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Graphical Abstract

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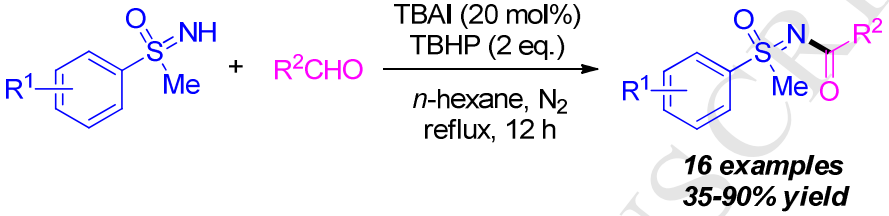

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ABSTRACT

A direct *N*-acylation of *N*H-sulfoximines and aldehydes has been developed under metal-free TBAI/TBHP oxidation system, affording *N*-acylsulfoximines in moderate to good yields.

1. Introduction

Recently, sulfoximines have been of great interest since the use of sulfoximine group as a pharmacophore for drug discovery (Figure 1).[1] For instance, aminopyrimidine BAY1000394 is a balanced pan-CDK inhibitor with potent, broad-spectrum antiproliferative activity against human cancer cell lines, and is currently being investigated in the phase I clinical trial for patients with advanced solid tumors.[1c,1d] Sulfoxaflor is another example that represents a novel insecticide targeting sap-feeding pests with unique resistance and mode of action characteristics.[1a] In addition, sulfoximine groups could act as the reusable directing groups in *ortho* C-H functionalizations.[2]

As one of the important classes of sulfoximine derivatives, the traditional approaches for the generation of *N*-acylsulfoximines were primarily relied on the acylations of *N*H-sulfoximines with acyl chlorides.[3] *N*-acylation can also be achieved *via* boric acid mediated cross-coupling of *N*H-sulfoximines with carboxylic acids.[4] Notably, Bolm's group[5] has had a great interest in *N*-acylsulfoximines. In 2013, they developed the copper-catalyzed oxidative *N*-acylations of sulfoximines with aldehydes[5a] and alkynes[5b]. More recently, they reported the MnO_2-mediated *N*-aroylation of *N*-chlorosulfoximines with methyl arenes.[5c] Though these synthetic strategies are efficient, the usage of pre-activated coupling partners or metal catalysts shows shortages in both industrial and green chemistry view.

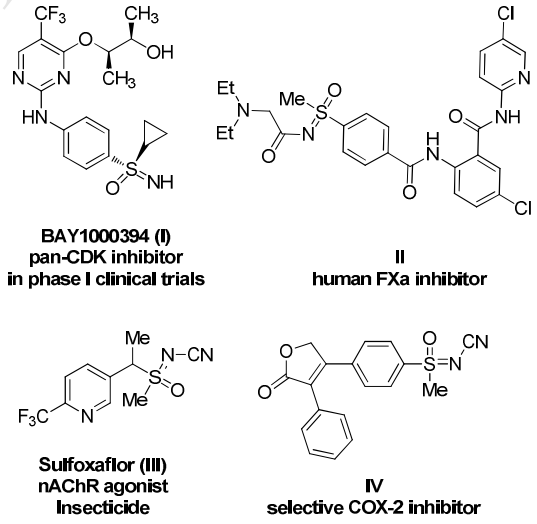

Figure 1. Selected examples of bioactive sulfoximines

On the other hand, the use of *n*-Bu_4NI (TBAI) as the catalyst in combination with *tert*-butyl hydroperoxide (TBHP) as a powerful metal-free oxidation system[6] has been the focus of recent interest, and widely used in various oxidative coupling reactions. It has been applied to the C-C[7], C-N[8], C-O[9], C-S[10] bonds formation. Therefore, our interest was focused on the C-N

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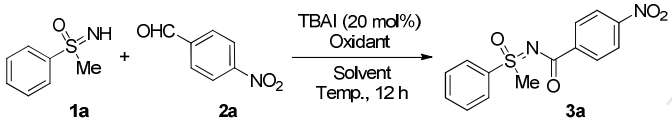
bonds formation for the generation of *N*-acylsulfoximines catalyzed by metal-free oxidation system.

Herein, we describe the first example of TBAI-catalyzed direct *N*-acylation of *N*H-sulfoximines with aldehydes as coupling partners, utilizing TBHP as the green terminal oxidant.

2. Results and discussion

Initially, 4-nitrobenzaldehyde **2a** was chosen as the coupling partner of the *N*-acylation. *N*H-sulfoximine **1a** was readily prepared *via* Bolm's method[5a] and added to a sealed tube with 4-nitrobenzaldehyde **2a** in the presence of TBAI (20 mol%) and TBHP (3.0 equiv., 70% aqueous solution) in CH_3CN at reflux in the air. To our delight, the acylation occurred, affording the *N*-acylsulfoximine **3a** in 16% yield (Table 1, entry 1). The reaction provided a slightly higher yield under anaerobic conditions (Table 1, entry 2). Solvents screening revealed that *n*-hexane was superior, delivering the *N*-acylsulfoximine **3a** in 49% yield (Table 1, entry 4). Gratifyingly, decreasing the amount of oxidant TBHP to 2.0 equivalents improved the yield to 56% (Table 1, entry 6). Lowering the reaction temperature reduced the yield significantly (Table 1, entries 8-9). In addition, only 7% yield of **3a** was obtained when TBPB was used as the oxidant instead of TBHP (Table 1, entry 10).

Table 1. Optimization of reaction conditions[a]

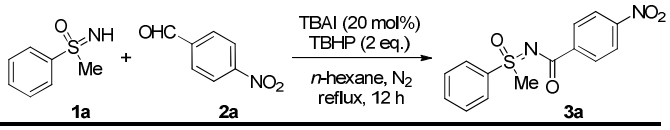


Entry	Oxidant	Solvent	Temp. (°C)	Yield(%)[b]
1[c]	TBHP (3 eq.)	CH_3CN	reflux	16
2	TBHP (3 eq.)	CH_3CN	reflux	25
3	TBHP (3 eq.)	DCE	reflux	37
4	TBHP (3 eq.)	*n*-hexane	reflux	49
5	TBHP (4 eq.)	*n*-hexane	reflux	46
6	TBHP (2 eq.)	*n*-hexane	reflux	56
7	TBHP (1 eq.)	*n*-hexane	reflux	29
8	TBHP (2 eq.)	*n*-hexane	60	38
9	TBHP (2 eq.)	*n*-hexane	25	trace
10	TBPB (2 eq.)	*n*-hexane	reflux	7

[a] Reaction conditions: All reactions were carried out with **1a** (0.45 mmol), **2a** (0.3 mmol), TBAI (20 mol%), TBHP (70% aqueous solution) in 1 mL solvent for 12h under N_2 atmosphere. [b] Isolated yield based on 4-nitrobenzaldehyde **2a**. [c] In the air.

Further optimization involved the screening of reactants ratios, catalyst loadings, and concentrations. A satisfactory result was obtained when 4.0 equivalents of 4-nitrobenzaldehyde **2a** was used (Table 2, entry 3). No further improvement in the yield was observed upon increasing the aldehyde quantity to 5.0 equivalents (Table 2, entry 4). Lowering the reaction concentration for ten folds led to a dramatically reduced yield (Table 2, entry 5). A decrease of catalyst loading reduced the product yield (Table 2, entries 6-7). The optimal reaction conditions were found consisted of *N*H-sulfoximine **1** (1.0 equiv.), aldehyde **2** (4.0 equiv.), TBAI (20 mol%), aqueous solution of TBHP (2.0 equiv.), *n*-hexane, reflux, 12h, under N_2 atmosphere.

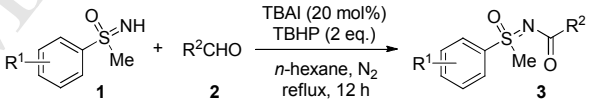
Table 2. Screening of the ratio of reactants and catalyst[a]



Entry	Sulfoximine 1a (equiv.)	Aldehyde 2a (equiv.)	TBAI (mol%)	Yield(%)[b]
1[c]	1.5	1.0	20	56
2	1.0	3.0	20	72
3	1.0	4.0	20	90
4	1.0	5.0	20	86
5[d]	1.0	4.0	20	44
6	1.0	4.0	15	79
7	1.0	4.0	10	64

[a] Reaction conditions: Reactions were carried out with **1a** (0.3 mmol), **2a** (1.0-5.0 eq.), TBAI (20 mol%), TBHP (70% aqueous solution) in 1 mL solvent reflux for 12h under N_2 atmosphere. [b] Isolated yield based on *N*H-sulfoximine **1a**. [c] Isolated yield based on 4-nitrobenzaldehyde **2a**. [d] In 10 mL solvent.

Table 3. Substrate scope of the TBAI/TBHP mediated direct *N*-acylation of sulfoximine **1** with aldehyde **2**[a]

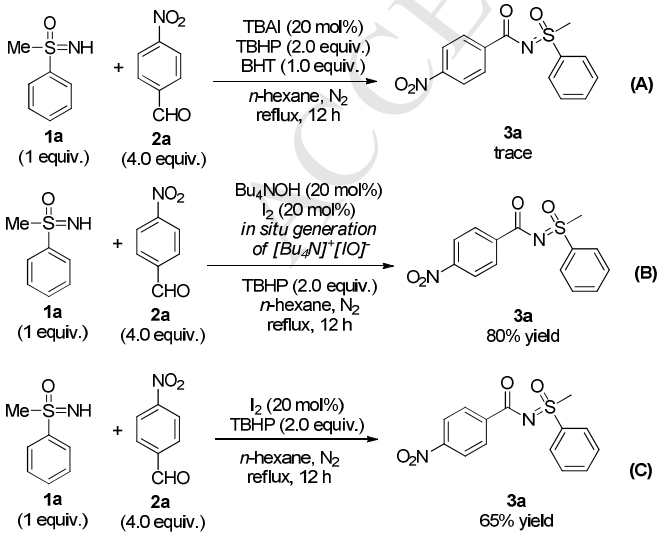


Entry	R^1	R^2	Yield (%)[b]
1	H (**1a**)	4-$NO_2C_6H_4$ (**2a**)	90 (**3a**)
2	H (**1a**)	3-$NO_2C_6H_4$ (**2b**)	66 (**3b**)
3	H (**1a**)	3-$CF_3C_6H_4$ (**2c**)	67 (**3c**)
4	H (**1a**)	4-FC_6H_4 (**2d**)	35 (**3d**)
5	H (**1a**)	4-ClC_6H_4 (**2e**)	49 (**3e**)
6	H (**1a**)	4-BrC_6H_4 (**2f**)	59 (**3f**)
7	H (**1a**)	4-MeC_6H_4 (**2g**)	56 (**3g**)
8	H (**1a**)	4-$OMeC_6H_4$ (**2h**)	60 (**3h**)
9	H (**1a**)	3-NO_2,4-$OMeC_6H_3$ (**2i**)	70 (**3i**)
10	H (**1a**)	Ph (**2j**)	46 (**3j**)
11	H (**1a**)	1-naphthyl (**2k**)	39 (**3k**)
12	H (**1a**)	Cy (**2l**)	74 (**3l**)
13	4-OMe (**1b**)	4-$NO_2C_6H_4$ (**2a**)	48 (**3m**)
14	4-OMe (**1b**)	3-NO_2,4-$OMeC_6H_3$ (**2i**)	48 (**3n**)
15	4-NO_2 (**1c**)	4-$NO_2C_6H_4$ (**2a**)	51 (**3o**)
16	4-NO_2 (**1c**)	3-NO_2,4-$OMeC_6H_3$ (**2i**)	47 (**3p**)

[a] Unless otherwise noted, the reaction was performed under N_2 atmosphere, with *N*H-sulfoximine **1** (0.3 mmol), aldehyde **2** (4.0 equiv.), TBAI (20 mol%) and aqueous solution of TBHP (2.0 equiv.), reflux in 1 mL *n*-hexane for 12 hours. [b] Isolated yields.

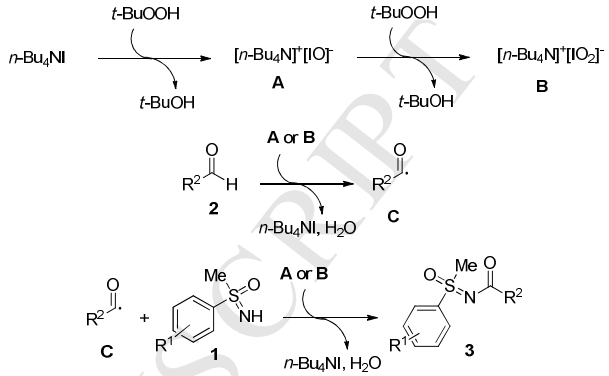
To examine the scope of this transformation, the optimized conditions were applied to the reactions of a variety of *N*H-sulfoximine **1** with aldehyde **2**. As shown in Table 3, all the reactions proceeded smoothly to generate *N*-acylsulfoximine **3** in moderate to good yields. The electron-deficient aromatic aldehydes **2a**-**2c** provided higher yields than halo substituted aromatic aldehydes **2d**-**2f** (Table 3, entries 1-3 *vs* 4-6). For electron-donating substituted benzaldehydes **2g** and **2h**, the reactions proceeded smoothly to afford the corresponding *N*-benzoylsulfoximines **3g** and **3h** in moderate yields (Table 3, entries 7-8). Interestingly, a good yield was obtained when nitro and methoxyl groups were at the 3- and 4-positions of the phenyl ring (Table 3, entry 9). In addition, electron-neutral benzaldehyde **2j** and 1-naphthaldehyde **2k** could also be employed, leading to *N*-acylsulfoximine **3j** in 46% and *N*-acylsulfoximine **3k** in 39% yields, respectively (Table 3, entries 10-11). Notably, alkyl aldehydes such as cyclohexanecarboxaldehyde **2l** afforded the desired *N*-acylsulfoximine **3l** in 74% yield (Table 3, entry 11). Moreover, *para*-methoxyl and *para*-nitro substituted *N*H-sulfoximines **1b** and **1c** performed well with 4-substituted or 3, 4-disubstituted benzaldehydes **2a** and **2i**, furnishing multi-functionalized *N*-acylsulfoximines **3m**-**3p** in moderate yields (Table 3, entries 13-16).

Several recent reports have proposed that a radical pathway and *in situ* generated ammonium hypoiodite ($[Bu_4N]^+[IO]^-$) or iodite ($[Bu_4N]^+[IO_2]^-$) from TBAI are involved in this catalysis system.[8f,9a] And in some other reports, *tert*-butoxyl or *tert*-butylperoxyl radicals[9c-e], generated from TBHP by iodide/iodinine catalysis cycle, are proposed as active species and trap H of aldehyde to form the acyl radical.[9c] To verify the reaction mechanism above, several control experiments were carried out (Scheme 1). When a stoichiometric amount of the radical scavenger 2, 6-di-*tert*-butyl-4-methylphenol (BHT) was added to the reaction mixture under the same reaction conditions, only trace amount of product **3a** was observed, which suggested that the reaction may indeed undergo a radical process (Scheme 1, A). In addition, The reaction performed well in the presence of 20 mol% of Bu_4NOH and iodine (*in situ* generation of $[Bu_4N]^+[IO]^-$), which indicated that hypoiodite or iodite was the catalytic species (Scheme 1, B). Interestingly, employing iodine only as the catalyst also afforded the desired product in 65% yield (Scheme 1, C). This result was significantly different from those reported by Yu[9f], in which replacing Bu_4NI with I_2 led to no desired product.



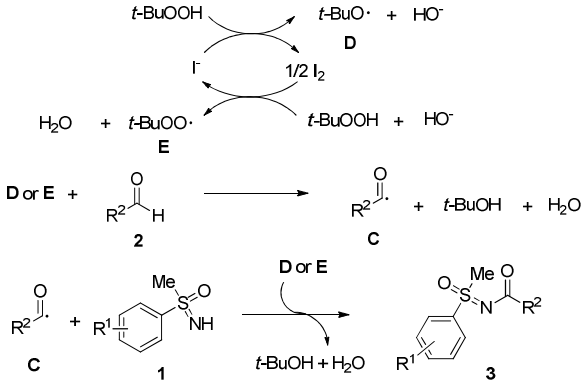
Scheme 1. Investigation of reaction mechanism.

Based on these observations and literature reports, two mechanism pathways were hypothesized. In pathway I (Scheme 2), TBAI was initially oxidized by TBHP to generate $[Bu_4N]^+[IO]^-$ **A** or $[Bu_4N]^+[IO_2]^-$ **B**, which subsequently induced the oxidative C(sp^2)-H bond activation of aldehyde **2** to form the acyl radical **C**. And the hypoiodite was reduced to TBAI and water. *N*H-sulfoximine **1** was liable to be activated by the hypoiodite species and coupled with acyl radical **C**, finally resulted in the formation of the *N*-acylsulfoximine **3**.



Scheme 2. The proposed pathway I.

Alternatively, in pathway II (Scheme 3), the *tert*-butoxyl radical **D** and *tert*-butylperoxy radical **E** were generated *via* iodide/ iodinine catalyzed redox process firstly. Secondly, these active radical species abstracted a hydrogen atom from the aldehyde **2** leading to acyl radical **C**. Similarly, the product *N*-acylsulfoximine **3** was formed *via* N-H bond cleavage of *N*H-sulfoximine **1** and C-N bond formation with acyl radical **C** in the presence of *tert*-butoxyl radical **D** and *tert*-butylperoxy radical **E**.



Scheme 3. The proposed pathway II.

3. Conclusion

In conclusion, we have developed the first example of metal-free direct *N*-acylation of *N*H-sulfoximines with aldehydes catalyzed by TBAI/TBHP oxidation system, affording *N*-acylsulfoximines in moderate to good yields. This straightforward protocol could be served as a practical alternative to the existing synthetic methods for the preparation of valuable *N*-acylsulfoximines. Two mechanism pathways were hypothesized, and studies to further elucidate the mechanism and applications of this reaction are ongoing in our laboratory.

4. Experimental section

4.1. General

Melting points were obtained in open capillary tubes using a micro melting point apparatus SGW X-4, which were uncalibrated. Mass spectra were recorded by the HP5989A service; HRMS (EI) spectra were obtained on a Finigann MAT8401 instrument. ^{1}H nuclear magnetic resonance (NMR) spectra were recorded using an internal deuterium lock for the residual protons in $CDCl_3$ (δ_H=7.26) at ambient temperatures on the following instruments: Bruker AVANCE DPX-400 (400 MHz). Data are presented as follows: Chemical shift (in ppm on the scale relative to δ_{TMS}=0), integration, multiplicity (s=singlet, d=doublet, t=triplet, q=quartet and m=multiplet), coupling constant (*J*/Hz) and interpretation. ^{13}C NMR spectra were recorded by broadband spin decoupling using an internal deuterium lock for $CDCl_3$ (δ=77.2) at ambient temperatures on the following instruments: Bruker AVANCE DPX-400 (100.6 MHz). Chemical shift values are reported in ppm on the scale (δ_{TMS}=0). All reagents and solvents were used as purchased if not otherwise stated.

4.2. General procedure for synthesis of *N*-acylsulfoximine 3

To a flame-dried 10 mL Schlenk tube under N_2 was added *N*H-sulfoximine **1** (0.3 mmol), aldehyde **3** (4.0 equiv.) and TBAI (20 mol%), followed by *n*-hexane (1 mL). TBHP (2.0 equiv., 70% aqueous solution) was added after the starting materials were dissolved. The reaction mixture was then heated to reflux. After completion, the reaction was cooled to room temperature and quenched with saturated $Na_2S_2O_3$, extracted by EA. The organic layer was washed by saturated brine, dried over anhydrous sodium sulfate. After the mixture was filtered and evaporated, the residue was purified by flash column chromatography to afford the desired *N*-acylsulfoximine **3**.

4.4.1. **3a**, [5a] Yellow solid (90%). Mp: 146-147 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 8.3 Hz, 2H), 8.25 (d, *J* = 8.0 Hz, 2H), 8.06 (d, *J* = 7.7 Hz, 2H), 7.73 (t, *J* = 7.0 Hz, 1H), 7.66 (t, *J* = 7.2 Hz, 2H), 3.51 (s, 3H).

4.4.2. **3b**, [5a] Yellow solid (66%). Mp: 123-124 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.98 (s, 1H), 8.46 (d, *J* = 7.5 Hz, 1H), 8.35 (d, *J* = 7.7 Hz, 1H), 8.06 (d, *J* = 7.5 Hz, 2H), 7.77-7.69 (m, 1H), 7.69-7.55 (m, 3H), 3.51 (s, 3H).

4.4.3. **3c**, [2c] White solid (67%). Mp: 117-118 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 7.9 Hz, 2H), 8.05 (d, *J* = 7.7 Hz, 2H), 7.75 – 7.60 (m, 5H), 3.48 (s, 3H).

4.4.4. **3d**, [5a] White solid (35%). Mp: 128-129 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22-8.14 (m, 2H), 8.05 (d, *J* = 7.8 Hz, 2H), 7.70 (t, *J* = 7.1 Hz, 1H), 7.62 (t, *J* = 7.5 Hz, 2H), 7.07 (t, *J* = 8.3 Hz, 2H), 3.46 (s, 3H).

4.4.5. **3e**, [5a] White solid (49%). Mp: 113-114 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.2 Hz, 2H), 8.05 (d, *J* = 7.8 Hz, 2H), 7.70 (t, *J* = 7.0 Hz, 1H), 7.63 (t, *J* = 7.5 Hz, 2H), 7.38 (d, *J* = 8.2 Hz, 2H), 3.47 (s, 3H).

4.4.6. **3f**, [5c] White solid (59%). Mp: 117-118 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08-7.99 (m, 4H), 7.70 (t, *J* = 7.3 Hz, 1H), 7.62 (t, *J* = 7.5 Hz, 2H), 7.54 (d, *J* = 8.3 Hz, 2H), 3.46 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.5, 138.9, 134.6, 134.1, 131.4, 131.2, 129.9, 127.3, 127.2, 44.5.

4.4.7. **3g**, [2a] White solid (56%). Mp: 168-169 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09-8.03 (m, 4H), 7.69 (t, *J* = 7.3 Hz, 1H), 7.61 (t, *J* = 7.6 Hz, 2H), 7.22 (d, *J* = 7.9 Hz, 2H), 3.46 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.5, 142.9, 139.3, 133.9, 133.1, 129.8, 129.7, 128.9, 127.3, 44.5, 21.8.

4.4.8. **3h**, [5a] White solid (60%). Mp: 138-139 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.5 Hz, 2H), 8.06 (d, *J* = 7.7 Hz, 2H), 7.69 (t, *J* = 7.1 Hz, 1H), 7.61 (t, *J* = 7.5 Hz, 2H), 6.90 (d, *J* = 8.6 Hz, 2H), 3.86 (s, 3H), 3.46 (s, 3H).

4.4.9. **3i**, Yellow oil (70%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (d, *J* = 2.1 Hz, 1H), 8.31 (dd, *J* = 8.8, 2.2 Hz, 1H), 8.04 (d, *J* = 7.5 Hz, 2H), 7.72 (t, *J* = 7.4 Hz, 1H), 7.64 (t, *J* = 7.5 Hz, 2H), 7.10 (d, *J* = 8.8 Hz, 1H), 4.02 (s, 3H), 3.47 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.7, 155.8, 139.2, 138.7, 135.1, 134.1, 129.9, 128.4, 127.2, 112.9, 56.9, 44.5; HRMS (EI): calcd for $C_{15}H_{14}N_2O_5S$ ([M]$^+$): 334.0623, found 334.0625.

4.4.10. **3j**, [5a] White solid (46%). Mp: 122-123 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, *J* = 7.8 Hz, 2H), 8.07 (d, *J* = 7.8 Hz, 2H), 7.70 (t, *J* = 7.1 Hz, 1H), 7.62 (t, *J* = 7.6 Hz, 2H), 7.52 (t, *J* = 7.0 Hz, 1H), 7.42 (t, *J* = 7.5 Hz, 2H), 3.47 (s, 3H).

4.4.11. **3k**, [5a] Colorless oil (39%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.00 (d, *J* = 8.6 Hz, 1H), 8.35 (d, *J* = 6.3 Hz, 1H), 8.10 (d, *J* = 7.2 Hz, 2H), 7.96 (d, *J* = 8.1 Hz, 1H), 7.85 (d, *J* = 7.6 Hz, 1H), 7.68 (d, *J* = 6.6 Hz, 1H), 7.67-7.58 (m, 2H), 7.57-7.46 (m, 3H), 3.49 (s, 3H).

4.4.12. **3l**, [4] Colorless oil (74%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 6.9 Hz, 1H), 7.91 (d, *J* = 7.0 Hz, 1H), 7.68-7.51 (m, 3H), 3.13 (s, 3H), 2.37 (m, 1H), 1.98-1.85 (m, 2H), 1.81-1.59 (m, 2H), 1.59-1.17 (m, 6H).

4.4.13. **3m**, White solid (48%). Mp: 141-142 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 8.9 Hz, 2H), 8.25 (d, *J* = 8.9 Hz, 2H), 7.59 (d, *J* = 7.9 Hz, 1H), 7.57-7.51 (m, 2H), 7.22 (d, *J* = 8.0 Hz, 1H), 3.90 (s, 3H), 3.49 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.2, 160.5, 150.2, 131.1, 130.6, 123.4, 120.4, 119.1, 112.3, 56.0, 44.5; HRMS (EI): calcd for $C_{15}H_{14}N_2O_5S$ ([M]$^+$): 334.0623, found 334.0622.

4.4.14. **3n**, Yellow oil (48%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (d, *J* = 2.1 Hz, 1H), 8.31 (dd, *J* = 8.8, 2.2 Hz, 1H), 7.63-7.47 (m, 3H), 7.23-7.17 (m, 1H), 7.10 (d, *J* = 8.8 Hz, 1H), 4.02 (s, 3H), 3.90 (s, 3H), 3.45 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.7, 160.5, 155.7, 139.9, 135.2, 131.0, 127.3, 120.3, 119.1, 112.9, 112.2, 56.9, 55.9, 44.6; HRMS (EI): calcd for $C_{16}H_{16}N_2O_6S$ ([M]$^+$): 364.0729, found 364.0729.

4.4.15. **3o**, White solid (51%). ^{1}H NMR (400 MHz, Acetone-D_6) δ 8.54 (d, *J* = 9.0 Hz, 2H), 8.42 (d, *J* = 9.0 Hz, 2H), 8.36-8.29 (m, 4H), 3.76 (s, 3H); ^{13}C NMR (100 MHz, DMSO-D_6) δ 171.3, 151.0, 150.2, 144.4, 140.9, 130.7, 129.5, 125.9, 124.0, 43.0; HRMS (EI): calcd for $C_{14}H_{11}N_3O_6S$ ([M]$^+$): 349.0369, found 349.0368.

4.4.16. **3p**, Yellow solid (47%). ^{1}H NMR (400 MHz, Acetone-D_6) δ 8.54 (s, 1H), 8.51 (s, 1H), 8.49 (d, *J* = 2.1 Hz, 1H), 8.39 (d, *J* = 9.0 Hz, 2H), 8.29 (dd, *J* = 8.8, 2.1 Hz, 1H), 7.42 (d, *J* = 9.0 Hz, 1H), 4.06 (s, 3H), 3.71 (s, 3H); ^{13}C NMR (100 MHz, DMSO-D_6) δ 175.5, 160.2, 155.7, 149.5, 143.8, 139.9, 134.3, 132.5, 130.9, 129.9, 119.4, 62.4, 47.9; HRMS (EI): calcd for $C_{15}H_{13}N_3O_7S$ ([M]$^+$): 379.0474, found 379.0473.

Acknowledgments

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Supplementary Material

The ^{1}H NMR and ^{13}C NMR copies of all compounds were attached as supplementary material.

Click here to remove instruction text...

TBHP/ TBAI catalyzed direct *N*-acylation of sulfoximines with aldehydes

Wen-Jing Qin, Yi Li, Xingxin Yu* and Wei-Ping Deng*

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Supplementary Material

^{1}H NMR and ^{13}C NMR spectra of *N*-acylsulfoximine **3**

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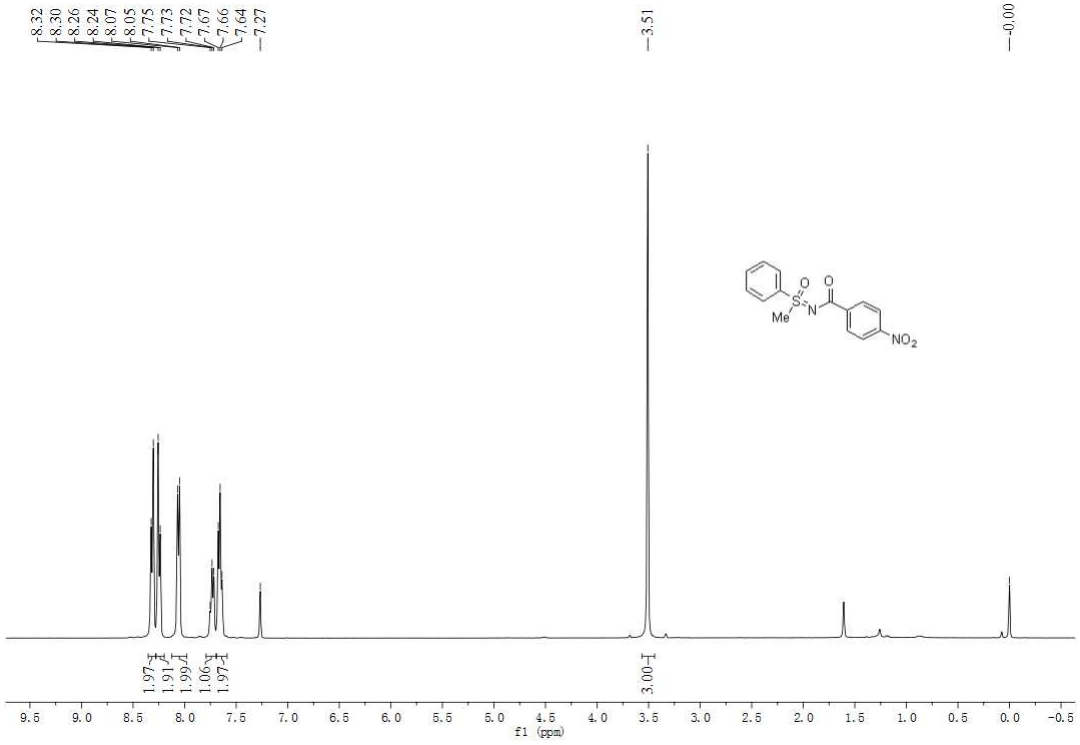
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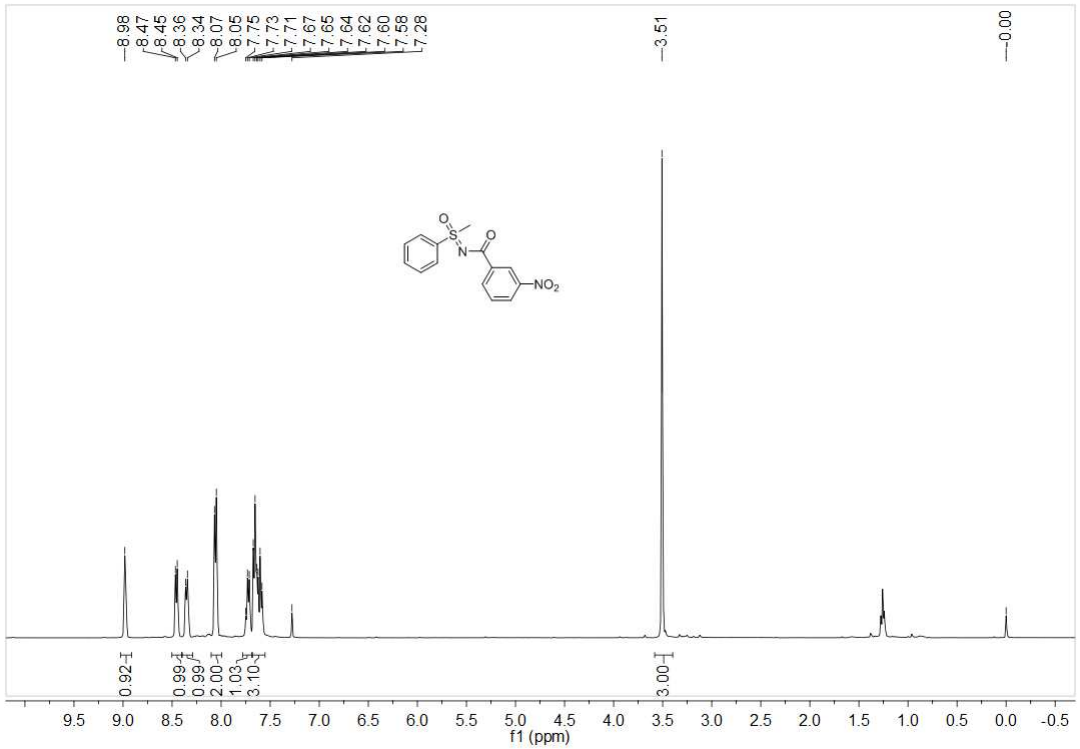
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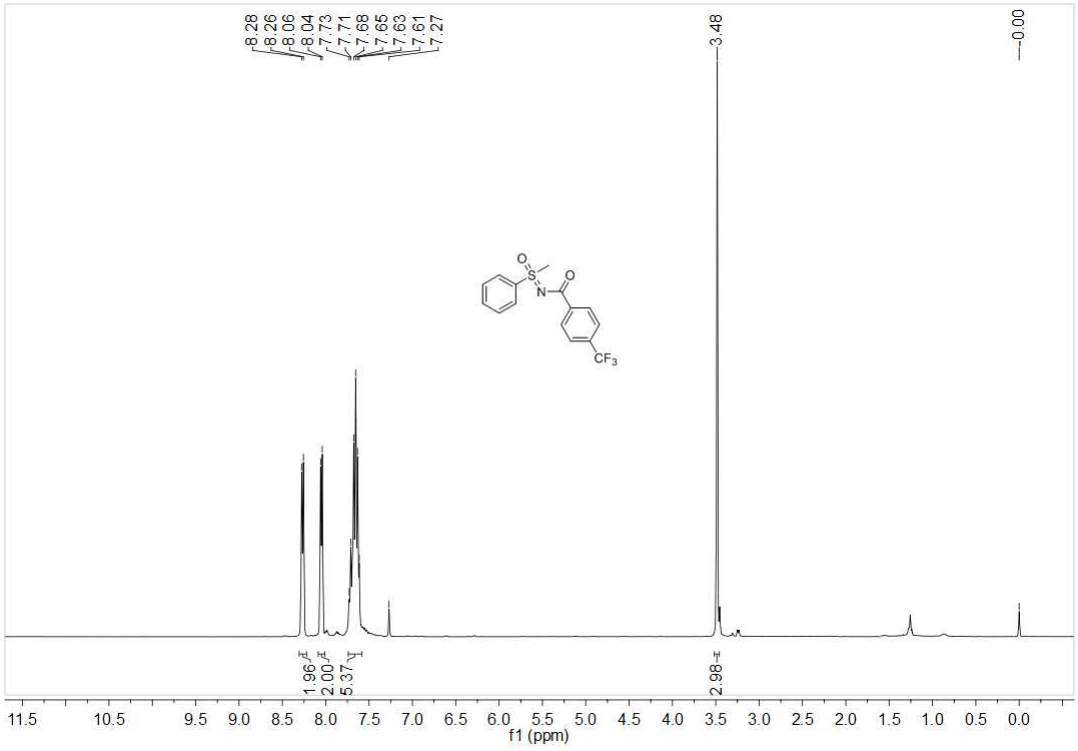
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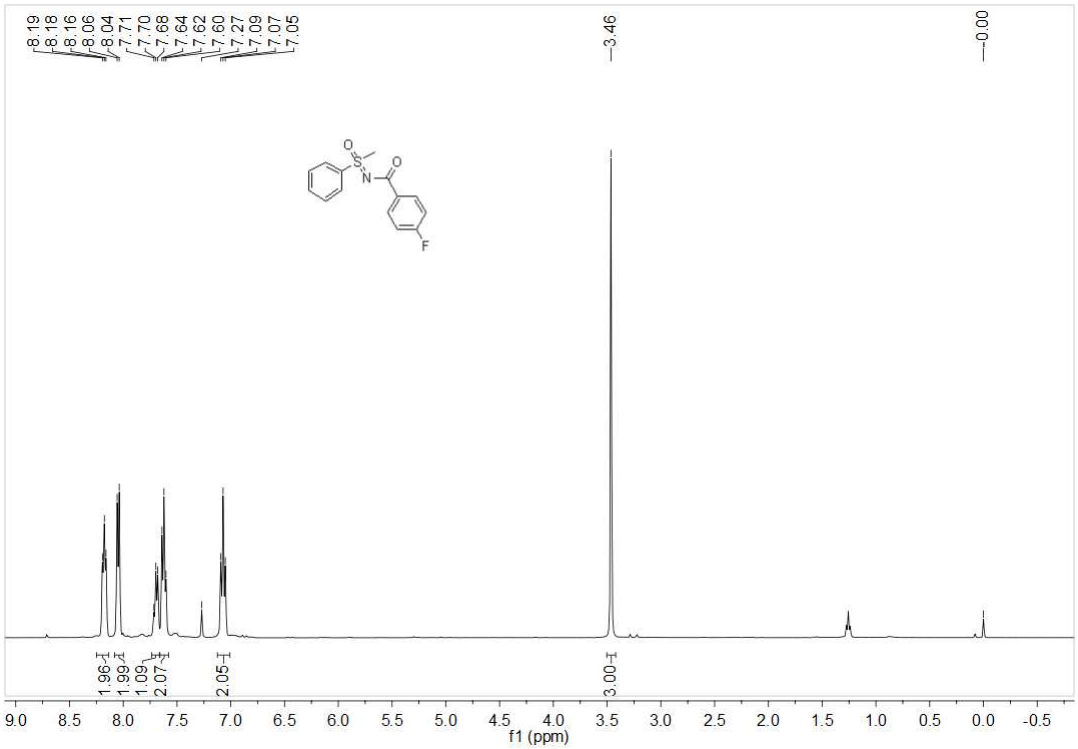
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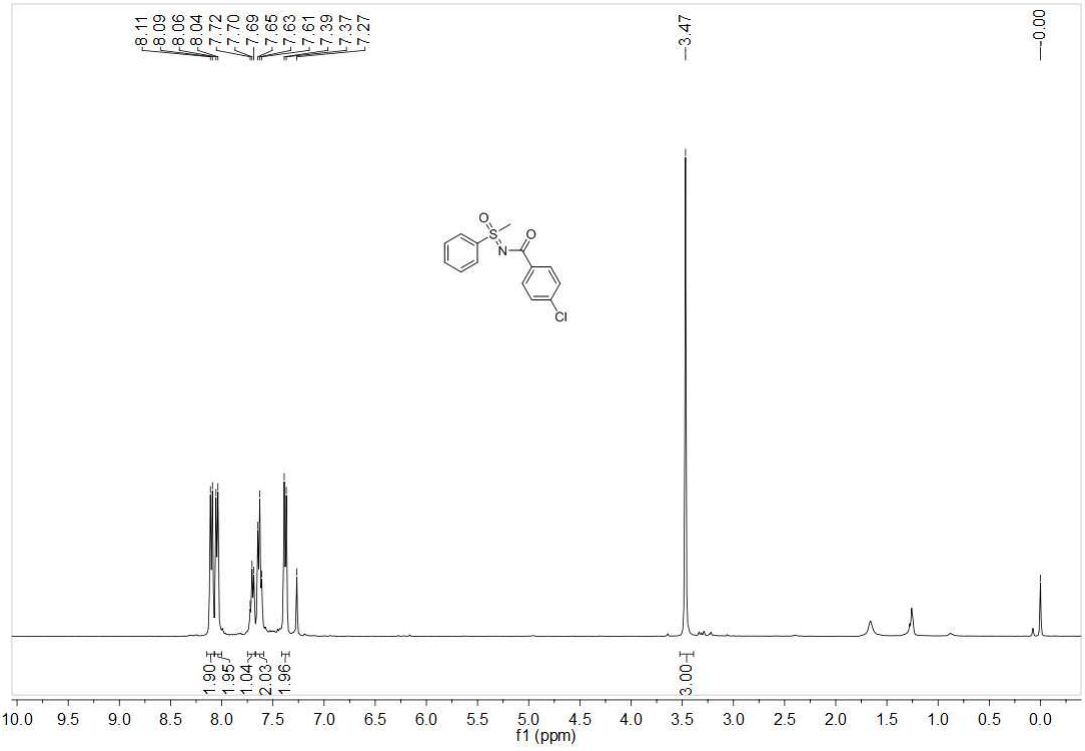
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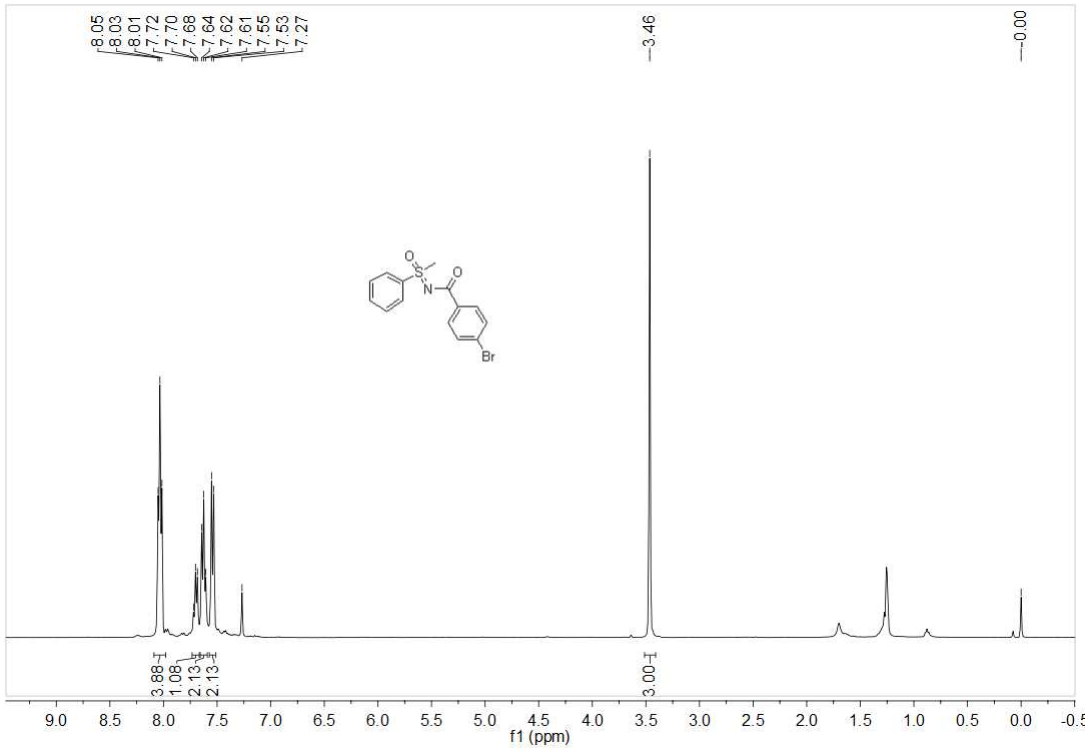
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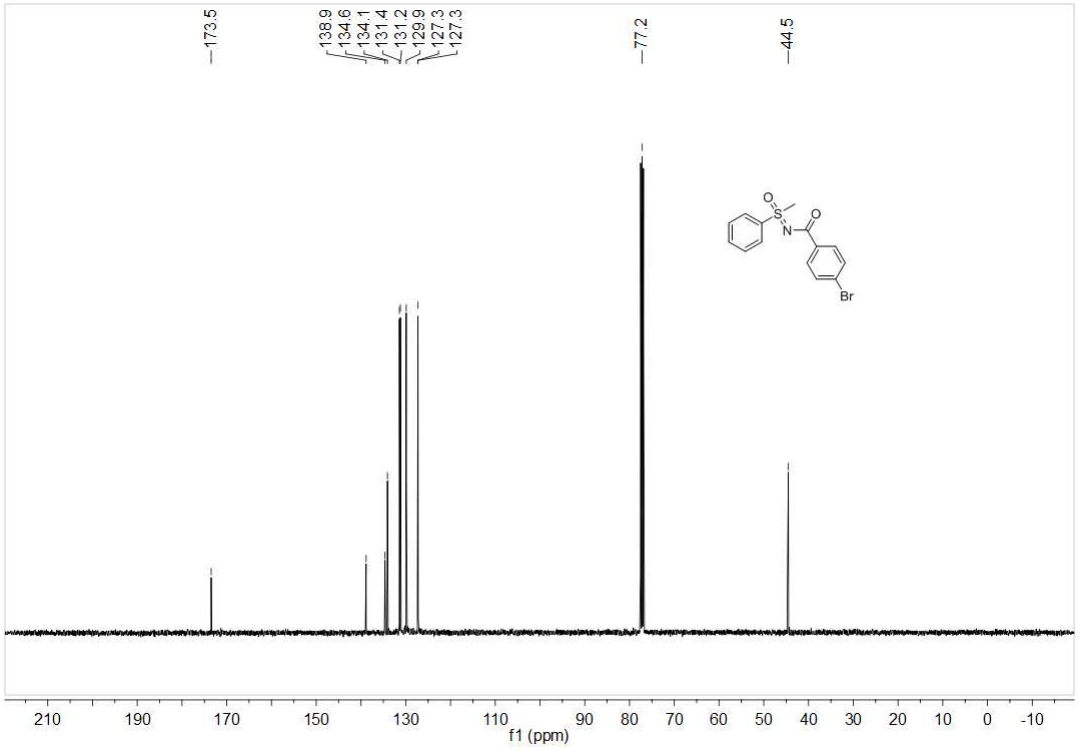
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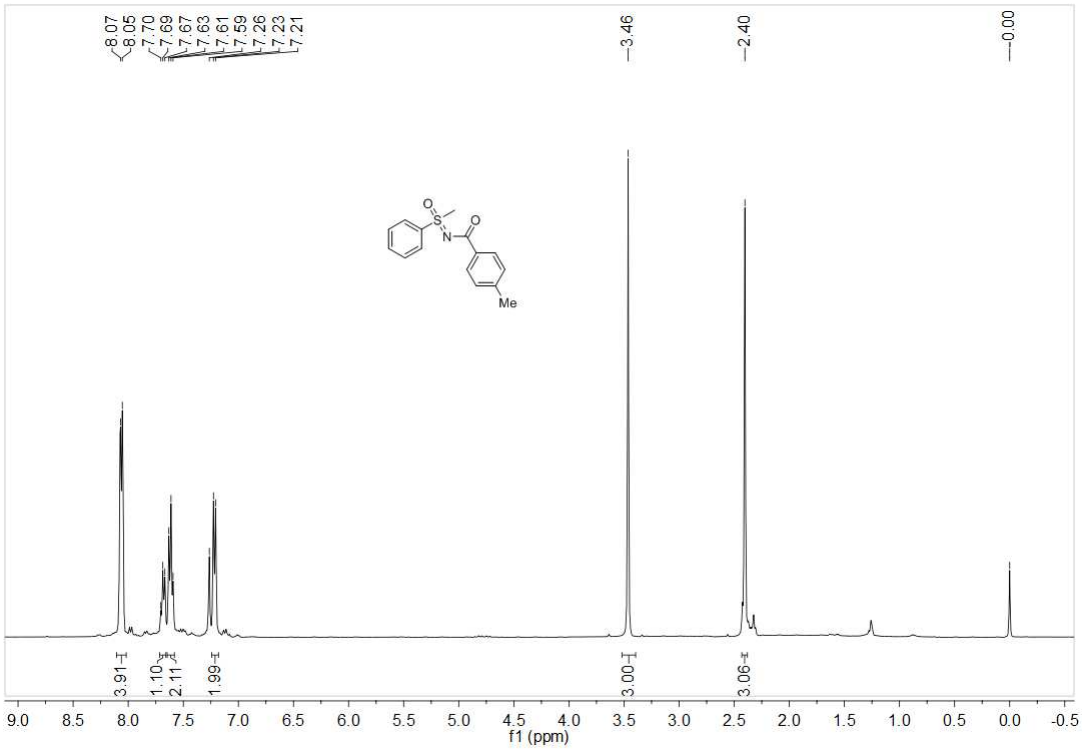
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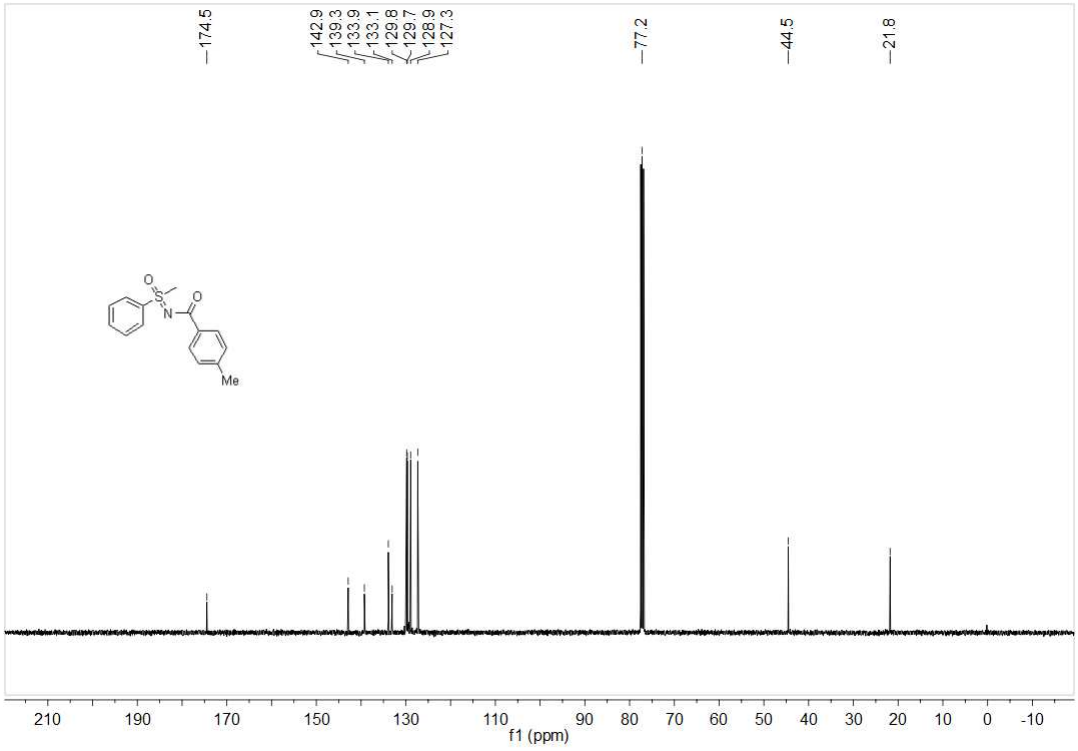
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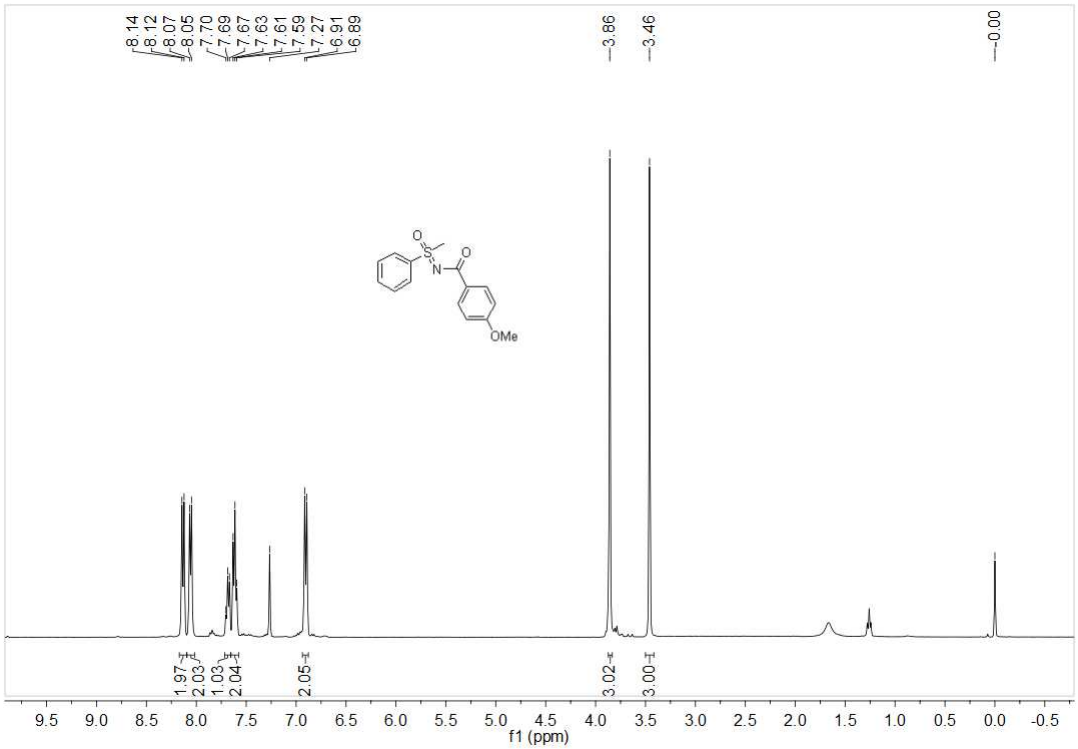
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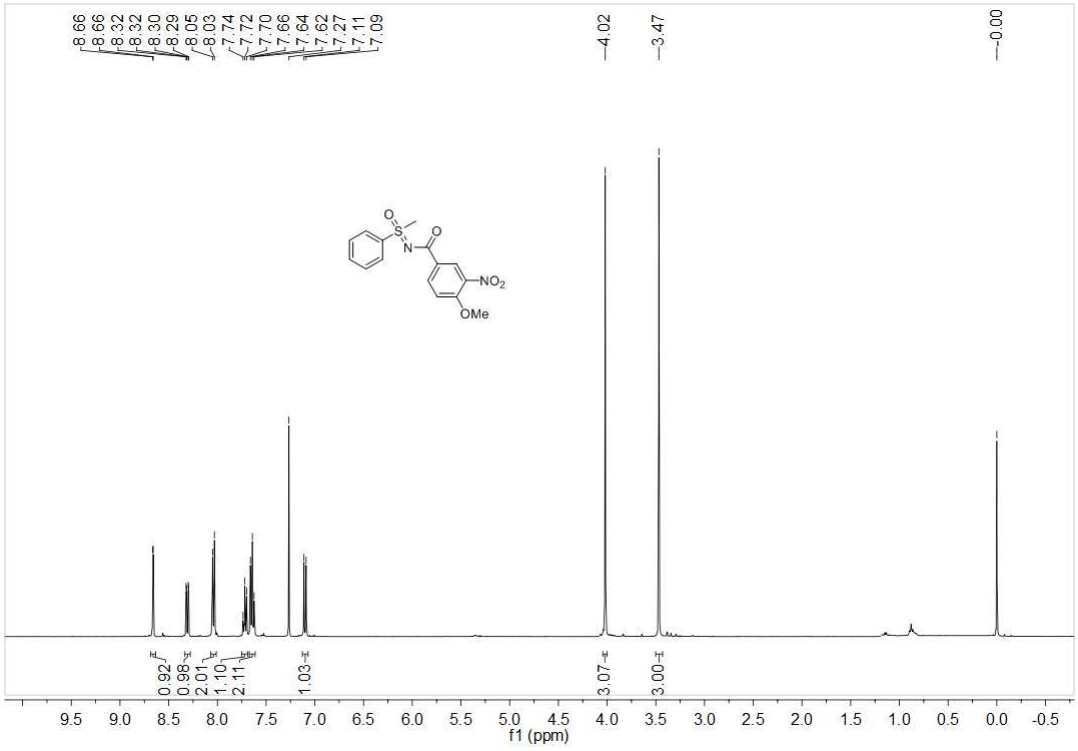
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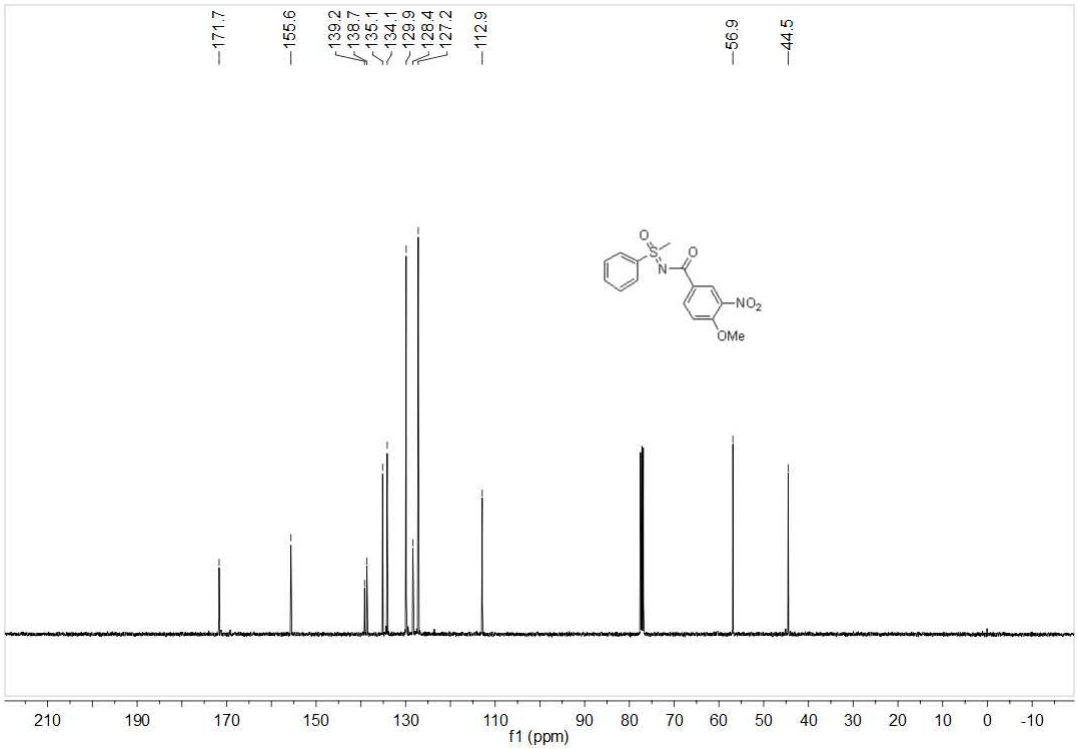
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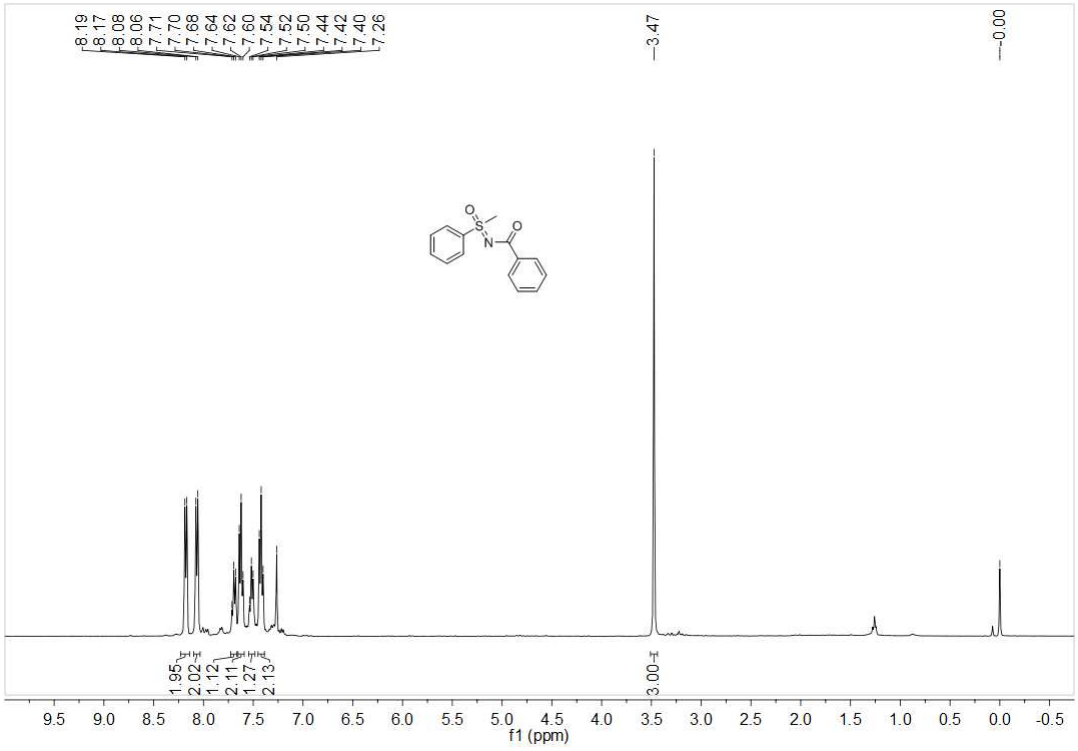
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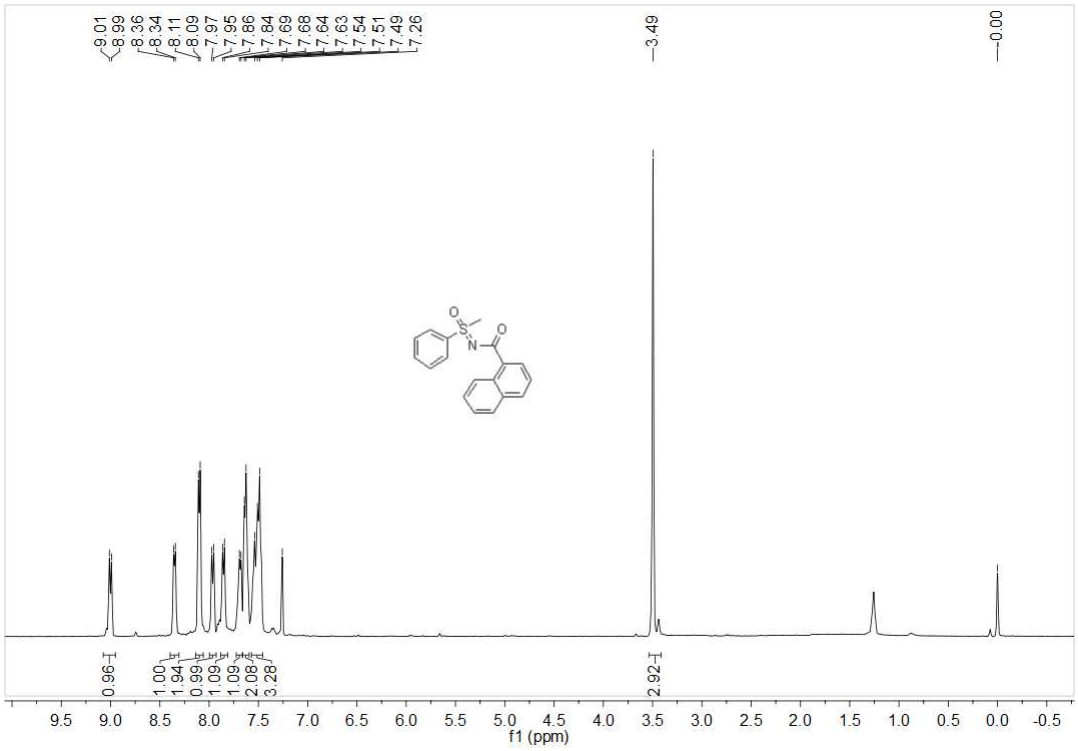
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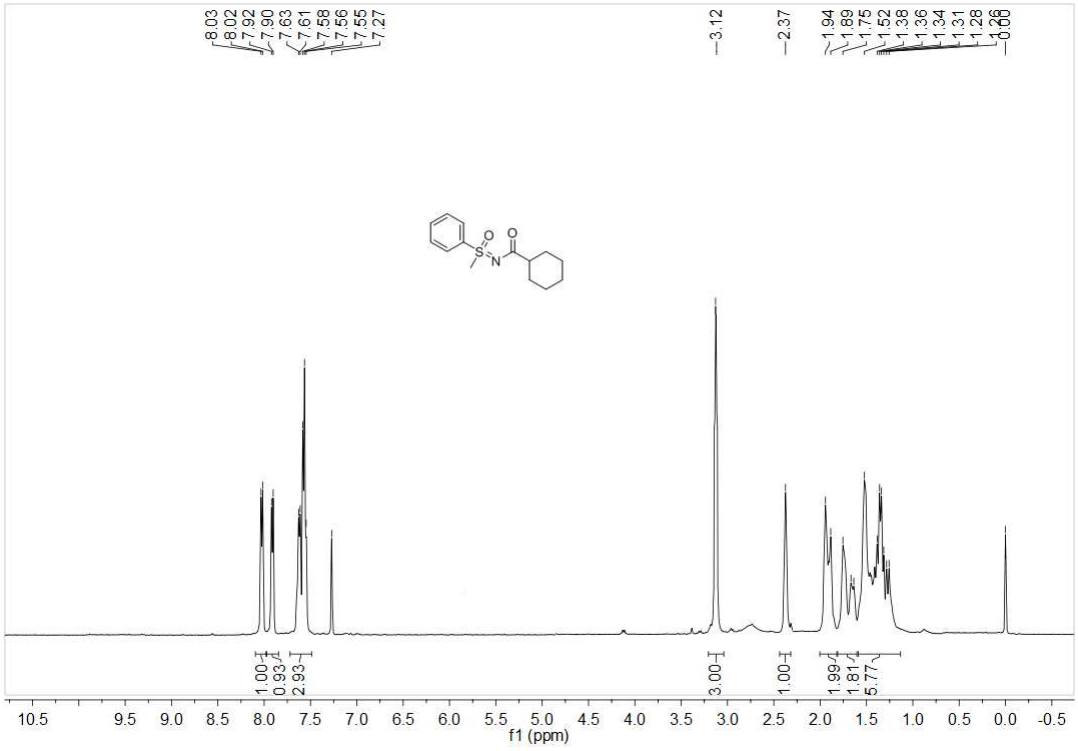
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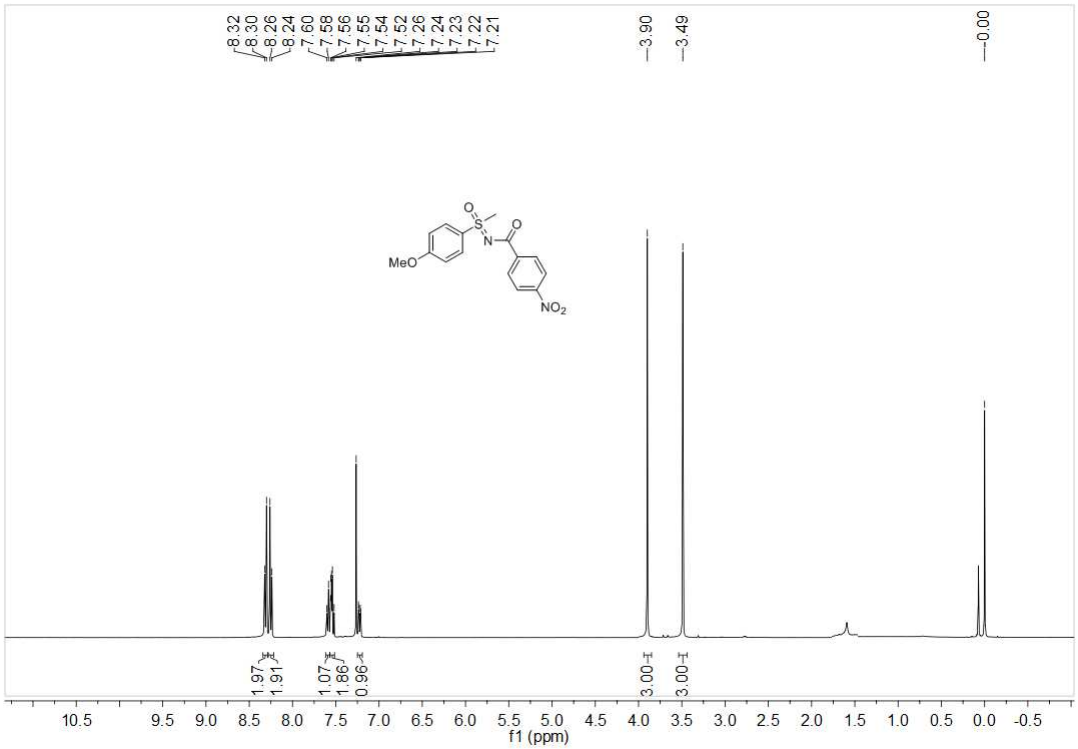
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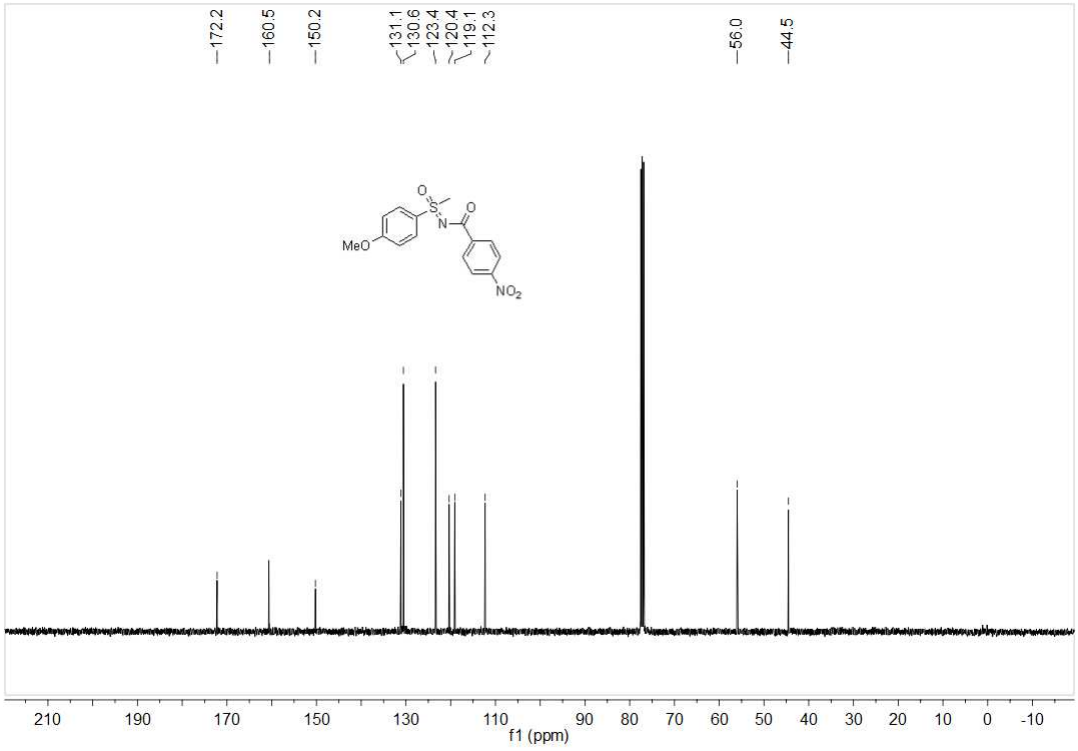
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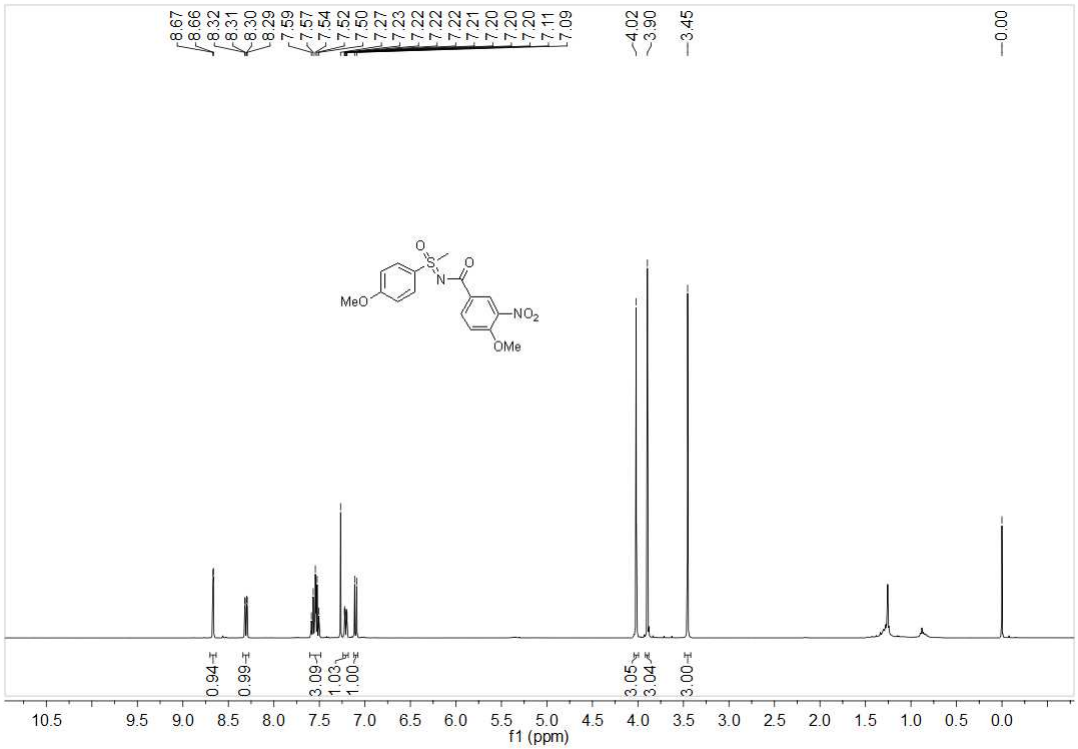
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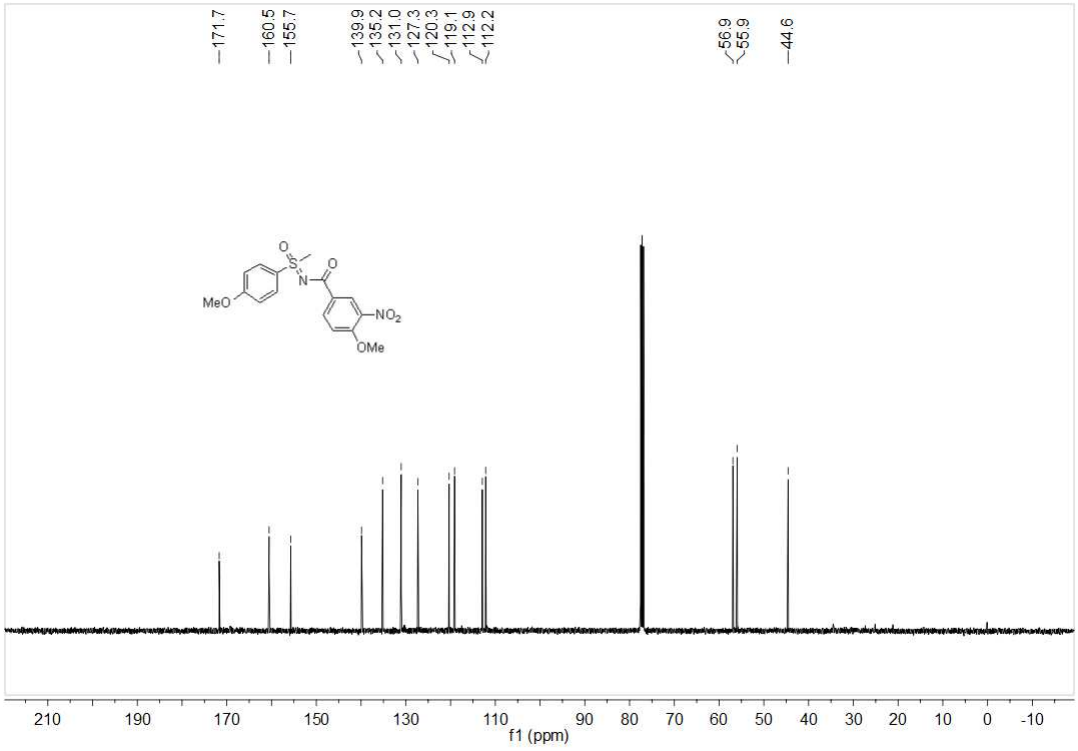
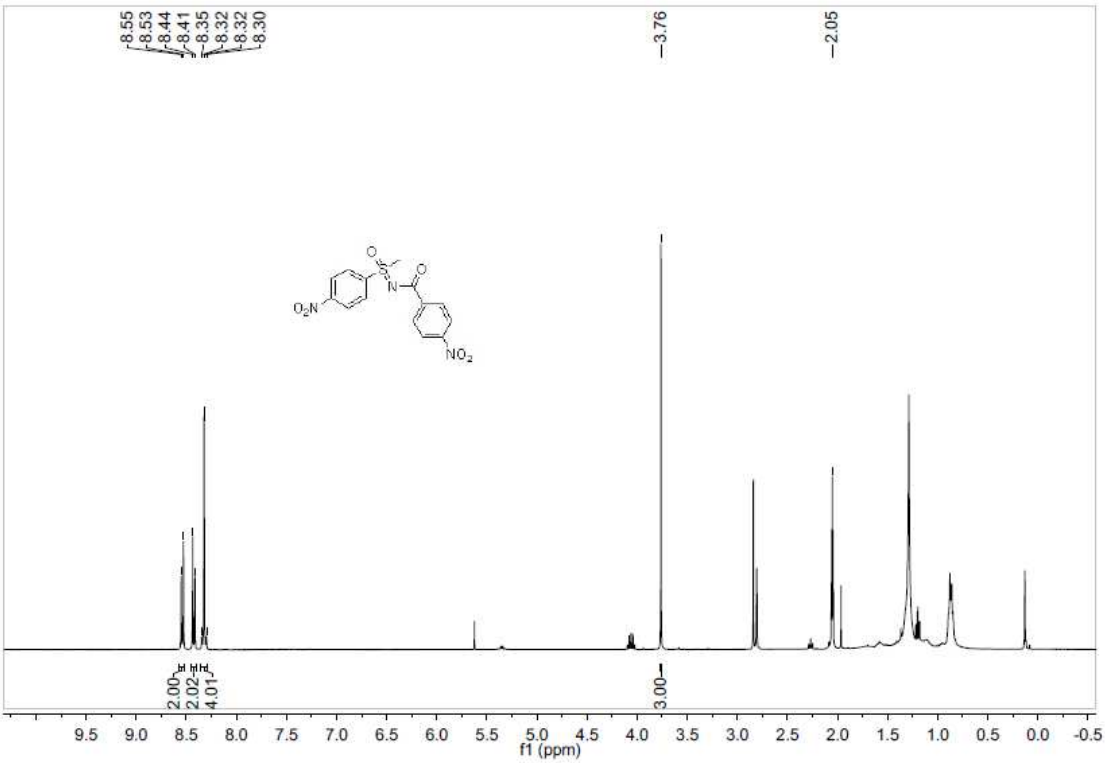
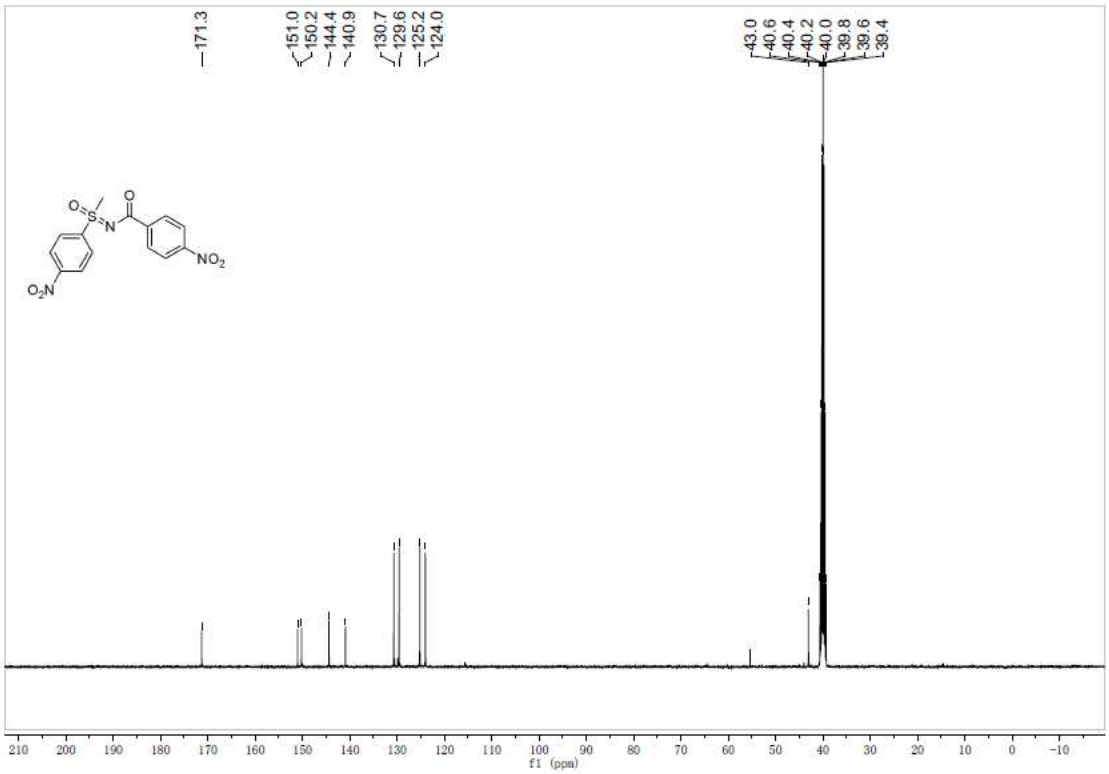
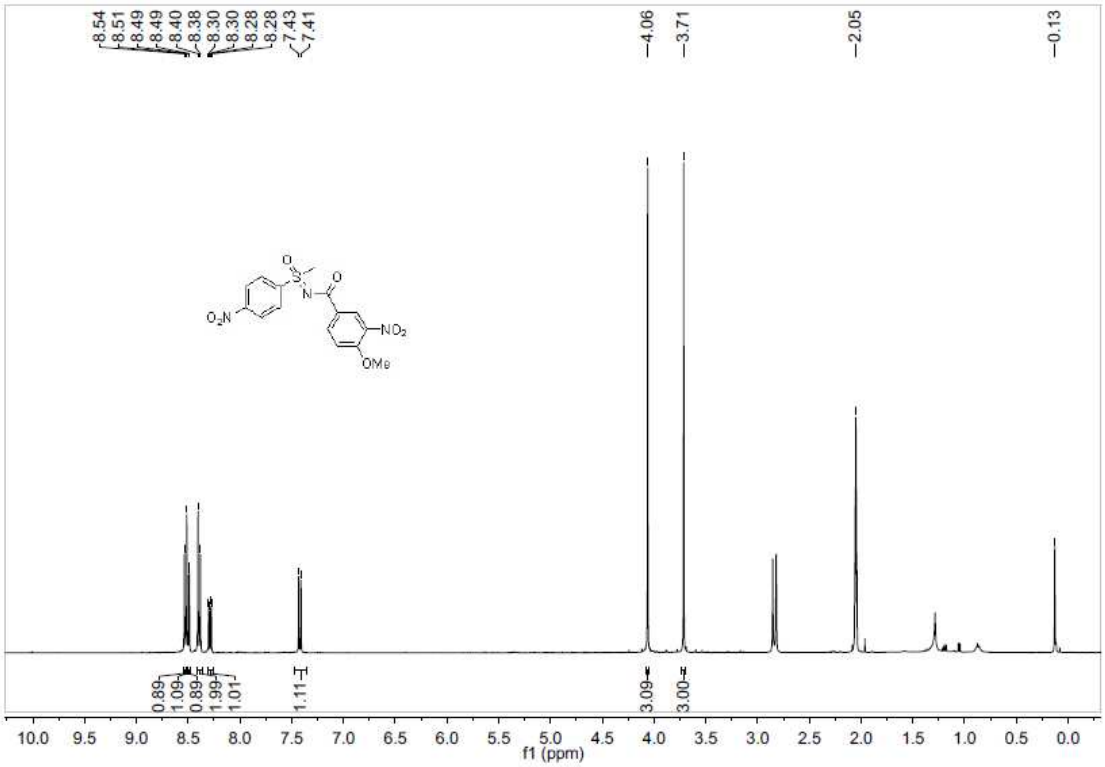
7.20
7.20
7.20
7.11
7.09
4.02
3.90
3.45
0.00
MeO
NO2
OMe
0.94
0.99
3.09
1.03
1.00
3.05
3.04
3.00
f1 (ppm)


171.7
160.5
155.7
139.9
135.2
131.0
127.3
120.3
119.1
112.9
112.2
56.9
55.9
44.6
MeO
NO2
OMe
f1 (ppm)


8.55
8.53
8.44
8.41
8.35
8.32
8.32
8.30
3.76
2.05
O2N
NO2
2.00
2.02
4.01
3.00
f1 (ppm)


171.3
151.0
150.2
144.4
140.9
130.7
129.6
125.2
124.0
43.0
40.6
40.4
40.2
40.0
39.8
39.6
39.4
f1 (ppm)


8.54
8.51
8.49
8.49
8.40
8.38
8.30
8.30
8.28
8.28
7.43
7.41
4.06
3.71
2.05
0.13
0.89
1.09
0.89
1.99
1.01
1.11
3.09
3.00
f1 (ppm)