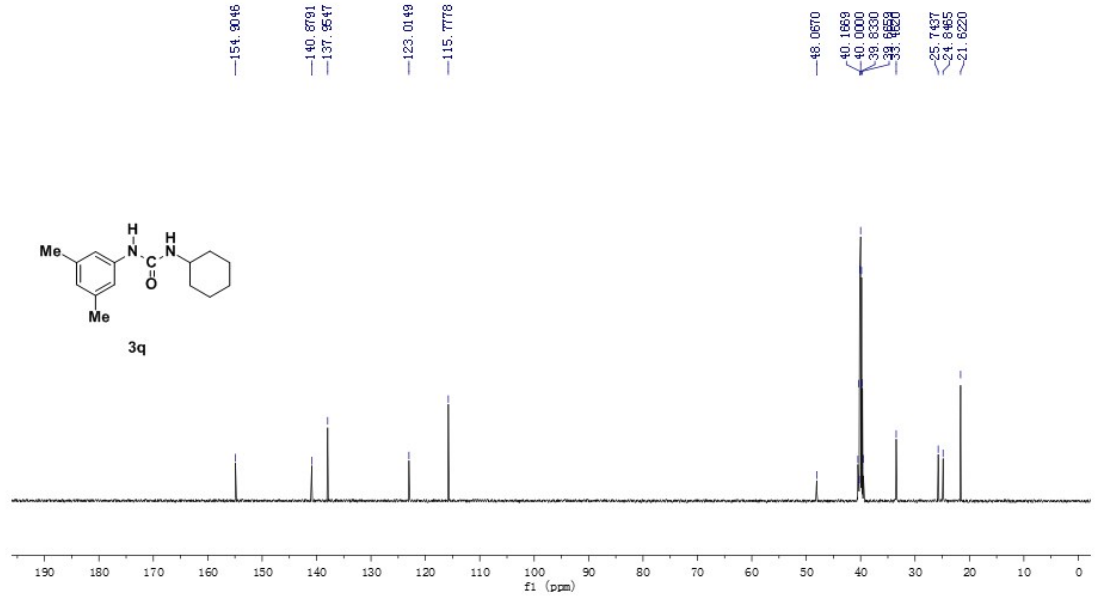
Me
3q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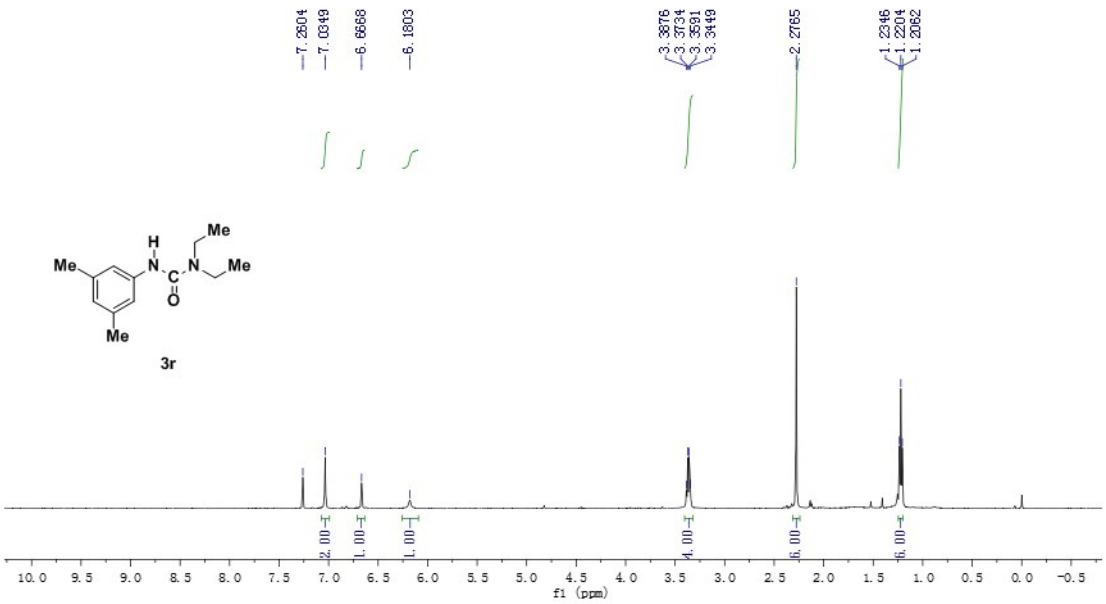
21.8220
f1 (ppm)
Me
Me
3q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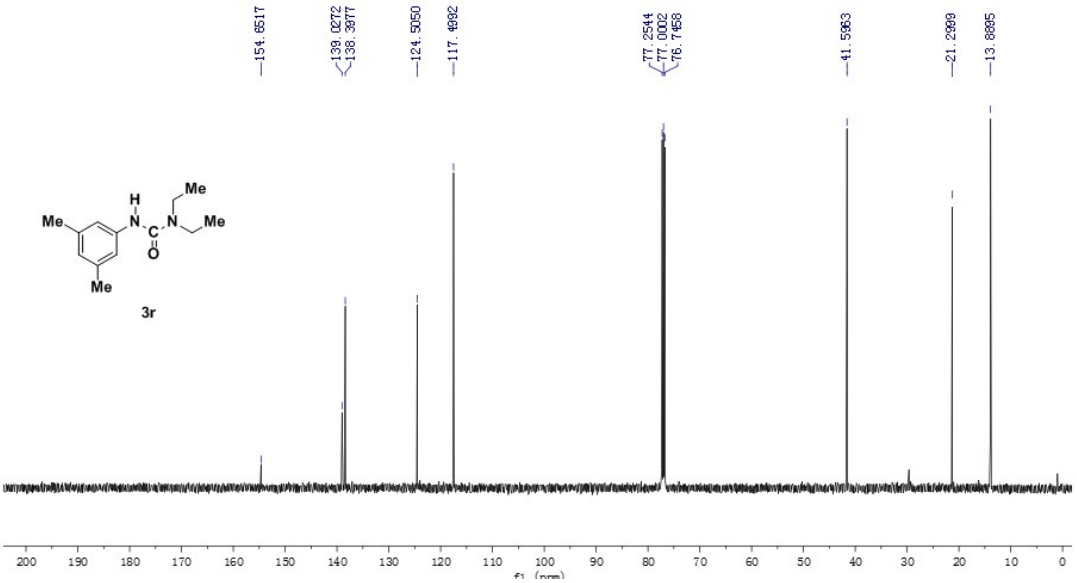
Me
H
N
C
O
N
Me
Me
Me
3r
2.00
1.00
1.00
4.00
6.00
6.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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N
C
O
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Me
Me
Me
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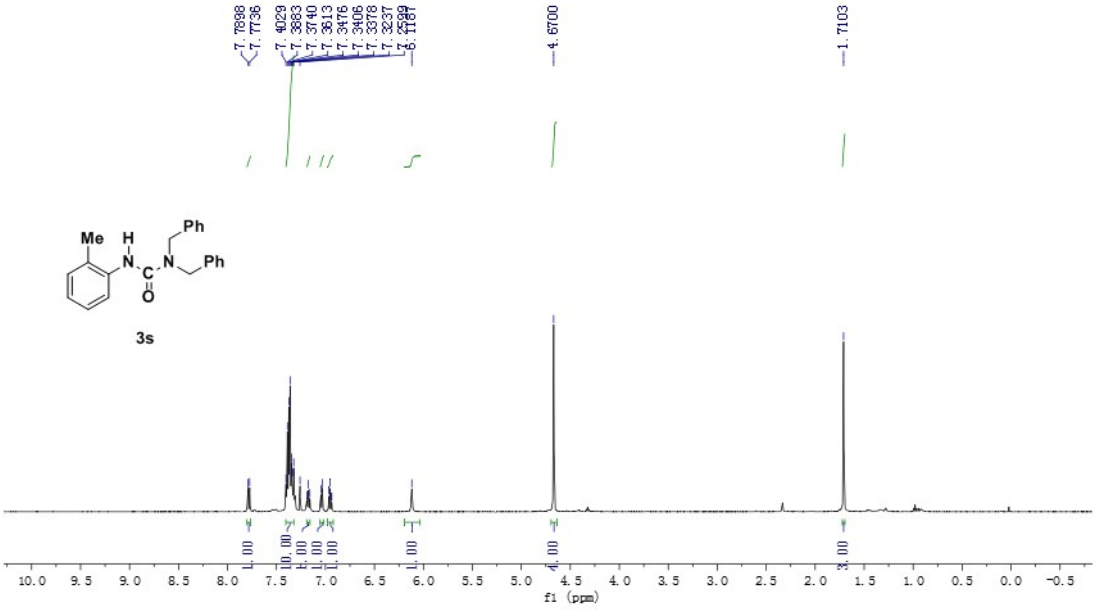
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7.3237
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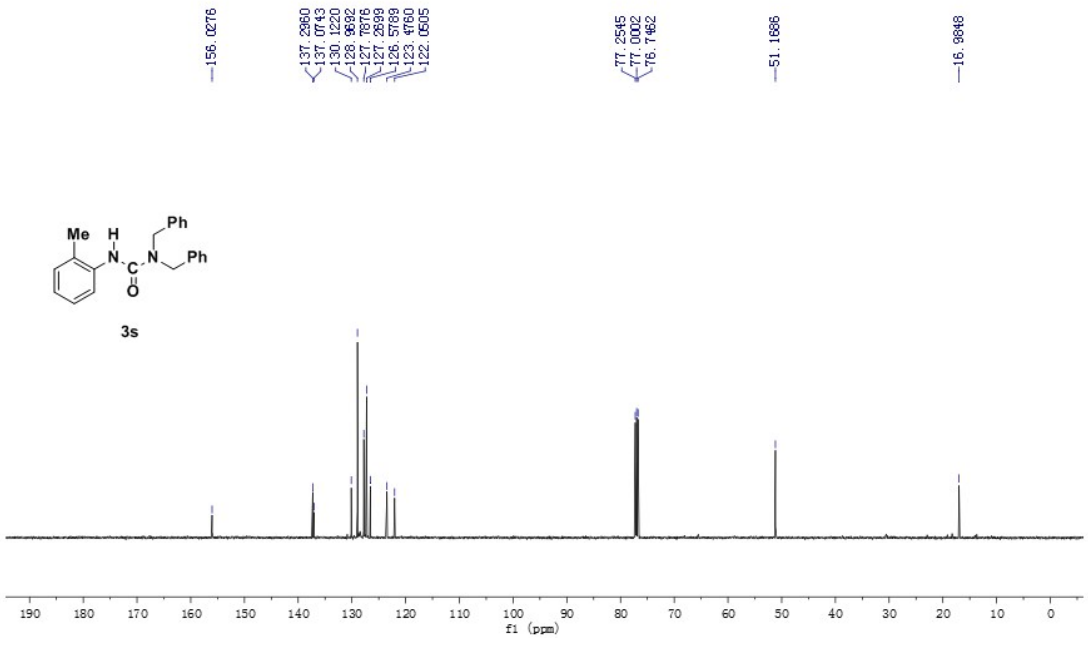
4.6700
1.7103
Me
H
N
C
O
N
Ph
Ph
3s
1.00
10.00
1.00
1.00
1.00
1.00
4.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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76.7462
51.1686
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C
O
N
Ph
Ph
3s
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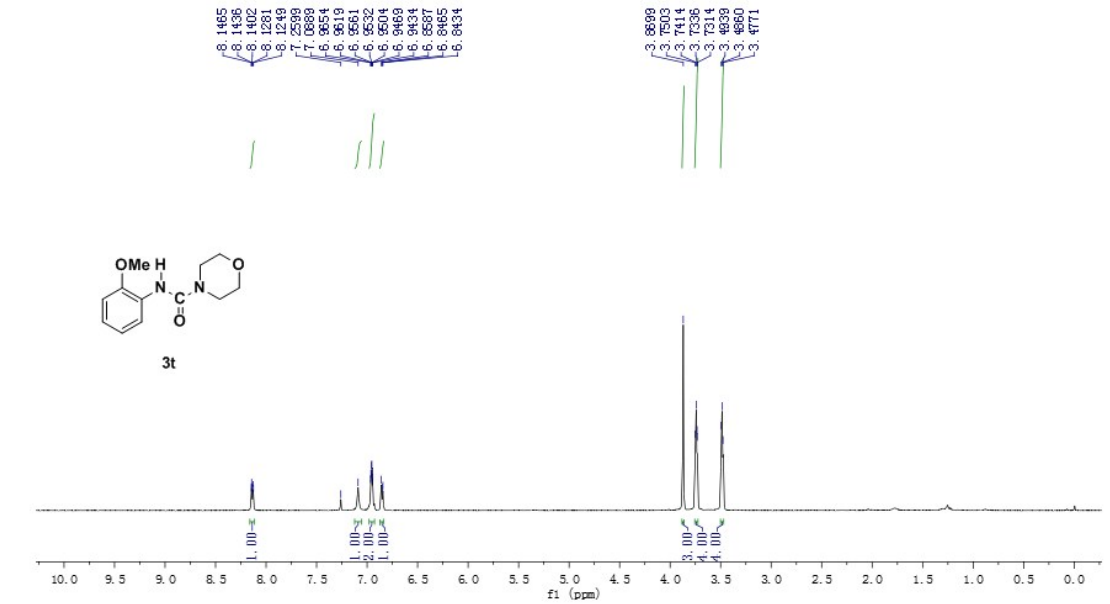
f1 (ppm)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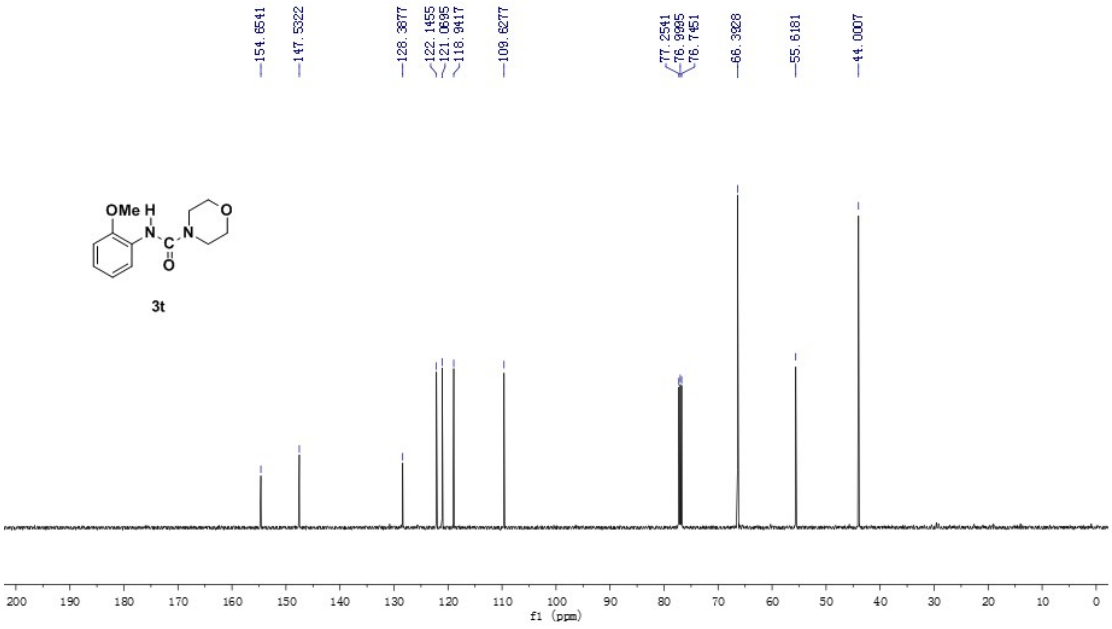
6.9504
6.9469
6.9434
6.6587
6.6455
6.6434
3.8699
3.7503
3.7414
3.7336
3.7314
3.4839
3.4660
3.4771
OMe
H
N
C
O
N
O
3t
1.00
1.00
2.00
1.00
3.00
4.00
4.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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109.6277
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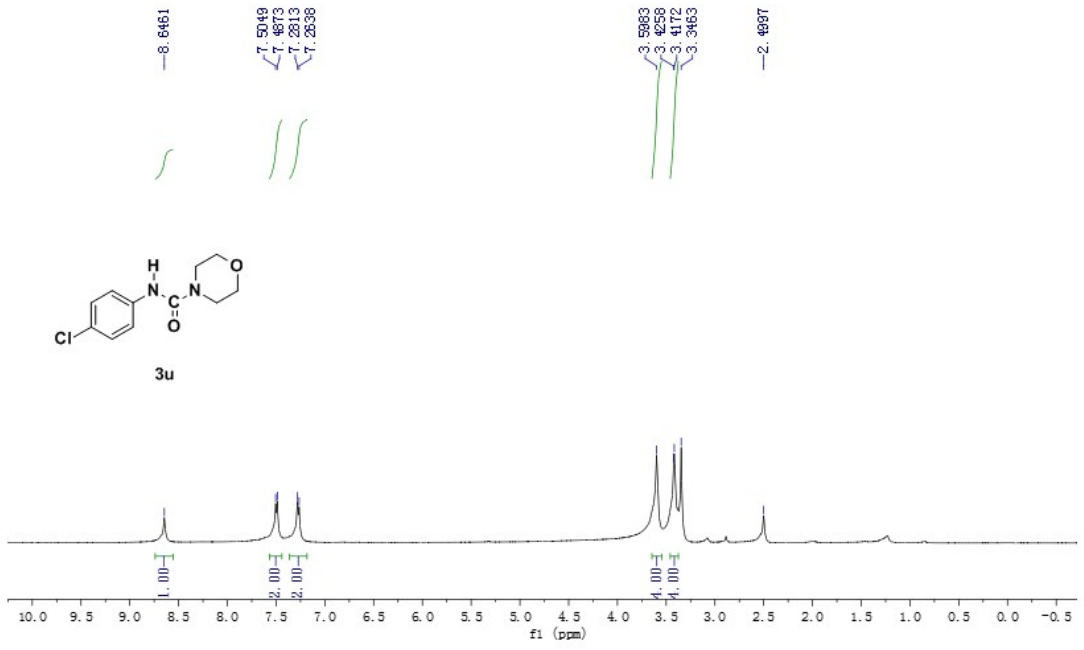
76.9995
76.7451
66.3928
55.6181
44.0007
OMe
H
N
C
O
N
O
3t
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.4873
7.2813
7.2638
3.5863
3.4258
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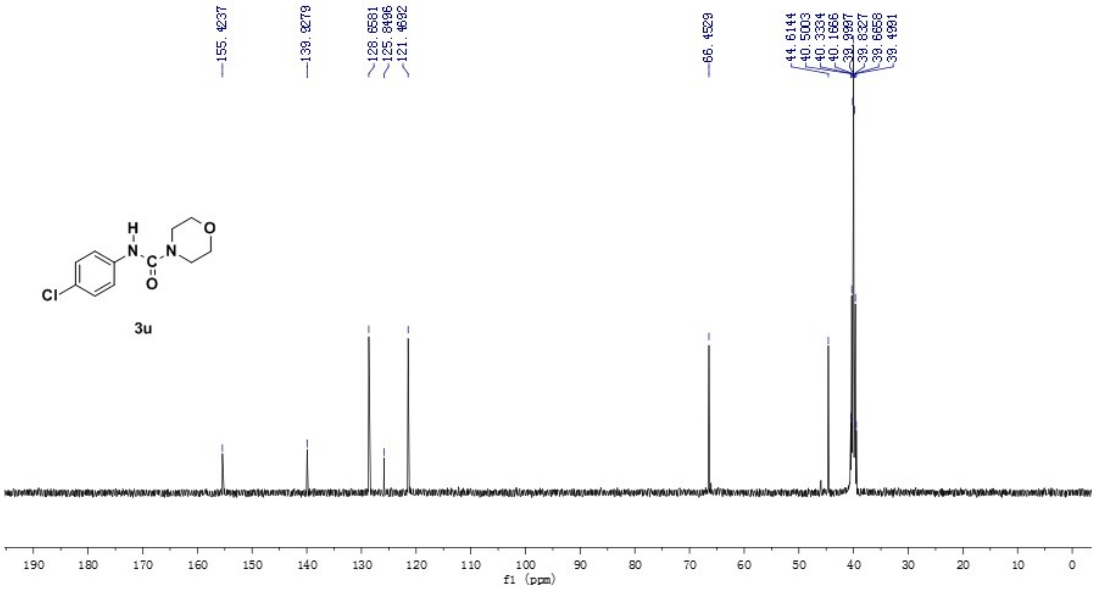
3.3463
2.4997
3u
1.00
2.00
2.00
4.00
4.00
f1 (ppm)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139.9279
128.8581
125.8496
121.4692
66.4529
44.6144
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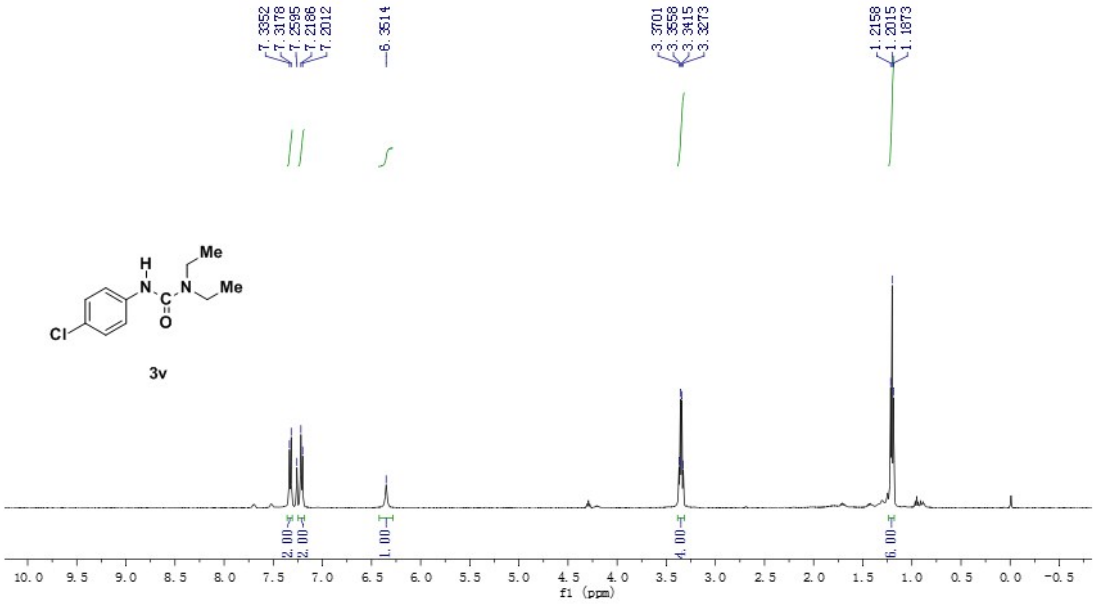
40.1666
39.9997
39.8327
39.6658
39.4991
3u
f1 (ppm)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7.2595
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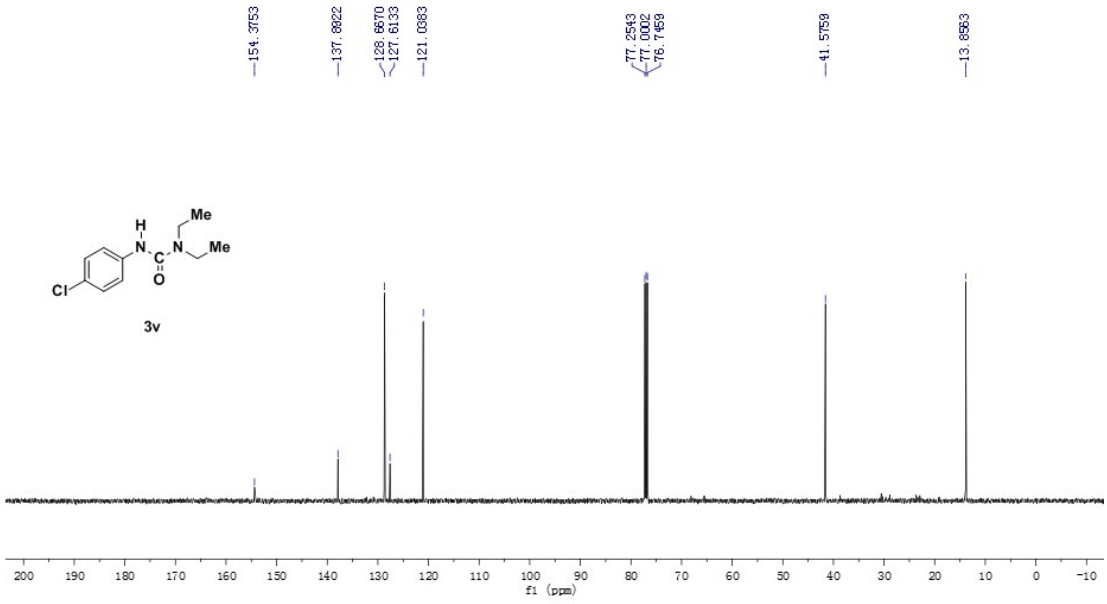
7.2012
6.3514
3.3701
3.3558
3.3415
3.3273
1.2158
1.2015
1.1873
Me
H
N
C
O
N
Me
Cl
3v
2.00
2.00
1.00
4.00
6.00
f1 (ppm)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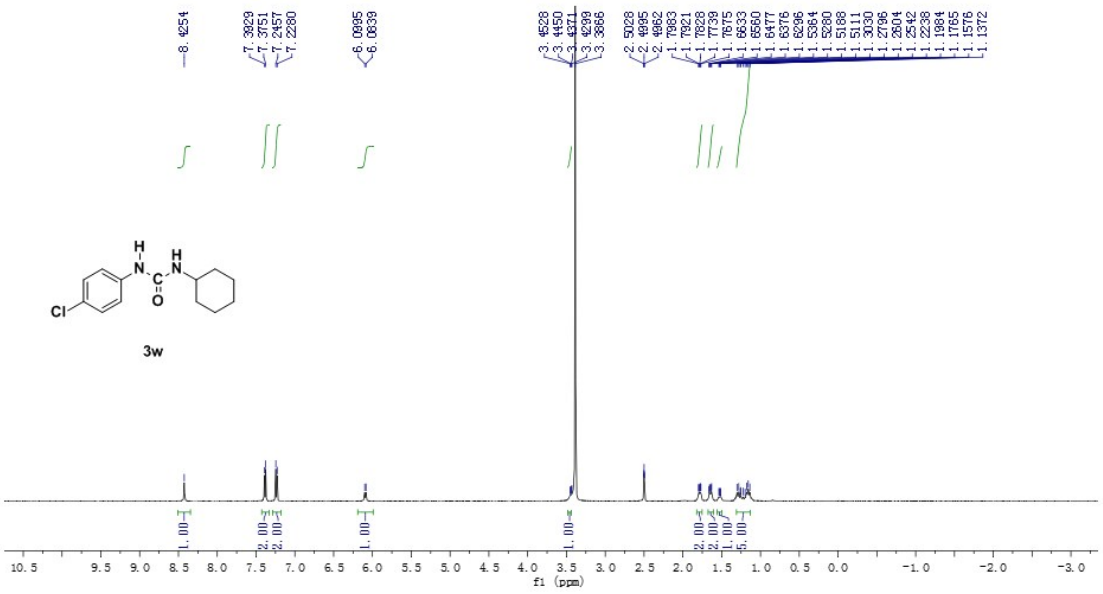
121.0383
77.2543
77.0002
76.7459
41.5759
13.8563
Me
H
N
C
O
N
Me
Cl
3v
f1 (ppm)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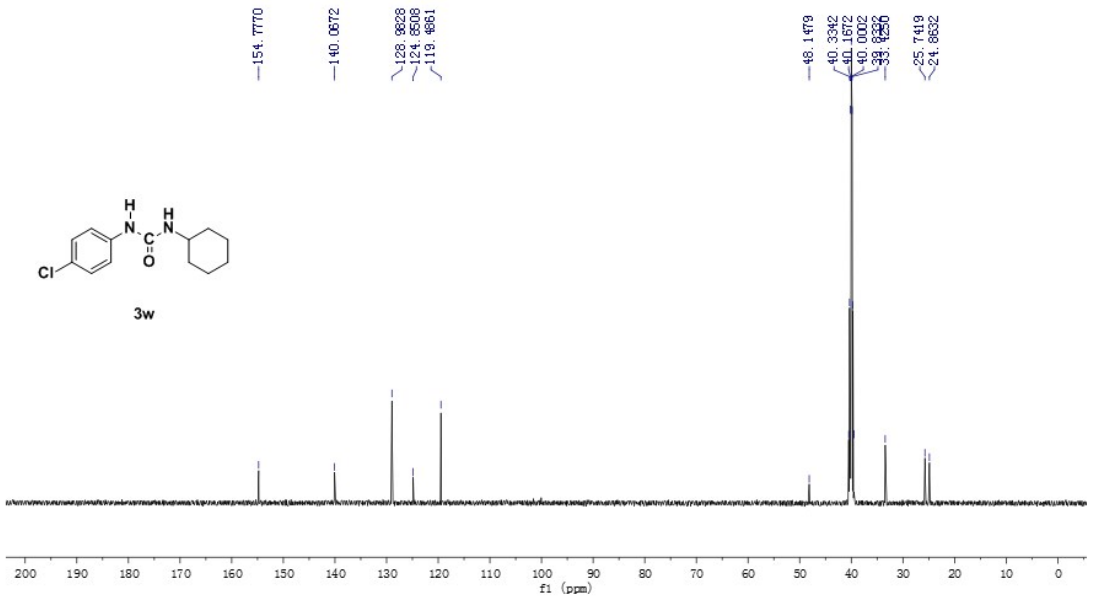
7.2457
7.2280
6.0995
6.0839
3.4528
3.4450
3.4371
3.4299
3.3866
2.5028
2.4995
2.4962
1.7983
1.7921
1.7828
1.7739
1.7675
1.6633
1.6560
1.6477
1.6376
1.6296
1.5364
1.5280
1.5188
1.5111
1.3030
1.2796
1.2604
1.2542
1.2238
1.1984
1.1765
1.1576
1.1372
1.00
2.00
2.00
1.00
1.00
2.00
2.00
1.00
5.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-1.0
-2.0
-3.0
f1 (ppm)
H
N
N
H
C
O
Cl
3w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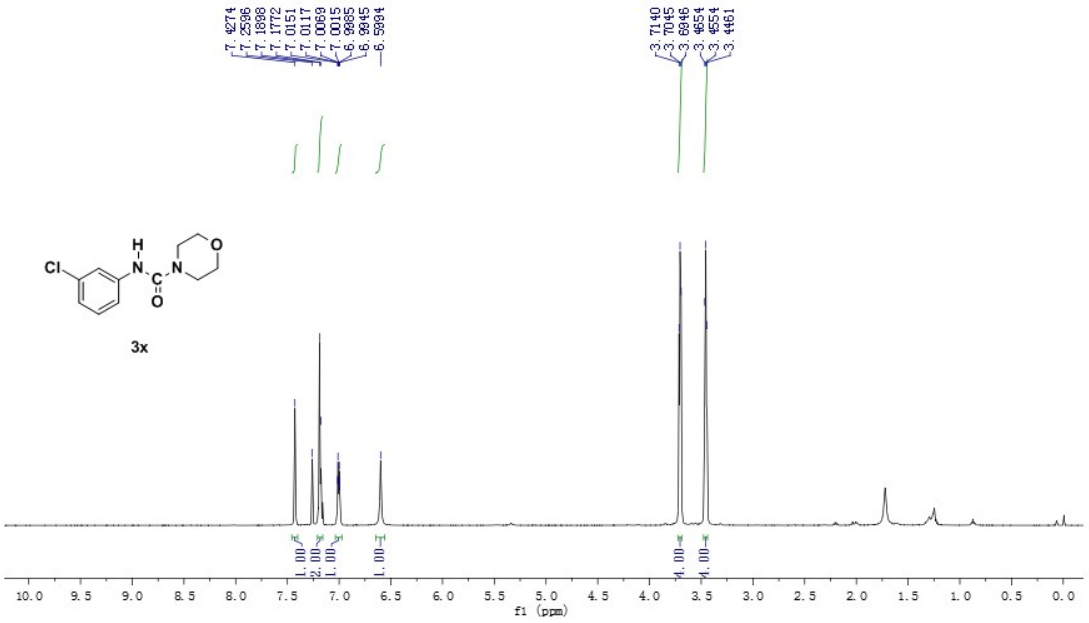
48.1479
40.3342
40.1672
40.0002
39.8332
39.6662
39.4992
39.3322
25.7419
24.8632
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
H
N
N
H
C
O
Cl
3w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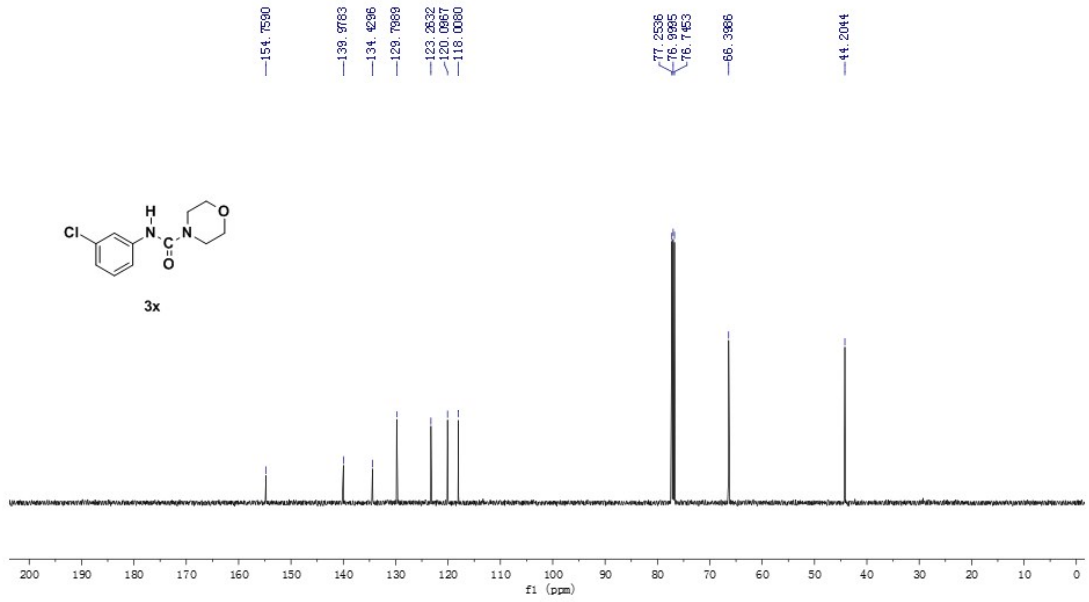
7.1898
7.1772
7.0151
7.0117
7.0069
7.0015
6.9985
6.9845
6.5994
3.7140
3.7045
3.6946
3.4654
3.4554
3.4461
Cl
H
N
C
O
O
N
3x
1.00
2.00
1.00
1.00
4.00
4.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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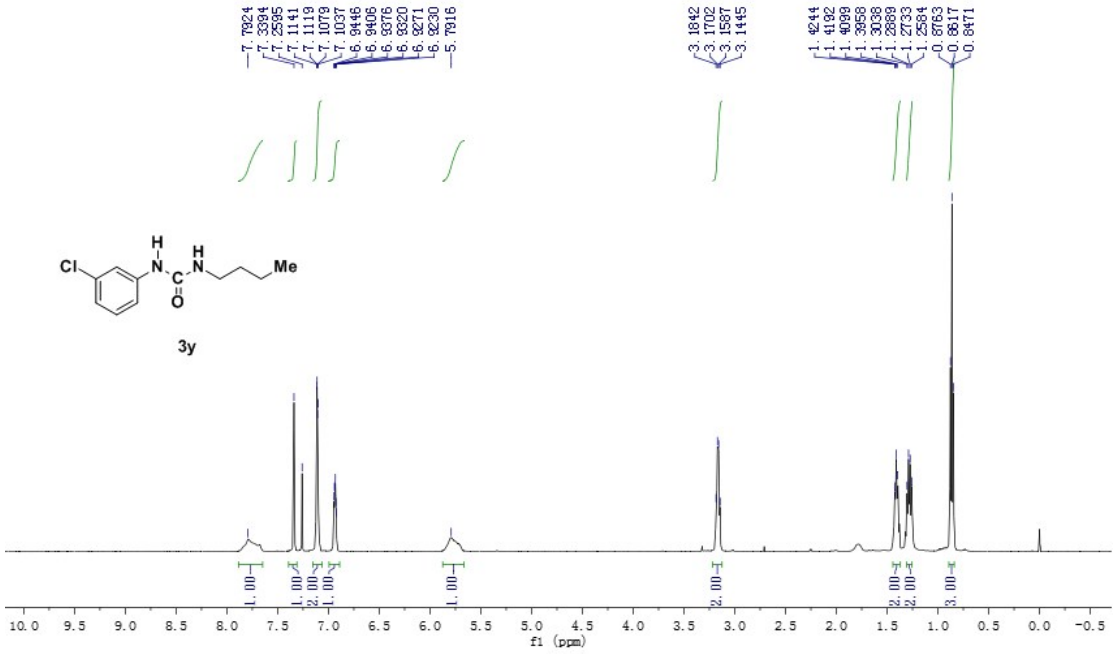
129.7989
123.2632
120.0967
118.0080
77.2536
76.9995
76.7453
66.3986
44.2044
Cl
H
N
C
O
O
N
3x
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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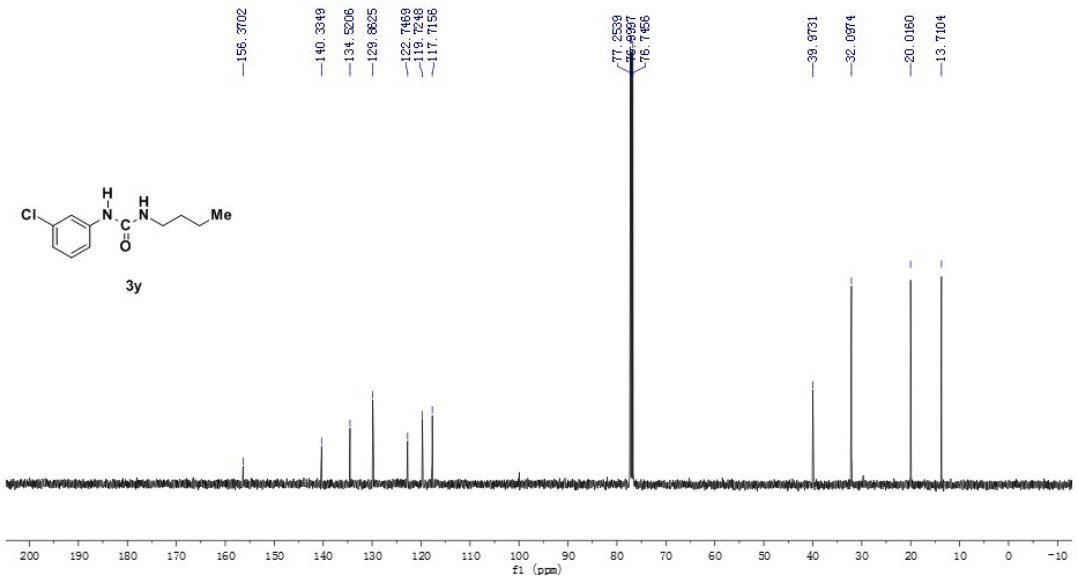
7.2595
7.1141
7.1119
7.1079
7.1037
6.9446
6.9406
6.9376
6.9320
6.9271
6.9230
5.7916
3.1842
3.1702
3.1587
3.1445
1.4244
1.4192
1.4099
1.3958
1.3038
1.2889
1.2733
1.2584
0.9763
0.8617
0.8471
Cl
H
N
C
O
H
N
Me
3y
1.00
1.00
2.00
1.00
1.00
2.00
2.00
2.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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119.7248
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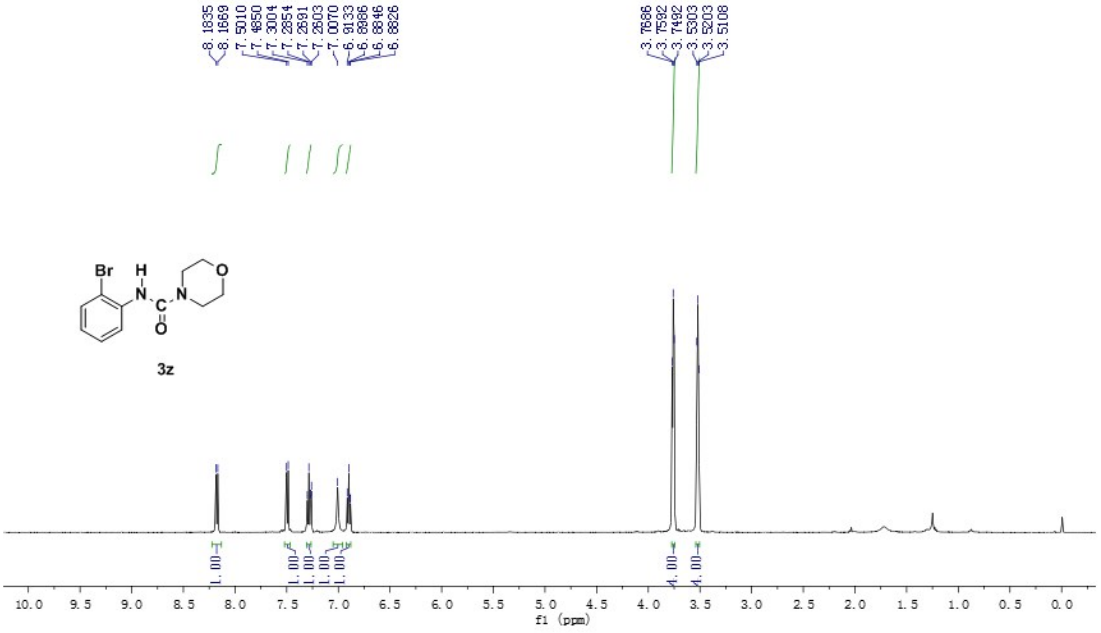
77.0397
76.7456
39.9731
32.0974
20.0160
13.7104
Cl
H
N
C
O
H
N
Me
3y
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.3004
7.2854
7.2691
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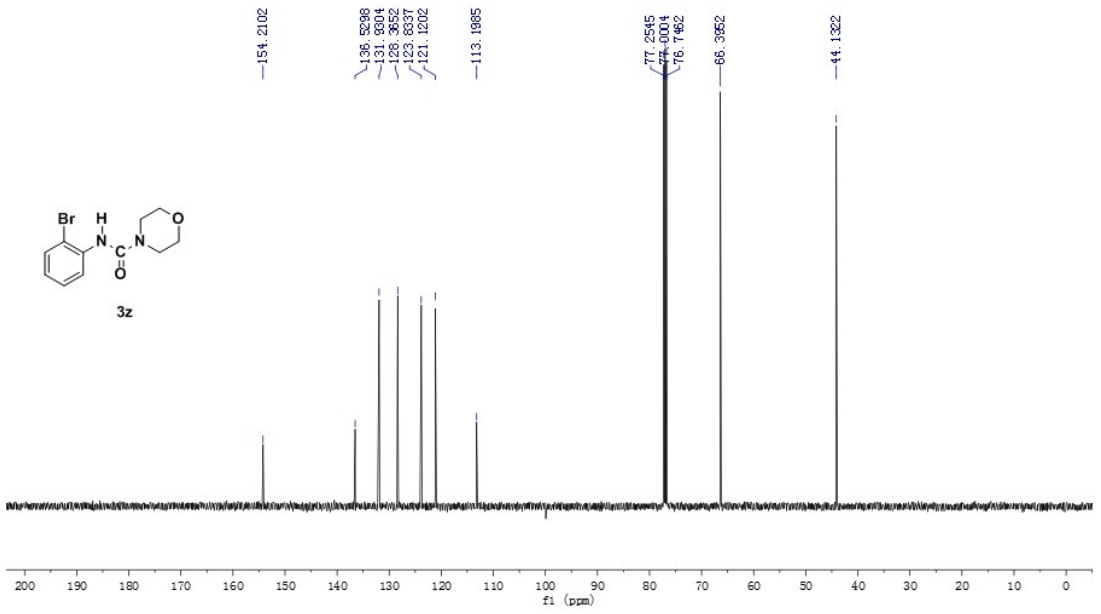
7.0070
6.9133
6.8986
6.8846
6.8826
3.7686
3.7592
3.7492
3.5303
3.5203
3.5108
Br
H
N
C
O
O
N
3z
1.00
1.00
1.00
1.00
1.00
4.00
4.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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131.9304
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121.1202
113.1985
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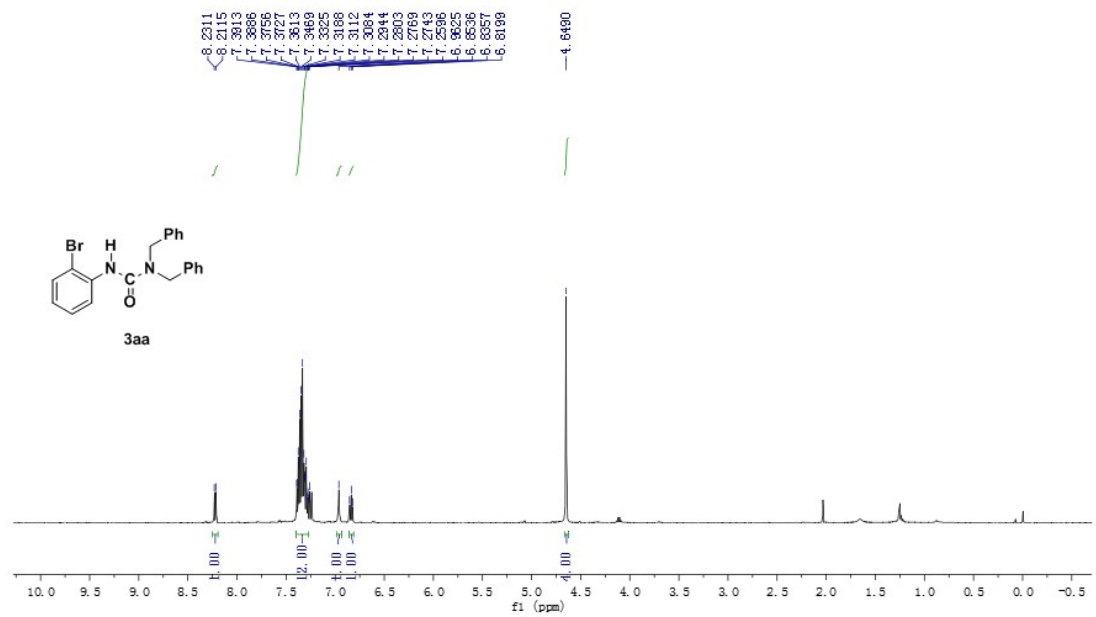
77.0004
76.7462
66.3552
44.1322
Br
H
N
C
O
O
N
3z
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.3686
7.3756
7.3727
7.3613
7.3469
7.3325
7.3188
7.3112
7.3084
7.2944
7.2803
7.2769
7.2743
7.2586
6.8625
6.8536
6.8357
6.8199
4.6490
Br
H
N
C
O
N
Ph
Ph
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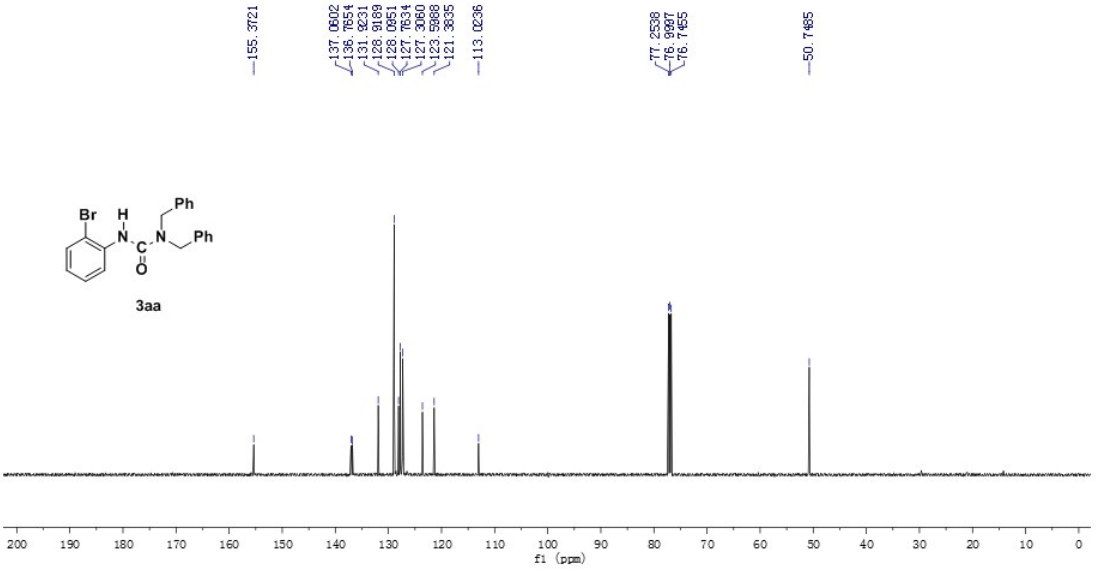
2.00
1.00
1.00
4.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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127.3060
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121.3835
113.0236
77.2538
76.9997
76.7455
50.7495
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N
C
O
N
Ph
Ph
3aa
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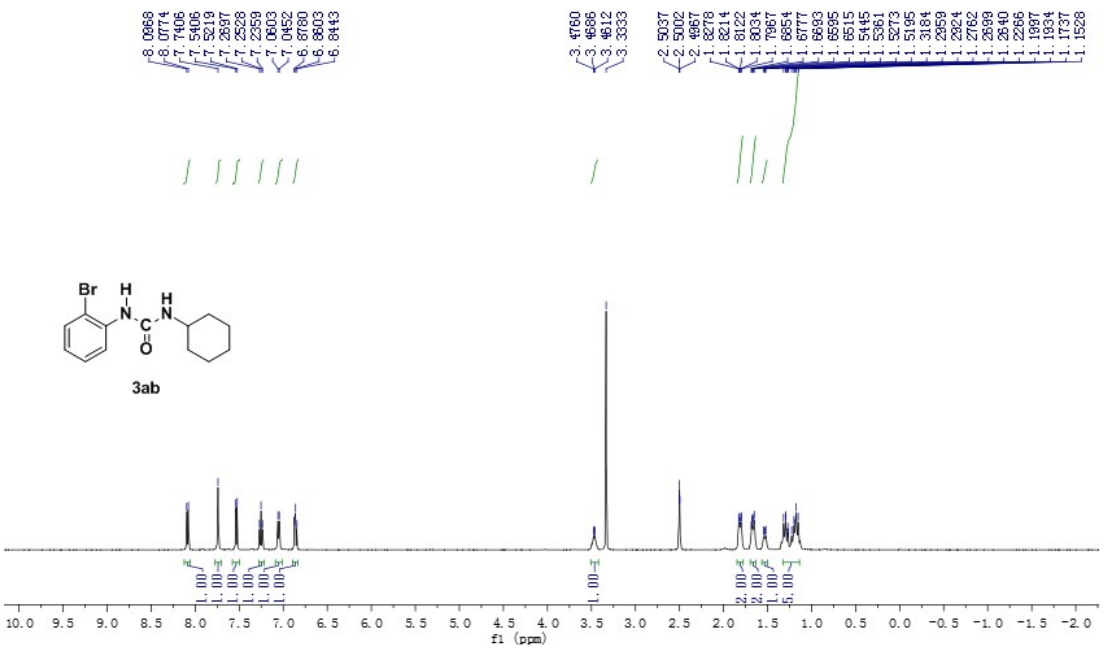
f1 (ppm)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6.8603
6.8443
3.4760
3.4686
3.4612
3.3333
2.5037
2.5002
2.4967
1.8278
1.8214
1.8122
1.8034
1.7967
1.6854
1.6777
1.6693
1.6595
1.6515
1.5445
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1.2824
1.2762
1.2599
1.2540
1.2266
1.1997
1.1934
1.1737
1.1528
Br
H
N
C
O
H
N
3ab
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1.00
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1.00
1.00
1.00
1.00
2.00
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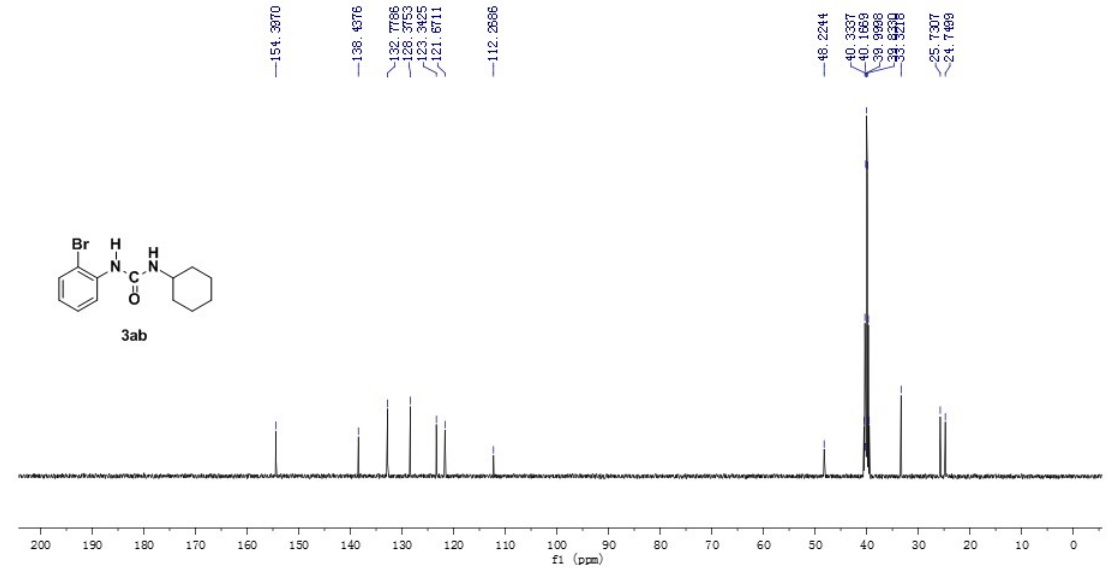
5.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)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40.1669
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25.7307
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Br
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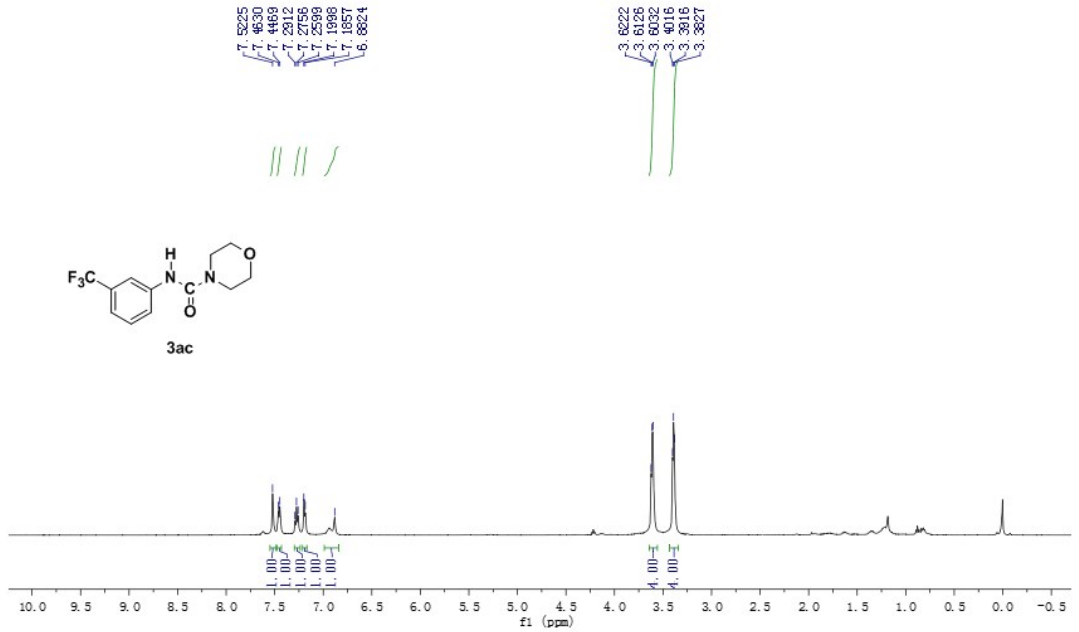
N
C
O
H
N
3ab
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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3.6128
3.6032
3.4016
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3ac
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1.00
1.00
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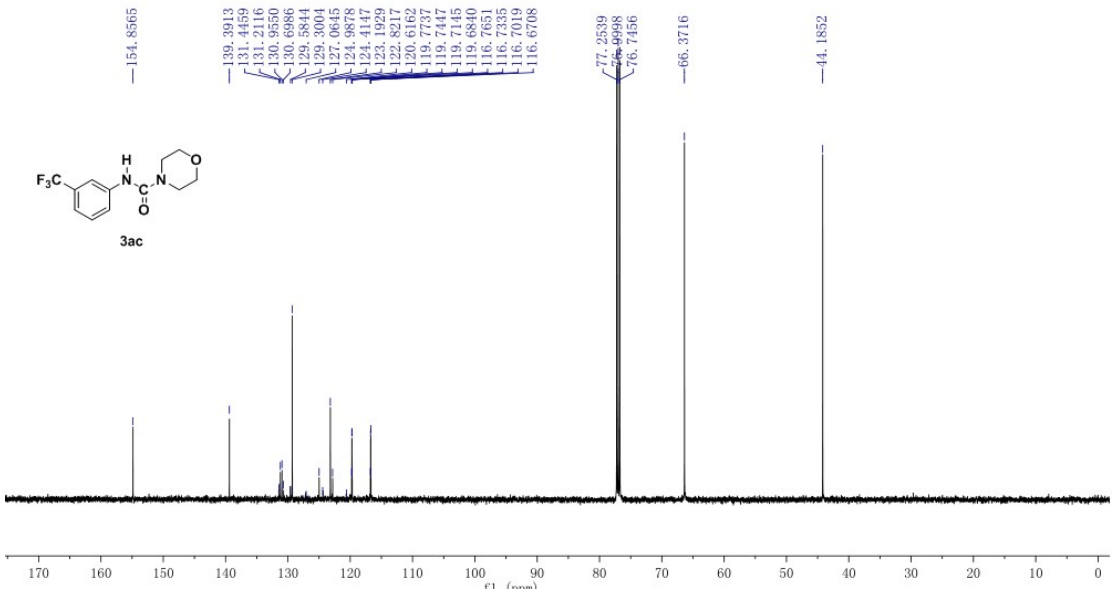
1.00
4.00
4.00
f1 (ppm)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119.7145
119.6840
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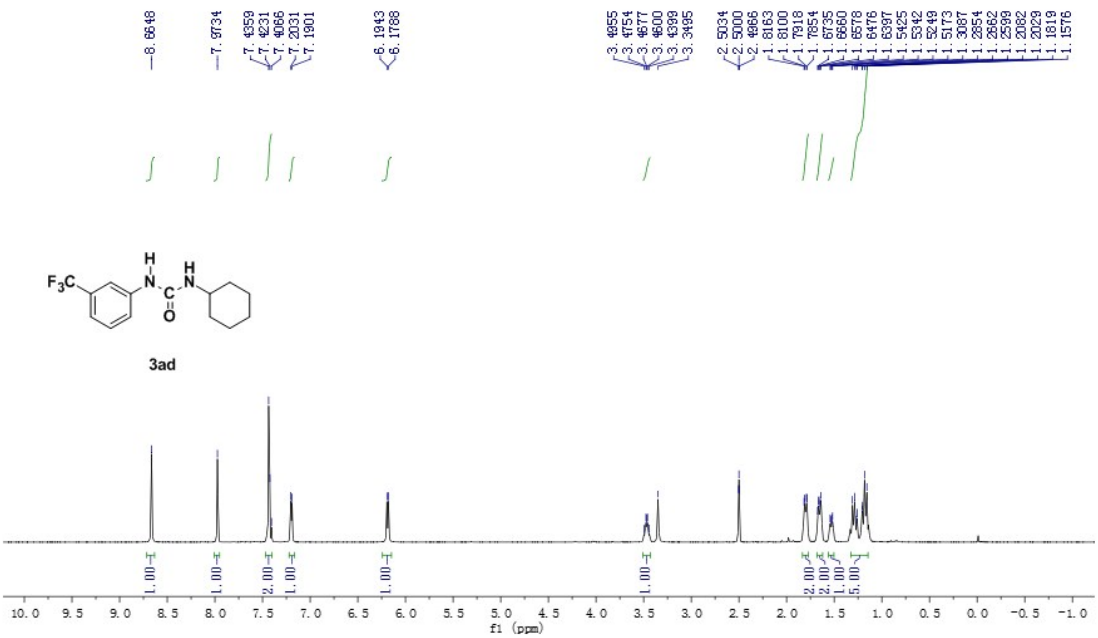
3ac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3.4754
3.4677
3.4600
3.4399
3.3495
2.5034
2.5000
2.4966
1.8163
1.8100
1.7918
1.7854
1.6735
1.6660
1.6578
1.6476
1.6397
1.5425
1.5342
1.5249
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1.2662
1.2599
1.2082
1.2029
1.1819
1.1576
F3C
H
N
C
O
N
H
3ad
1.00
1.00
2.00
1.00
1.00
1.00
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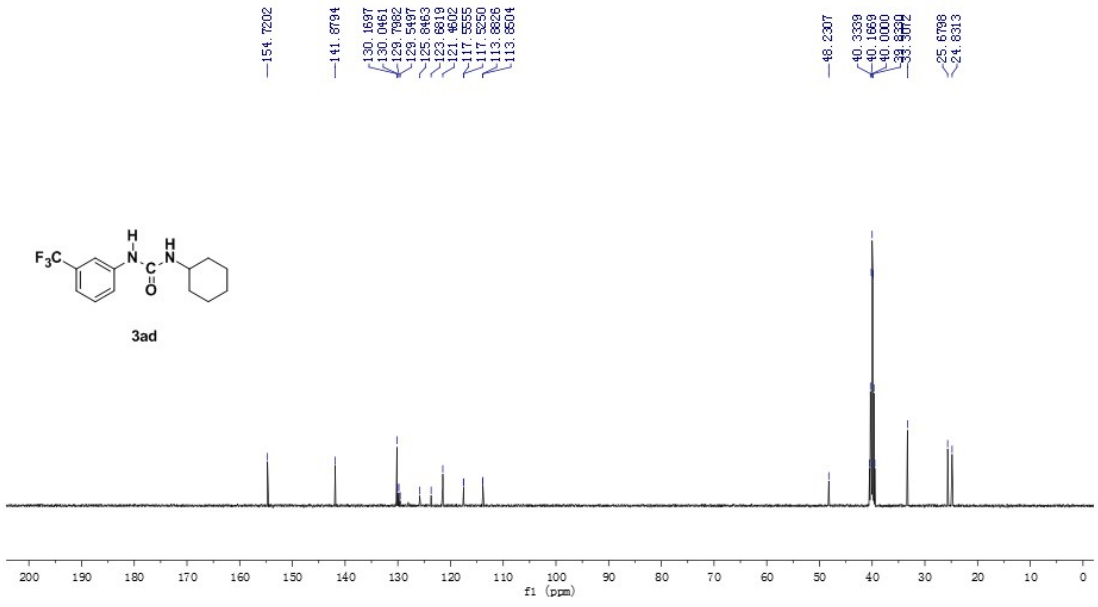
5.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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113.8826
113.8504
48.2307
40.3339
40.1868
40.0000
39.8330
33.3072
25.6798
24.8313
F3C
H
N
C
O
N
H
3ad
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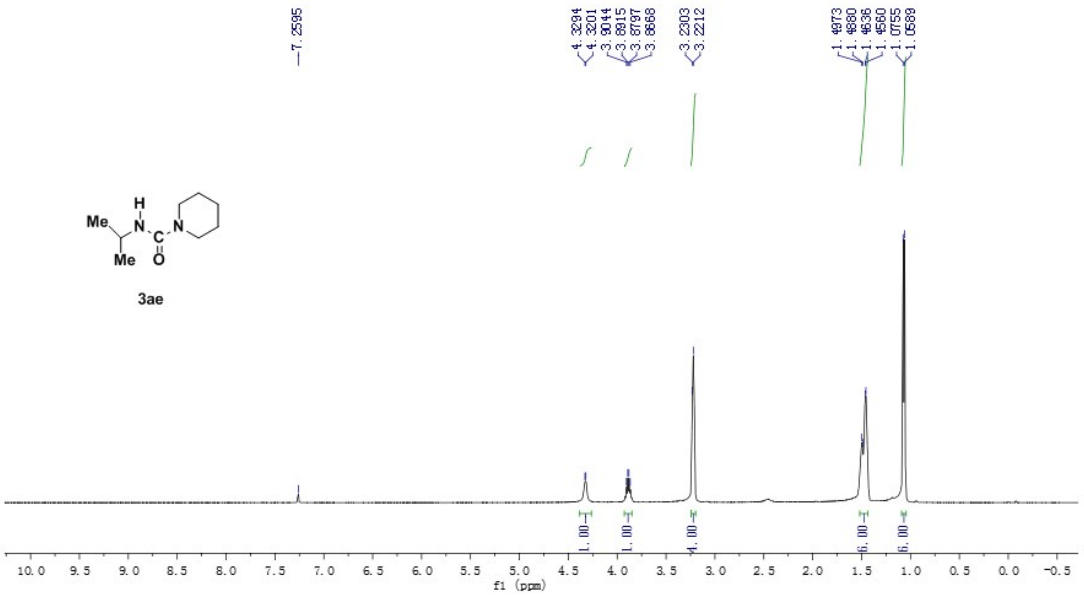
f1 (ppm)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3.2212
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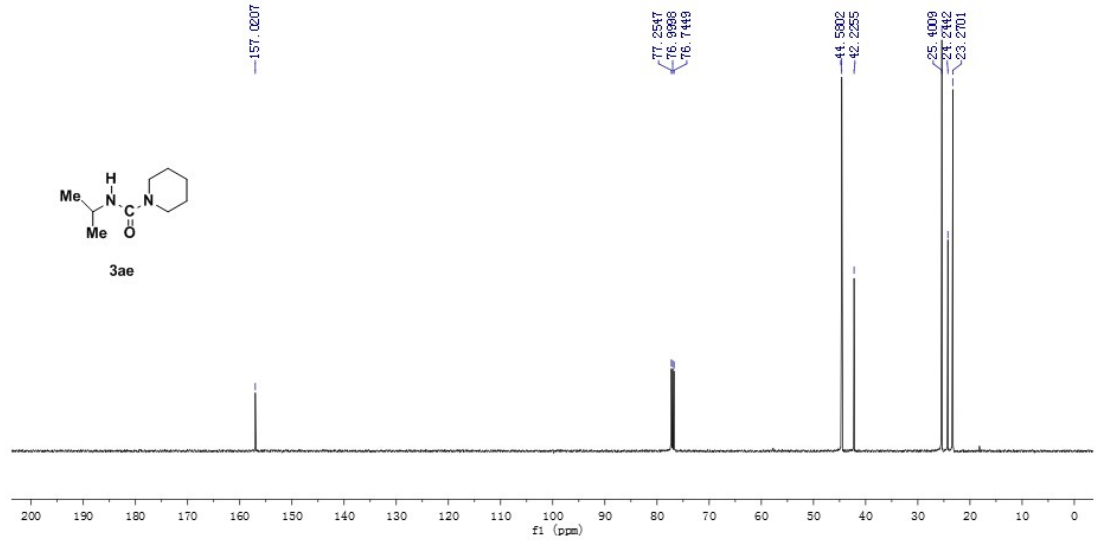
1.4880
1.4636
1.4560
1.0755
1.0689
Me
H
N
C
O
N
Me
3ae
1.00
1.00
4.00
6.00
6.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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25.4009
24.2442
23.2701
Me
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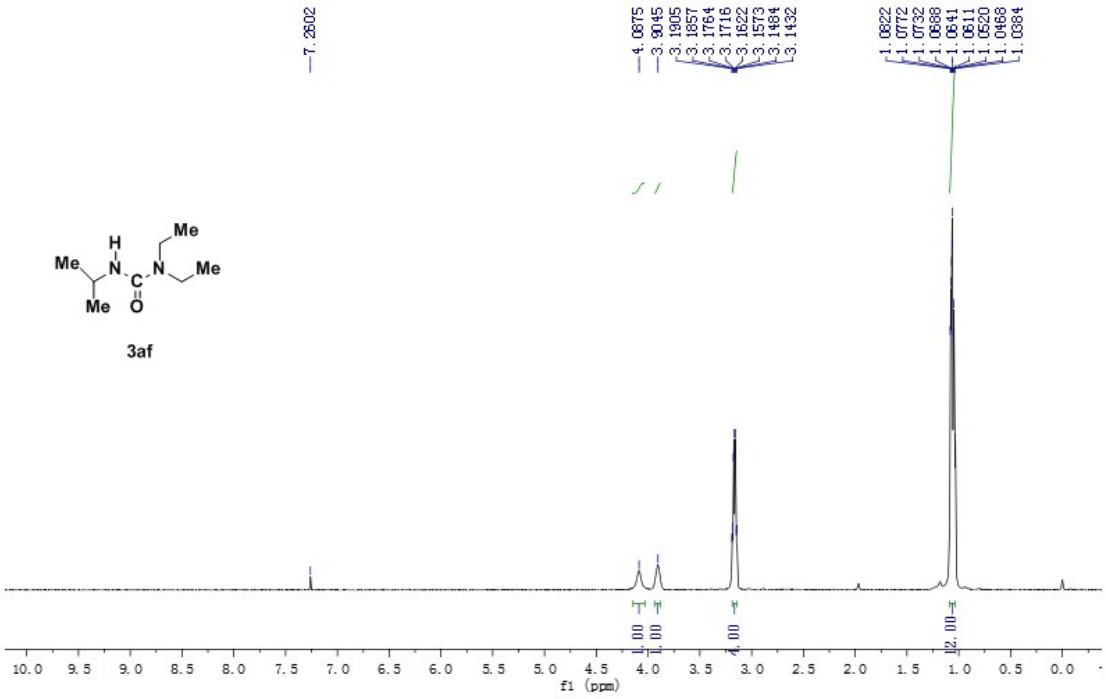
N
C
O
N
Me
3ae
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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1.0772
1.0732
1.0688
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Me
H
N
Me
Me
C
O
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Me
3af
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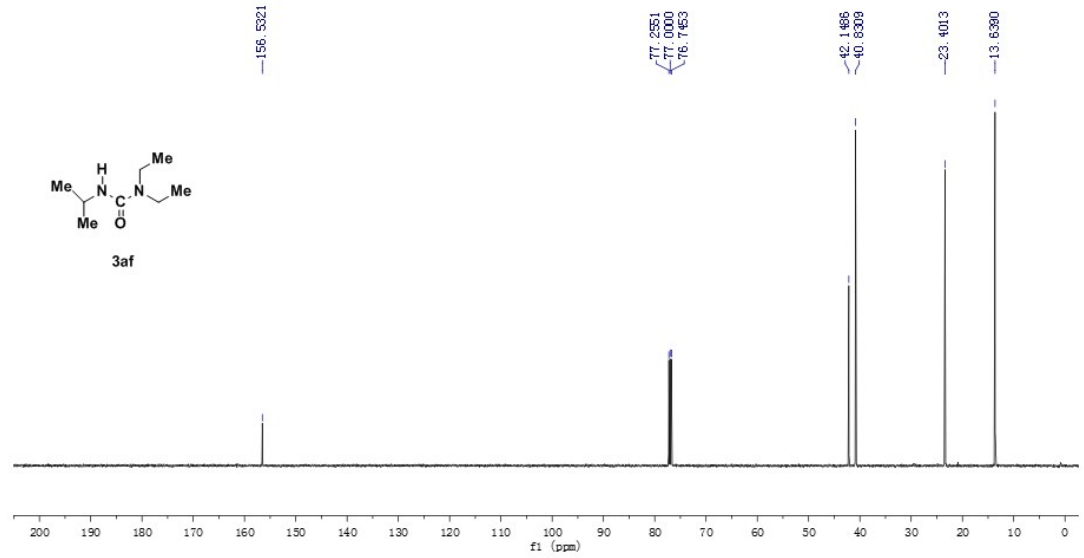
1.00
4.00
12.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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H
N
Me
Me
C
O
N
Me
3af
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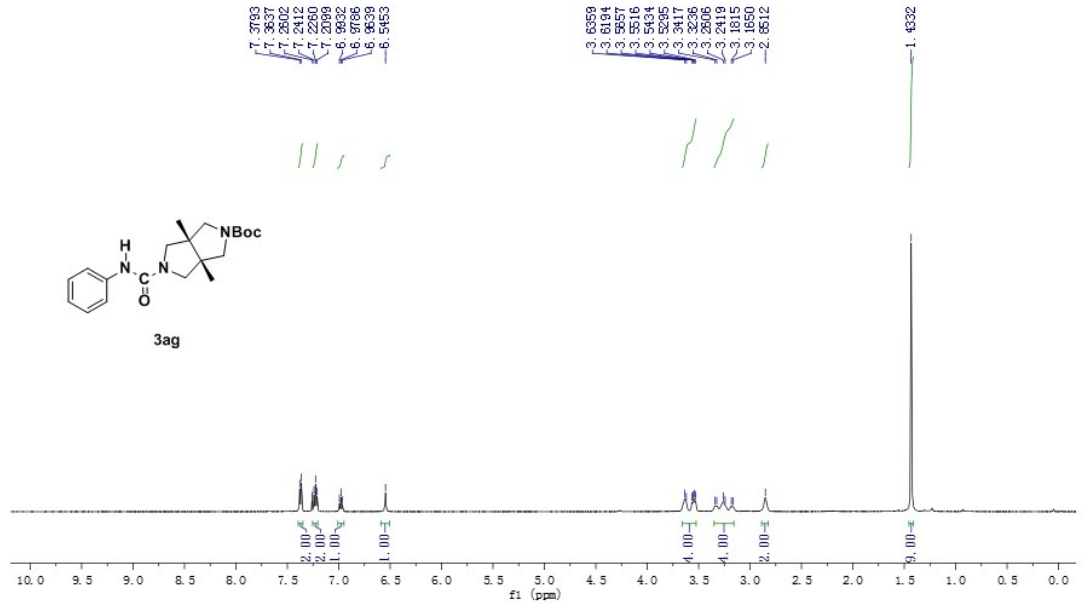
f1 (ppm)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3.6194
3.5857
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3.5434
3.5295
3.3417
3.3236
3.2506
3.2419
3.1815
3.1650
2.8512
1.4332
NBoc
H
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C
O
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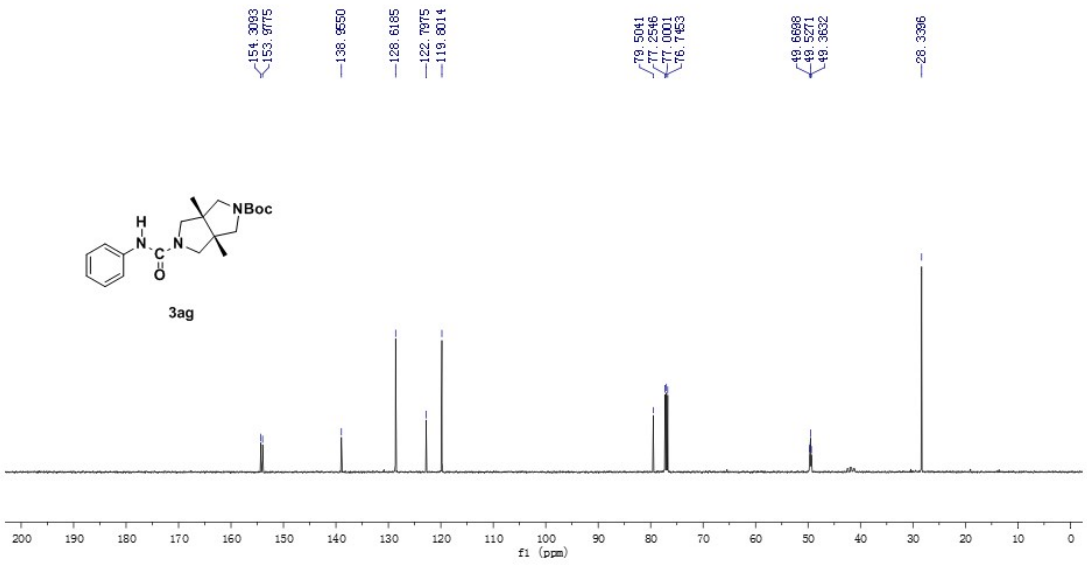
2.00
2.00
1.00
1.00
4.00
4.00
2.00
9.00
f1 (ppm)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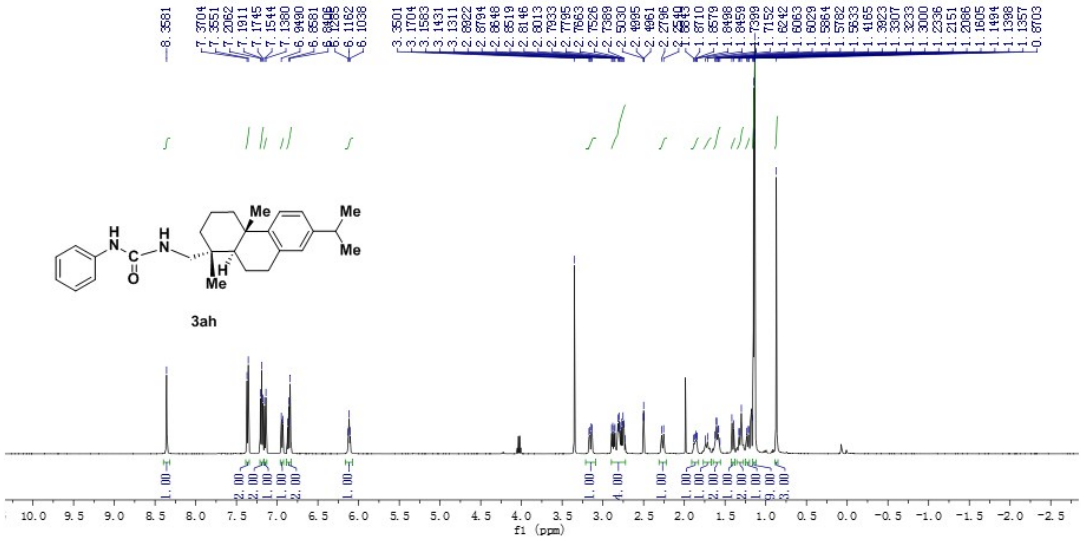
NBoc
H
N
C
O
3ag
f1 (ppm)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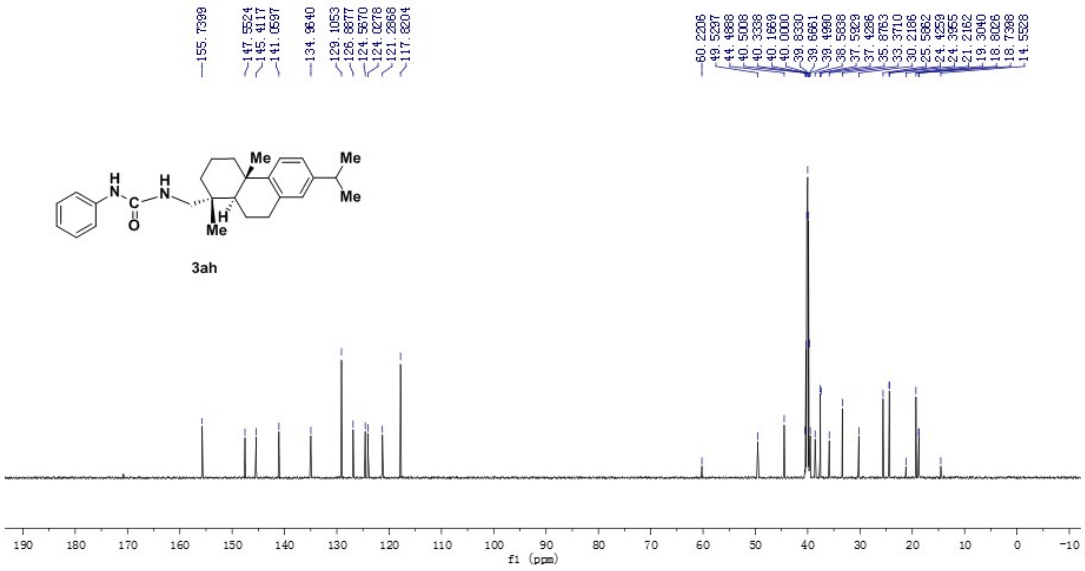
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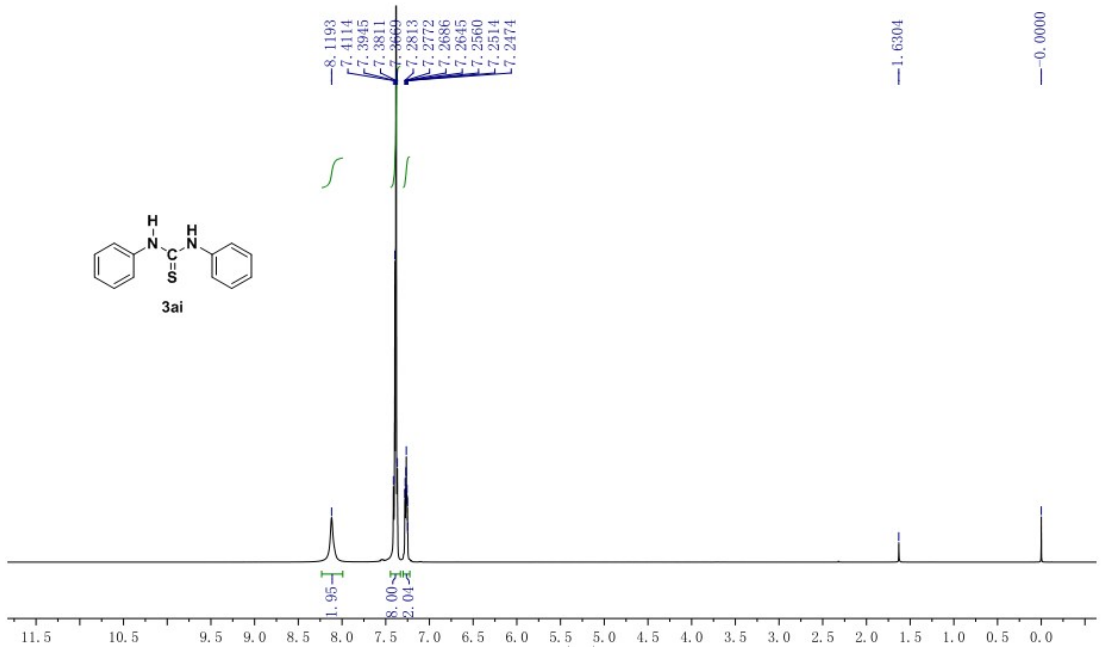
f1 (ppm)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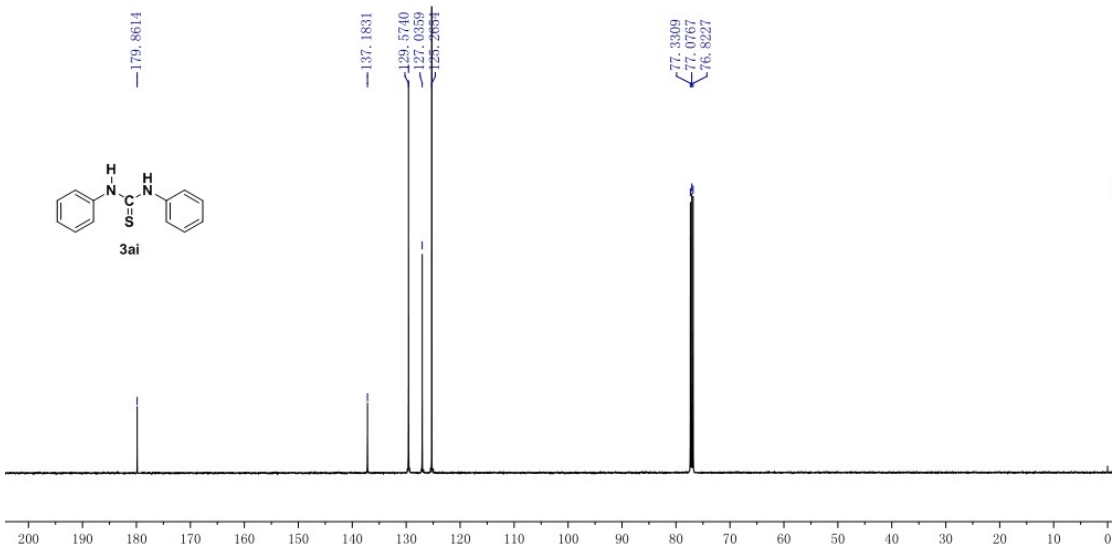
7.3811
7.3669
7.2813
7.2772
7.2686
7.2645
7.2560
7.2514
7.2474
1.6304
0.0000
1.95
8.00
2.04
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
3ai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129.5740
127.0359
125.2634
77.3309
77.0767
76.8227
200
190
180
170
160
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140
130
120
110
100
90
80
70
60
50
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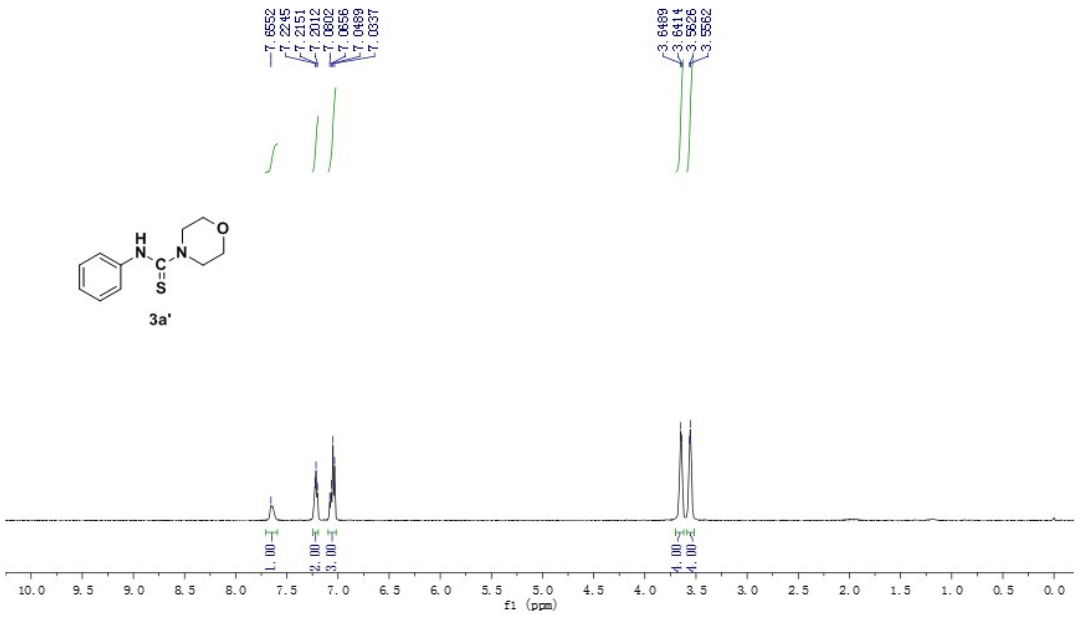
30
20
10
0
3ai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3.6489
3.6414
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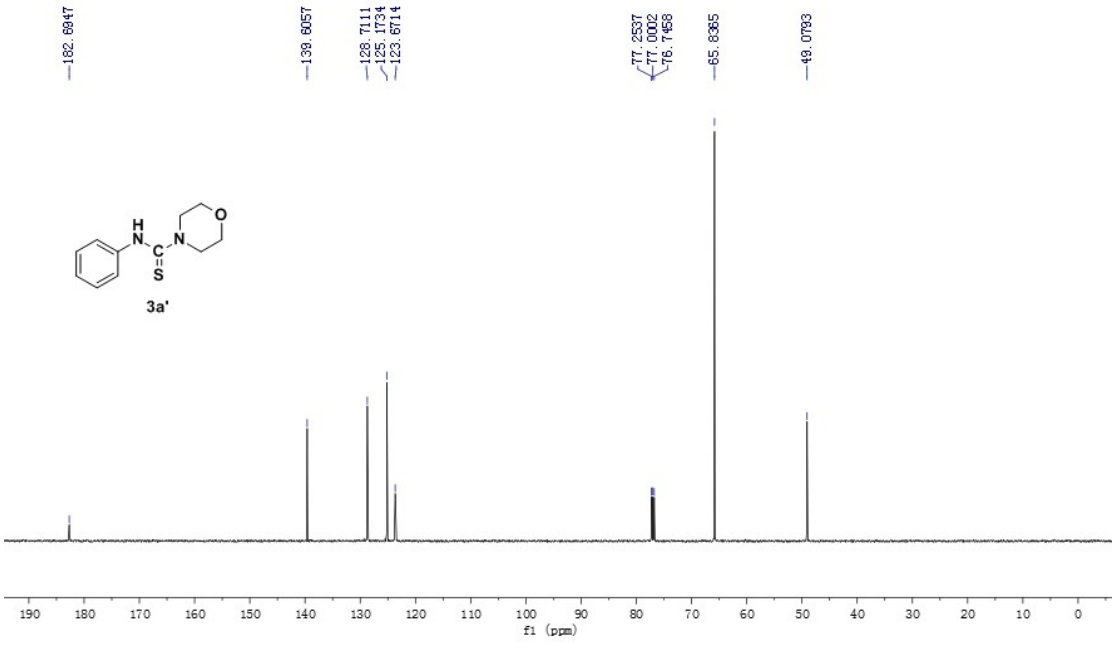
3.5582
3a'
1.00
2.00
3.00
4.00
4.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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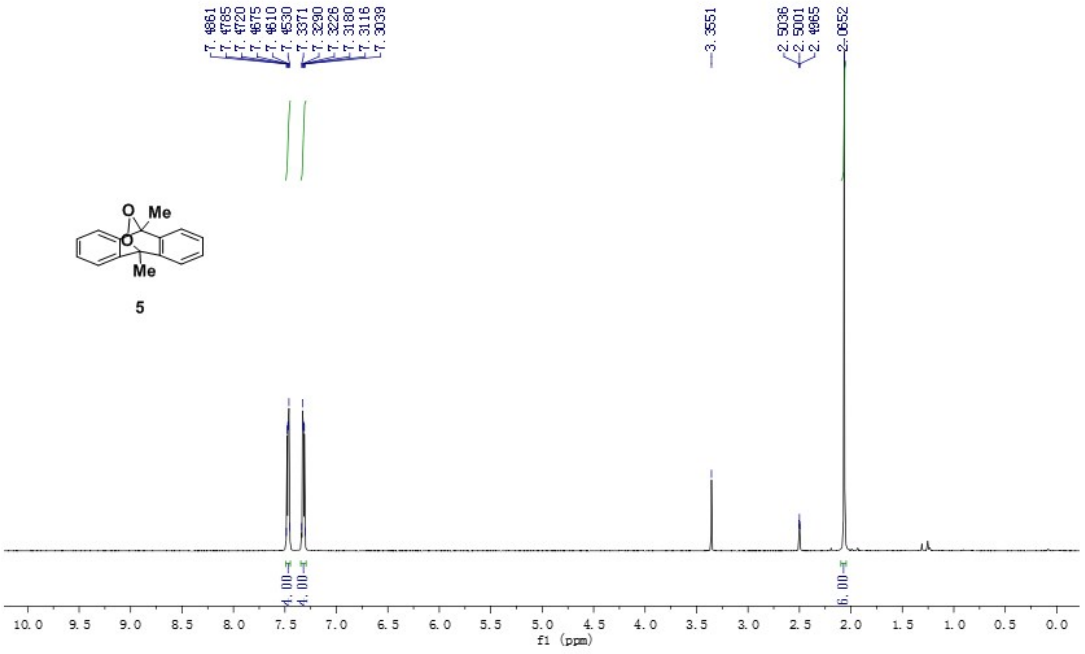
49.0793
3a'
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.4610
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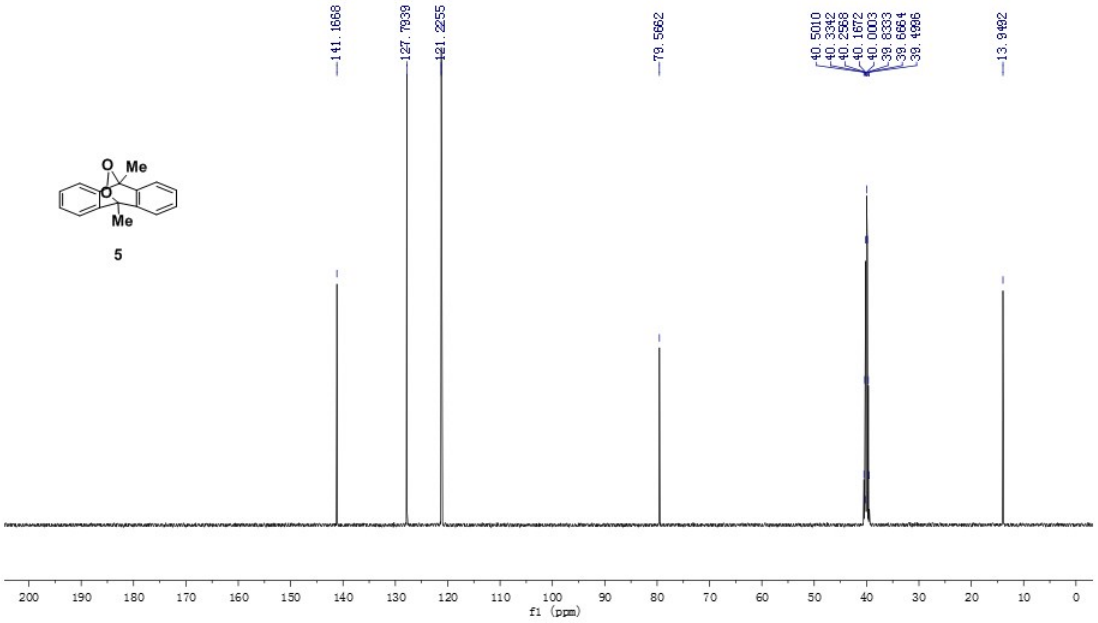
7.3226
7.3180
7.3116
7.3039
3.3551
2.5036
2.5001
2.4965
2.0652
O
Me
O
Me
5
4.00
4.00
6.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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79.5662
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40.0003
39.8333
39.6664
39.4996
13.9492
O
Me
O
Me
5
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

DFT studies

Computational methods

Density functional theory (DFT) calculations were performed with G09 program[1] and M06-2X method.[2] Geometry optimization was performed with basis set of Lanl2DZ[3] and related effective core potential for Br and 6-31G(d) for the rest atoms. At the same level of theory, frequency analysis and intrinsic reaction coordinates (IRC) analysis[4] were performed based on the optimized structures to calculated thermodynamic corrections and to ensure that the optimized the structures are minima (no imaginary frequency) or transition states (only one imaginary frequency) connecting correct intermediates. Solution-phase single-point energies were further calculated based on optimized structure with the larger basis set of SDD[5] and related effective core potential for Br and 6-311++G(d,p) for the rest atoms. 'Ultrafine' grid as assigned to all calculations to avoid possible grid errors.[6] 1.9 kcal/mol was added to the Gibbs free energy of all species to account for the standard-state change from 1 atm. to 1 M at 298.15 K. The solution-phase single-point energy was added by thermodynamic correction for Gibbs free energy and 1.9 kcal/mol to get the solution-phase Gibbs free energy referring to 1 M and 298.15 K for mechanistic discussion.

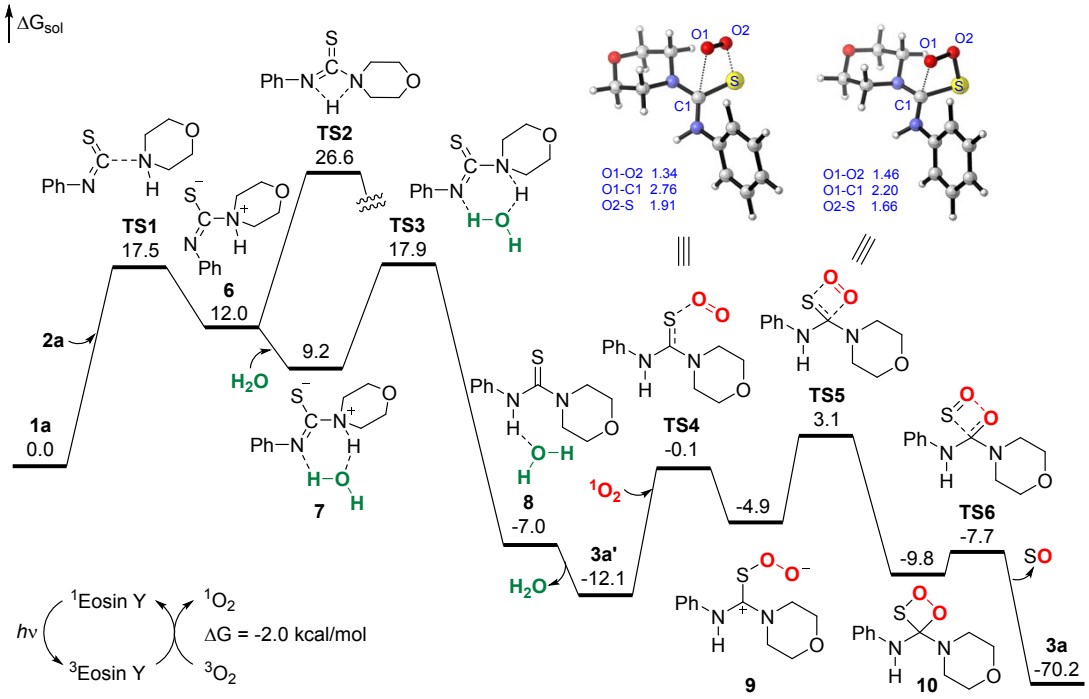


Figure S5. Calculated solution-phase Gibbs free energy profile of the transformation of **1a** and **2b** to **3b** (in kcal/mol).

1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Revision D.01; Gaussian, Inc., Wallingford, CT, 2013.

2. Zhao, Y.; Truhlar, D. G. The M06 Suite of Density Functionals for Main Group Thermochemistry, Thermochemical Kinetics, Noncovalent Interactions, Excited states,

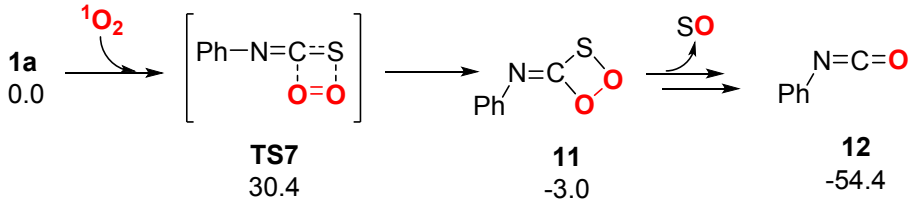
and Transition Elements: Two New Functionals and Systematic Testing of Four M06-ClassFunctionals and 12 Other Functionals. *Theor. Chem. Acc.* **2008**, *120*, 215–241.

3. Hay, P. J.; Wadt, W. R. Ab Initio Effective Core Potentials for Molecular Calculations. Potentials for the Transition Metal Atoms Sc to Hg. *J. Chem. Phys*. **1985**, *82*, 270–283.

4. Fukui, K. The Path of Chemical Reactions-The IRC Approach. *Acc. Chem. Res.* **1981**, *14*, 363–368.

5. Igel-Mann, G.; Stoll, H.; Preuss, H. Pseudopotentials for main group elements (Illa through VIIa). *Mol. Phys*. **1988**, *65*, 1321–1328.

6. For the comments on utilizing ultrafine grid in DFT calculations, see: (a) Grafenstein, J.; Izotov, D.; Cremer, D. Avoiding Singularity Problems Associated with Meta-GGA (Generalized Gradient Approximation) Exchange and Correlation Functionals Containing the Kinetic Energy Density. *J. Chem. Phys.* **2007**, *127*, 214103. (b) Johnson, E. R.; Becke, A. D.; Sherrill, C. D.; DiLabio, G. A. Oscillations in Meta-Generalized-Gradient Approximation Potential Energy Surfaces for Dispersion-bound Complexes. *J. Chem. Phys*. **2009**, *131*, 034111. (c) Wheeler, S. E.; Houk, K. N. Integration Grid Errors for Meta-GGA-Predicted Reaction Energies: Origin of Grid Errors for the M06 Suite of Functionals. *J. Chem. Theory Comput*. **2010**, *6*, 395–404.



Scheme S1. Calculated Results of the Formation of Isocyanatobenzene from 1a (in kcal/mol).

Table S3. Calculated thermodynamic corrections for Gibbs free energies (ΔG_{cor} in hartree), solution-phase single-point energies (ΔE_{sol} in hartree) and Solution-

phase Gibbs free energies (ΔG_{sol} in hartree)

species	ΔG_{cor}	ΔE_{sol}	ΔG_{sol}
1a	0.069404	-722.63703	-722.5645981
2a	0.109039	-287.7611651	-287.6490983
^{3}Eosin Y	0.170718	-1196.218897	-1196.045151
^{1}Eosin Y	0.174214	-1196.28589	-1196.108648
$^3O_2$	-0.015873	-150.3204421	-150.3332873
$^1O_2$	-0.014856	-150.2611514	-150.2729795
TS1	0.199527	-1010.388296	-1010.185741
4	0.203997	-1010.401534	-1010.194509
TS2	0.198221	-1010.372514	-1010.171265
5	0.224805	-1086.850127	-1086.622294
H_2O	0.003557	-76.42921704	-76.4226322
TS3	0.220975	-1086.831733	-1086.60773
6	0.222705	-1086.873293	-1086.64756
3a'	0.201844	-1010.437864	-1010.232992
TS4	0.206466	-1160.696336	-1160.486842
7	0.207254	-1160.704755	-1160.494473
TS5	0.208138	-1160.692885	-1160.481719
8	0.209283	-1160.714591	-1160.502281
TS6	0.208666	-1160.710581	-1160.498887
3a	0.206033	-687.491557	-687.2824962
SO	-0.018091	-473.3010632	-473.3161263
TS7	0.069785	-872.8619227	-872.7891098
9	0.075164	-872.9205519	-872.84236
10	0.072704	-399.6838174	-399.6080856

Cartesian coordinates of optimized structures (in angstrom)

1a

N	-0.91732400	-0.00003300	-0.00001600
C	-2.09109100	-0.00002400	-0.00000600
S	-3.69416700	0.00001400	0.00001400
C	0.46351300	-0.00001600	-0.00002700
C	1.14802200	-1.21877800	-0.00001500
C	1.14799500	1.21876900	-0.00001500
C	2.53820300	-1.20828400	0.00000800
H	0.58785400	-2.14766300	-0.00001500
C	2.53817700	1.20830700	0.00000800
H	0.58780800	2.14764300	-0.00001500
C	3.23453400	0.00002000	0.00002000
H	3.07820600	-2.14951000	0.00002200
H	3.07816200	2.14954600	0.00002200

H	4.31979000	0.00003200	0.00004200

2a

C	1.19520800	0.71440800	0.20131700
C	1.16712100	-0.75282300	-0.19805800
C	-1.16730100	-0.75253600	-0.19807600
C	-1.19503000	0.71468800	0.20133300
H	1.20382100	-0.83370000	-1.29612300
H	2.02180300	-1.28877900	0.22292500
H	1.24606600	0.77501500	1.30243600
H	2.08902700	1.19324300	-0.21065300
H	-1.20399700	-0.83340200	-1.29614200
H	-2.02211500	-1.28829200	0.22289100
H	-2.08873400	1.19375200	-0.21062000
H	-1.24585900	0.77529700	1.30245400
O	-0.00017600	-1.39067400	0.29273100
N	0.00016300	1.36362400	-0.33614300
H	0.00027100	2.34446500	-0.06510800

^{3}Eosin Y

C	3.47048400	-1.46400600	-0.16015900
C	2.09315700	-1.93486100	-0.09888600
C	1.01196100	-1.06797700	-0.12816300
C	1.20077000	0.32107000	-0.22195600
C	2.51972200	0.81967300	-0.31105000
C	3.59664300	-0.02580000	-0.27738900
C	0.01878900	1.18553000	-0.24761000
C	-1.24651700	0.56420000	-0.18118800
C	-1.33329400	-0.85303300	-0.09089500
C	-2.55256200	-1.50370900	-0.01206200
C	-3.75845300	-0.79073500	-0.01099900
C	-3.66849400	0.61193300	-0.08128900
C	-2.47161400	1.27910000	-0.15729200
H	2.67352600	1.88719300	-0.42038200
H	-2.45471200	2.36185400	-0.18962600
O	-0.22343700	-1.63051000	-0.06940700
O	4.43790900	-2.24377200	-0.11782800
O	-4.90523800	-1.47373300	0.06236300
H	-5.66369600	-0.86353900	0.06021800
Br	5.38287100	0.69158600	-0.38934200
Br	1.80088500	-3.81608300	0.02331000
Br	-5.32574500	1.63748800	-0.05729600
Br	-2.60737400	-3.42851200	0.10437800
C	0.15154700	2.65018100	-0.39611900

C	0.79247700	3.48413700	0.54464100
C	-0.35731500	3.23843600	-1.56282200
C	0.92944600	4.85095700	0.28969400
C	-0.23413300	4.60393400	-1.79798900
H	-0.84188000	2.60349500	-2.29915200
C	0.41707500	5.41511300	-0.87174100
H	1.43304400	5.46674400	1.02725200
H	-0.63810100	5.02973100	-2.71100500
H	0.52361000	6.47975100	-1.05150800
C	1.34424600	3.01320000	1.85129200
O	2.15286500	3.63540500	2.50172700
O	0.83620800	1.84511100	2.26795700
H	1.26586000	1.63391000	3.12086900

[1]Eosin Y

C	3.78536500	-0.97495900	-0.04435800
C	2.47771100	-1.62929800	-0.02809700
C	1.30663600	-0.94353900	-0.09000600
C	1.27361200	0.50024200	-0.18402500
C	2.54154800	1.19136000	-0.17608300
C	3.69474700	0.50406400	-0.11158800
C	0.06681400	1.14759300	-0.24383200
C	-1.15098700	0.37015500	-0.22301500
C	-1.04765400	-1.02540400	-0.11976600
C	-2.18044100	-1.83286000	-0.08160100
C	-3.45577900	-1.27067400	-0.14661600
C	-3.54462400	0.13118700	-0.25926800
C	-2.43281400	0.93737500	-0.30013300
H	2.53705000	2.27486400	-0.21634200
H	-2.54257300	2.01213000	-0.39710500
O	0.14934200	-1.64394800	-0.05987900
O	4.84561500	-1.57480300	-0.00089500
O	-4.51056400	-2.08554300	-0.10370300
H	-5.33907600	-1.57667100	-0.15687000
Br	5.38718000	1.44848500	-0.09573900
Br	2.46680100	-3.55467700	0.09086500
Br	-5.31427500	0.93588900	-0.36061900
Br	-1.99734100	-3.74449700	0.05871500
C	-0.01190800	2.62499200	-0.41575500
C	-0.47648900	3.51104100	0.57406800
C	0.35206700	3.13530200	-1.66546500
C	-0.57607100	4.87431100	0.28889000
C	0.25681100	4.49787900	-1.93467700
H	0.70334000	2.45157300	-2.43238000

C	-0.21104400	5.37065900	-0.95665600
H	-0.93708500	5.53951200	1.06582600
H	0.54664800	4.87198800	-2.91123900
H	-0.28904300	6.43326700	-1.16091700
C	-0.87283800	3.09916100	1.95452500
O	-1.50278700	3.80157500	2.71041500
O	-0.44066900	1.87797600	2.29464700
H	-0.75752000	1.69774600	3.20232800

$^3O_2$

O	0.00000000	0.00000000	0.59841000
O	0.00000000	0.00000000	-0.59841000

$^1O_2$

O	0.00000000	0.00000000	0.59828500
O	0.00000000	0.00000000	-0.59828500

TS1

N	-0.65914100	1.33205000	-0.64414600
C	0.50025300	1.45823400	-0.27446100
S	1.81588100	2.42696200	-0.24641900
C	-1.79448900	0.61163600	-0.28376600
C	-2.59779900	0.05784300	-1.28758500
C	-2.16768200	0.48715400	1.06112100
C	-3.74556600	-0.64655300	-0.94153100
H	-2.30356600	0.17790900	-2.32548700
C	-3.32282400	-0.21549700	1.39261700
H	-1.56322400	0.95887800	1.83124900
C	-4.11195700	-0.78892200	0.39724200
H	-4.35923400	-1.08349500	-1.72327200
H	-3.60749200	-0.30884300	2.43620200
H	-5.01087700	-1.33648200	0.66151500
C	2.29190500	-0.39618700	1.35046600
C	3.34632000	-0.72422000	0.30208100
C	1.77859600	-1.72423100	-1.07893000
C	0.66096200	-1.50201100	-0.07736900
H	3.46041000	0.11755800	-0.39360300
H	4.30521900	-0.90521000	0.79403900
H	2.28946000	-1.17780300	2.12192100
H	2.52164700	0.56256600	1.82320200
H	1.83448500	-0.87047800	-1.77394800
H	1.58705900	-2.63148700	-1.65667000
H	-0.28882900	-1.35874700	-0.59720900
H	0.57443700	-2.38514600	0.57029800

O	3.01733200	-1.89831200	-0.41853700
N	0.95549500	-0.31129200	0.74031300
H	0.26695300	-0.25290900	1.49028600

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N	-0.68108400	1.47499500	-0.44281900
C	0.52707900	1.20518500	-0.12653300
S	1.89532300	2.19976500	-0.29530600
C	-1.79475500	0.65945700	-0.18289700
C	-2.50491300	0.09428700	-1.25241300
C	-2.26638000	0.46751800	1.12517400
C	-3.64384900	-0.66681800	-1.01295800
H	-2.14780800	0.26014200	-2.26477500
C	-3.41113000	-0.29432300	1.35420900
H	-1.73786200	0.93399300	1.95352000
C	-4.10284000	-0.86686400	0.28997100
H	-4.17834900	-1.10481000	-1.85071000
H	-3.76349100	-0.43252500	2.37211100
H	-4.99457500	-1.45822600	0.47133100
C	1.86153200	-0.43348600	1.44018900
C	3.20033300	-0.75373700	0.78958700
C	2.20398400	-1.42347300	-1.18918700
C	0.79568300	-1.26251400	-0.65185600
H	3.62243900	0.13683200	0.31446500
H	3.87891300	-1.09543100	1.57488800
H	1.53615900	-1.28175800	2.04780800
H	1.92519700	0.45994200	2.06101300
H	2.54888500	-0.49846100	-1.67142500
H	2.20024800	-2.22549900	-1.93074900
H	0.09292900	-0.96084400	-1.42930100
H	0.46043500	-2.19746000	-0.19657900
O	3.08390500	-1.80404000	-0.15115300
N	0.75035300	-0.22225300	0.44514000
H	-0.11289400	-0.42040500	0.96657000

TS2

N	0.67180700	-0.52908800	-0.00001000
C	-0.37130100	0.27855200	-0.00005700
S	-0.61624900	1.92943300	-0.00017100
C	2.04942200	-0.29036800	-0.00001000
C	2.86713100	-1.43116500	-0.00004500
C	2.63941600	0.98119900	0.00003600
C	4.24949700	-1.30522900	-0.00003600
H	2.39604600	-2.40969600	-0.00007900

C	4.02861500	1.09303500	0.00004600
H	2.01722700	1.86700100	0.00006600
C	4.83868500	-0.03973200	0.00001000
H	4.86910300	-2.19682600	-0.00006400
H	4.47845200	2.08146100	0.00008400
H	5.91948600	0.06039400	0.00001800
C	-2.25852700	-0.86846800	-1.22744400
C	-3.48967300	0.02400300	-1.16246300
C	-3.48957500	0.02410400	1.16260300
C	-2.25842600	-0.86836300	1.22755900
H	-3.20009400	1.08319700	-1.18046500
H	-4.13028000	-0.18121300	-2.02380900
H	-2.57157700	-1.91460000	-1.30013200
H	-1.63169100	-0.62617600	-2.08910800
H	-3.19999100	1.08330000	1.18048700
H	-4.13010900	-0.18103400	2.02402200
H	-1.63151500	-0.62599800	2.08914800
H	-2.57147100	-1.91448800	1.30036400
O	-4.24877800	-0.25612400	0.00011500
N	-1.43168600	-0.77263800	0.00001800
H	-0.27580300	-1.42058000	0.00003400

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N	0.64454000	0.61473800	0.07852200
C	-0.29020500	-0.10047800	-0.44186900
S	-0.30142000	-1.57369200	-1.27479700
C	1.97993600	0.17616800	0.13070100
C	2.97670300	1.02409600	-0.36481800
C	2.34865300	-1.02952900	0.74091200
C	4.31795400	0.65963500	-0.27834400
H	2.68716600	1.96661600	-0.82171300
C	3.69161200	-1.38033500	0.83789800
H	1.57791200	-1.67897500	1.14324300
C	4.68236600	-0.54338100	0.32342300
H	5.07952300	1.32356400	-0.67666700
H	3.96552100	-2.31481200	1.31904200
H	5.72839800	-0.82395400	0.39746100
C	-2.01387700	0.76197400	1.19686100
C	-2.74523900	-0.49068500	1.63469900
C	-3.56932100	-0.90732100	-0.48972800
C	-2.79795100	0.26170600	-1.08743700
H	-2.09055700	-1.37198000	1.55803300
H	-3.05153900	-0.37600600	2.67666900
H	-2.67831200	1.62697600	1.27149300

H	-1.10677800	0.93989200	1.77410300
H	-2.99101800	-1.83358700	-0.57473500
H	-4.50214300	-1.01809400	-1.04770600
H	-2.44264100	0.02944500	-2.09050700
H	-3.43428500	1.14949700	-1.11854200
O	-3.91472400	-0.67099700	0.86232600
N	-1.61605300	0.66082700	-0.25476700
H	-1.36914400	1.63835900	-0.51485800
O	-0.43095200	3.19579800	-0.28814200
H	-0.71386600	3.65321500	0.52020500
H	0.24670600	2.55044900	0.00768800

H_2O

O	0.00000000	0.00000000	0.11979000
H	0.00000000	0.76100000	-0.47916000
H	0.00000000	-0.76100000	-0.47916000

TS3

N	0.71227200	0.60580900	0.02864900
C	-0.32462900	-0.13031300	-0.30896800
S	-0.39398800	-1.70287700	-0.89459500
C	2.05591800	0.18125000	0.06762200
C	3.01987000	1.07063200	-0.42028800
C	2.46031300	-1.02829700	0.64279900
C	4.37103900	0.74439400	-0.35697600
H	2.69861400	2.01433300	-0.85249700
C	3.81451300	-1.34301500	0.70859500
H	1.71902600	-1.70915900	1.04410300
C	4.77429800	-0.46530100	0.20559500
H	5.10846200	1.44008500	-0.74558600
H	4.12054700	-2.28155400	1.16098700
H	5.82821500	-0.71982400	0.25799100
C	-2.09367600	0.59661400	1.27375600
C	-3.04836400	-0.56912600	1.44964900
C	-3.64454600	-0.58255200	-0.79301700
C	-2.64855100	0.52150200	-1.12951900
H	-2.52524900	-1.52701100	1.31883500
H	-3.47173700	-0.53562600	2.45642400
H	-2.63278800	1.53279900	1.45243400
H	-1.24556600	0.53821900	1.95978000
H	-3.19509900	-1.57012100	-0.94301000
H	-4.50870800	-0.48118800	-1.45452700
H	-2.19436800	0.35532100	-2.10744800
H	-3.17097800	1.48329000	-1.14142200

O	-4.12195700	-0.46084100	0.53504800
N	-1.55864000	0.68122000	-0.12572500
H	-1.13430700	1.84940600	-0.16482000
O	-0.32025100	2.80989000	-0.05718800
H	-0.46197300	3.23001100	0.80844500
H	0.41484200	1.85073100	0.08500600

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N	0.57118200	0.36735000	-0.08217900
C	-0.40750500	-0.52314800	-0.41484000
S	-0.07159600	-2.11384700	-0.92037000
C	1.94509100	0.09767500	0.10512800
C	2.87085400	0.96862200	-0.47556500
C	2.39142400	-0.94798000	0.91910900
C	4.23431100	0.78448800	-0.25670000
H	2.51465800	1.78783900	-1.09397200
C	3.75520100	-1.13199200	1.11948000
H	1.67096500	-1.60533500	1.39181400
C	4.68357100	-0.27033200	0.53367200
H	4.94464500	1.46740200	-0.71285300
H	4.09383900	-1.94849700	1.75020700
H	5.74617700	-0.41739600	0.69928500
C	-2.03978500	1.18598400	0.39761600
C	-3.13280500	0.84051900	1.40733600
C	-3.86610300	-0.96725600	0.14903800
C	-2.82692400	-0.68850300	-0.92460400
H	-2.70980900	0.17360800	2.17454500
H	-3.48533400	1.75492400	1.89094200
H	-2.40330500	1.93926700	-0.31203500
H	-1.18773800	1.58942700	0.94229100
H	-3.45976000	-1.68213200	0.88153800
H	-4.76657300	-1.39270600	-0.30026600
H	-2.51204100	-1.60886800	-1.41186000
H	-3.25447100	-0.00777800	-1.67183200
O	-4.25007200	0.23176900	0.79743100
N	-1.66339300	-0.02898900	-0.33347100
H	-0.42514200	3.24709100	-1.49570900
O	0.25205100	3.13626800	-0.80824500
H	-0.00058000	3.76639400	-0.11378800
H	0.36566200	1.35702100	-0.25434000

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N	0.48358000	0.44968200	-0.19029200
C	-0.41393700	-0.57659500	-0.08724100

S	0.03910900	-2.12422700	0.45525400
C	1.89220000	0.37566400	-0.07576100
C	2.64115100	-0.53943800	-0.82072500
C	2.53982900	1.30708800	0.73752400
C	4.02830300	-0.53426200	-0.72286500
H	2.13600000	-1.24224400	-1.47340100
C	3.93067400	1.31487500	0.81727000
H	1.94998800	2.02121000	1.30577600
C	4.67994600	0.39013900	0.09461600
H	4.60447300	-1.24948700	-1.30198300
H	4.42483100	2.04400100	1.45196400
H	5.76334600	0.39257500	0.16047600
N	-1.67744000	-0.26262300	-0.43791600
C	-2.09886800	0.98428900	-1.08530900
C	-2.83921700	-1.07773300	-0.08685800
C	-3.02360100	1.74960500	-0.14745700
H	-1.24760000	1.58847400	-1.39524000
H	-2.65650200	0.70547200	-1.98727200
C	-3.75638400	-0.25210100	0.81008300
H	-2.51261900	-1.98102700	0.42426500
H	-3.36276100	-1.35181800	-1.01020600
H	-2.47214500	2.04087100	0.76032400
H	-3.39980800	2.65004800	-0.63872200
O	-4.14753900	0.95930600	0.18995900
H	-3.23828300	-0.04112000	1.75860400
H	-4.67088000	-0.81024100	1.02460700
H	0.11298100	1.38786800	-0.08512400

TS4

N	0.65096500	-0.89878700	-0.41224200
C	-0.30463100	0.05112600	-0.51490700
S	0.11429300	1.59469200	-1.16902500
C	2.03237100	-0.67315100	-0.16195400
C	2.42963200	0.30138000	0.75832700
C	2.97017700	-1.48940300	-0.78951300
C	3.78444900	0.47157100	1.01916100
H	1.67270800	0.91104900	1.24920300
C	4.32362900	-1.32137500	-0.50328200
H	2.63706000	-2.24502600	-1.49498600
C	4.73431100	-0.33779700	0.39309700
H	4.09958800	1.23045500	1.72865500
H	5.05598500	-1.95822800	-0.98946300
H	5.78955600	-0.20476200	0.60955400
O	-0.63354200	2.00763900	1.40699100

O	-0.74251800	2.59462900	0.21209900
N	-1.51928400	-0.19976500	-0.06211900
C	-1.80660500	-1.18861000	0.98920400
C	-2.69096600	0.62909100	-0.35995000
C	-3.01257500	-2.02531000	0.59291300
H	-0.93888100	-1.81590800	1.18529300
H	-2.03520400	-0.60957300	1.89126300
C	-3.86874400	-0.28224100	-0.68327500
H	-2.47647400	1.27544400	-1.20919000
H	-2.87721300	1.24603000	0.52443000
H	-2.77862100	-2.61841800	-0.30418200
H	-3.27106500	-2.70363600	1.40907900
O	-4.13519100	-1.19916300	0.35964900
H	-3.66650200	-0.82456900	-1.61956800
H	-4.76680600	0.32515200	-0.81669700
H	0.34913700	-1.86974700	-0.40730500

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N	0.63205400	-0.87928600	-0.41992000
C	-0.32990200	0.05854400	-0.44536600
S	0.11223300	1.65035600	-1.04969900
C	2.02200600	-0.67486600	-0.17506500
C	2.45010000	0.29614600	0.73492100
C	2.93014000	-1.52505700	-0.80116400
C	3.81169700	0.42149800	0.98795700
H	1.71444800	0.94749500	1.20698000
C	4.28942800	-1.39748200	-0.52294400
H	2.57036300	-2.27685300	-1.49773700
C	4.73395800	-0.42230500	0.36606700
H	4.15429100	1.17638400	1.68912200
H	4.99866900	-2.06083700	-1.00788700
H	5.79356600	-0.32152700	0.57866000
O	-0.35155000	2.17907500	1.36750600
O	-0.72629100	2.56876000	0.02072400
N	-1.54934400	-0.22220400	-0.03622900
C	-1.84178500	-1.26913100	0.95881100
C	-2.70970600	0.64138700	-0.28692800
C	-3.07265400	-2.05340600	0.53458800
H	-0.98726700	-1.92909900	1.09647500
H	-2.04085000	-0.74767700	1.90256300
C	-3.90973600	-0.23120600	-0.63220700
H	-2.49600700	1.31274600	-1.11656500
H	-2.87593400	1.23397800	0.61793300
H	-2.86712900	-2.59757000	-0.39957600

H	-3.33223600	-2.77238600	1.31456200
O	-4.17898700	-1.19043200	0.37012300
H	-3.73204000	-0.73222000	-1.59594600
H	-4.79625800	0.40021900	-0.72381900
H	0.33503400	-1.85187000	-0.45538100

TS5

N	0.63882200	-0.81742500	-0.25783200
C	-0.32396200	0.11500800	-0.30003700
S	0.10962200	1.70462700	-1.01757100
C	2.04228600	-0.63613600	-0.10408900
C	2.56584300	0.37398900	0.70615400
C	2.88161600	-1.55434400	-0.73512600
C	3.94679400	0.46922000	0.85163400
H	1.87846000	1.05468000	1.20251900
C	4.25995100	-1.45382800	-0.56749500
H	2.45286000	-2.33839000	-1.35299200
C	4.79761200	-0.43791000	0.21979700
H	4.36071800	1.25430100	1.47735400
H	4.91157500	-2.16972400	-1.05863600
H	5.87263600	-0.35714200	0.34623300
O	-0.24178100	1.54430000	1.37249000
O	-0.53642900	2.48373400	0.30044200
N	-1.59939200	-0.27335600	-0.17747200
C	-1.94545100	-1.30884200	0.81482300
C	-2.69194000	0.69754700	-0.32301200
C	-3.27433200	-1.95052800	0.45065000
H	-1.18219400	-2.08420500	0.86988400
H	-2.01207400	-0.80996000	1.79095200
C	-3.98193200	-0.03879100	-0.64379600
H	-2.45920600	1.39250100	-1.12968500
H	-2.77633000	1.25335600	0.61762300
H	-3.17011900	-2.49606800	-0.49957100
H	-3.56014000	-2.65646300	1.23363200
O	-4.30256500	-0.98907100	0.35298700
H	-3.89329300	-0.53426400	-1.62272700
H	-4.80579700	0.67731600	-0.68514600
H	0.34023100	-1.78851900	-0.28554100

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N	0.60111400	-0.74186600	-0.10676800
C	-0.33558500	0.28694200	-0.03749500
S	0.02907500	1.88117900	-1.00322600
C	1.99874100	-0.60943800	-0.03485000

C	2.65718900	0.49901400	0.51391100
C	2.75864800	-1.68146000	-0.52541500
C	4.05009000	0.51955100	0.55639200
H	2.09972400	1.33827800	0.90818200
C	4.14604900	-1.64785600	-0.47102000
H	2.24785000	-2.54164400	-0.95097700
C	4.80481200	-0.54420300	0.06981400
H	4.54569700	1.38722200	0.98183800
H	4.71300700	-2.48937500	-0.85764700
H	5.88880400	-0.51522200	0.11098200
O	-0.15403400	1.05080400	1.19163300
O	-0.07014400	2.39009000	0.64572200
N	-1.64700600	-0.22606600	-0.23355100
C	-1.98474500	-1.38212400	0.62784700
C	-2.72572900	0.76599800	-0.11073200
C	-3.32703300	-1.95018500	0.19416600
H	-1.23221300	-2.16557100	0.53902000
H	-2.04038900	-1.06937900	1.68183800
C	-4.04215400	0.12876600	-0.52333900
H	-2.52569900	1.61472800	-0.76559700
H	-2.80063700	1.12828800	0.92551800
H	-3.24585700	-2.32300600	-0.83892000
H	-3.60374100	-2.78098000	0.84778900
O	-4.35693700	-0.98782500	0.28383700
H	-3.98621800	-0.17370500	-1.58067000
H	-4.85431100	0.85024500	-0.40621900
H	0.29725000	-1.51780100	-0.68651900

TS6

N	-0.62182800	-0.78596300	-0.20097900
C	0.34902700	0.19376200	-0.17645100
S	0.08567400	1.67747500	1.21814500
C	-2.01389600	-0.60644000	-0.11575100
C	-2.66824200	0.61459100	-0.32333200
C	-2.77223600	-1.75144600	0.16964800
C	-4.05835700	0.66868900	-0.23608100
H	-2.11318200	1.51491600	-0.55018100
C	-4.15692700	-1.68092500	0.24694700
H	-2.26341400	-2.69854300	0.33193200
C	-4.81250300	-0.46687200	0.04576200
H	-4.55333500	1.62222800	-0.39499900
H	-4.72309200	-2.58023800	0.46975400
H	-5.89427700	-0.40822300	0.10817600
O	0.07766600	1.23138700	-1.13634600

O	-0.05765900	2.42484000	-0.33381300
N	1.64506000	-0.25948000	-0.22781400
C	2.07202300	-1.65572300	-0.28965600
C	2.68216800	0.69297600	-0.62229900
C	3.39391500	-1.81314500	0.45380600
H	1.35682100	-2.32232800	0.19366600
H	2.18728900	-1.96652600	-1.33735800
C	3.95672600	0.41457200	0.15559000
H	2.33985600	1.70907000	-0.42041100
H	2.87910300	0.59859000	-1.69896500
H	3.22502100	-1.64315500	1.52827200
H	3.77460600	-2.82728400	0.31133400
O	4.37948300	-0.92368500	-0.02596500
H	3.78775700	0.61530600	1.22518900
H	4.76257800	1.05920900	-0.20340200
H	-0.32524100	-1.71509900	0.06811400

3a

N	0.60936500	0.38318200	-0.03075700
C	-0.34386100	-0.61310800	-0.08930800
C	2.00290700	0.21420400	-0.02620500
C	2.64380900	-0.99163700	0.28921500
C	2.78013400	1.34651400	-0.31180700
C	4.03613800	-1.04530300	0.30598200
H	2.05786100	-1.87143900	0.51286000
C	4.16740600	1.27703400	-0.28673300
H	2.28369300	2.28304800	-0.55377700
C	4.80858300	0.07767300	0.02072100
H	4.51934500	-1.98671900	0.55136500
H	4.74780200	2.16699000	-0.51128600
H	5.89219500	0.02086100	0.03817300
O	-0.06005200	-1.80137100	-0.18478200
N	-1.65328300	-0.17028300	-0.06540400
C	-2.67442900	-1.21496100	0.00716200
C	-2.07026500	1.06383400	0.60490100
C	-3.99600500	-0.67115600	-0.50819200
H	-2.35543600	-2.06322800	-0.59783500
H	-2.79390200	-1.55464700	1.04680000
C	-3.42397600	1.50017700	0.06366500
H	-1.36358900	1.87656500	0.43473000
H	-2.14464200	0.89313700	1.68880400
H	-3.90519900	-0.43499700	-1.57987200
H	-4.78409100	-1.41686200	-0.37834800
O	-4.39403000	0.48373400	0.20727500

H	-3.32037100	1.77618600	-0.99727200
H	-3.78099300	2.36934000	0.62137200
H	0.30475300	1.33293700	-0.19893100

SO

S	0.00000000	0.00000000	0.49938600
O	0.00000000	0.00000000	-0.99877300

TS7

N	0.15370000	-0.26485000	-0.23798600
C	1.30141600	-0.38105100	-0.32381800
S	2.95077800	-0.57767200	-0.64784400
C	-1.21684200	-0.11871000	-0.10994400
C	-1.79926700	1.09280200	-0.49018400
C	-1.96086200	-1.18726100	0.39605000
C	-3.17436000	1.22946600	-0.35393500
H	-1.17844000	1.89349500	-0.87711300
C	-3.33453400	-1.02788200	0.52085900
H	-1.46189900	-2.10808000	0.67786900
C	-3.93735400	0.17438500	0.14835200
H	-3.65096900	2.16056800	-0.64054200
H	-3.93486900	-1.84276300	0.91050500
H	-5.01146200	0.29057600	0.25094800
O	2.93094900	1.39653700	0.88757400
O	3.52906300	0.10501500	0.73560800

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N	0.33021300	-0.88240000	-0.14623400
C	1.38349700	-0.23239800	-0.04058700
S	3.08629500	-0.68226400	-0.08130700
C	-0.98635700	-0.38200900	-0.08103200
C	-1.32068800	0.97486800	-0.18859800
C	-1.99973900	-1.33291200	0.08211500
C	-2.65532700	1.36354100	-0.11905600
H	-0.55151300	1.72445100	-0.34020000
C	-3.32948600	-0.93425200	0.15808400
H	-1.72411900	-2.38055200	0.15133300
C	-3.66216400	0.41614600	0.05892300
H	-2.90674300	2.41618400	-0.20484900
H	-4.10704000	-1.68012600	0.29059000
H	-4.70004800	0.72866900	0.11524400
O	1.63763500	1.10502600	0.17789900
O	3.07721900	1.02578600	0.20876800

12

N	1.44519200	-0.60762500	-0.00003000
C	2.52610700	-0.07921700	-0.00003300
C	0.08713900	-0.26450100	-0.00001200
C	-0.32094400	1.07242300	-0.00001400
C	-0.85414100	-1.29421100	0.00000200
C	-1.67899600	1.37123500	-0.00000100
H	0.42609800	1.86067800	-0.00002900
C	-2.21056900	-0.98126100	0.00001500
H	-0.51418600	-2.32460100	0.00000200
C	-2.62755000	0.34855700	0.00001400
H	-1.99555400	2.40958800	-0.00000400
H	-2.94290400	-1.78253400	0.00002600
H	-3.68607400	0.58793900	0.00002400
O	3.63374900	0.30801900	0.00004700