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Electronic Supplementary Information for

# Catalytic Substitution/Cyclization Sequences of *O*-Substituted Isocyanates: Synthesis of 1‑Alkoxybenzimidazolones and 1-Alkoxy-3,4-dihydroquinazolin-2(1H)-ones

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## Supporting Information

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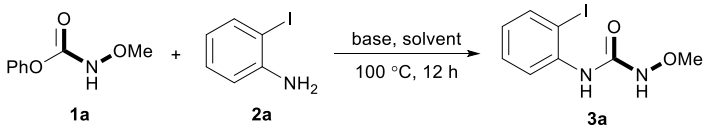
## 1. General Information

Purification of reaction products was carried out by flash column chromatography using SiliCycle silica gel (40-63 μm), unless otherwise noted. Analytical thin layer chromatography (TLC) was performed on aluminum plates, cut to size. Visualization was accomplished with UV light, ceric ammonium molybdate or $KMnO_4$ stains. $^1H$ NMR and $^{13}C$ NMR spectra were recorded on Bruker AVANCE 300 MHz and 400 MHz spectrometers at ambient temperature, unless otherwise indicated. Spectral data was reported in ppm using solvent as the reference ($CDCl_3$ at 7.26 ppm or DMSO-$d_6$ at 2.50 ppm for $^1H$ NMR and $CDCl_3$ at 77.0 ppm or DMSO-$d_6$ at 39.5 for $^{13}C$ NMR). 1H NMR data was reported as: multiplicity (ap = apparent, br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), integration and coupling constant(s) in Hz. Infrared spectra were recorded on all neat samples on a Nicolet 6700 FT-IR spectrometer in the 4000-600 $cm^{-1}$ region. High resolution mass spectroscopy (HRMS) was performed at the Ottawa-Carleton Mass Spectroscopy Centre on the Kratos Concept-11A mass spectrometer for Electron Impact (EI) and Waters Micromass Q-TOF I for electrospray ionization (ESI). Unless otherwise noted, all commercially available materials were purchased from commercial sources and used without further purification. All air- and moisture-sensitive reactions were carried out in oven-dried glassware under an atmosphere of argon unless otherwise noted.

## 2. Details for Conditions Optimization

We selected the readily accessible phenyl methoxycarbamate **1a** and 2-iodoaniline **2a** as model substrates to optimize the *O*-isocyanate substitution reaction (Table S1). Gratifyingly, substitution proceeded in the presence of several bases to afford the desired mixed *N*-methoxyurea **3a** upon heating at 100 °C (Table S1). Different bases were screened to minimize the trimerization of *in situ* generated reactive *O*-isocyanate (entries 1-6). While the strong base DBU only gave trace amount of the desired product, other organic bases and $K_2CO_3$ provided *N*-methoxyurea **3a** in encouraging yields. DABCO emerged as the optimal base (entry 6, 86% yield) and subsequently, the ratio of **1a** to **2a** was varied (entries 6-8): using a slight excess (1.5 equiv) of 2-iodoaniline **2a** yielded the best result, which is in line with the reduced nucleophilicity of this aniline derivative. Then solvent effects were examined to further improve the reaction efficiency (entries 9-11), and the use of *p*-xylene as solvent further improved the formation of product **3a** (entry 11, 94% yield). When a catalytic amount of base was used (5 mol%), a comparable isolated yield of product **3a** was obtained (entry 12, 89% yield). Interestingly, no reaction occured in the absence of base at 100 °C (entry 13).

**Table S1.** Optimization of reaction conditions for substitution[a]

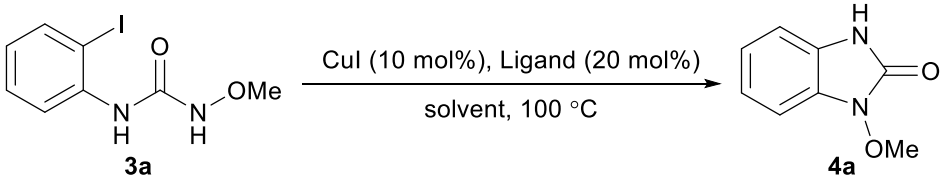



1a 2a 3a

| Entry | Base | Base (eq.) | Solvent | Ratio (**1a**:**2a**) | Yield (%)[b] |
|---|---|---|---|---|---|
| 1 | DBU | 1.0 | $PhCF_3$ | 1:1.5 | trace |
| 2 | $Et_3N$ | 1.0 | $PhCF_3$ | 1:1.5 | 63 |
| 3 | *i*-$Pr_2NEt$ | 1.0 | $PhCF_3$ | 1:1.5 | 72 |
| 4 | DMAP | 1.0 | $PhCF_3$ | 1:1.5 | 68 |
| 5 | $K_2CO_3$ | 1.0 | $PhCF_3$ | 1:1.5 | 64 |
| 6 | DABCO | 1.0 | $PhCF_3$ | 1:1.5 | 84 |
| 7 | DABCO | 1.0 | $PhCF_3$ | 1:1.2 | 80 |
| 8 | DABCO | 1.0 | $PhCF_3$ | 1:1.0 | 76 |
| 9 | DABCO | 1.0 | $(CH_2Cl)_2$ | 1:1.5 | 59 |
| 10 | DABCO | 1.0 | Benzene | 1:1.5 | 75 |
| 11 | DABCO | 1.0 | *p*-xylene | 1:1.5 | 94 (92)[c] |
| 12[d] | DABCO | 0.05 | *p*-xylene | 1:1.5 | (89)[c] |
| 13[e] | -- | 1.0 | *p*-xylene | 1:1.5 | 0 |

[a] Reaction conditions: **1a** (0.1 mmol), **2a** (0.1-0.15 mmol), solvent (1.0 mL). [b] Determined by $^1H$ NMR analysis of the crude reaction mixture using 1,3,5-trimethoxybenzene as an internal standard. [c] Isolated yield in parentheses. [d] DABCO (5 mol%). [e] Without base.

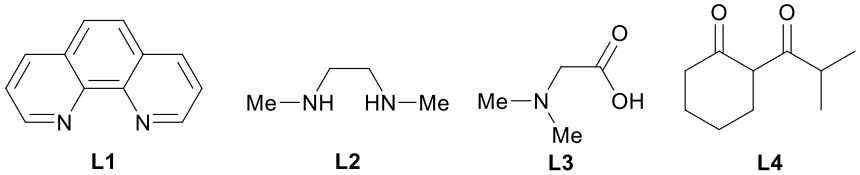
**Table S2.** Optimization of reaction conditions for cyclization[a]




3a 4a

| Entry | Ligand | Base | Time | Solvent | Yield (%)[b] |
|---|---|---|---|---|---|
| 1 | **L1** | DABCO | 4 h | DMSO | 96 |
| 2 | **L2** | DABCO | 4 h | DMSO | >98 (87)[c] |
| 3 | **L3** | DABCO | 4 h | DMSO | 76 |
| 4 | **L4** | DABCO | 4 h | DMSO | 70 |
| 5 | **L2** | $K_2CO_3$ | 4 h | DMSO | 0 |
| 6 | **L2** | $K_3PO_4$ | 4 h | DMSO | 0 |
| 7 | **L2** | $Et_3N$ | 4 h | DMSO | 99 |
| 8 | **L2** | *i*-$Pr_2NEt$ | 4 h | DMSO | 90 |
| 9 | **L2** | DMAP | 4 h | DMSO | 51 |
| 10 | **L2** | DABCO | 12 h | DMF | 52 |
| 11 | **L2** | DABCO | 36 h | $CH_3CN$ | 32 |
| 12 | **L2** | DABCO | 36 h | 1,4-Dioxane | 66 |
| 13[c] | **L2** | DABCO | 4 h | DMSO | 19 |
| 14[d] | -- | DABCO | 4 h | DMSO | 63 |
| 15[e] | -- | DABCO | 4 h | DMSO | < 5 |

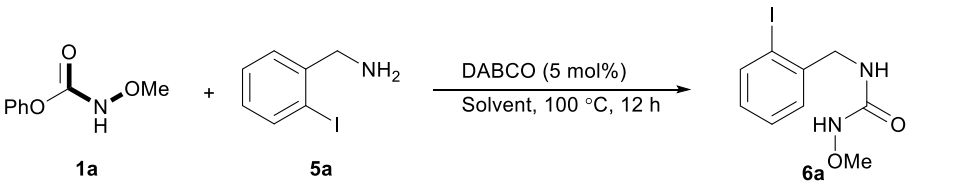
[a] Reaction conditions: **3a** (0.1 mmol), base (0.2 mmol), solvent (1.0 mL). [b] Determined by $^1H$ NMR analysis of the crude reaction mixture using 1,3,5-trimethoxybenzene as an internal standard. [c] Without CuI. [d] Without **L2**. [e] Without CuI and **L2**.




L1 L2 L3 L4

**Scheme S1.** Optimization of reaction conditions for the one pot synthesis of 1-Methoxy-3,4-dihydroquinazolin-2(1H)-one[a]

***Substitution***




**1a** 0.1 mmol

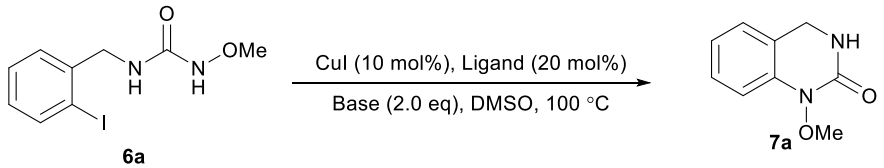
**5a** 0.15 mmol

**6a**

Solvent: p-xylene, 90% yield

**Solvent: $PhCF_3$, >98% yield**

***Cyclization***




**6a** 0.1 mmol

**7a**

L2, DABCO, 0% yield

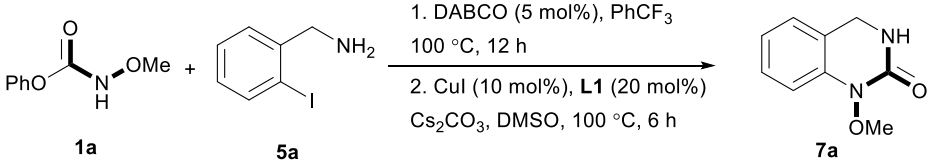
L1, DABCO, trace

L1, $K_2CO_3$, 50% yield

**L1, $Cs_2CO_3$, >98% yield**

L1, $K_3PO_4$, 40% yield

***One pot reaction***




**1a** 0.2 mmol

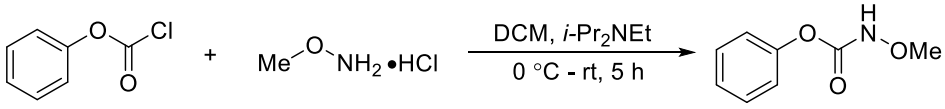
**5a** 0.3 mmol

**7a** 95% yield (isolated)

[a]Determined by $^1H$ NMR analysis of the crude reaction mixture using 1,3,5-trimethoxybenzene as an internal standard.

## 3. Preparation and Spectral Data of Substrates

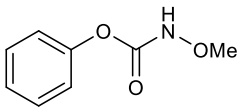
### 3.1 Representative Procedure for the Preparation of Carbamate




*O*-Methyl-hydroxylamine hydrochloride (1.67 g, 20.0 mmol) was dissolved in $CH_2Cl_2$ (100 mL) in a 250 mL round-bottom flask under Argon. The solution was cooled to 0 °C, then *i*-$Pr_2NEt$ (7.3 mL, 44.0 mmol) was added and phenyl chloroformate (3.13 g, 20.0 mmol) was added dropwise over 15 min. The resulting solution was stirred at room temperature for 5 h. The mixture was transferred to a separatory funnel containing water (50 mL), organic phase was separated and aqueous phases were extracted with $CH_2Cl_2$ (50 mL x 2). The combined organic layers were washed with brine, dried over $Na_2SO_4$, filtered, and concentrated. The residue was purified by flash silica gel chromatography (Hexane/EtOAc/$CH_2Cl_2$ 15:1:1) to afford the title compound as a white solid (2.0 g, 60% yield).

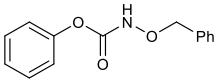
### 3.2 Spectral Data of Carbamate 1a-e

**Phenyl methoxycarbamate (1a)**



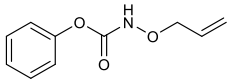

Synthesized according to general procedure using *O*-methyl-hydroxylamine hydrochloride. The title compound was purified by flash silica gel chromatography (Hexane/EtOAc/$CH_2Cl_2$ 15:1:1) to give **1a** (2.0 g, 60% yield) as a white solid. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.88 (s, 1H), 7.43 – 7.33 (m, 2H), 7.25-7.21 (m, 1H), 7.19 – 7.12 (m, 2H), 3.82 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 155.5, 150.3, 129.5, 125.9, 121.4, 64.8. IR (ATR): 3250, 2984, 2942, 1719, 1591, 1473, 1438, 1294, 1266, 1196, 1162, 1100, 1027, 995, 916, 836, 792, 729, 688, 609 $cm^{-1}$. HRMS (EI): Exact mass calculated for: $C_8H_9NO_3$ $[M]^+$: 167.05824, found 167.05487.

**Phenyl (benzyloxy)carbamate (1b)**



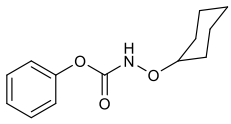

Synthesized according to general procedure using *O*-benzyl-hydroxylamine[S1]. The title compound was purified by flash silica gel chromatography (Hexane/EtOAc = 10:1-7:1) to give **1b** (0.620 g, 60% yield) as a white solid. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.66 (s, 1H), 7.45 – 7.41 (m, 2H), 7.39 (td, *J* = 3.9, 1.6 Hz, 2H), 7.38 – 7.36 (m, 2H), 7.36 – 7.33 (m, 1H), 7.25 – 7.19 (m, 1H), 7.16 – 7.10 (m, 2H), 4.95 (s, 2H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 155.3, 150.4, 135.2, 129.5, 129.3, 128.8, 128.7, 125.9, 121.4, 78.9. IR (ATR): 3288, 3065, 3041, 2941, 2880, 1729, 1593, 1472, 1455, 1248, 1204, 1163, 1100, 1071, 1022, 997, 978, 909, 845, 787, 746, 697, 687, 644 $cm^{-1}$. HRMS (ESI): Exact mass calculated for: $C_{14}H_{13}NNaO_3$ $[M+Na]^+$: 266.0788, found 266.0812.

**Phenyl (allyloxy)carbamate (1c)**



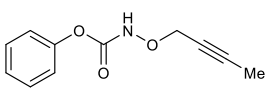
Synthesized according to general procedure using *O*-allyl-hydroxylamine hydrochloride. The title compound was purified by flash silica gel chromatography (Hexane/EtOAc = 15:1-12:1) to give **1c** (0.268 g, 63% yield) as a colorless oil. $^1$H NMR (300 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.43 – 7.27 (m, 2H), 7.24 – 7.17 (m, 1H), 7.17 – 7.10 (m, 2H), 6.09 – 5.89 (m, 1H), 5.44 – 5.26 (m, 2H), 4.42 (dt, *J* = 6.4, 1.1 Hz, 2H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 155.4, 150.4, 132.1, 129.4, 125.8, 121.4, 120.7, 77.9. IR (ATR): 3265, 1733, 1592, 1473, 1363, 1240, 1198, 1163, 1085, 1023, 995, 931, 906, 790, 753, 688 cm$^{-1}$. HRMS (ESI): Exact mass calculated for: $C_{10}H_{11}NNaO_3$ $[M+Na]^+$: 216.0631, found 216.0627.

**Phenyl (cyclohexyloxy)carbamate (1d)**



Synthesized according to general procedure using *O*-cyclohexyl-hydroxylamine[S2]. The title compound was purified by flash silica gel chromatography (Hexane/EtOAc = 10:1-5:1) to give **1d** (0.425 g, 60% yield) as a white solid. $^1$H NMR (300 MHz, $CDCl_3$) δ 7.46 (s, 1H), 7.39 – 7.31 (m, 2H), 7.23 – 7.17 (m, 1H), 7.17 – 7.07 (m, 2H), 3.86 (tt, *J* = 9.3, 3.8 Hz, 1H), 2.06 – 1.94 (m, 2H), 1.84 – 1.70 (m, 2H), 1.58 – 1.53 (m, 1H), 1.50-1.38 (m, 2H), 1.36 – 1.19 (m, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 155.7, 150.5, 129.4, 125.7, 121.4, 83.8, 30.5, 25.6, 23.7. IR (ATR) 3250, 2938, 2855, 1730, 1591, 1475, 1454, 1366, 1295, 1246, 1206, 1167, 1100, 1073, 1039, 1019, 992, 947, 897, 888, 781, 758, 737, 687, 622 cm$^{-1}$. HRMS (ESI): Exact mass calculated for: $C_{13}H_{17}NNaO_3$ $[M+Na]^+$: 258.1101, found 258.1116.

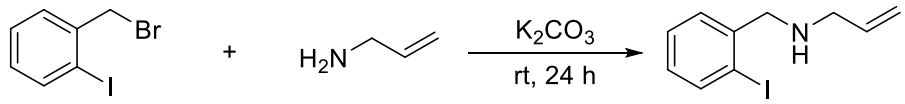
**Phenyl (but-2-yn-1-yloxy)carbamate (1e)**



Synthesized according to general procedure using O-(but-2-yn-1-yl)hydroxylamine[S3]. The title compound was purified by flash silica gel chromatography (Hexane/EtOAc = 10:1-7:1) to give **1e** (0.750 g, 50% yield) as a white solid. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.86 (s, 1H), 7.41 – 7.30 (m, 2H), 7.24 – 7.18 (m, 1H), 7.18 – 7.10 (m, 2H), 4.53 (q, *J* = 2.3 Hz, 2H), 1.88 (t, *J* = 2.4 Hz, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 155.0, 150.3, 129.5, 125.9, 121.3, 84.8, 73.1, 64.9, 3.7. IR (ATR): 3249, 2923, 2228, 1729, 1592, 1474, 1438, 1363, 1255, 1208, 1165, 1144, 1089, 1027, 1004, 936, 908, 818, 790, 753, 721, 688, 621, 607 cm$^{-1}$. HRMS (ESI): Exact mass calculated for: $C_{11}H_{11}NNaO_3$ $[M+Na]^+$: 228.0631, found 228.0637.

**3.3 Preparation of Substituted 2-iodobenzylamine**

(2-Iodophenyl)methanamine **5a**[S4] and *N*-(2-iodobenzyl)aniline **5b**[S5] were prepared according to literature procedures. Substituted 2-iodobenzylamine **5c-f** were prepared by following the procedures:

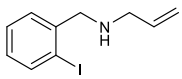



**General Procedure**: To a suspension of $K_2CO_3$ (0.829 g, 6.0 mmol) in allylamine (3.0 mL, 40.0 mmol), was added 1-(bromomethyl)-2-iodobenzene (1.48 g, 5.0 mmol) slowly over a period of 15 min. The resulting suspension was stirred at room temperature for 24 hours. The reaction mixture was filtered off over a Celite® pad and washed with dichloromethane. Filtrate was concentrated in vacuo and purification by column chromatography on silica gel ($CH_2Cl_2$: MeOH 20:0 to 20:1) afforded pure *N*-(2-iodobenzyl)prop-2-en-1-amine as a yellow oil (1.23 g, 90% yield).

[S1] J. T. Welch and K. W. Seper, *J. Org. Chem.*, 1988, **53**, 2991-2999.
[S2] M. K. Christensen, K. D. Erichsen, U. H. Olesen, J. Tjørnelund, P. Fristrup, A. Thougaard, S. J. Nielsen, M. Sehested, P. B. Jensen, E. Loza, I. Kalvinsh, A. Garten, W. Kiess and F. Björkling, *J. Med. Chem.,* 2013, **56**, 9071-9088.
[S3] S. M. Bromidge, F. Brown, F. Cassidy, M. S. G. Clark, S. Dabbs, M. S. Hadley, J. Hawkins, J. M. Loudon, C. B. Naylor, B. S. Orlek and G. J. Riley, *J. Med. Chem.*, 1997, **40**, 4265-4280.
[S4] J.M. Antonio, JR. Barbosa et al. (Boehringer Ingelheim Pharmaceuticals, Inc.), *U.S. Pat. Appl. Publ.*, 2006025433, **2006**.
[S5] A. M. Linsenmeier, C. M. Williams and S. Bräse, *J. Org. Chem.*, 2011, **76**, 9127-9132.

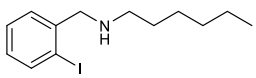
### 3.4 Spectral Data of Substituted 2-iodobenzylamine 5c-5g and N-(2-bromobenzyl)cyclopropanamine 11

***N*-(2-Iodobenzyl)prop-2-en-1-amine (5c)**




Synthesized according to general procedure using allylamine. The title compound was purified by flash silica gel chromatography ($CH_2Cl_2$: MeOH 20:0 to 20:1) to give **5c** (1.23 g, 90% yield) as a yellow oil. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.82 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.38 (dd, *J* = 7.6, 1.8 Hz, 1H), 7.32 (td, *J* = 7.4, 1.2 Hz, 1H), 6.95 (td, *J* = 7.8, 1.9 Hz, 1H), 6.00-5.90 (m, 1H), 5.25-5.20 (m, 1H), 5.17 – 5.09 (m, 1H), 3.82 (s, 2H), 3.28 (dt, *J* = 6.0, 1.5 Hz, 2H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 142.1, 139.5, 136.6, 129.8, 128.8, 128.3, 116.3, 99.6, 57.5, 51.6. IR (ATR): 3059, 2816, 1642, 1562, 1435, 1258, 1196, 1098, 1044, 1010, 928, 916, 820, 745, 646 cm$^{-1}$. HRMS (EI): Exact mass calculated for: $C_{10}H_{12}IN$ $[M]^+$: 273.00144, found 272.99785.

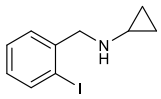
***N*-(2-Iodobenzyl)prop-2-en-1-amine (5d)**




Synthesized according to general procedure using hexan-1-amine. The title compound was purified by flash silica gel chromatography ($CH_2Cl_2$: MeOH 20:0 to 20:1) to give **5d** (1.43 g, 90% yield) as a yellow oil. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.79 (dd, *J* = 7.9,

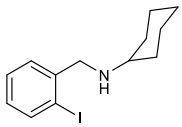
1.2 Hz, 1H), 7.43 – 7.15 (m, 2H), 6.92 (td, *J* = 7.6, 1.9 Hz, 1H), 3.78 (s, 2H), 2.60 (t, *J* = 7.2 Hz, 2H), 1.58 – 1.41 (m, 3H), 1.41 – 1.14 (m, 6H), 0.90 – 0.71 (m, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 142.4, 139.4, 129.6, 128.7, 128.2, 99.6, 58.3, 49.2, 31.7, 30.1, 27.0, 22.6, 14.0. IR (ATR): 3057, 2953, 2923, 2853, 1585, 1562, 1456, 1435, 1377, 1192, 1122, 1043, 1010, 820, 745, 647, 602 cm$^{-1}$. HRMS (EI): Exact mass calculated for: $C_{13}H_{20}IN$ $[M]^+$: 317.06404, found 317.06062.

**_N_-(2-Iodobenzyl)cyclopropanamine (5e)**



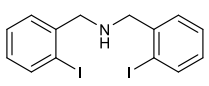
Synthesized according to general procedure using cyclopropanamine. The title compound was purified by flash silica gel chromatography ($CH_2Cl_2$: MeOH 20:0 to 20:1) to give **5e** (1.28 g, 94% yield) as a yellow oil. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.81 (dd, *J* = 7.9, 1.1 Hz, 1H), 7.35 – 7.13 (m, 2H), 6.93 (td, *J* = 7.6, 1.9 Hz, 1H), 3.85 (s, 2H), 2.11-2.06 (m, 2H), 0.46-0.38 (m, 4H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 142.4, 139.5, 130.0, 128.8, 128.2, 99.7, 58.0, 6.6. IR (ATR): 3084, 3004, 2926, 1683, 1585, 1562, 1463, 1434, 1371, 1339, 1210, 1159, 1042, 1009, 929, 826, 744, 646, 606 cm$^{-1}$. HRMS (EI): Exact mass calculated for: $C_{10}H_{12}IN$ $[M]^+$: 273.00144, found 272.99867.

**_N_-(2-Iodobenzyl)cyclohexanamine (5f)**



Synthesized according to general procedure using cyclopropanamine. The title compound was purified by flash silica gel chromatography ($CH_2Cl_2$: MeOH 20:0 to 20:1) to give **5f** (1.40 g, 89% yield) as a yellow oil. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.79 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.39 – 7.15 (m, 2H), 6.91 (td, *J* = 7.6, 1.8 Hz, 1H), 3.80 (s, 2H), 2.49-2.42 (m, 1H), 2.04 – 1.82 (m, 2H), 1.75-1.70 (m, 2H), 1.62-1.57 (m, 1H), 1.30-1.08 (m, 5H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 142.8, 139.4, 129.7, 128.6, 128.3, 99.6, 56.1, 55.4, 33.5, 26.1, 25.0. IR (ATR) 3056, 2922, 2849, 1584, 1562, 1447, 1435, 1346, 1258, 1196, 1122, 1043, 1010, 887, 820, 791, 745, 646 cm$^{-1}$. HRMS (EI): Exact mass calculated for: $C_{13}H_{18}IN$ $[M]^+$: 315.04839, found 315.04698.

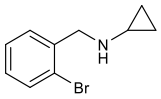
**Bis(2-iodobenzyl)amine (5g)**



Synthesized according to the following procedure: to a suspension of 1-(bromomethyl)-2-iodobenzene (1.48 g, 5.0 mmol) in ethanol (25 mL), ammonia solution (28% wt) (3.3 mL, 25.0 mmol) was added, the resulting solution was stirred overnight. The solution was concentrated under reduced pressure, and the resulting liquid was extracted with $CH_2Cl_2$. The combined organic layers were washed with brine, dried over $Na_2SO_4$, filtered, and concentrated. The residue was purified by flash silica gel chromatography (Hexane/EtOAc 10:1) to afford the title compound **5g** as colorless oil (0.224 g, 20% yield). $^1$H NMR (400 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 7.9, 1.2 Hz, 2H), 7.44 (dd, *J* = 7.6, 1.8 Hz, 2H), 7.34 (td, *J* = 7.5, 1.3 Hz, 2H), 6.97 (td, *J* = 7.6, 1.8 Hz, 2H), 3.85 (s, 4H),

1.92 (s, 1H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 142.0, 139.5, 129.8, 128.9, 128.3, 99.8, 57.5. IR (ATR): 3048, 2883, 2837, 1585, 1560, 1462, 1433, 1368, 1356, 1300, 1232, 1200, 1128, 1098, 1044, 1010, 959, 939, 859, 745, 648 $cm^{-1}$. HRMS (EI): Exact mass calculated for: $C_{14}H_{13}I_2N$ $[M]^+$: 448.91374, found 448.91435.

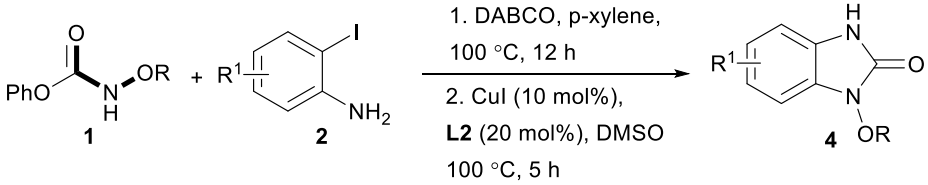
***N*-(2-bromobenzyl)cyclopropanamine 11**



Synthesized according to general procedure using 1-bromo-2-(bromomethyl)benzene and cyclopropanamine. The title compound was purified by flash silica gel chromatography ($CH_2Cl_2$: MeOH 20:0 to 20:1) to give **11** (1.01 g, 89% yield) as a yellow oil. $^1$H NMR (300 MHz, $CDCl_3$) δ 7.56 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.38 (ddd, *J* = 7.5, 1.8, 0.5 Hz, 1H), 7.29 (td, *J* = 7.4, 1.3 Hz, 1H), 7.18 – 7.09 (m, 1H), 3.94 (s, 2H), 2.17 (d, *J* = 10.9 Hz, 1H), 2.14 – 2.02 (m, 1H), 0.53 – 0.38 (m, 4H). $^{13}$C NMR (76 MHz, CDCl3) δ 139.3, 132.8, 130.6, 128.6, 127.3, 124.1, 53.6, 29.7, 6.5. IR (ATR): 3085, 3006, 2929, 1568, 1468, 1437, 1372, 1342, 1212, 1159, 1024, 930, 826, 745, 655, 606 $cm^{-1}$. HRMS (EI): Exact mass calculated for: $C_{10}H_{12}BrN$ $[M]^+$: 225.01531, found 225.01378.

## 4. One pot synthesis of 1-Alkoxybenzimidazolones

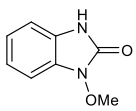
### 4.1 General procedure for one pot synthesis of 1-Alkoxybenzimidazolones




**General Procedure**: A mixture of carbamate **1** (0.20 mmol, 1.0 equiv), 2-iodoaniline **2** (0.30 mmol, 1.5 equiv), DABCO (0.0450 g, 0.40 mmol) in p-xylene (2.0 mL) was stirred at 100 $^o$C for 12 h under argon. Then the solvent was removed under reduced pressure. To the residue was added CuI (0.0038 g, 0.02 mmol), N,N'-Dimethyl-1,2-ethanediamine **L2** (0.0035 g, 0.04 mmol) and DMSO (2.0 mL). Then the reaction was stirred at 100 $^o$C for 5 h under argon. After cooling to room temperature, the reaction mixture was diluted with water (10 mL) and extracted with EtOAc (20 mL x 3). The combined organic layer was dried over $Na_2SO_4$ and concentrated. The residue was purified by flash chromatography (n-hexane: EtOAc 2:1 - 1:1) on silica gel to afford the title compound **4**.

### 4.2 Spectral data of 1-Alkoxybenzimidazolones

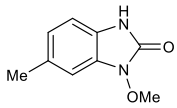
**1-Methoxy-1,3-dihydro-2H-benzo[d]imidazol-2-one (4a)**



Synthesized according to general procedure using phenyl methoxycarbamate **1a** and 2-iodoaniline **2a**. The residue was purified by column chromatography (n-hexane/EtOAc = 2:1 – 1:1) to give **4a** (0.0290 g, 87% yield) as a white solid. $^1$H NMR (300 MHz, $CDCl_3$) δ

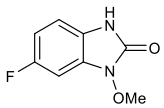
9.53 (brs, 1H), 7.16-7.10 (m, 2H), 7.11 (d, $J$ = 3.8 Hz, 2H), 4.13 (s, 3H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 151.0, 127.3, 125.1, 122.1, 121.5, 110.0, 106.8, 64.6. IR (ATR): 3142, 3016, 2946, 1694, 1624, 1477, 1451, 1422, 1383, 1300, 1272, 1203, 1170, 1103, 1020, 995, 953, 916, 884, 768, 732, 681, 636 cm$^{-1}$. HRMS (EI): Exact mass calculated for: $C_8H_8N_2O_2$ $[M]^+$: 164.05858, found 164.05747.

**1-Methoxy-6-methyl-1,3-dihydro-2H-benzo[d]imidazol-2-one (4b)**



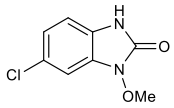

Synthesized according to general procedure using phenyl methoxycarbamate **1a** and 2-iodo-4-methylaniline **2b**. The residue was purified by column chromatography (*n*-hexane/EtOAc = 2:1 – 1:1) to give **4b** (0.0330 g, 92% yield) as a white solid. $^1$H NMR (300 MHz, $CDCl_3$) δ 9.64 (br s, 1H), 7.04 – 6.93 (m, 2H), 6.90 (dd, $J$ = 8.0, 1.6 Hz, 1H), 4.11 (s, 3H), 2.41 (s, 3H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 151.2, 130.8, 127.4, 122.9, 122.5, 109.8, 107.3, 64.5, 21.5. IR (ATR): 3150, 2921, 2851, 1700, 1495, 1457, 1425, 1379, 1295, 1273, 1202, 1184, 1147, 1121, 958, 904, 852, 794, 754, 726, 685 cm$^{-1}$. HRMS (EI): Exact mass calculated for: $C_9H_{10}N_2O_2$ $[M]^+$: 178.07423, found 178.07257.

**6-Fluoro-1-methoxy-1,3-dihydro-2H-benzo[d]imidazol-2-one (4c)**



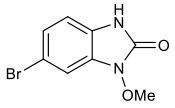

Synthesized according to general procedure using phenyl methoxycarbamate **1a** and 4-fluoro-2-iodoaniline **2c**. The residue was purified by column chromatography (n-hexane/EtOAc = 2:1 – 1:1) to give **4c** (0.030 g, 82% yield) as a white solid. $^1$H NMR (300 MHz, DMSO-$d_6$) δ 11.03 (br s, 1H), 7.05 (dd, $J$ = 8.5, 2.5 Hz, 1H), 6.95 (dd, $J$ = 8.5, 4.5 Hz, 1H), 6.80 (m, 1H), 3.92 (s, 3H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 159.5, 157.1, 151.4, 128.0, 127.8, 121.3, 110.7, 110.6, 108.3, 108.1, 95.5, 95.2, 64.8. IR (ATR): 3219, 2956, 2921, 2851, 1757, 1687, 1635, 1490, 1467, 1432, 1413, 1299, 1241, 1190, 1180, 1140, 1095, 1013, 954, 907, 831, 800, 738, 676 cm$^{-1}$. HRMS (EI): Exact mass calculated for: $C_8H_7FN_2O_2$ $[M]^+$: 182.04916, found 182.04671.

**6-Chloro-1-methoxy-1,3-dihydro-2H-benzo[d]imidazol-2-one (4d)**



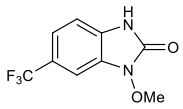

Synthesized according to general procedure using phenyl methoxycarbamate **1a** and 4-chloro-2-iodoaniline **2d**. The residue was purified by column chromatography (n-hexane/EtOAc = 2:1 – 1:1) to give **4d** (0.0330 g, 83% yield) as a white solid. $^1$H NMR (400 MHz, DMSO-$d_6$) δ 11.15 (br s, 1H), 7.20 (s, 1H), 7.05 – 6.94 (m, 2H), 3.93 (s, 3H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 151.0, 128.3, 125.9, 124.0, 121.8, 111.2, 106.9, 64.9. IR (ATR): 3207, 2948, 1733, 1670, 1478, 1428, 1397, 1279, 1245, 1195, 1158, 1112, 1062, 1017, 957, 891, 841, 800, 766, 660 cm$^{-1}$. HRMS (EI): Exact mass calculated for: $C_8H_7ClN_2O_2$ $[M]^+$: 198.01961, found 198.01473.

**6-Bromo-1-methoxy-1,3-dihydro-2H-benzo[d]imidazol-2-one (4e)**



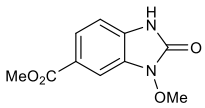
Synthesized according to general procedure using phenyl methoxycarbamate **1a** and 4-bromo-2-iodoaniline **2e**. The residue was purified by column chromatography (n-hexane/EtOAc = 2:1 – 1:1) to give **4e** (0.0365 g, 75% yield) as a white solid. $^{1}$H NMR (300 MHz, $CDCl_3$) δ 9.60 (br s, 1H), 7.30-7.29 (m, 1H), 7.23 (dd, *J* = 8.3, 1.9 Hz, 1H), 7.00 – 6.95 (m, 1H), 4.12 (s, 3H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 150.8, 128.6, 124.6, 124.4, 113.4, 111.7, 109.5, 64.9. IR (ATR): 3200, 2942, 1699, 1608, 1478, 1431, 1378, 1280, 1195, 1169, 1114, 1049, 1021, 956, 885, 802, 766, 675 cm$^{-1}$. HRMS (EI): Exact mass calculated for: $C_8H_7BrN_2O_2$ $[M]^+$: 241.96909, found 241.97053.

**1-Methoxy-6-(trifluoromethyl)-1,3-dihydro-2H-benzo[d]imidazol-2-one (4f)**



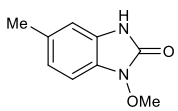
Synthesized according to general procedure using phenyl methoxycarbamate **1a** and 2-iodo-4-(trifluoromethyl)aniline **2f**. The residue was purified by column chromatography (n-hexane/EtOAc = 2:1 – 1:1) to give **4f** (0.0420 g, 90% yield) as a white solid. $^{1}$H NMR (300 MHz, $CDCl_3$) δ 9.79 (brs, 1H), 7.41-7.37 (m, 2H), 7.18 (dd, *J* = 8.6, 0.7 Hz, 1H), 4.14 (s, 3H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 151.1, 128.3, 127.4, 125.1 (q, *J* = 271.5 Hz), 122.3 (q, *J* = 32.1 Hz), 119.4 (q, *J* = 4.1 Hz), 110.2, 103.7 (q, *J* = 4.0 Hz), 65.1. IR (ATR): 3200, 3022, 2953, 2850, 1705, 1641, 1480, 1433, 1316, 1262, 1203, 1168, 1101, 1048, 953, 898, 865, 816, 786, 739, 688, 665 cm$^{-1}$. HRMS (EI): Exact mass calculated for: $C_9H_7F_3N_2O_2$ $[M]^+$: 232.04596, found 232.04555.

**Methyl 3-methoxy-2-oxo-2,3-dihydro-1H-benzo[d]imidazole-5-carboxylate (4g)**



Synthesized according to general procedure using phenyl methoxycarbamate 1a and methyl 4-amino-3-iodobenzoate **2g**. The residue was purified by column chromatography (n-hexane/EtOAc = 2:1 – 1:1) to give **4g** (0.0310 g, 70% yield) as a white solid. $^{1}$H NMR (300 MHz, $CDCl_3$) δ 9.47 (br s, 1H), 7.86 (dd, *J* = 8.2, 1.6 Hz, 1H), 7.82 (dt, *J* = 1.6, 0.7 Hz, 1H), 7.12 (d, *J* = 8.4 Hz, 1H), 4.13 (s, 3H), 3.92 (s, 3H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 166.6, 151.1, 129.3, 127.2, 124.3, 123.0, 109.9, 107.2, 65.0, 52.5. IR (ATR): 3190, 3005, 2924, 2849, 1705, 1633, 1611, 1471, 1440, 1284, 1249, 1198, 1166, 1094, 1020, 968, 950, 899, 874, 820, 758, 722, 689, 674 cm$^{-1}$. HRMS (EI): Exact mass calculated for: $C_{10}H_{10}N_2O_4$ $[M]^+$: 222.06406, found 222.06360.

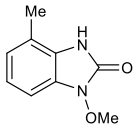
**1-Methoxy-5-methyl-1,3-dihydro-2H-benzo[d]imidazol-2-one (4h)**



Synthesized according to general procedure using phenyl methoxycarbamate **1a** and methyl 2-iodo-5-methylaniline **2h**. The residue was purified by column chromatography (n-hexane/EtOAc = 2:1 – 1:1) to give **4h** (0.0240 g, 68% yield) as a white solid. $^{1}$H NMR (300 MHz, $CDCl_3$) δ 9.05 (br s, 1H), 7.05 – 6.97 (m, 1H), 6.96 – 6.86 (m, 2H), 4.08 (s, 3H), 2.36 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 152.2, 132.1, 124.8, 124.4, 122.5, 110.9, 106.7, 64.6, 21.4. IR (ATR): 3115, 2919, 2850, 1700, 1636, 1505, 1470, 1437,

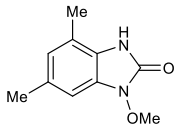
1427, 1385, 1293, 1207, 1168, 1013, 956, 939, 853, 787, 778 724, 695 $cm^{-1}$. HRMS (EI): Exact mass calculated for: $C_9H_{10}N_2O_2$ $[M]^+$: 178.07423, found 178.07497.

**1-Methoxy-4-methyl-1,3-dihydro-2H-benzo[d]imidazol-2-one (4i)**



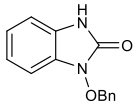

Synthesized according to general procedure using phenyl methoxycarbamate **1a** and methyl 2-iodo-5-methylaniline **2i**. The residue was purified by column chromatography (n-hexane/EtOAc = 2:1 – 1:1) to give **4i** (0.0175 g, 49% yield) as a white solid. $^1$H NMR (300 MHz, $CDCl_3$) δ 9.34 (brs, 1H), 7.07 – 7.00 (m, 1H), 6.99-6.95 (m, 1H), 6.92-6.88 (m, 1H), 4.09 (s, 3H), 2.37 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 152.2, 126.6, 123.4, 123.2, 121.8, 120.3, 104.5, 64.6, 15.9. IR (ATR): 3206, 3020, 2921, 2851, 1700, 1463, 1428, 1378, 1352, 1300, 1221, 1200, 1175, 1154, 993, 965, 890, 864, 760, 730, 720, 646 $cm^{-1}$. HRMS (EI): Exact mass calculated for for: $C_9H_{10}N_2O_2$ $[M]^+$: 178.07423, found 178.07502.

**1-Methoxy-4-methyl-1,3-dihydro-2H-benzo[d]imidazol-2-one (4j)**



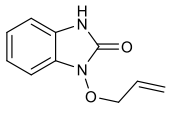

Synthesized according to general procedure using phenyl methoxycarbamate **1a** and methyl 2-iodo-4,6-dimethylaniline **2j**. The residue was purified by column chromatography (*n*-hexane/EtOAc = 2:1 – 1:1) to give **4j** (0.0170 g, 45% yield) as a white solid. $^1$H NMR (300 MHz, $CDCl_3$) δ 9.38 (br, 1H), 6.80 (d, $J$ = 1.5 Hz, 1H), 6.77 – 6.68 (m, 1H), 4.09 (s, 3H), 2.38 (s, 3H), 2.34 (s, 3H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 151.4, 130.7, 127.1, 123.9, 121.6, 119.5, 104.8, 64.4, 21.4, 16.1. IR (ATR): 3146, 3012, 2919, 2857, 1699, 1629, 1463, 1456, 1425, 1374, 1302, 1198, 1181, 1143, 974, 957, 892, 827, 803, 763, 728, 713, 631 $cm^{-1}$. HRMS (EI): Exact mass calculated for: $C_{10}H_{12}N_2O_2$ $[M]^+$: 192.08988, found 192.09368.

**1-(Benzyloxy)-1,3-dihydro-2H-benzo[d]imidazol-2-one (4k)**




Synthesized according to general procedure using phenyl (benzyloxy)carbamate **1b** and 2-iodoaniline **2a**. The residue was purified by column chromatography (n-hexane/EtOAc = 2:1 – 1:1) to give **4k** (0.0400 g, 82% yield) as a white solid. $^1$H NMR (400 MHz, DMSO-$d_6$) δ 10.98 (s, 1H), 7.49 (dd, $J$ = 6.4, 2.9 Hz, 2H), 7.36 (dd, $J$ = 4.9, 1.7 Hz, 3H), 6.93 (d, $J$ = 6.6 Hz, 3H), 6.88 – 6.81 (m, 1H), 5.14 (s, 2H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 151.6, 134.9, 130.4, 129.5, 129.0, 128.2, 125.0, 121.9, 121.4, 109.9, 107.1, 78.7. IR (ATR): 3137, 3065, 3020, 2832, 1699, 1477, 1455, 1396, 1297, 1273, 1198, 1172, 998, 954, 910, 847, 772, 726, 697, 688, 643 $cm^{-1}$. HRMS (EI): Exact mass calculated for: $C_{14}H_{12}N_2O_2$ $[M]^+$: 240.08988, found 240.08702.

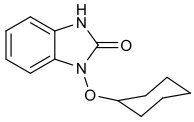
**1-(Allyloxy)-1,3-dihydro-2H-benzo[d]imidazol-2-one (4l)**




Synthesized according to general procedure using phenyl (allyloxy)carbamate **1c** and 2-iodoaniline **2a**. The residue was purified by column chromatography (n-hexane/EtOAc = 2:1 – 1:1) to give **4l** (0.0315 g, 83% yield) as a white solid. $^1$H NMR (300 MHz, $CDCl_3$) δ

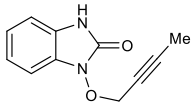
9.05 (brs, 1H), 7.13 – 7.07 (m, 4H), 6.23-6.10 (m, 1H), 5.54 – 5.29 (m, 2H), 4.79-4.77 (m, 2H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 151.5, 132.5, 128.3, 125.0, 122.1, 121.9, 121.5, 109.9, 107.2, 77.7. IR (ATR): 3145, 3022, 2923, 1701, 1646, 1478, 1421, 1388, 1299, 1200, 1175, 994, 938, 883, 773, 734, 724, 689 cm$^{-1}$. HRMS (EI): Exact mass calculated for: $C_{10}H_{10}N_2O_2$ $[M]^+$: 190.07423, found 190.07159.

**1-(Cyclohexyloxy)-1,3-dihydro-2H-benzo[d]imidazol-2-one (4m)**



Synthesized according to general procedure using phenyl (cyclohexyloxy)carbamate **1d** and 2-iodoaniline **2a**. The residue was purified by column chromatography (n-hexane/EtOAc = 2:1 – 1:1) to give **4m** (0.0350 g, 75% yield) as a white solid. $^1$H NMR (400 MHz, $CDCl_3$) δ 10.31 (s, 1H), 7.17 – 7.09 (m, 3H), 7.09 – 7.03 (m, 1H), 4.40-4.33 (m, 1H), 2.25 – 2.06 (m, 2H), 1.91 – 1.80 (m, 2H), 1.65-1.56 (m, 3H), 1.37-1.21 (m, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 153.2, 128.9, 124.3, 121.8, 121.6, 110.2, 107.5, 85.4, 31.2, 25.4, 24.0. IR (ATR): 3145, 3072, 3028, 2937, 2851, 1702, 1478, 1447, 1385, 1367, 1298, 1199, 1170, 1012, 996, 936, 926, 898, 882, 845, 765, 723, 688, 642 cm$^{-1}$. HRMS (EI): Exact mass calculated for: $C_{13}H_{16}N_2O_2$ $[M]^+$: 232.12118, found 232.12050.

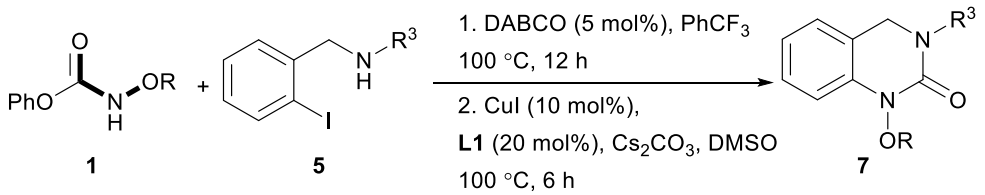
**1-(But-2-yn-1-yloxy)-1,3-dihydro-2H-benzo[d]imidazol-2-one (4n)**



Synthesized according to general procedure using phenyl (but-2-yn-1-yloxy)carbamate **1e** and 2-iodoaniline **2a**. The residue was purified by column chromatography (n-hexane/EtOAc = 2:1 – 1:1) to give **4n** (0.0340 g, 84% yield) as a white solid. $^1$H NMR (400 MHz, $CDCl_3$) δ 9.92 (brs, 1H), 7.26 – 7.23 (m, 1H), 7.13 – 7.09 (m, 1H), 7.09 – 7.03 (m, 2H), 4.87 (q, $J$ = 2.3 Hz, 2H), 1.77 (t, $J$ = 2.4 Hz, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 152.7, 128.4, 124.1, 122.2, 121.8, 110.1, 108.0, 86.4, 72.8, 65.5, 3.7. IR (ATR): 3149, 3031, 2914, 2245, 1694, 1630, 1478, 1451, 1388, 1298, 1276, 1202, 1175, 1161, 999, 936, 886, 821, 764, 730, 683, 638 cm$^{-1}$. HRMS (EI): Exact mass calculated for: $C_{11}H_{10}N_2O_2$ $[M]^+$: 202.07423, found 202.07704.

## 5. One pot synthesis of 1-Alkoxy-3,4-dihydroquinazolin-2(1H)-ones

### 5.1 General procedure for one pot synthesis of 1-Alkoxy-3,4-dihydroquinazolin -2(1H)-ones

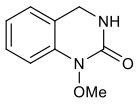



**General Procedure**: A mixture of carbamate **1** (0.20 mmol, 1.0 equiv), 2-iodobenzylamine **2** (0.30 mmol, 1.5 equiv), DABCO (0.0011 g, 0.01 mmol) in $PhCF_3$ (2.0 mL) was stirred at 100 °C for 12 h under argon. Then the solvent was

removed under reduced pressure. To the residue was added CuI (0.0038 g, 0.02 mmol), 1,10-phenanthroline **L1** (0.0072 g, 0.04 mmol), $Cs_2CO_3$ (0.130 g, 0.4 mmol) and DMSO (2.0 mL). Then the reaction was stirred at 100 °C for 5 h under argon. After cooling to room temperature, the reaction mixture was diluted with water (10 mL) and extracted with EtOAc (20 mL x 3). The combined organic layer was dried over $Na_2SO_4$ and concentrated. The residue was purified by flash chromatography on silica gel to afford the title compound **7**.

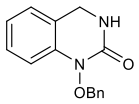
### 5.2 Spectral data of 1-Alkoxy-3,4-dihydroquinazolin-2(1H)-ones

**1-Methoxy-3,4-dihydroquinazolin-2(1H)-one (7a)**



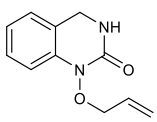

Synthesized according to general procedure using phenyl methoxycarbamate **1a** and (2-iodophenyl)methanamine **5a**. The residue was purified by column chromatography (n-hexane/EtOAc = 2:1 – 1:1) to give **7a** (0.0340 g, 95% yield) as a white solid. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.26 (td, *J* = 8.2, 1.6 Hz, 1H), 7.18 – 7.10 (m, 1H), 7.06-7.04 (m, 1H), 6.99-6.97 (m, 1H), 6.51 (brs, 1H), 4.34 (s, 2H), 3.93 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 155.5, 138.8, 128.3, 125.4, 122.9, 118.4, 111.1, 63.4, 42.7. IR (ATR): 3211, 3105, 2970, 2922, 2852, 1690, 1606, 1595, 1461, 1393, 1313, 1260, 1234, 1197, 1147, 1108, 1061, 964, 762, 745, 705, 674 cm$^{-1}$. HRMS (EI): Exact mass calculated for: $C_9H_{10}N_2O_2$ $[M]^+$: 178.07423, found 178.07459.

**1-(Benzyloxy)-3,4-dihydroquinazolin-2(1H)-one (7b)**




Synthesized according to general procedure using phenyl (benzyloxy)carbamate **1b** and (2-iodophenyl)methanamine **5a**. The residue was purified by column chromatography (n-hexane/EtOAc = 2:1 – 1:1) to give **7b** (0.0355 g, 70% yield) as a white solid. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.50 (m, 2H), 7.40 – 7.30 (m, 3H), 7.24 – 7.19 (m, 1H), 7.16 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.05 – 7.01 (m, 1H), 7.00-6.96 (m, 1H), 6.10 (brs, 1H), 5.10 (s, 2H), 4.34 (d, *J* = 2.1 Hz, 2H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 155.5, 139.4, 134.8, 129.6, 128.8, 128.5, 128.2, 125.2, 122.8, 118.4, 111.5, 77.9, 42.7. IR (ATR): 3235, 3113, 2923, 1688, 1606, 1497, 1460, 1405, 1321, 1268, 1198, 1154, 1111, 1055, 1008, 907, 850, 746, 734, 632 cm$^{-1}$. HRMS (EI): Exact mass calculated for: $C_{15}H_{14}N_2O_2$ $[M]^+$: 254.10553, found 254.10541.

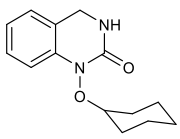
**1-(Allyloxy)-3,4-dihydroquinazolin-2(1H)-one (7c)**




Synthesized according to general procedure using phenyl (allyloxy)carbamate **1c** and (2-iodophenyl)methanamine **5a**. The residue was purified by column chromatography (n-hexane/EtOAc = 2:1 – 1:1) to give **7c** (0.0340 g, 83% yield) as a white solid. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.29 – 7.24 (m, 1H), 7.17 (dd, *J* = 8.1, 1.1 Hz, 1H), 7.09 – 6.92 (m, 2H), 6.23 (brs, 1H), 6.10 (m, 1H), 5.39 (dq, *J* = 17.2, 1.4 Hz, 1H), 5.31-5.27 (m, 1H), 4.58 (d, *J* = 6.4 Hz, 2H), 4.33 (d, *J* = 1.8 Hz, 2H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 155.7, 139.5, 131.9, 128.2, 125.3, 122.8, 120.5, 118.5, 111.5, 76.8, 42.7. IR (ATR): 3226, 3110, 2925, 1690, 1475, 1465, 1417, 1388, 1318, 1284, 1201, 1170, 1142, 1115, 1062,

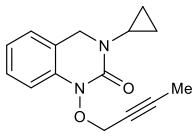
996, 958, 927, 848, 735, 632, 614 $cm^{-1}$. HRMS (EI): Exact mass calculated for: $C_{11}H_{12}N_2O_2$ $[M]^+$: 204.08988, found 204.08855.

**1-(Cyclohexyloxy)-3,4-dihydroquinazolin-2(1H)-one (7d)**



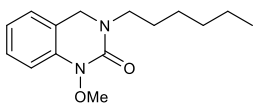
Synthesized according to general procedure using phenyl (cyclohexyloxy)carbamate **1d** and (2-iodophenyl)methanamine **5a**. The residue was purified by column chromatography (n-hexane/EtOAc = 2:1 – 1:1) to give **7d** (0.0240 g, 49% yield) as a yellow solid. $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.29 – 7.24 (m, 1H), 7.23 – 7.19 (m, 1H), 7.04 (dd, *J* = 7.4, 1.4 Hz, 1H), 7.00-6.96 (m, 1H), 5.82 (s, 1H), 4.31 (s, 2H), 4.04-3.97 (m, 1H), 2.09 (m, 2H), 1.80 (m, 2H), 1.60 – 1.45 (m, 3H), 1.32 – 1.21 (m, 3H). $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 156.4, 140.7, 128.1, 125.0, 122.6, 118.9, 111.9, 83.4, 42.7, 30.8, 25.6, 24.2. IR (ATR): 3374, 2950, 2293, 2855, 2817, 1713, 1678, 1608, 1493, 1462, 1450, 1421, 1366, 1309, 1258, 1236, 1193, 1109, 1050, 1037, 1015, 946, 757, 745, 720, 691, 622 $cm^{-1}$. HRMS (EI): Exact mass calculated for: $C_{14}H_{18}N_2O_2$ $[M]^+$: 246.13683, found 246.13813.

**1-(But-2-yn-1-yloxy)-3-cyclopropyl-3,4-dihydroquinazolin-2(1H)-one (7e)**



Synthesized according to general procedure using phenyl (but-2-yn-1-yloxy)carbamate **1e** and *N*-(2-iodobenzyl)cyclopropan -amine **5e**. The residue was purified by column chromatography (n-hexane/EtOAc = 10:1 – 6:1) to give **7e** (0.0430 g, 84% yield) as a yellow oil. $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.25 – 7.22 (m, 2H), 7.05-7.03 (m, 1H), 6.98- 6.94 (m, 1H), 4.68 (q, *J* = 2.4 Hz, 2H), 4.27 (s, 2H), 2.66-2.61 (m, 1H), 1.76 (t, *J* = 2.4 Hz, 3H), 0.85 – 0.80 (m, 2H), 0.65-0.67 (m, 2H). $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 155.5, 139.5, 128.2, 124.8, 122.5, 117.9, 111.8, 84.5, 73.4, 64.1, 48.8, 29.9, 7.5, 3.7. IR (ATR): 3243, 2920, 2238, 1669, 1606, 1494, 1464, 1417, 1362, 1271, 1198, 1116, 1072, 1012, 908, 834, 750, 708, 668 $cm^{-1}$. HRMS (EI): Exact mass calculated for: $C_{15}H_{16}N_2O_2$ $[M]^+$: 256.12118, found 256.12165.

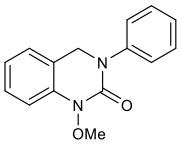
**3-Hexyl-1-methoxy-3,4-dihydroquinazolin-2(1H)-one (7f)**



Synthesized according to general procedure using phenyl methoxycarbamate **1a** and *N*-(2-iodobenzyl)hexan-1-amine **5d**. The residue was purified by column chromatography (n-hexane/EtOAc = 10:1 – 6:1) to give **7f** (0.0500 g, 95% yield) as a yellow oil. $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.25 (t, *J* = 7.8 Hz, 1H), 7.11 (d, *J* = 8.0 Hz, 1H), 7.04 (d, *J* = 7.2 Hz, 1H), 6.97 (t, *J* = 7.4 Hz, 1H), 4.25 (s, 2H), 3.90 (s, 3H), 3.48 – 3.32 (t, *J* = 8 Hz, 2H), 1.57 (m, 2H), 1.27 (m, 6H), 0.87 – 0.82 (t, *J* = 8 Hz, 3H). $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 154.2, 139.4, 128.4, 125.0, 122.4, 117.6, 110.9, 63.3, 47.9, 47.7, 31.5, 27.2, 26.4, 22.5, 14.0. IR (ATR): 2929, 2857, 1715, 1667, 1611, 1465, 1429, 1395, 1318, 1264, 1205, 1096, 1046, 1025, 752, 737, 708, 690, 679 $cm^{-1}$. HRMS (EI): Exact mass calculated for: $C_{15}H_{22}N_2O_2$ $[M]^+$: 262.16813, found 260.16500.

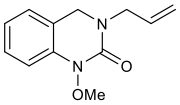
**1-Methoxy-3-phenyl-3,4-dihydroquinazolin-2(1H)-one (7g)**

Synthesized according to general procedure using phenyl methoxycarbamate **1a** and



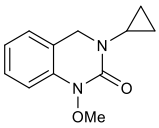
*N*-(2-iodobenzyl)aniline **5b**. The residue was purified by column chromatography (n-hexane/EtOAc = 10:1 – 6:1) to give **7g** (0.0500 g, 90% yield) as a yellow oil. $^{1}$H NMR (300 MHz, $CDCl_3$) δ 7.43 – 7.38 (m, 1H), 7.37 (dd, *J* = 1.5, 1.0 Hz, 3H), 7.35 – 7.31 (m, 1H), 7.27 – 7.19 (m, 2H), 7.16 – 6.98 (m, 2H), 4.70 (s, 2H), 3.97 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 153.7, 141.9, 138.9, 128.9, 128.7, 126.2, 125.2, 125.0, 122.9, 118.0, 111.1, 63.5, 50.4. IR (ATR): 2933, 1675, 1597, 1491, 1463, 1405, 1309, 1249, 1216, 1196, 1170 1068, 1005, 965, 752, 737, 706, 693, 655, 638 cm$^{-1}$. HRMS (EI): Exact mass calculated for: $C_{15}H_{14}N_2O_2$ [M]$^{+}$: 254.10553, found 254.10827.

**3-Allyl-1-methoxy-3,4-dihydroquinazolin-2(1H)-one (7h)**



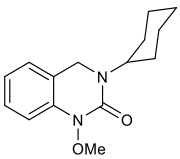
Synthesized according to general procedure using phenyl methoxycarbamate **1a** and *N*-(2-iodobenzyl)prop-2-en-1-amine **5c**. The residue was purified by column chromatography (n-hexane/EtOAc = 10:1 – 6:1) to give **7h** (0.0390 g, 89% yield) as a yellow oil. $^{1}$H NMR (300 MHz, $CDCl_3$) δ 7.32 – 7.24 (m, 1H), 7.12 (m, 1H), 7.07 – 7.02 (m, 1H), 6.98 (m, 1H), 5.86-5.73 (m, 1H), 5.32 – 5.13 (m, 2H), 4.22 (s, 2H), 4.07 (t, *J* = 1.4 Hz, 1H), 4.05 (t, *J* = 1.4 Hz, 1H), 3.92 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 154.0, 139.2, 132.6, 128.4, 125.2, 122.6, 118.2, 117.5, 111.0, 63.3, 50.0, 47.0. IR (ATR): 2933, 1674, 1610, 1464, 1434, 1417, 1386, 1318, 1262, 1205, 1156, 1096, 1045, 1032, 994, 965, 928, 740, 708, 679, 641 cm$^{-1}$. HRMS (EI): Exact mass calculated for: $C_{12}H_{14}N_2O_2$ [M]$^{+}$: 218.10553, found 218.10419.

**3-Cyclopropyl-1-methoxy-3,4-dihydroquinazolin-2(1H)-one (7i)**



Synthesized according to general procedure using phenyl methoxycarbamate **1a** and *N*-(2-iodobenzyl)cyclopropanamine **5e**. The residue was purified by column chromatography (n-hexane/EtOAc = 10:1 – 6:1) to give **7i** (0.0410 g, 94% yield) as a yellow oil. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.27 – 7.22 (m, 1H), 7.13 – 7.07 (m, 1H), 7.08-7.06 (m, 1H), 6.97 (td, *J* = 7.4, 1.2 Hz, 1H), 4.26 (s, 2H), 3.91 (s, 3H), 2.66-2,60 (m, 1H), 0.87 – 0.79 (m, 2H), 0.71 – 0.60 (m, 2H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 155.3, 138.7, 128.4, 125.0, 122.5, 118.3, 110.8, 63.3, 48.7, 29.9, 7.5. IR (ATR): 3011, 2934, 1668, 1605, 1493, 1463, 1417, 1363, 1271, 1198, 1077, 1021, 965, 920, 833, 750, 665 cm$^{-1}$. HRMS (EI): Exact mass calculated for: $C_{12}H_{14}N_2O_2$ [M]$^{+}$: 218.10553, found 218.10117.

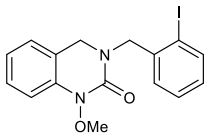
**3-Cyclohexyl-1-methoxy-3,4-dihydroquinazolin-2(1H)-one (7j)**



Synthesized according to general procedure using phenyl methoxycarbamate **1a** and *N*-(2-iodobenzyl)cyclohexanamine **5f**. The residue was purified by column chromatography (n-hexane/EtOAc = 10:1 – 6:1) to give **7j** (0.0440 g, 85% yield) as a yellow oil. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.18 (m, 1H), 7.17 – 7.09 (m, 1H), 7.09 – 7.03 (m, 1H), 6.97 (td, *J* = 7.4, 1.1 Hz, 1H), 4.31-4.23 (m, 1H), 4.15 (s, 2H), 3.91 (s, 3H), 1.84 – 1.76 (m, 2H), 1.72 (d, *J* = 10.5 Hz, 2H), 1.66 (m, 1H), 1.51 – 1.42 (m, 2H), 1.42 – 1.32 (m, 2H), 1.16 – 1.01 (m, 1H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 154.4,

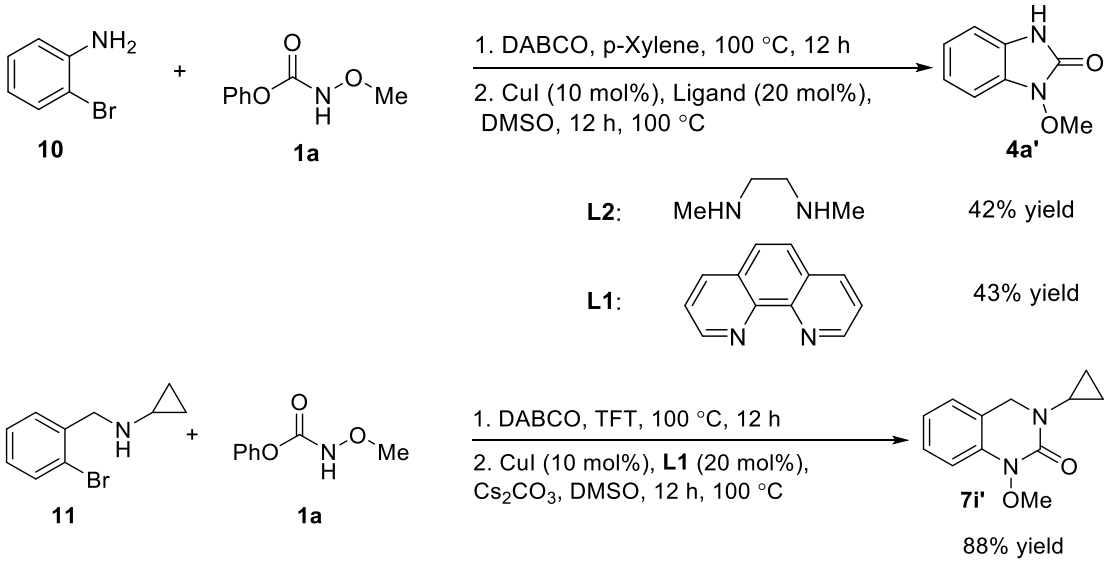
139.6, 128.3, 125.0, 122.4, 118.1, 110.8, 63.3, 53.8, 42.1, 29.9, 25.7, 25.6. IR (ATR): 2928, 2853, 1725, 1673, 1598, 1495, 1463, 1419, 1375, 1321, 1304, 1253, 1208, 1180, 1132, 1093, 1030, 1001, 984, 966, 896, 885, 795, 748, 712, 677, 646 $cm^{-1}$. HRMS (EI): Exact mass calculated for: $C_{15}H_{20}N_2O_2$ $[M]^+$: 260.15248, found 260.15005.

**3-(2-Iodobenzyl)-1-methoxy-3,4-dihydroquinazolin-2(1H)-one (7k)**



Synthesized according to general procedure using phenyl methoxycarbamate **1a** and bis(2-iodobenzyl)amine **5g**. The residue was purified by column chromatography (n-hexane/EtOAc = 10:1 – 6:1) to give **7k** (0.0710 g, 90% yield) as a yellow oil. $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 7.9, 1.1 Hz, 1H), 7.32 – 7.25 (m, 2H), 7.25 – 7.22 (m, 1H), 7.17 (d, *J* = 8.0 Hz, 1H), 7.01 – 6.97 (m, 2H), 6.94 (dd, *J* = 7.4, 1.7 Hz, 1H), 4.73 (s, 2H), 4.25 (s, 2H), 3.97 (s, 3H). $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 154.3, 139.6, 139.0, 138.5, 129.3, 128.7, 128.6, 128.4, 125.3, 122.7, 117.3, 111.1, 98.9, 63.4, 55.7, 47.7. IR (ATR): 2926, 1668, 1609, 1464, 1435, 1354, 1318, 1268, 1208, 1154, 1098, 1032, 1012, 965, 738, 679, 651 $cm^{-1}$. HRMS (EI): Exact mass calculated for: $C_{16}H_{15}IN_2O_2$ $[M]^+$: 394.01782, found 394.01395.

## 6. Procedure for bromo substituted substrates



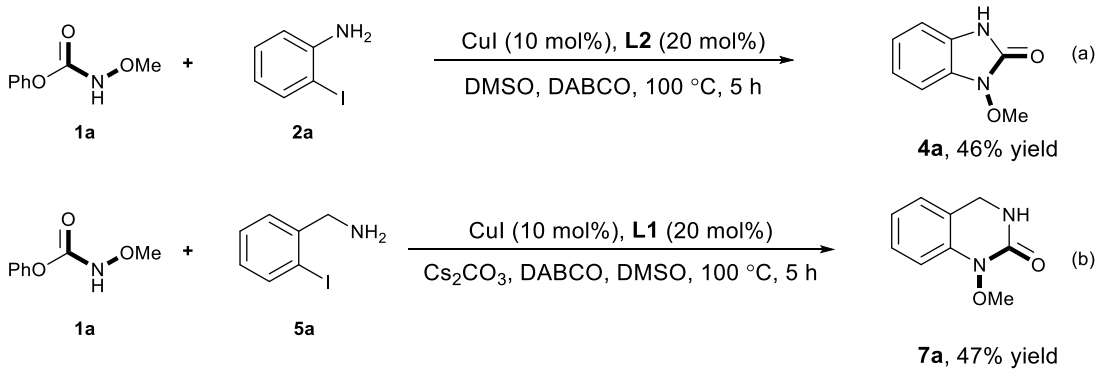

**Procedure for one-pot reaction of phenyl methoxycarbamate 1a and 2-bromoaniline 10**: A mixture of phenyl methoxycarbamate **1a** (0.0334 g, 0.20 mmol,), 2-bromoaniline **10** (0.0516 g, 0.30 mmol), DABCO (0.0450 g, 0.40 mmol) in p-xylene (2.0 mL) was stirred at 100 $^oC$ for 12 h under argon. Then the solvent was removed under reduced pressure. To the residue was added CuI (0.0038 g, 0.02 mmol), N,N'-Dimethyl-1,2-ethanediamine **L2** (0.0035 g, 0.04 mmol) and DMSO (2.0 mL). Then the reaction was stirred at 100 $^oC$ for 12 h under argon. After cooling to room temperature, the reaction mixture was diluted with water (10 mL) and extracted with EtOAc (20 mL x 3). The combined organic layer was dried over $Na_2SO_4$ and

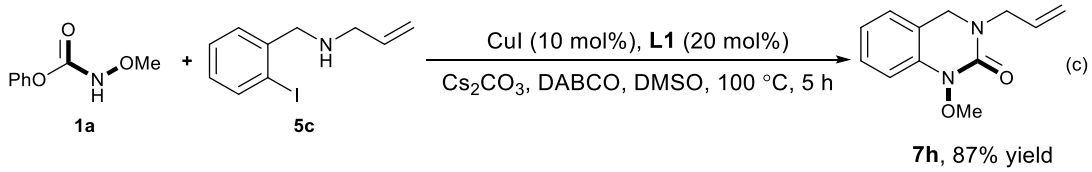
concentrated. The residue was purified by flash chromatography (n-hexane: EtOAc 2:1 - 1:1) on silica gel to afford the title compound **4a**' (0.0138 g, 42%). The spectral data was in excellent agreement with the data listed above.

**Procedure for one-pot reaction of phenyl methoxycarbamate 1a and 2-bromoaniline 10**: A mixture of phenyl methoxycarbamate **1a** (0.0334 g, 0.20 mmol,), 2-bromoaniline **10** (0.0516 g, 0.30 mmol), DABCO (0.0450 g, 0.40 mmol) in p-xylene (2.0 mL) was stirred at 100 $^{o}$C for 12 h under argon. Then the solvent was removed under reduced pressure. To the residue was added CuI (0.0038 g, 0.02 mmol), 1,10-phenanthroline **L1** (0.0072 g, 0.04 mmol) and DMSO (2.0 mL). Then the reaction was stirred at 100 $^{o}$C for 12 h under argon. After cooling to room temperature, the reaction mixture was diluted with water (10 mL) and extracted with EtOAc (20 mL x 3). The combined organic layer was dried over $Na_2SO_4$ and concentrated. The residue was purified by flash chromatography (n-hexane: EtOAc 2:1 - 1:1) on silica gel to afford the title compound **4a**' (0.0141 g, 43%). The spectral data was in excellent agreement with the data listed above.

**Procedure for one-pot reaction of phenyl methoxycarbamate 1a and N-(2-bromobenzyl)cyclopropanamine 11**: A mixture of phenyl methoxycarbamate **1a** (0.0334 g, 0.20 mmol,), N-(2-bromobenzyl)cyclopropanamine **11** (0.0678 g, 0.30 mmol), DABCO (0.0011 g, 0.01 mmol) in $PhCF_3$ (2.0 mL) was stirred at 100 °C for 12 h under argon. Then the solvent was removed under reduced pressure. To the residue was added CuI (0.0038 g, 0.02 mmol), 1,10-phenanthroline **L1** (0.0072 g, 0.04 mmol), $Cs_2CO_3$ (0.130 g, 0.4 mmol) and DMSO (2.0 mL). Then the reaction was stirred at 100 °C for 12 h under argon. After cooling to room temperature, the reaction mixture was diluted with water (10 mL) and extracted with EtOAc (20 mL x 3). The combined organic layer was dried over $Na_2SO_4$ and concentrated. The residue was purified by flash chromatography on silica gel to afford the title compound **7i**' (0.0384 g, 88%). The spectral data was in excellent agreement with the data listed above.

## 7. Cascade Reactions



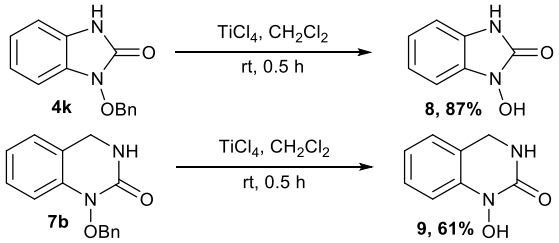



**Procedure for cascade reaction of phenyl methoxycarbamate 1a and 2-iodoaniline 2a**: A mixture of phenyl methoxycarbamate **1a** (0.0334 g, 0.20 mmol,), 2-iodoaniline **2a** (0.0660 g, 0.30 mmol), DABCO (0.0440 g, 0.40 mmol), CuI (0.0038 g, 0.02 mmol), N,N'-Dimethyl-1,2-ethanediamine **L2** (0.0035 g, 0.04 mmol) in DMSO (2.0 mL) was stirred at 100 °C for 5 h under argon. After cooling to room temperature, the reaction mixture was diluted with water (10 mL) and extracted with EtOAc (20 mL x 3). The combined organic layer was dried over $Na_2SO_4$ and concentrated. The residue was purified by flash chromatography (n-hexane/EtOAc = 1:1 – 1:2) on silica gel to afford the title compound **4a** as a white solid (0.0151 g, 46% yield). The spectral data was in excellent agreement with the data listed above.

**Procedure for cascade reaction of phenyl methoxycarbamate 1a and 2-iodobenzylamine 5a**: A mixture of phenyl methoxycarbamate **1a** (0.0334 g, 0.20 mmol,), 2-iodobenzylamine **5a** (0.0700 g, 0.30 mmol), DABCO (0.0011 g, 0.01 mmol), CuI (0.0038 g, 0.02 mmol), 1,10-phenanthroline **L1** (0.0072 g, 0.04 mmol), $Cs_2CO_3$ (0.130 g, 0.40 mmol) in DMSO (2.0 mL) was stirred at 100 °C for 5 h under argon. After cooling to room temperature, the reaction mixture was diluted with water (10 mL) and extracted with EtOAc (20 mL x 3). The combined organic layer was dried over $Na_2SO_4$ and concentrated. The residue was purified by flash chromatography (n-hexane/EtOAc = 2:1 – 1:1) on silica gel to afford the title compound **7a** as a white solid (0.0167 g, 47% yield). The spectral data was in excellent agreement with the data listed above.

**Procedure for cascade reaction of phenyl methoxycarbamate 1a and 2-iodobenzylamine 5a**: A mixture of phenyl methoxycarbamate **1a** (0.0334 g, 0.20 mmol,), *N*-(2-iodobenzyl)prop-2-en-1-amine **5c** (0.0820 g, 0.30 mmol), DABCO (0.0011 g, 0.01 mmol), CuI (0.0038 g, 0.02 mmol), 1,10-phenanthroline **L1** (0.0072 g, 0.04 mmol), $Cs_2CO_3$ (0.130 g, 0.40 mmol) in DMSO (2.0 mL) was stirred at 100 °C for 5 h under argon. After cooling to room temperature, the reaction mixture was diluted with water (10 mL) and extracted with EtOAc (20 mL x 3). The combined organic layer was dried over $Na_2SO_4$ and concentrated. The residue was purified by flash chromatography (n-hexane/EtOAc = 10:1 – 6:1) on silica gel to afford the title compound **7h** as a yellow oil (0.0379 g, 87% yield). The spectral data was in excellent agreement with the data listed above.

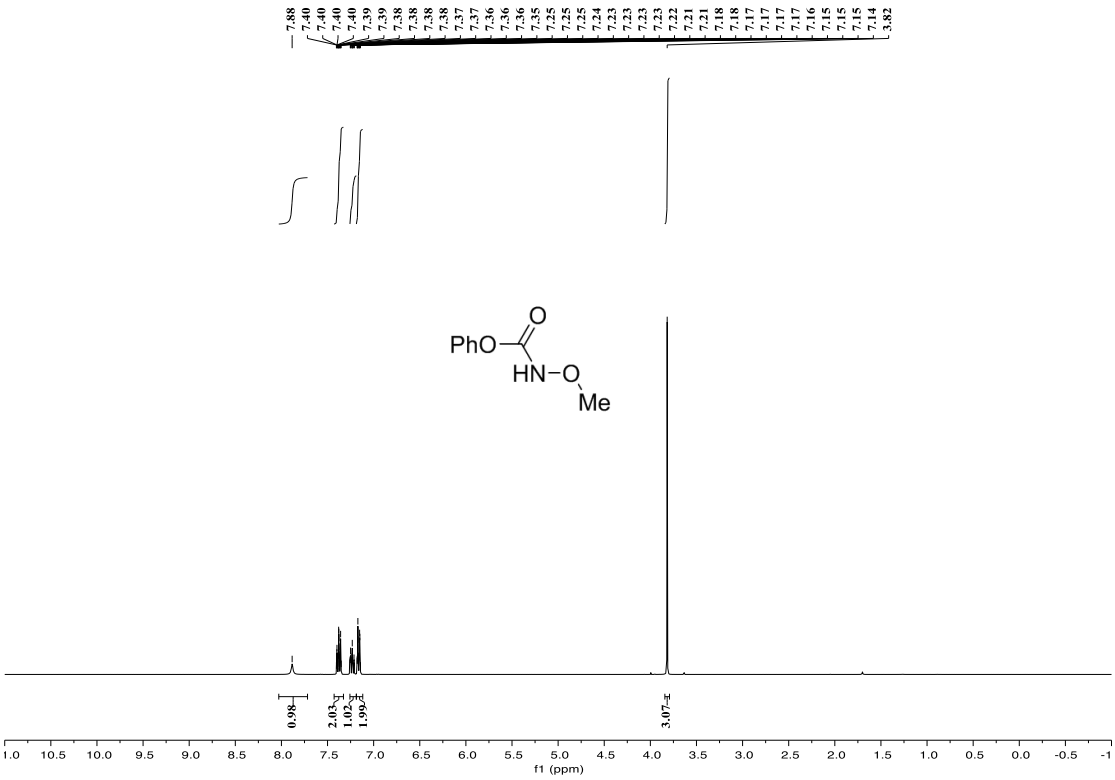
## 8. Removal of benzyl group

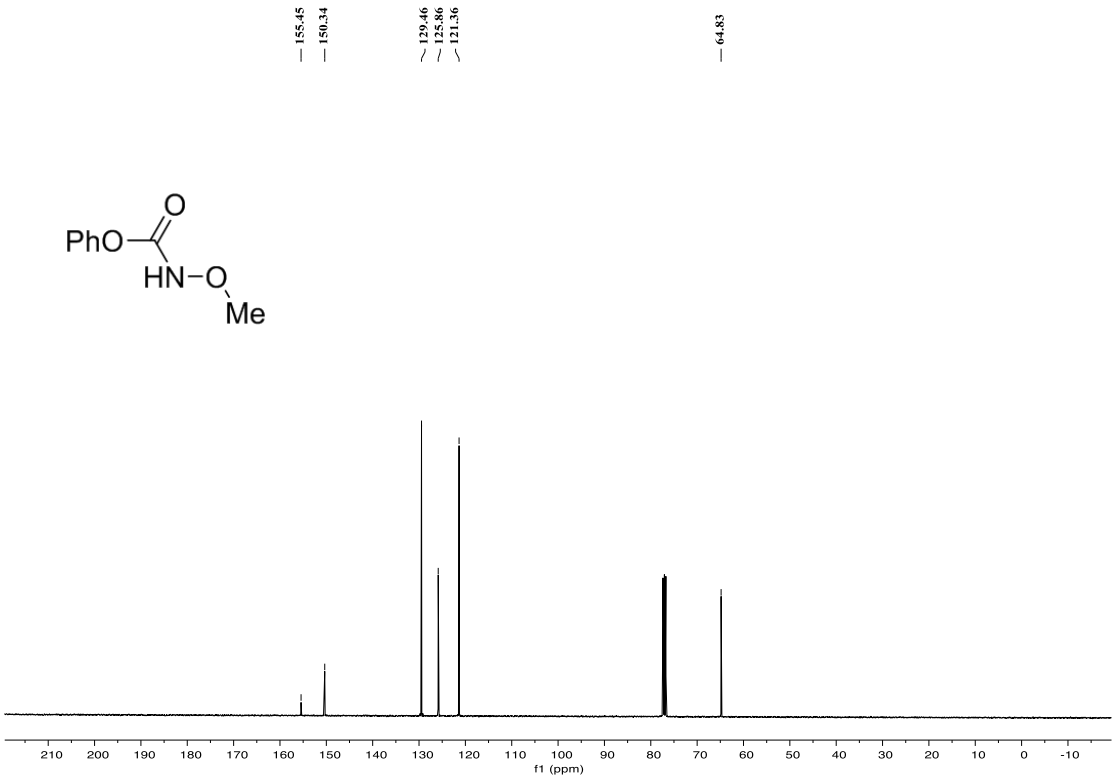


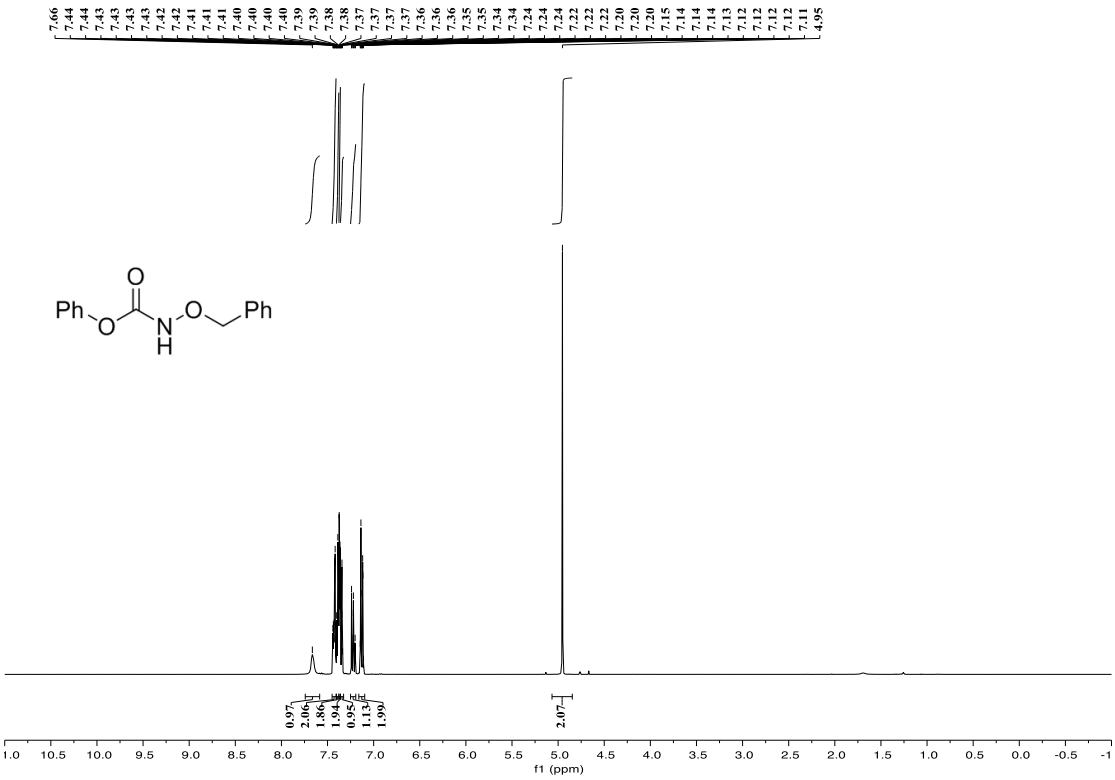

**Procedure for removal of benzyl group of 1-benzyloxybenzimidazolones 4k**: To a solution of 1-benzyloxybenzimidazolones **4k** (0.0270 g, 0.11 mmol) in $CH_2Cl_2$ (2 mL), $TiCl_4$ (0.059 mL, 0.55 mmol) was added slowly and the resulting red solution was stirred at room temperature for 0.5 h under argon. Then the reaction mixture was diluted with ethyl acetate (10 mL) and quenched with 2 N HCl (5 mL). Aqueous phase was separated and extracted with ethyl acetate. The combined organic layer was dried over $Na_2SO_4$ and concentrated. The residue was purified by flash chromatography ($CH_2Cl_2$/MeOH = 10:0 – 10:1) on silica gel to afford the title compound **8** as a white solid (0.0144 g, 87% yield). $^1$H NMR (300 MHz, $CD_3OD$) δ 7.22 – 6.94 (m, 4H). $^{13}$C NMR (76 MHz, $CD_3OD$) δ 152.8, 129.2, 124.3, 121.27, 121.30, 109.3, 106.4. IR (ATR): 3131, 2902, 2289, 2162, 1662, 1525, 1475, 1295, 1214, 1186, 1085, 996, 912, 888, 842, 732, 682, 640, 567 cm$^{-1}$. HRMS (EI): Exact mass calculated for: $C_7H_6N_2O_2$ $[M]^+$: 150.04293, found 150.04113.

**Procedure for removal of benzyl group of 1-benzyloxy-3,4-dihydroquinazolin-2(1H)-ones 7b**: To a solution of 1-benzyloxy-3,4-dihydroquinazolin-2(1H)-ones **7b** (0.0430 g, 0.17 mmol) in $CH_2Cl_2$ (4 mL), $TiCl_4$ (0.091 mL, 0.85 mmol) was added slowly and the resulting red solution was stirred at room temperature for 0.5 h under argon. Then the reaction mixture was diluted with ethyl acetate (10 mL) and quenched with 2 N HCl (5 mL). Aqueous phase was separated and extracted with ethyl acetate. The combined organic layer was dried over $Na_2SO_4$ and concentrated. The residue was purified by flash chromatography ($CH_2Cl_2$/MeOH = 10:0 – 15:1) on silica gel to afford the title compound **9** as a white solid (0.0169 g, 61% yield). $^1$H NMR (300 MHz, $CD_3OD$) δ 7.32 – 7.20 (m, 2H), 7.11 (dd, J = 7.1, 1.1 Hz, 1H), 7.00 (ddd, J = 7.4, 6.3, 2.2 Hz, 1H), 4.31 (s, 2H). $^{13}$C NMR (76 MHz, $CD_3OD$) δ 157.2, 140.7, 127.7, 124.7, 122.3, 118.7, 111.0, 41.7. IR (ATR): 3078, 2919, 2366, 2162, 1652, 1609, 1514, 1474, 1319, 1287, 1201, 1180, 1063, 982, 919, 843, 735, 699, 623, 549 cm$^{-1}$. HRMS (EI): Exact mass calculated for: $C_8H_8N_2O_2$ $[M]^+$: 164.05858, found 164.05940.

# 9. Copies of $^{1}$H NMR and $^{13}$C NMR Spectra

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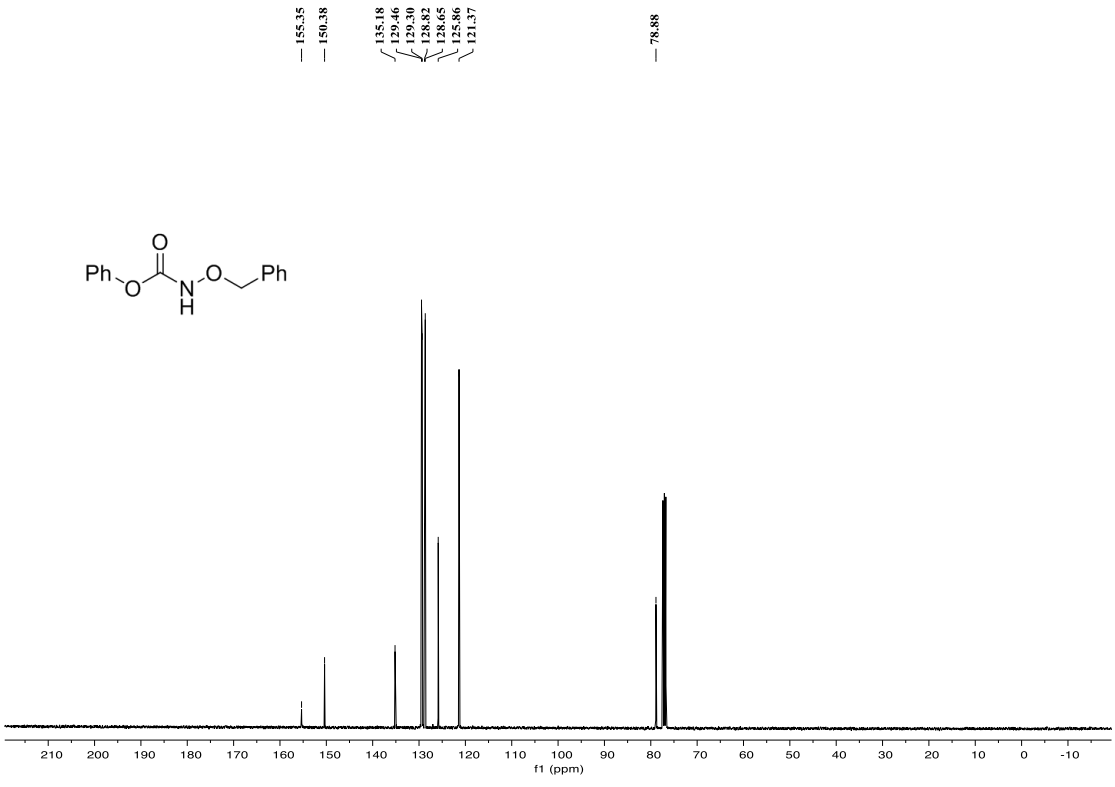
Ph O O N H O Ph
0.97 2.06 1.86 1.94 0.95 1.13 1.99 2.07
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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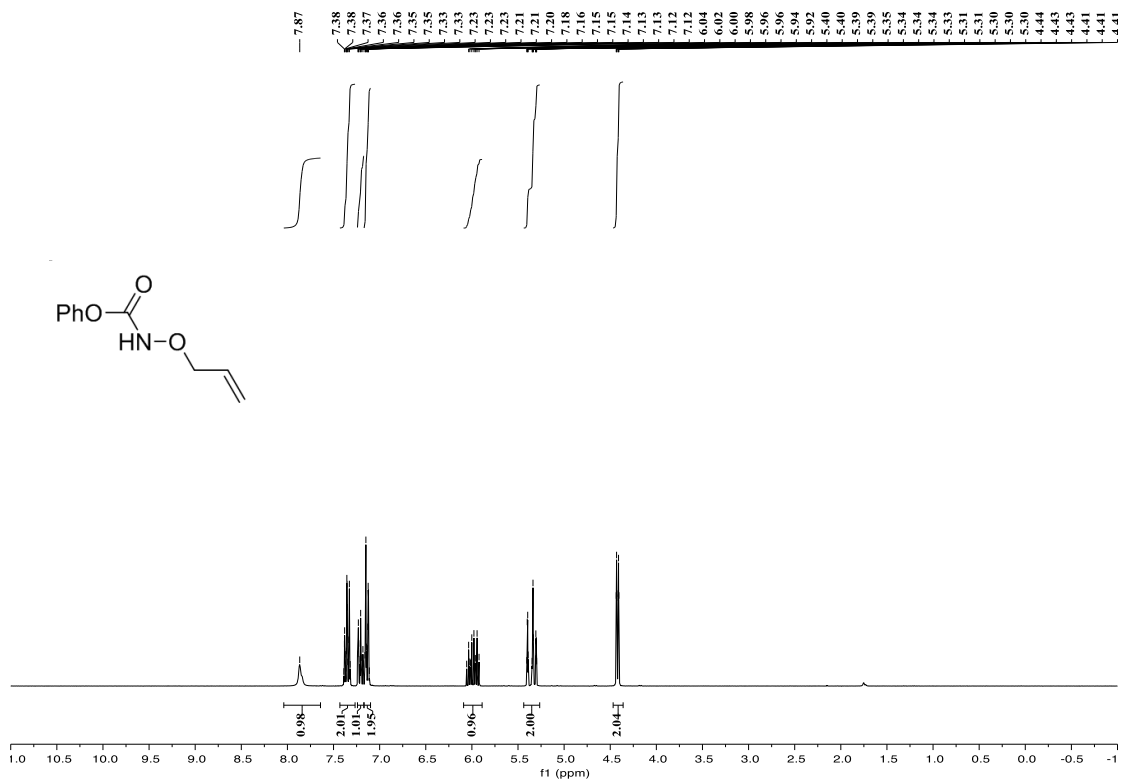
f1 (ppm)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6.02
6.00
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4.41
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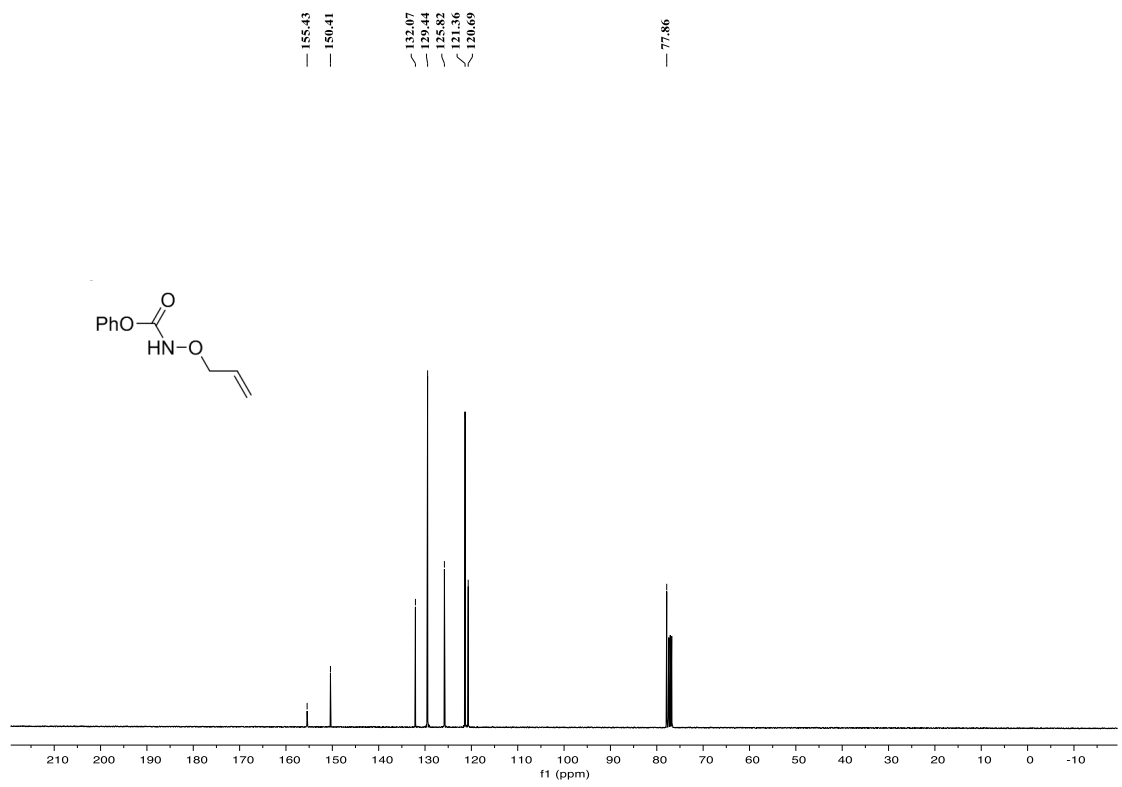
f1 (ppm)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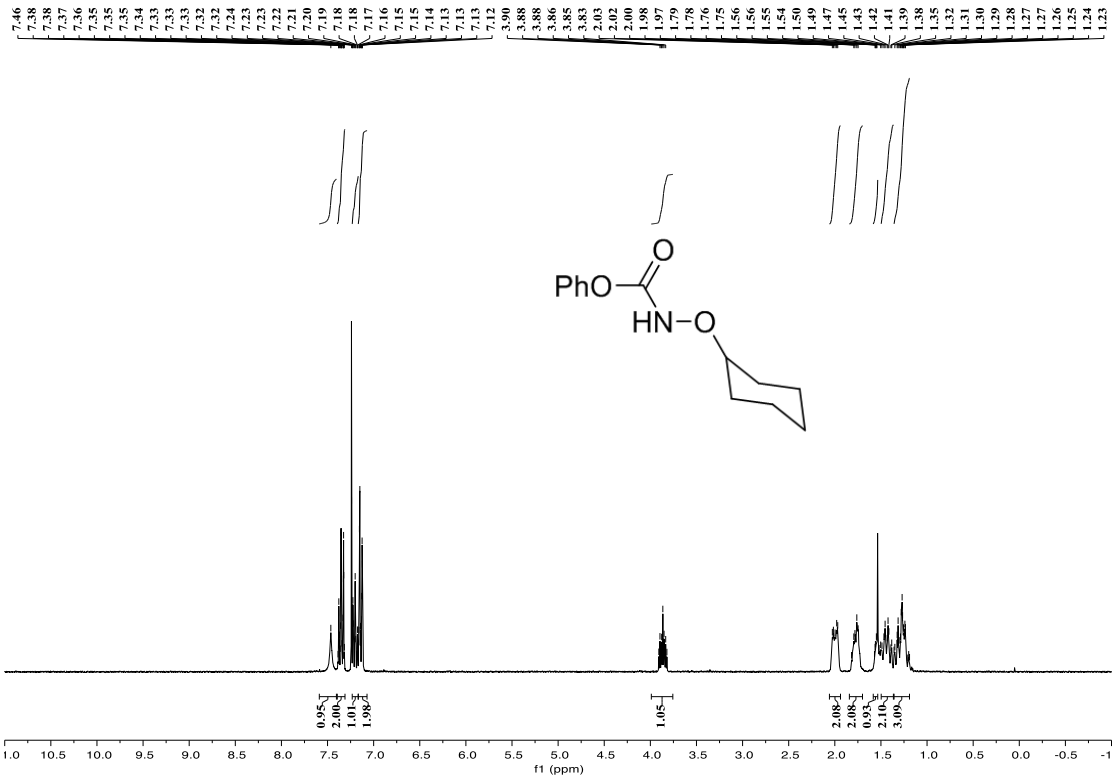
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3.90 3.88 3.88 3.86 3.85 3.83 2.03 2.02 2.00 1.98 1.97 1.79 1.78 1.76 1.75 1.56 1.56 1.55 1.54 1.50 1.49 1.47 1.45 1.43 1.42 1.41 1.39 1.38 1.35 1.32 1.31 1.30 1.29 1.28 1.27 1.27 1.26 1.25 1.24 1.23
PhO
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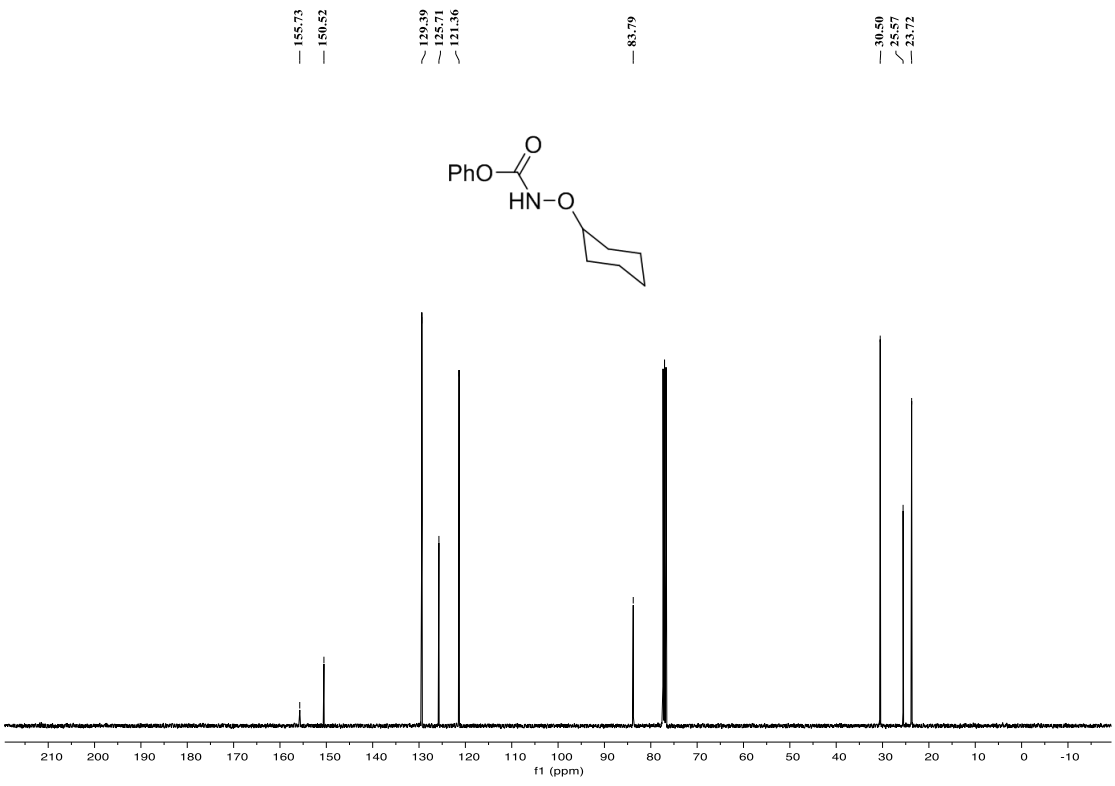
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HN−O
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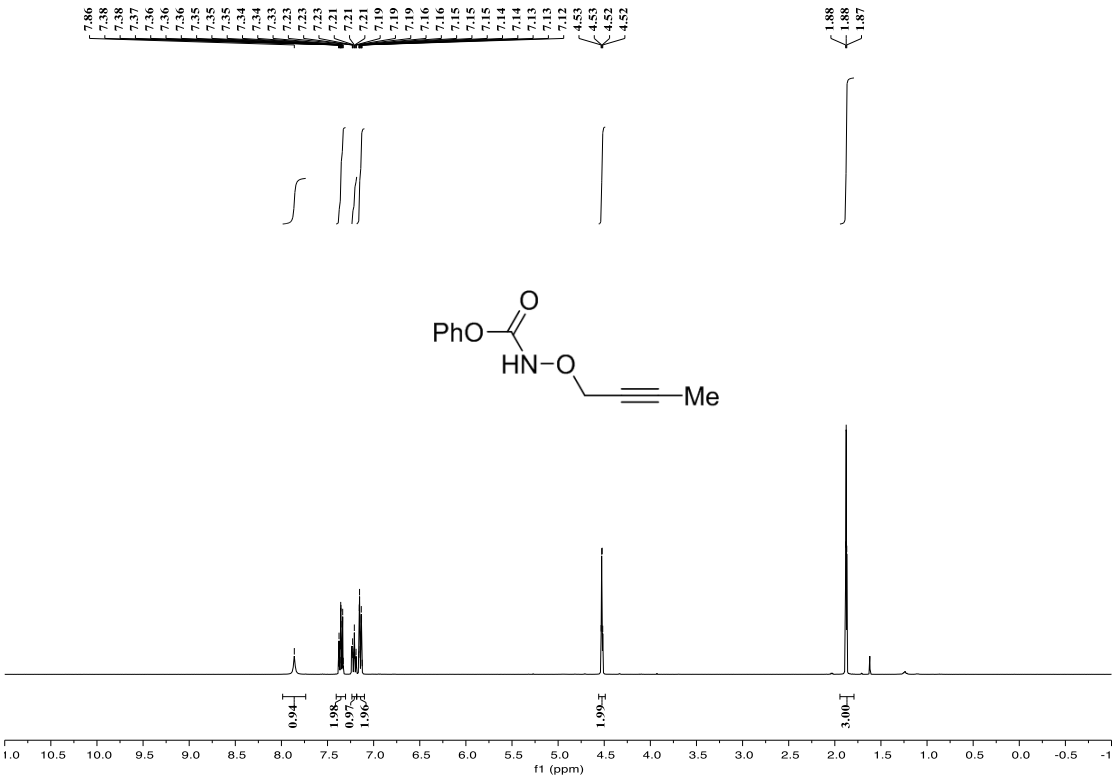
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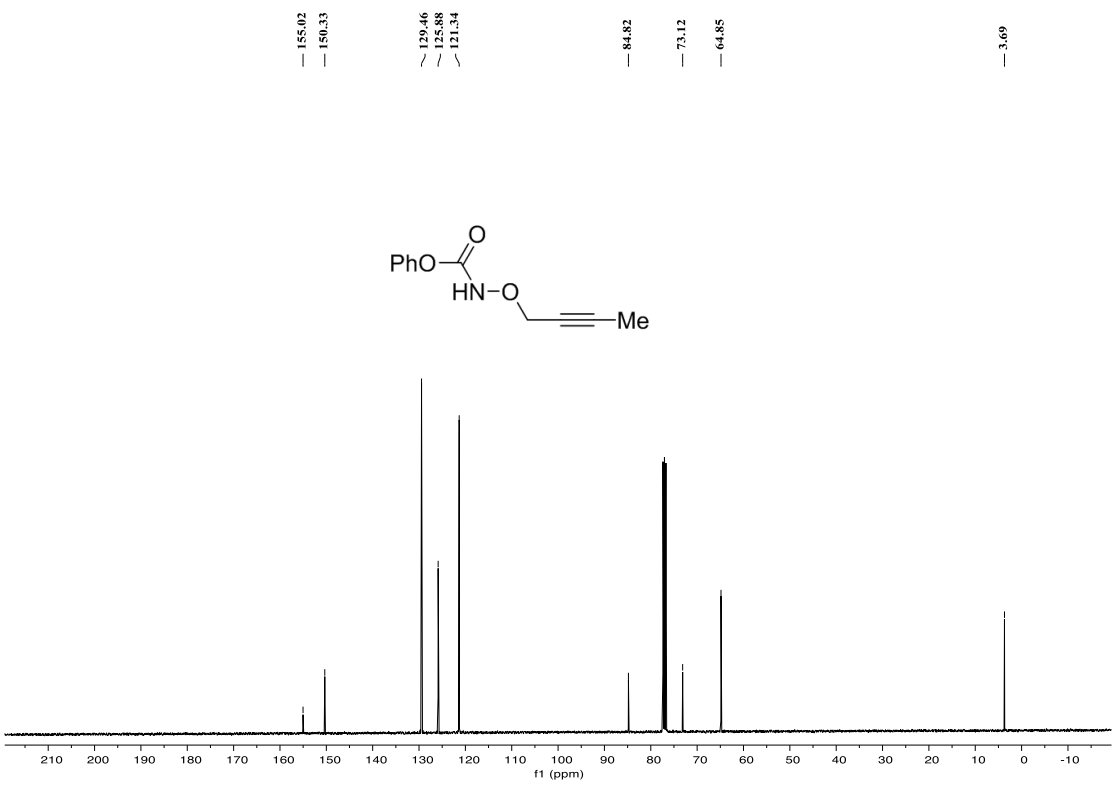
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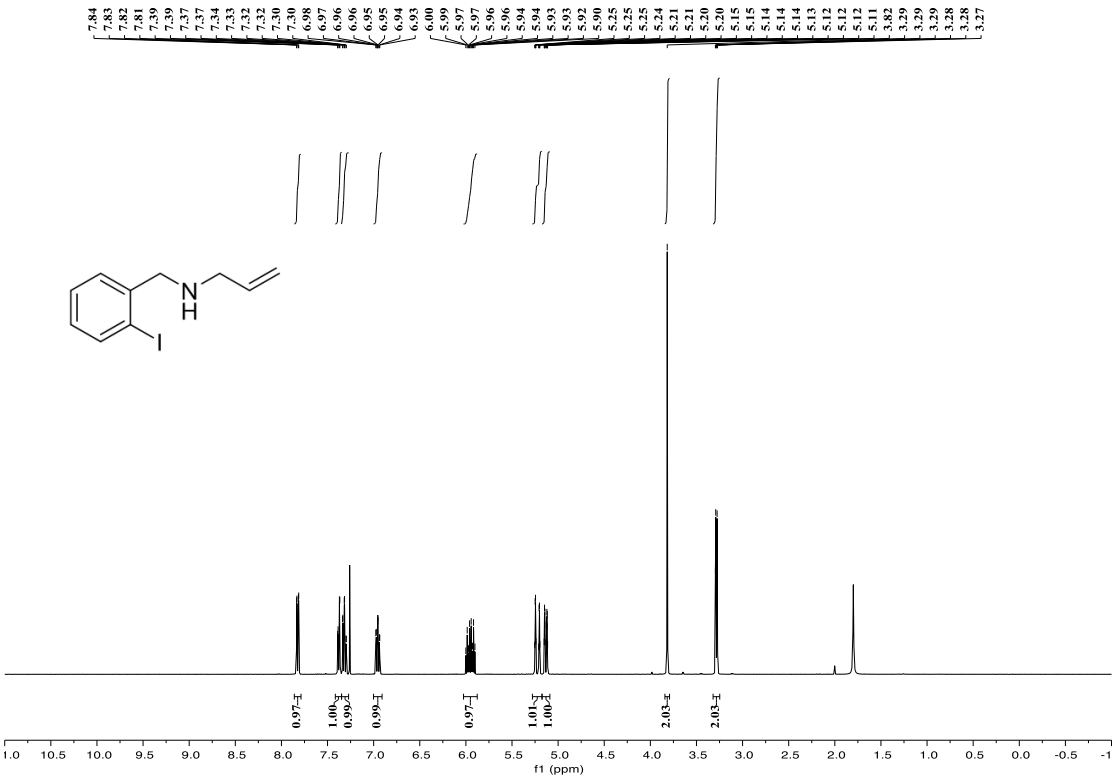
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H
I
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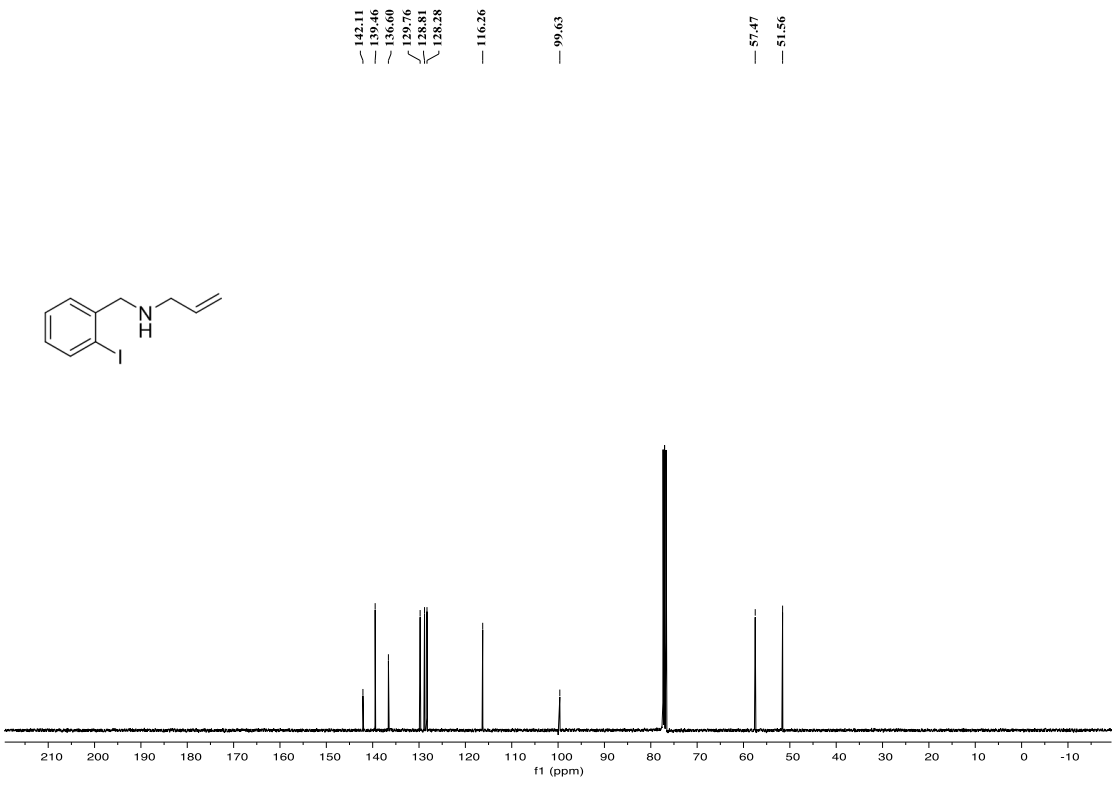
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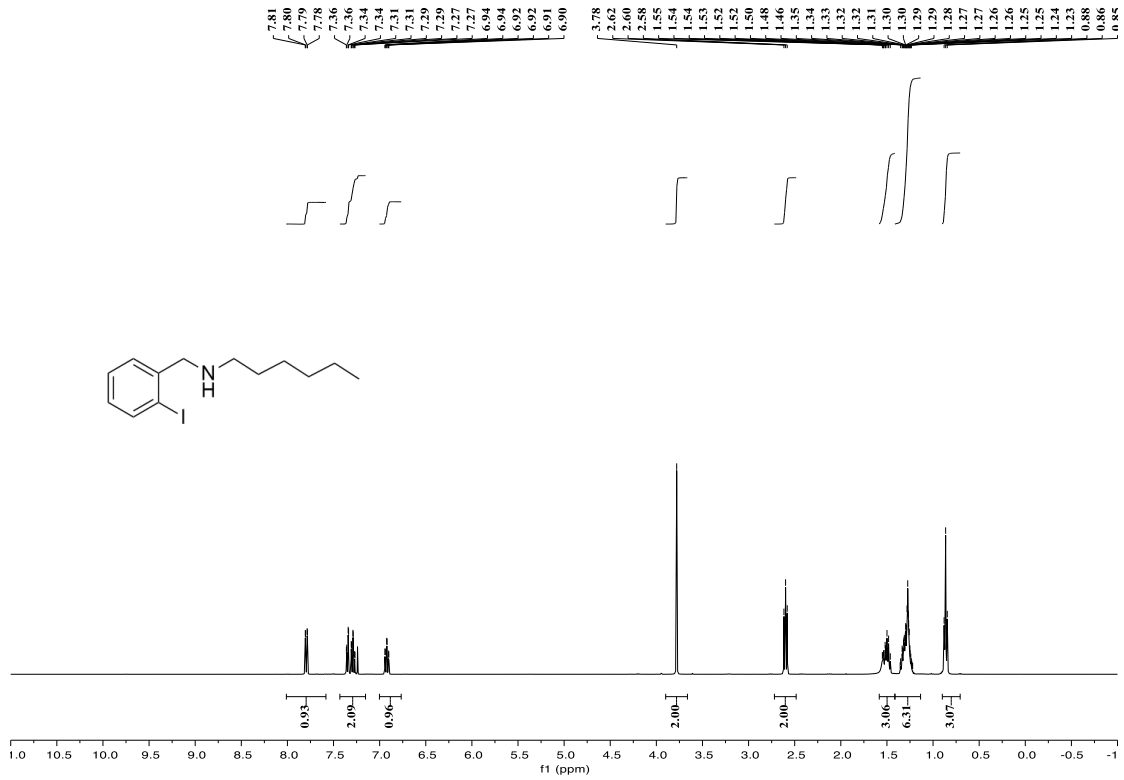
N
H
I
f1 (ppm)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H
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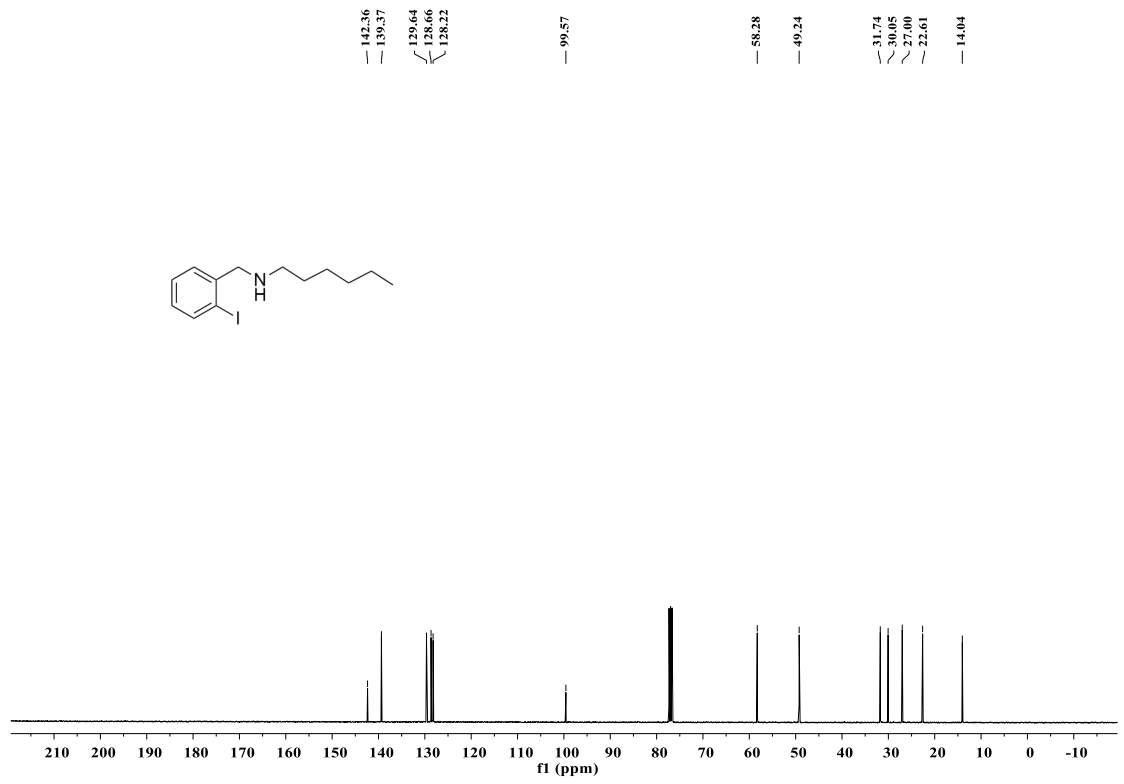
0.96
2.00
2.00
3.06
6.31
3.07
f1 (ppm)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139.37
129.64
128.66
128.22
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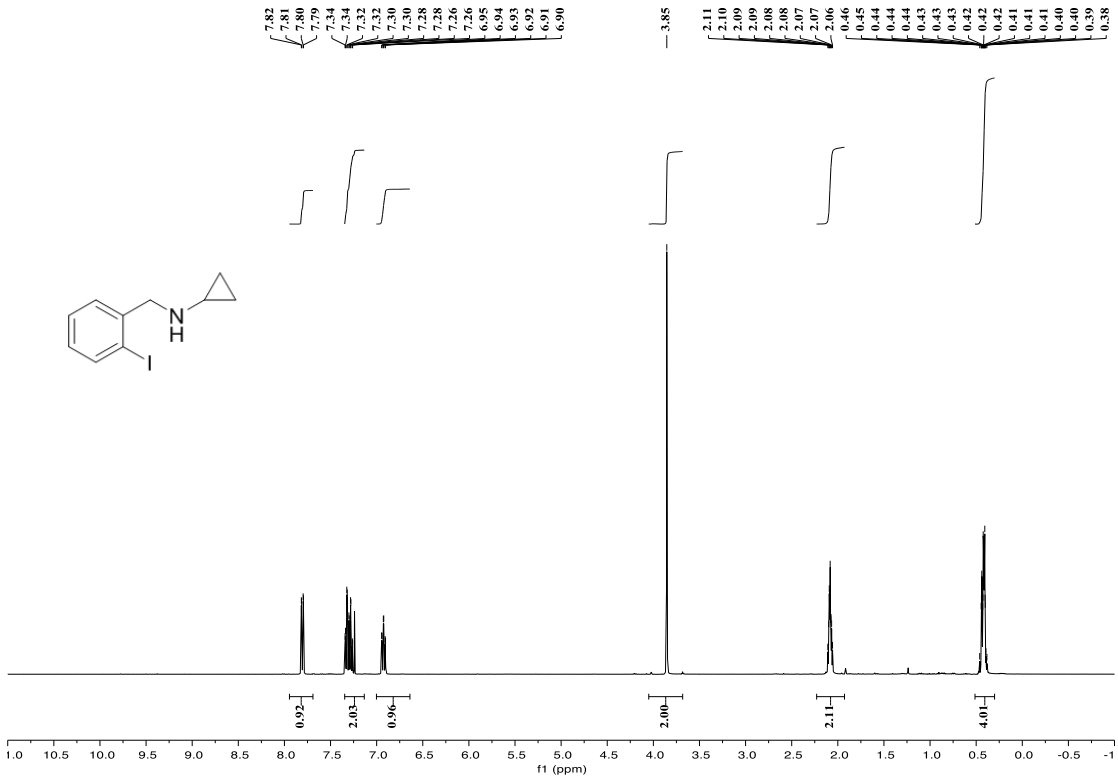
58.28
49.24
31.74
30.05
27.00
22.61
14.04
N
H
I
f1 (ppm)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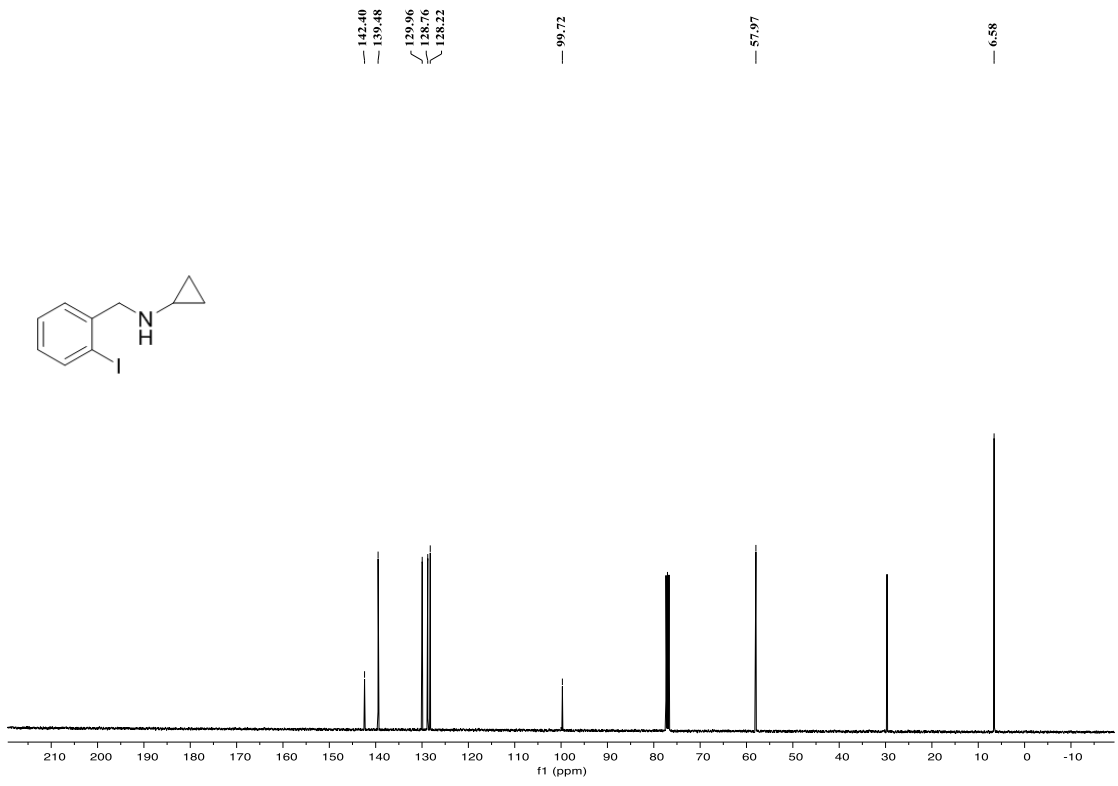
7.81
7.80
7.79
7.34
7.34
7.32
7.32
7.30
7.30
7.28
7.28
7.26
6.95
6.94
6.93
6.92
6.91
6.90
3.85
2.11
2.10
2.09
2.09
2.08
2.08
2.07
2.07
2.06
0.46
0.45
0.44
0.44
0.44
0.43
0.43
0.43
0.42
0.42
0.42
0.41
0.41
0.41
0.40
0.40
0.39
0.38
N
H
I
0.92
2.03
0.96
2.00
2.11
4.01
f1 (ppm)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139.48
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128.22
99.72
57.97
6.58
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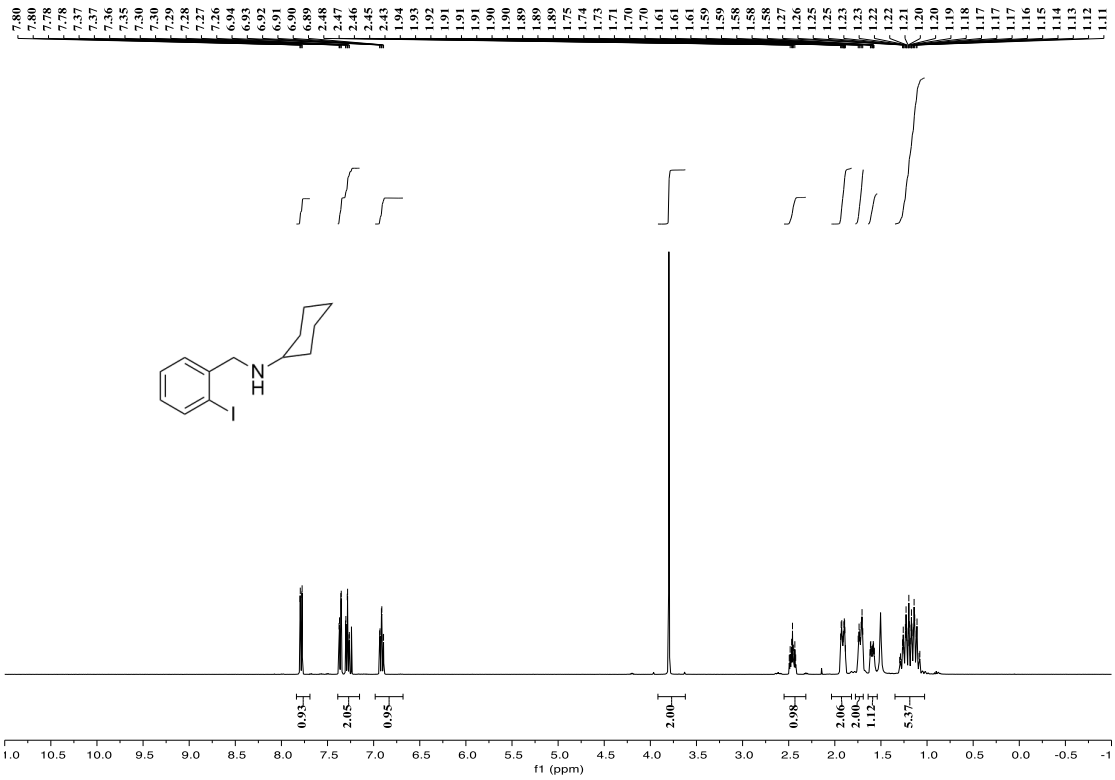
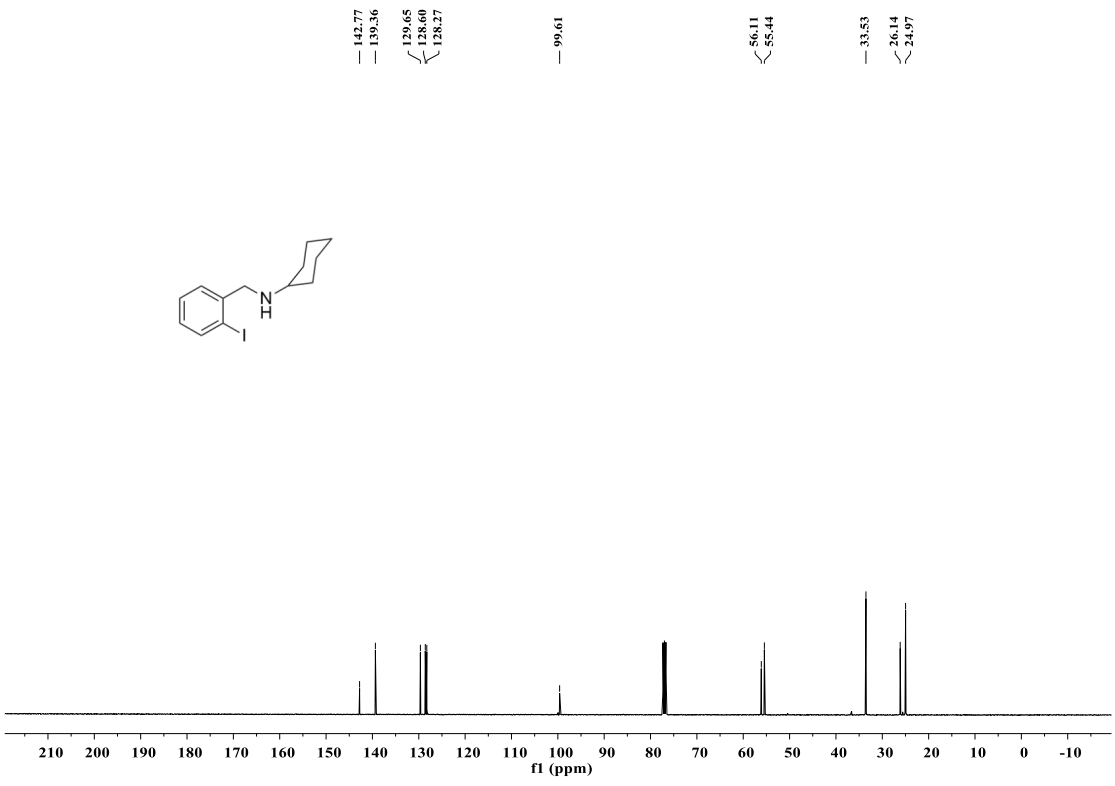
H
I
f1 (ppm)


7.80 7.80 7.78 7.78 7.37 7.37 7.36 7.35 7.30 7.30 7.29 7.28 7.27 7.26 6.94 6.93 6.92 6.91 6.90 6.89 2.48 2.47 2.46 2.45 2.43 1.94 1.93 1.92 1.91 1.91 1.91 1.90 1.90 1.89 1.89 1.89 1.75 1.74 1.73 1.71 1.70 1.70 1.61 1.61 1.61 1.59 1.59 1.58 1.58 1.58 1.27 1.26 1.25 1.25 1.23 1.23 1.22 1.22 1.21 1.20 1.20 1.19 1.18 1.17 1.17 1.17 1.16 1.15 1.14 1.13 1.12 1.11
N
H
I
0.93 2.05 0.95 2.00 0.98 2.06 2.00 1.12 5.37
f1 (ppm)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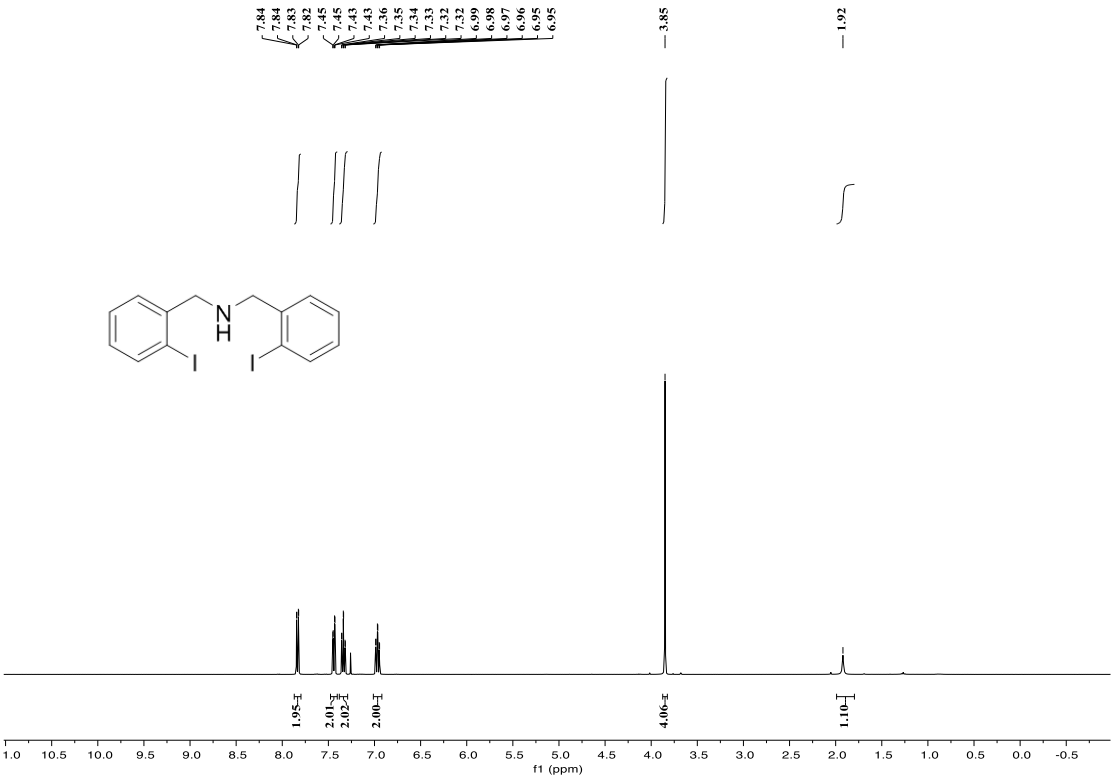
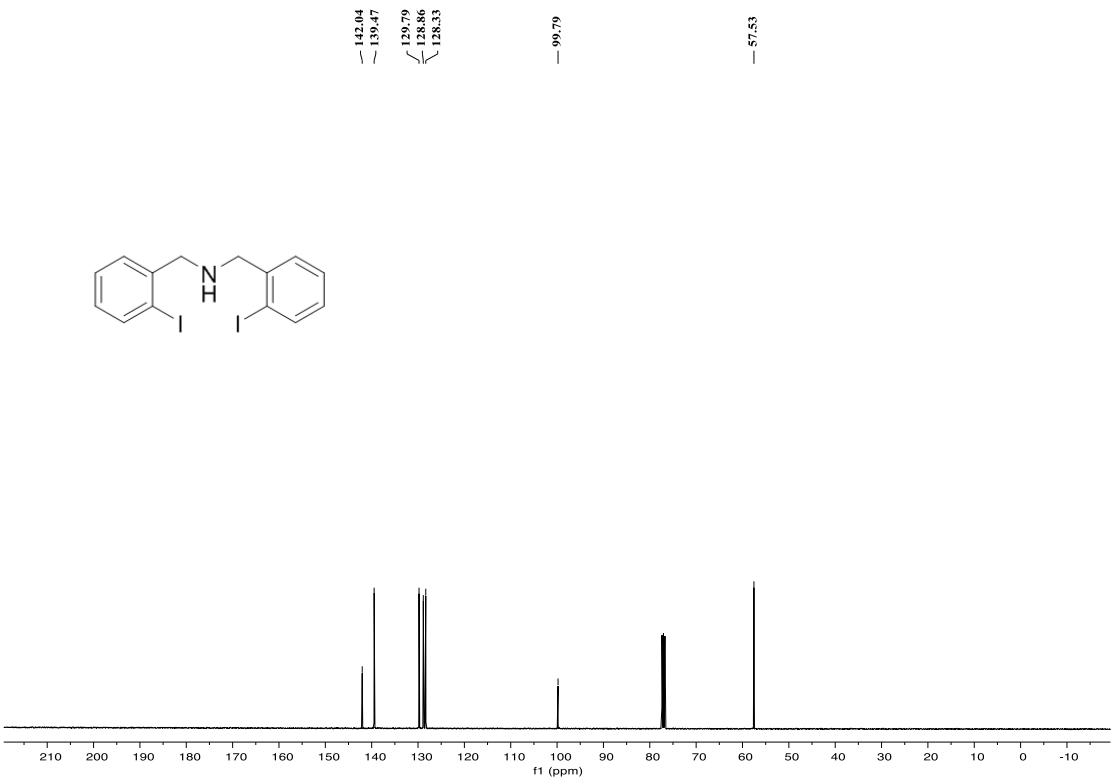
56.11
55.44
33.53
26.14
24.97
N
H
I
f1 (ppm)


7.84
7.84
7.83
7.82
7.45
7.45
7.43
7.43
7.36
7.35
7.34
7.33
7.32
7.32
6.99
6.98
6.97
6.96
6.95
6.95
3.85
1.92
N
H
I
I
1.95
2.01
2.02
2.00
4.06
1.10
f1 (ppm)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129.79
128.86
128.33
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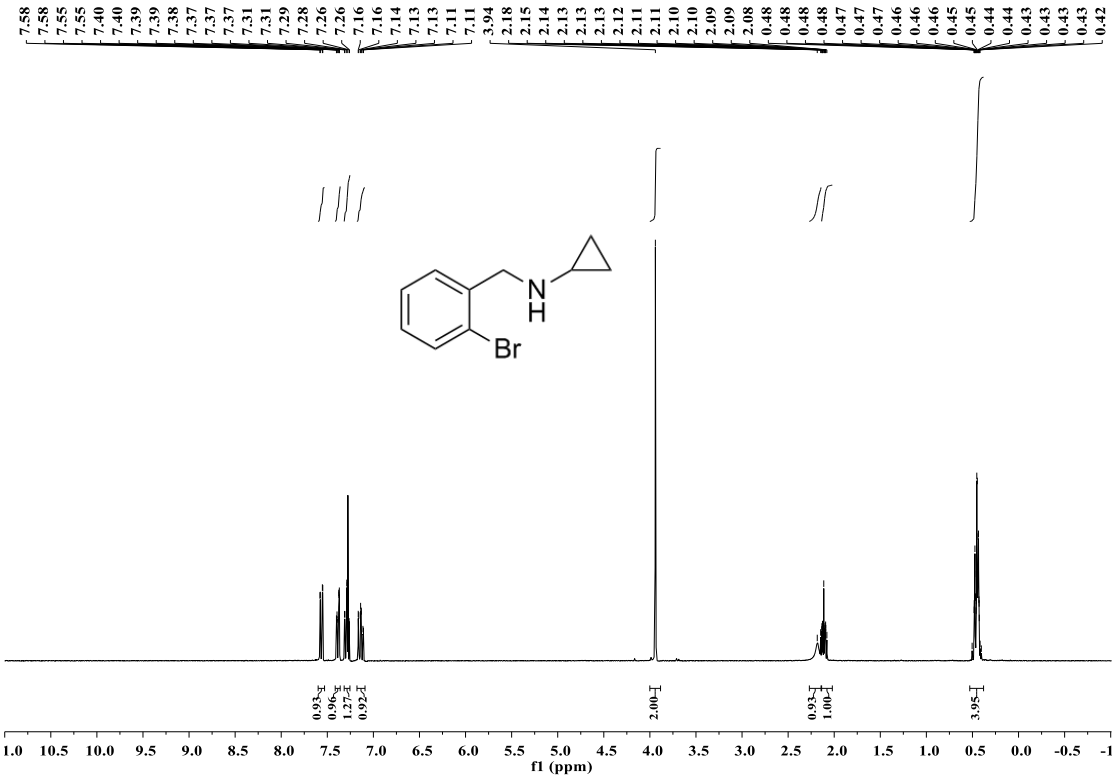
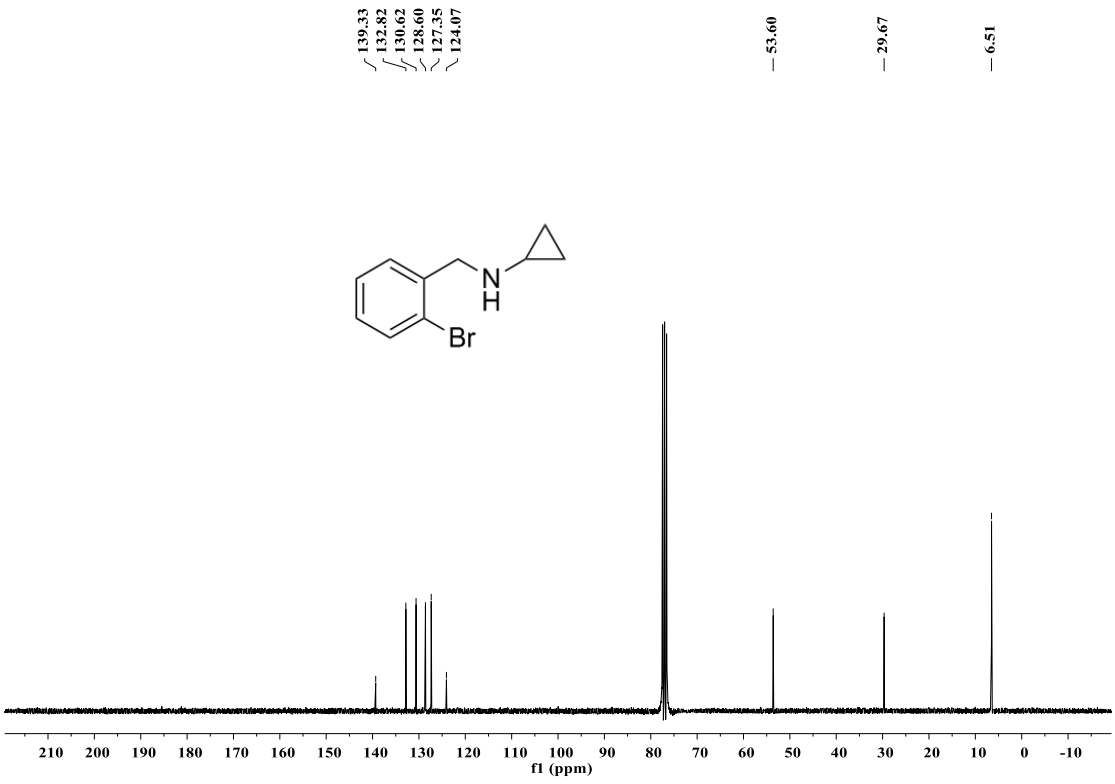
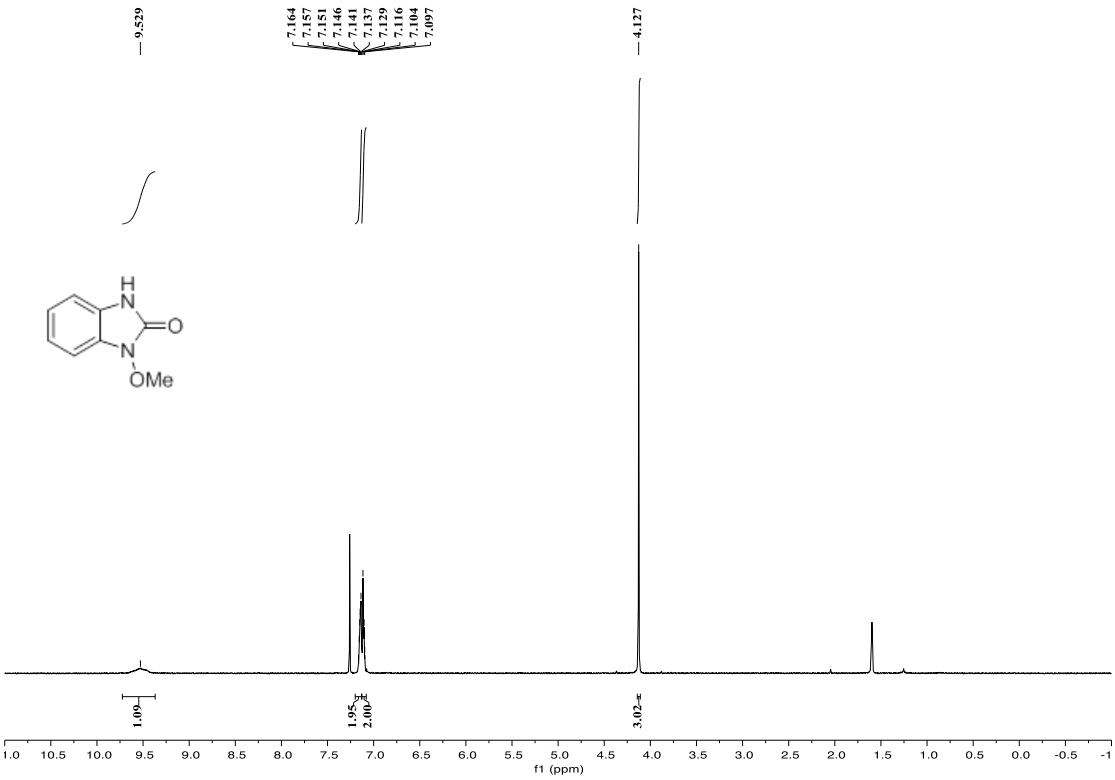
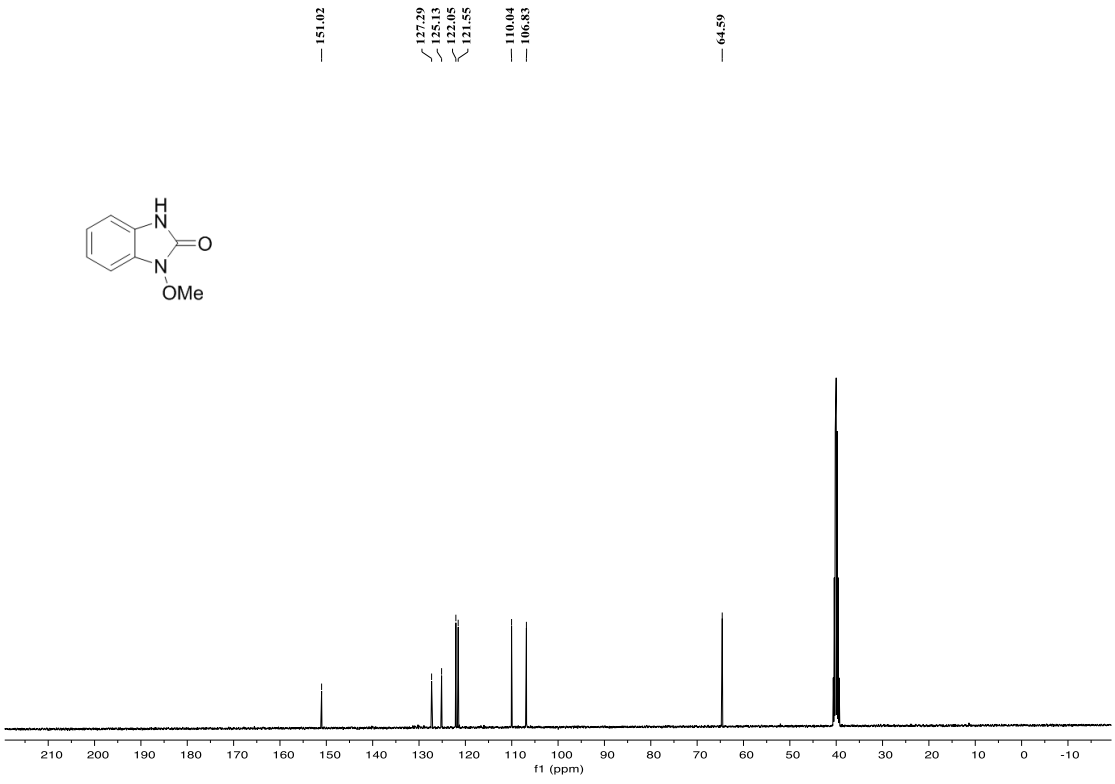
57.53
N
H
I
I
f1 (ppm)


7.58 7.58 7.55 7.55 7.40 7.40 7.39 7.39 7.38 7.37 7.37 7.37 7.31 7.31 7.29 7.28 7.26 7.26 7.16 7.16 7.14 7.13 7.13 7.11 7.11
3.94 2.18 2.15 2.14 2.13 2.13 2.13 2.12 2.11 2.11 2.10 2.10 2.09 2.09 2.08 0.48 0.48 0.48 0.47 0.47 0.46 0.46 0.46 0.45 0.45 0.44 0.44 0.43 0.43 0.43 0.42
N
H
Br
0.93 0.96 1.27 0.92 2.00 0.93 1.00 3.95
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


139.33 132.82 130.62 128.60 127.35 124.07
53.60 29.67 6.51
N
H
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


9.529
7.164
7.157
7.151
7.146
7.141
7.137
7.129
7.116
7.104
7.097
4.127
H
N
O
N
OMe
1.09
1.95
2.00
3.02
f1 (ppm)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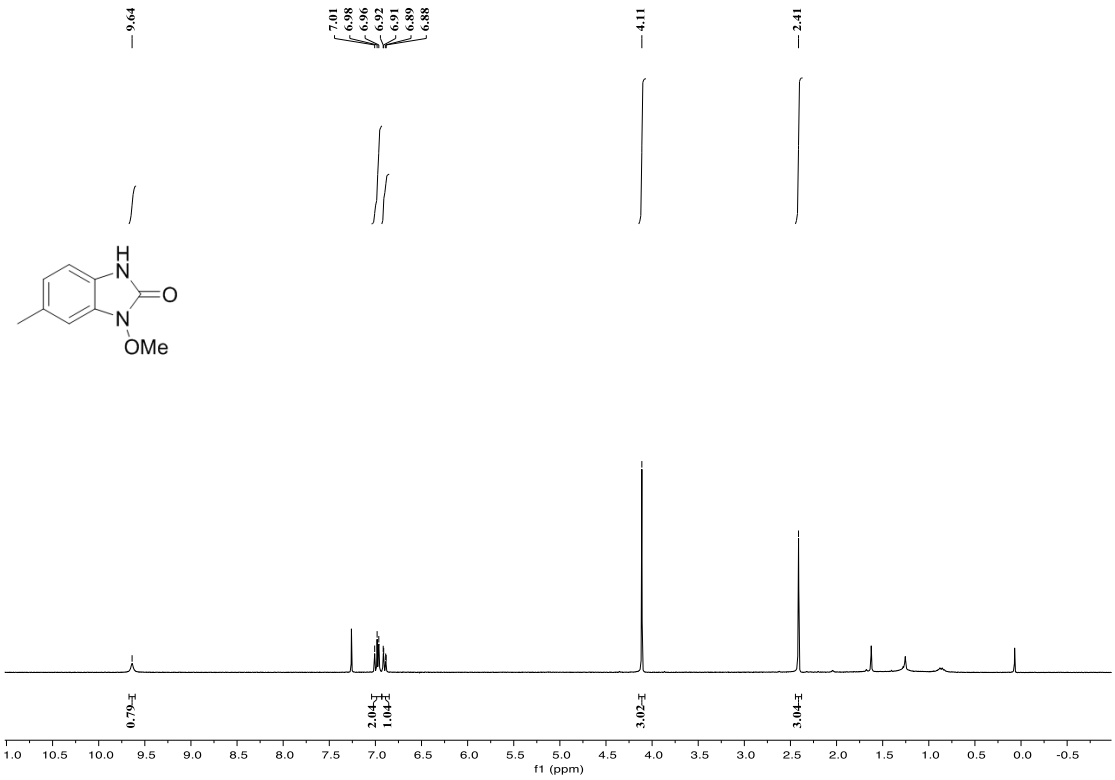
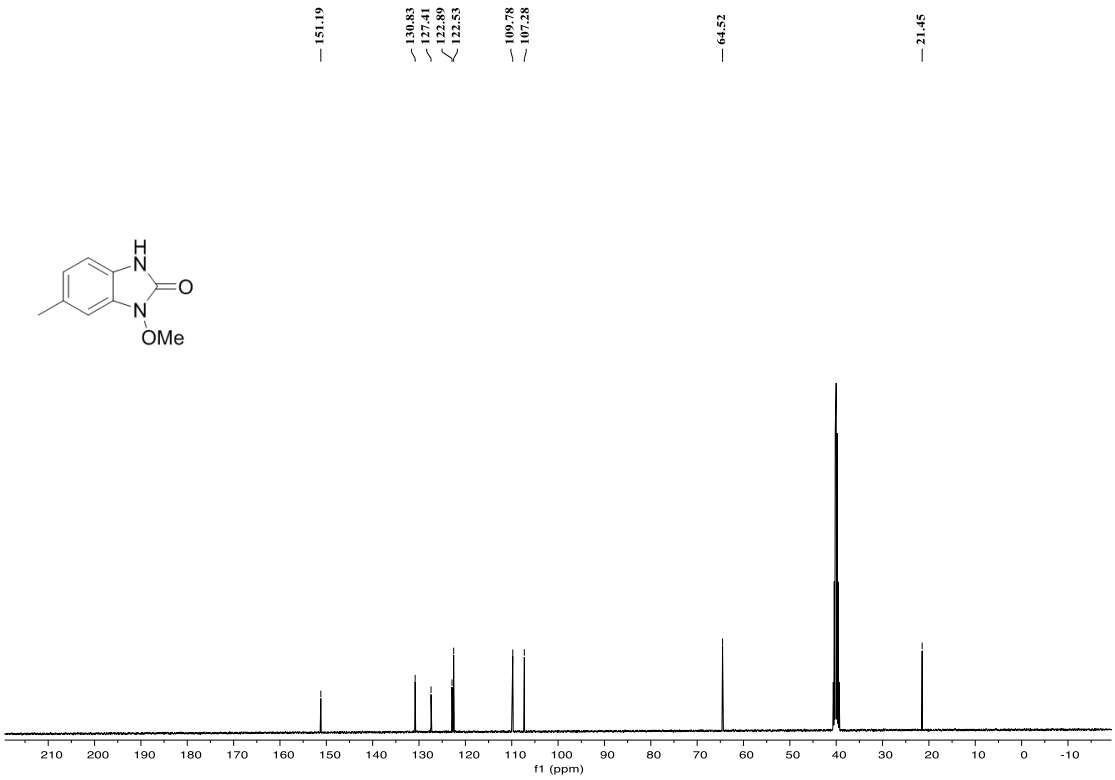
127.29
125.13
122.05
121.55
110.04
106.83
64.59
H
N
O
N
OMe
f1 (ppm)


9.64
7.01
6.98
6.96
6.92
6.91
6.89
6.88
4.11
2.41
H
N
O
N
OMe
0.79
2.04
1.04
3.02
3.04
f1 (ppm)


151.19
130.83
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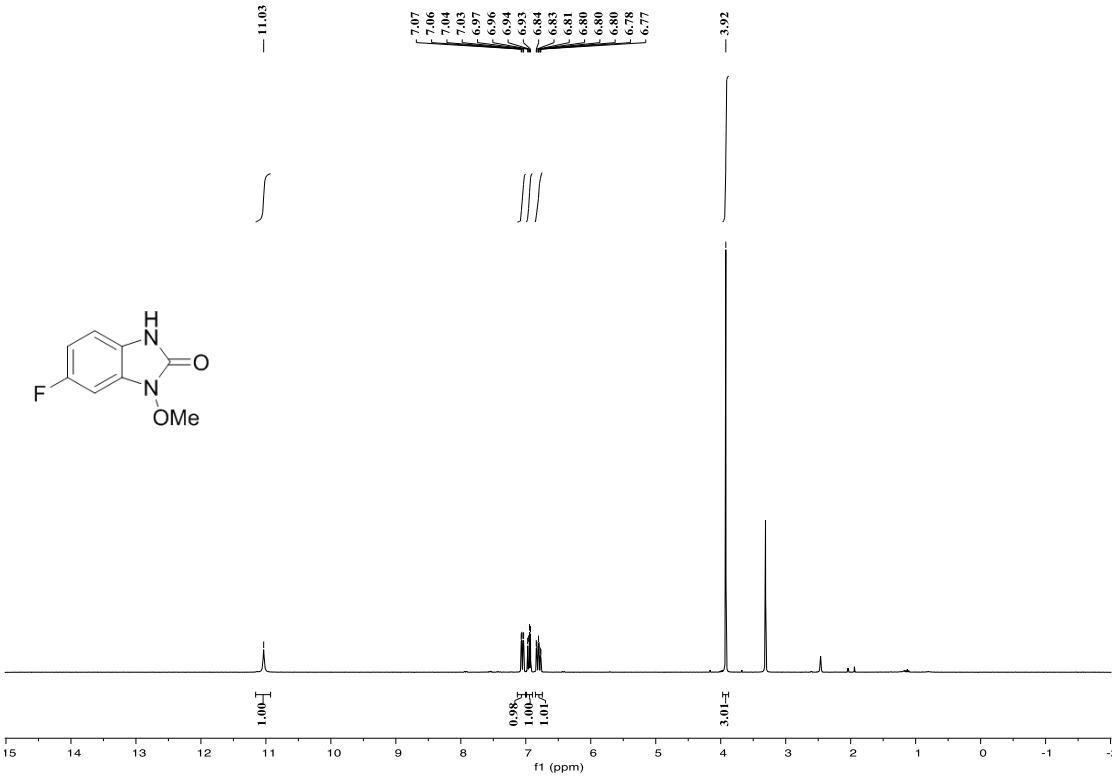
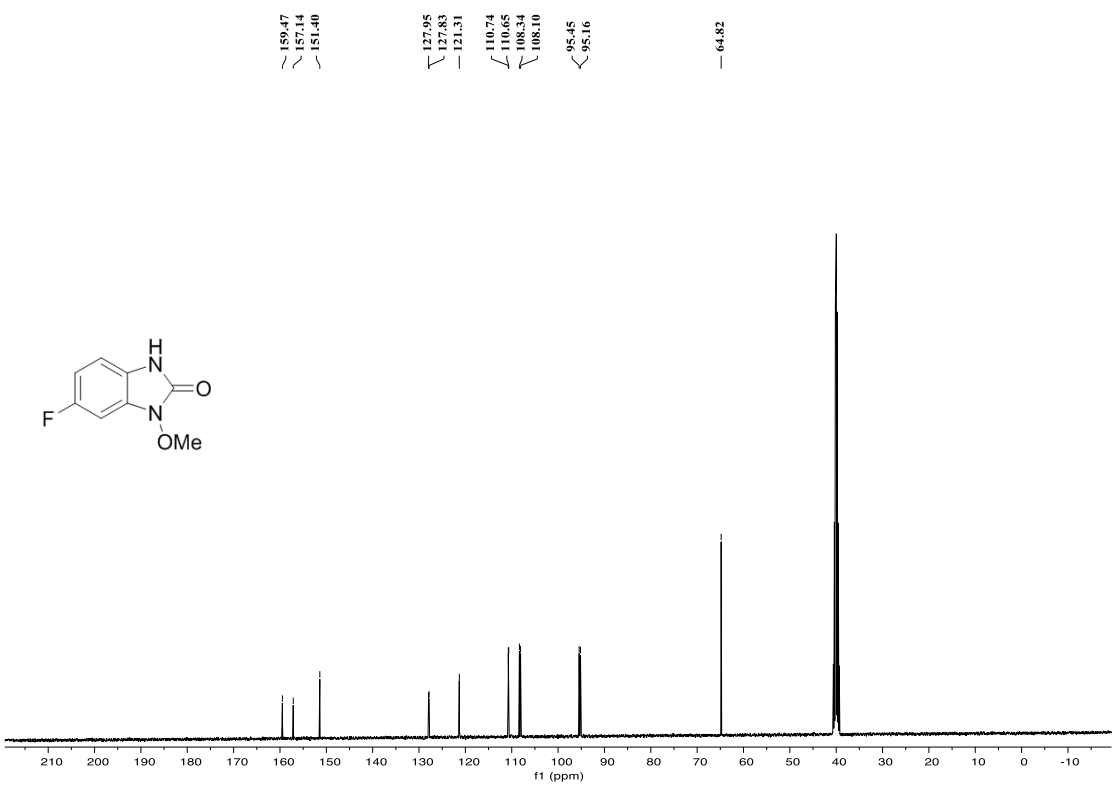
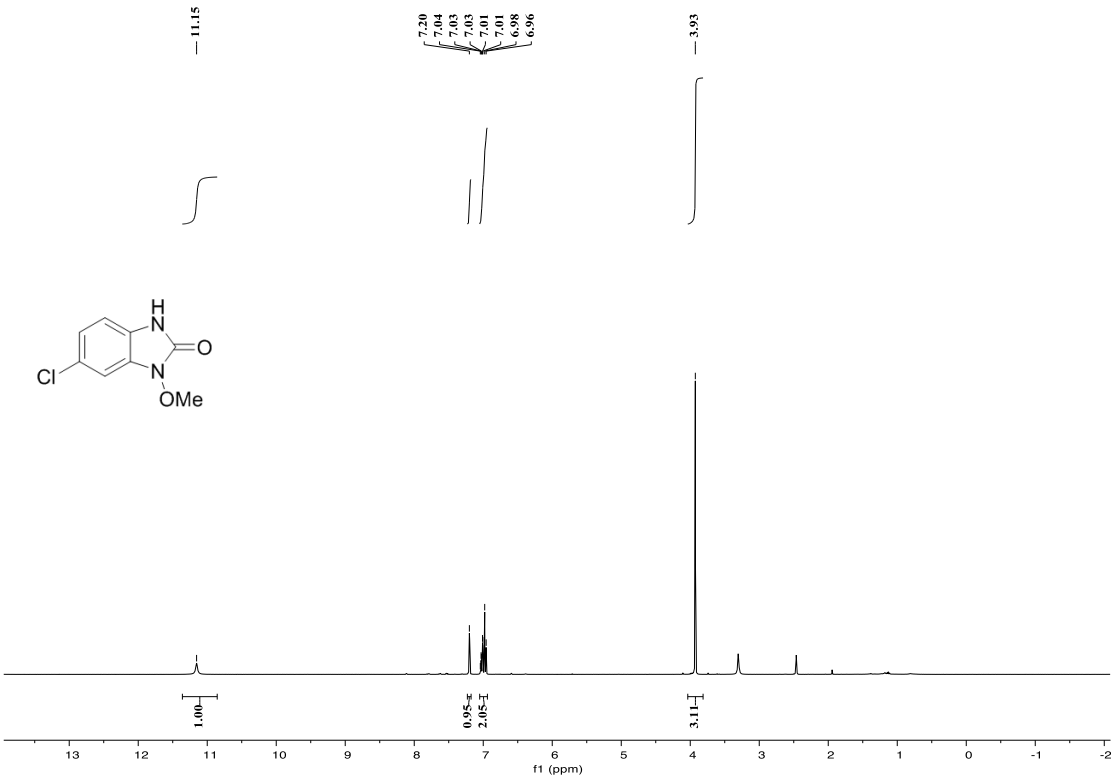
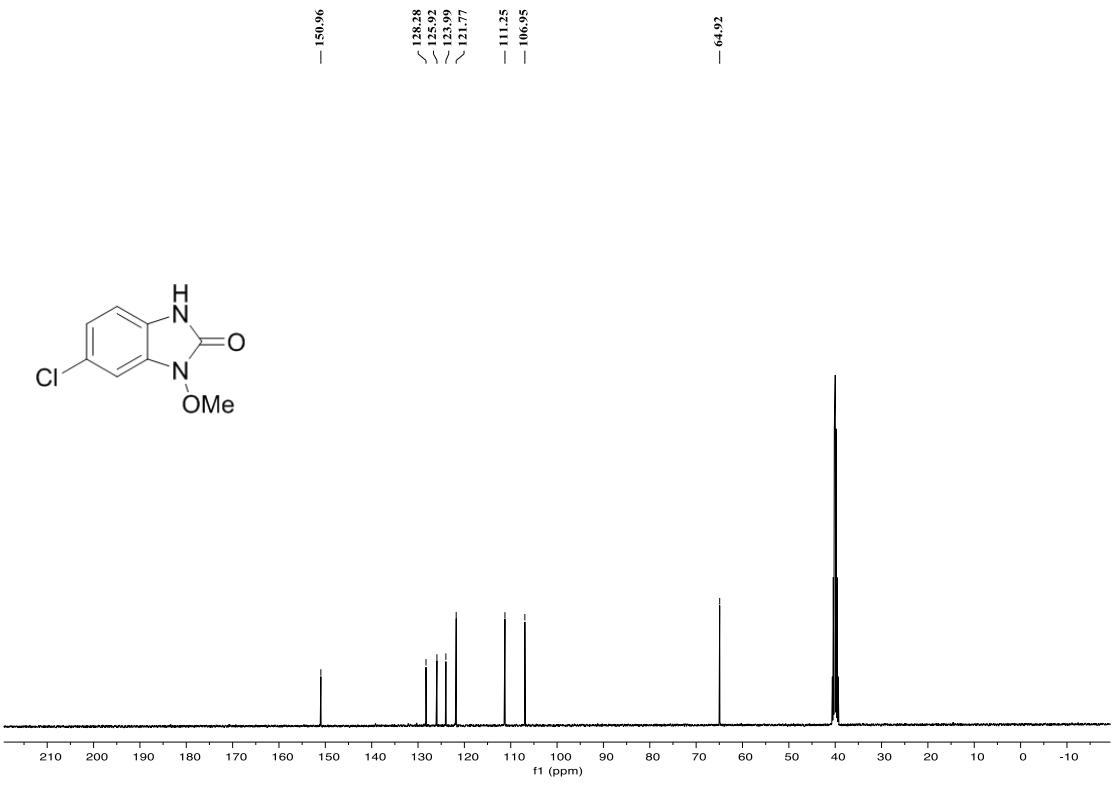
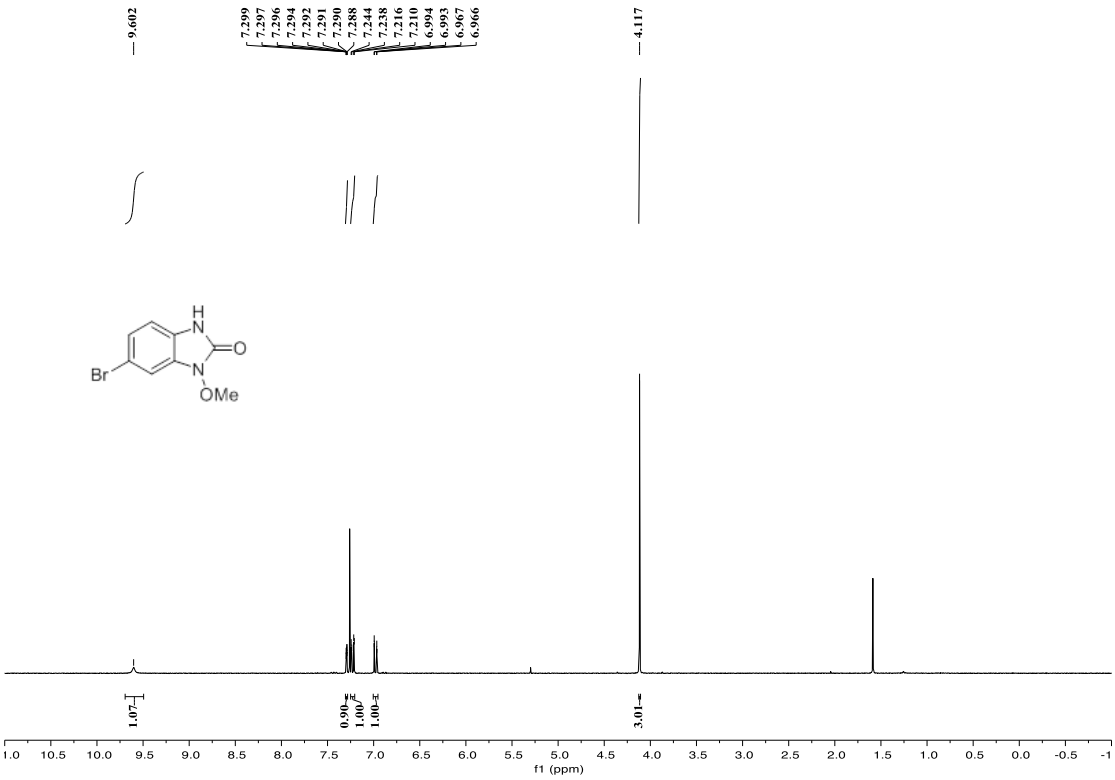
122.53
109.78
107.28
64.52
21.45
H
N
O
N
OMe
f1 (ppm)


11.03
7.07
7.06
7.04
7.03
6.97
6.96
6.94
6.93
6.84
6.83
6.81
6.80
6.80
6.80
6.78
6.77
3.92
1.00
0.98
1.00
1.01
3.01
f1 (ppm)


159.47
157.14
151.40
127.95
127.83
121.31
110.74
110.65
108.34
108.10
95.45
95.16
64.82
f1 (ppm)


11.15
7.20
7.04
7.03
7.03
7.01
7.01
6.98
6.96
3.93
H
N
O
Cl
N
OMe
1.00
0.95
2.05
3.11
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)


150.96
128.28
125.92
123.99
121.77
111.25
106.95
64.92
H
N
O
Cl
N
OMe
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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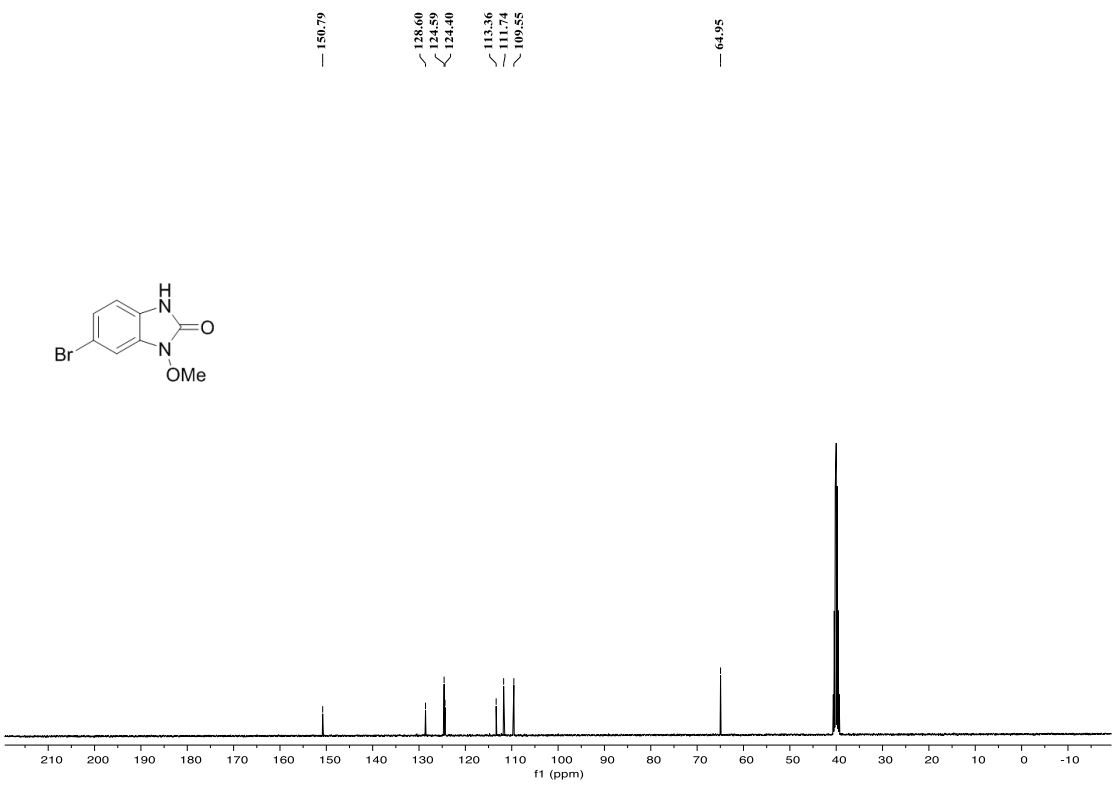
7.297
7.296
7.294
7.292
7.291
7.290
7.288
7.244
7.238
7.216
7.210
6.994
6.993
6.967
6.966
4.117
Br
N
H
O
N
OMe
1.07
0.90
1.00
1.00
3.01
f1 (ppm)


150.79
128.60
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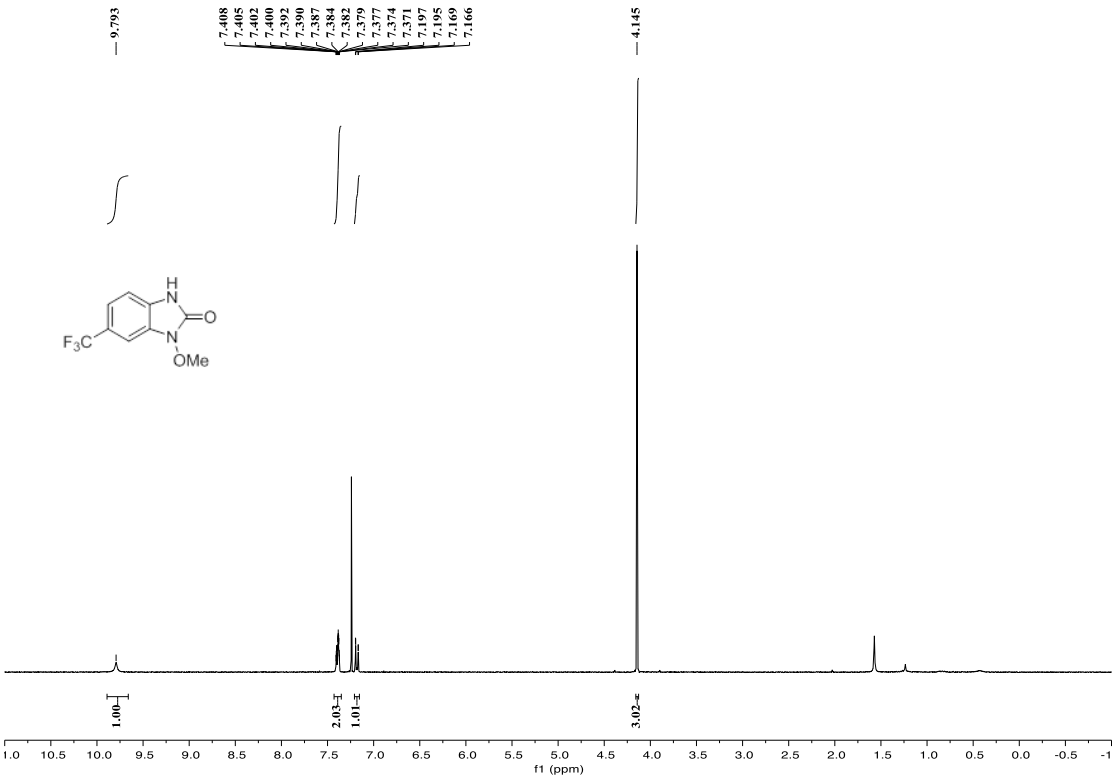
124.40
113.36
111.74
109.55
64.95
Br
N
H
O
N
OMe
f1 (ppm)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7.392
7.390
7.387
7.384
7.382
7.379
7.377
7.374
7.371
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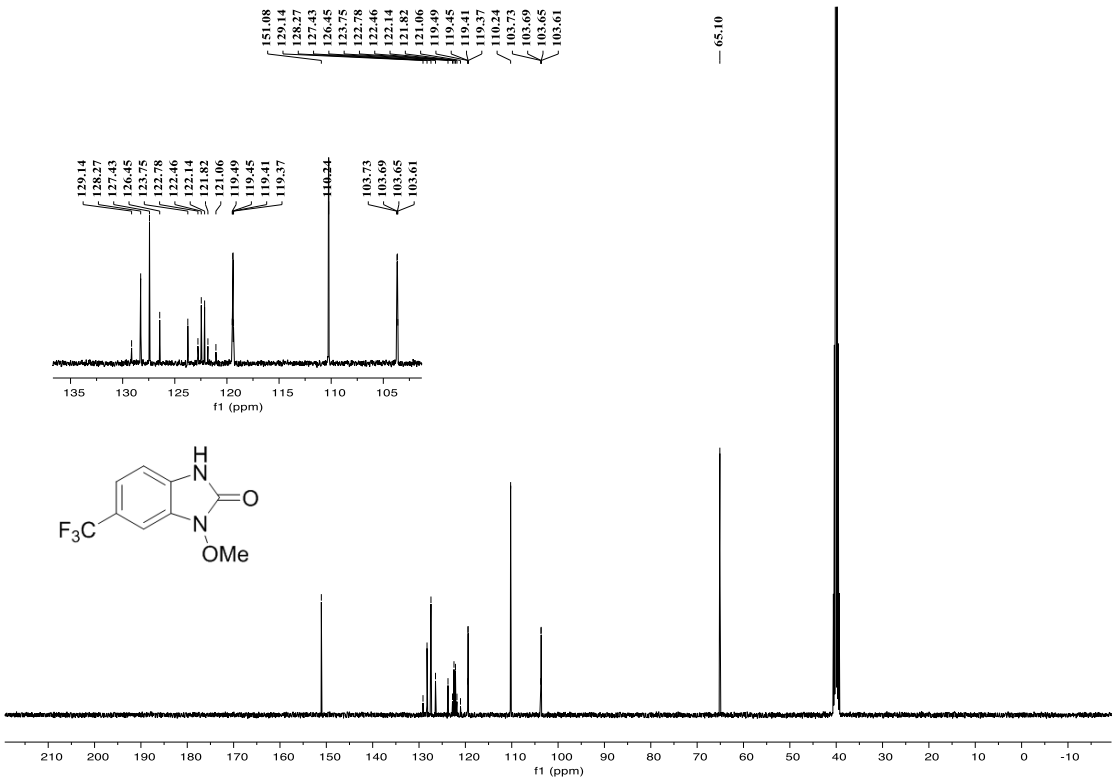
7.195
7.169
7.166
4.145
1.00
2.03
1.01
3.02
f1 (ppm)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127.43
126.45
123.75
122.78
122.46
122.14
121.82
121.06
119.49
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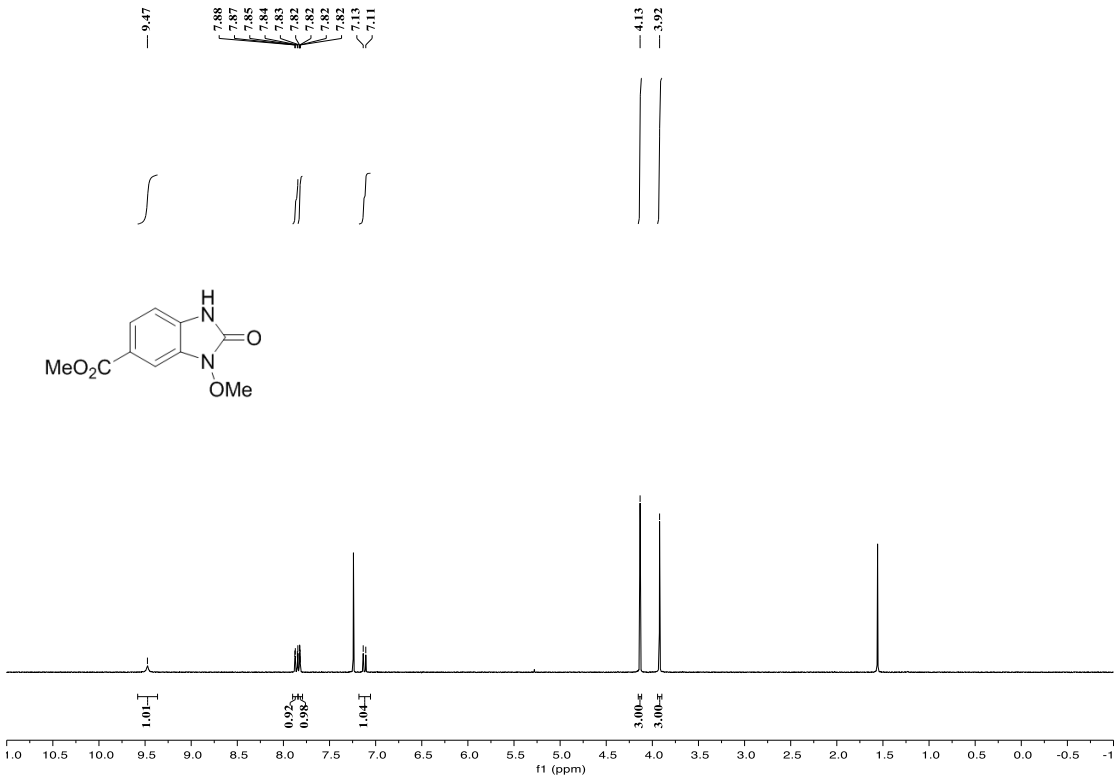
103.69
103.65
103.61
65.10
f1 (ppm)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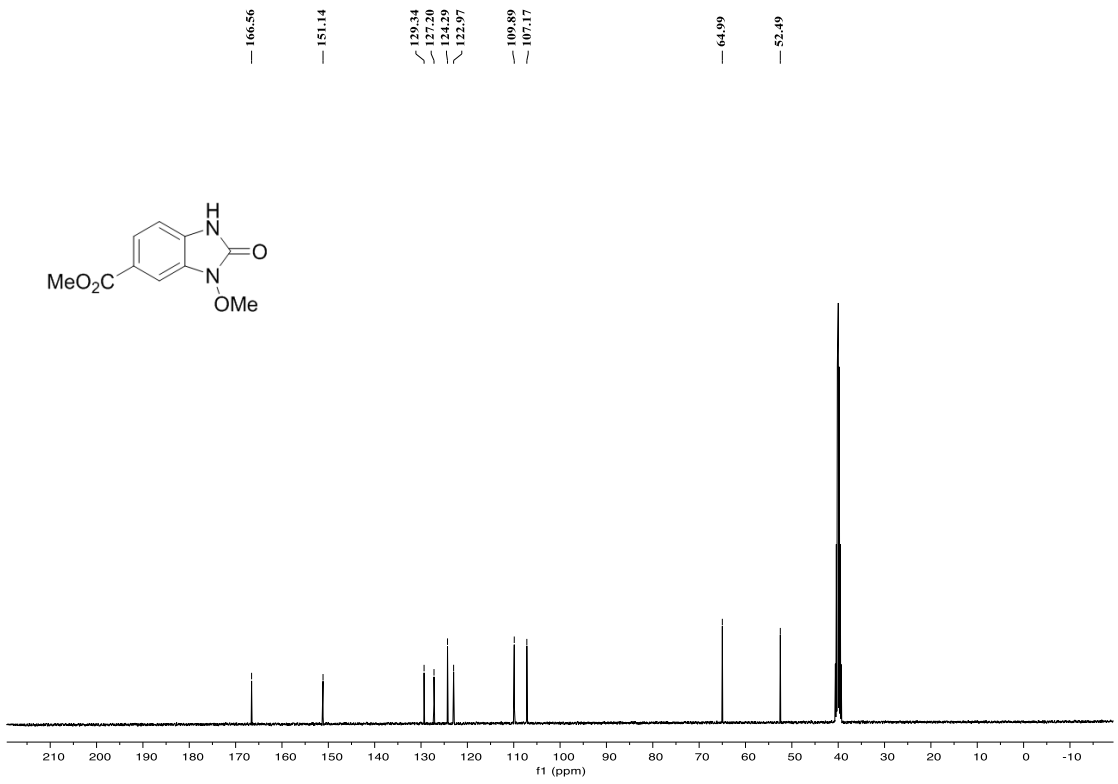
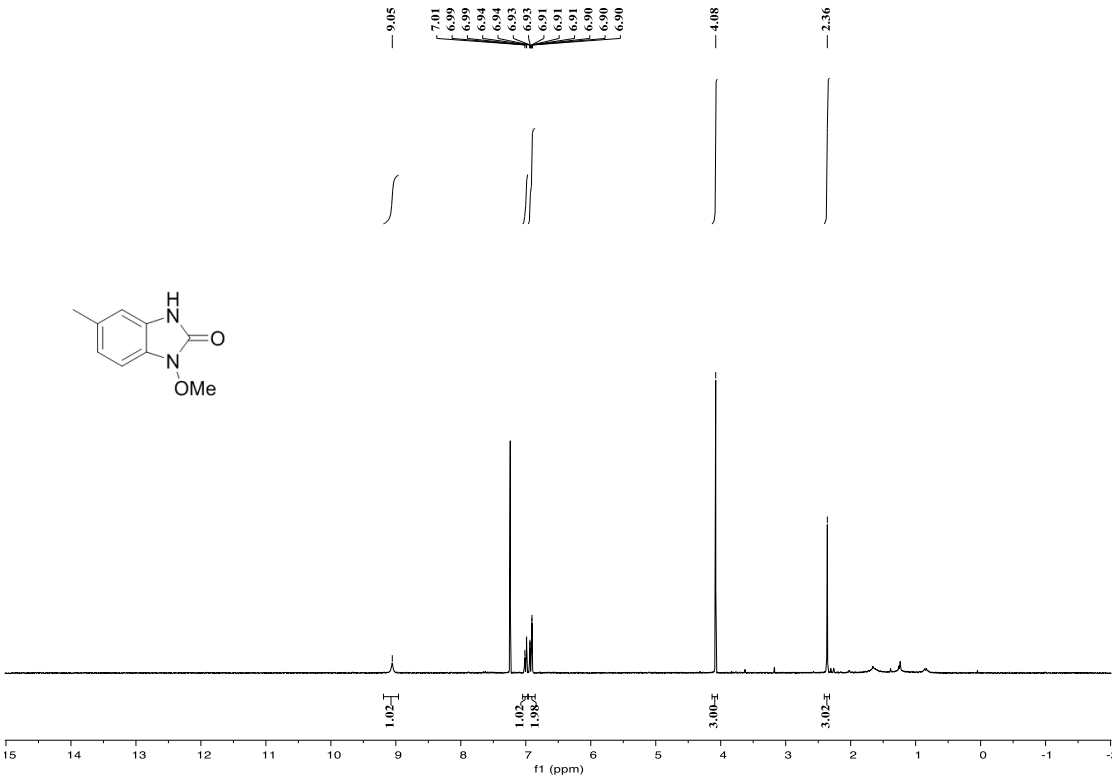
7.87
7.85
7.84
7.83
7.82
7.82
7.82
7.82
7.13
7.11
4.13
3.92
MeO2C
H
N
O
N
OMe
1.01
0.92
0.98
1.04
3.00
3.00
f1 (ppm)


166.56
151.14
129.34
127.20
124.29
122.97
109.89
107.17
64.99
52.49
MeO2C
H
N
O
N
OMe
f1 (ppm)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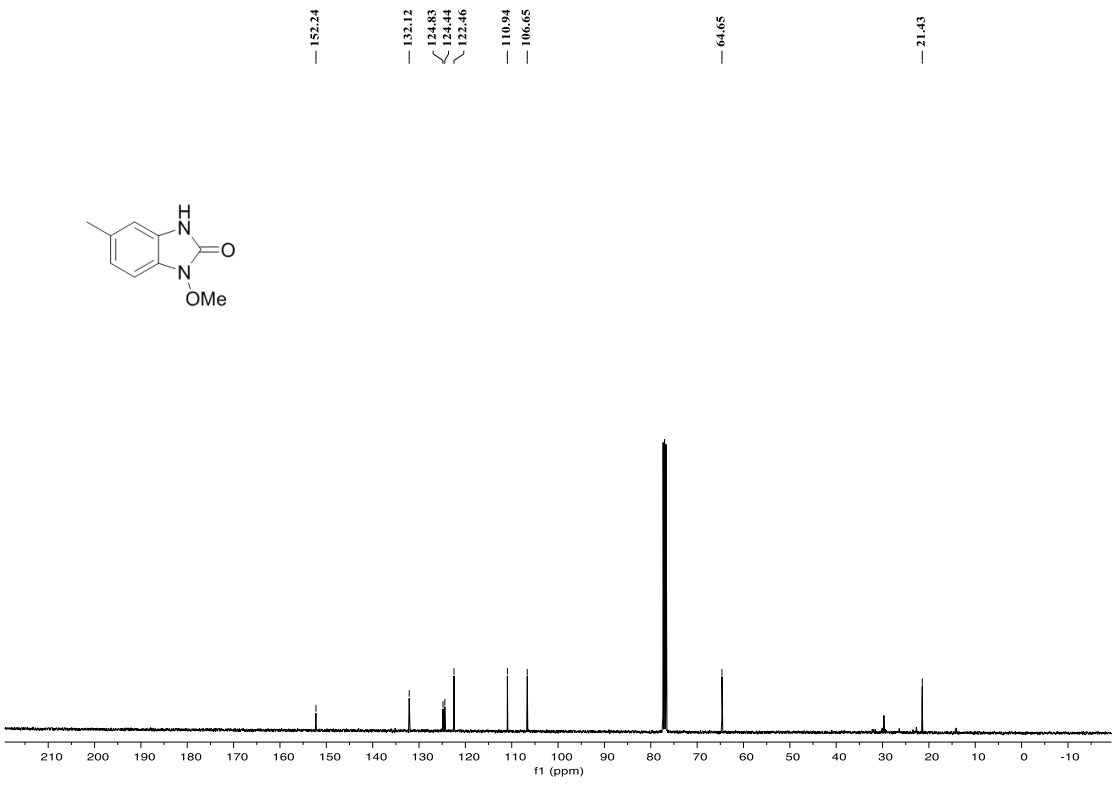
7.01
6.99
6.99
6.94
6.94
6.93
6.93
6.91
6.91
6.91
6.90
6.90
6.90
4.08
2.36
H
N
O
N
OMe
1.02
1.02
1.98
3.00
3.02
f1 (ppm)


152.24
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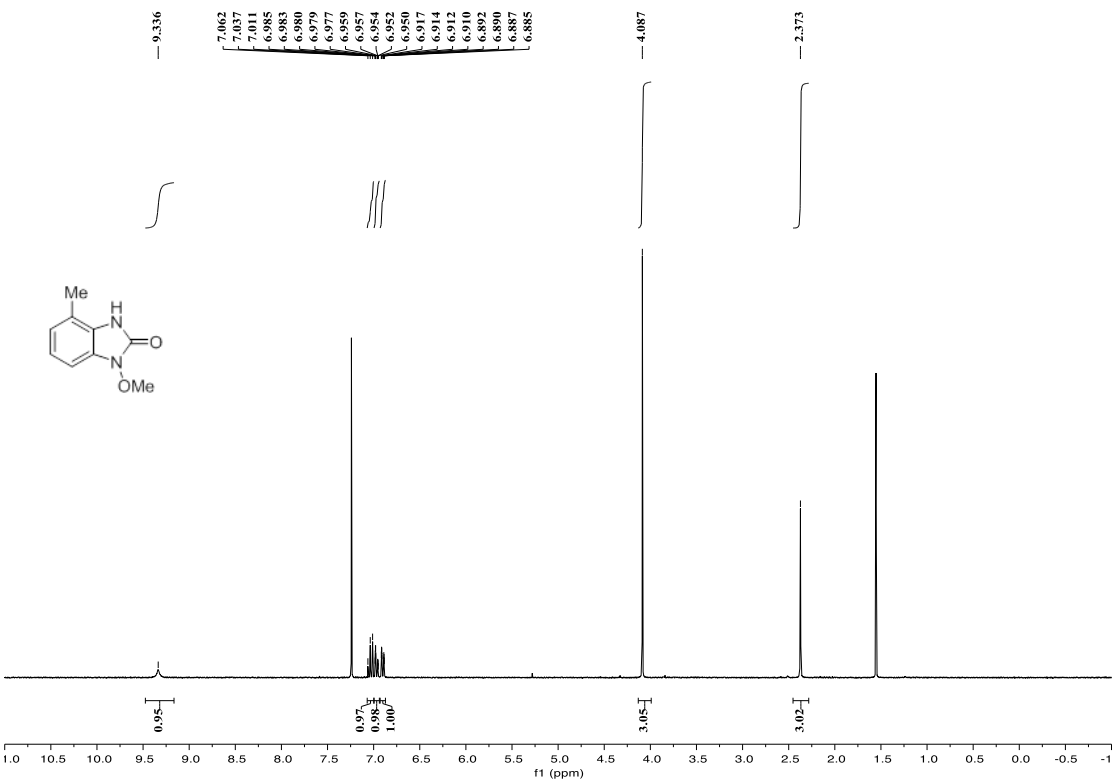
124.44
122.46
110.94
106.65
64.65
21.43
H
N
O
N
OMe
f1 (ppm)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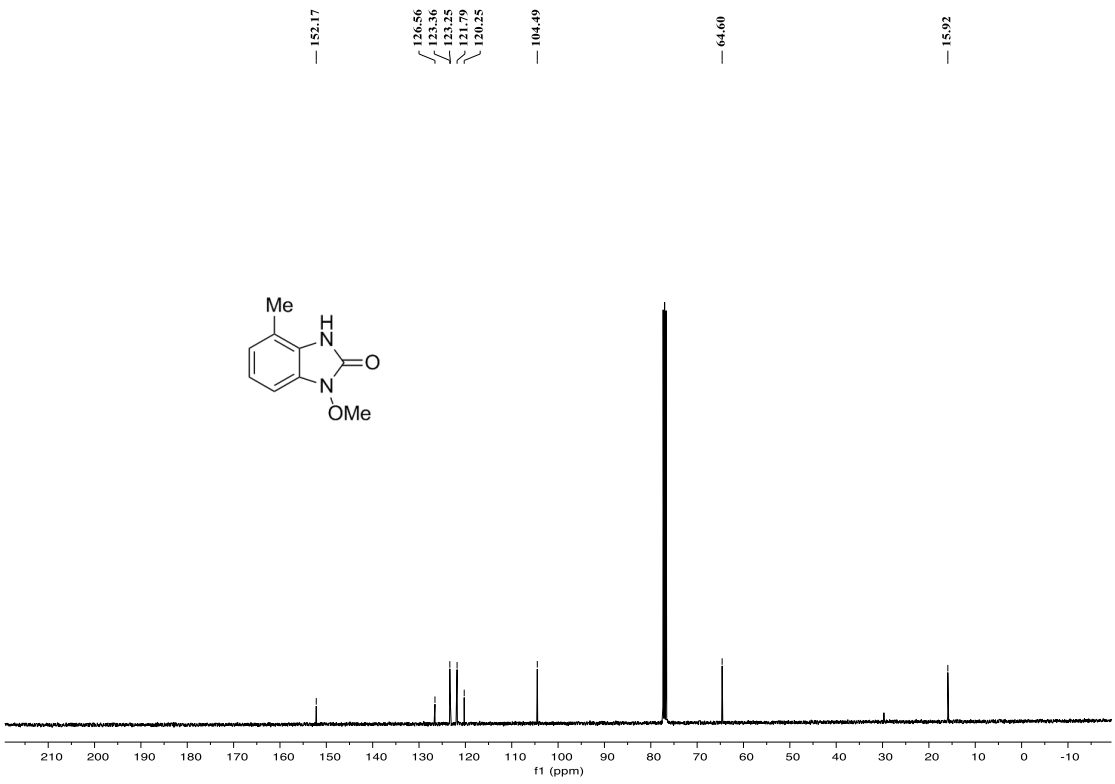
6.977
6.959
6.957
6.954
6.952
6.950
6.917
6.914
6.912
6.910
6.892
6.890
6.887
6.885
4.087
2.373
Me
H
N
O
N
OMe
0.95
0.97
0.98
1.00
3.05
3.02
f1 (ppm)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120.25
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64.60
15.92
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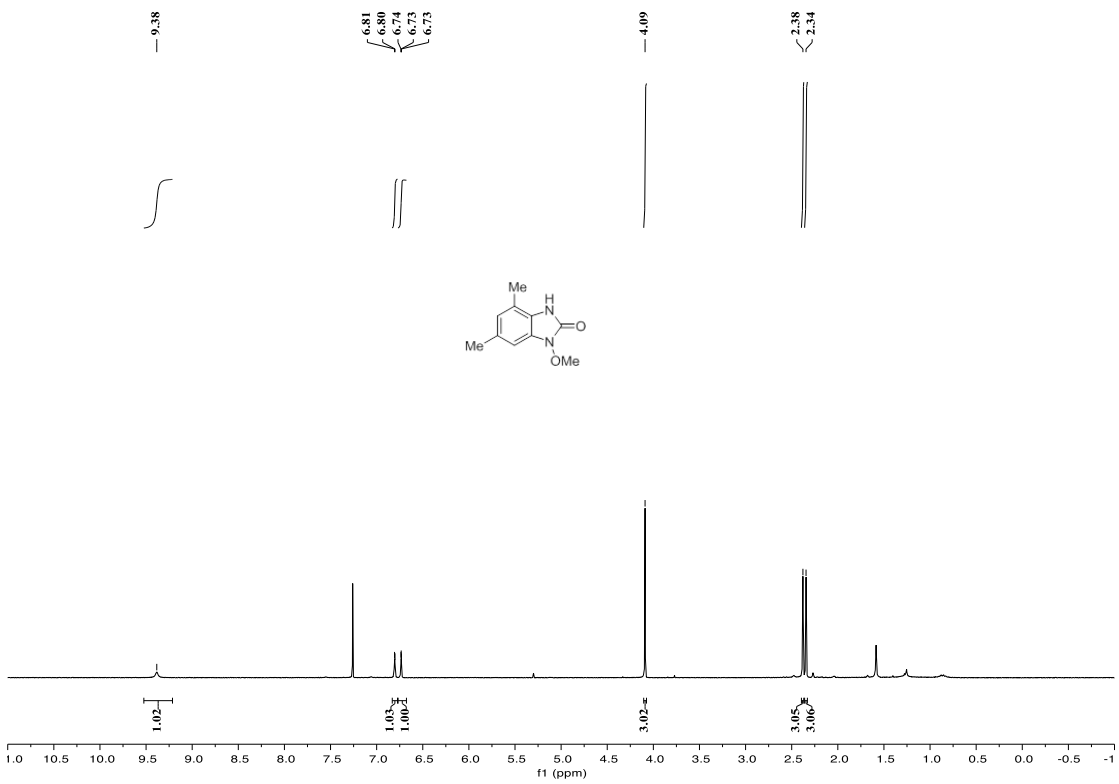
H
N
O
N
OMe
f1 (ppm)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6.73
6.73
4.09
2.38
2.34
Me
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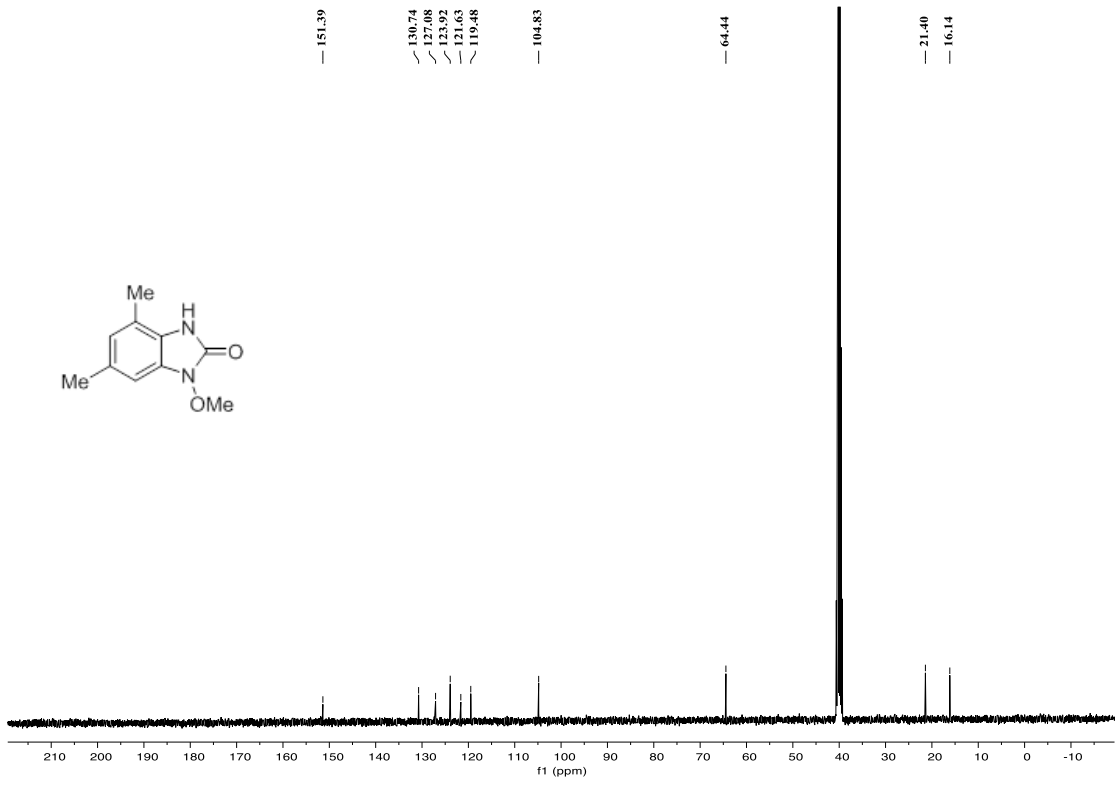
N
O
Me
N
OMe
1.02
1.03
1.00
3.02
3.05
3.06
f1 (ppm)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130.74
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121.63
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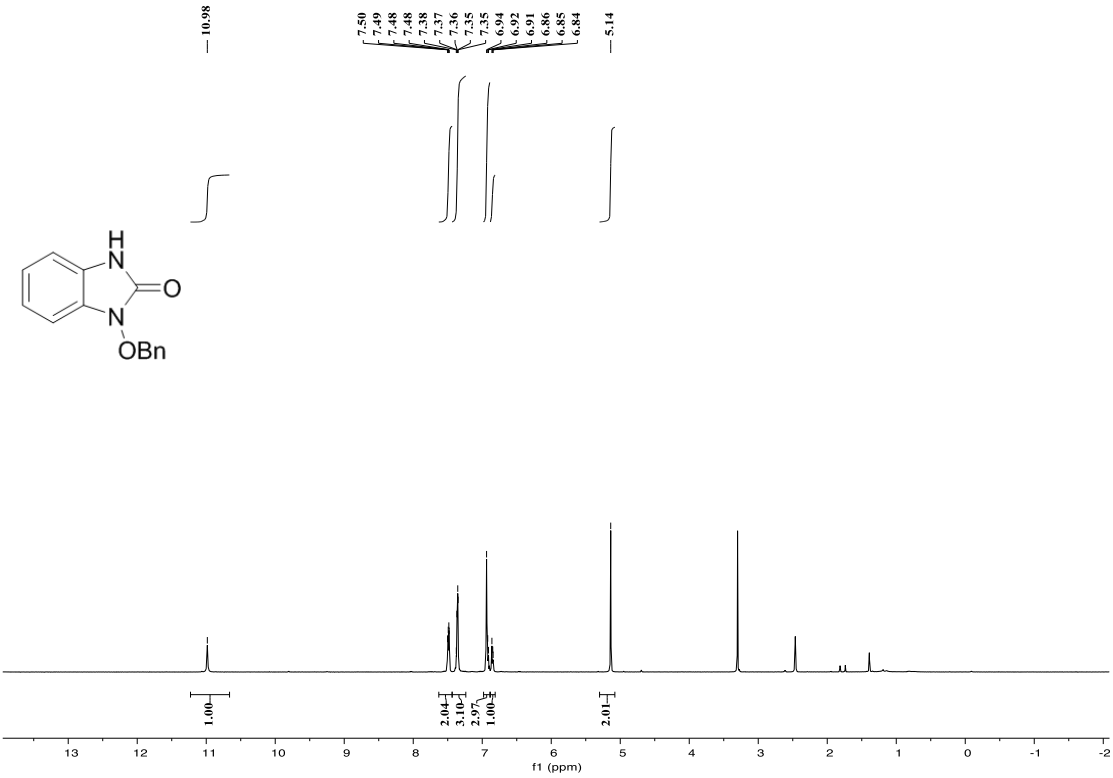
104.83
64.44
21.40
16.14
Me
H
N
O
Me
N
OMe
f1 (ppm)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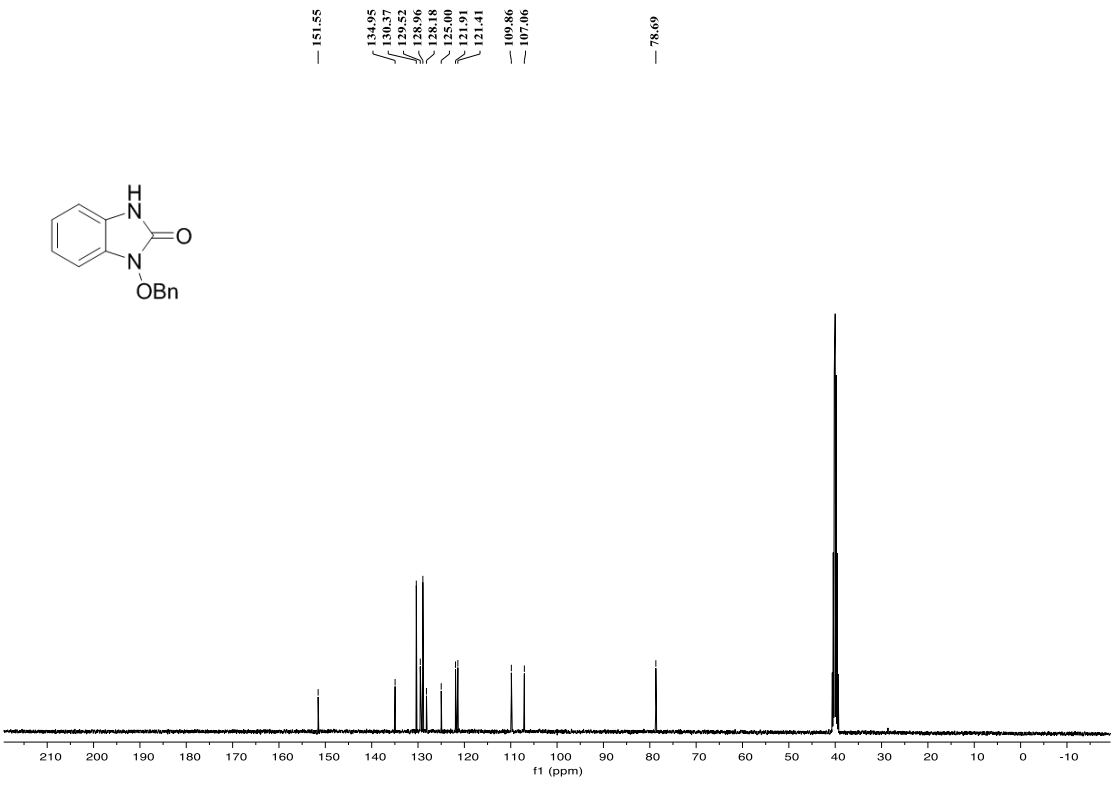
7.48
7.38
7.37
7.36
7.35
7.35
6.94
6.92
6.91
6.86
6.85
6.84
5.14
H
N
O
N
OBn
1.00
2.04
3.10
2.97
1.00
2.01
f1 (ppm)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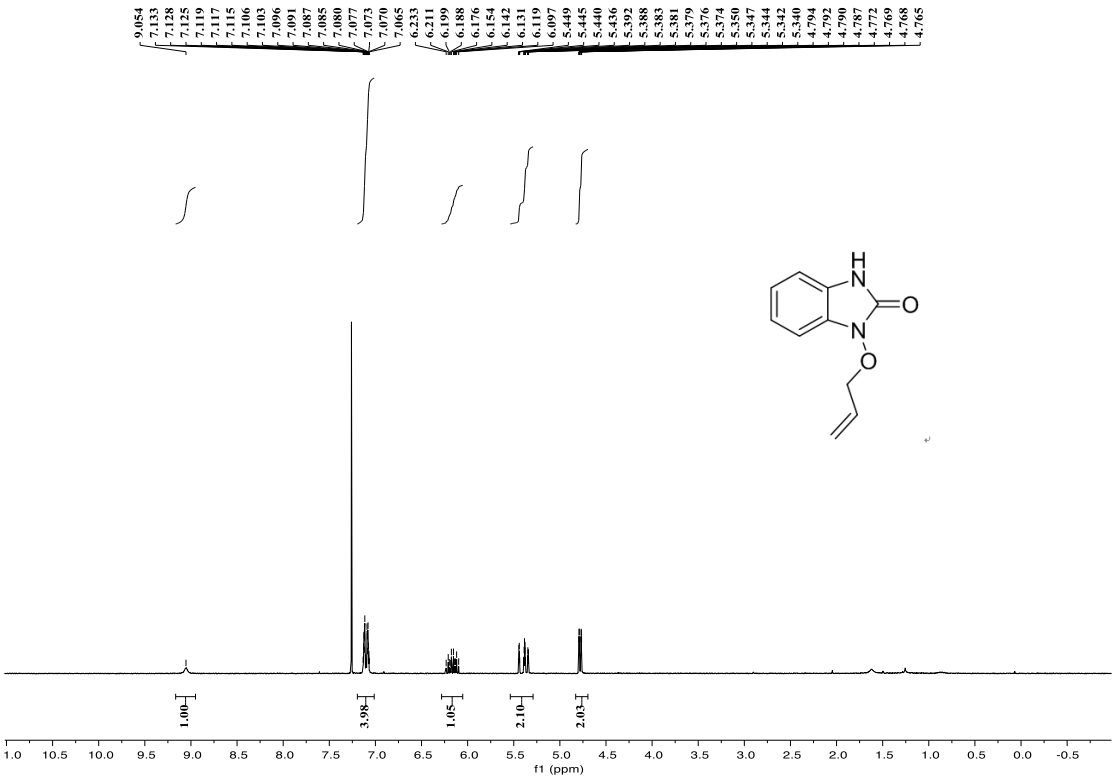
129.52
128.96
128.18
125.00
121.91
121.41
109.86
107.06
78.69
H
N
O
N
OBn
f1 (ppm)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7.080
7.077
7.073
7.070
7.065
6.233
6.211
6.199
6.188
6.176
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6.119
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5.388
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5.381
5.379
5.376
5.374
5.350
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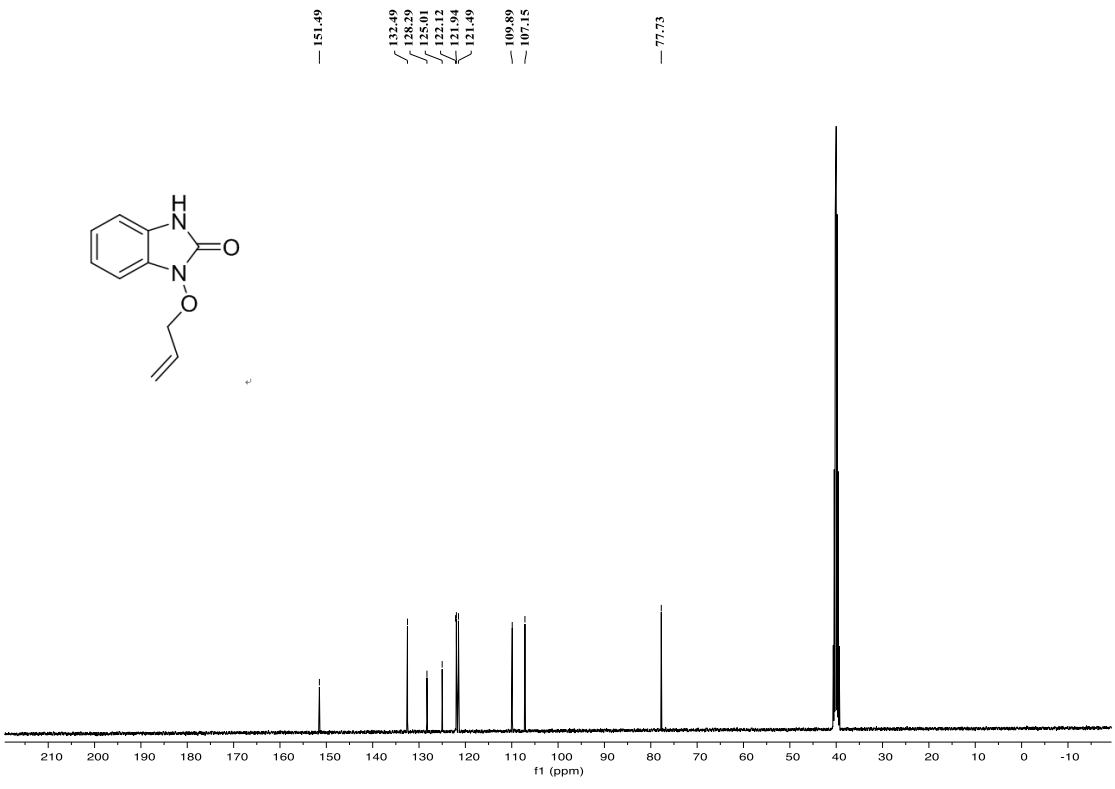
4.790
4.787
4.772
4.769
4.768
4.765
1.00
3.98
1.05
2.10
2.03
f1 (ppm)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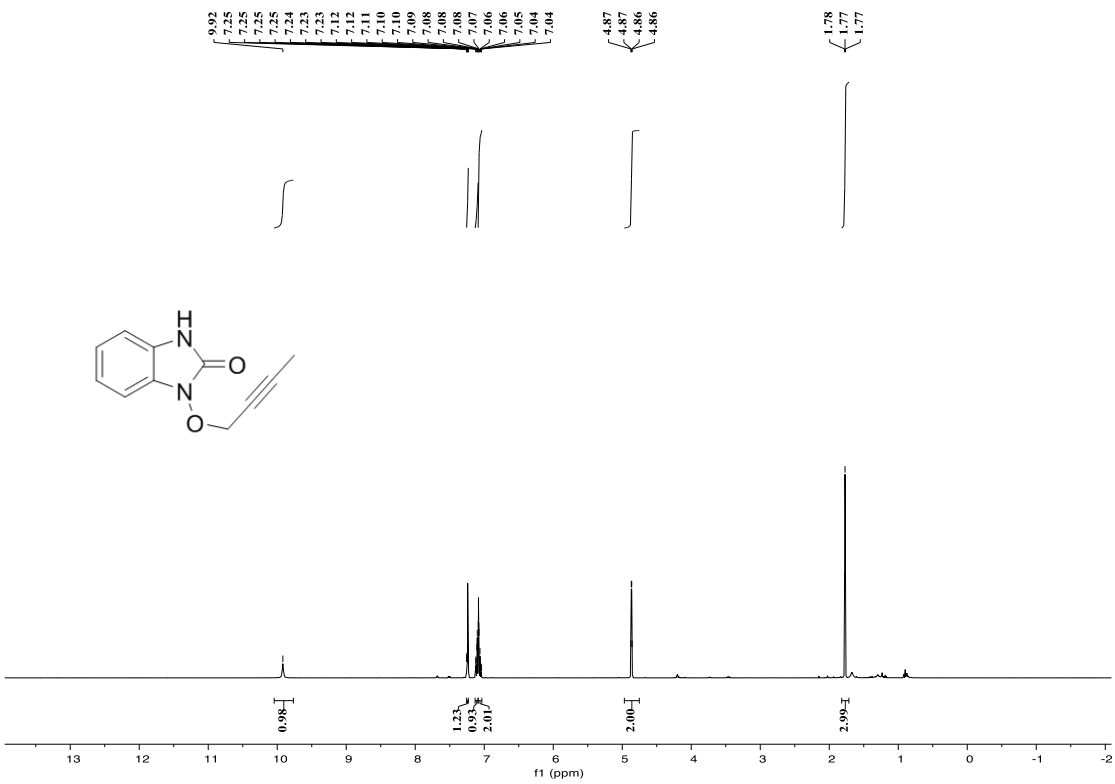
77.73
f1 (ppm)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7.09
7.08
7.08
7.08
7.07
7.06
7.06
7.05
7.04
7.04
4.87
4.87
4.86
4.86
1.78
1.77
1.77
H
N
O
N
O
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0.93
2.01
2.00
2.99
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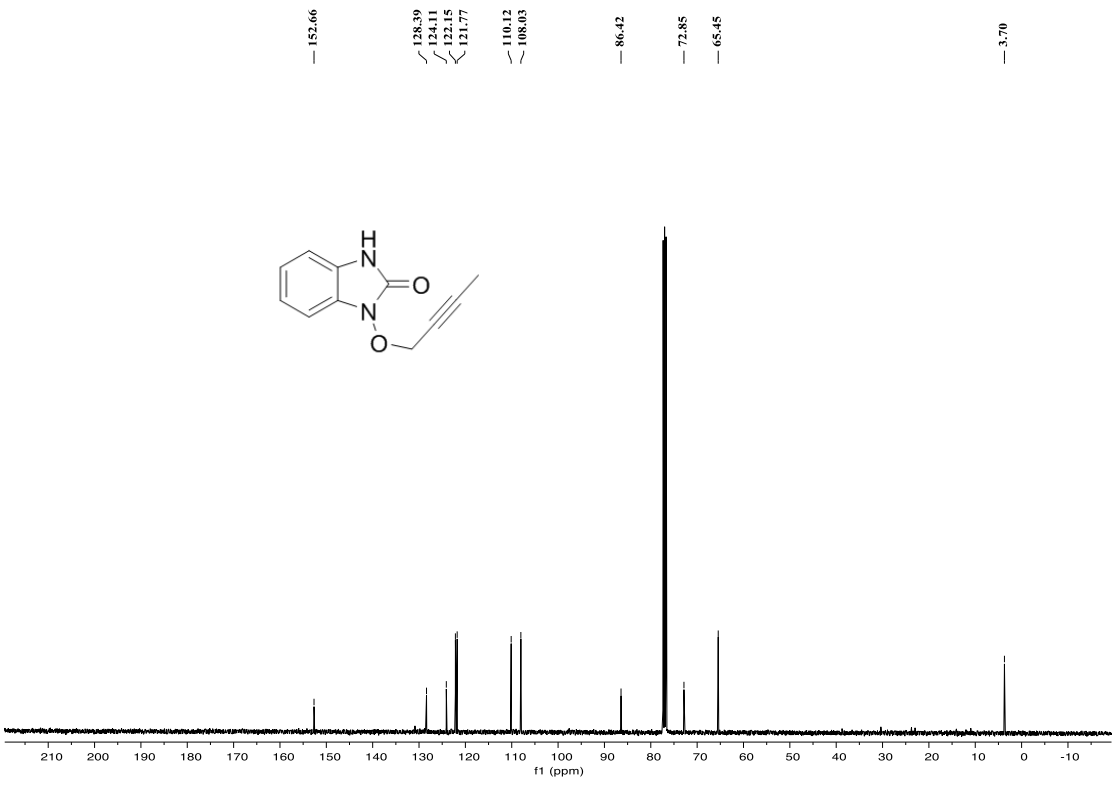
f1 (ppm)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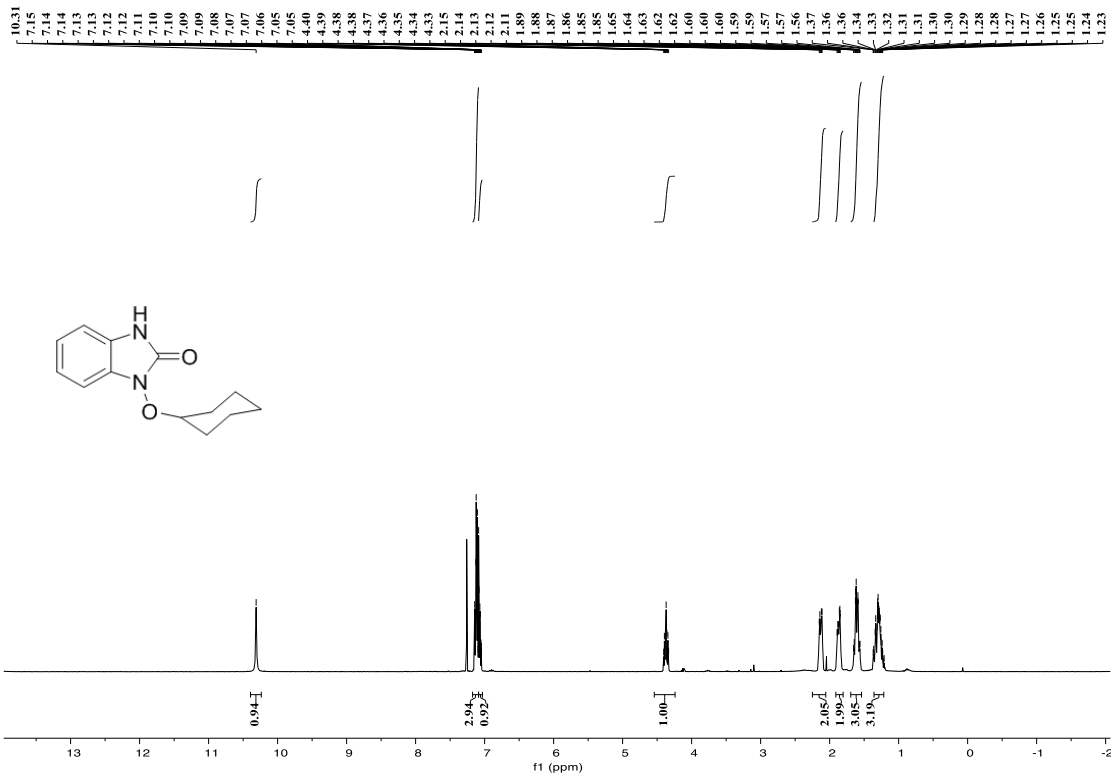
f1 (ppm)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7.05
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4.38
4.37
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4.35
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4.33
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2.14
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1.88
1.87
1.86
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1.24
1.23
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O
N
O
0.94
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3.05
3.19
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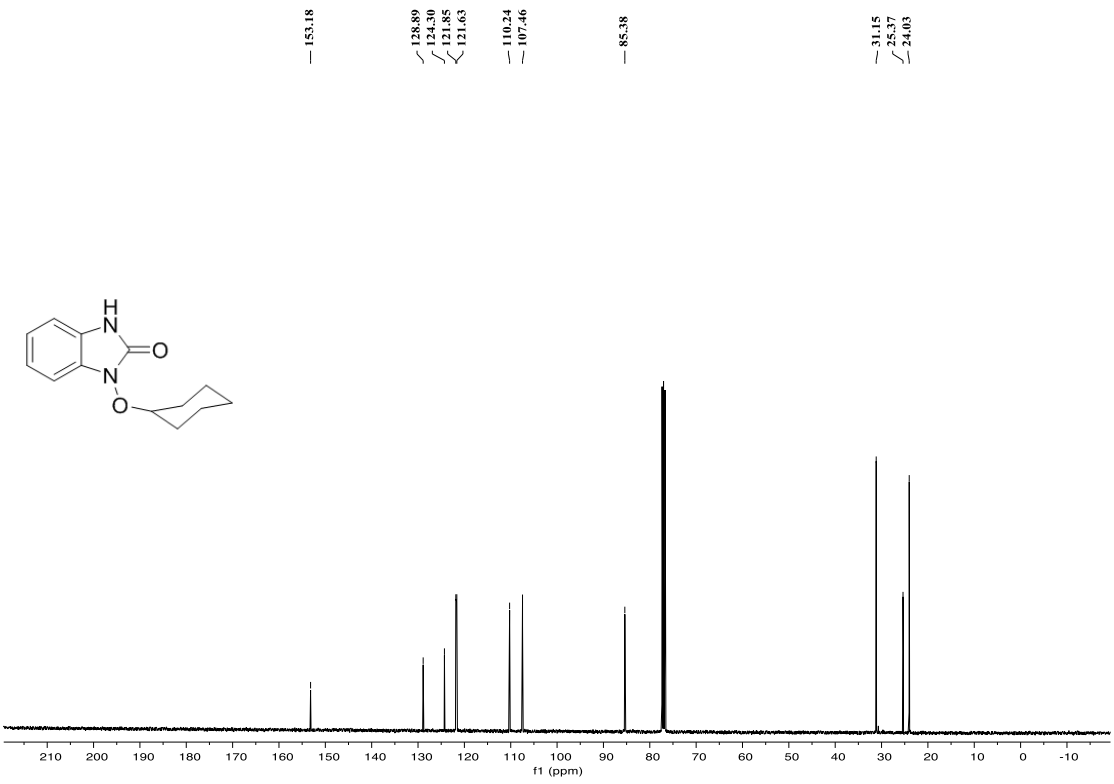
f1 (ppm)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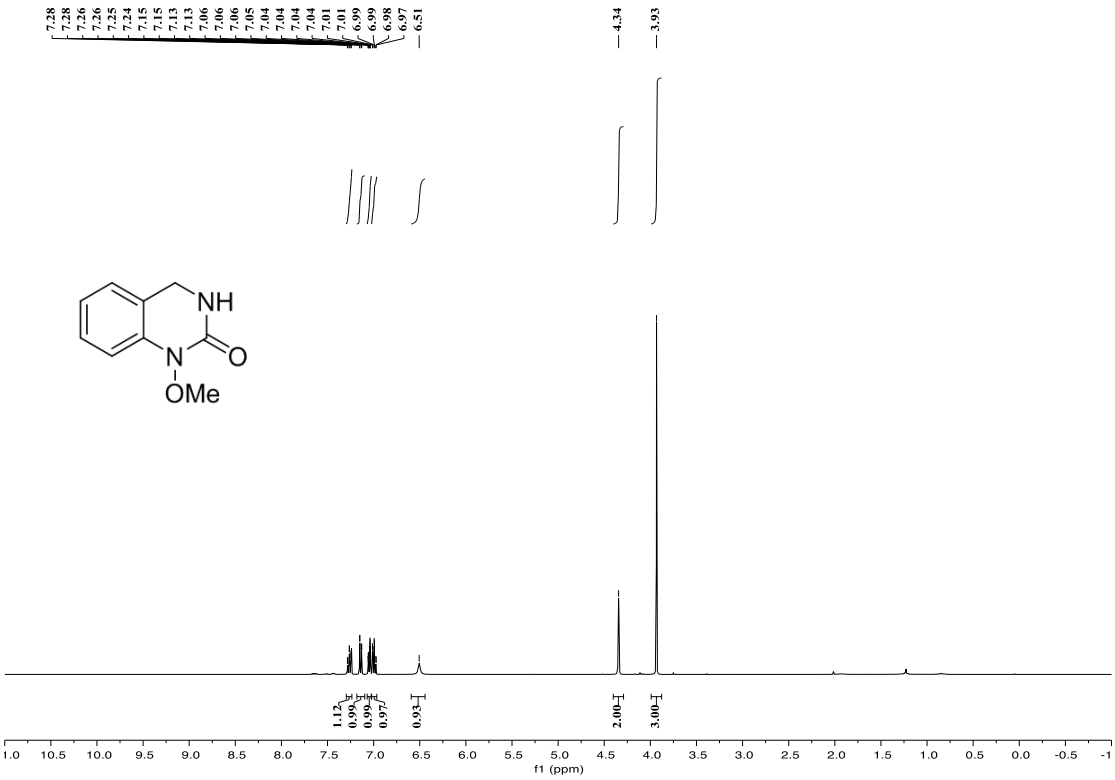
f1 (ppm)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7.04
7.04
7.04
7.04
7.01
7.01
6.99
6.99
6.98
6.97
6.51
4.34
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OMe
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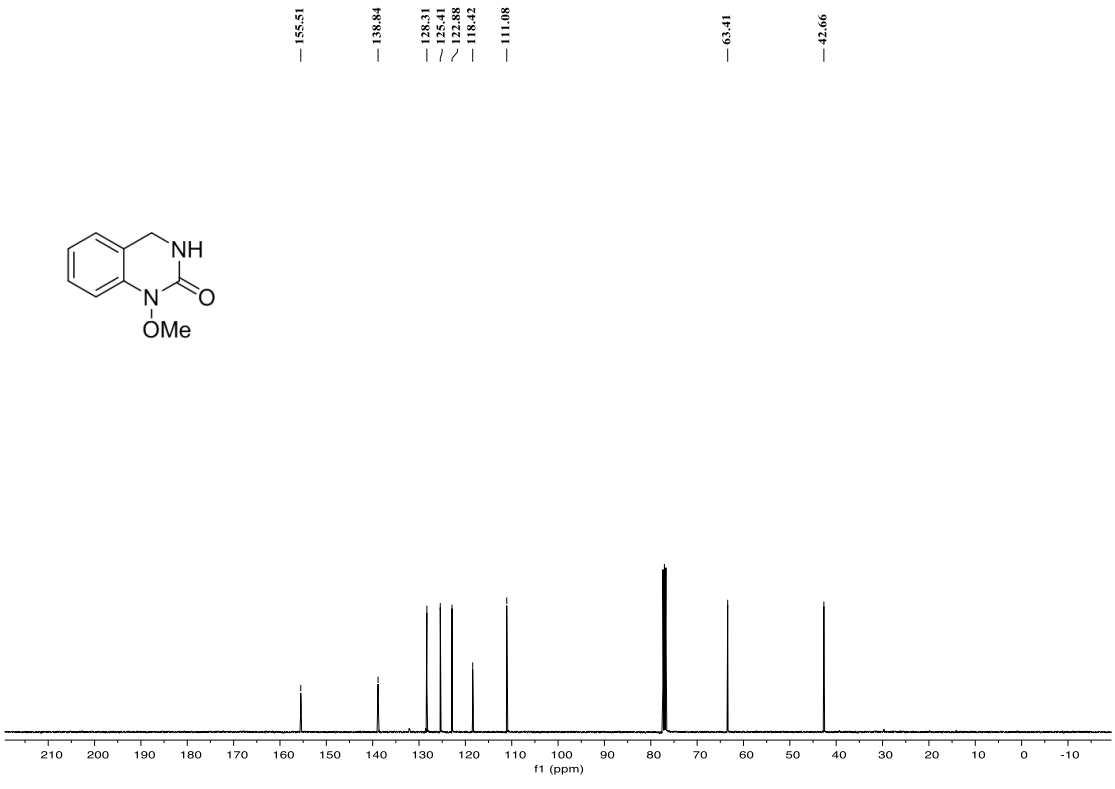
3.00
f1 (ppm)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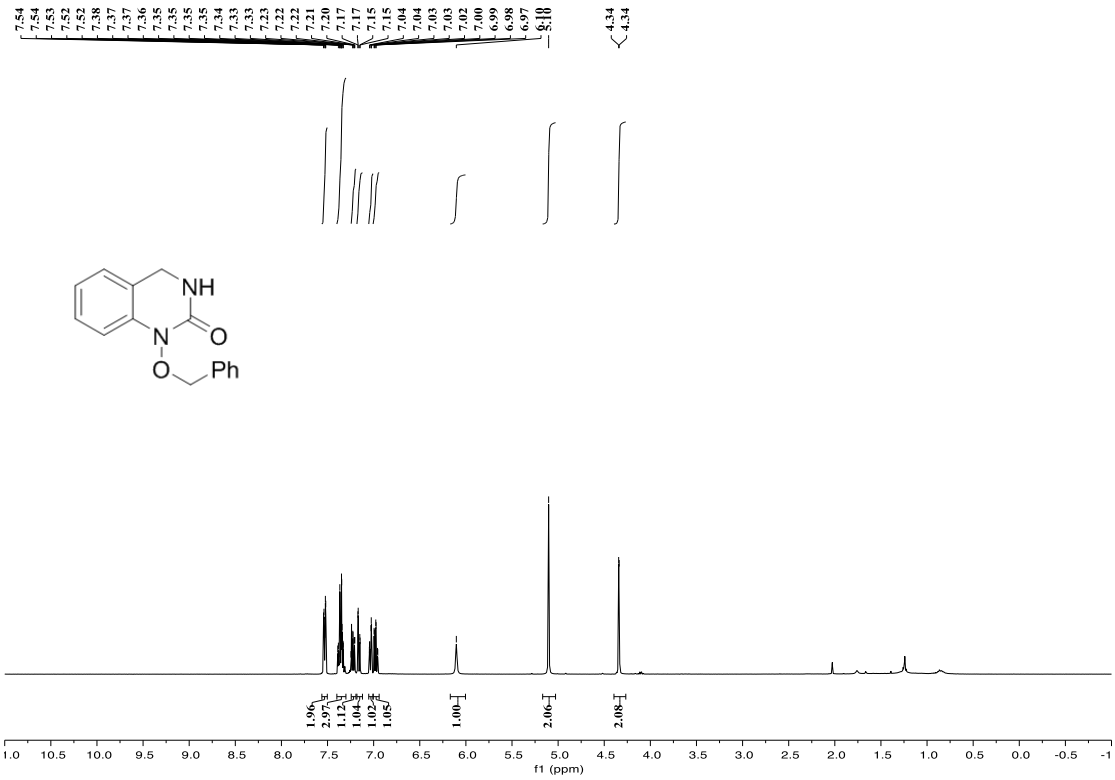
O
OMe
f1 (ppm)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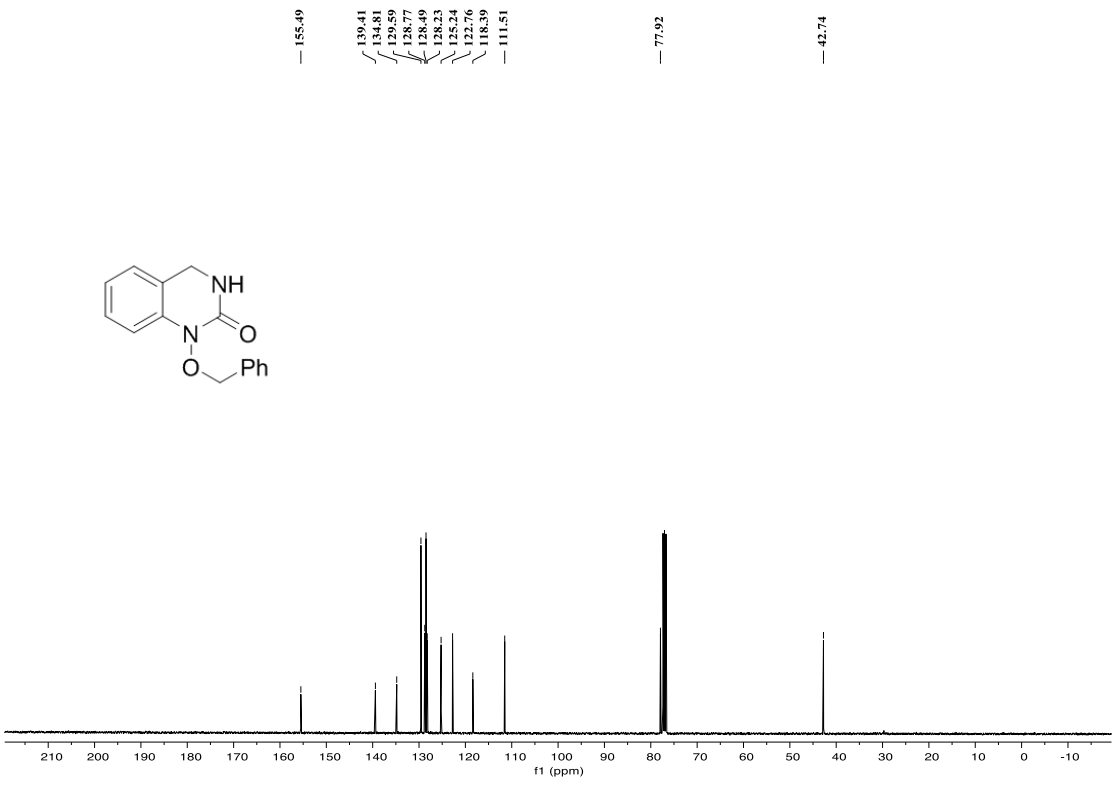
7.17
7.15
7.15
7.04
7.04
7.03
7.03
7.02
7.00
6.99
6.98
6.97
5.10
5.10
4.34
4.34
NH
N
O
O
Ph
1.96
2.97
1.12
1.04
1.02
1.05
1.00
2.06
2.08
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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O
Ph
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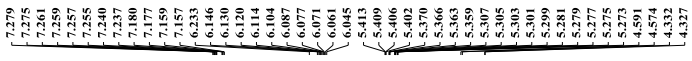
f1 (ppm)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7.157
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6.146
6.130
6.120
6.114
6.104
6.087
6.077
6.071
6.061
6.045
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5.409
5.406
5.402
5.370
5.366
5.363
5.359
5.307
5.305
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5.279
5.277
5.275
5.273
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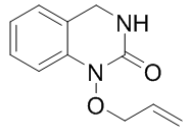
4.574
4.332
4.327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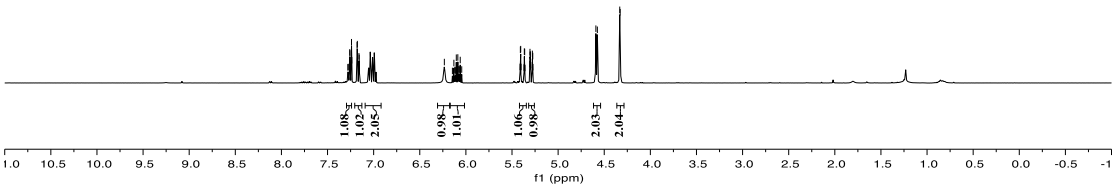
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1.02
2.05
0.98
1.01
1.06
0.98
2.03
2.04
f1 (ppm)


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120.54
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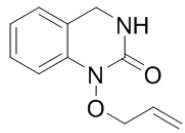
76.83
42.66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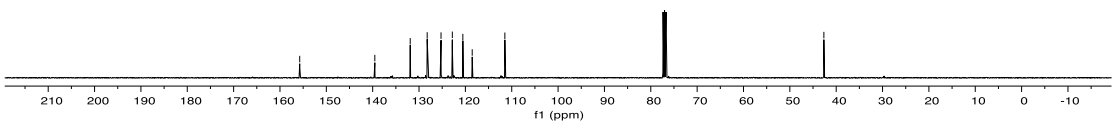
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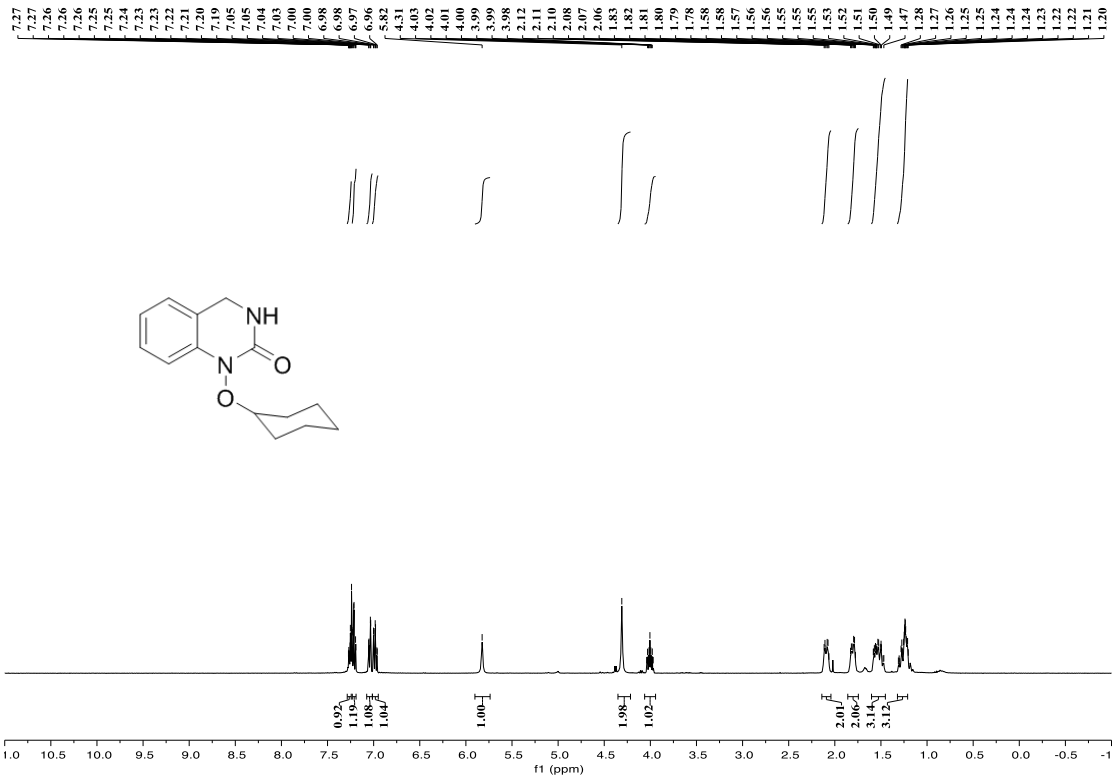
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NH
N
O
O
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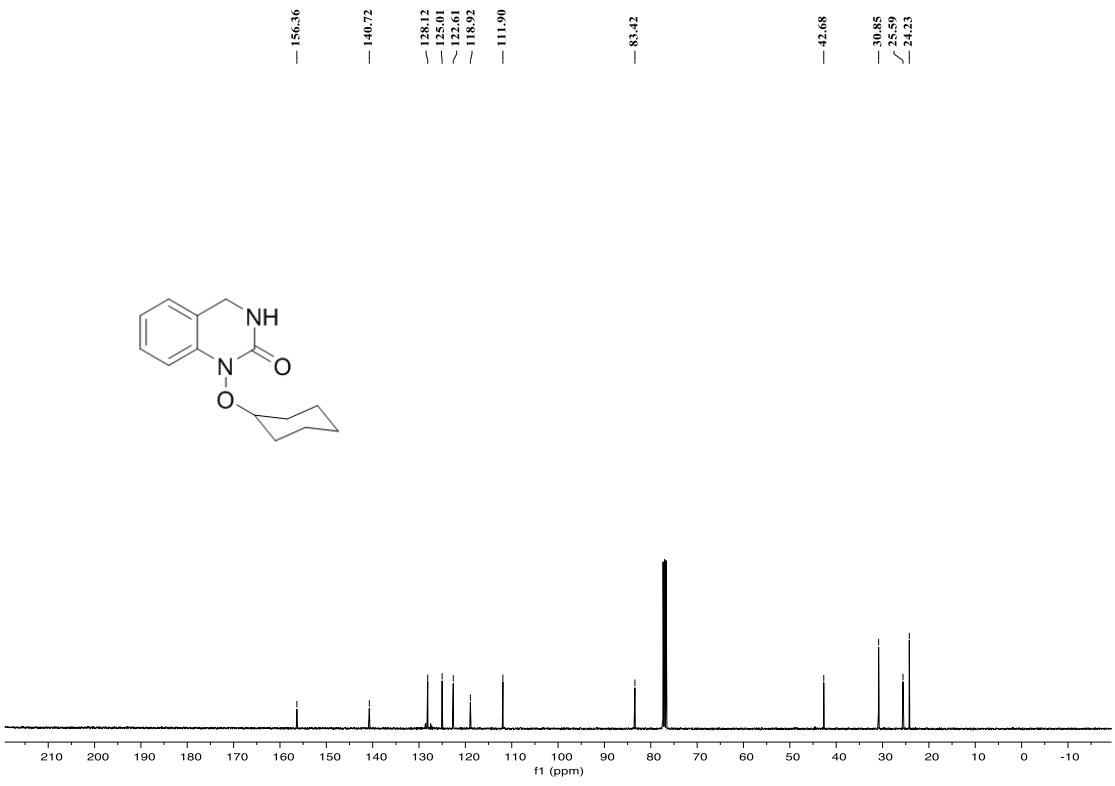
1.04
1.00
1.98
1.02
2.01
2.06
3.14
3.12
f1 (ppm)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24.23
NH
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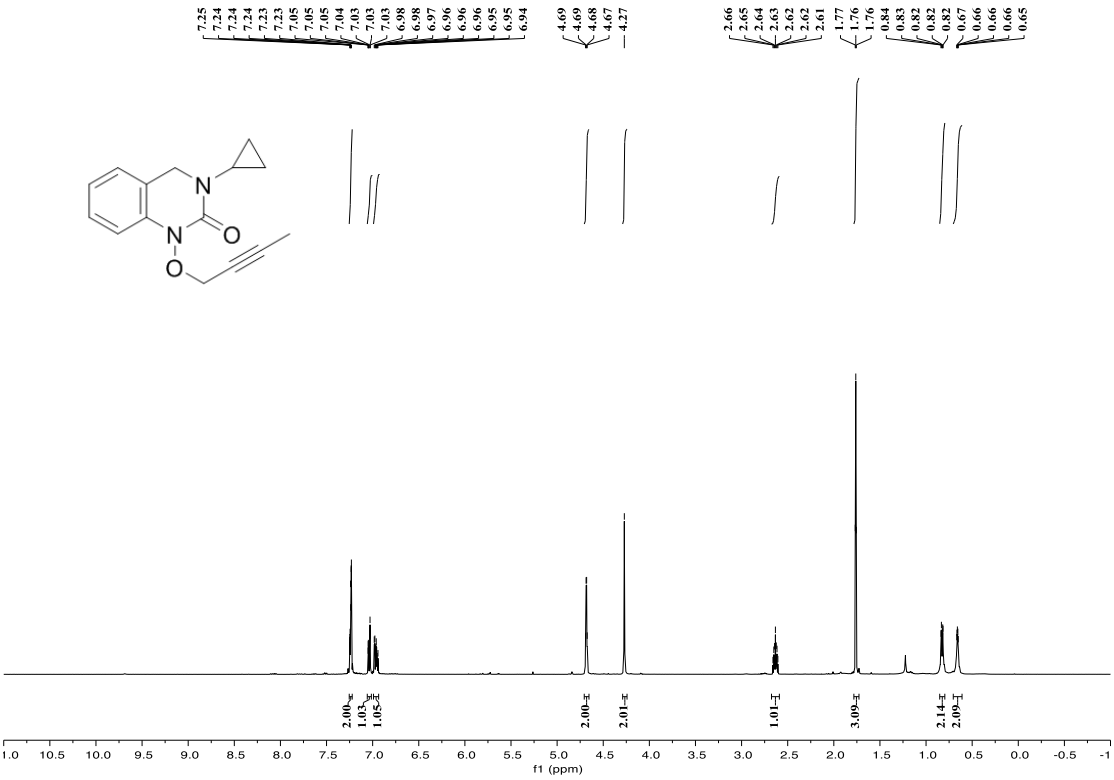
O
O
f1 (ppm)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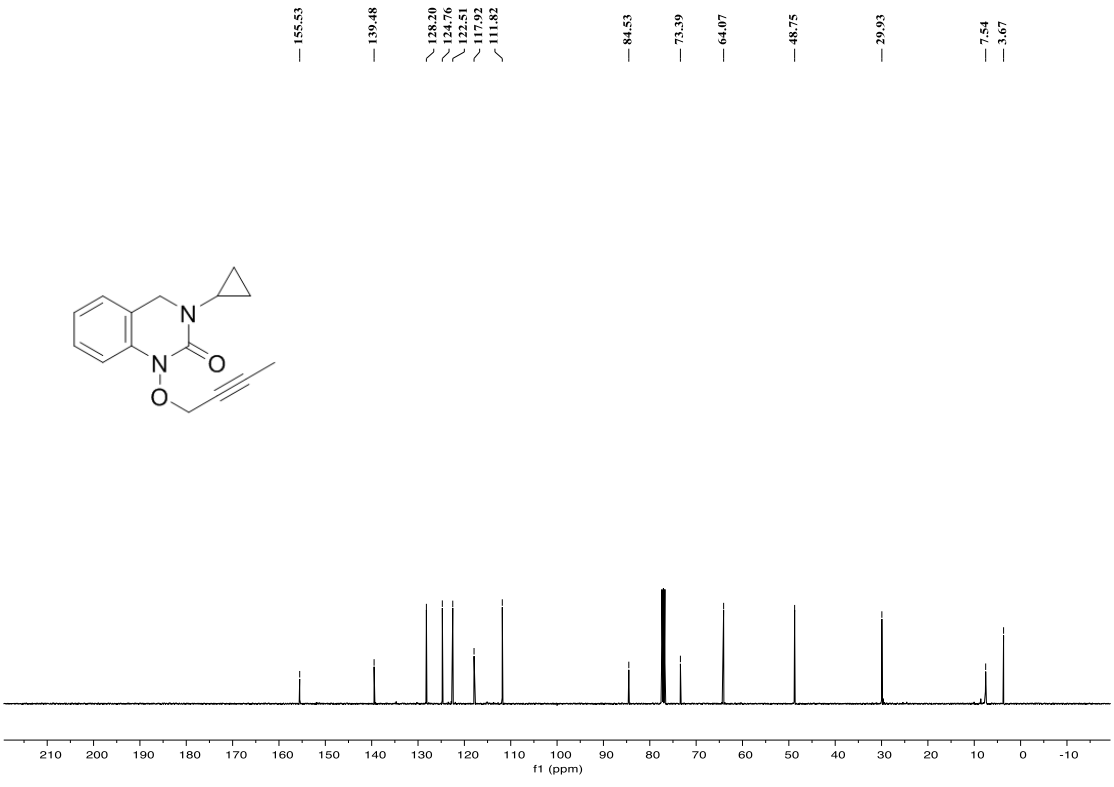
4.69 4.69 4.68 4.67 4.27
2.66 2.65 2.64 2.63 2.62 2.62 2.61
1.77 1.76 1.76 0.84 0.83 0.82 0.82 0.82 0.67 0.66 0.66 0.66 0.65
2.00 1.03 1.05 2.00 2.01 1.01 3.09 2.14 2.09
f1 (ppm)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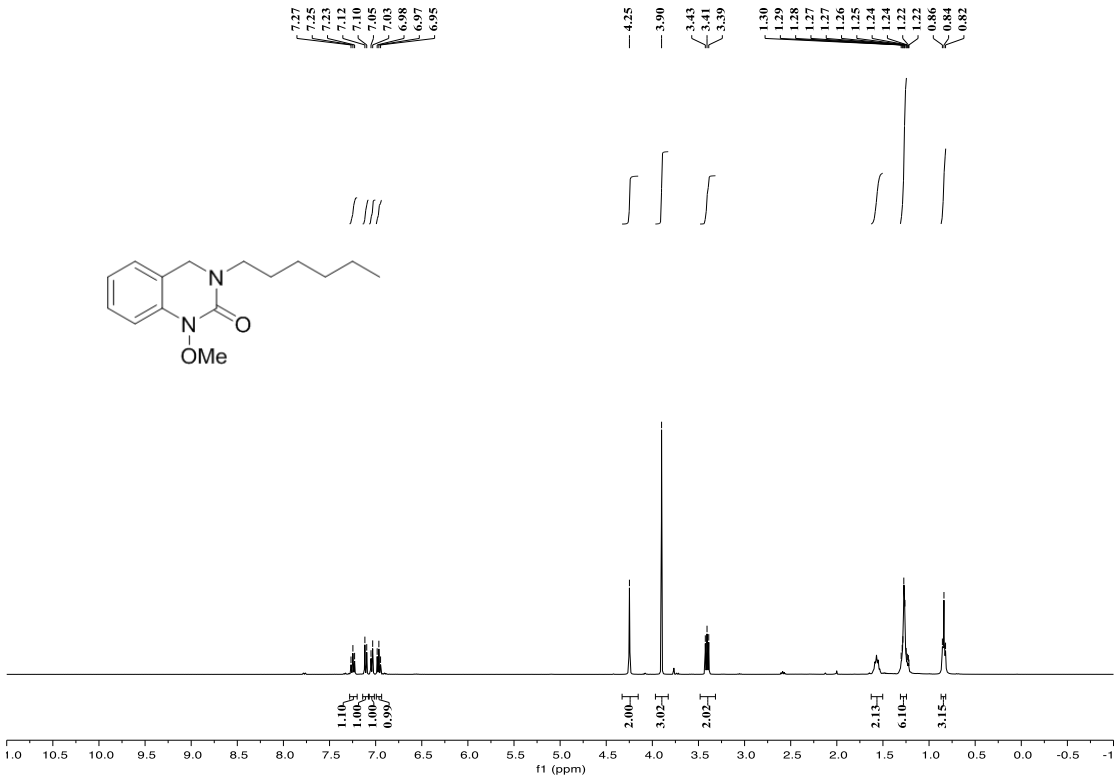
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6.95
4.25
3.90
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1.29
1.28
1.27
1.27
1.26
1.25
1.24
1.24
1.22
1.22
0.86
0.84
0.82
N
N
O
OMe
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1.00
0.99
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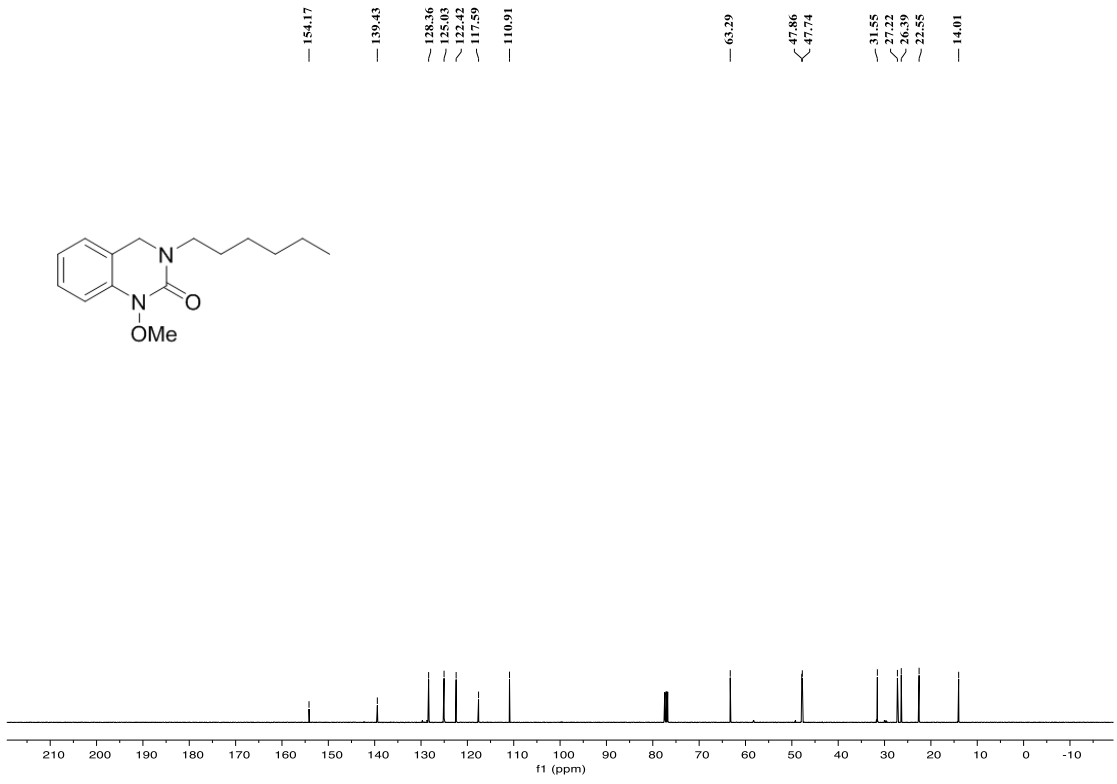
3.02
2.02
2.13
6.10
3.15
f1 (ppm)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26.39
22.55
14.01
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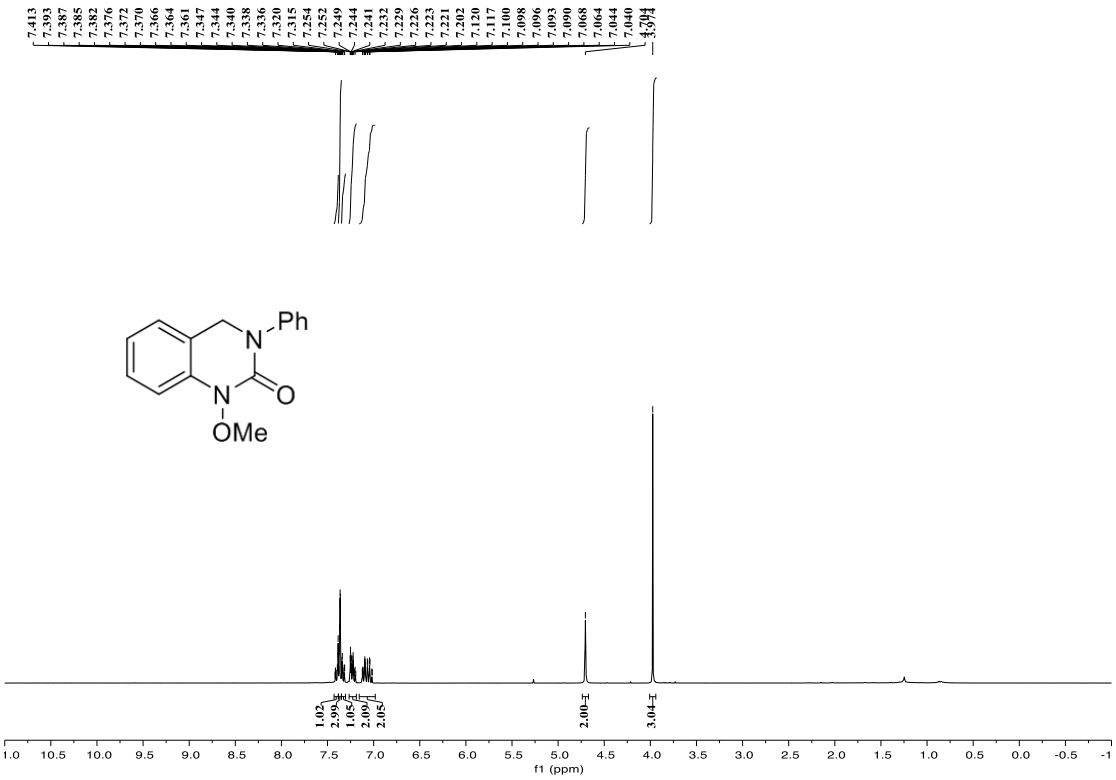
OMe
f1 (ppm)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7.040
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1.05
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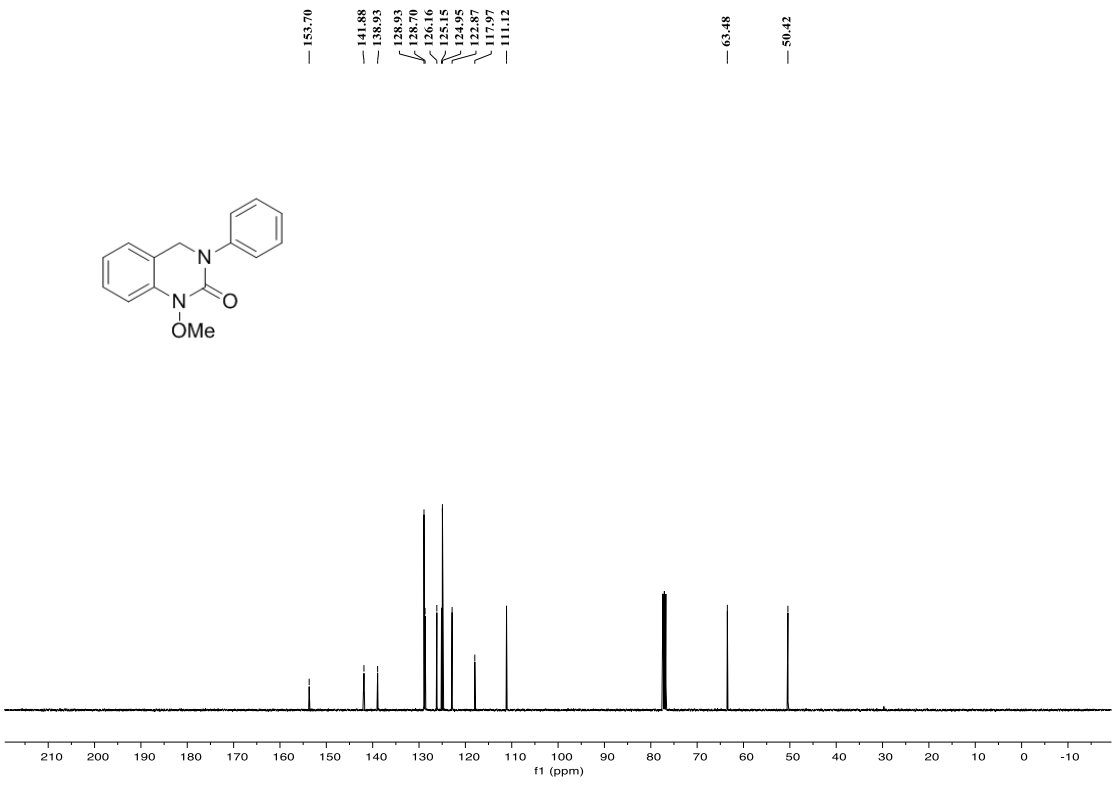
2.00
3.04
f1 (ppm)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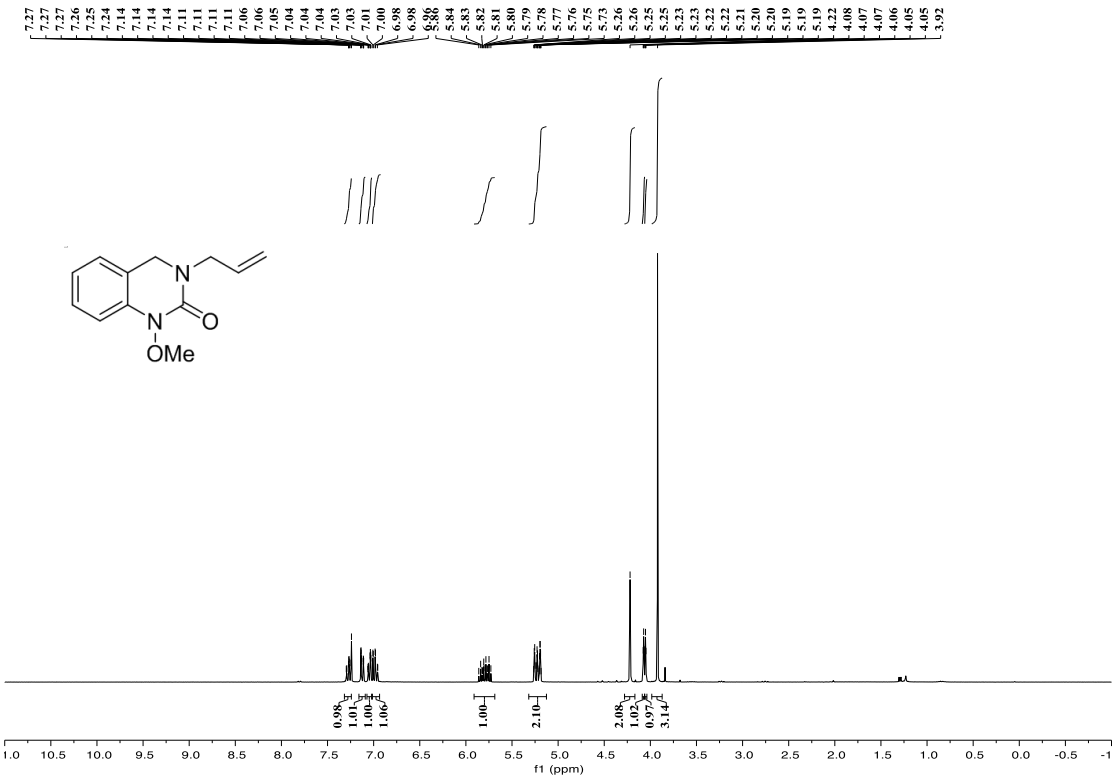
OMe
f1 (ppm)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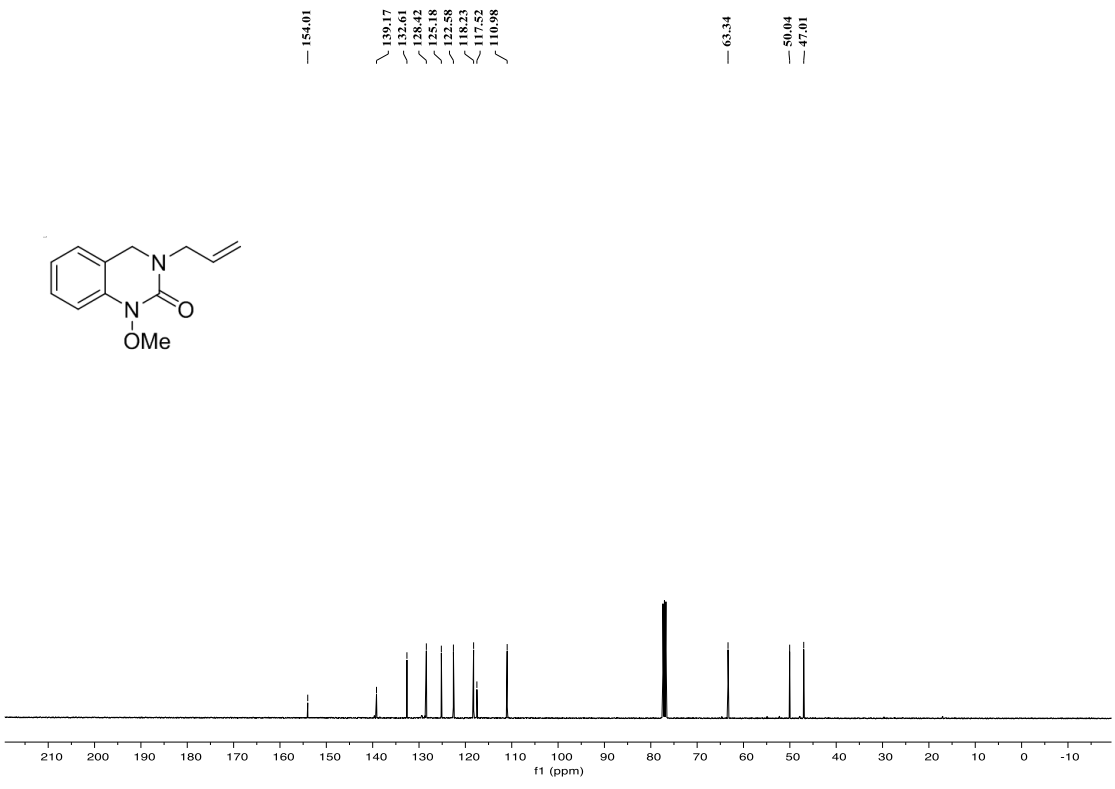
f1 (ppm)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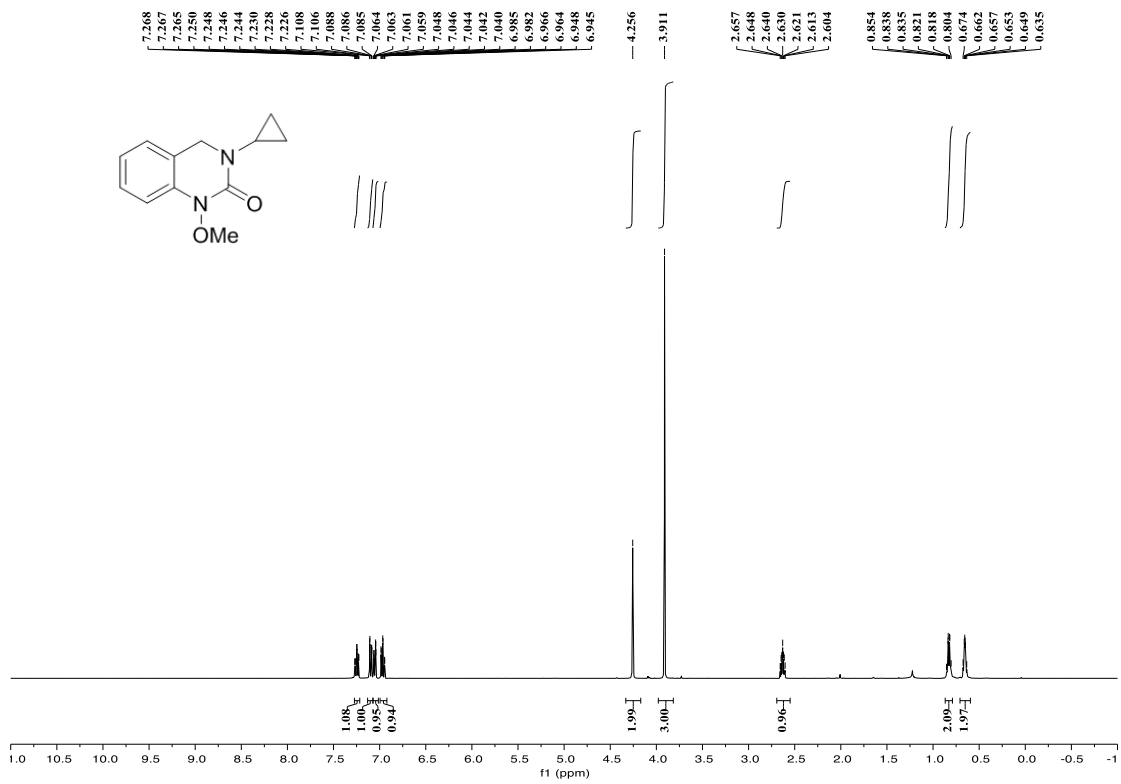
f1 (ppm)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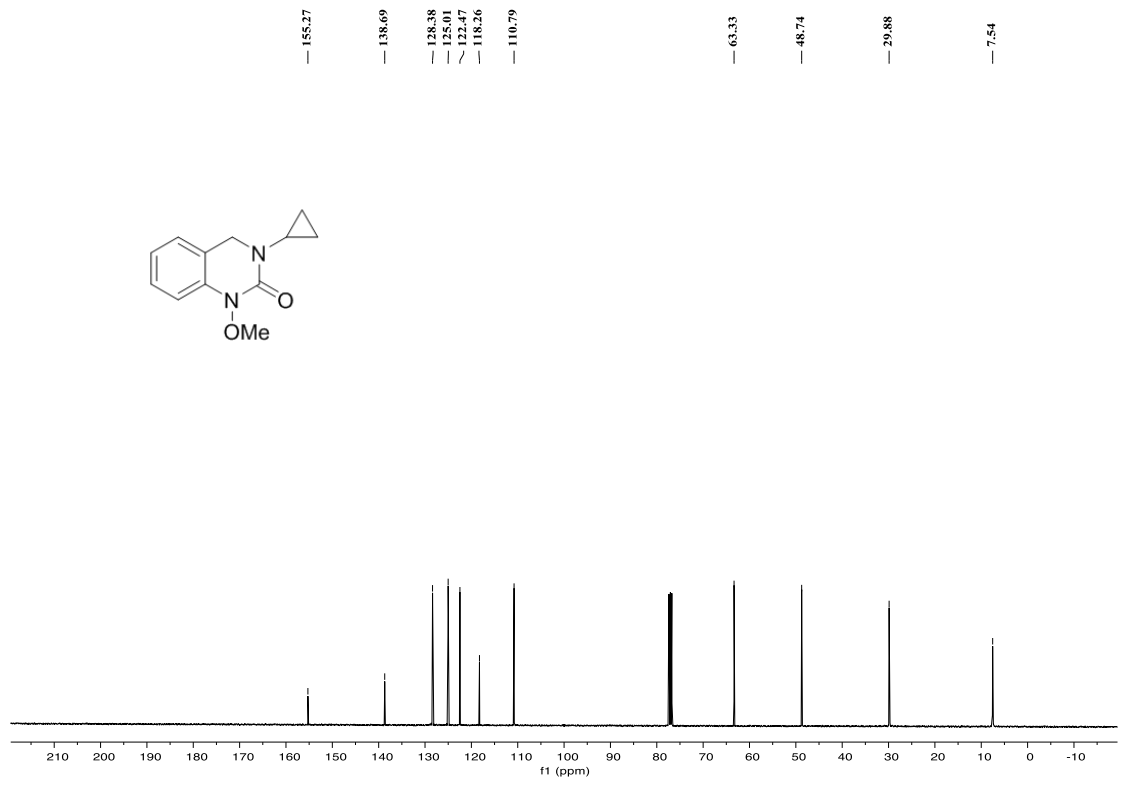
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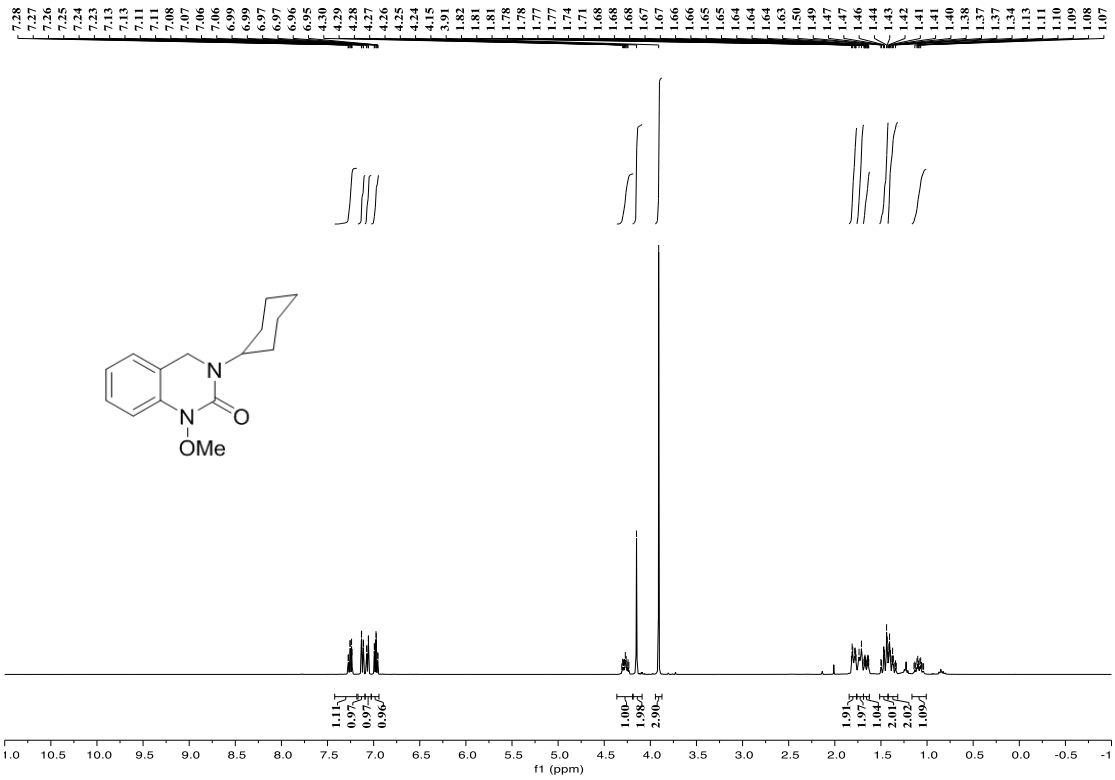
OMe
f1 (ppm)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N
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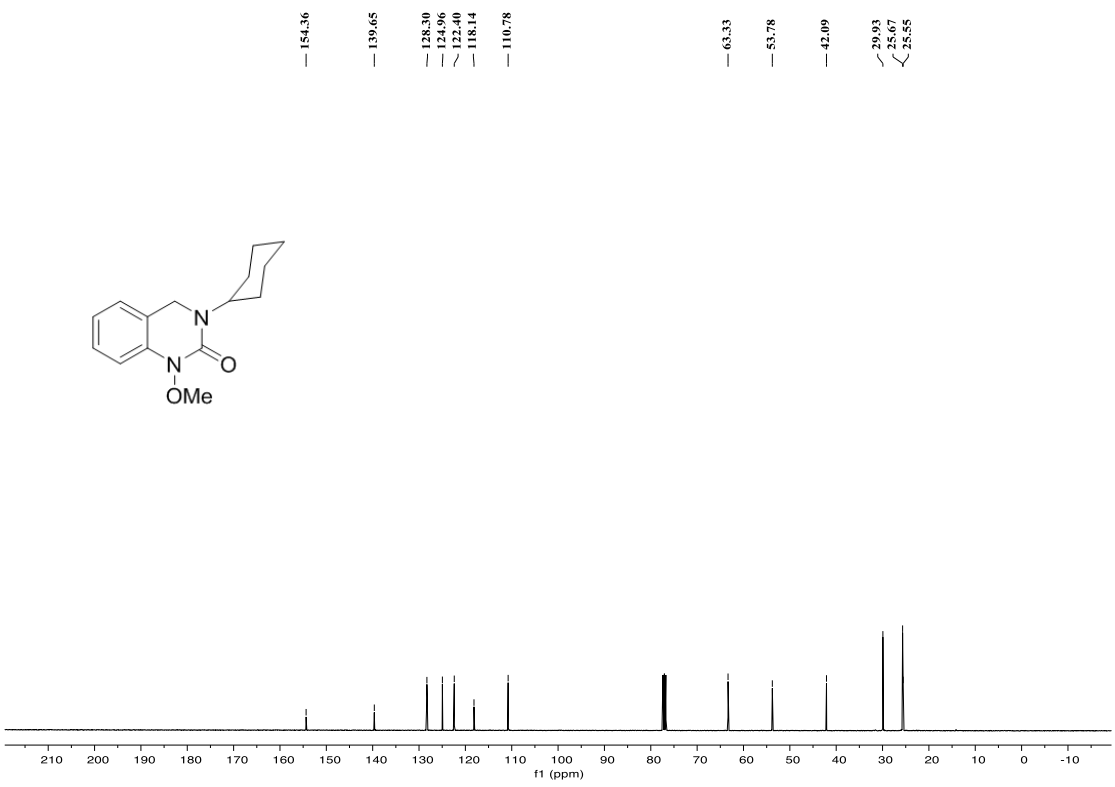
1.00 1.98 2.90
1.91 1.97 1.04 2.01 2.02 1.09
f1 (ppm)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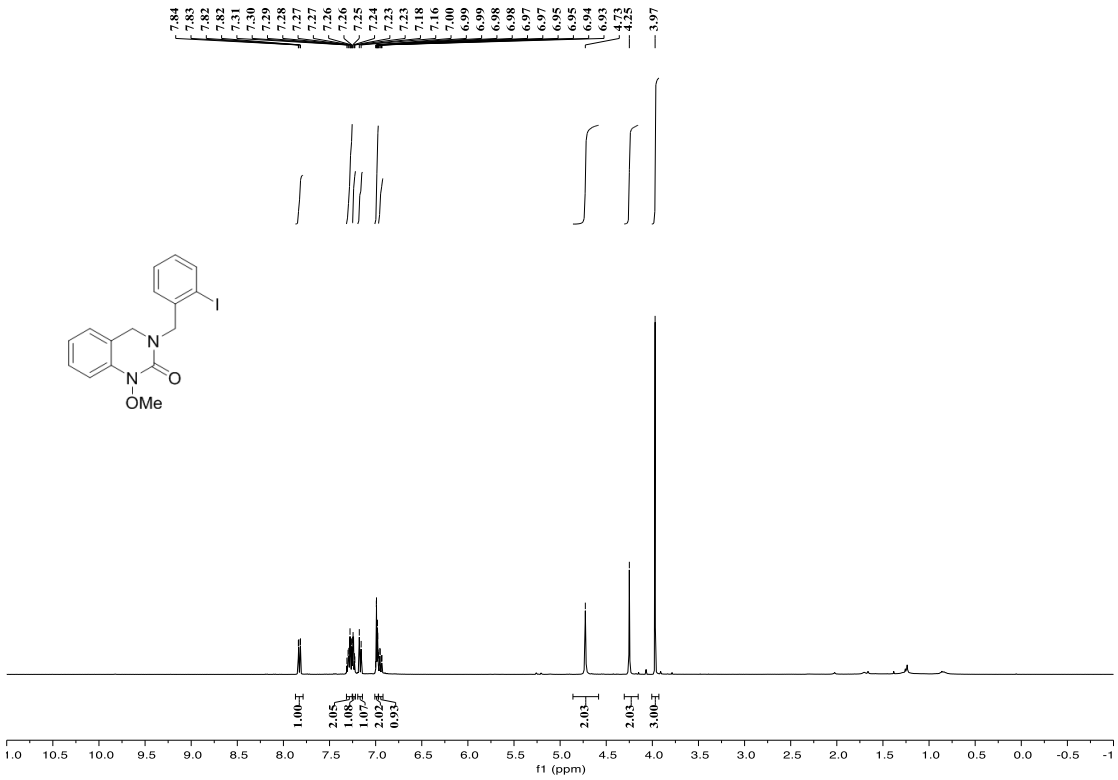
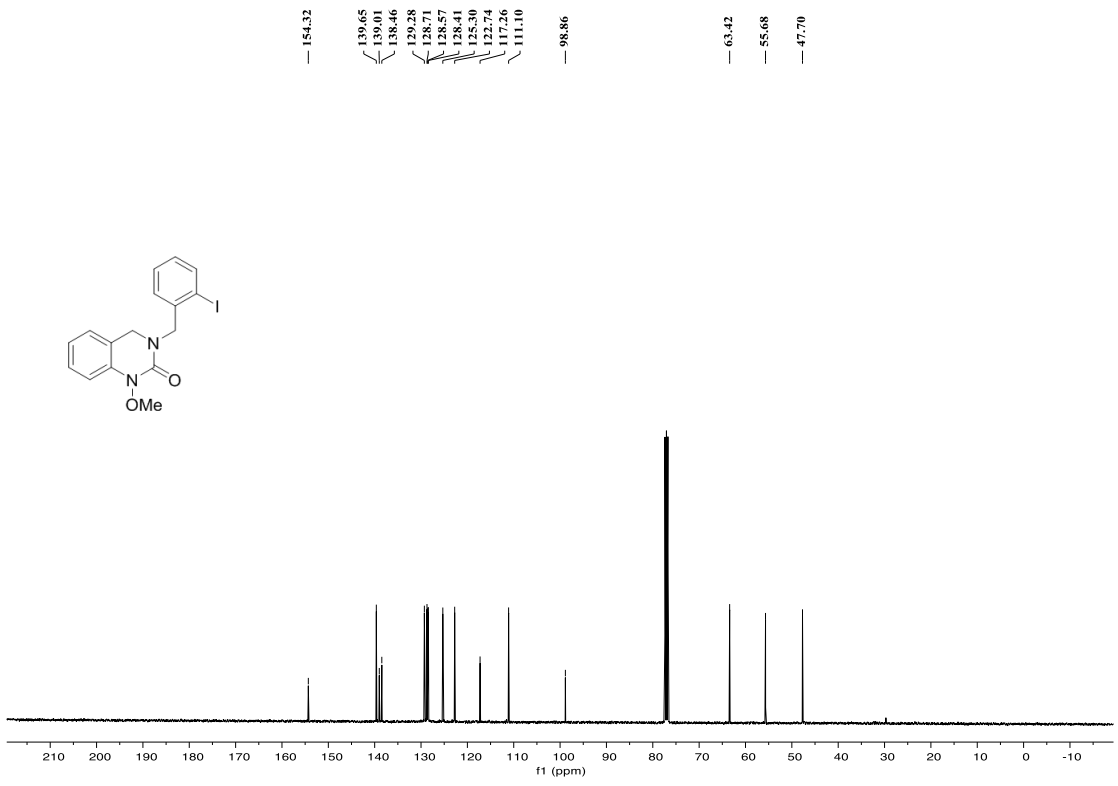
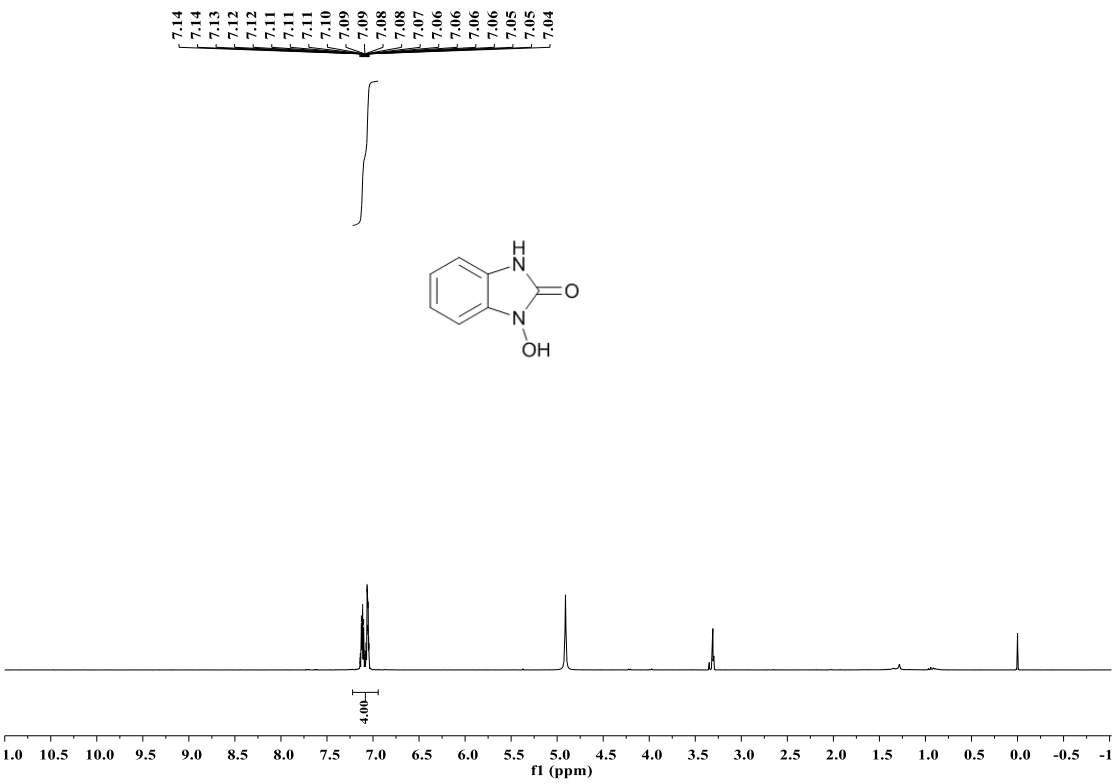
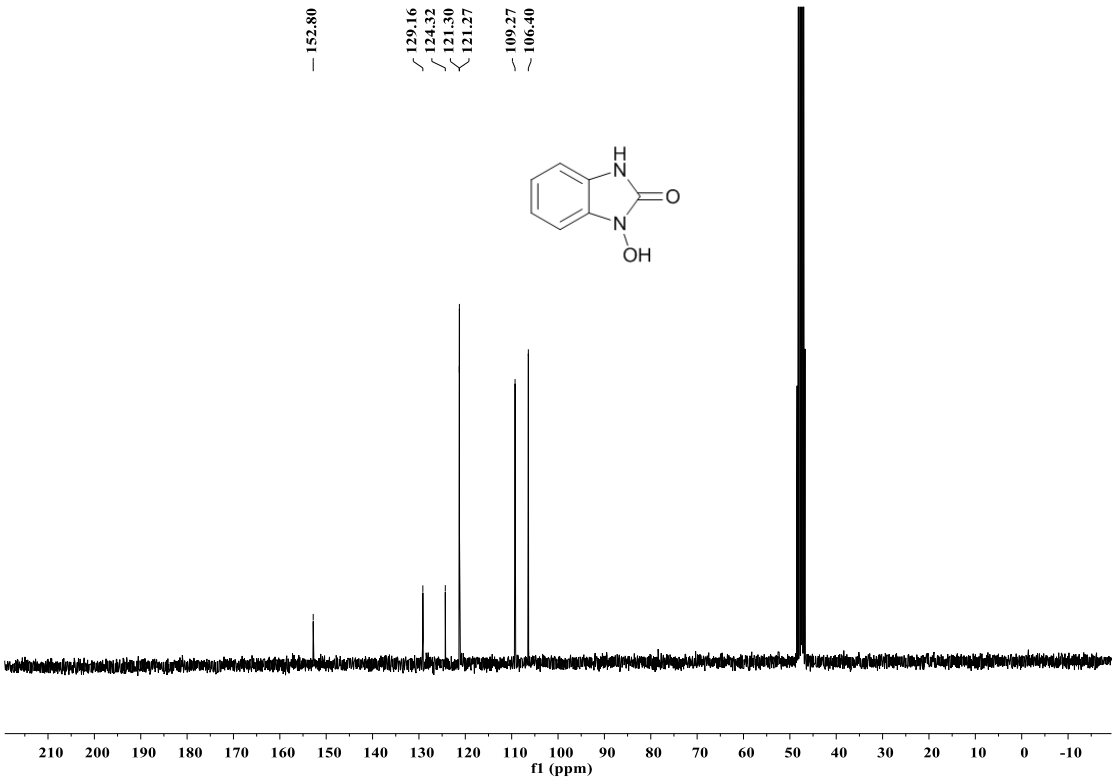
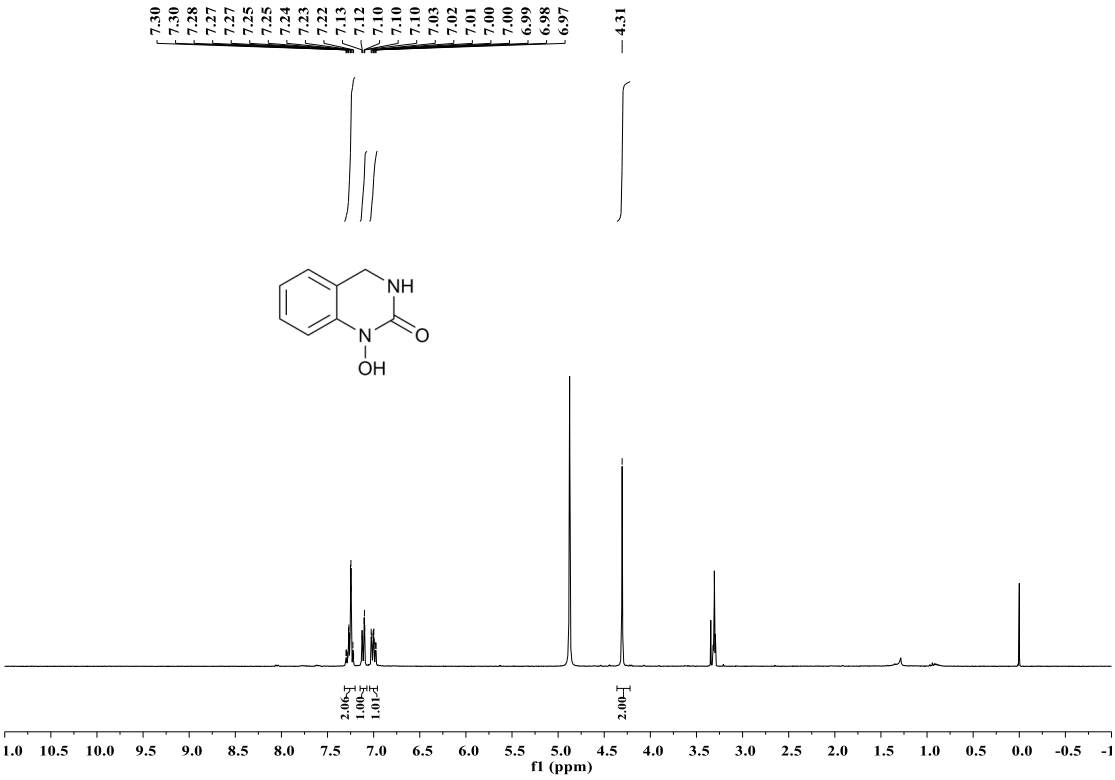
OMe
f1 (ppm)

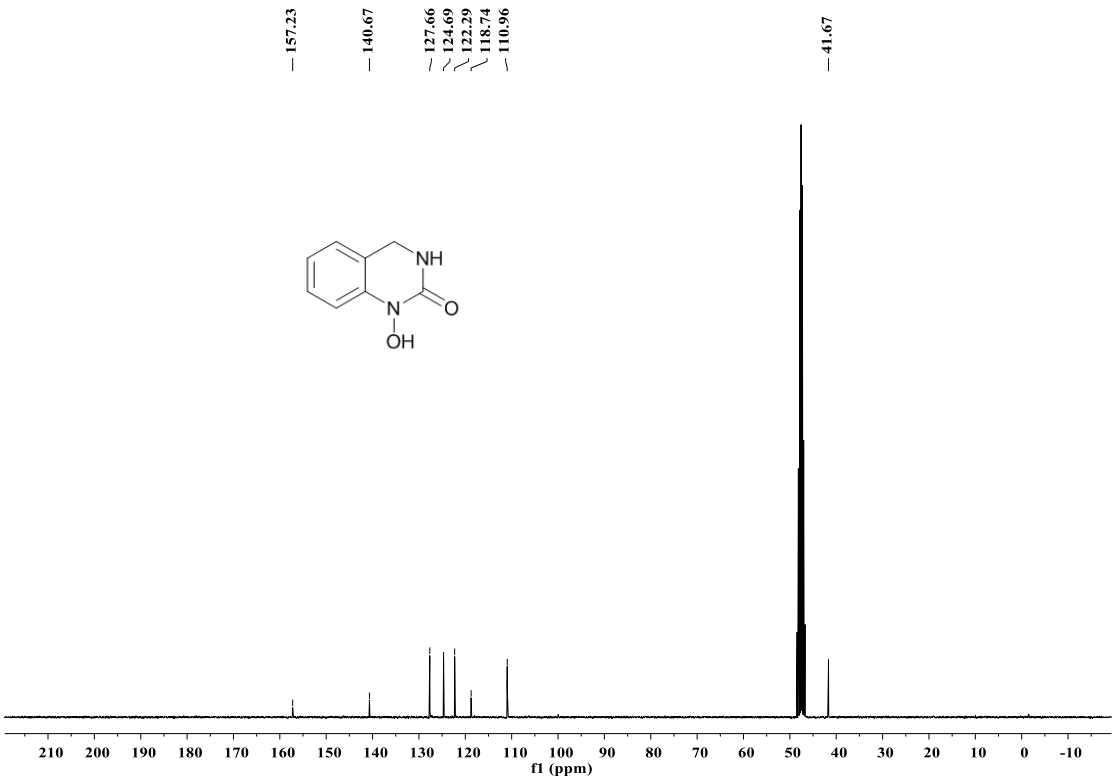

7.84
7.83
7.82
7.82
7.31
7.30
7.29
7.28
7.27
7.27
7.26
7.26
7.25
7.24
7.23
7.23
7.18
7.16
7.00
6.99
6.99
6.98
6.98
6.97
6.97
6.95
6.95
6.94
6.93
4.73
4.25
3.97
I
N
N
O
OMe
1.00
2.05
1.08
1.07
2.02
0.93
2.03
2.03
3.00
f1 (ppm)


154.32
139.65
139.01
138.46
129.28
128.71
128.57
128.41
125.30
122.74
117.26
111.10
98.86
63.42
55.68
47.70
I
N
N
O
OMe
f1 (ppm)


7.14
7.14
7.13
7.12
7.12
7.11
7.11
7.11
7.10
7.09
7.09
7.08
7.08
7.07
7.06
7.06
7.06
7.06
7.05
7.05
7.04
H
N
O
N
OH
4.00
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


152.80
129.16
124.32
121.30
121.27
109.27
106.40
H
N
O
N
OH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.30
7.30
7.28
7.27
7.27
7.25
7.25
7.24
7.23
7.22
7.13
7.12
7.10
7.10
7.10
7.03
7.02
7.01
7.00
7.00
6.99
6.98
6.97
4.31
NH
N
O
OH
2.06
1.00
1.01
2.00
f1 (ppm)


157.23
140.67
127.66
124.69
122.29
118.74
110.96
41.67
NH
N
O
OH
f1 (ppm)

## 10. Full reference of 10:

10. Compound **III**: A. B. Dounay, M. Anderson, B. M. Bechle, B. M. Campbell, M. M. Claffey, A. Evdokimov, E. Evrard, K. R. Fonseca, X. Gan, S. Ghosh, M. M. Hayward, W. Horner, J. Y. Kim, L. A. McAllister, J. Pandit, V. Paradis, V. D. Parikh, M. R. Reese, S. Rong, M. A. Salafia, K. Schuyten, C. A. Strick, J. B. Tuttle, J. Valentine, H. Wang, L. E. Zawadzke and P. R. Verhoest, *ACS. Med. Chem. Lett.,* 2012, **3**, 187.

## 11. Unsuccessful substrates: