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Transition-metal-free Regioselective Construction of 1,5-Diaryl-1,2,3-triazoles through Dehydrative Cycloaddition of Alcohols with Arylazides Mediated by SO_2F_2

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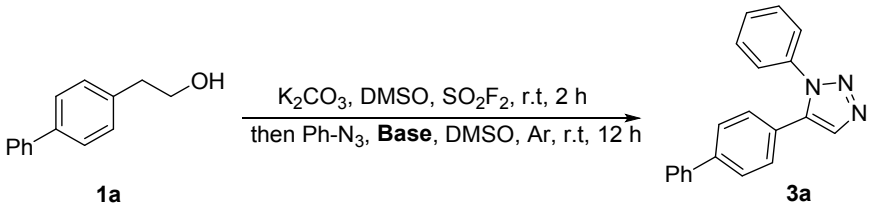
1. General Information

Unless otherwise specified, NMR spectra were recorded in $CDCl_3$ on a 500 MHz (for

^{1}H), 471 MHz (for ^{19}F), 126 MHz (for ^{13}C) spectrometer. All chemical shifts were reported in ppm relative to TMS (^{1}H NMR, 0 ppm) as internal standards. The HPLC experiments were carried out on a Waters e2695 instrument (column: J&K, RP-C18, 5 μm, 4.6 × 150 mm), and the yields of the products were determined by using the corresponding pure compounds as the external standards. The coupling constants were reported in Hertz (Hz). The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad, dd = doublet of doublets. HRMS experiments were performed on a TOF-Q ESI or CI/EI instrument. Melting points were measured and uncorrected. Reagents used in the reactions were all purchased from commercial sources and used without further purification.

2. Screening the Optimized Reaction Conditions for One-Pot Synthesis of 1,5-Disubstituted Triazole

Table 1 Screening the base[a]



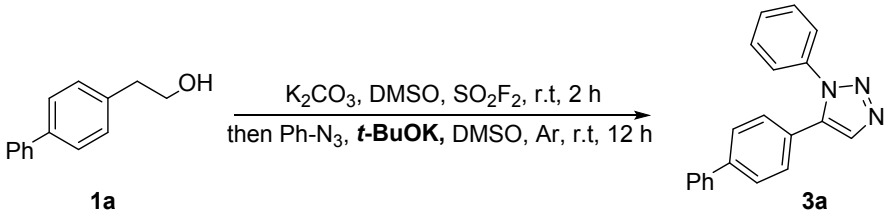
1a **3a**

Entry	Base (2.0 eq.)	Yield (**3a**, %)[b]
1	***t*-BuOK**	**40**
2	CsF	<5
3	KOH	25
4	KNO_3	n.d.

5	KF	n.d.
6	K_2CO_3	<5
7	CH_3COOK	n.d.
8	K_3PO_4	n.d.

[a]Reaction conditions: 4-biphenylethanol (**1a**, 0.4 mmol), K_2CO_3 (0.8 mmol, 2.0 eq.), DMSO (3.0 mL) were added to a reaction tube (10 mL) and SO_2F_2 was introduced into the reaction mixture through a balloon before reacting at room temperature for 2 h. The SO_2F_2 balloon was removed from reaction, phenyl-azide (**2a**, 2 eq.), another base (2.0 eq.) and DMSO (0.5 mL) were subsequently added, then the reaction mixture was allowed to stir at room temperature for 12 h under argon atmosphere. [b]The yield was determined by HPLC using **3a** as the external standard (t_R = 5.509 min, λ_{max} = 276.0 nm, acetonitrile/water = 70 : 30 (v / v)).

Table 2 Screening the amount of base[a]

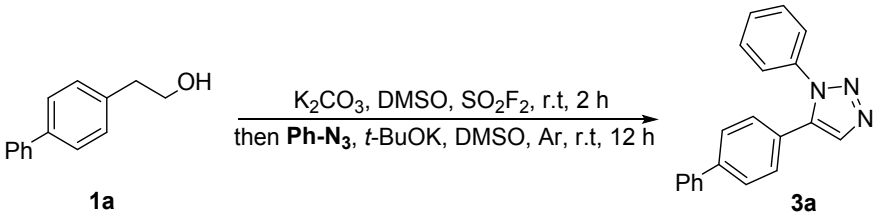


1a **3a**

Entry	*t*-BuOK (X eq.)	Yield (**3a**, %)[b]
1	1.0	<5
2	2.0	40
3	**3.0**	**82**
4	4.0	87
5	4.5	83
6	5.0	68

[a]Reaction conditions: 4-biphenylethanol (**1a**, 0.4 mmol), K_2CO_3 (0.8 mmol, 2.0 eq.), DMSO (3.0 mL) were added to a reaction tube (10 mL) and SO_2F_2 was introduced into the reaction mixture through a balloon before reacting at room temperature for 2 h. The SO_2F_2 balloon was removed from reaction, phenyl azide (**2a**, 2 eq.), *t*-BuOK (X eq.) and DMSO (0.5 mL) were subsequently charged, then the reaction stirred at room temperature for 12 h under argon atmosphere. [b]The yield was determined by HPLC using **3a** as the external standard (t_R = 5.509 min, λ_{max} = 276.0 nm, acetonitrile/water = 70 : 30 (v / v)).

Table 3 Screening the amount of azidobenzene[a]



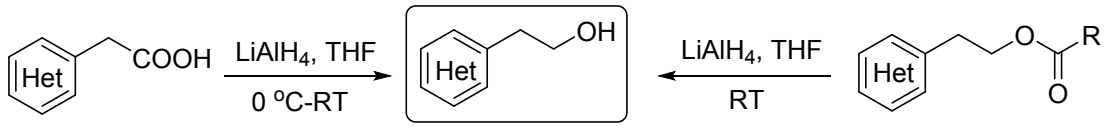
Entry	Ph-N_3 (X eq.)	Yield (**3a**, %)[b]
1	1.0	77
2	**1.5**	**82**
3	2.0	84
4	3.0	73

[a]Reaction conditions: 4-biphenylethanol (**1a**, 0.4 mmol), K_2CO_3 (0.8 mmol, 2.0 eq.), DMSO (3.0 mL) were added to a reaction tube (10 mL) and SO_2F_2 was introduced into the reaction mixture through a balloon before reacting at room temperature for 2 h. The SO_2F_2 balloon was removed from reaction, phenyl azide (**2a**, X eq.), *t*-BuOK (3 eq.) and DMSO (0.5 mL) were subsequently charged, then the reaction stirred at room temperature for 12 h under argon atmosphere. [b]The yield was determined by HPLC using **3a** as the external standard (t_R = 5.509 min, λ_{max} = 276.0 nm, acetonitrile/water = 70 : 30 (v / v)).

3. General Procedures.

3.1 General Procedure for Synthesis Aryl Ethanols.

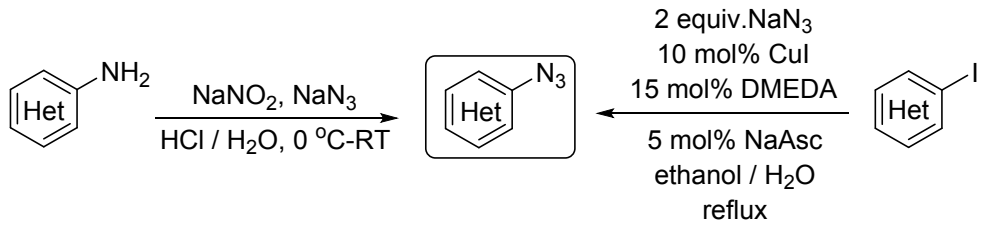
1a and **1c** were prepared according to the literatures.[1,2] **1j-1t** were prepared according to the literatures.[3~9] Others were all purchased from commercial sources and used without further purification.



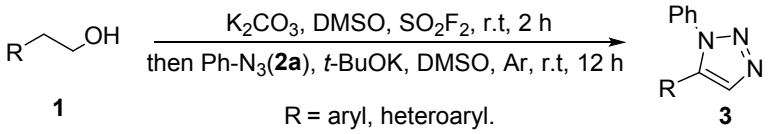
3.2 General Procedure for Synthesis Aryl Azides.

2ba-2bx were all prepared according to the literatures.[10,11] **2by** was prepared according to the literature.[12] (**Caution**: extraction should never be performed with halogenated solvents such as DCM or $CHCl_3$ as these solvents can react with residual sodium azide to form diazidomethane or azidoform which are highly shock sensitive

and energetic explosives.).



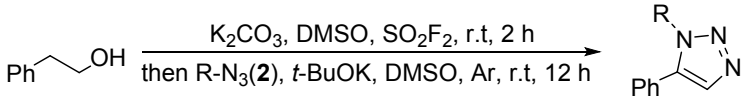
3.3 General Procedure for Synthesis 1,5-Disubstituted Triazole.



1 R = aryl, heteroaryl. **3**

Procedure A

Aryl ethanol (**1**, 1.0 mmol), K_2CO_3 (2.0 mmol, 2.0 eq., 277 mg), DMSO (0.13 M) were added to a reaction tube (25 mL) and SO_2F_2 was introduced into the reaction mixture through a balloon before reacting at room temperature for 2 h, the SO_2F_2 balloon was removed from reaction, then azido benzene (**2a**, 1.5 mmol, 1.5 eq., 179 mg), *t*-BuOK (3 mmol, 3.0 eq., 337 mg) were subsequently added and the mixture was stirred at room temperature for 12 h under argon atmosphere before extracted with ethyl acetate (3×50 mL) and the combined organic layers was dried over anhydrous sodium sulfate, filtered and concentrated under reduced pressure. The crude products were further purified by column chromatography on silica gel by gradient elution with petroleum ether/ethyl acetate (85/15 to 50/50) as eluent to obtain pure triazoles **3**.



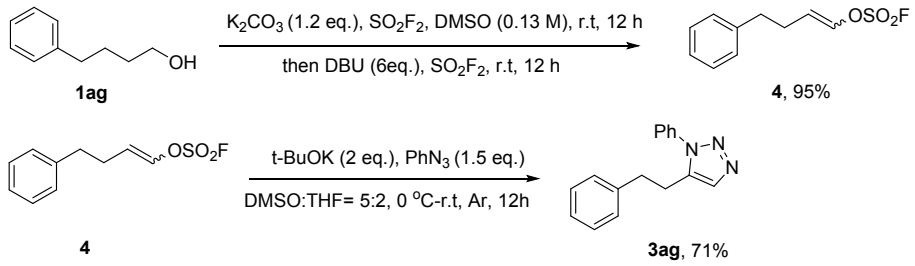
1b R = aryl, heteroaryl **3**

Procedure B

Phenyl ethanol (**1b**, 1.0 mmol), K_2CO_3 (2.0 mmol, 2.0 eq., 277 mg), DMSO (0.13 M) were added to a reaction tube (25 mL) and SO_2F_2 was introduced into the reaction mixture through a balloon before reacting at room temperature for 2 h, the SO_2F_2 balloon was removed from reaction, then aryl azide (**2**, 1.5 mmol, 1.5 eq., 179 mg), *t*-

BuOK (3 mmol, 3.0 eq., 337 mg) were subsequently added and mixture was stirred at room temperature for 12 h under argon atmosphere. The reaction mixture was extracted with ethyl acetate (3×50 mL) and the combined organic layers was dried over anhydrous sodium sulfate, filtered and concentrated under reduced pressure. The crude products were further purified by column chromatography on silica gel by gradient elution with petroleum ether/ethyl acetate (85/15 to 50/50) as eluent to obtain pure triazoles **3**.

3.4 General Procedure for Synthesis 1,5-Disubstituted Triazole through Alkyl Alcohol.



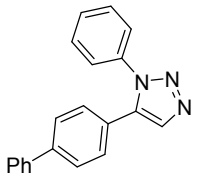
In first step, 4-phenylbutan-1-ol (**1ag**, 1.0 mmol), K_2CO_3 (1.2 mmol, 1.2 eq., 166 mg), DMSO (0.13 M) were added to a reaction tube (25 mL) and SO_2F_2 was introduced into the reaction mixture through a balloon before reacting at room temperature for 12 h, then added DBU (6 eq., 6 mmol, 914 mg) into the reaction tube and SO_2F_2 was introduced into the reaction mixture through a balloon stirred for another 12 h. The reaction mixture was extracted with ethyl acetate (3×50 mL) and the combined organic layers was dried over anhydrous sodium sulfate, filtered and concentrated under reduced pressure. The crude products were further purified by column chromatography on silica gel by gradient elution with petroleum ether/ethyl acetate (90/10 to 80/20) as eluent to obtain isomer **4**.

In second step, 4-phenylbut-1-en-1-yl sulfurofluoridate (**4**, 1 mmol, 230.3 mg) was added to a reaction tube (25 mL), then *t*-BuOK (2 mmol, 2.0 eq., 225 mg) and azido benzene (**2a**, 1.5 mmol, 1.5 eq., 179 mg) were subsequently added at 0 ℃ and mixture was stirred at room temperature for 12 h under argon atmosphere in mixed solvent DMSO : THF = 5:2 (v / v). The reaction mixture was extracted with ethyl acetate

(3×50 mL) and the combined organic layers was dried over anhydrous sodium sulfate, filtered and concentrated under reduced pressure. The crude products were further purified by column chromatography on silica gel by gradient elution with petroleum ether/ethyl acetate (85/15 to 50/50) as eluent to obtain pure triazoles **3ag**.

4. Product Characterization.

5-([1,1'-biphenyl]-4-yl)-1-phenyl-1H-1,2,3-triazole (3a).



3a

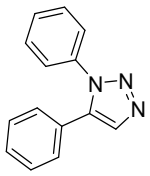
According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Yellow solid, 214 mg, 72% yield, mp 157.8-159.0 °C.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.92 (s, 1H), 7.59-7.57 (m, 4H), 7.47-7.41 (m, 7H), 7.37 (t, J = 7.3 Hz, 1H), 7.30 (d, J = 8.2 Hz, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 142.0, 139.9, 137.5, 136.7, 133.5, 129.5, 129.4, 128.98 128.96, 128.0, 127.5, 127.0, 125.6, 125.3.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{20}H_{15}N_3$: 298.1266, found: 298.1265.

1,5-diphenyl-1H-1,2,3-triazole (3b). [13]

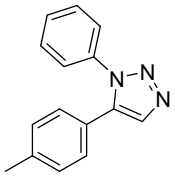


3b

According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Yellow solid, 190 mg, 86% yield, mp 104.0-106.0 ℃ (lit. 113-114 ℃).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 (s, 1H), 7.44-7.41 (m, 3H), 7.38-7.32 (m, 5H), 7.23-7.21 (m, 2H).

1-phenyl-5-(p-tolyl)-1H-1,2,3-triazole (3c). [16]

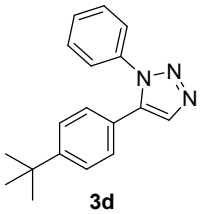


3c

According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Yellow solid, 183 mg, 78% yield, mp 142.0-143.5 ℃ (lit. 141-142 ℃).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (s, 1H), 7.45-7.43 (m, 3H), 7.38-7.36 (m, 2H), 7.16-7.11 (m, 4H), 2.36 (s, 3H).

5-(4-(tert-butyl) phenyl)-1-phenyl-1H-1,2,3-triazole (3d).



3d

According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Orange liquid, 140 mg, 51% yield, mp 157.0-158.0 °C.

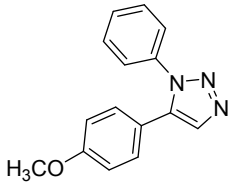
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (s, 1H), 7.45-7.43 (m, 3H), 7.39-7.34 (m, 4H), 7.15 (d, J = 8.3 Hz, 2H), 1.31 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 152.5, 137.8, 136.8, 133.3, 129.4, 129.3, 128.2, 125.9,

125.3, 123.7, 34.8, 31.2.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{18}H_{19}N_3$: 278.3710, found: 278.3712.

5-(4-methoxyphenyl)-1-phenyl-1H-1,2,3-triazole (3e). [16]

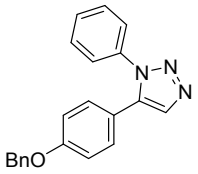


3e

According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Orange liquid, 226 mg, 90% yield, mp 61.0-63.0 ℃ (lit. 97-98 ℃).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79 (s, 1H), 7.43-7.42 (m, 3H), 7.37-7.35 (m, 2H), 7.13 (d, J = 8.7 Hz, 2H), 6.85 (d, J = 8.7 Hz, 2H), 3.79 (s, 3H).

5-(4-(benzyloxy) phenyl)-1-phenyl-1H-1,2,3-triazole (3f).



3f

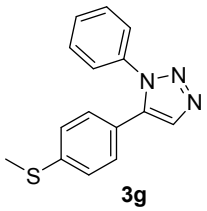
According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Yellow solid, 186 mg, 57% yield, mp 95.8-97.3 °C.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.81 (s, 1H), 7.45-7.34 (m, 10H), 7.15 (dt, J_1 = 8.8 Hz, J_2 = 2.8 Hz, 2H), 6.94 (dt, J_1 = 8.9 Hz, J_2 = 2.6 Hz, 2H), 5.06 (s, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 159.5, 137.6, 136.7, 136.4, 133.0, 130.0, 129.4, 129.2, 128.7, 128.2, 127.5, 125.3, 119.2, 115.2, 70.1.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{21}H_{17}N_3O$: 328.1372, found: 328.1370.

5-(4-(methylthio) phenyl)-1-phenyl-1H-1,2,3-triazole (3g).



3g

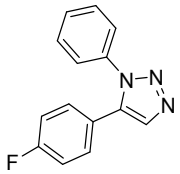
According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Yellow solid, 165 mg, 62% yield, mp 103.8-105.3 °C.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 (s, 1H), 7.43 (t, J = 2.5 Hz, 3H), 7.36-7.34 (m, 2H), 7.19-7.15 (m, 2H), 7.11 (d, J = 8.6 Hz, 2H), 2.45 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 140.7, 137.4, 136.6, 133.2, 129.5, 129.3, 128.8, 126.1, 125.3, 122.9, 15.1.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{15}H_{13}N_3S$: 268.0830, found: 268.0830.

5-(4-fluorophenyl)-1-phenyl-1H-1,2,3-triazole (3h). [15]



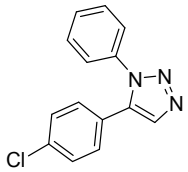
3h

According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Yellow solid, 175 mg, 74% yield, mp 89.0-91.0 ℃ (lit. 100-103 ℃).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 (s, 1H), 7.43-7.33 (m, 5H), 7.21-7.16 (m, 2H), 7.03 (t, J = 8.4 Hz, 2H).

^{19}F NMR (471 MHz, $CDCl_3$) δ –110.9- –111.0 (m, Ar-F).

5-(4-chlorophenyl)-1-phenyl-1H-1,2,3-triazole (3i). [16]

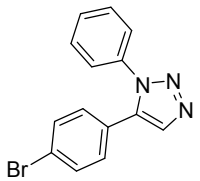


3i

According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Orange solid, 190 mg, 75% yield, mp 114.0-116.0 ℃ (lit. 105-106 ℃).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (s, 1H), 7.45-7.42 (m, 3H), 7.34-7.30 (m, 4H), 7.15 (d, J = 8.3 Hz, 2H).

5-(4-bromophenyl)-1-phenyl-1H-1,2,3-triazole (3j). [13]

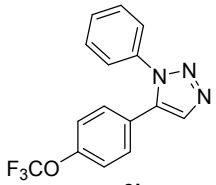


3j

According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Yellow solid, 178 mg, 60% yield, mp 139.5-141.5 ℃ (lit. 151-152 ℃).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.49-7.44 (m, 5H), 7.36-7.34 (m, 2H), 7.09 (dt, J_1 = 8.4 Hz, J_2 = 1.7 Hz, 2H).

1-phenyl-5-(4-(trifluoromethoxy) phenyl)-1H-1,2,3-triazole (3k).



3k

According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Orange liquid, 175 mg, 58% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.47-7.43 (m, 3H), 7.36-7.34 (m, 2H), 7.27-7.25 (m, 2H), 7.19 (d, J = 8.2 Hz, 2H).

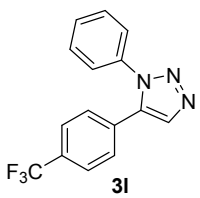
^{13}C NMR (126 MHz, $CDCl_3$) δ 149.8, 136.4 (d, J = 22.7 Hz), 133.6, 130.2, 129.6, 125.4, 125.3, 121.2.

In the ^{13}C NMR spectrum of **3k**, theoretically, there should be eleven peaks. Due to the compact overlaying, it is difficult to specify the overlaying peaks.

^{19}F NMR (471 MHz, $CDCl_3$) δ –57.8 (s, 3F).

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{15}H_{10}F_3N_3O$: 306.0776, found: 306.0770.

1-phenyl-5-(4-(trifluoromethyl)phenyl)-1H-1,2,3-triazole (3l).



3l

According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as

eluent for column chromatography. Orange liquid, 140 mg, 49% yield.

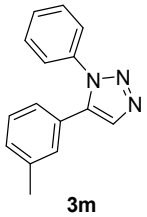
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.91 (s, 1H), 7.59 (d, J = 8.3 Hz, 2H), 7.47-7.43 (m, 3H), 7.36-7.33 (m, 4H).

^{19}F NMR (471 MHz, $CDCl_3$) δ –62.9 (s, 3F).

^{13}C NMR (126 MHz, $CDCl_3$) δ 136.4, 136.3, 133.8, 131.4, 131.1, 130.4, 129.64, 129.61, 128.9, 125.9 (q, J = 3.6 Hz), 125.3, 124.8, 122.6.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{15}H_{10}F_3N_3$: 290.0827, found: 290.0830.

1-phenyl-5-(m-tolyl)-1H-1,2,3-triazole (3m). [15]

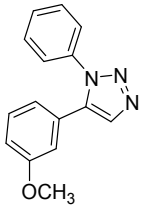


3m

According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Orange solid, 173 mg, 74% yield, mp 104.0-106.0 ℃ (lit. 109-113 ℃).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (s, 1H), 7.44-7.42 (m, 3H), 7.38-7.36 (m, 2H), 7.21-7.18 (m, 2H), 7.08 (s, 1H), 6.96 (d, J = 7.4 Hz, 1H), 2.30 (s, 3H).

5-(3-methoxyphenyl)-1-phenyl-1H-1,2,3-triazole (3n).



3n

According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Yellow solid, 189 mg, 76% yield, mp 95.5-97.0 °C.

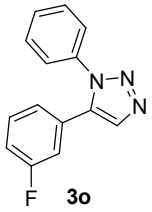
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (s, 1H), 7.44-7.43 (m, 3H), 7.38-7.36 (m, 2H), 7.24 (t, J = 8.0 Hz, 1H), 6.89 (dd, J_1 = 8.3 Hz, J_2 = 2.0 Hz, 1H), 6.80 (d, J = 7.6 Hz, 1H), 6.72 (t, J = 1.9 Hz, 1H), 3.67 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 159.7, 137.6, 136.6, 133.4, 130.0, 129.4, 129.3, 127.9,

125.3, 121.0, 115.0, 114.0, 55.2.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{15}H_{13}N_3O$: 252.1059, found: 252.1050.

5-(3-fluorophenyl)-1-phenyl-1H-1,2,3-triazole (3o).



3o

According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Yellow solid, 172 mg, 72% yield, mp 116.0-117.2 °C.

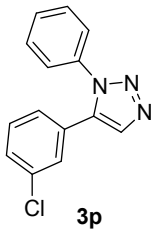
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.45-7.44 (m, 3H), 7.35-7.28 (m, 3H), 7.05 (t, J = 7.7 Hz, 1H), 7.00 (d, J = 7.5 Hz, 1H), 6.91 (d, J = 9.4 Hz, 1H).

^{19}F NMR (471 MHz, $CDCl_3$) δ –111.30- –111.35 (m, Ar-F).

^{13}C NMR (126 MHz, $CDCl_3$) δ 162.6 (d, J = 247.9 Hz), 136.60, 136.58, 136.3, 133.6, 130.7 (d, J = 9.1 Hz), 129.5 (d, J = 2.8 Hz), 128.7 (d, J = 8.1 Hz), 125.2, 124.4 (d, J = 2.7 Hz), 116.3 (d, J = 20.8 Hz), 115.5 (d, J = 23.6 Hz).

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{14}H_{10}FN_3$: 240.0859, found: 240.0860.

5-(3-chlorophenyl)-1-phenyl-1H-1,2,3-triazole (3p). [15]

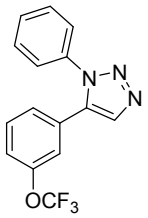


3p

According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Orange solid, 186 mg, 73% yield, 78.0-80.0 ℃, (lit. 85-87 ℃).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 (s, 1H), 7.47-7.44 (m, 3H), 7.36-7.34 (m, 3H), 7.26 (t, J = 7.8 Hz, 2H), 7.06 (d, J = 7.8 Hz, 1H).

1-phenyl-5-(3-(trifluoromethoxy) phenyl)-1H-1,2,3-triazole (3q).



3q

According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Red liquid, 150 mg, 50% yield.

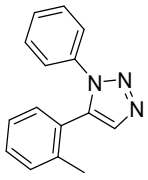
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.91 (s, 1H), 7.49-7.44 (m, 3H), 7.39 (t, J = 8.1 Hz, 1H), 7.35 (d, J = 7.7 Hz, 2H), 7.21 (t, J = 8.1 Hz, 2H), 7.03 (s, 1H).

^{19}F NMR (471 MHz, $CDCl_3$) δ –57.97 (s, 3F).

^{13}C NMR (126 MHz, $CDCl_3$) δ 149.3, 136.2 (d, J = 17.2 Hz), 133.6, 130.5, 129.64, 129.58, 129.3, 128.7, 126.9, 125.3, 125.2, 121.7, 121.0.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{15}H_{10}F_3N_3O$: 306.0776, found: 306.0776.

1-phenyl-5-(o-tolyl)-1H-1,2,3-triazole (3r). [16]

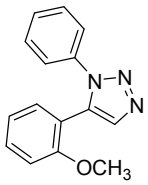


3r

According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Orange solid, 200 mg, 86% yield, mp 61.0-63.0 ℃ (lit. 81-82 ℃).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.75 (s, 1H), 7.32-7.28 (m, 6H), 7.20-7.14 (m, 3H), 1.96 (s, 3H).

5-(2-methoxyphenyl)-1-phenyl-1H-1,2,3-triazole (3s). [15]



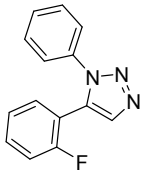
3s

According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Orange solid, 185 mg, 74% yield, mp 86.5-88.0

℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 (s, 1H), 7.39-7.30 (m, 6H), 7.23 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 6.97 (td, J_1 = 7.7 Hz, J_2 = 0.9 Hz, 1H), 6.83 (d, J = 8.3 Hz, 1H), 3.40 (s, 3H).

5-(2-fluorophenyl)-1-phenyl-1H-1,2,3-triazole (3t). [17]



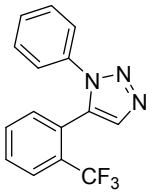
3t

According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Yellow solid, 181 mg, 76% yield, mp 103.0-105.0 ℃ (lit. 97-99 ℃).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.91 (s, 1H), 7.41-7.33 (m, 6H), 7.19-7.07 (m, 3H).

^{19}F NMR (471 MHz, $CDCl_3$) δ –111.87- –111.92 (m, Ar-F).

1-phenyl-5-(2-(trifluoromethyl)phenyl)-1H-1,2,3-triazole (3u).



3u

According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Orange solid, 100 mg, 35% yield.

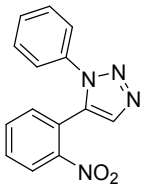
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (s, 1H), 7.79 (d, J = 7.6 Hz, 1H), 7.54 (t, J = 7.6 Hz, 1H), 7.49 (t, J = 7.5 Hz, 1H), 7.35-7.33 (m, 3H), 7.30-7.27 (m, 2H), 7.15 (d, J = 7.5 Hz, 1H).

^{19}F NMR (471 MHz, $CDCl_3$) δ –58.7 (s, 3F).

^{13}C NMR (126 MHz, $CDCl_3$) δ 136.3, 135.2, 134.1, 132.7, 131.8, 130.1, 129.8, 129.3 129.1, 126.7 (q, J = 3.5 Hz), 125.9, 124.6, 122.3.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{15}H_{10}F_3N_3$: 290.0827, found: 290.0827.

5-(2-nitrophenyl)-1-phenyl-1H-1,2,3-triazole (3v).[26]

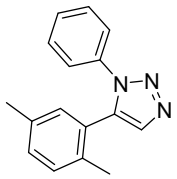


3v

According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Black solid, 45 mg, 17% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.24 (s, 1H), 8.12 (d, J = 7.7 Hz, 1H), 7.85 (d, J = 8.1 Hz, 1H), 7.78 (d, J = 7.9 Hz, 2H), 7.70 (t, J = 7.5 Hz, 1H), 7.54 (q, J = 8.2 Hz, 3H), 7.47 (t, J = 7.3 Hz, 1H).

5-(2,5-dimethylphenyl)-1-phenyl-1H-1,2,3-triazole (3w).



3w

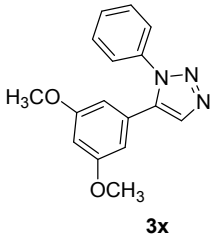
According to general procedure A, 4 eq. *t*-BuOK was used, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Yellow solid, 150 mg, 61% yield, mp 121.8-123.2 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (s, 1H), 7.36-7.31 (m, 5H), 7.13 (d, J = 7.2 Hz, 1H), 7.08 (d, J = 7.7 Hz, 1H), 7.02 (s, 1H), 2.30 (s, 3H), 1.89 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 137.1, 136.9, 135.8, 134.4, 134.1, 131.0, 130.61, 130.57, 129.2, 128.7, 126.6, 123.7, 20.8, 19.3.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{16}H_{15}N_3$: 250.1266, found: 250.1260.

5-(3,5-dimethoxyphenyl)-1-phenyl-1H-1,2,3-triazole (3x).



3x

According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Yellow solid, 190 mg, 68% yield, mp 148.0-149.2

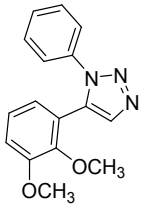
℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (s, 1H), 7.44-7.37 (m, 5H), 6.43 (s, 1H), 6.32 (d, J = 2.0 Hz, 2H), 3.64 (s, 6H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 160.9, 137.7, 136.7, 133.3, 129.4, 129.3, 128.3, 125.3, 106.7, 101.3, 55.3.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{16}H_{15}N_3O_2$: 282.1164, found: 282.1160.

5-(2,3-dimethoxyphenyl)-1-phenyl-1H-1,2,3-triazole (3y).



3y

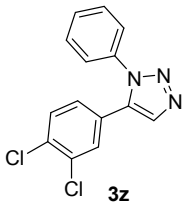
According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Orange solid, 126 mg, 45% yield, mp 78.5-80.0 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 (s, 1H), 7.37 (s, 5H), 7.03 (t, J = 8.0 Hz, 1H), 6.97 (d, J = 8.0 Hz, 1H), 6.73 (d, J = 7.7 Hz, 1H), 3.85 (s, 3H), 3.51 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 153.0, 147.0, 137.2, 134.7, 134.1, 129.2, 128.9, 124.2, 124.1, 122.6, 121.4, 114.0, 60.5, 55.9.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{16}H_{15}N_3O_2$: 282.1164, found: 282.1164.

5-(3,4-dichlorophenyl)-1-phenyl-1H-1,2,3-triazole (3z).



3z

According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Orange solid, 130 mg, 45% yield, mp 125.3-126.7 °C.

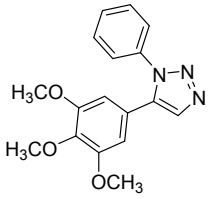
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.49 (d, J = 5.2 Hz, 3H), 7.41-7.36 (m, 4H), 7.00 (d, J = 7.5 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 136.1, 135.6, 133.8, 133.7, 133.3, 131.0, 130.3, 129.8,

129.7, 127.7, 126.7, 125.2.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{14}H_9Cl_2N_3$: 290.0174, found: 290.0170.

1-phenyl-5-(3,4,5-trimethoxyphenyl)-1H-1,2,3-triazole (3aa).



3aa

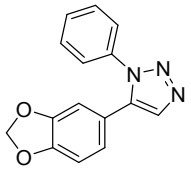
According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Orange liquid, 127 mg, 41% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (s, 1H), 7.46-7.45 (m, 3H), 7.39-7.38 (m, 2H), 6.38 (s, 2H), 3.84 (s, 3H), 3.65 (s, 6H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 153.4, 138.8, 137.8, 136.7, 132.9, 129.4, 129.3, 125.5, 121.8, 105.9, 60.9, 56.0.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{17}H_{17}N_3O_3$: 312.1270, found: 312.1270.

5-(benzo[d] [1,3] dioxol-5-yl)-1-phenyl-1H-1,2,3-triazole (3ab).



3ab

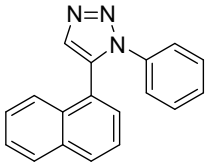
According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Orange solid, 195 mg, 74% yield, mp 133.0-134.5 °C.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79 (s, 1H), 7.44 (t, J = 3.4 Hz, 3H), 7.38-7.36 (m, 2H), 6.77 (d, J = 8.1 Hz, 1H), 6.73 (dd, J_1 = 8.3 Hz, J_2 = 1.7 Hz, 1H), 6.63 (d, J = 1.6 Hz, 1H), 5.98 (s, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 148.5, 148.1, 137.6, 136.6, 133.2, 129.4 (d, J = 17.2 Hz), 125.2, 122.9, 121.9, 120.2, 109.4, 108.8 (d, J = 7.3 Hz), 101.6.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{15}H_{11}N_3O_2$: 266.0851, found: 266.0850.

5-(naphthalen-1-yl)-1-phenyl-1H-1,2,3-triazole (3ac). [14]

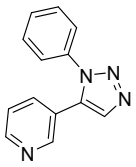


3ac

According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Yellow liquid, 200 mg, 74% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (s, 1H), 7.92 (d, J = 8.2 Hz, 1H), 7.89 (d, J = 8.1 Hz, 1H), 7.64 (d, J = 8.2 Hz, 1H), 7.50 (td, J_1 = 6.9 Hz, J_2 = 1.1 Hz, 1H), 7.44 (td, J_1 = 7.2 Hz, J_2 = 1.5 Hz, 2H), 7.32-7.22 (m, 6H).

3-(1-phenyl-1H-1,2,3-triazol-5-yl) pyridine (3ad).



3ad

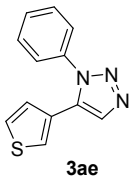
According to general procedure A, 4 eq. *t*-BuOK was used, petroleum ether / ethyl acetate = 50 : 50 (v / v) as eluent for column chromatography. Yellow solid, 115 mg, 72% yield, mp 152.9-154.0 °C.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.57 (dd, J_1 = 4.9 Hz, J_2 = 1.4 Hz, 1H), 8.51 (d, J = 1.7 Hz, 1H), 7.91 (s, 1H), 7.48-7.41 (m, 4H), 7.33-7.31 (m, 2H), 7.24 (t, J = 4.1 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 150.3, 149.1, 136.1, 135.7, 134.7, 133.7, 130.0, 129.7, 125.3, 123.5, 123.2.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{13}H_{10}N_4$: 223.0905, found: 223.0900.

1-phenyl-5-(thiophen-3-yl)-1H-1,2,3-triazole (3ae).



3ae

According to general procedure A, 4 eq. *t*-BuOK was used, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Orange solid, 155 mg, 69% yield, mp 89.5-91.0 ℃.

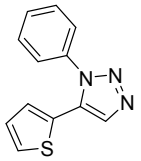
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.48 (d, J = 5.5 Hz, 3H), 7.41-7.40 (m,

2H), 7.32-7.31 (m, 1H), 7.14 (s, 1H), 6.92 (d, J = 4.8 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 136.7, 133.6, 132.8, 129.7, 129.5, 127.0, 126.8, 126.7, 125.6, 124.7.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{12}H_9N_3S$: 228.0517, found: 228.0515.

1-phenyl-5-(thiophen-2-yl)-1H-1,2,3-triazole (3af). [18]

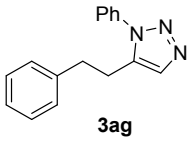


3af

According to general procedure A, 4 eq. *t*-BuOK was used, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Orange solid, 186 mg, 82% yield, mp 97.5-99.0 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.53-7.48 (m, 3H), 7.42 (d, J = 7.2 Hz, 2H), 7.34 (d, J = 5.0 Hz, 1H), 6.98 (t, J = 3.8 Hz, 1H), 6.92 (d, J = 3.3 Hz, 1H).

5-phenethyl-1-phenyl-1H-1,2,3-triazole (3ag).



3ag

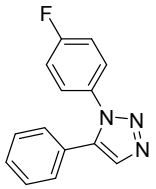
According to **general procedure 3.4**, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Orange solid, 167 mg, 67% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69-7.67 (m, 2H), 7.56 (s, 1H), 7.52-7.48 (m, 2H), 7.43-7.40 (m, 1H), 7.32-7.29 (m, 2H), 7.24-7.21 (m, 3H), 3.16-3.13 (m, 2H), 3.09-3.06 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 148.0, 141.1, 137.3, 129.7, 128.53, 128.50, 126.2, 120.4, 119.2, 35.5, 27.5.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{16}H_{15}N_3$: 250.1266, found: 250.1260.

1-(4-fluorophenyl)-5-phenyl-1H-1,2,3-triazole (3ba). [22]



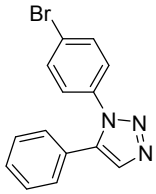
3ba

According to general procedure B, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Yellow solid, 190 mg, 80% yield, mp 155.0-157.0 ℃ (lit. 140-141 ℃).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (s, 1H), 7.40-7.33 (m, 5H), 7.21 (d, J = 6.9 Hz, 2H), 7.12 (t, J = 8.4 Hz, 2H).

^{19}F NMR (471 MHz, $CDCl_3$) δ –111.12- –111.18 (m, Ar-F).

1-(4-bromophenyl)-5-phenyl-1H-1,2,3-triazole (3bb). [21]

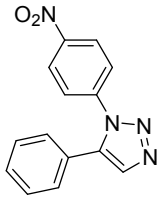


3bb

According to general procedure B, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Orange solid, 272 mg, 91% yield, mp 88.0-90.0 ℃ (lit. 100-102 ℃).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (s, 1H), 7.52 (d, J = 8.5 Hz, 2H), 7.35 (q, J = 7.2 Hz, 3H), 7.23-7.20 (m, 4H).

1-(4-nitrophenyl)-5-phenyl-1H-1,2,3-triazole (3bc). [22]



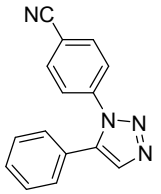
3bc

According to general procedure B, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Red solid, 185 mg, 70% yield, mp 151.0-153.0 ℃, (lit. 164-165 ℃).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.29 (d, J = 8.9 Hz, 2H), 7.88 (s, 1H), 7.58 (d, J = 8.9

Hz, 2H), 7.47-7.40 (m, 3H), 7.24 (d, *J* = 7.3 Hz, 2H).

4-(5-phenyl-1H-1,2,3-triazol-1-yl) benzonitrile (3bd). [23]

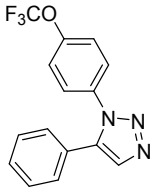


3bd

According to general procedure B, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Orange solid, 170 mg, 70% yield, mp 115.0-117.0 °C.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.75-7.70 (m, 2H), 7.52 (d, *J* = 8.5 Hz, 2H), 7.46-7.39 (m, 3H), 7.23 (d, *J* = 7.2 Hz, 2H).

5-phenyl-1-(4-(trifluoromethoxy) phenyl)-1H-1,2,3-triazole (3be).



3be

According to general procedure B, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Yellow solid, 245 mg, 81% yield, mp 89.7-91.5 °C.

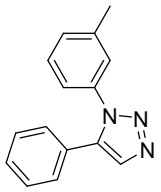
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.43-7.37 (m, 5H), 7.28 (d, *J* = 8.6 Hz, 2H), 7.23 (d, *J* = 6.5 Hz, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 149.4, 137.9, 134.9, 133.7, 129.6, 129.1, 128.7, 126.6, 126.4, 122.4, 121.7.

^{19}F NMR (471 MHz, $CDCl_3$) δ –57.9 (s, 3F).

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{15}H_{10}F_3N_3O$: 306.0776, found: 306.0775.

5-phenyl-1-(m-tolyl)-1H-1,2,3-triazole (3bf). [24]

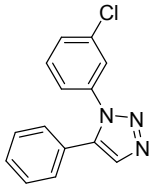


3bf

According to general procedure B, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Orange liquid, 230 mg, 98% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (s, 1H), 7.34-7.30 (m, 3H), 7.25-7.20 (m, 5H), 7.04 (d, J = 7.6 Hz, 1H), 2.33 (s, 3H).

1-(3-chlorophenyl)-5-phenyl-1H-1,2,3-triazole (3bg). [18]

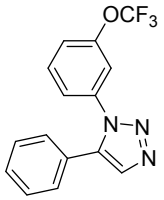


3bg

According to general procedure B, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Orange liquid, 254 mg, 99% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (s, 1H), 7.46 (s, 1H), 7.41-7.31 (m, 5H), 7.22 (d, J = 6.9 Hz, 2H), 7.18 (d, J = 7.9 Hz, 1H).

5-phenyl-1-(3-(trifluoromethoxy) phenyl)-1H-1,2,3-triazole (3bh).



3bh

According to general procedure B, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Yellow liquid, 190 mg, 63% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (s, 1H), 7.46 (t, J = 8.2 Hz, 1H), 7.40-7.34 (m, 4H), 7.28 (d, J = 8.3 Hz, 1H), 7.23-7.22 (m, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 149.3, 136.2 (d, J = 20.0 Hz), 133.7, 130.5, 129.65, 129.58, 128.7, 126.9, 125.3, 121.7, 121.0.

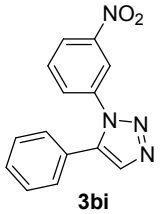
In the ^{13}C NMR spectrum of **3bh**, theoretically, there should be thirteen peaks. Due to

the compact overlaying, it is difficult to specify the overlaying peaks.

^{19}F NMR (471 MHz, $CDCl_3$) δ –58.0 (s, 3F).

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{15}H_{10}F_3N_3O$: 306.0776, found: 306.0780.

1-(3-nitrophenyl)-5-phenyl-1H-1,2,3-triazole (3bi). [25]

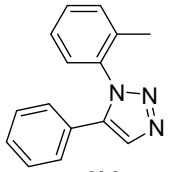


3bi

According to general procedure B, 4 eq. *t*-BuOK was used, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Orange solid, 160 mg, 61% yield, mp 110.0-112.0 ℃ (lit. 133-134 ℃).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.31-8.30 (m, 2H), 7.90 (s, 1H), 7.70 (d, J = 8.1 Hz, 1H), 7.63 (t, J = 8.7 Hz, 1H), 7.46-7.39 (m, 3H), 7.25 (d, J = 7.0 Hz, 2H).

5-phenyl-1-(o-tolyl)-1H-1,2,3-triazole (3bj). [19]

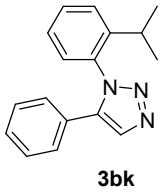


3bj

According to general procedure B, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Orange solid, 160 mg, 68% yield, mp 73.0-75.0 ℃ (lit. 71-73 ℃).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.93 (s, 1H), 7.39 (t, J = 6.3 Hz, 1H), 7.30-7.25 (m, 6H), 7.16 (d, J = 6.9 Hz, 2H), 1.93 (s, 3H).

1-(2-isopropylphenyl)-5-phenyl-1H-1,2,3-triazole (3bk).



3bk

According to general procedure B, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Yellow solid, 220 mg, 84% yield, mp 107.5-108.8

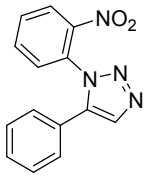
°C.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.94 (s, 1H), 7.49 (t, J = 7.5 Hz, 1H), 7.42 (d, J = 7.6 Hz, 1H), 7.31-7.24 (m, 5H), 7.17-7.16 (m, 2H), 2.46 (hept, J = 6.8 Hz, 1H), 0.97 (br s, 6H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 145.7, 139.0, 134.5, 132.2, 130.7, 129.1, 128.8, 127.9, 127.8, 127.1, 126.7, 126.6, 28.0, 22.3.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{17}H_{17}N_3$: 264.1422, found: 264.1425.

1-(2-nitrophenyl)-5-phenyl-1H-1,2,3-triazole (3bl).



3bl

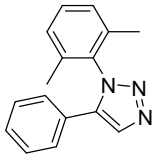
According to general procedure A, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Black liquid, 70 mg, 27% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 (dt, J = 8.0 Hz, J = 1.4 Hz, 1H), 7.89 (s, 1H), 7.74-7.66 (m, 2H), 7.45 (dt, J = 7.6 Hz, J = 1.2 Hz, 1H), 7.38-7.31 (m, 3H), 7.21 (d, J = 7.0 Hz, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 145.4, 139.4, 133.9, 133.7, 132.7, 131.6, 131.0, 130.1, 129.7, 129.6, 129.1, 128.4, 125.7, 124.3.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{14}H_{10}N_4O_2$: 267.0804, found: 267.0810.

1-(2,6-dimethylphenyl)-5-phenyl-1H-1,2,3-triazole (3bm).



3bm

According to general procedure B, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Yellow solid, 130 mg, 53% yield, mp 58.8-60.5 °C.

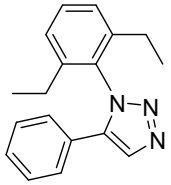
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.33-7.28 (m, 4H), 7.16 (d, J = 7.5 Hz, 4H), 1.93 (s, 6H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 138.3, 135.9, 135.3, 132.2, 130.2, 129.2, 129.0, 128.7,

126.9, 126.6, 17.6.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{16}H_{15}N_3$: 250.1266, found: 250.1268.

1-(2,6-diethylphenyl)-5-phenyl-1H-1,2,3-triazole (3bn).



3bn

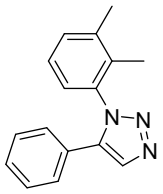
According to general procedure B, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Orange solid, 145 mg, 53% yield, mp 78.9-80.6 °C.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.44 (t, J = 7.8 Hz, 1H), 7.32-7.23 (m, 5H), 7.16 (d, J = 7.5 Hz, 2H), 2.18 (hept, J = 7.4 Hz, 4H), 1.01 (t, J = 7.5 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 141.5, 138.6, 134.3, 132.1, 130.6, 129.2, 129.0, 127.0, 126.8, 126.6, 24.1, 14.1.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{18}H_{19}N_3$: 278.1579, found: 278.1580.

1-(2,3-dimethylphenyl)-5-phenyl-1H-1,2,3-triazole (3bo).



3bo

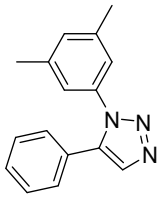
According to general procedure B, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Yellow liquid, 127 mg, 51% yield, mp 61.7-63.2 °C.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.93 (s, 1H), 7.29-7.25 (m, 4H), 7.20-7.16 (m, 3H), 7.11 (d, J = 7.8 Hz, 1H), 2.29 (s, 3H), 1.80 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 138.79, 138.76, 136.0, 133.9, 132.3, 131.6, 129.1, 128.9, 127.7, 126.7, 126.3, 125.3, 20.3, 14.1.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{16}H_{15}N_3$: 250.1266, found: 250.1270.

1-(3,5-dimethylphenyl)-5-phenyl-1H-1,2,3-triazole (3bp).



3bp

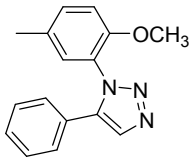
According to general procedure B, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Orange solid, 185 mg, 75% yield, mp 85.5-87.0 °C.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (s, 1H), 7.37-7.33 (m, 3H), 7.24 (d, J = 7.0 Hz, 2H), 7.07 (s, 1H), 6.97 (s, 2H), 2.30 (s, 6H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 139.3, 137.7, 136.5, 133.2, 130.9, 129.2, 128.8, 128.5, 126.9, 123.0, 120.5, 21.2.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{16}H_{15}N_3$: 250.1266, found: 250.1265.

1-(2-methoxy-5-methylphenyl)-5-phenyl-1H-1,2,3-triazole (3bq).



3bq

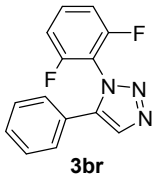
According to general procedure B, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Yellow solid, 216 mg, 82% yield, mp 157.7-159.2 °C.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 (s, 1H), 7.29 (d, J = 5.4 Hz, 4H), 7.24-7.21 (m, 3H), 6.81 (d, J = 8.4 Hz, 1H), 3.40 (s, 3H), 2.34 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 151.4, 139.3, 132.1, 131.8, 130.7, 129.1, 128.9, 128.7, 128.6, 127.6, 127.4, 125.4, 55.5, 20.3.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{16}H_{15}N_3O$: 266.1215, found: 266.1215.

1-(2,6-difluorophenyl)-5-phenyl-1H-1,2,3-triazole (3br).



3br

According to general procedure B, petroleum ether / ethyl acetate = 85 : 15 (v / v) as

eluent for column chromatography. Yellow solid, 233 mg, 91% yield, mp 117.5-119.0 ℃.

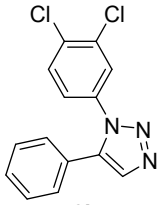
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.92 (s, 1H), 7.51-7.45 (m, 1H), 7.39-7.33 (m, 3H), 7.25 (d, J = 7.8 Hz, 2H), 7.06 (t, J = 8.2 Hz, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 158.0 (dd, J_1 = 256.2 Hz, J_2 = 2.7 Hz), 140.3, 132.2 (d, J = 9.1 Hz), 132.1 (d, J = 10.0 Hz), 129.7, 129.0, 127.7, 126.0, 112.4 (d, J_1 = 3.7 Hz), 112.3 (d, J = 3.6 Hz).

^{19}F NMR (471 MHz, $CDCl_3$) δ –117.44- –117.47 (m, Ar-F).

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{14}H_9F_2N_3$: 258.0765, found: 258.0760.

1-(3,4-dichlorophenyl)-5-phenyl-1H-1,2,3-triazole (3bs).



3bs

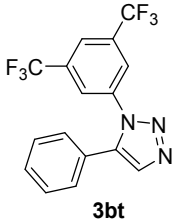
According to general procedure B, 4 eq. *t*-BuOK was used, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Yellow solid, 125 mg, 44% yield, mp 96.3-97.5 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (s, 1H), 7.59 (d, J = 2.3 Hz, 1H), 7.48 (d, J = 8.5 Hz, 1H), 7.43-7.39 (m, 3H), 7.24 (d, J = 6.7 Hz, 2H), 7.14 (dd, J_1 = 8.6 Hz, J_2 = 2.3 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 137.8, 135.7, 133.7, 133.64, 133.61, 131.0, 129.8, 129.2, 128.7, 126.9, 126.1, 124.1.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{14}H_9Cl_2N_3$: 290.0174, found: 290.0170.

1-(3,5-bis(trifluoromethyl)phenyl)-5-phenyl-1H-1,2,3-triazole (3bt). [20]



3bt

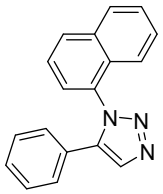
According to general procedure B, 4 eq. *t*-BuOK was used, petroleum ether / ethyl acetate = 65 : 35 (v / v) as eluent for column chromatography. Yellow solid, 206 mg,

58% yield, mp 140.0-142.0 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.92 (s, 1H), 7.89 (s, 1H), 7.85 (s, 2H), 7.49-7.42 (m, 3H), 7.24 (d, J = 7.4 Hz, 2H).

^{19}F NMR (471 MHz, $CDCl_3$) δ –63.2 (s, 6F).

1-(naphthalen-1-yl)-5-phenyl-1H-1,2,3-triazole (3bu). [24]

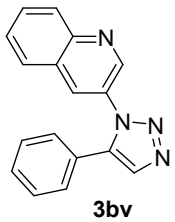


3bu

According to general procedure B, 4 eq. *t*-BuOK was used, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Orange solid, 225 mg, 83% yield, mp 128.0-130.0 ℃ (lit.127-129 ℃).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05 (s, 1H), 8.01 (d, J = 8.2 Hz, 1H), 7.94 (d, J = 8.3 Hz, 1H), 7.56-7.43 (m, 4H), 7.38 (d, J = 8.4 Hz, 1H), 7.23 (d, J = 7.4 Hz, 1H), 7.18 (t, J = 7.6 Hz, 2H), 7.13 (d, J = 7.5 Hz, 2H).

3-(5-phenyl-1H-1,2,3-triazol-1-yl) quinoline (3bv).



3bv

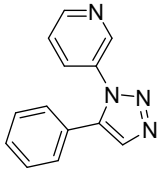
According to general procedure B, petroleum ether / ethyl acetate = 65 : 35 (v / v) as eluent for column chromatography. Orange solid, 180 mg, 67% yield, mp 134.5-136.0 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.80 (d, J = 2.1 Hz, 1H), 8.29 (d, J = 2.0 Hz, 1H), 8.14 (d, J = 8.4 Hz, 1H), 7.93 (s, 1H), 7.85-7.79 (m, 2H), 7.63 (t, J = 7.3 Hz, 1H), 7.41-7.34 (m, 3H), 7.26 (d, J = 7.1 Hz, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 147.6, 146.3, 138.2, 133.8, 131.2, 130.9, 130.2, 129.8, 129.6, 129.3, 128.7, 128.3, 128.1, 127.3, 126.2.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{17}H_{12}N_4$: 273.1062, found: 273.1060.

3-(5-phenyl-1H-1,2,3-triazol-1-yl) pyridine (3bw). [24]

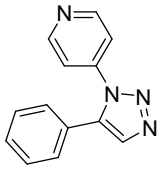


3bw

According to general procedure B, petroleum ether / ethyl acetate = 50 : 50 (v / v) as eluent for column chromatography. Yellow solid, 174 mg, 79% yield, mp 112.0-114.0 ℃ (lit. 112.0-114.0 ℃).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.68 (d, J = 4.8 Hz, 1H), 8.63 (d, J = 2.0 Hz, 1H), 7.88 (s, 1H), 7.74 (d, J = 8.2 Hz, 1H), 7.42-7.36 (m, 4H), 7.22 (d, J = 7.0 Hz, 2H)

4-(5-phenyl-1H-1,2,3-triazol-1-yl) pyridine (3bx). [19]

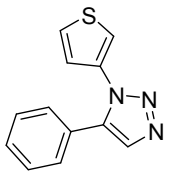


3bx

According to general procedure B, petroleum ether / ethyl acetate = 50 : 50 (v / v) as eluent for column chromatography. Yellow solid, 180 mg, 81% yield, mp 204.0-206.0 ℃ (lit. 199-201 ℃).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.67 (d, J = 6.0 Hz, 2H), 7.85 (s, 1H), 7.47-7.40 (m, 3H), 7.33 (d, J = 6.1 Hz, 2H), 7.26 (d, J = 7.1 Hz, 2H).

5-phenyl-1-(thiophen-3-yl)-1H-1,2,3-triazole (3by).



3by

According to general procedure B, petroleum ether / ethyl acetate = 85 : 15 (v / v) as eluent for column chromatography. Black solid, 180 mg, 80% yield, mp 103.0-105.0 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (s, 1H), 7.42-7.38 (m, 3H), 7.36-7.34 (m, 1H), 7.32-7.28 (m, 3H), 7.06 (d, J = 5.0 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 137.7, 134.7, 133.2, 129.6, 128.9, 128.7, 126.7, 126.4, 123.7, 119.3.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{12}H_9N_3S$: 228.0517, found: 228.0517.

5. References.

[1] I. P. Holmes, S. Gaines, S. P. Watson, O. Lorthioir, A. Walker, S. J. Baddeley, S. Herbert, D. Egan, M. A. Convery, O. M. P. Singh, J. W. Gross, J. M. Strelow, R. H. Smith, A. J. Amour, D. Brown and S. L. Martin, *Bioorg. Med. Chem. Lett.,* 2009, **19**, 5760-5763.

[2] N. Eleftheriadis, H. Poelman, N. G. J. Leus, B. Honrath, C. G. Neochoritis, A. Dolga, A. Domling and F. J. Dekker, *Eur. J. Med. Chem.,* 2016, **122**, 786-801.

[3] E. Szymanska, K. Frydenvang, A. Contreras-Sanz, D. S. Pickering, E. Frola, Z. Serafimoska, B. Nielsen, J. S. Kastrup, T. N. Johansen, *J. Med. Chem.,* 2011, **54**, 7289-7298.

[4] S. Das, K. Moller, K. Junge and M. Beller, *Chem. Eur. J.,* 2011, **17**, 7414-7417.

[5] Q. Xie, C. Ni, R. Zhang, L. Li, J. Rong and J. Hu, *Angew. Chem., Int. Ed*., 2017, **56**, 1-6.

[6] R. O. Silva, A. S. de Oliveira, L. F. N. Lemes, L. de Camargo Nascente, P. C. do

Nascimento Nogueira, E. R. Silveira, G. D. Brand, G. Vistoli, A. Cilia, E. Poggesi, M. Buccioni, G. Marucci, M. L. Bolognesi and L. A. S. Romeiro, *Eur. J. Med. Chem*., 2016, **122**, 601-610.

[7] M. Leiendecker, A. Chatupheeraphat and M. Rueping, *Org. Chem. Front.,* 2015, **2**, 350-353.

[8] E. Castagnetti and M. Schlosser, *Eur. J. Org. Chem.,* 2001, 691-695.

[9] R. Yoshida, K. Isozaki, T. Yokoi, N. Yasuda, K. Sadakane, T. Iwamoto, H. Takaya and M. Nakamura, *Org. Biomol. Chem.,* 2016, **14**, 7468-7479.

[10] S. W. Kwok, J. R. Fotsing, R. J. Fraser, V. O. Rodionov and V. V. Fokin, *Org. Lett.,* 2010**, 12**, 4217-4219.

[11] N. Chandna, F. Kaur, S. Kumar and N. Jain, *Green. Chem.,* 2017, **19**, 4268-4371.

[12] S. Potratz, A. Mishra and P. Bäuerle, *Beilstein. J. Org. Chem.,* 2012, **8**, 683-692.

[13] L. K. Rasmussen, B. C. Boren and V. V. Fokin, *Org. Lett*., 2007, **9**, 5337-5339.

[14] D. Liu, W. Gao, Q. Dai and X. Zhang, *Org. Lett*., 2005, **7**, 4907-4910.

[15] U. F. Röhrig, S. R. Majjigapu, A. Grosdidier, S. Bron, V. Stroobant, L. Pilotte, D. Colau, P. Vogel, B. J. Van den Eynde, V. Zoete and O. Michielin, *J. Med. Chem.,* 2012, **55**, 5270-5290.

[16] G. Cheng, X. Zeng, J. Shen, X. Wang and X. Cui, *Angew. Chem., Int. Ed.,* 2013, **52**, 13265-13268.

[17] F. Gang, Y. Che, Z. Du, H. Feng and Y. Fu, *Synlett.,* 2017, **28**, 1624-1629.

[18] L. Hong, W. Lin, F. Zhang, R. Liu and X. Zhou, *Chem. Commun.,* 2013, **49**, 5589-5591.

[19] K. D. B. Yamajala, M. Patil and S. Banerjee, *J. Org. Chem.,* 2015, **80**, 3003-3011.

[20] P. Zardi, A. Savoldelli, D. M. Carminati, A. Caselli, F. Ragaini and E. Gallo, *ACS Catal.,* 2014, **4**, 3820-3823.

[21] L. Wu, Y. Chen, M. Tang, X. Song, G. Chen, X. Song and Q. Lin, *Synlett.,* 2012, **23**, 1529-1533.

[22] N. Kumar, M. Y. Ansari, R. Kantb and A. Kumar, *Chem. Commun.,* 2018, **54**, 2627-2630.

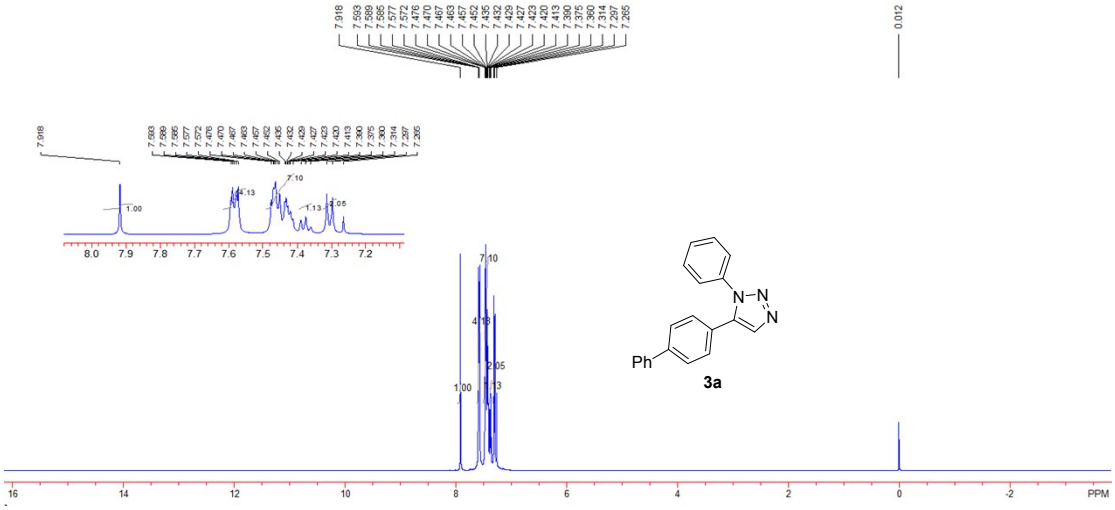
[23] C. D. Smith and M. F. Greaney, *Org. Lett.,* 2013, **15**, 4826-4829.

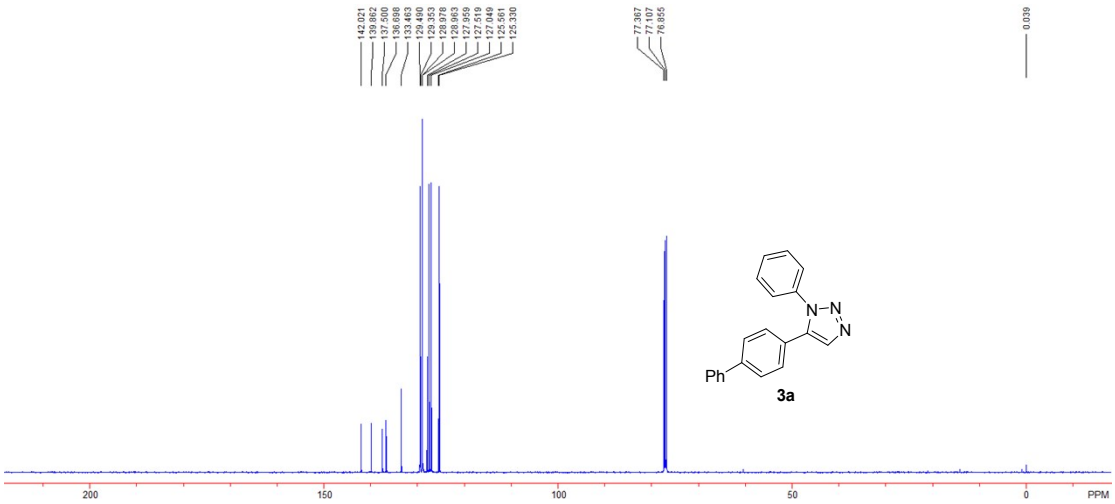
[24] L. Wu, Y. Chen, J. Luo, Q. Sun, M. Peng and Q. Lin, *Tetrahedron. Lett.,* 2014, **55**, 3847-3850.

[25] K. A. Durugkar, R. G. Gonnade, C.V. Ramana. *Tetrahedron.,* 2009, **65**, 3974-3979.

[26] A. D. Nino, P. Merino, V. Algieri, M. Nardi, M. L. D. Gioia, B. Russo, M. A. Tallarida and L. Maiuolo, *Catalysts.*, 2018, **8**, 364-376.

6. NMR Spectra.

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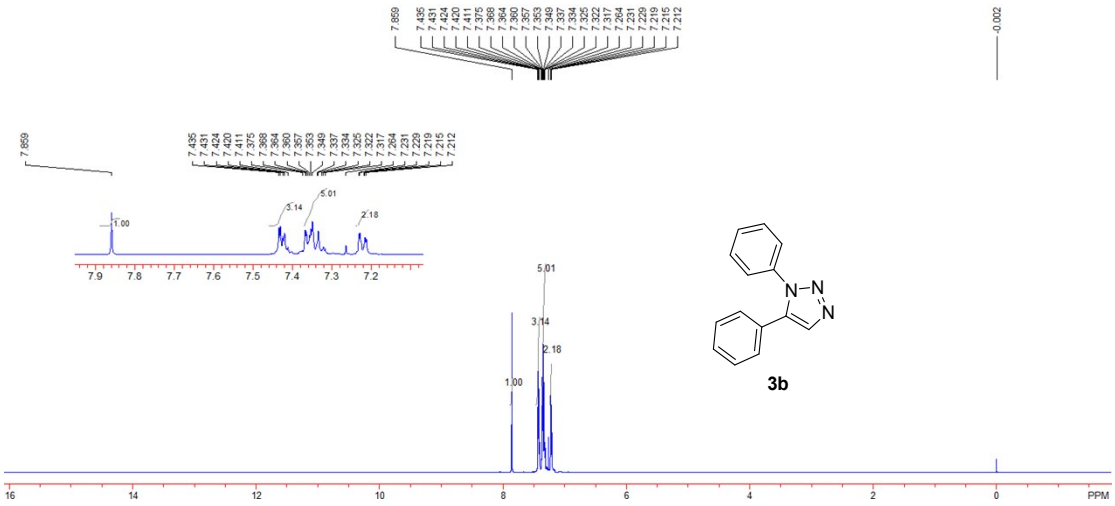
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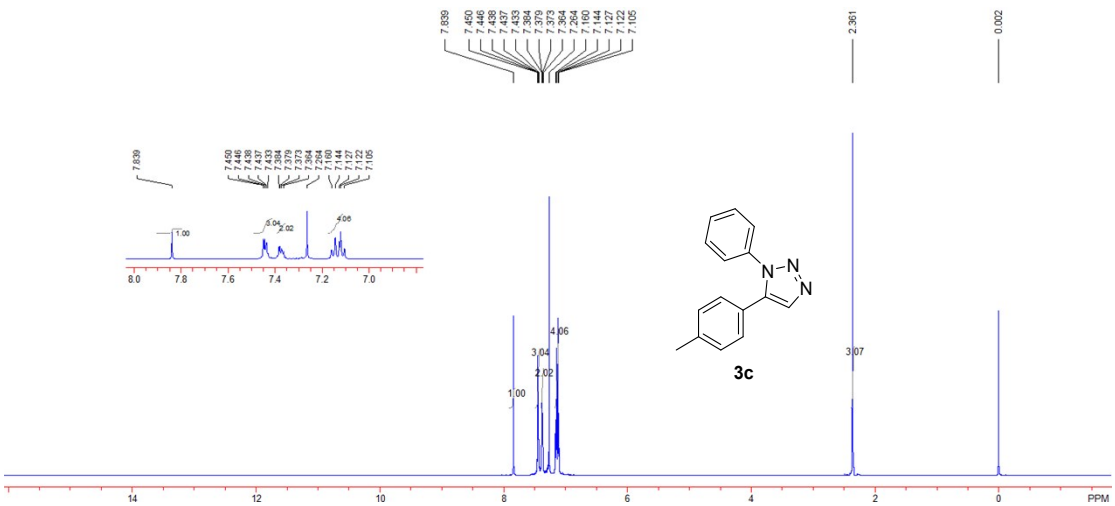
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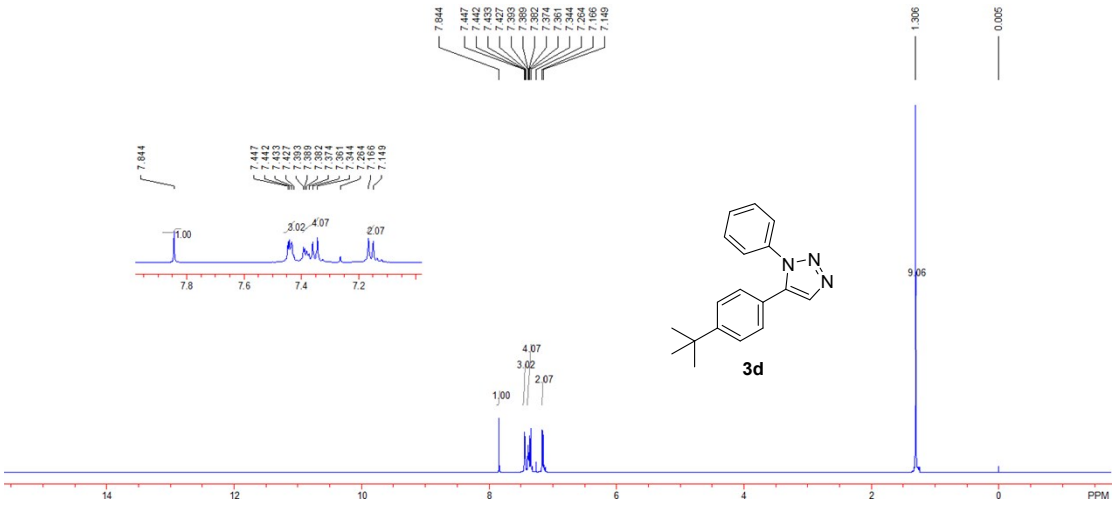
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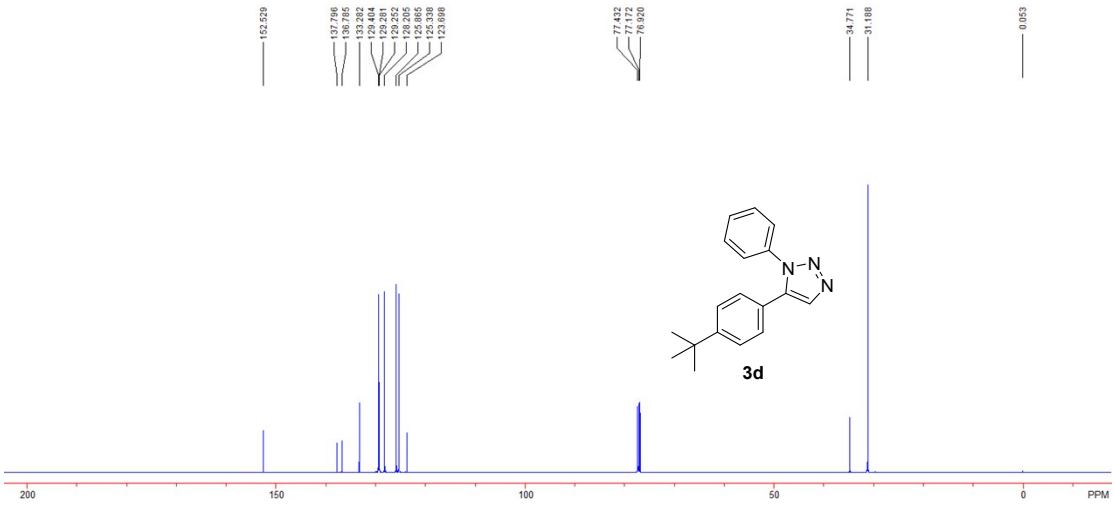
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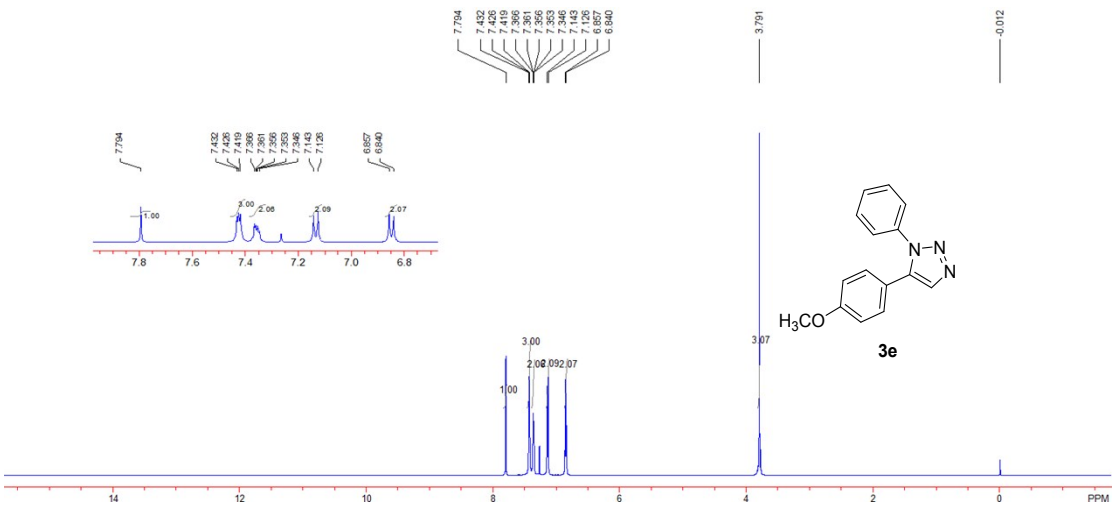
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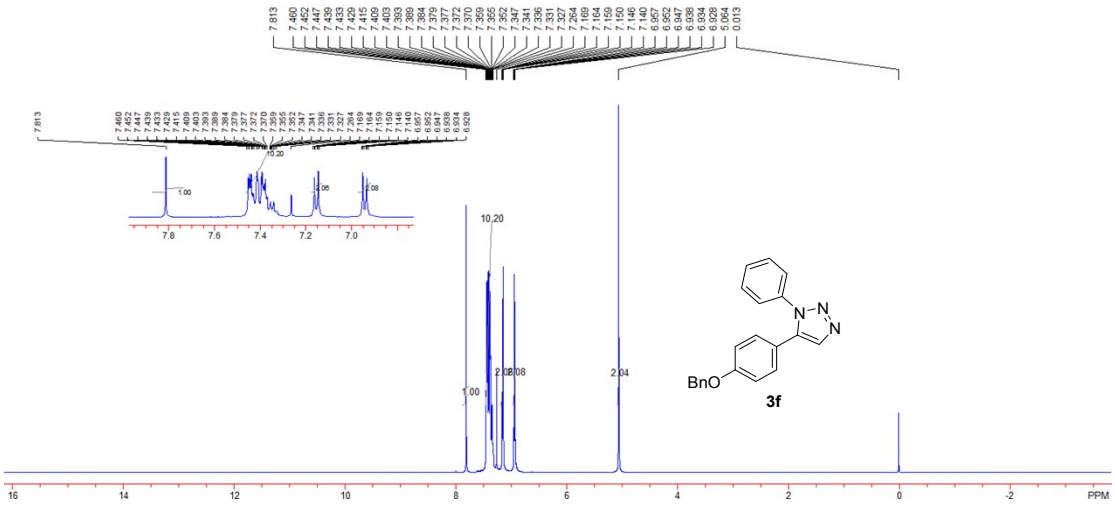
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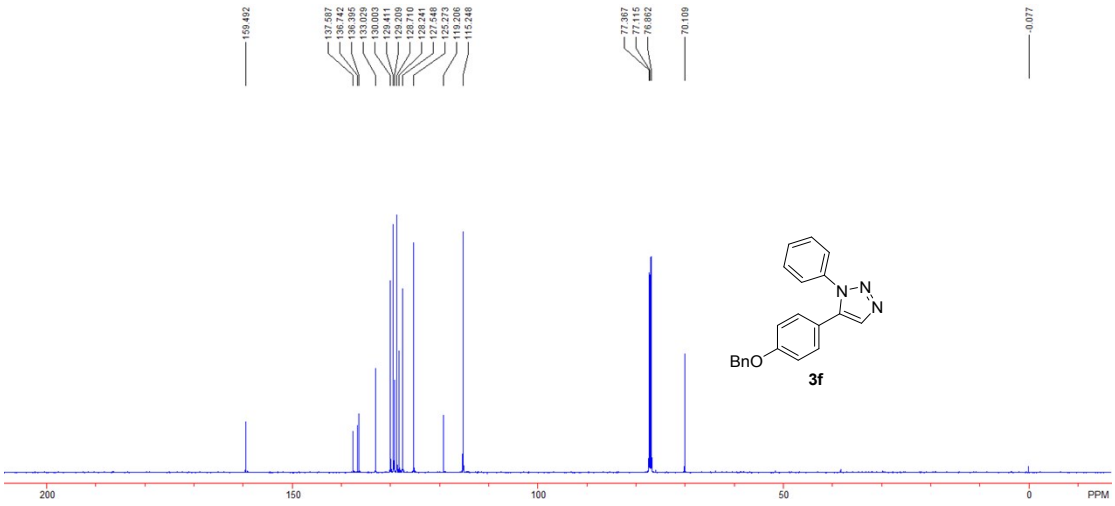
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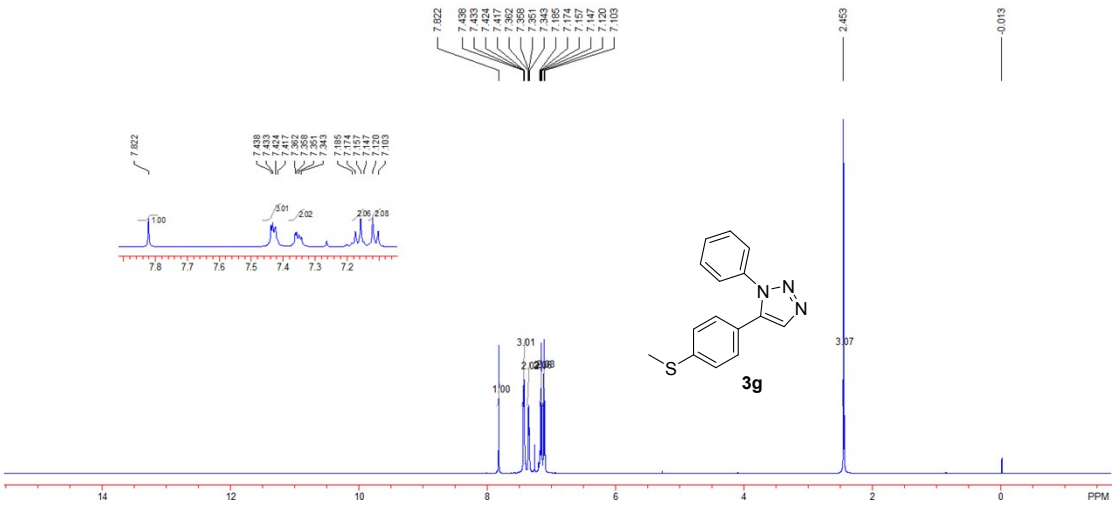
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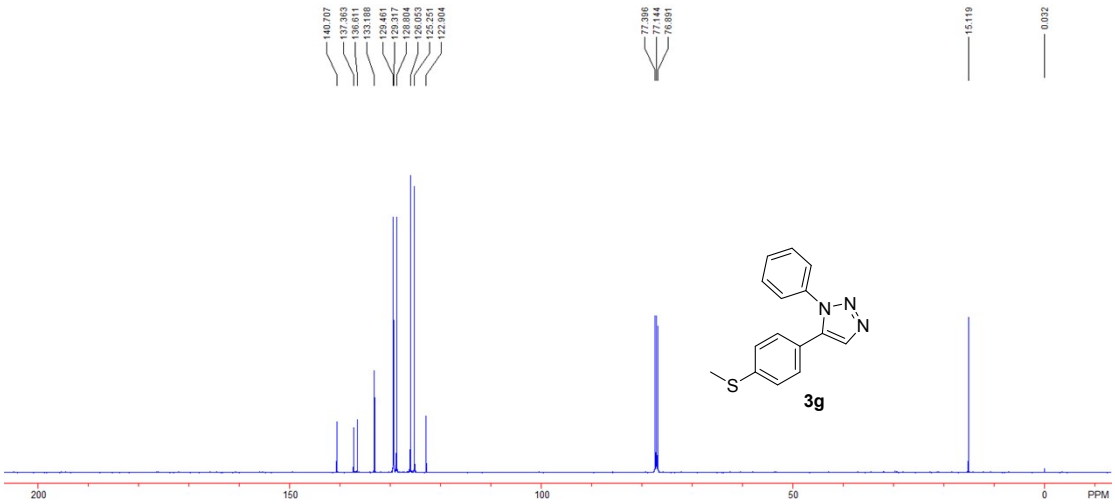
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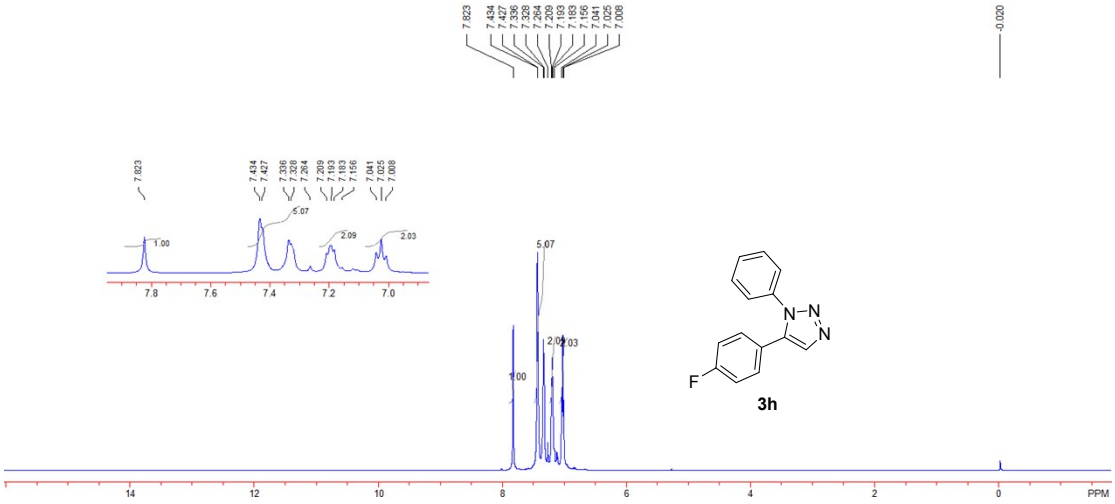
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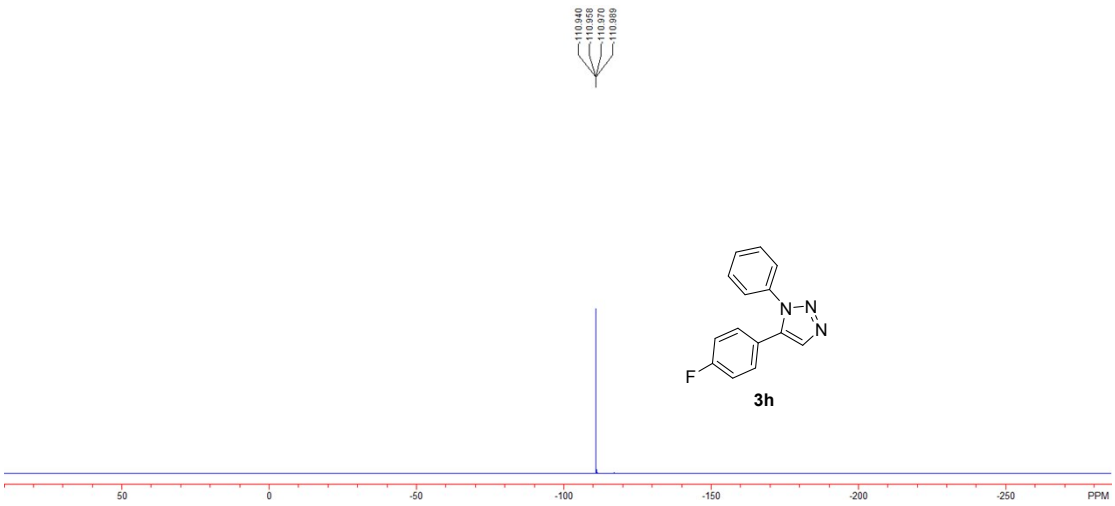
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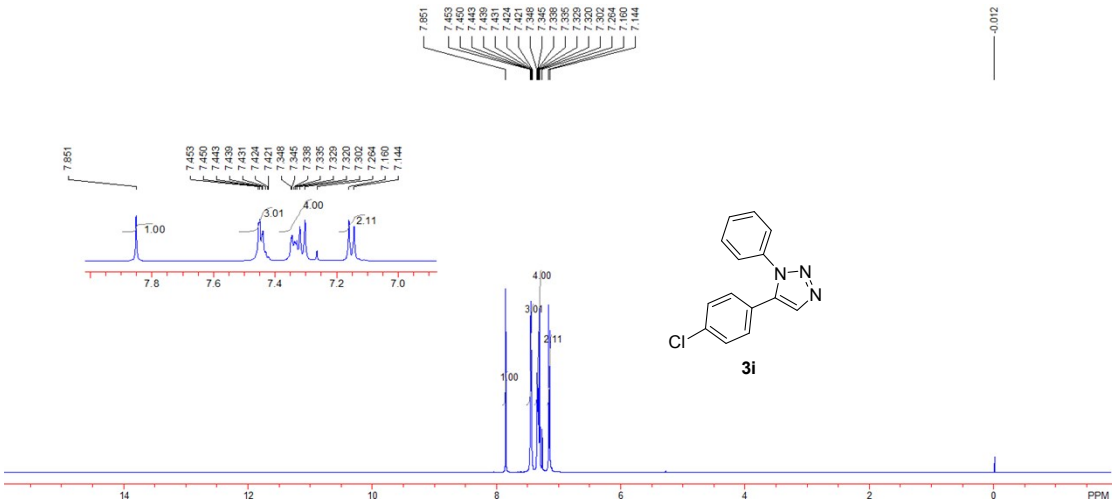
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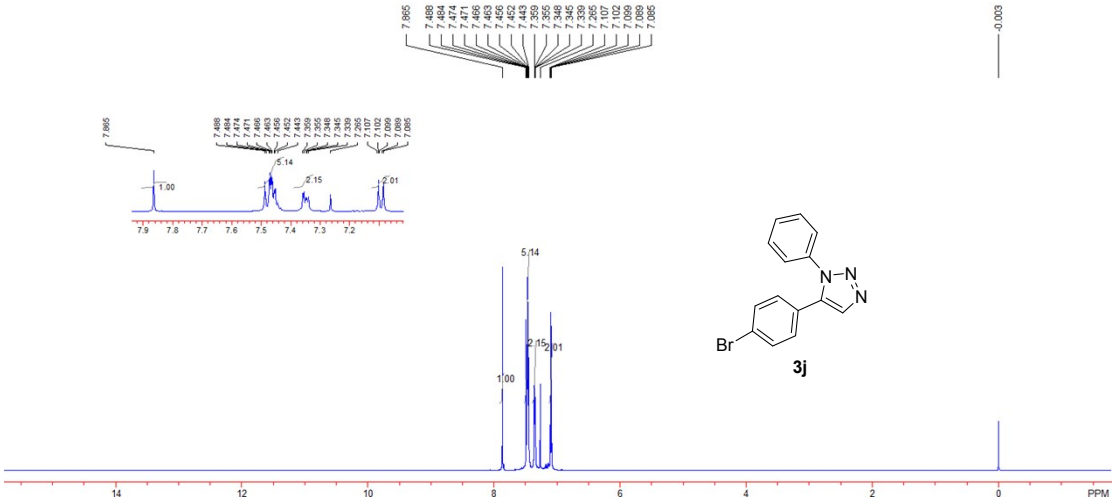
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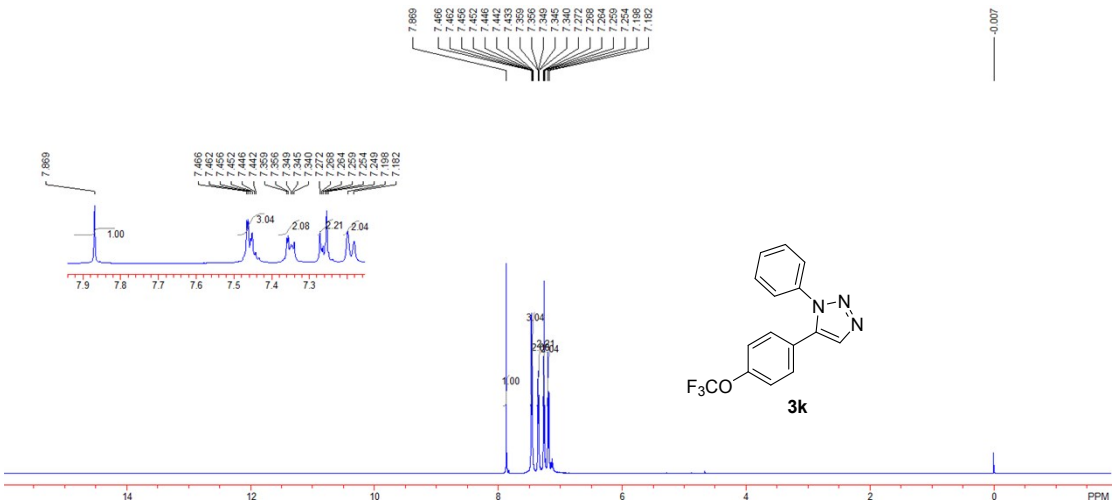
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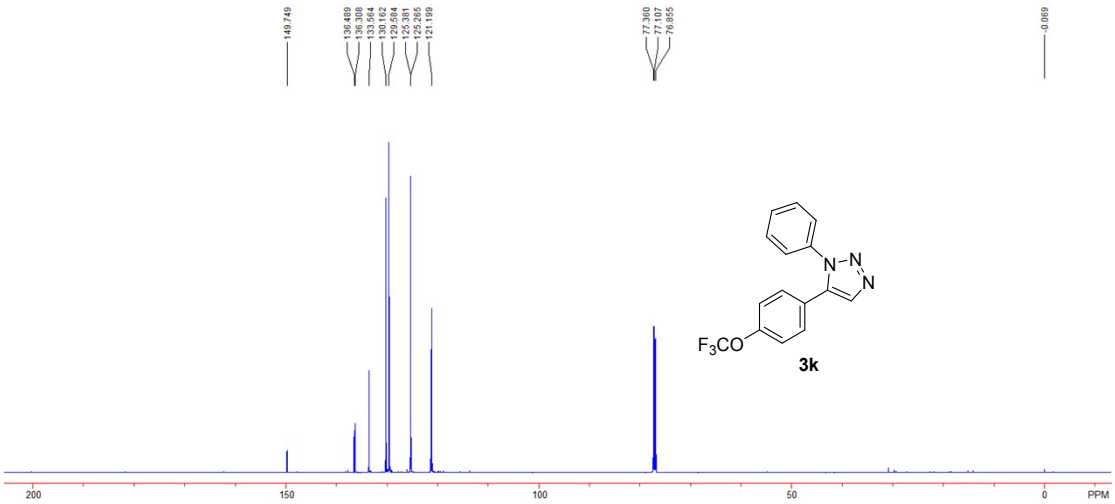
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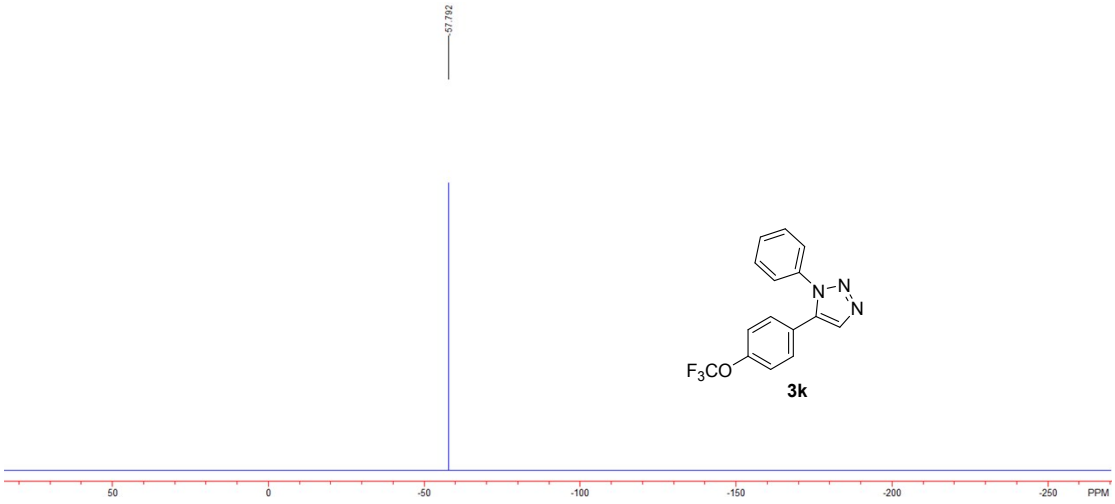
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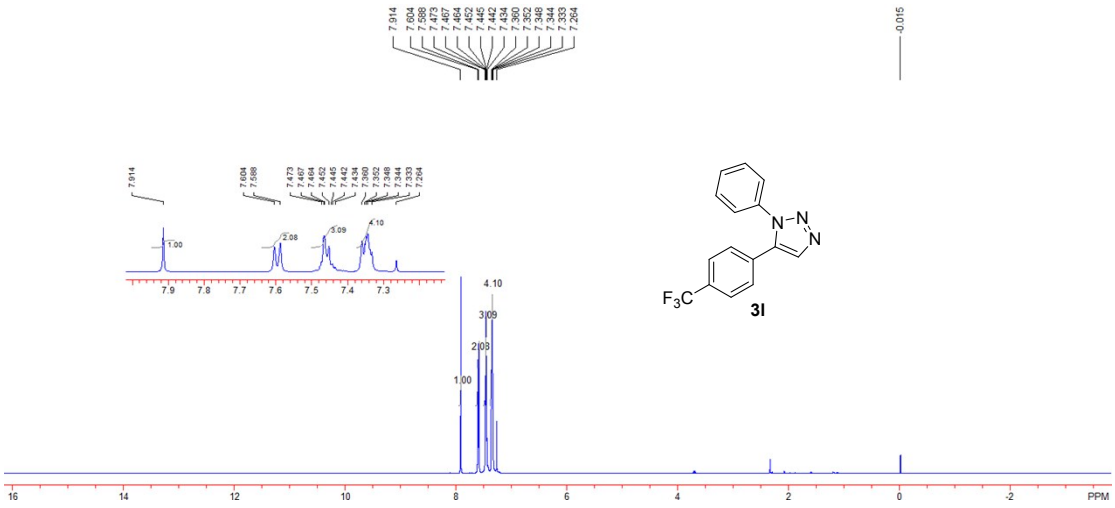
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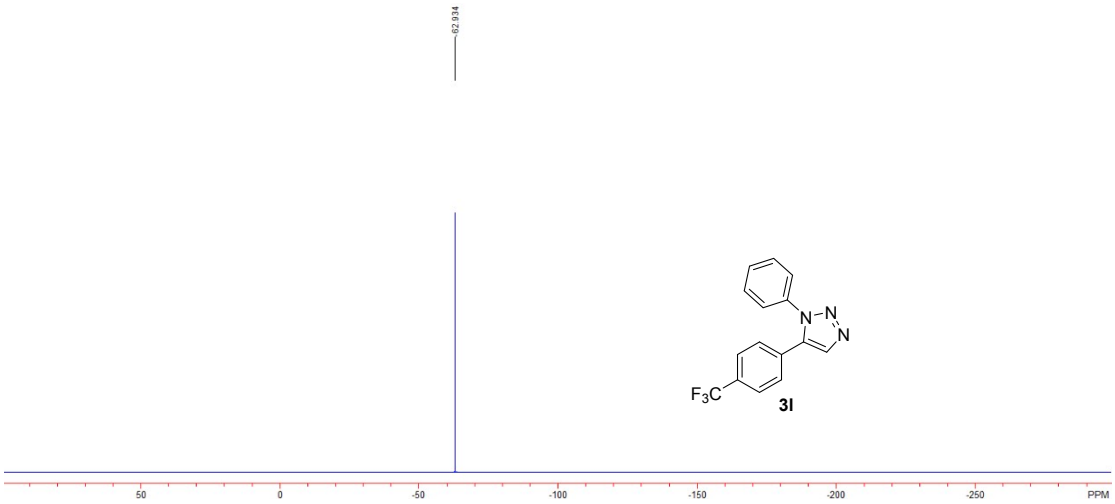
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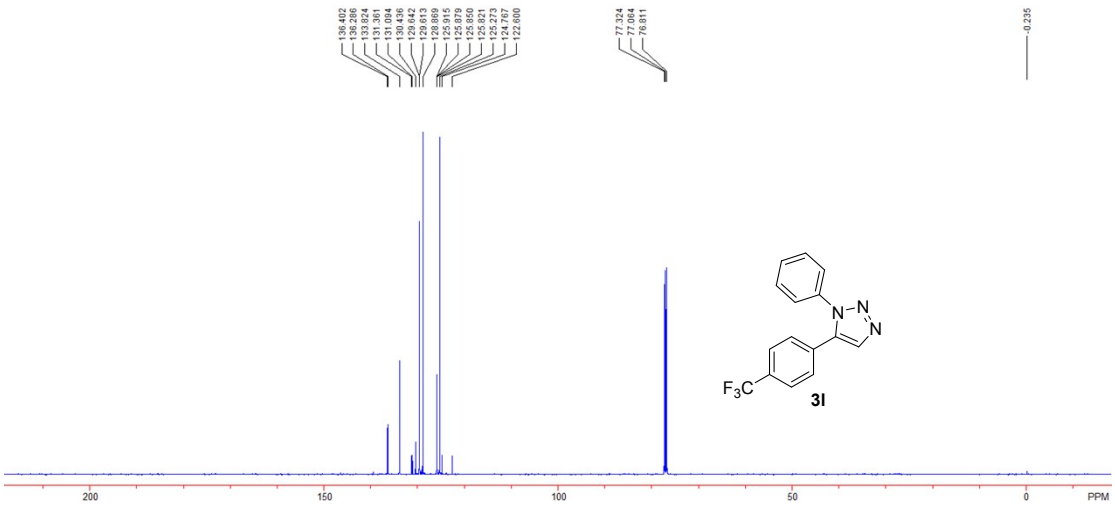
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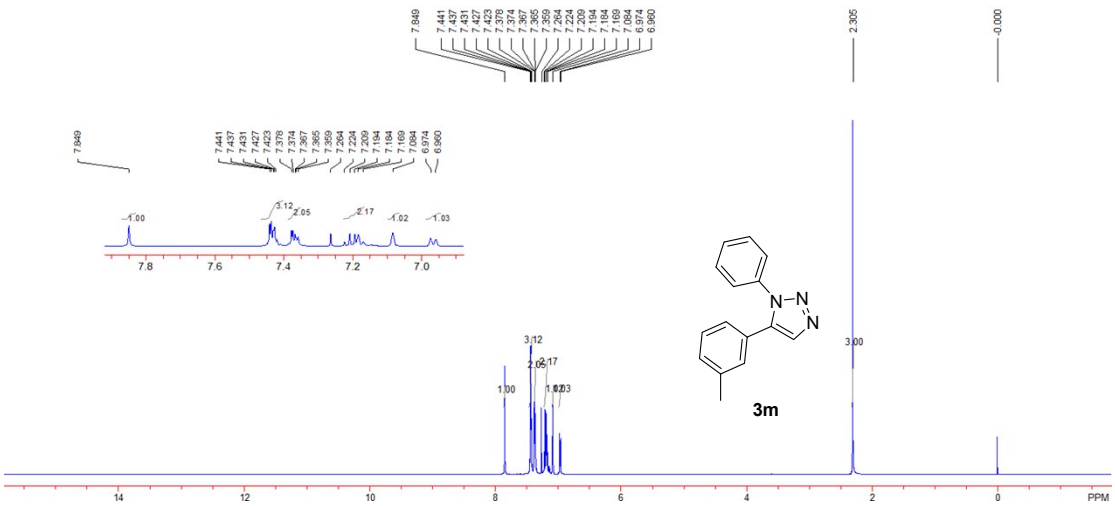
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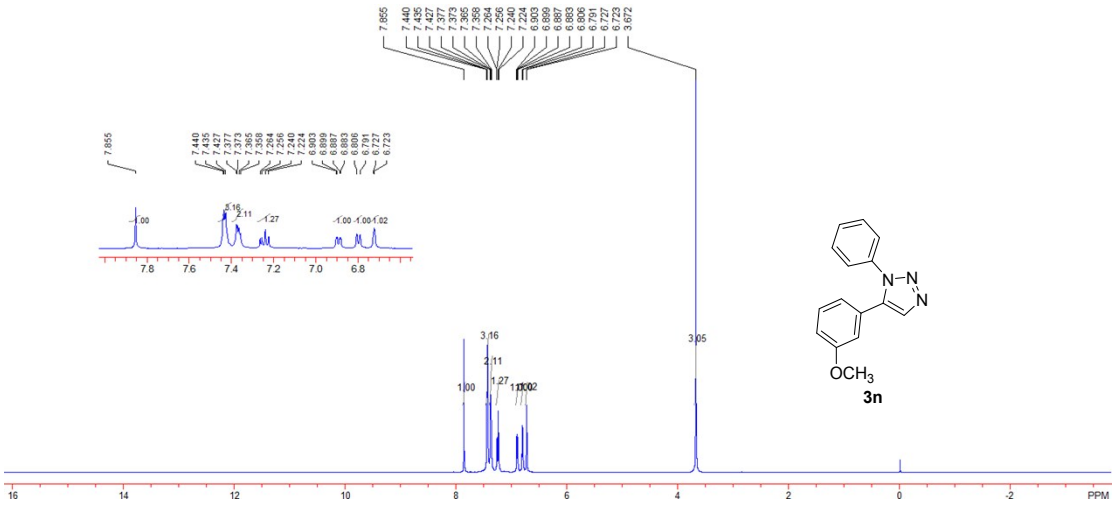
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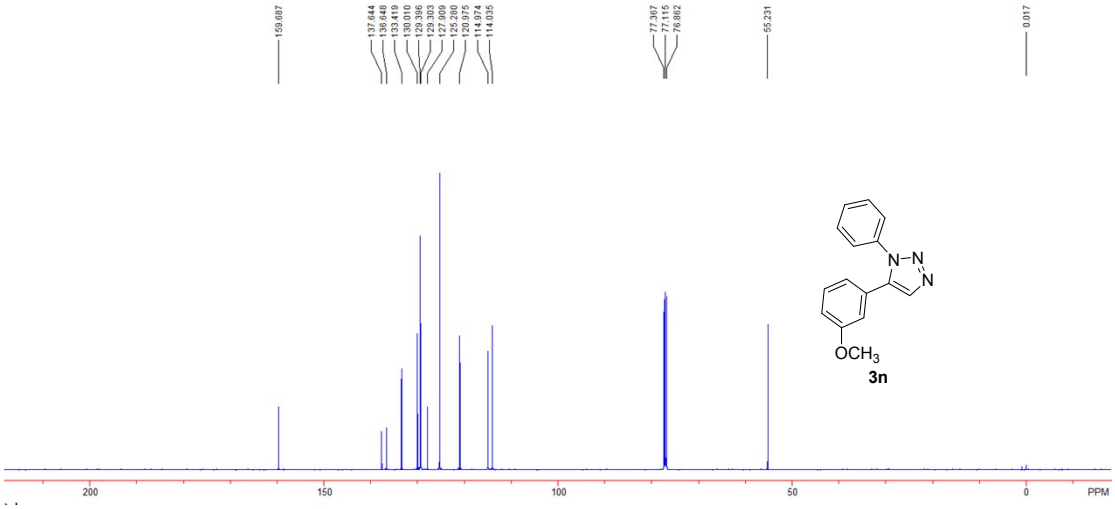
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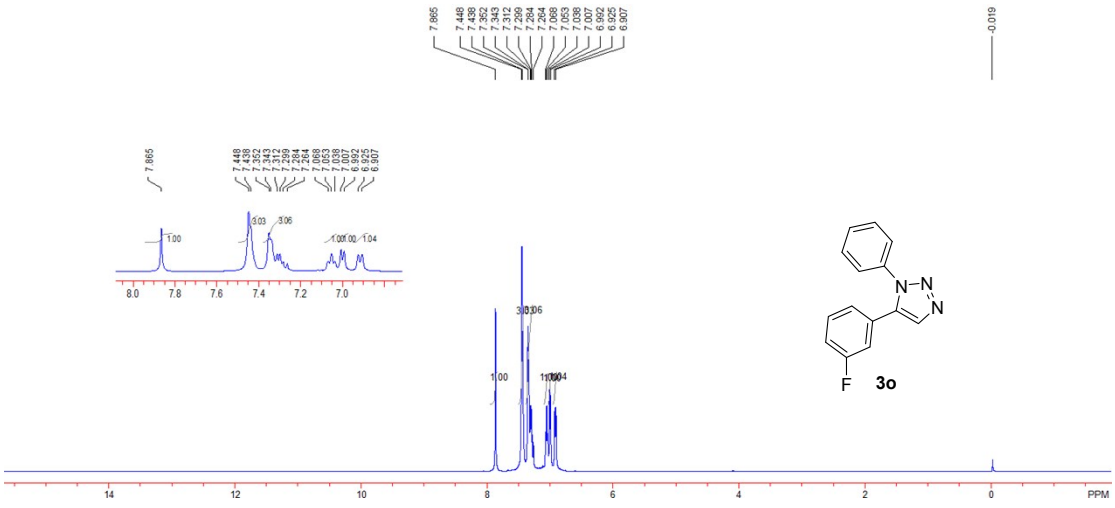
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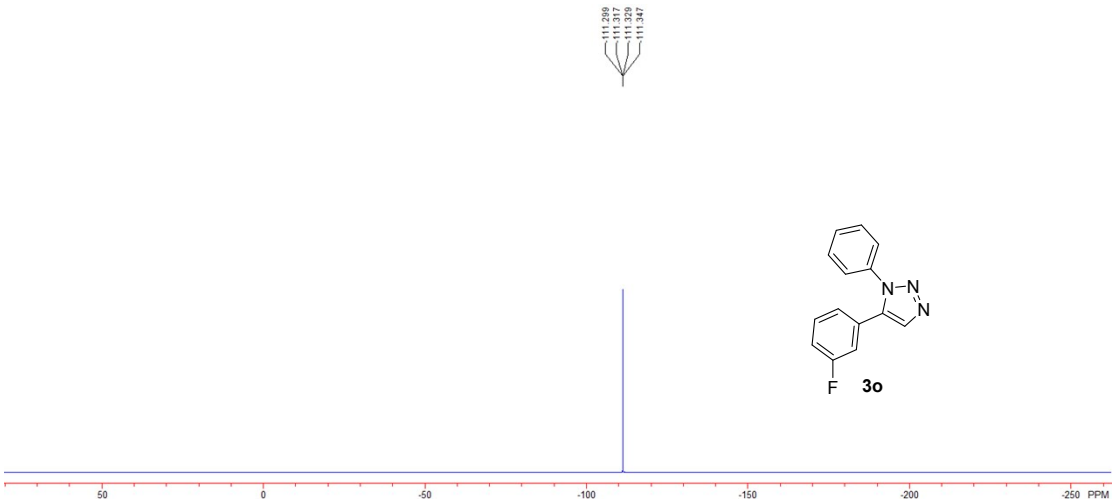
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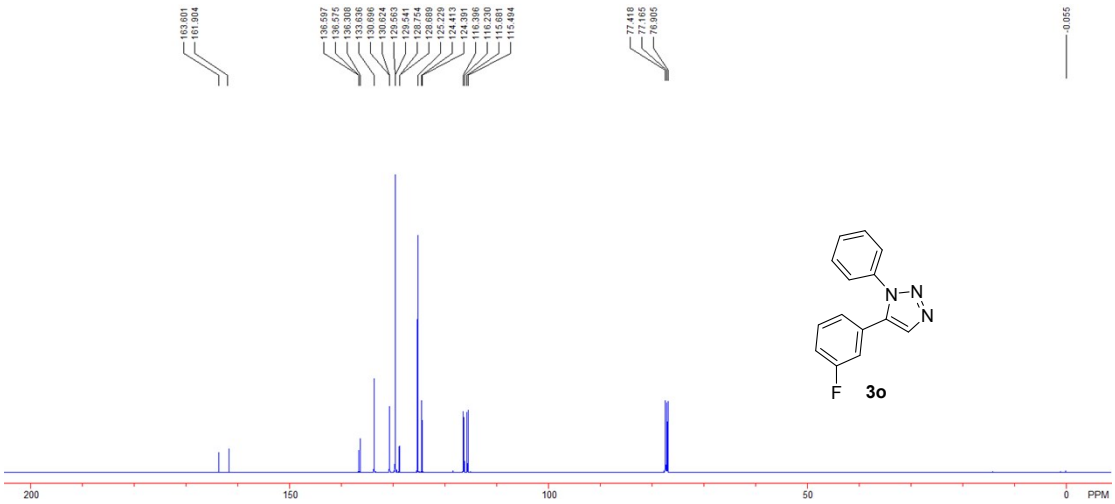
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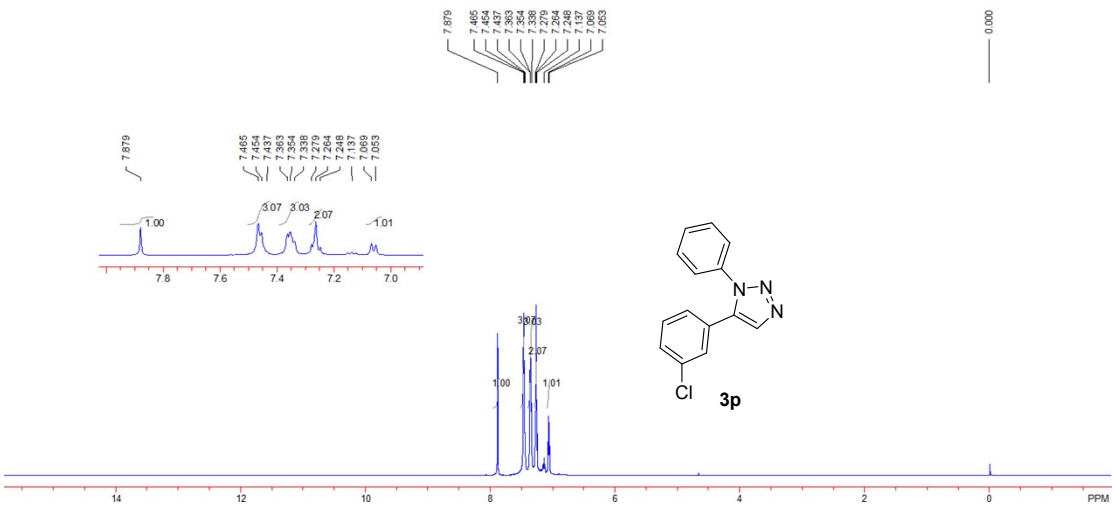
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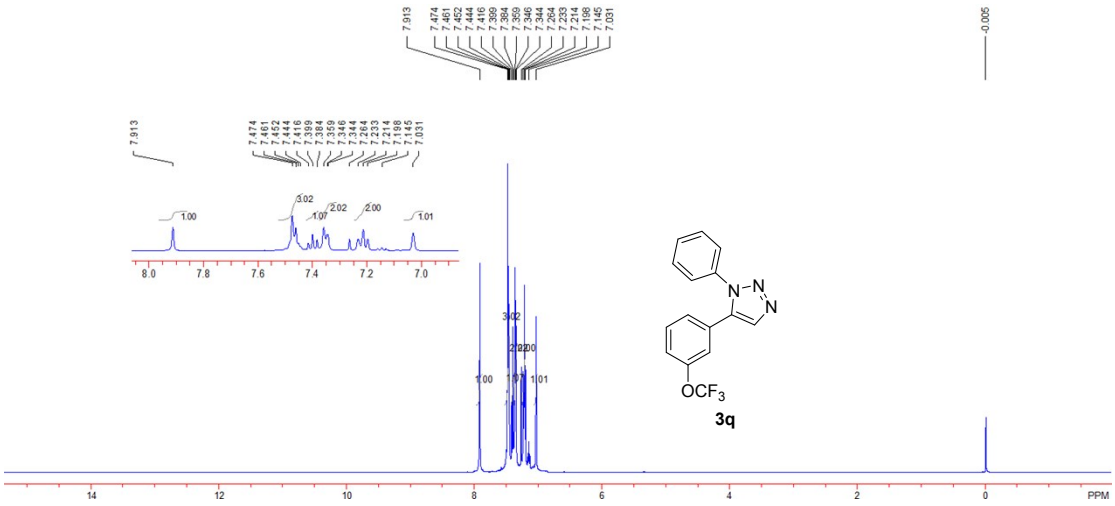
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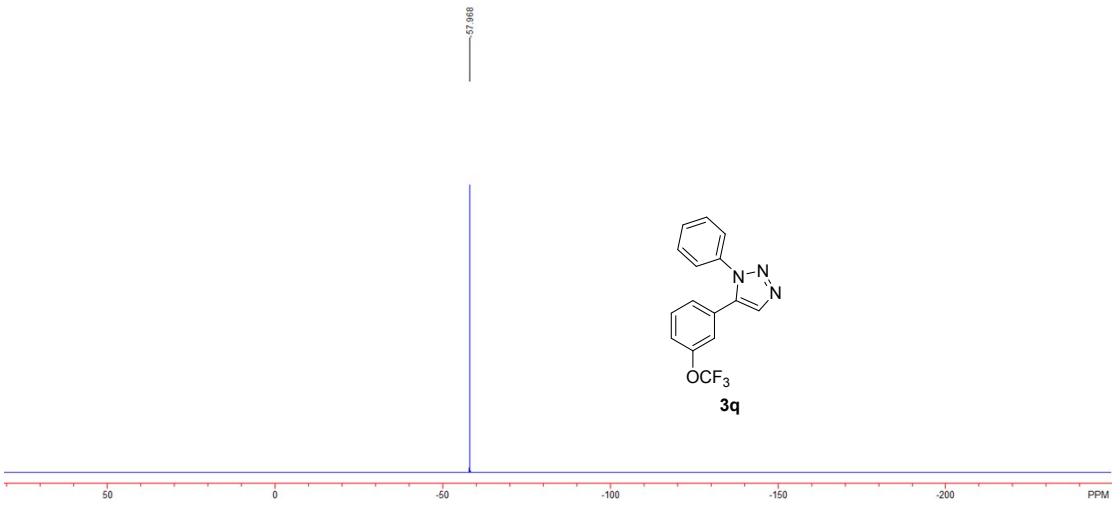
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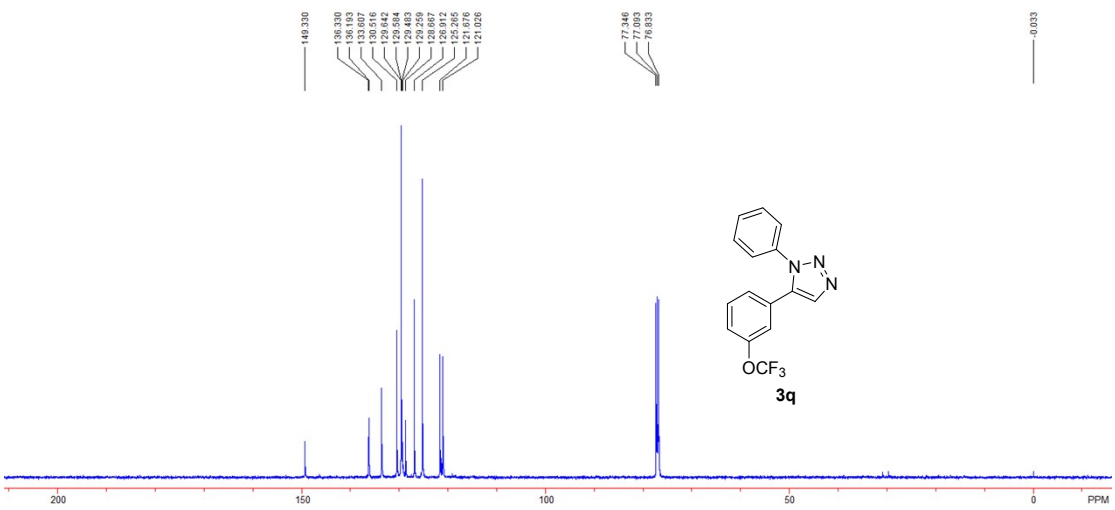
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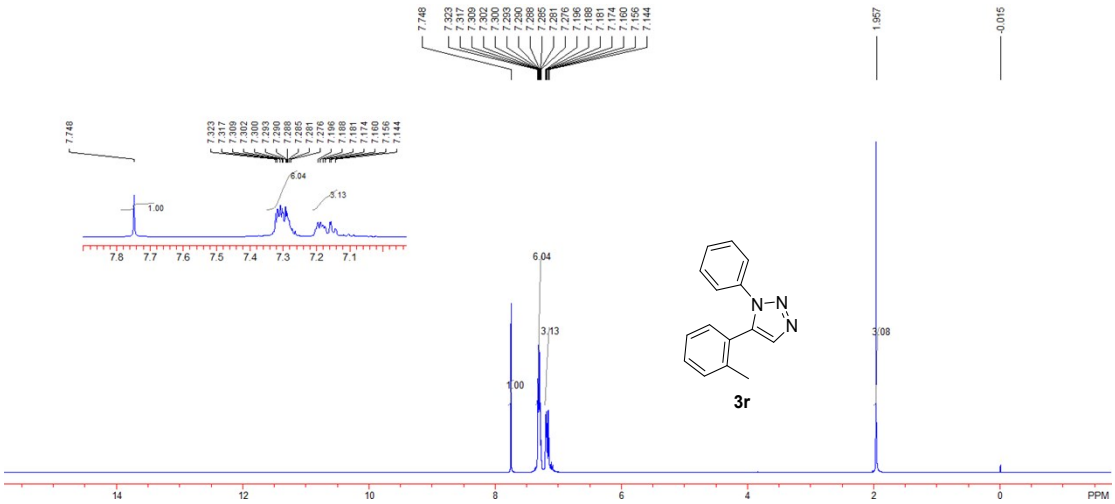
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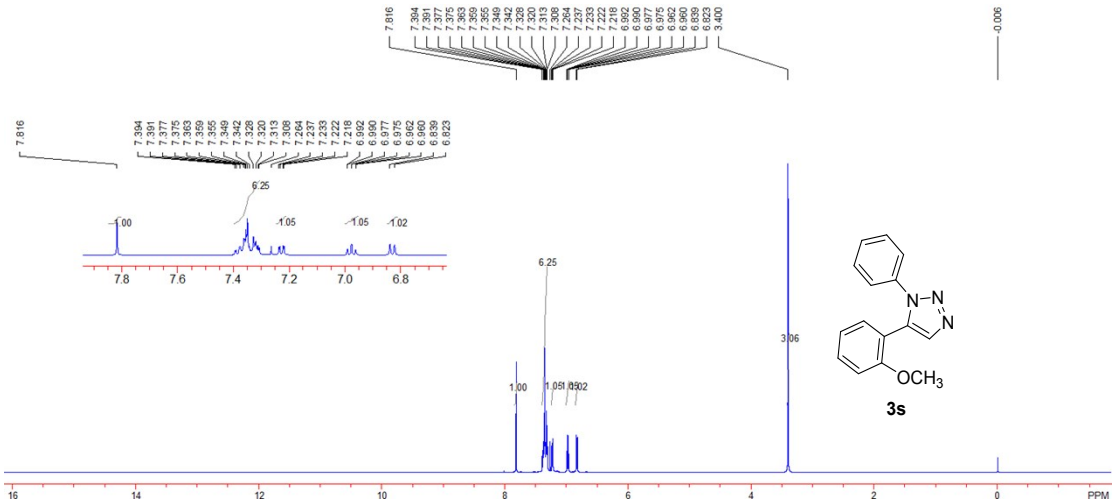
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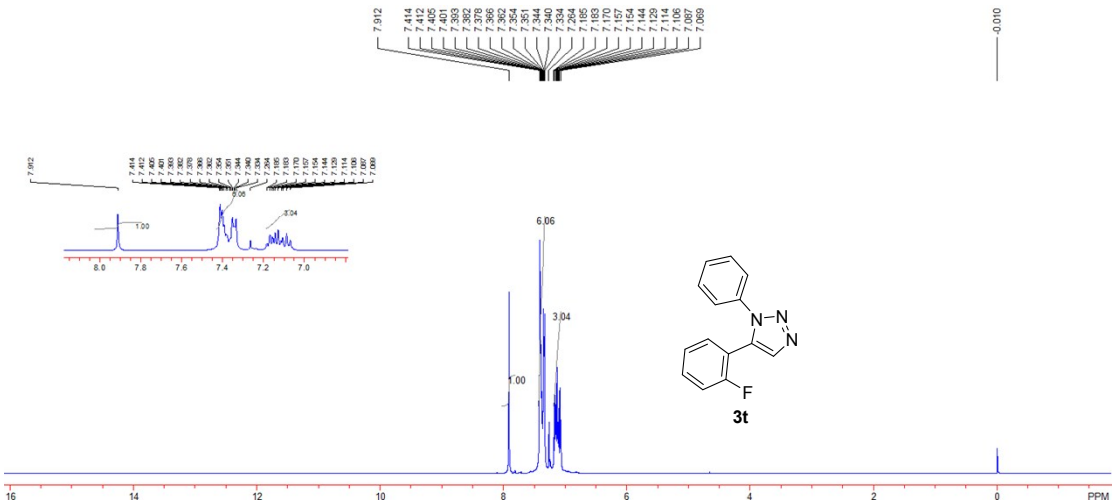
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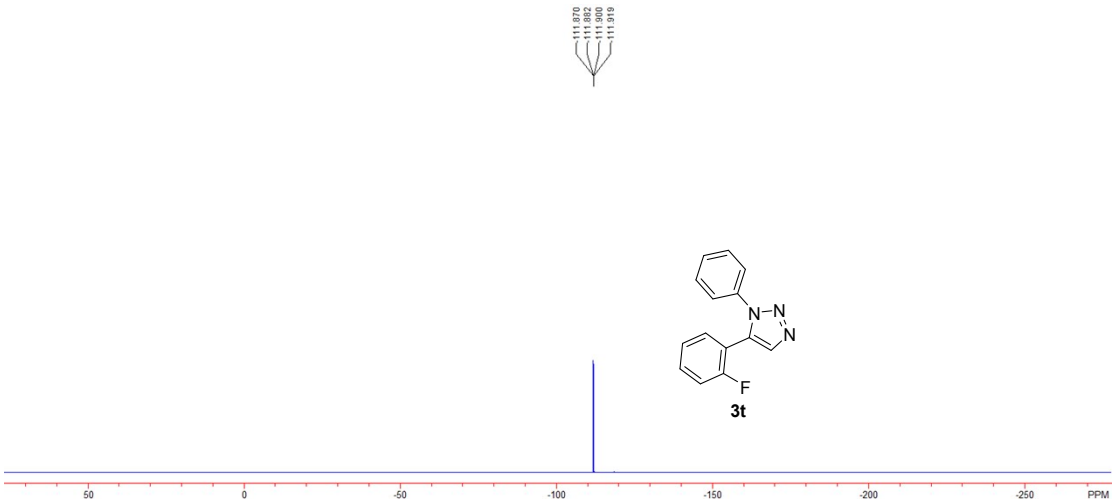
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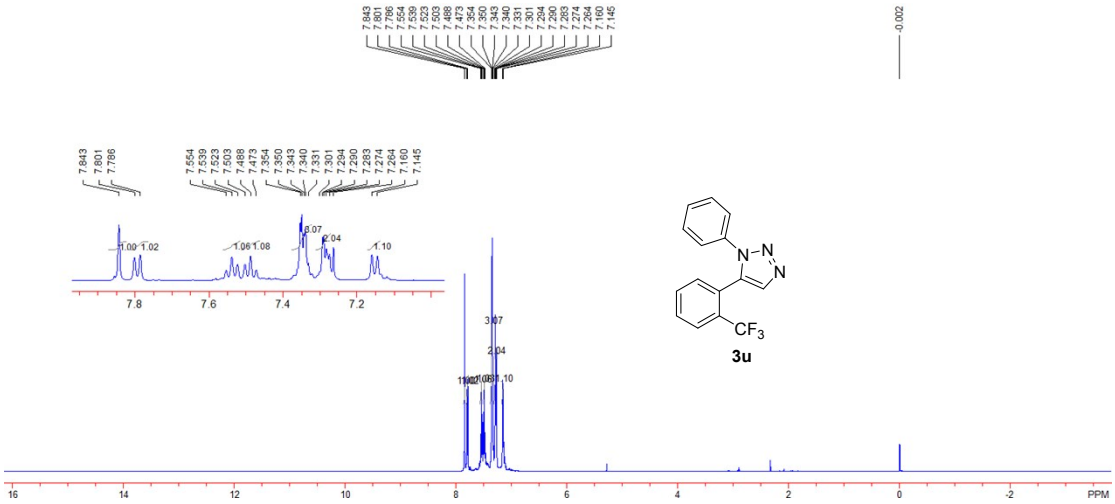
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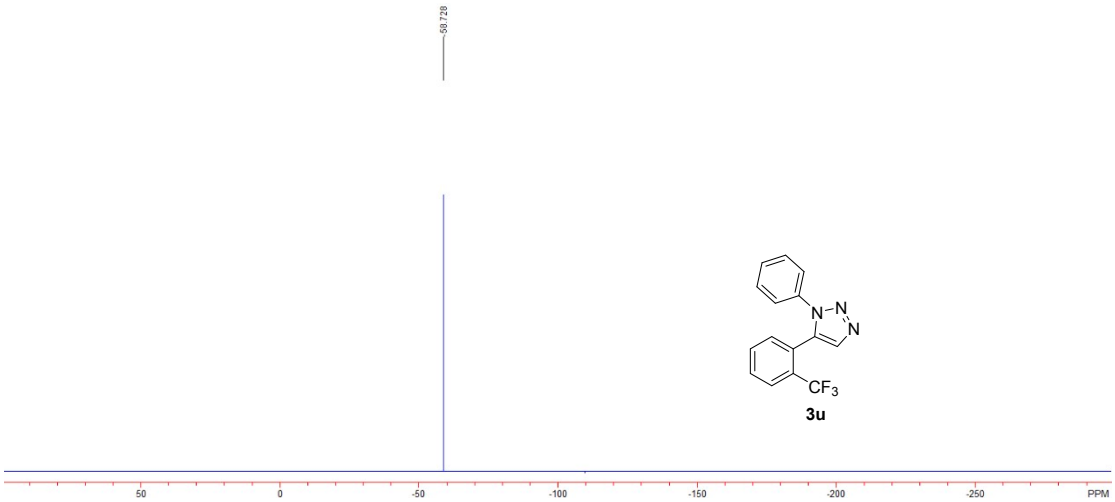
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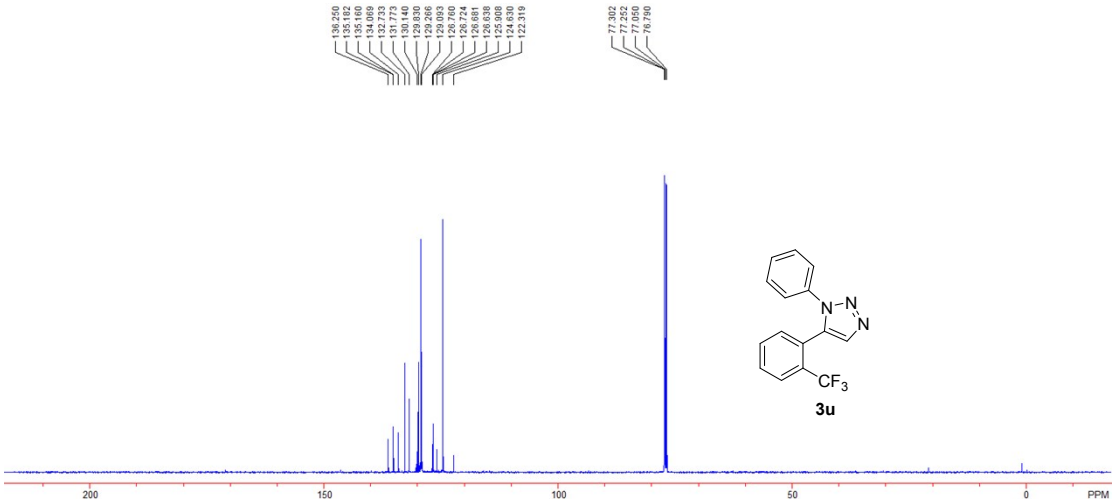
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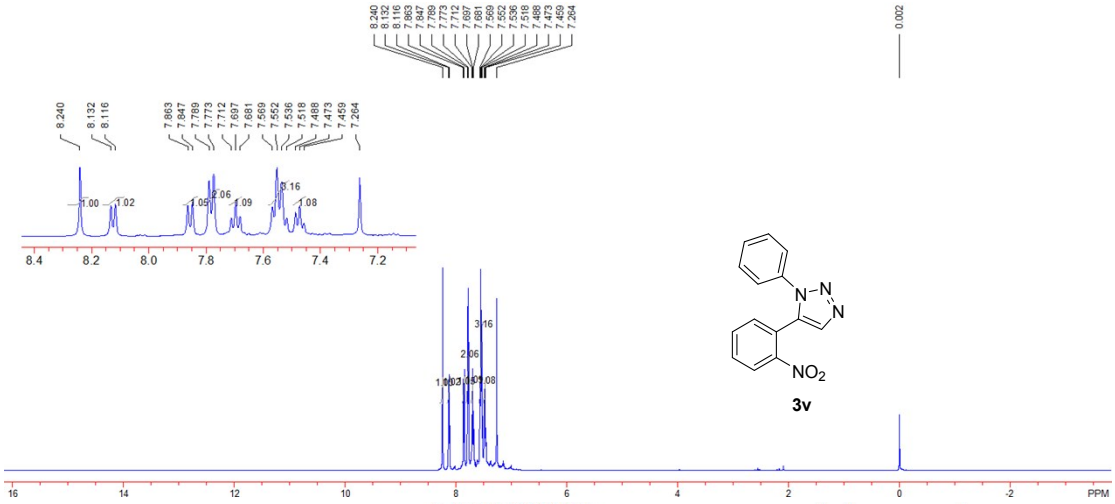
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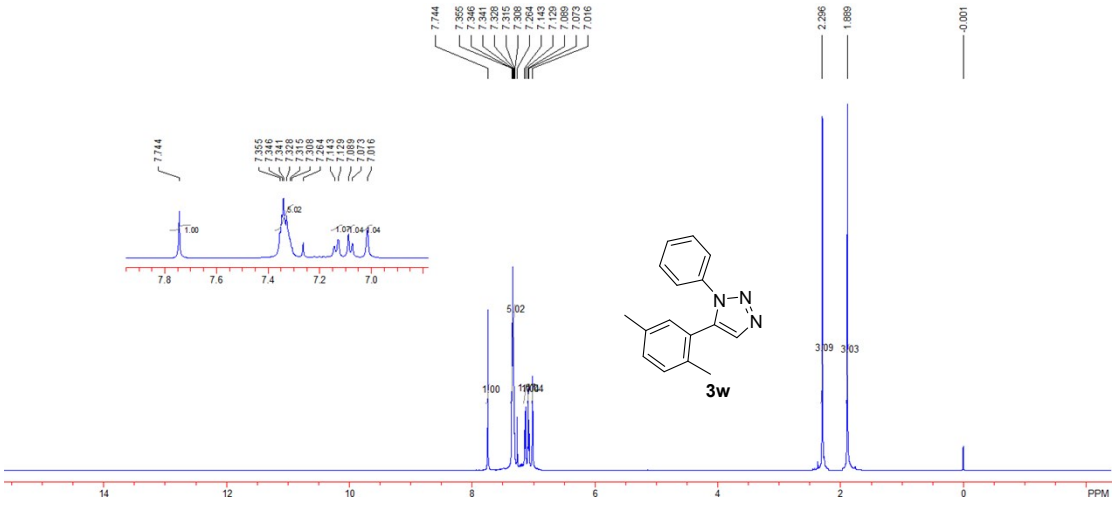
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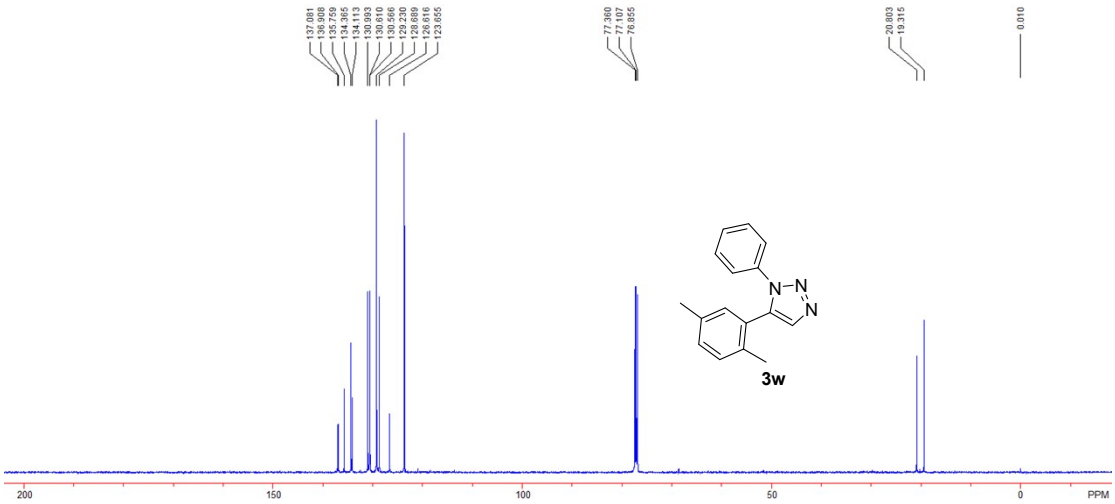
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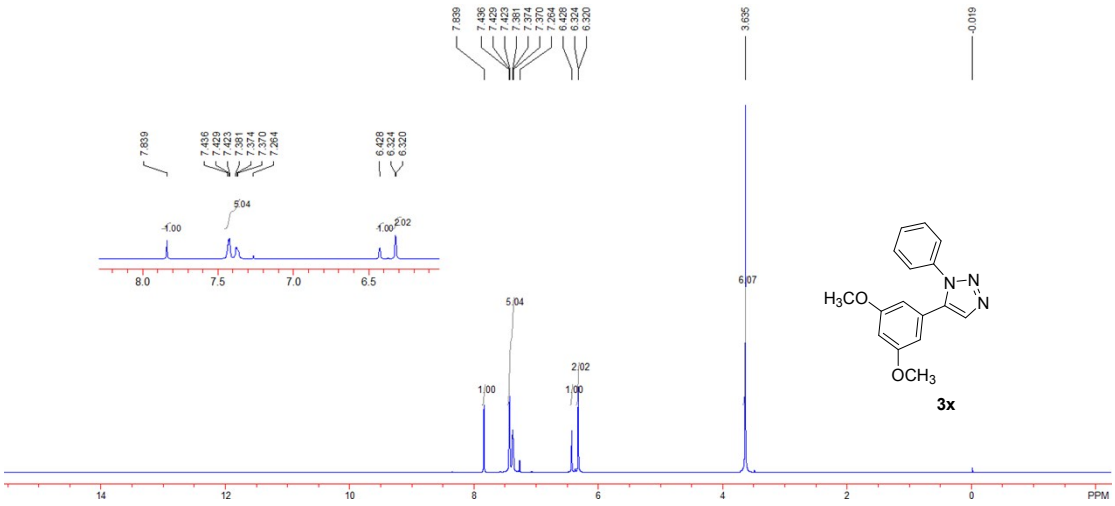
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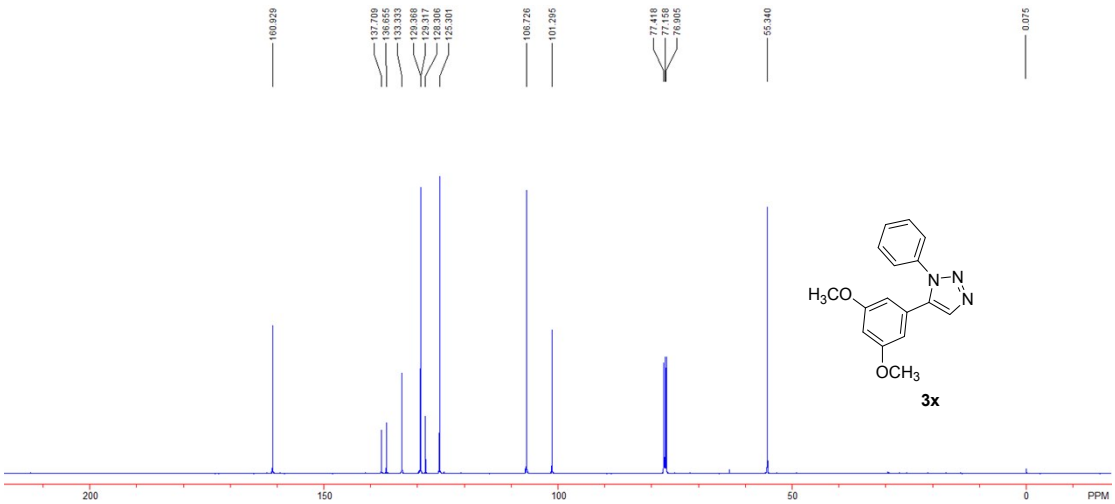
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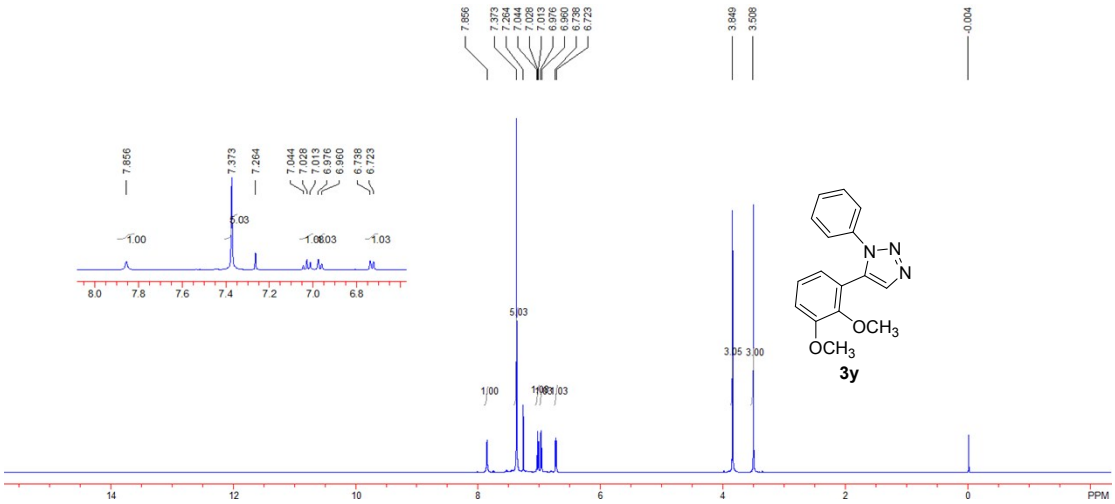
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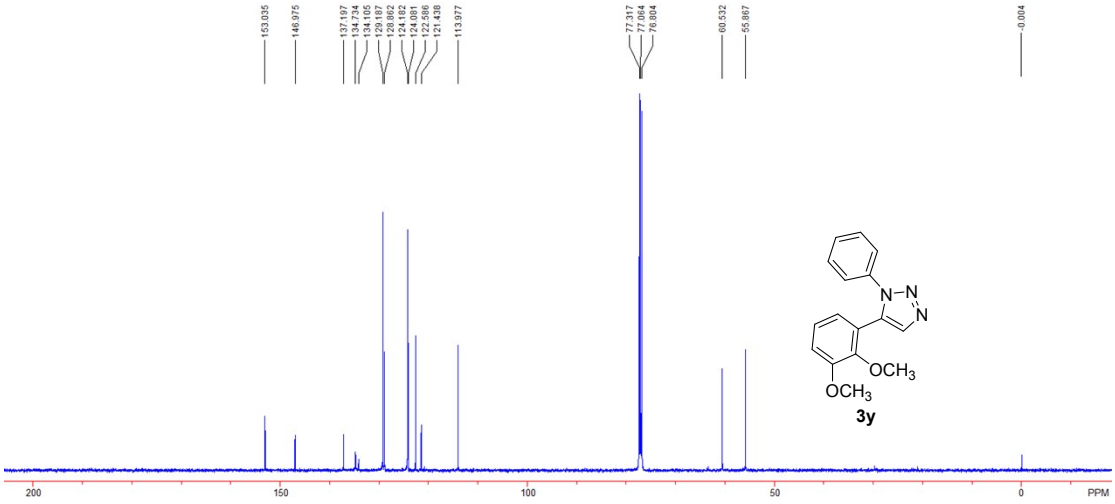
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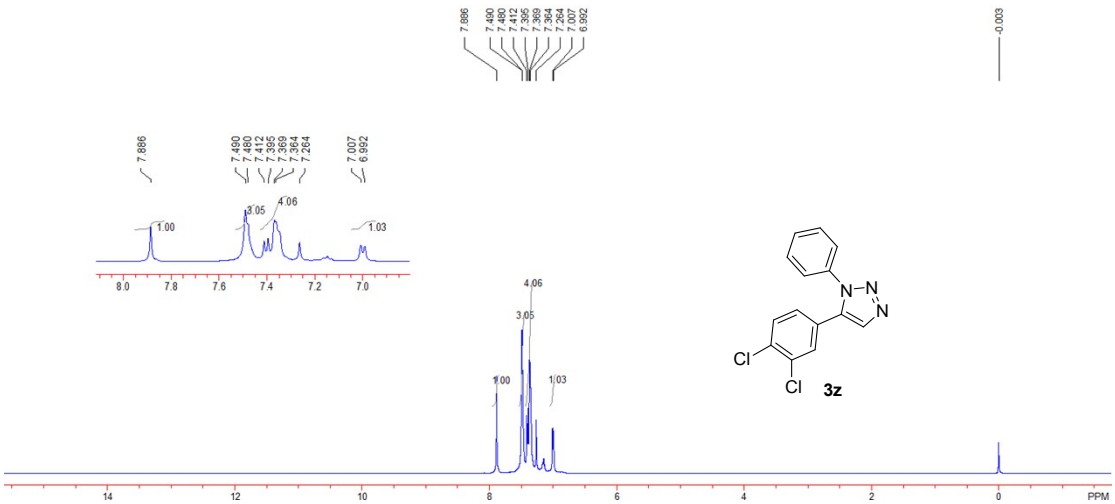
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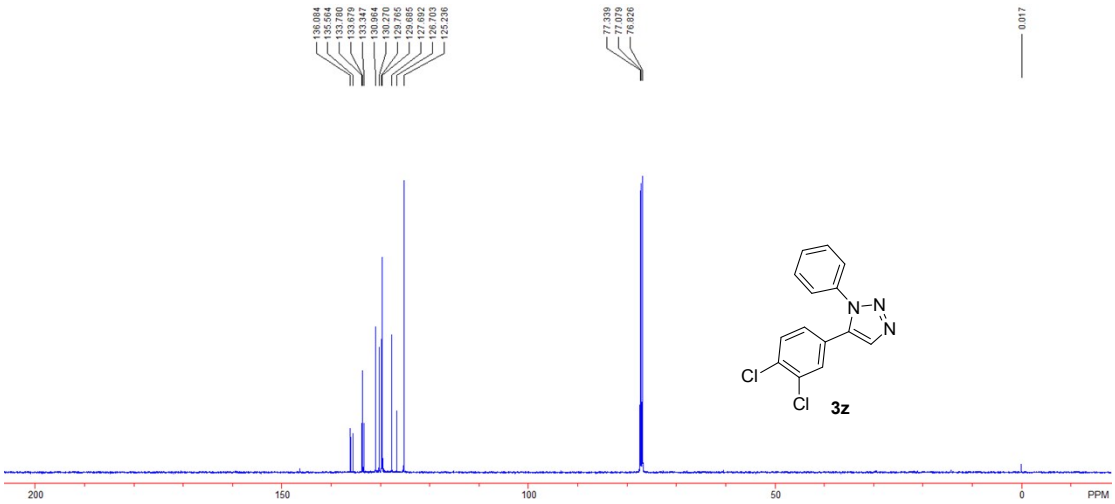
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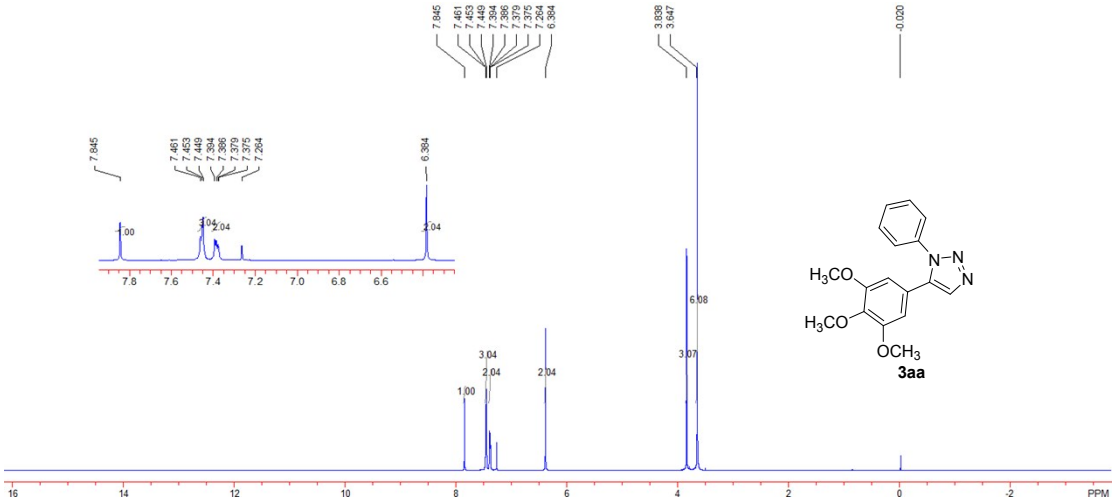
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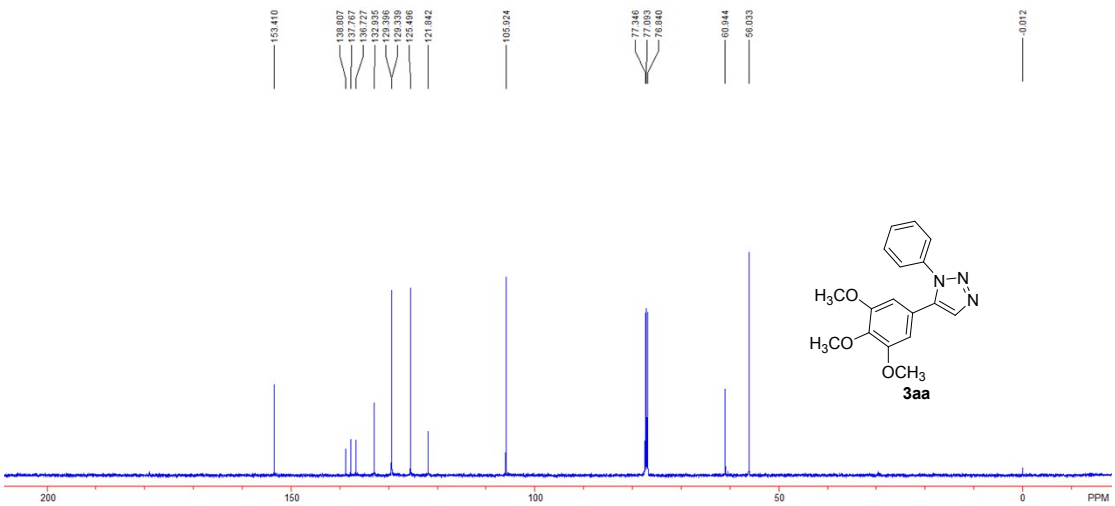
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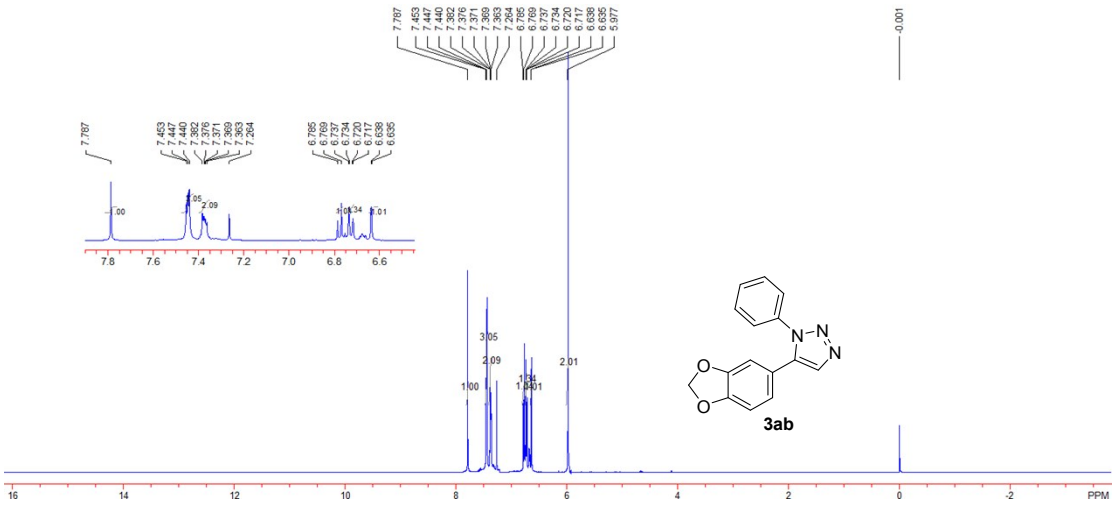
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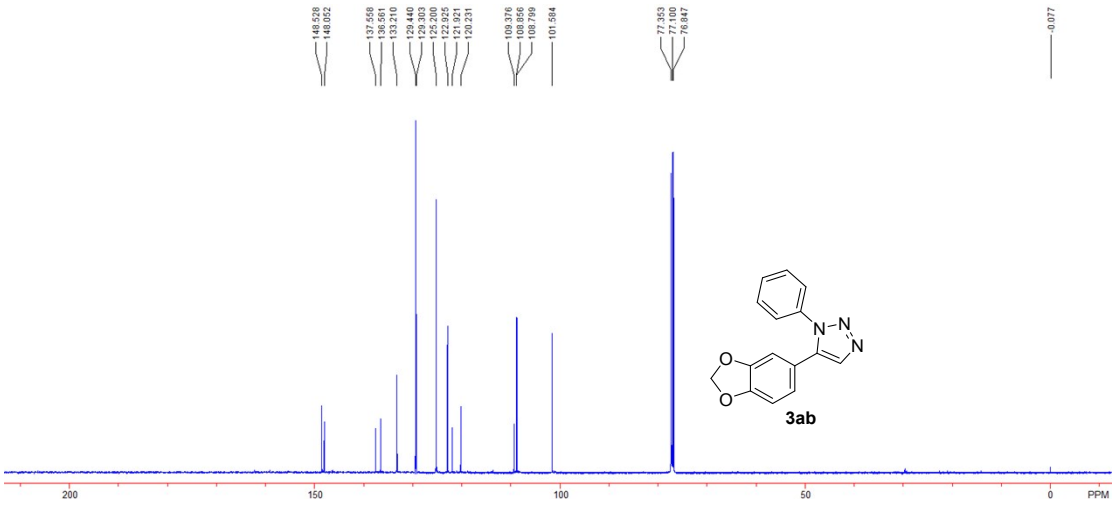
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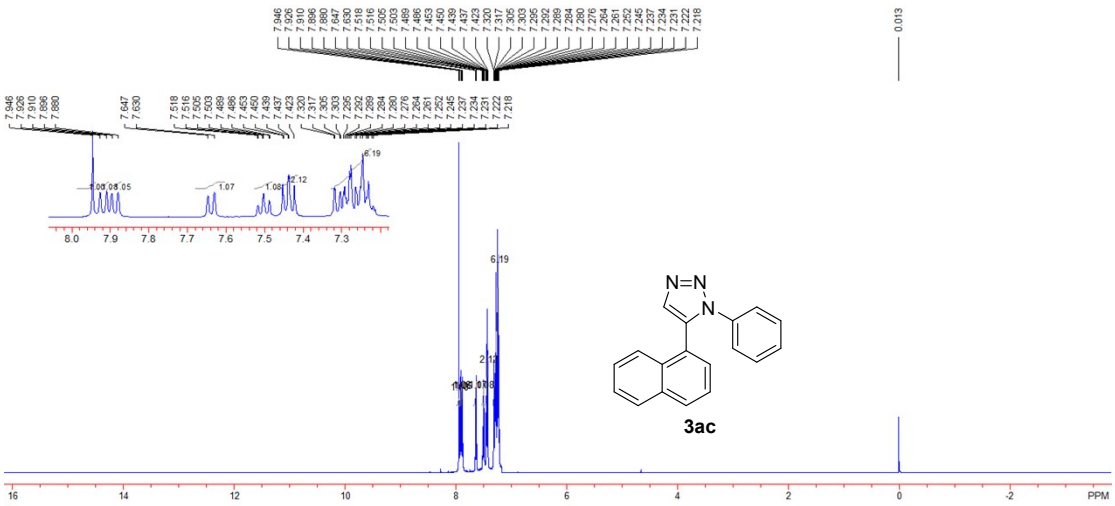
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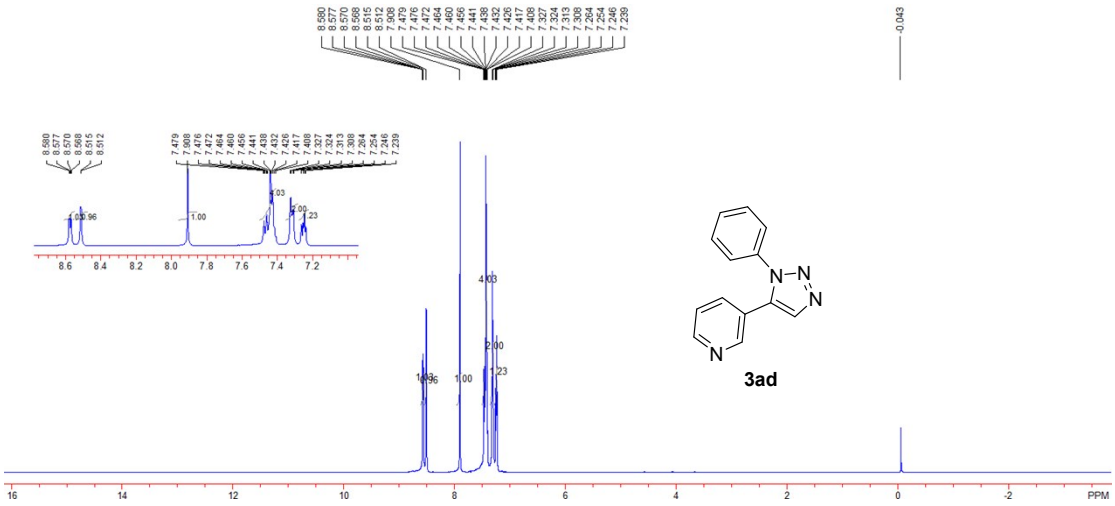
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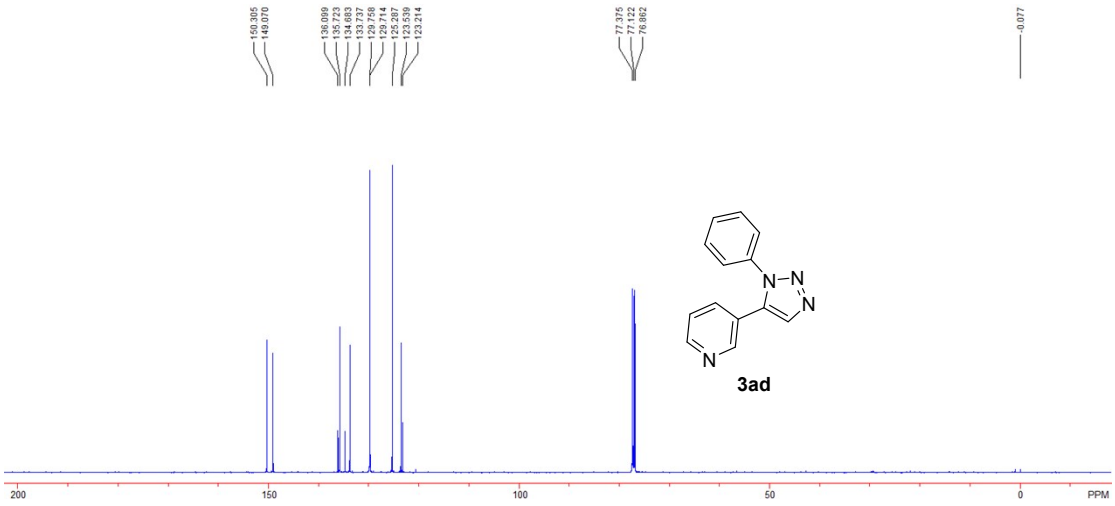
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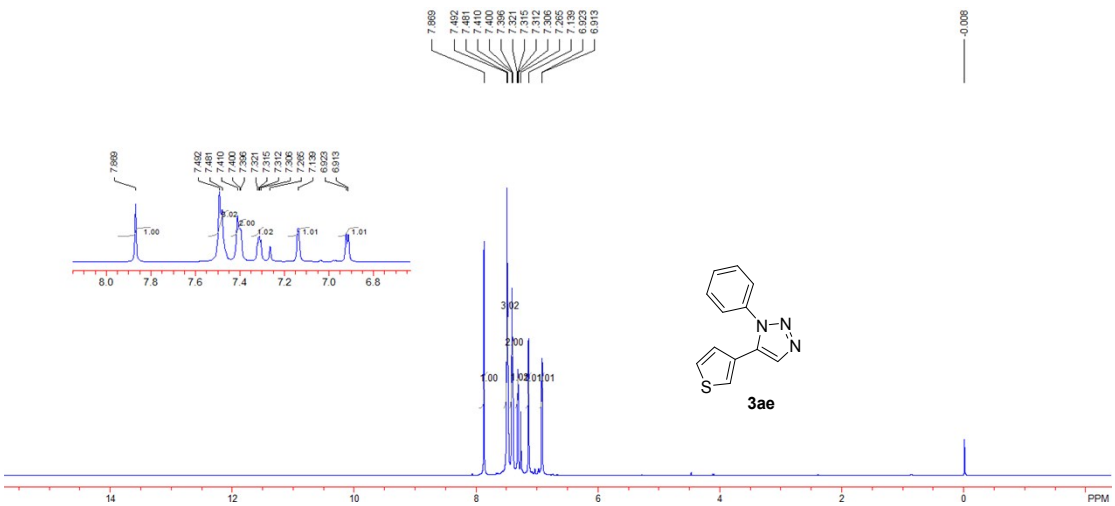
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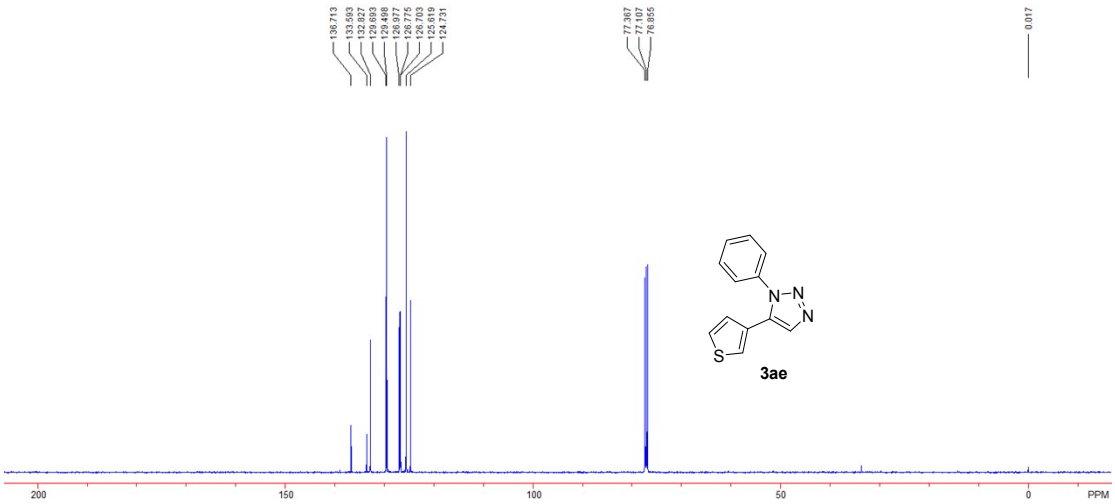
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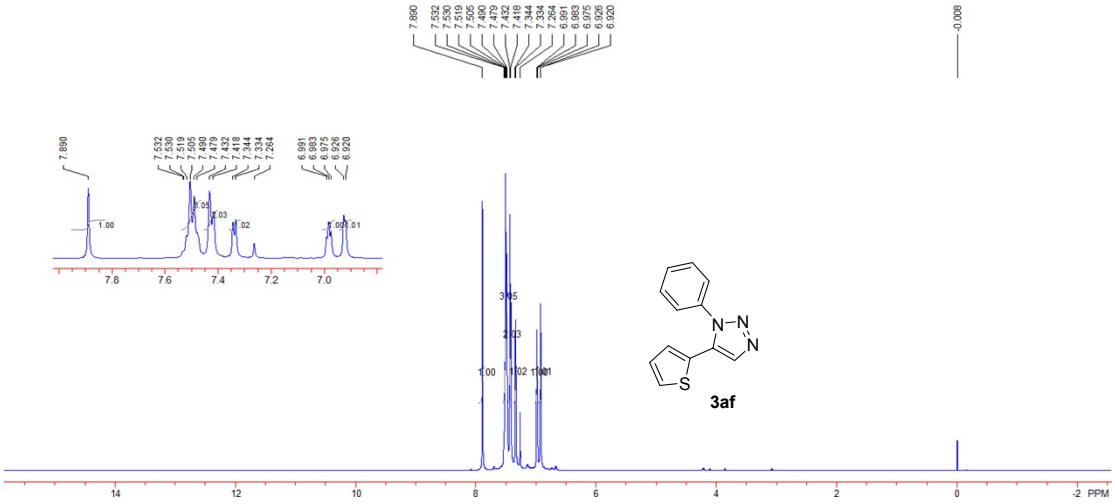
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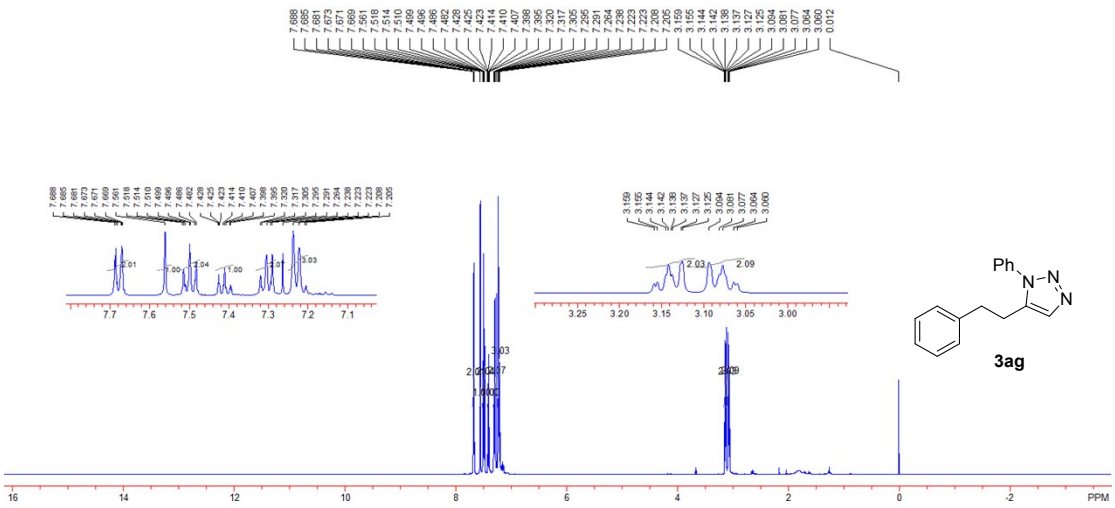
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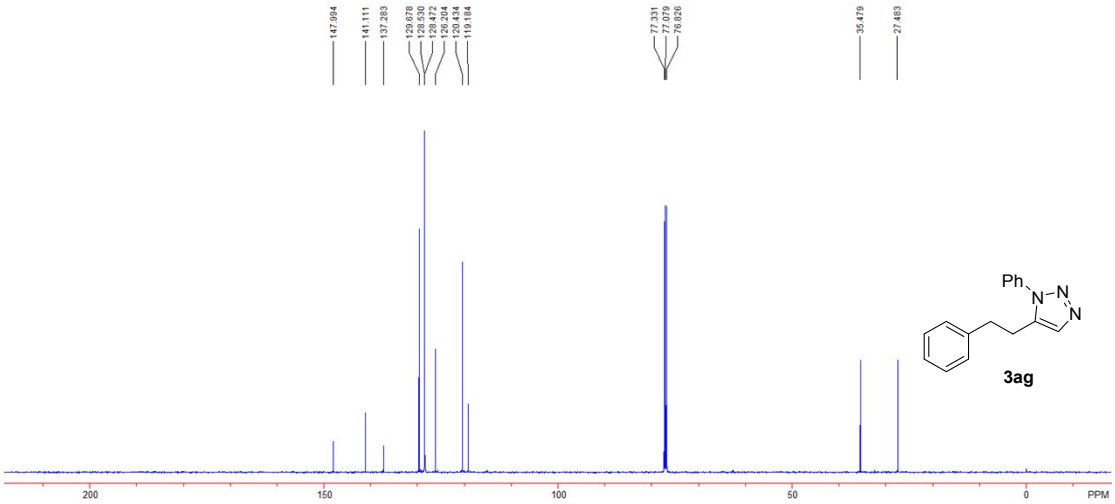
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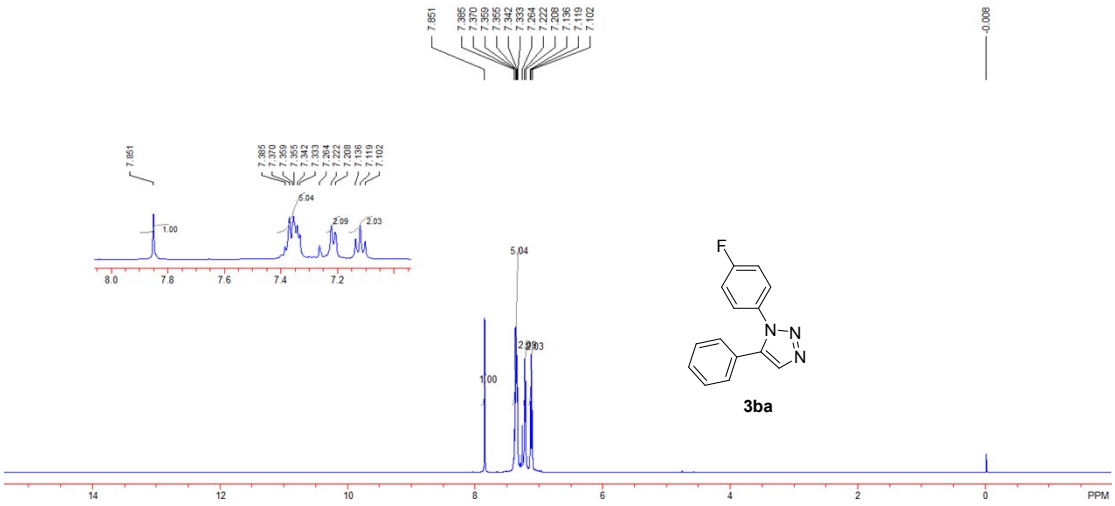
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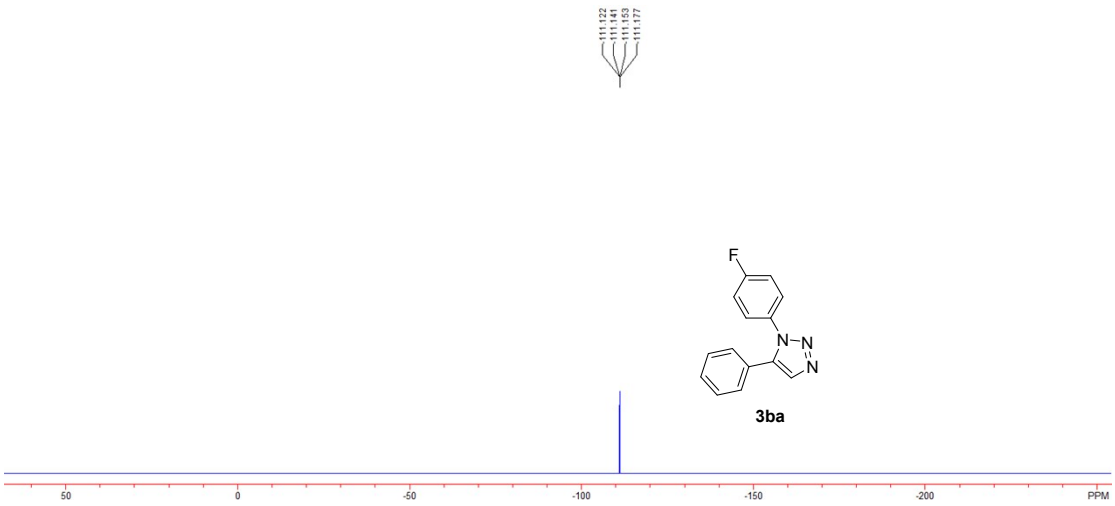
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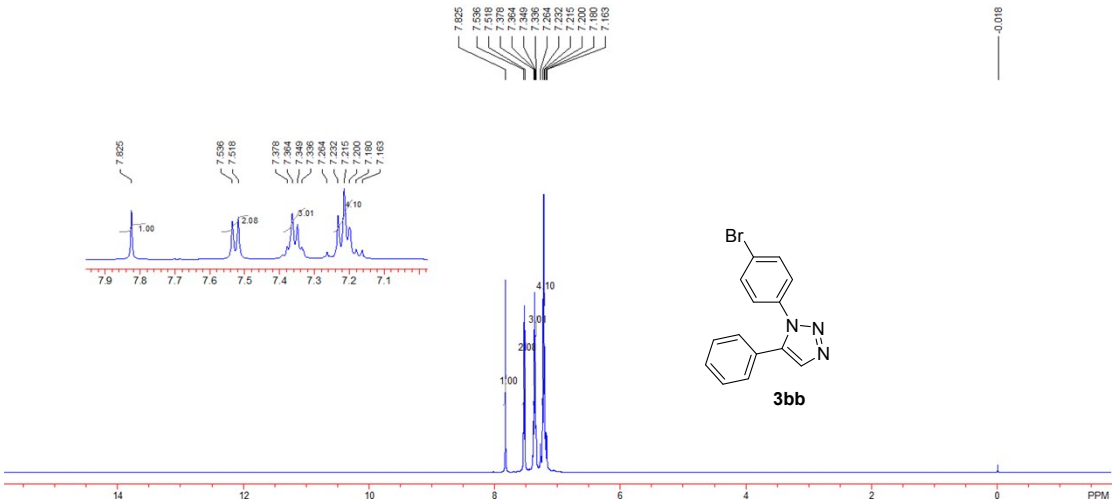
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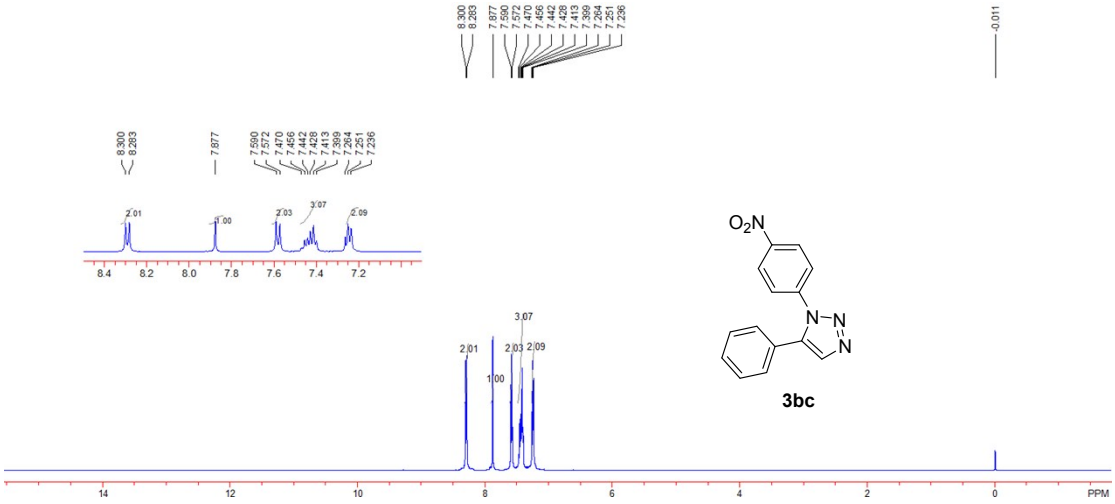
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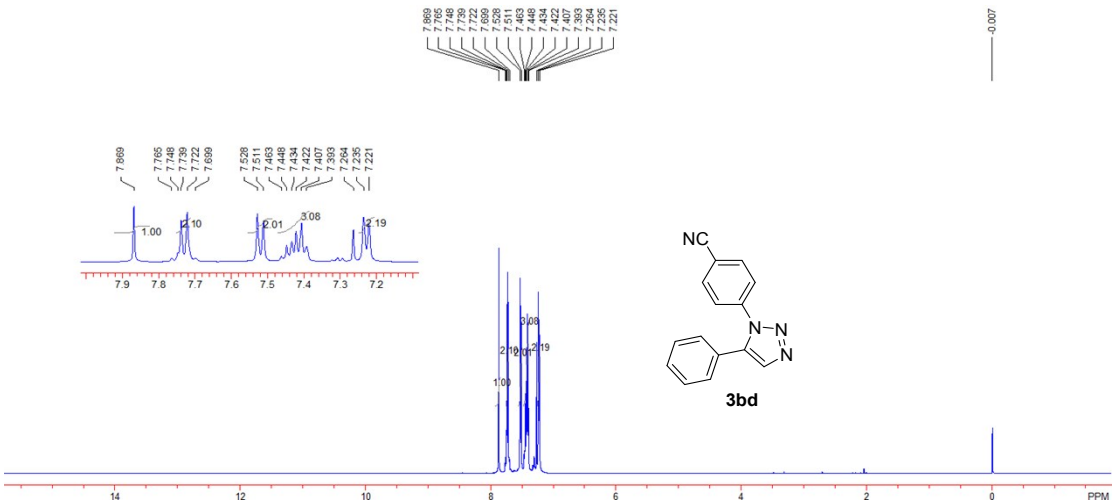
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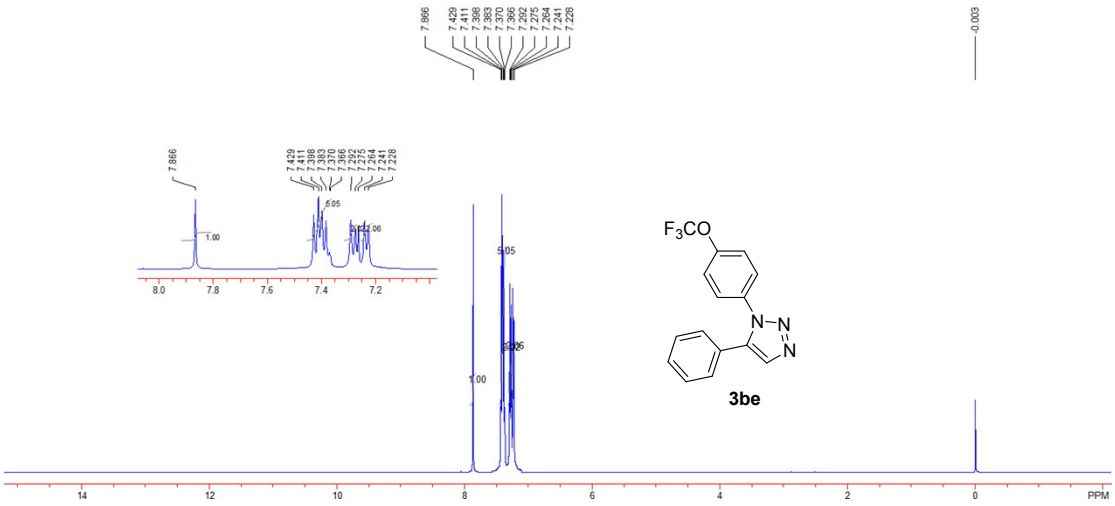
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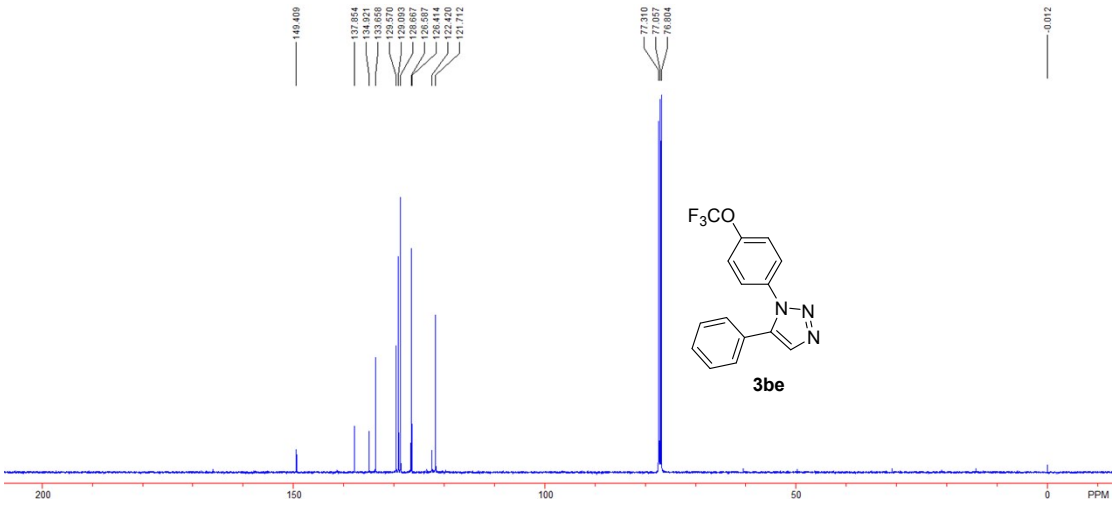
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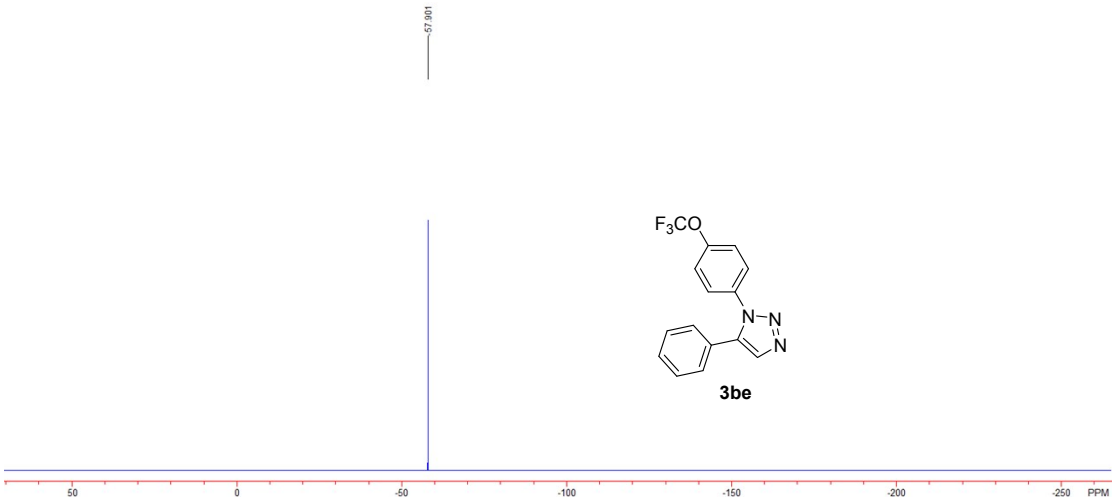
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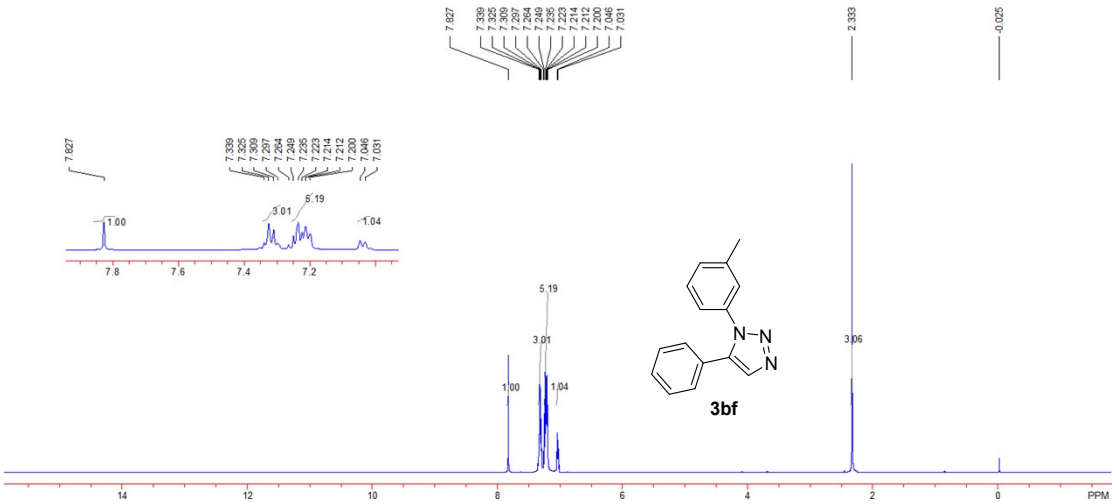
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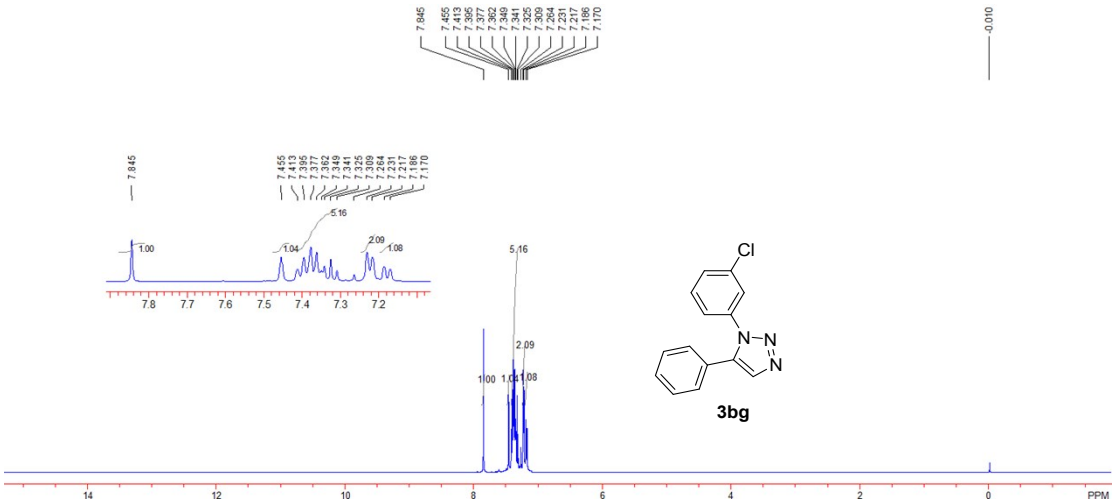
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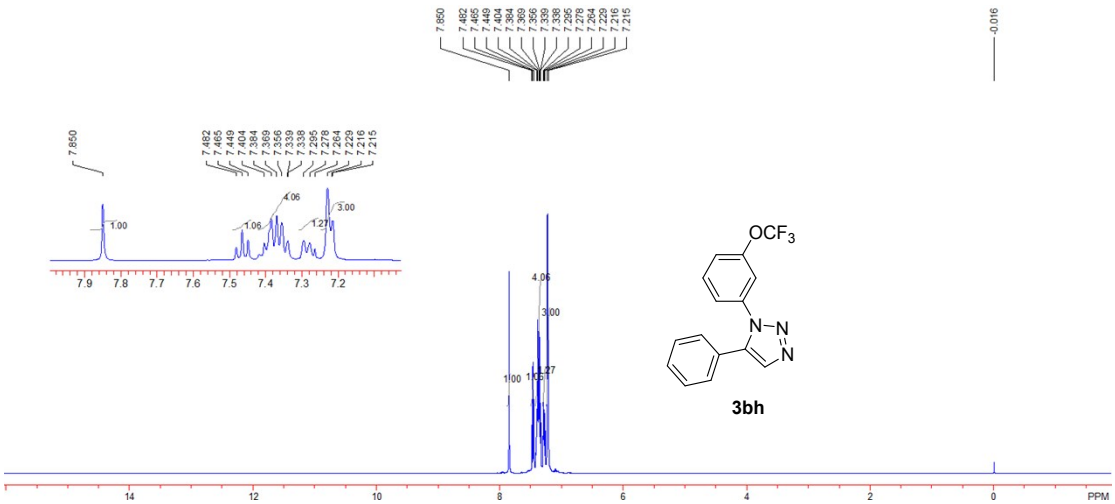
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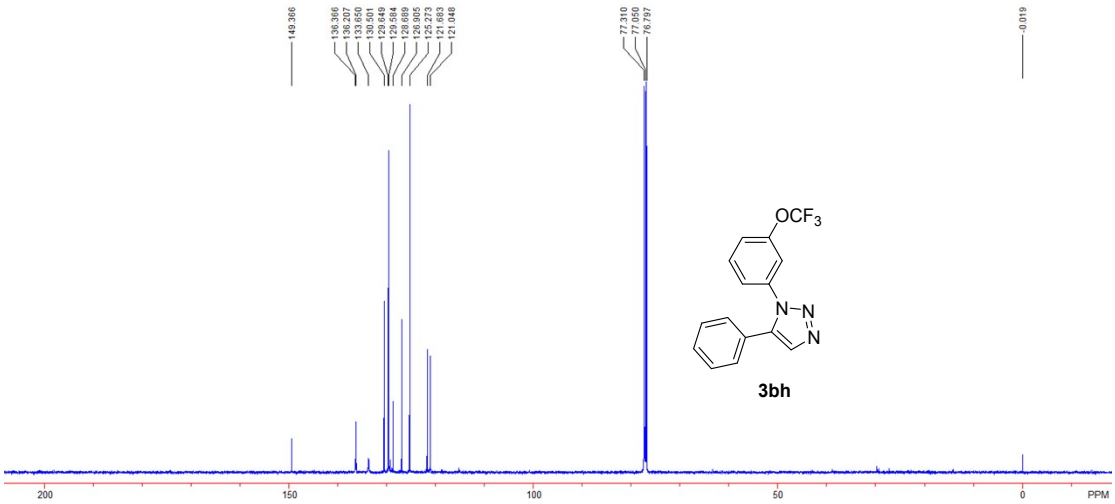
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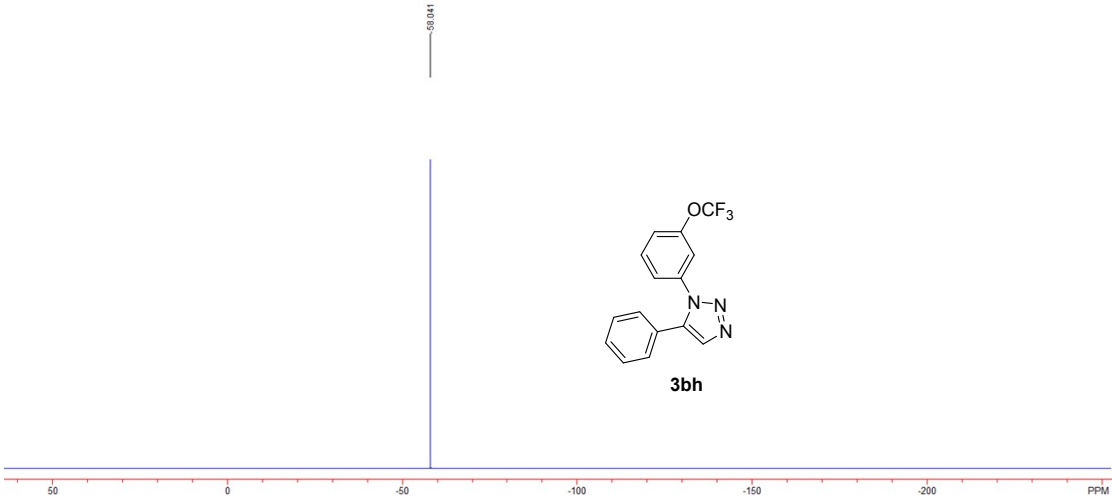
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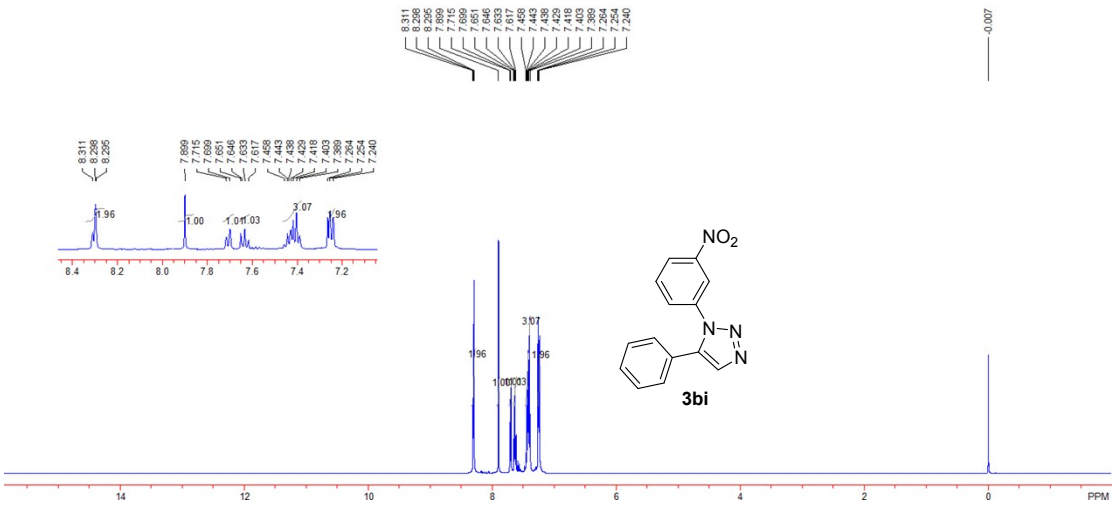
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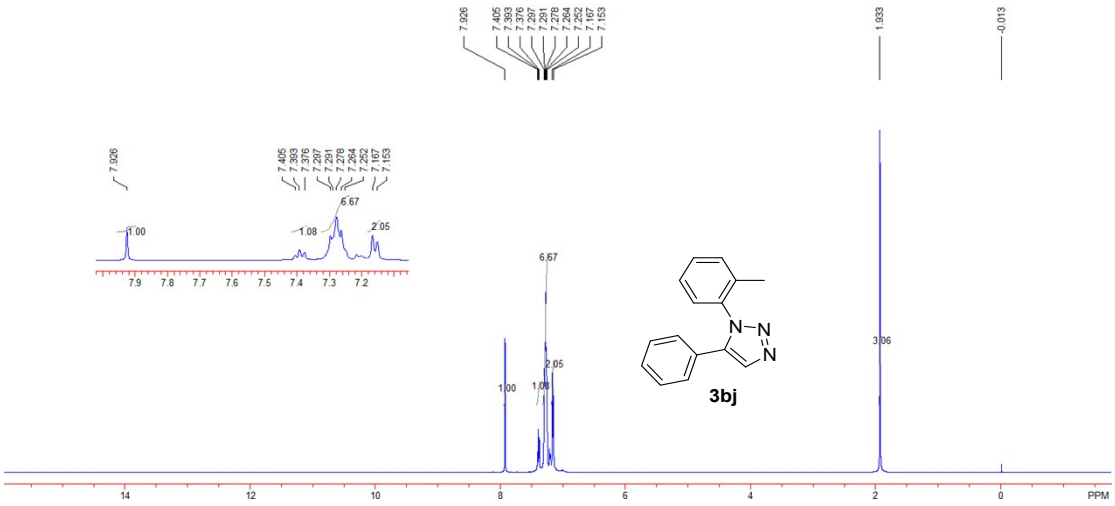
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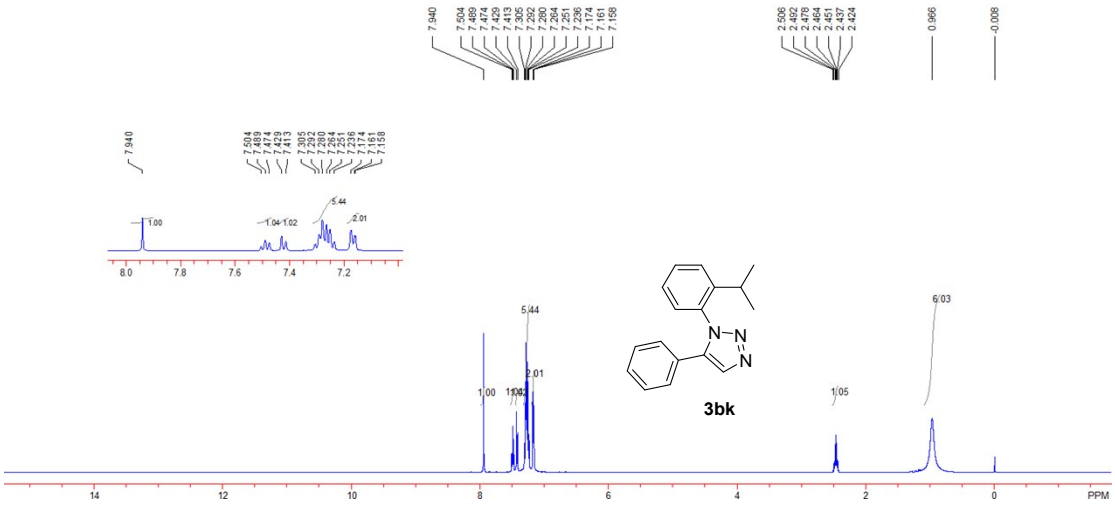
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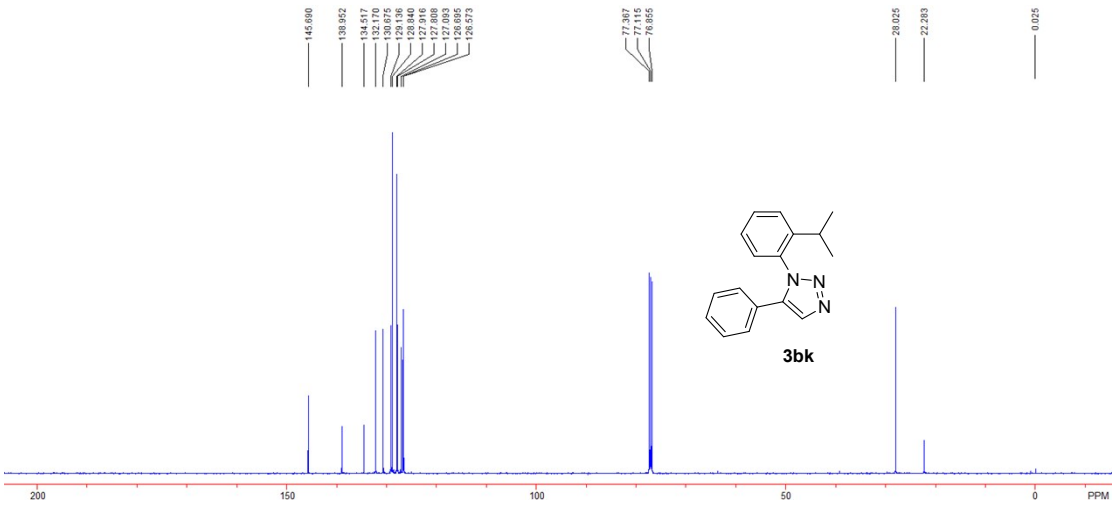
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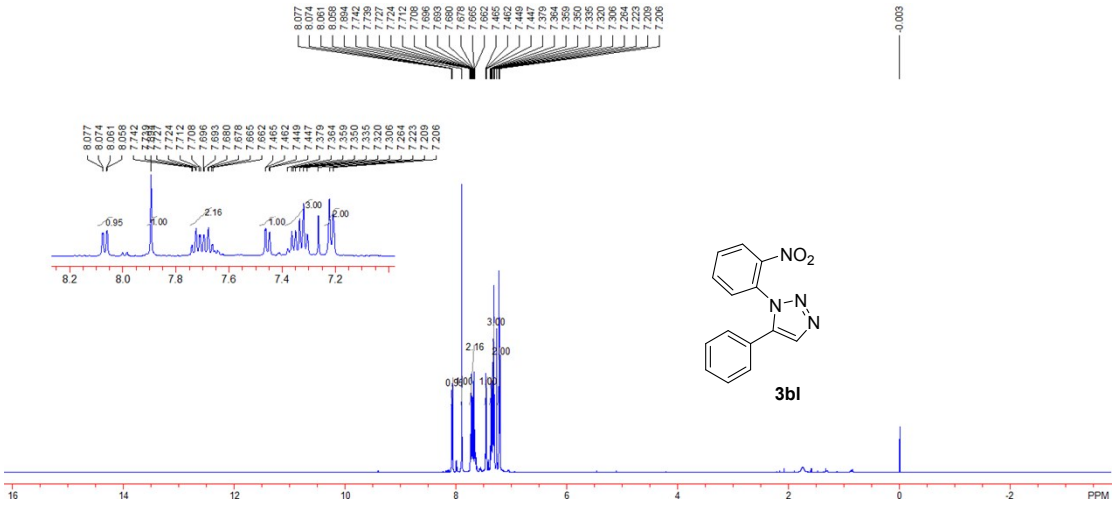
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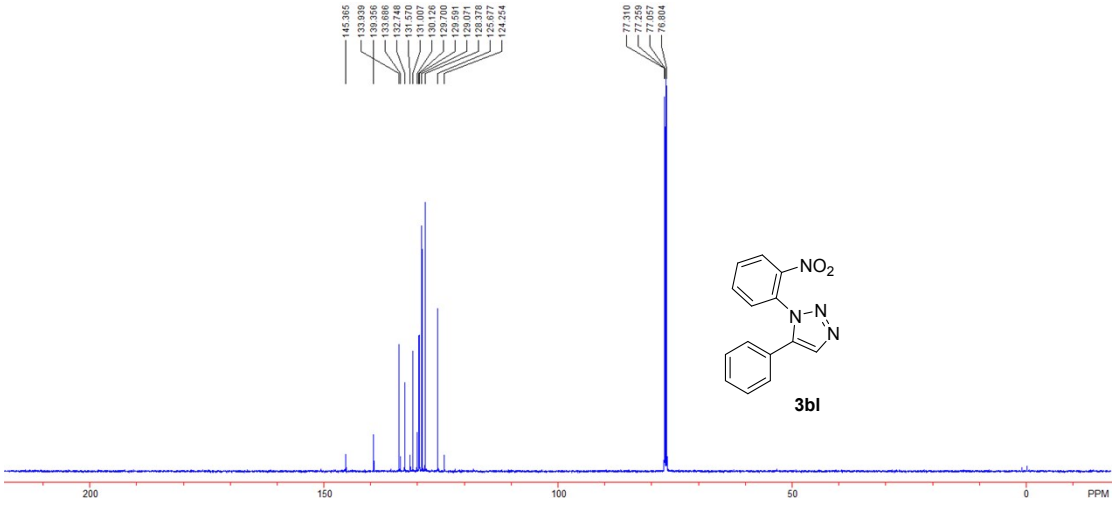
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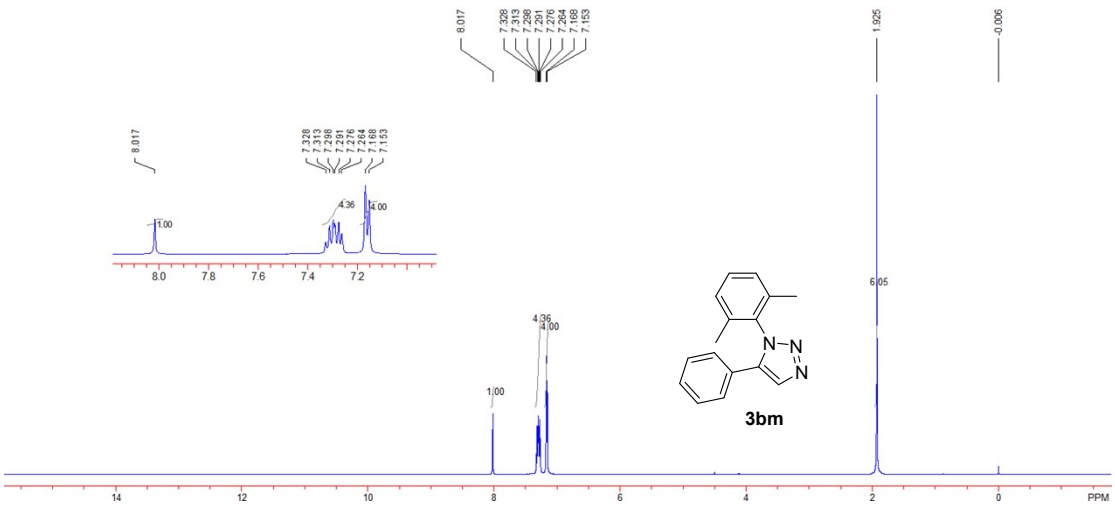
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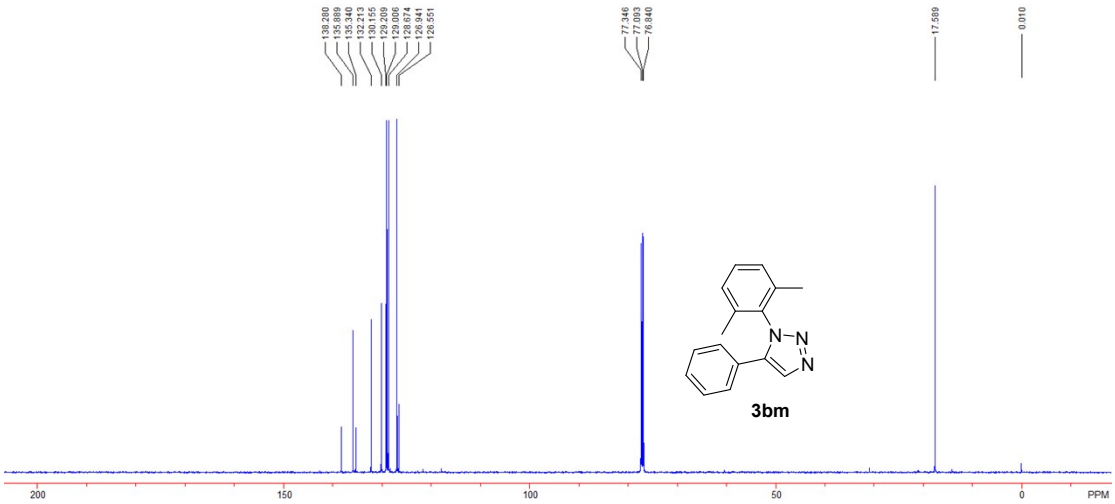
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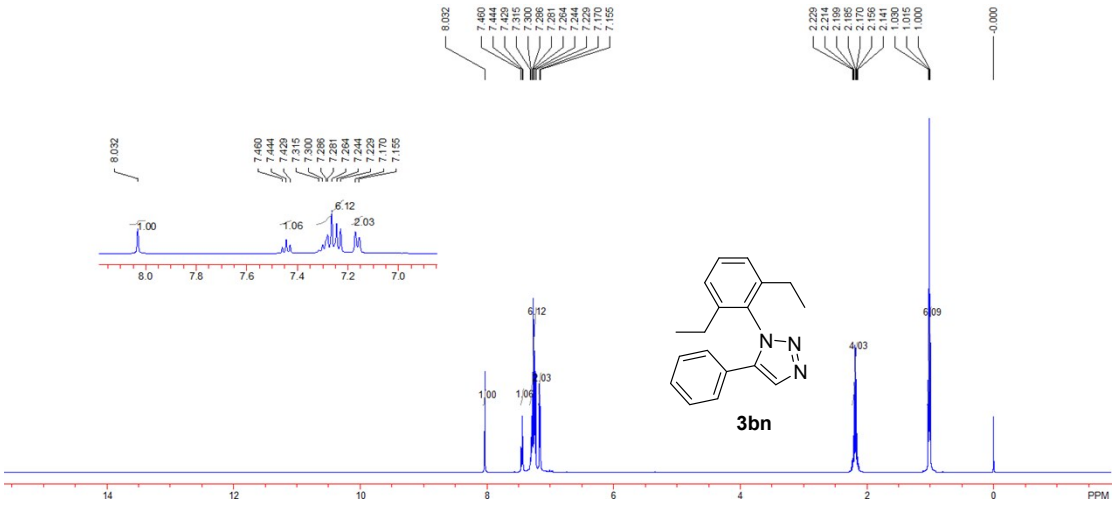
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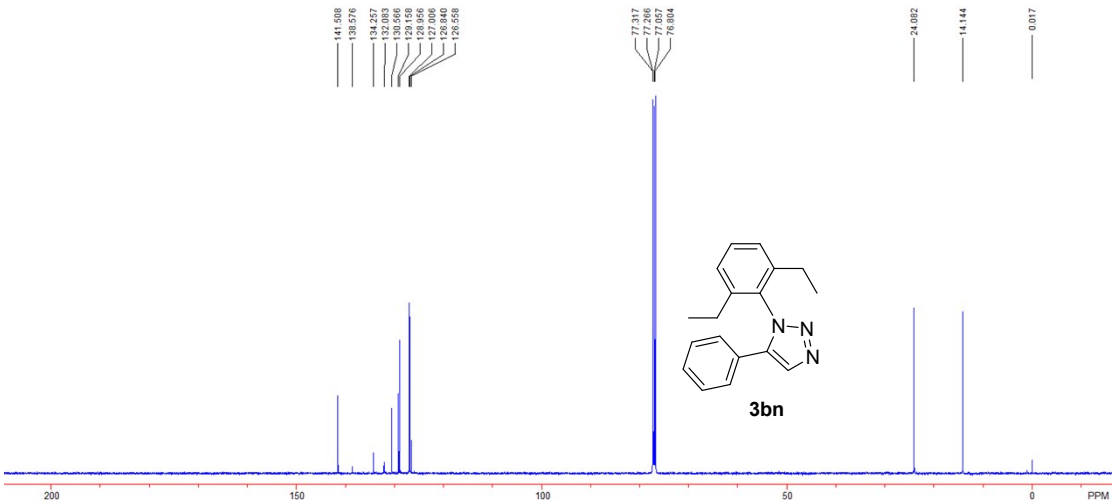
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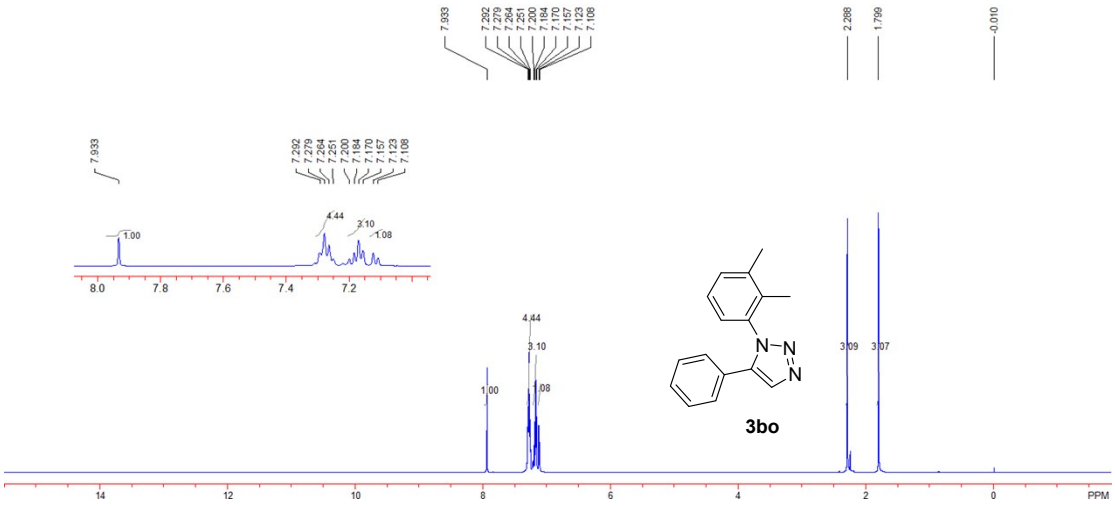
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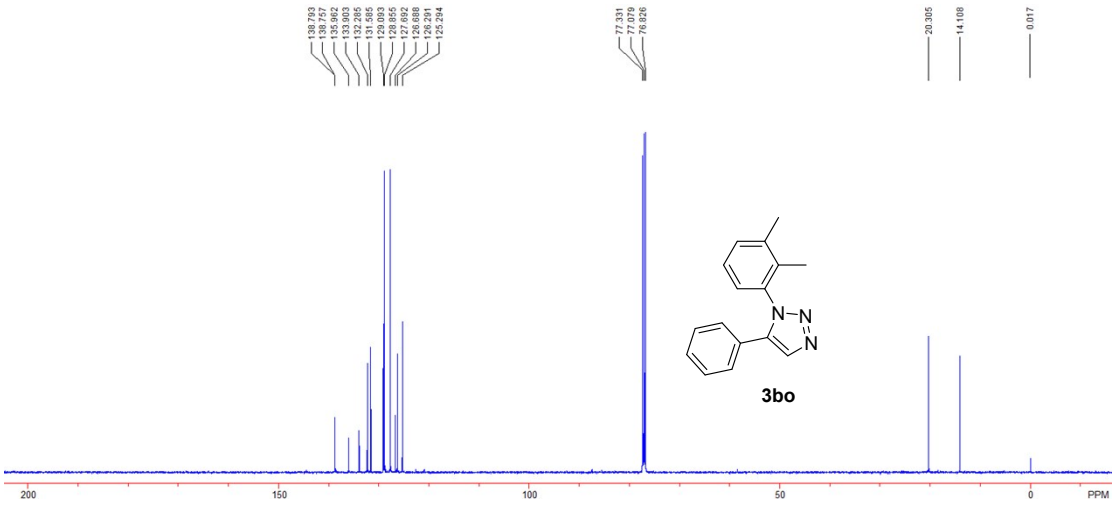
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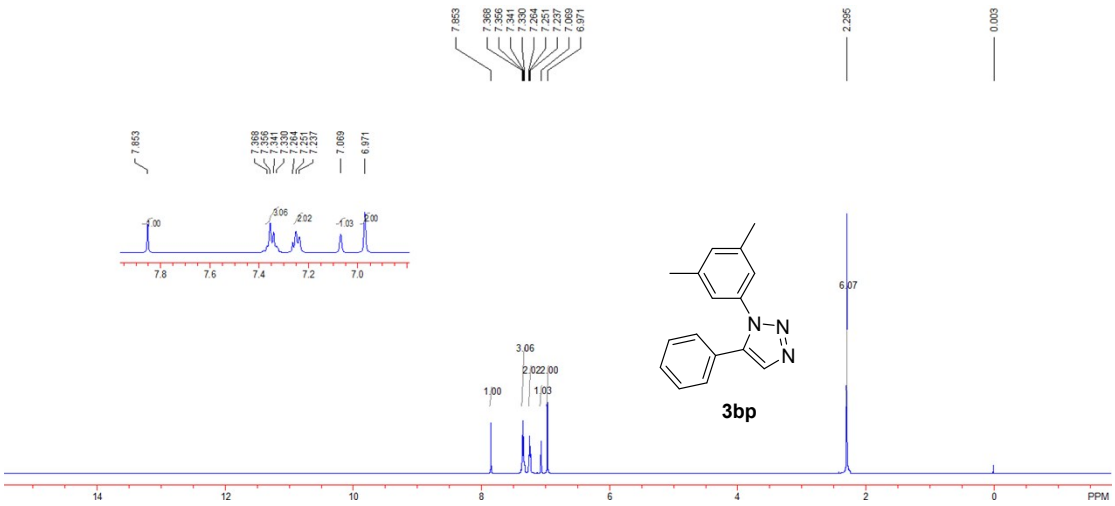
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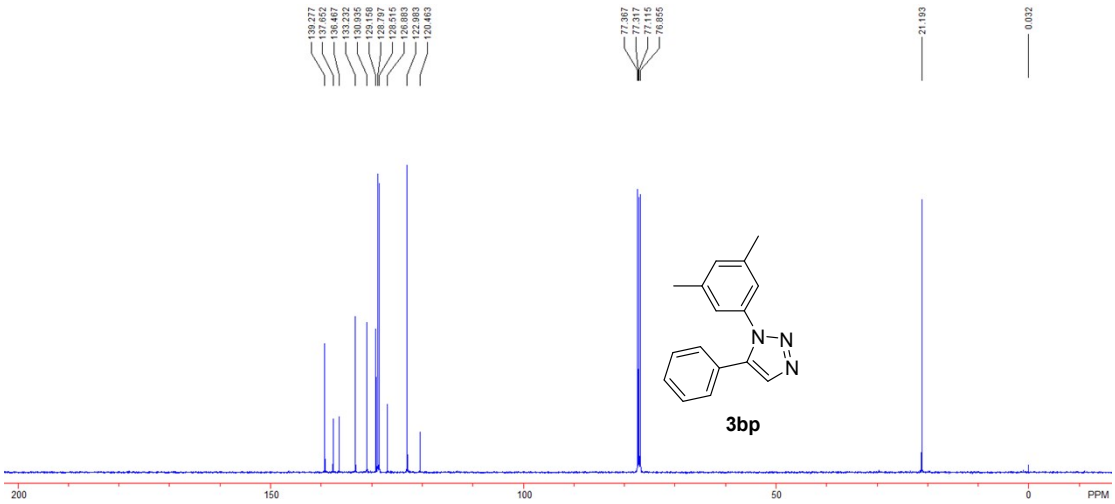
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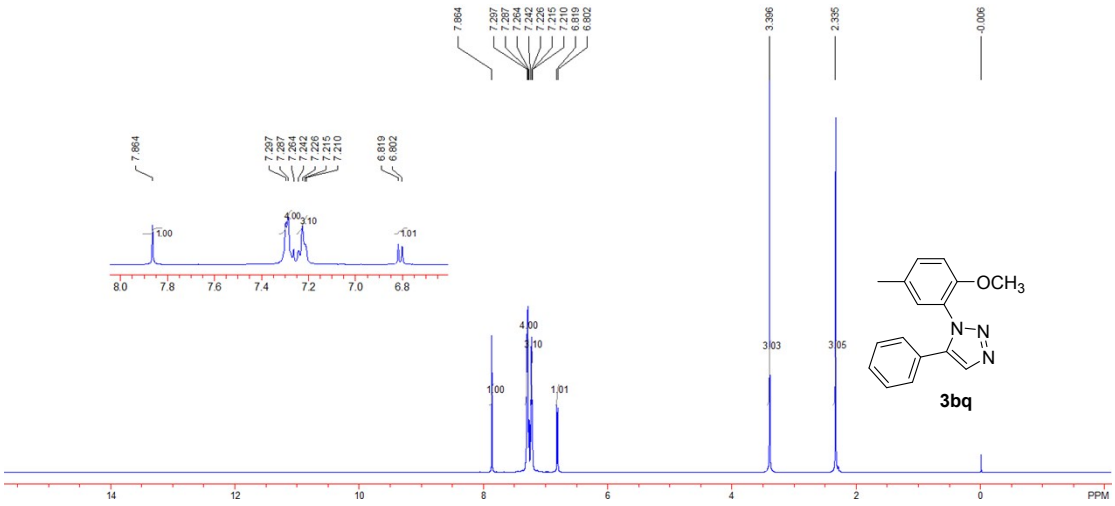
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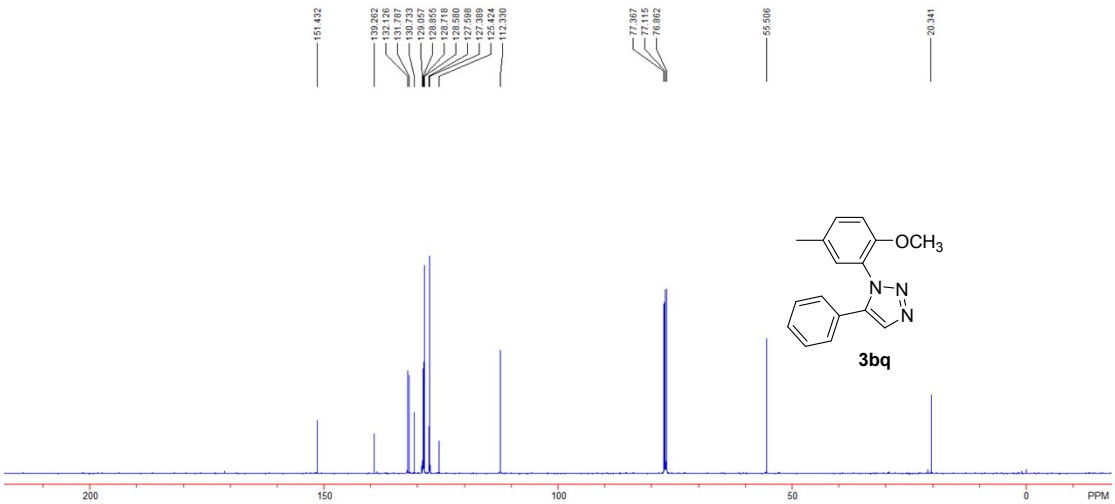
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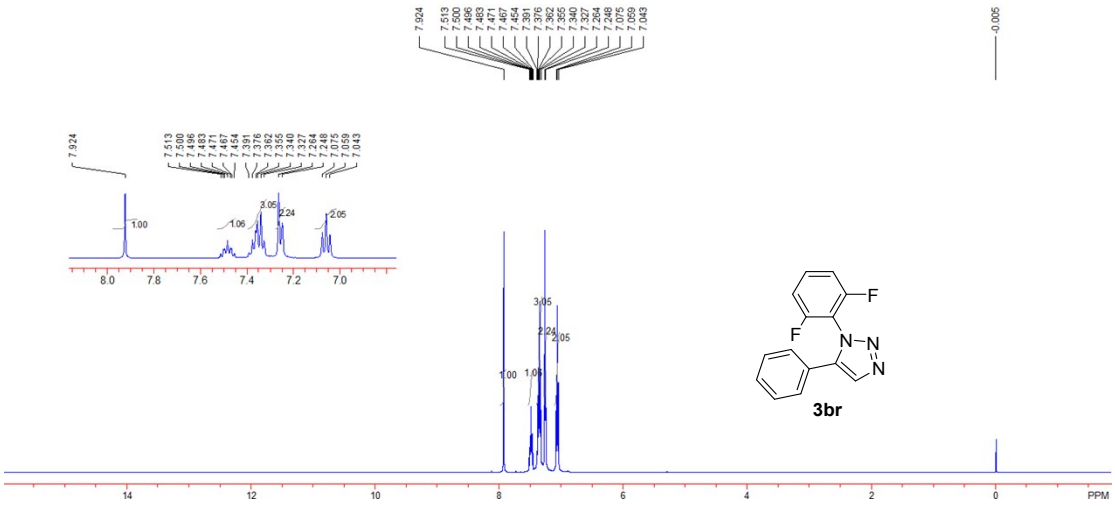
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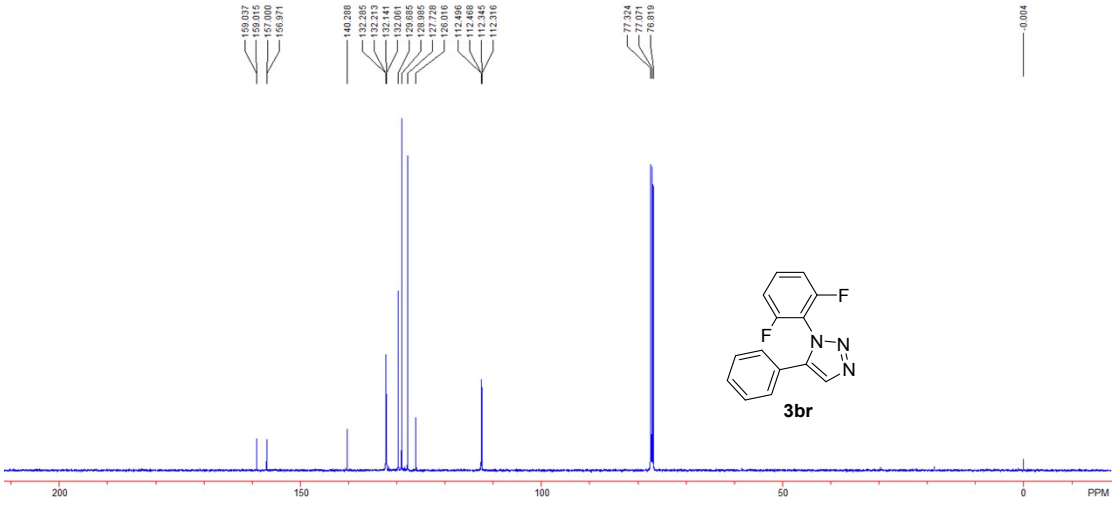
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112.345
112.316
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F
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N
N
3br
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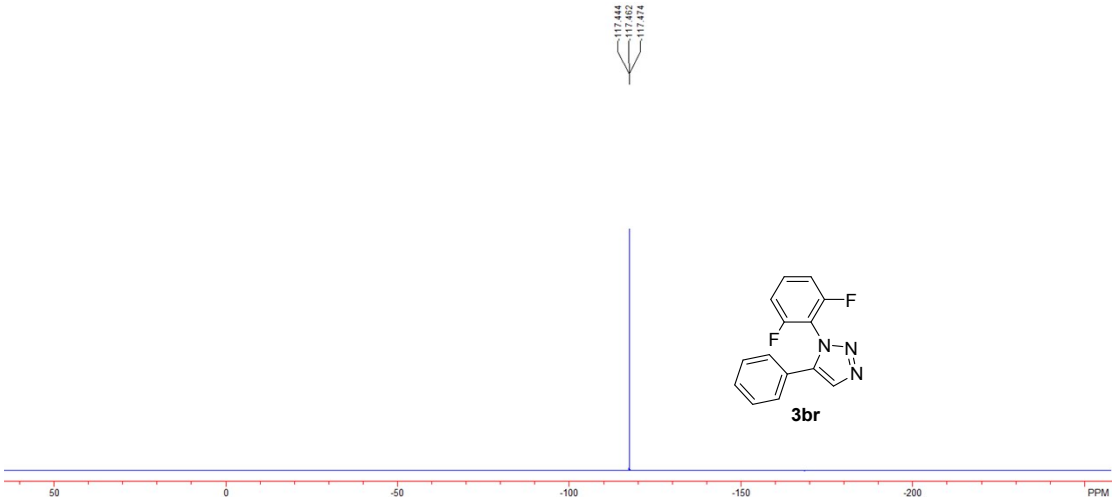
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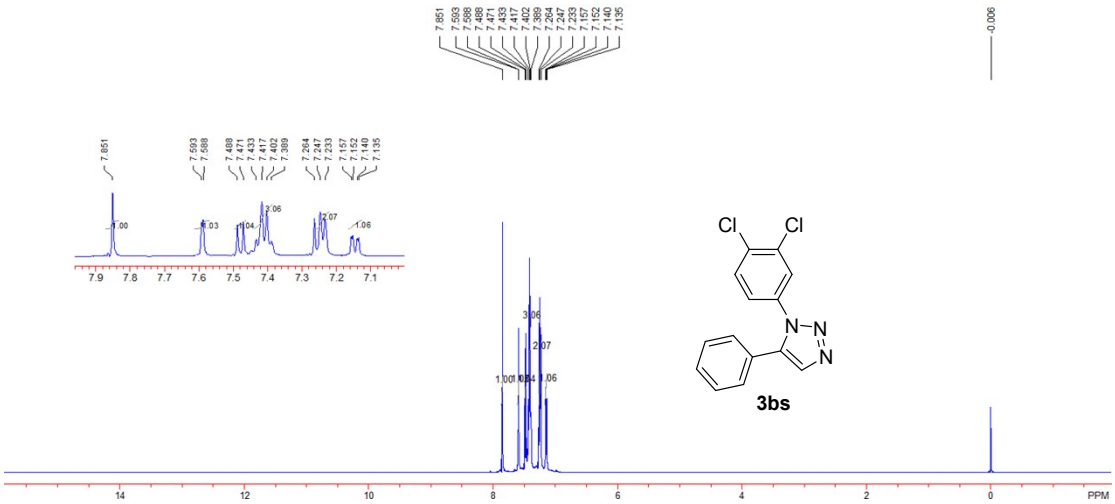
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7.402
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7.157
7.152
7.140
7.135
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Cl
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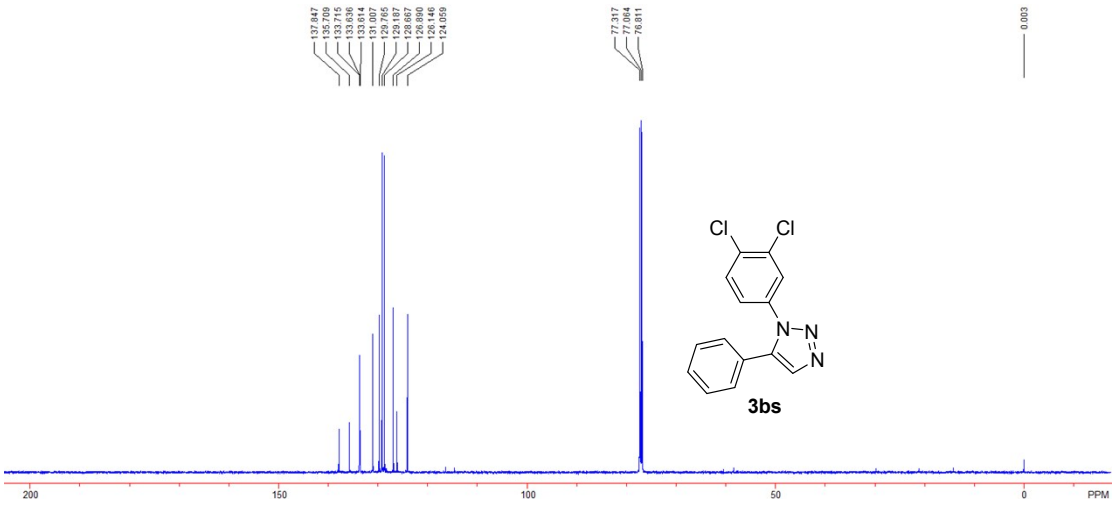
N
3bs
PPM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3bs
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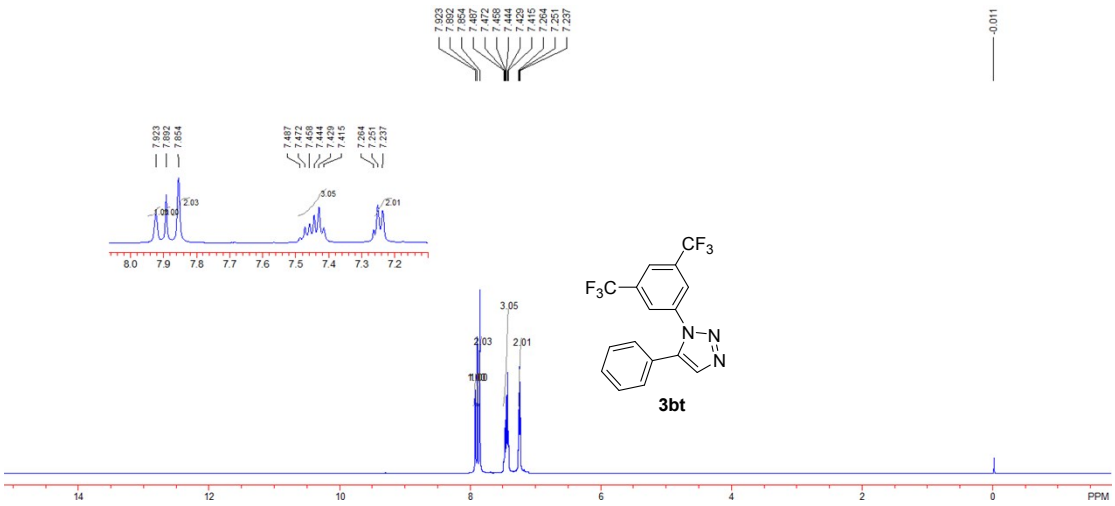
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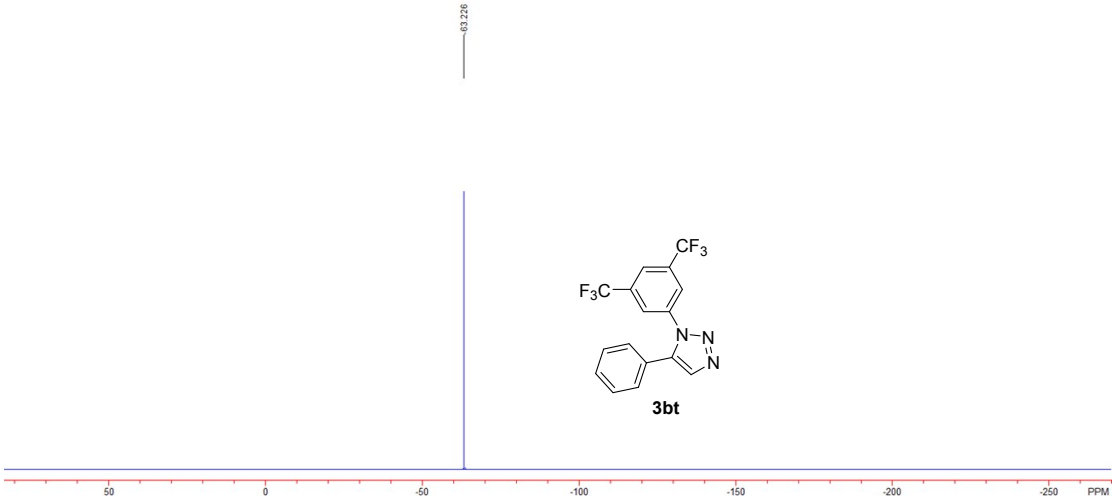
PPM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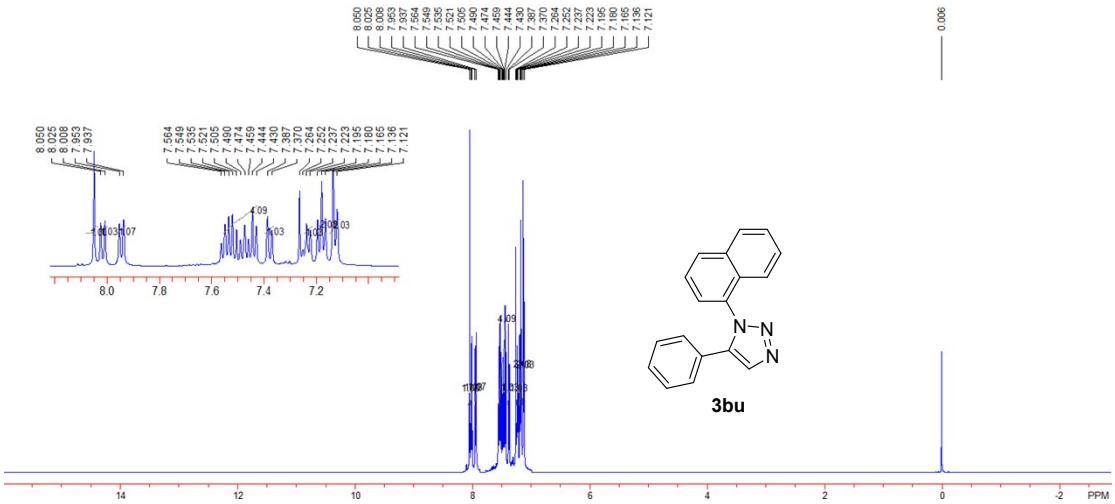
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7.444
7.430
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7.264
7.252
7.237
7.223
7.195
7.180
7.165
7.136
7.121
0.006
4.09
2.03
1.07
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7.4
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3bu
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10
8
6
4
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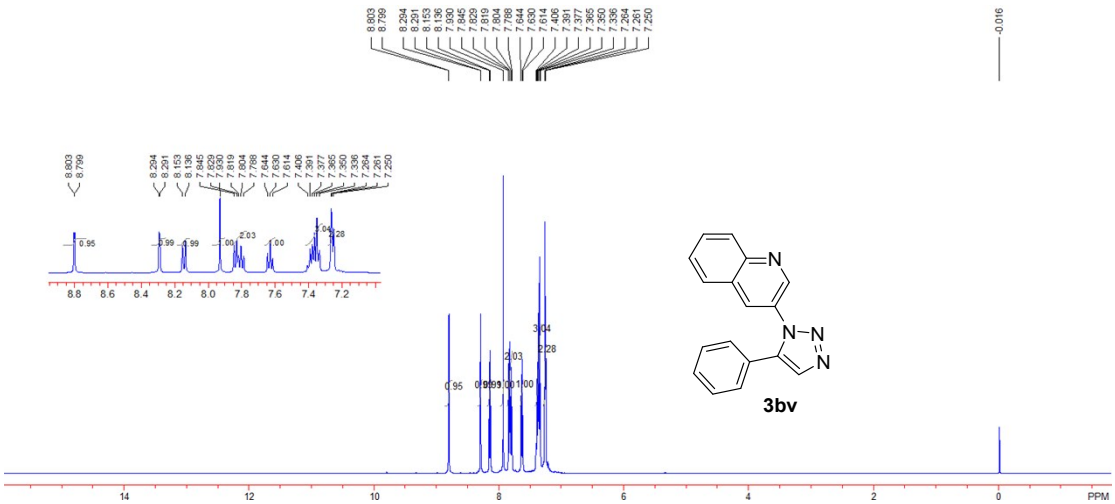
-2
PPM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7.614
7.406
7.391
7.377
7.365
7.360
7.336
7.264
7.261
7.250
-0.016
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0.99
0.99
1.00
2.03
1.00
3.04
2.28
8.8
8.6
8.4
8.2
8.0
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7.2
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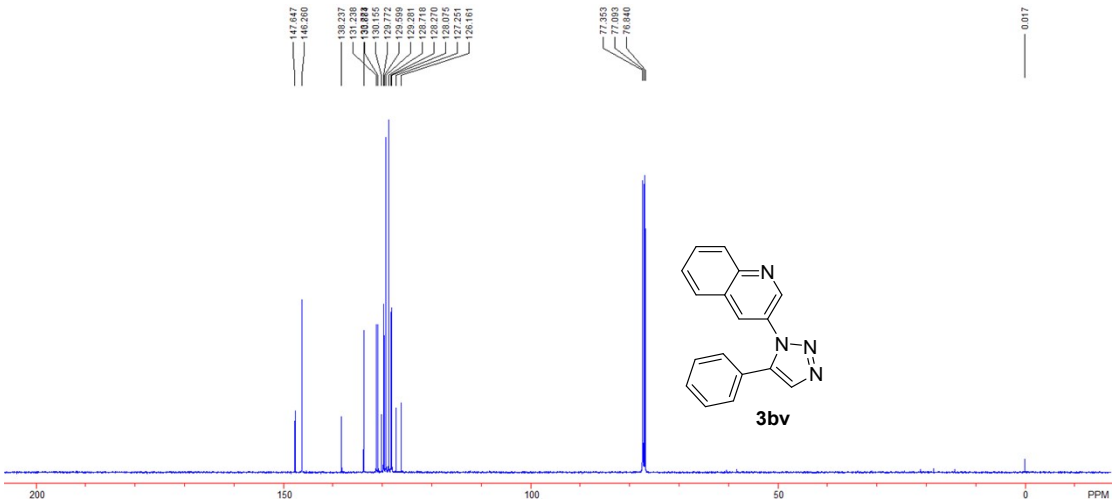
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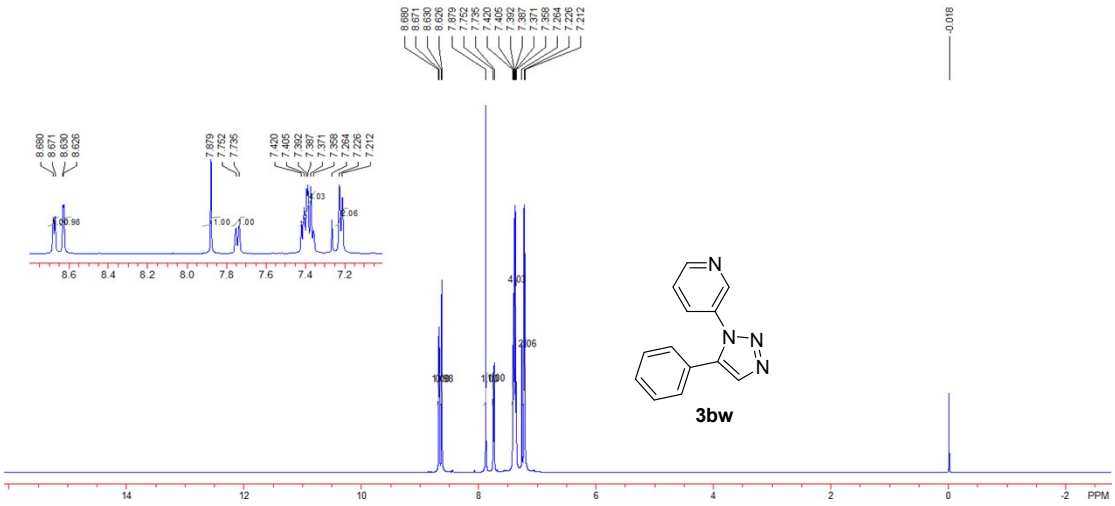
77.093
76.840
0.017
3bv
200
150
100
50
0
PPM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7.358
7.264
7.226
7.212
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2.06
1.00
1.00
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8
6
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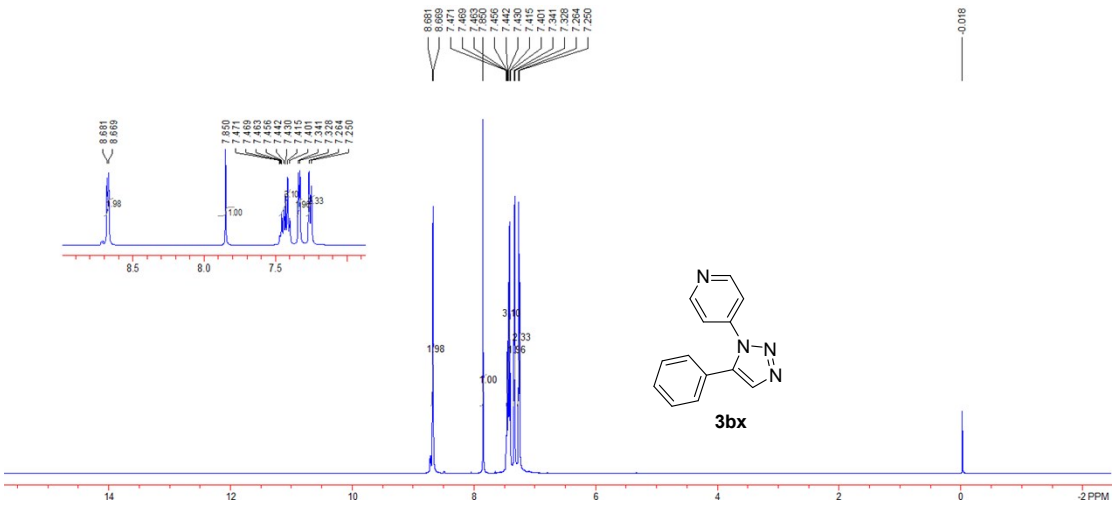
-2
PPM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7.264
7.250
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2.33
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3bx
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10
8
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2
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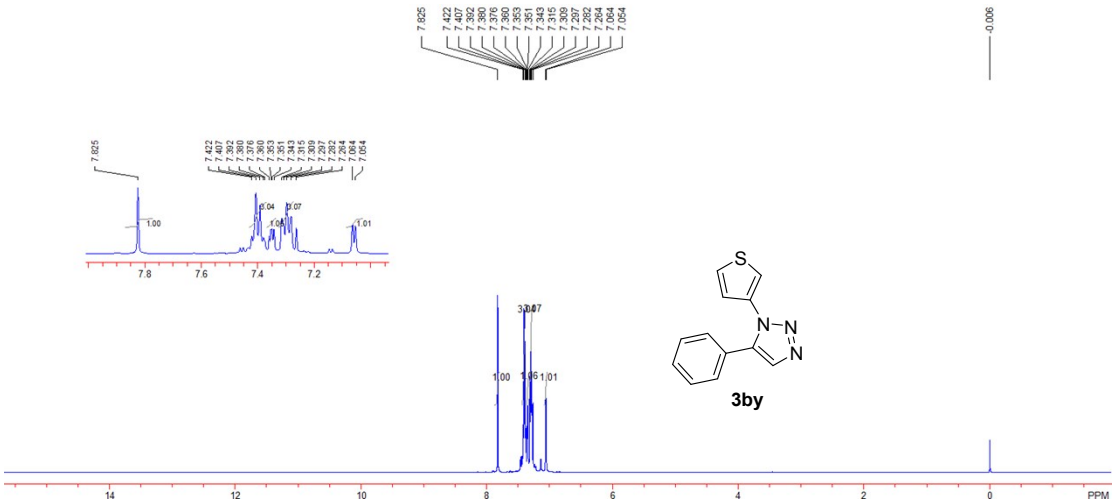
-2 PPM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7.343
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7.297
7.282
7.264
7.064
7.054
-0.006
1.00
1.04
1.07
1.01
7.8
7.6
7.4
7.2
3.07
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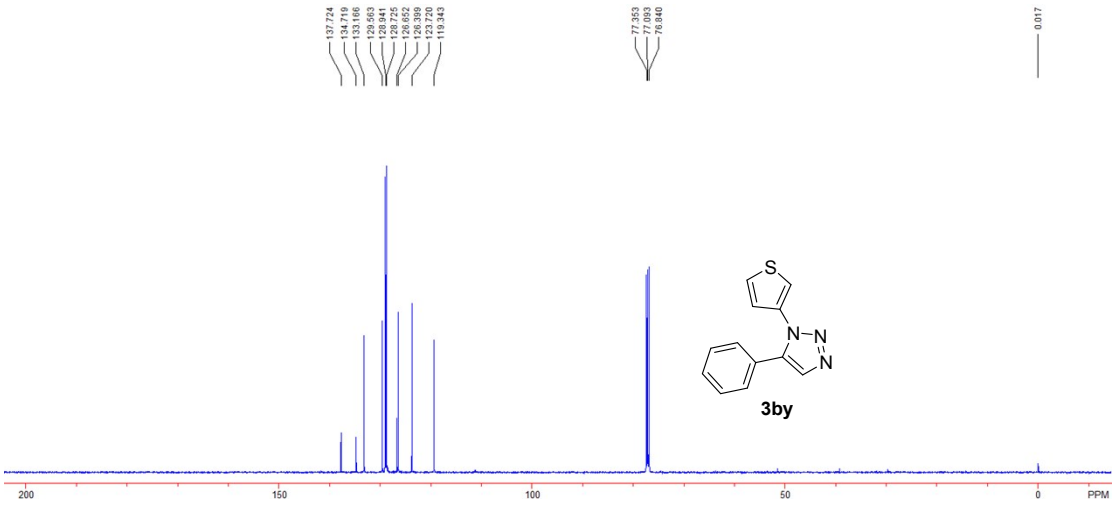
3by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76.840
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200
150
100
50
0
PPM
S
N
N
N
3by