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Radical oxyamination of vinyl azides with *N*-hydroxyphthalimide under the action of [bis(trifluoroacetoxy)iodo]benzene

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General Information

^{1}H and ^{13}C spectra were recorded on Bruker AVANCE II 300 spectrometer (300.13 MHz and 75.47 MHz, respectively) in $CDCl_3$ and DMSO-d_6. Chemical shifts were reported in parts per million (ppm), and the residual solvent peak was used as an internal reference: ^{1}H ($CDCl_3$ δ = 7.26 ppm; DMSO-d_6 δ = 2.50 ppm), ^{13}C ($CDCl_3$ δ = 77.16 ppm; DMSO-d_6 δ = 39.52 ppm). Multiplicity was indicated as follows: s (singlet), d (doublet), dd (doublet of doublet), ddd (doublet of doublet of doublet), t (triplet), q (quartet), m (multiplet).

High-resolution mass spectra (HRMS) were measured on a Bruker micrOTOF II instrument using electrospray ionization (ESI). The measurements were performed in a positive ion mode (interface capillary voltage – 4500 V); mass range from *m*/*z* 50 to *m*/*z* 3000 Da; external calibration with Electrospray Calibrant Solution.

Methanol (MeOH) was distilled over magnesium turnings. Acetone was distilled over $KMnO_4$ and stored over molecular sieves 4 Å. Acetonitrile (MeCN) was distilled over P_2O_5. Dichloromethane (DCM) and dichloroethane (DCE) were distilled over K_2CO_3. Toluene (PhMe) was distilled over sodium metal. Tetrahydrofuran (THF) was distilled over $LiAlH_4$. Ethanol (EtOH), trifluoroethanol (TFE) and glacial acetic acid (AcOH) were used as supplied without further purification. *N*-Hydroxyphthalimide (NHPI) **2** and [bis(acetoxy)iodo]benzene $PhI(OAc)_2$ were commercial reagents and used as supplied without further purification.

Vinyl azides **1a-n**[S1] and [bis(trifluoroacetoxy)iodo]benzene $PhI(OCOCF_3)_2$[S2] were synthesized according to the literature.

All the obtained products **3a–n** were characterized using ^{1}H, ^{13}C NMR spectroscopy and HRMS ESI. For the previously described compounds **3a-d,f,h** all the characterization data was in a good agreement with the literature.

General procedure 1

Optimization of the reaction conditions for the synthesis of *O,O'*-bis(phthalimido)-modified 2-(hydroxyimino)ethanol 3a from α-phenylvinyl azide 1a and *N*-hydroxyphthalimide 2 (see Table 1, entries 1-16). To a solution of vinyl azide **1a** (73 mg, 0.5 mmol, 1.0 equiv.) and *N*-hydroxyphthalimide **2** (163 mg, 1.0 mmol, 2.0 equiv.) in MeOH, acetone, MeCN, DCM, DCE, EtOH, PhMe, TFE, THF or AcOH (5.0 ml), oxidant (0.5–1.0 mmol) was added, and the mixture was stirred at 20–25 °C for 5–30 min. The reaction mixture was concentrated under reduced pressure. The yield of product **3a** was determined by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as the internal standard.

General procedure 2

Synthesis of *O,O'*-bis(phthalimido)-modified 2-(hydroxyimino)ethanols 3a-n (see Scheme 1). To a solution of vinyl azide **1a-n** (0.5 mmol, 1.0 equiv.) and *N*-hydroxyphthalimide **2** (163 mg, 1.0 mmol, 2.0 equiv.) in MeOH (5.0 ml), $PhI(OCOCF_3)_2$ (258 mg, 0.6 mmol) was added, and the mixture was stirred at 20–25 °C for 20 min. The resulted precipitate was filtered, washed with MeOH (2×5 mL) and dried under vacuum to give pure *O*-phthalimide oximes **3a-n**.

Scale up experiment for synthesis of *O,O'*-bis(phthalimido)-modified 2-(hydroxyimino)ethanol 3a (see Table 1, entry 15). To a solution of vinyl azide**1a** (1.45 g, 10.0 mmol, 1.0 equiv.) and *N*-hydroxyphthalimide **2** (3.26 g, 20.0 mmol, 2.0 equiv.) in MeOH (100.0 ml), $PhI(OCOCF_3)_2$ (5.16 g, 12.0 mmol) was added, and the mixture was stirred at 20–25 °C for 20 min. The resulted precipitate was filtered, washed with MeOH (2×30 ml) and dried under vacuum to give pure *O*-phthalimide oxime **3a** (67%, 2.95 g).

Analytical data for *O,O'*-bis(phthalimido)-modified 2-(hydroxyimino)ethanols 3a-n

2-(((2-((1,3-Dioxoisoindolin-2-yl)oxy)-1-phenylethylidene)amino)oxy)isoindoline-1,3-dione **(3a)**.[S3] White solid, mp 141-143 °C (dec.).Yield 70% (156 mg); mixture of two stereoisomers with the ratio of 0.72:1. ^{1}H NMR ($CDCl_3$), δ: 8.08-7.96 (m, 1.55H), 7.96-7.63 (m, 16.83H), 7.63-7.36 (m, 5.60H), 5.63 (s, 2.00H), 5.05 (s, 1.43H). ^{13}C NMR ($CDCl_3$), δ: 163.3, 163.2, 162.5, 162.5, 134.8, 134.7, 134.6, 134.5, 131.4, 131.0, 130.9, 129.5, 129.3, 129.2, 129.0, 129.0, 128.9, 128.7, 128.6, 128.0, 124.0, 123.9, 123.8, 123.8, 68.3.

2-(((2-((1,3-Dioxoisoindolin-2-yl)oxy)-1-(*p*-tolyl)ethylidene)amino)oxy)isoindoline-1,3-dione **(3b)**.[S3] White solid, mp 131-133 °C (dec.). Yield 52% (164 mg); mixture of two stereoisomers with the ratio of 0.85:1. ^{1}H NMR ($CDCl_3$), δ: 7.96-7.65 (m, 20.27H), 7.38-7.15 (m, 4.39H), 5.58 (s, 2.00H), 5.02 (s, 1.70H), 2.40 (s, 2.62H), 2.37 (s, 2.98H). ^{13}C NMR ($CDCl_3$), δ: 163.2, 163.1, 162.4, 162.4, 156.8, 155.7, 141.3, 141.2, 134.6, 134.6, 134.5, 134.4, 129.3, 129.3, 129.1, 129.1, 128.9, 128.8, 128.4, 127.7, 126.3, 123.8, 123.7, 123.7, 67.2, 21.6, 21.5.

2-(((2-((1,3-Dioxoisoindolin-2-yl)oxy)-1-(*m*-tolyl)ethylidene)amino)oxy)isoindoline-1,3-dione **(3c)**.[S3] White solid, mp 135-137 °C (dec.). Yield 69% (157 mg); mixture of two stereoisomers with the ratio of 0.84:1. ^{1}H NMR ($CDCl_3$), δ: 7.90-7.70 (m, 16.17H), 7.69-7.62 (m, 2.15H), 7.44-7.34 (m, 1.20H), 7.33-7.23 (m, 3.17H), 5.59 (s, 2.00H), 5.03 (s, 1.68H), 2.44 (s, 2.49), 2.38 (s, 2.95H). ^{13}C NMR (75, 47 MHz, $CDCl_3$), δ: 163.3, 163.1, 162.5, 157.2, 156.1, 138.5, 138.3, 134.7,

134.7, 134.6, 134.5, 131.8, 131.6, 131.3, 129.6, 129.2, 129.1, 129.0, 128.6, 128.5, 126.4, 125.2, 123.9, 123.8, 123.8, 68.4, 21.6, 21.5.

2-(2-(4-(*tert*-Butyl)phenyl)-2-(((1,3-dioxoisoindolin-2-yl)oxy)imino)ethoxy)isoindoline-1,3-dione **(3d)**.[S3] White solid, mp 135-137 °C (dec.). Yield 51% (171 mg); mixture of two stereoisomers with the ratio of 0.43:1. ^{1}H NMR ($CDCl_3$), δ: 7.99-7.89 (m, 0.83H), 7.90-7.66 (m, 13.85H), 7.56-7.48 (m, 0.86H), 7.48-7.39 (m, 2.04H), 5.59 (s, 2.00H), 5.03 (s, 0.85H), 1.33 (s, 3.89H), 1.31 (s, 9.02H). ^{13}C NMR ($CDCl_3$), δ: 163.3, 163.2, 162.5, 162.5, 156.9, 155.6, 154.4, 134.7, 134.7, 134.6, 134.5, 129.2, 129.2, 129.1, 128.9, 128.6, 127.7, 125.7, 125.5, 123.9, 123.8, 123.8, 68.3, 35.1, 35.0, 31.3.

2-(((2-((1,3-Dioxoisoindolin-2-yl)oxy)-1-(4-methoxyphenyl)ethylidene)amino)oxy)isoindoline-1,3-dione **(3e)**.[S3] White solid, mp 118-120 °C (dec.). Yield 40% (94 mg); mixture of two stereoisomers with the ratio of 0.92:1. ^{1}H NMR ($CDCl_3$), δ: 8.00 (d, J = 8.7 Hz, 2.08H), 7.92-7.53 (m, 20.45H), 7.07-6.81 (m, 4.71H), 5.58 (s, 2.00H), 5.01 (s, 1.84H), 3.93-3.71 (m, 5.78H). ^{13}C NMR ($CDCl_3$), δ: 163.3, 163.2, 162.6, 161.9, 161.5, 160.7, 155.1, 137.6, 134.7, 134.7, 134.6, 134.5, 131.6, 130.4, 129.6, 129.3, 129.2, 129.1, 129.0, 123.9, 123.8, 123.8, 121.7, 114.0, 68.2, 55.5.

4-(2-((1,3-Dioxoisoindolin-2-yl)oxy)-1-(((1,3-dioxoisoindolin-2-yl)oxy)imino)ethyl)phenyl acetate **(3f)**. White solid, mp 145-147 °C (dec.). Yield 68% (170 mg); mixture of two stereoisomers with the ratio of 0.76:1. ^{1}H NMR (DMSO-d_6), δ: 8.01 (d, J = 8.7 Hz, 1.74H), 7.93-7.84 (m, 16.95H), 7.38 (d, J = 8.7 Hz, 1.65H), 7.28 (d, J = 8.7 Hz, 2.11H), 5.64 (s, 2.00H), 5.14 (s, 1.51H), 2.35-2.27 (m, 5.69). ^{13}C NMR (DMSO-d_6), δ: 169.1, 162.3, 156.0, 152.5, 152.0, 135.4, 135.3, 134.8, 130.6, 129.0, 128.3, 128.2, 123.8, 123.7, 123.4, 122.2, 122.0, 24.6. HRMS (ESI), *m/z:* (M+K) 538.0648 (calc. for $C_{26}H_{17}N_3O_8$, *m/z:*538.0647).

2-(((2-((1,3-Dioxoisoindolin-2-yl)oxy)-1-(4-fluorophenyl)ethylidene)amino)oxy)isoindoline-1,3-dione **(3g)**.[S3] White solid, mp 144-146 °C (dec.). Yield 79% (145 mg); mixture of two stereoisomers with the ratioof 0.84:1. ^{1}H NMR (DMSO-d_6), δ: 8.06-7.94 (m, 1.74H), 7.95-7.78 (m, 16.84H), 7.49-7.39 (m, 1.78H), 7.38-7.28 (m, 2.16H), 5.64 (s, 2.00H), 5.14 (s, 1.67H). ^{13}C NMR (DMSO-d_6), δ: 162.9, 162.7, 162.3, 156.4, 155.3, 135.4, 135.4, 134.8, 131.9, 131.8, 130.2, 130.1, 128.6, 128.3, 128.2, 128.2, 127.5, 127.5, 125.3, 123.8, 123.8, 123.4, 123.4, 115.9, 115.7, 115.6, 115.4, 75.8, 67.2. HRMS (ESI), *m/z:* (M+NH_4) 477.1212 (calc. for $C_{24}H_{14}FN_3O_6$, *m/z:* 477.1205).

2-(((2-((1,3-Dioxoisoindolin-2-yl)oxy)-1-(2-fluorophenyl)ethylidene)amino)oxy)isoindoline-1,3-dione**(3h)**. White solid, mp 149-151 °C (dec.). Yield 68% (156 mg); mixture of two stereoisomers with the ratio of 0.58:1. ^{1}H NMR (DMSO-d_6), δ: 7.97-7.78 (m, 13.86H), 7.72-7.65 (m, 1.10H), 7.64-7.53 (m, 1,70H), 7.45-7.28 (m, 3.29H), 5.63 (s, 2.00H), 5.16 (s, 1.16H). ^{13}C NMR (DMSO-d_6), δ: 162.6, 162.6, 162.2, 162.1, 160.7, 158.9, 157.7, 155.7, 152.5, 135.4, 135.3, 134.8, 134.8, 132.9, 132.9, 130.9, 130.0, 128.6, 128.4, 128.2, 124.7, 124.6, 123.9, 123.7, 123.3, 118.7, 118.6, 117.0, 116.8, 116.3, 116.1, 116.0, 75.3, 70.3. HRMS (ESI), *m/z:* (M+Na) 482.0760 (calc. for $C_{24}H_{14}FN_3O_6$, *m/z:*482.0759).

2-(2-(3-Chlorophenyl)-2-(((1,3-dioxoisoindolin-2-yl)oxy)imino)ethoxy)isoindoline-1,3-dione **(3i)**. White solid, mp 117-120 °C (dec.). Yield 79% (188 mg); mixture of two stereoisomers with the ratio of 0.78:1. ^{1}H NMR (DMSO-d_6), δ: 8.15-7.71 (m, 16.77H), 7.69-7.46 (m, 3.91H), 5.65 (s, 2.00H), 5.15 (s, 1.56H). ^{13}C NMR (DMSO-d_6), δ: 162.8, 162.2, 162.0, 155.6, 155.1, 135.3, 135.3, 134.8, 133.4, 133.1, 133.0, 130.7, 130.5, 130.5, 130.3, 128.6, 128.1, 127.5, 127.3, 126.2, 124.2, 123.7, 123.3, 76.8, 68.2. HRMS (ESI), *m/z:* (M+NH_4) 493.0910 (calc. for $C_{24}H_{14}ClN_3O_6$, *m/z:*493.0909).

2-(2-(2-Chlorophenyl)-2-(((1,3-dioxoisoindolin-2-yl)oxy)imino)ethoxy)isoindoline-1,3-dione **(3j)**. White solid, mp 133-135 °C (dec.). Yield 67% (159 mg); mixture of two stereoisomers with the ratio of 0.39:1. ^{1}H NMR (DMSO-d_6), δ: 8.02-7.74 (m, 12.27H), 7.69-7.42 (m, 5.70H), 5.64 (s, 2.00H), 5.13 (s, 0,77H). ^{13}C NMR (DMSO-d_6), δ: 162.5, 162.1, 158.5, 135.4, 135.2, 134.7, 132.2, 131.8, 131.8, 131.4, 129.9, 129.6, 129.6, 128.6, 128.4, 128.1, 127.2, 123.8, 123.7, 123.3, 123.2, 75.3, 70.0. HRMS (ESI), *m/z:* (M+NH_4) 493.0905 (calc. for $C_{24}H_{14}ClN_3O_6$, *m/z:*493.0909).

2-(2-(4-Bromophenyl)-2-(((1,3-dioxoisoindolin-2-yl)oxy)imino)ethoxy)isoindoline-1,3-dione **(3k)**. White solid, mp 148-150 °C (dec.). Yield 72% (187 mg); mixture of two stereoisomers with the ratio of 0.88:1. ^{1}H NMR (DMSO-d_6), δ: 7.90-7.69 (m, 23.09H), 5.63 (s, 2.00H), 5.13 (s, 1.76). ^{13}C NMR (DMSO-d_6), δ: 162.9, 162.7, 162.2, 155.9, 155.4, 135.4, 135.4, 134.9, 131.7, 131.5, 131.1, 130.2, 129.6, 128.6, 128.3, 128.2, 128.0, 124.7, 124.5, 123.9, 123.8, 123.4, 123.4, 76.1, 67.1. HRMS (ESI), *m/z:* (M+NH_4) 539.0369 (calc. for $C_{24}H_{14}BrN_3O_6$, *m/z:*539.0385).

2-(2-(3-Bromophenyl)-2-(((1,3-dioxoisoindolin-2-yl)oxy)imino)ethoxy)isoindoline-1,3-dione **(3l)**. White solid, mp 141-143 °C (dec.). Yield 62% (161 mg); mixture of two stereoisomers with the ratio of 0.83:1.^{1}H NMR (DMSO-d_6), δ: 8.15 (s, 0.88H), 8.02 (s, 0.81H), 7.96-7.70 (m, 19.23H), 7.55 (t, J = 7.9 Hz, 1.17H), 7.46 (t, J = 7.9 Hz, 0.99H), 5.64 (s, 1.66H), 5.14 (s, 2.00H). ^{13}C NMR (DMSO-d_6), δ: 162.8, 162.6, 162.2, 162.1, 155.6, 155.1, 135.4, 135.3, 134.8, 133.7, 133.4, 131.4, 131.1, 130.7, 130.6, 130.1, 128.6, 128.3, 128.2, 127.9, 126.6, 123.8, 123.7, 123.4, 123.4, 121.8, 121.6, 76.9, 69.5. HRMS (ESI), *m/z:* (M+NH_4) 537.0393 (calc. for $C_{24}H_{14}BrN_3O_6$, *m/z:*537.0404).

2-(2-(1*H*-Benzo[*d*]imidazol-1-yl)-2-(((1,3-dioxoisoindolin-2-yl)oxy)imino)ethoxy)isoindoline-1,3-dione **(3m)**. White solid, mp 134-137 °C (dec.). Yield 51% (123 mg); mixture of two stereoisomers with the ratio of 0.16:1.^{1}H NMR (DMSO-d_6), δ: 8.94 (s, 1.02H), 0.18 (s, 0.18H), 8.04-7.70 (m, 11.34H), 7.47-7.25 (m, 2.34H), 5.92 (s, 2.00H), 5.48 (s, 0.32H). ^{13}C NMR (DMSO-d_6), δ: 163.0, 162.0, 150.7, 143.7, 142.9, 135.4, 134.9, 130.8, 128.6, 128.2, 124.9, 124.2, 123.9, 123.5, 120.0, 116.0, 115.3, 66.6. HRMS (ESI), *m/z:* (M+Na) 504.0908 (calc. for $C_{25}H_{15}N_5O_6$, *m/z:*504.0915).

Methyl 3-((1,3-dioxoisoindolin-2-yl)oxy)-2-(((1,3-dioxoisoindolin-2-yl)oxy)imino)propanoate **(3n)**. White solid, mp 145-147 °C (dec.). Yield 51% (108 mg); mixture of two stereoisomers with the ratio of 0.12:1.^{1}H NMR (DMSO-d_6), δ: 7.94-7.84 (m, 9.01H), 5.27 (s, 2.00H), 5.07 (s, 0.24H), 3.95 (s, 0.40H), 3.83 (s, 3.00H). ^{13}C NMR (DMSO-d_6), δ: 163.2, 161.8, 160.5, 150.0, 135.5, 135.0, 128.6, 128.0, 124.0, 123.5, 66.3, 53.2. HRMS (ESI), *m/z:* (M+NH_4) 441.1033 (calc. for $C_{20}H_{13}N_3O_8$, *m/z:*441.1041).

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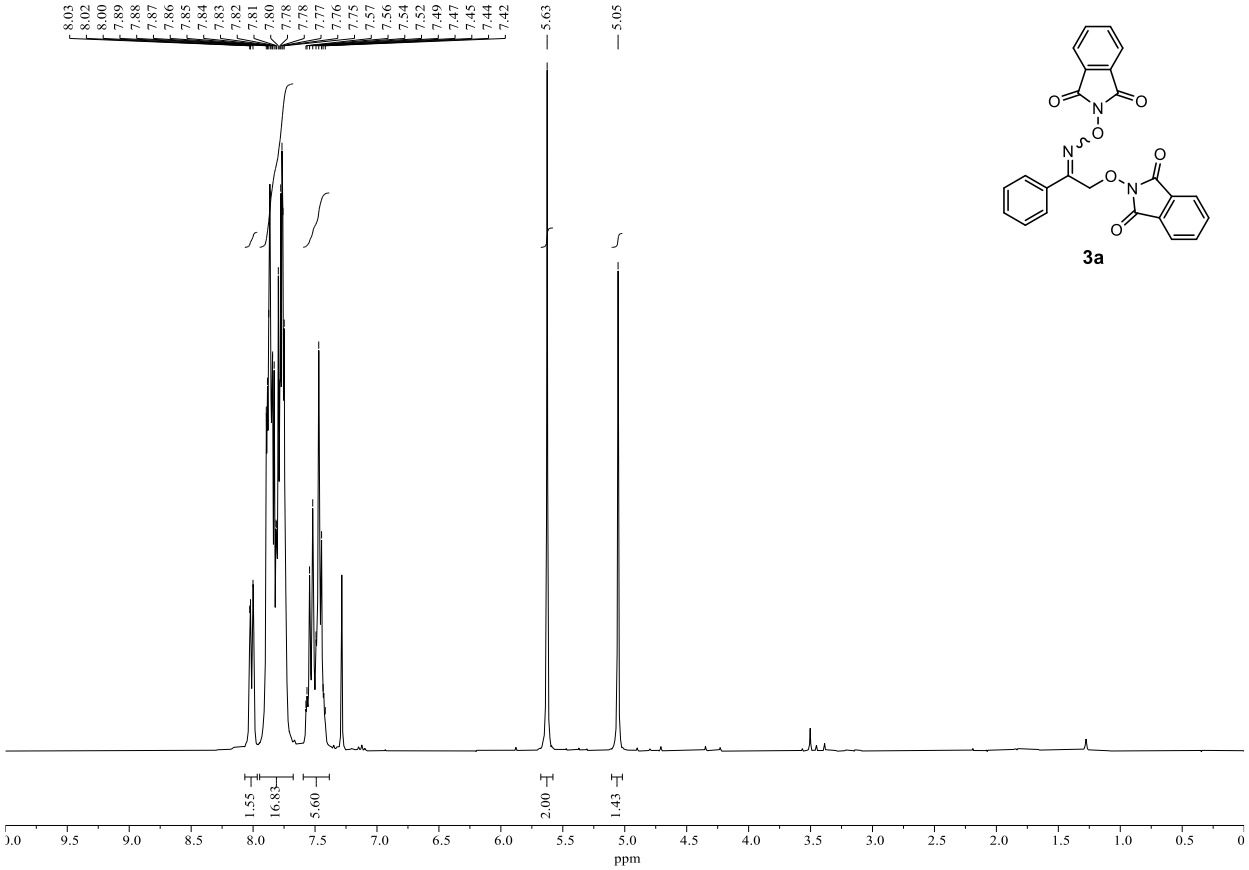
NMR spectra of synthesized compounds



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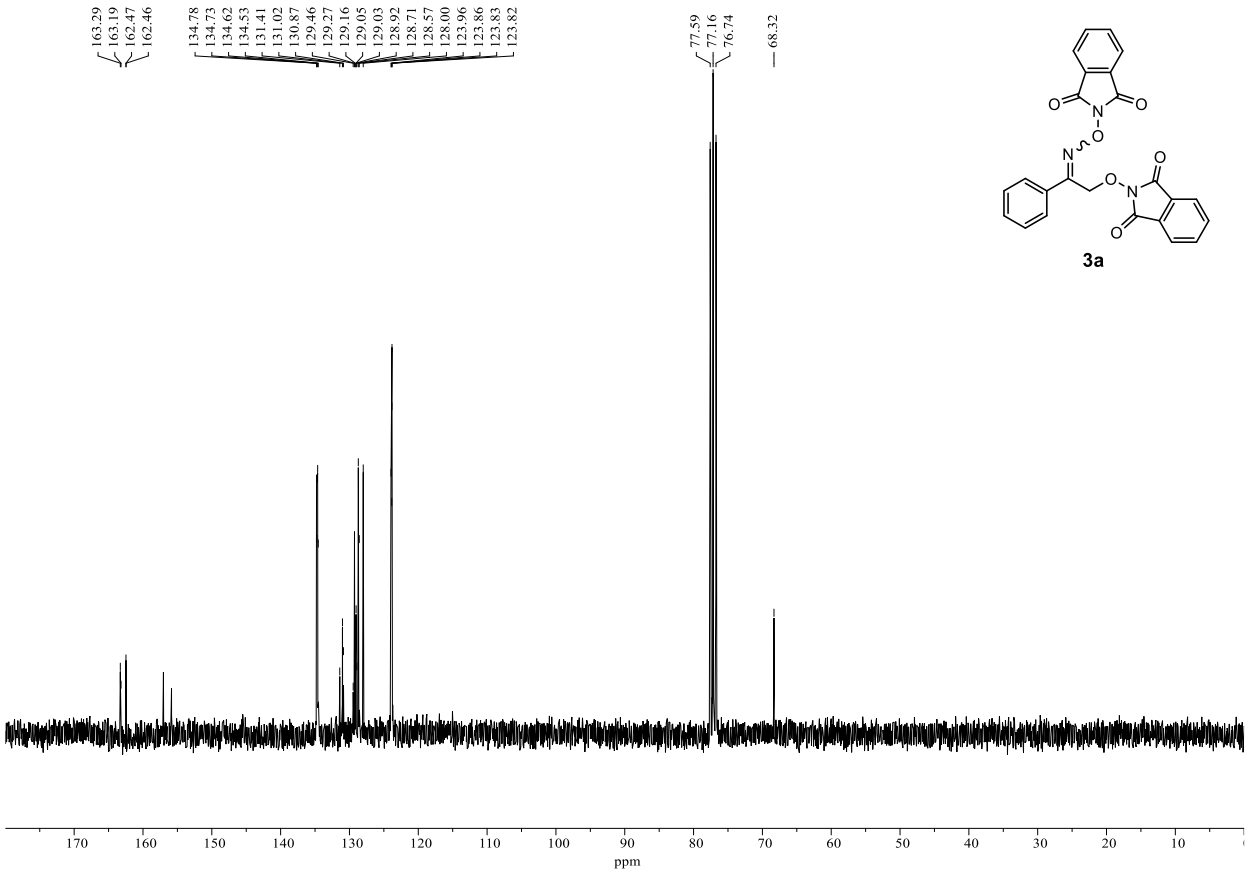

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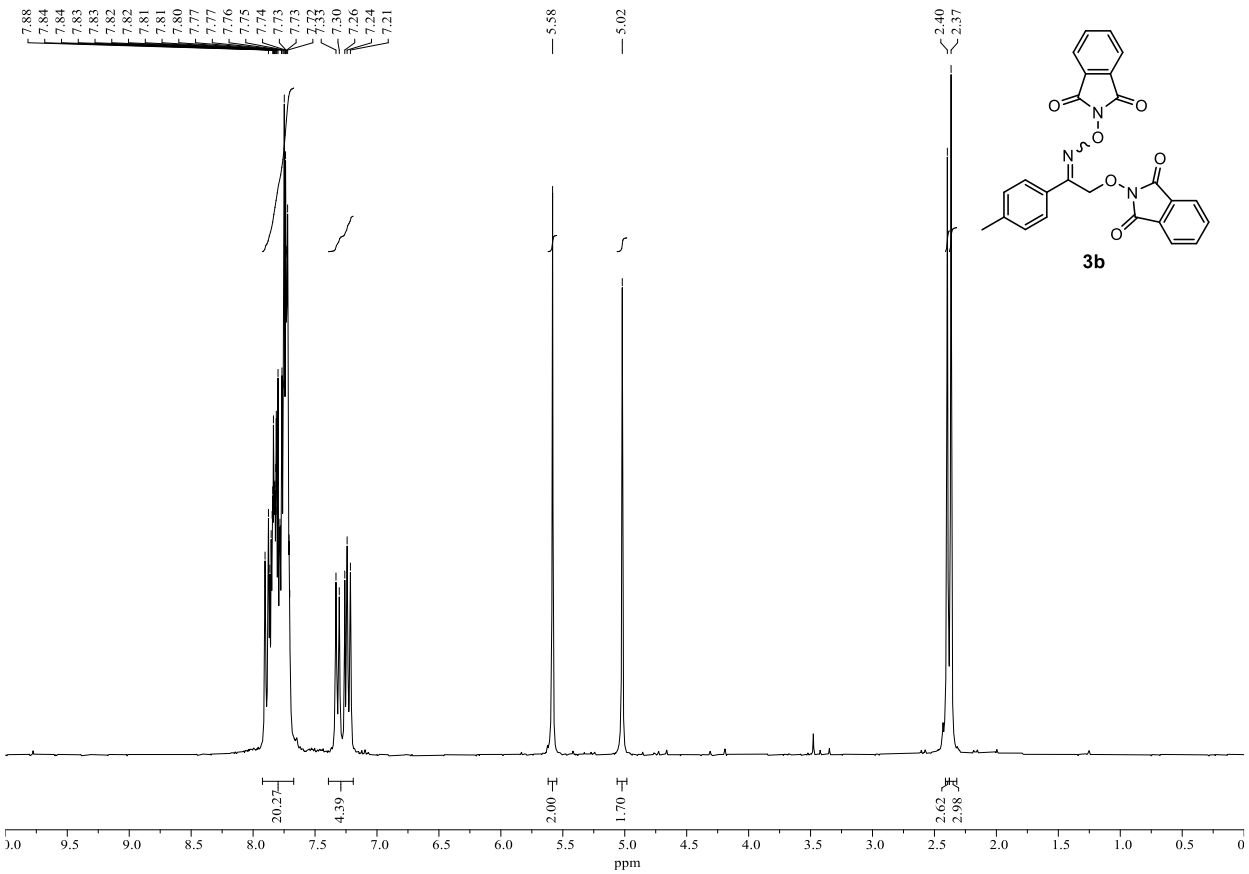
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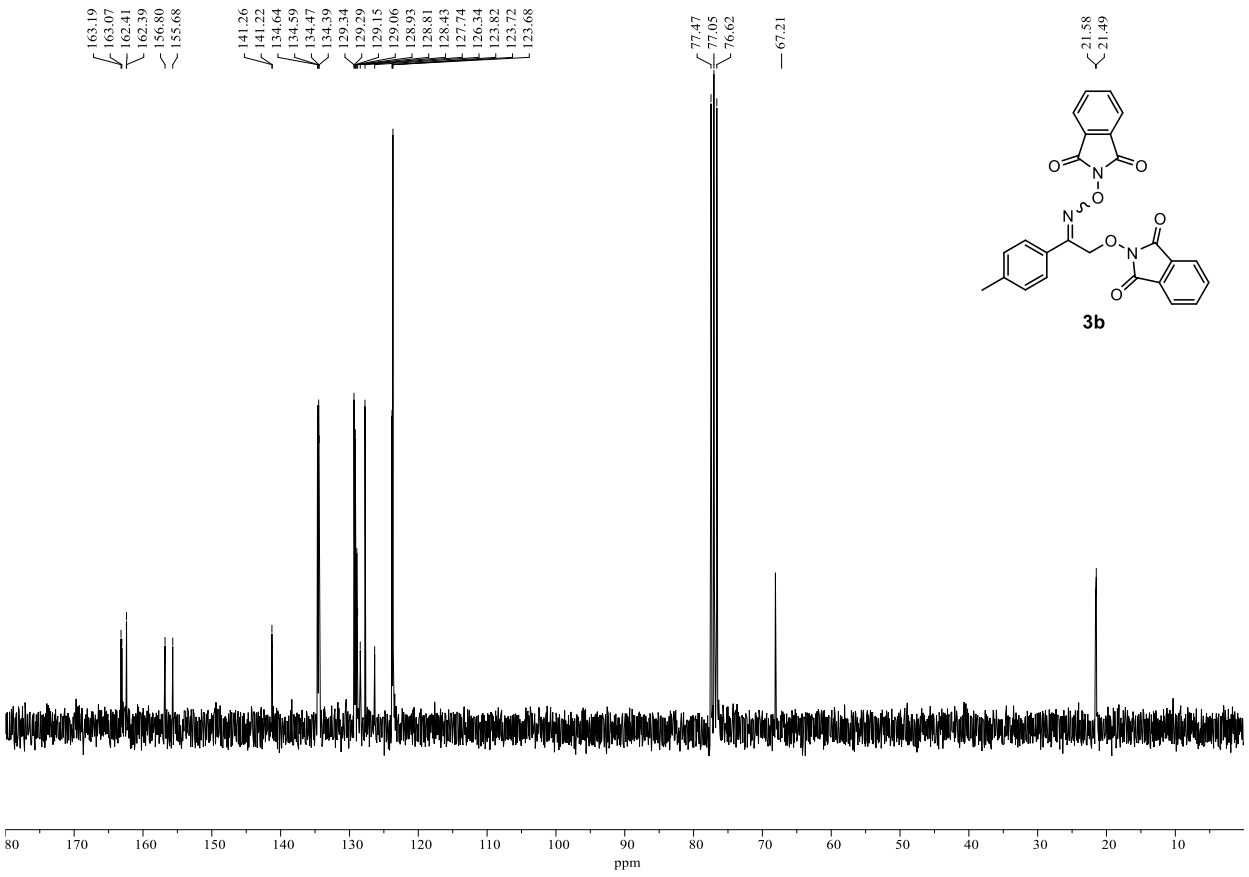
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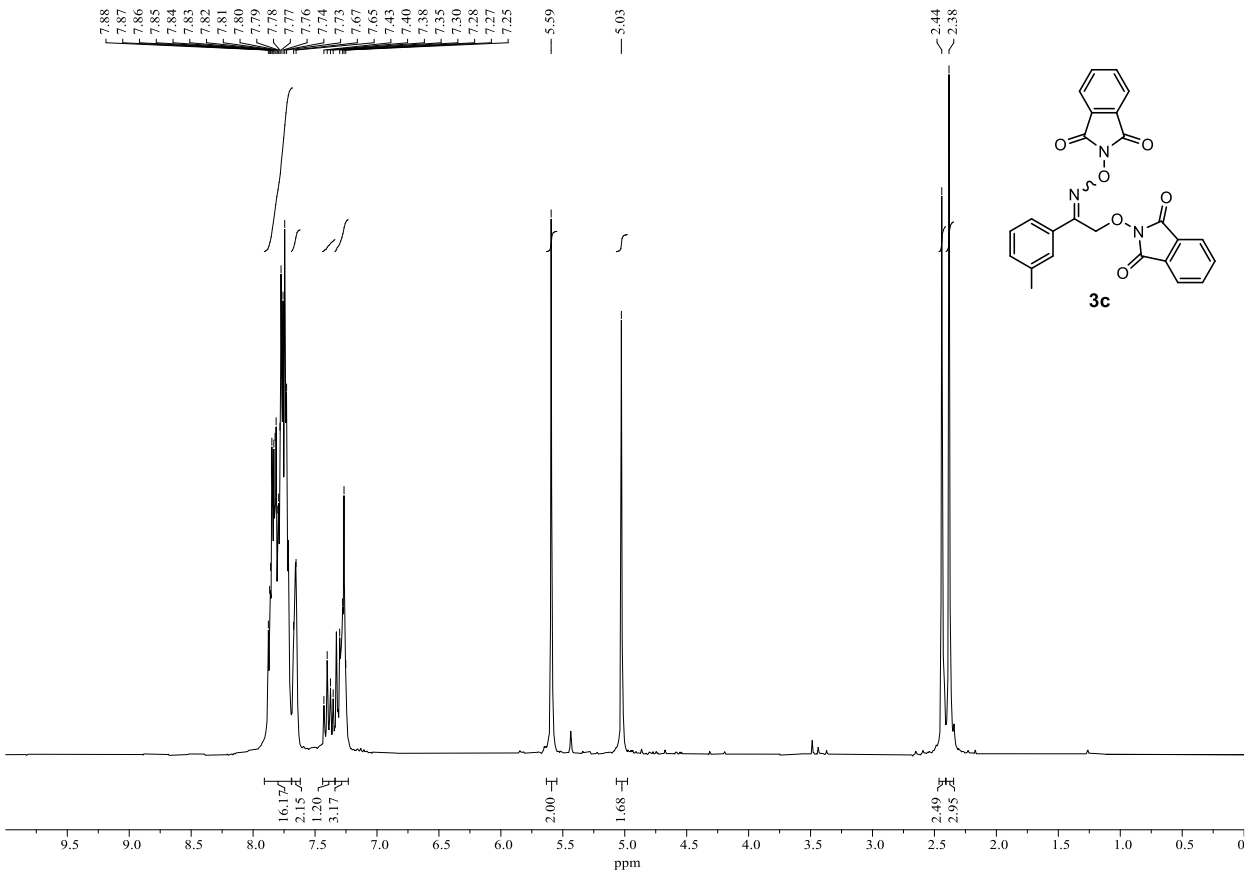
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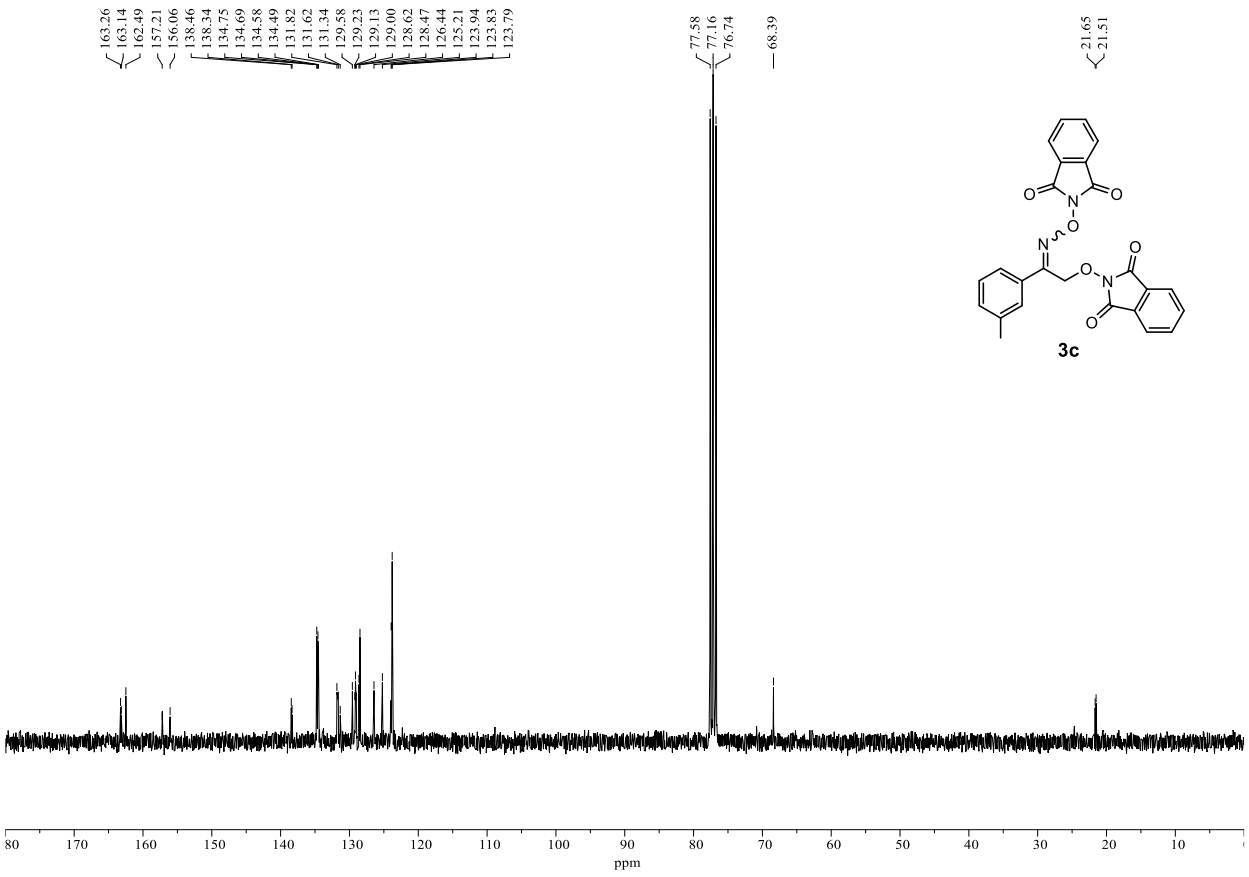
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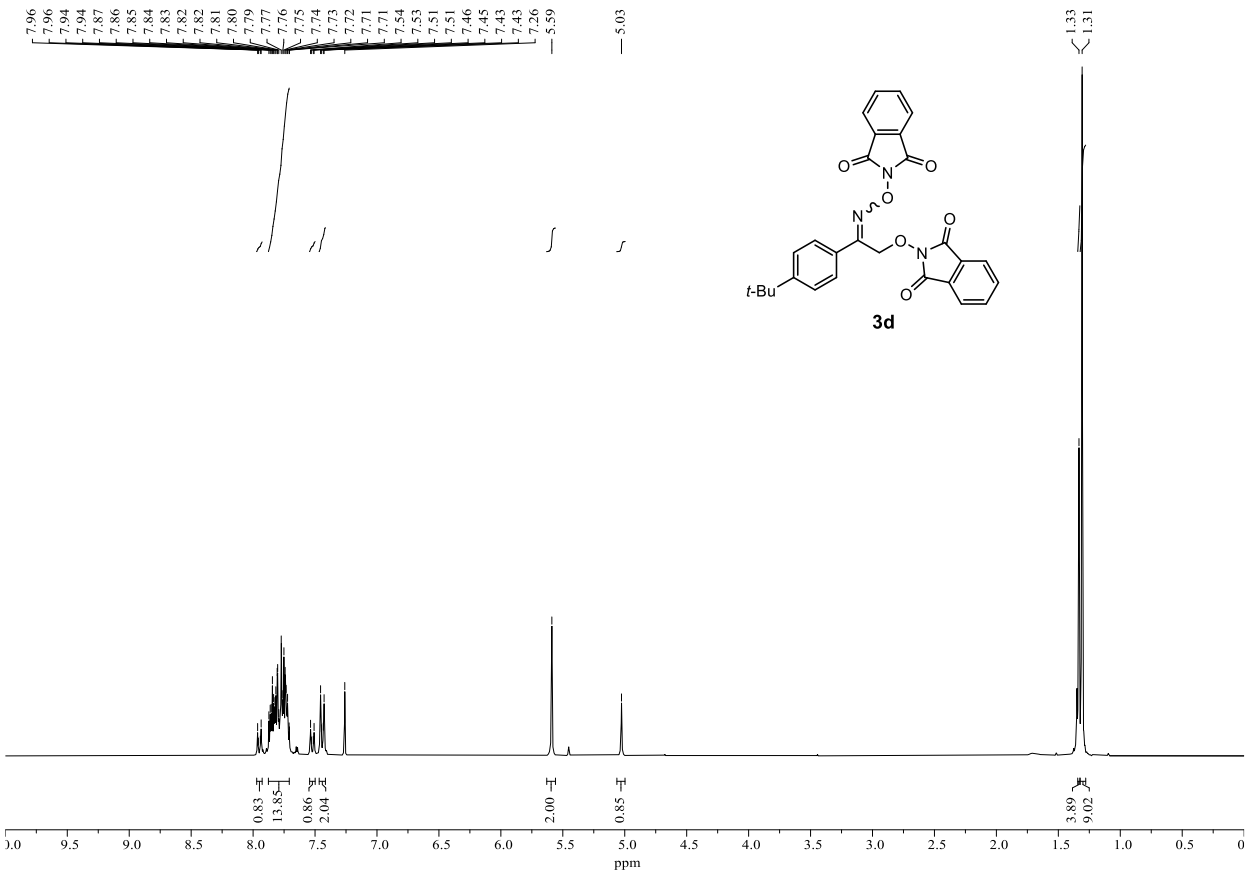
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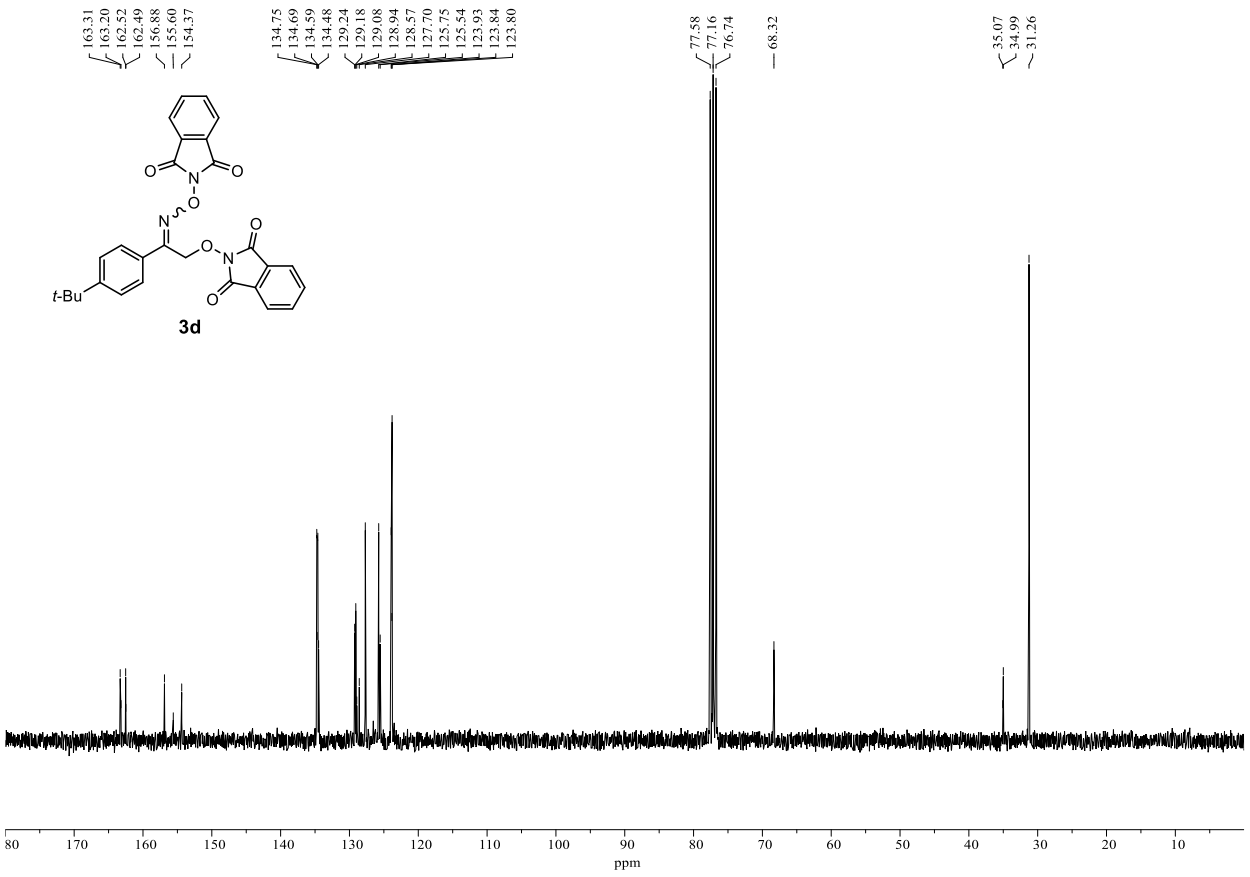
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134.75
134.69
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129.24
129.18
129.08
128.94
128.57
127.70
125.75
125.54
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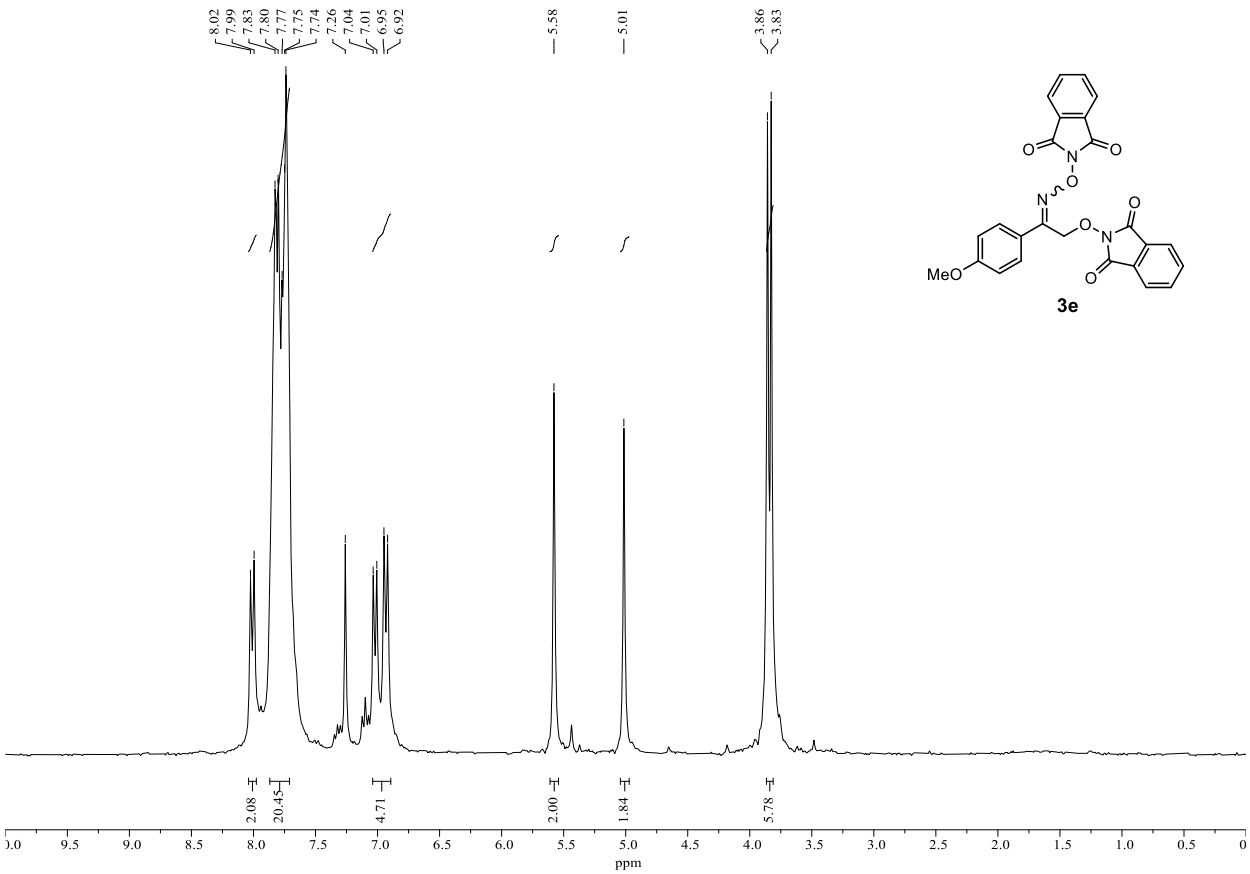
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MeO
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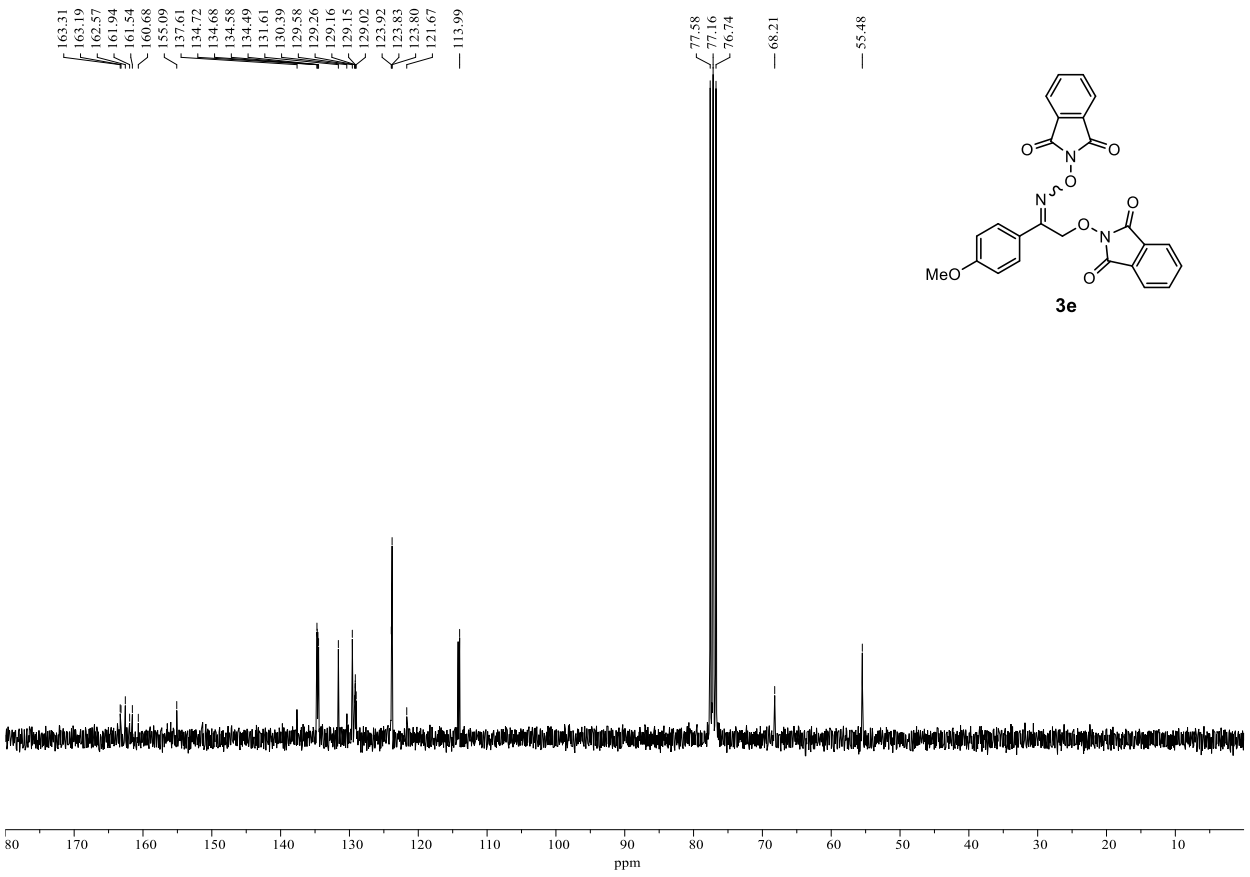
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129.26
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ppm
MeO
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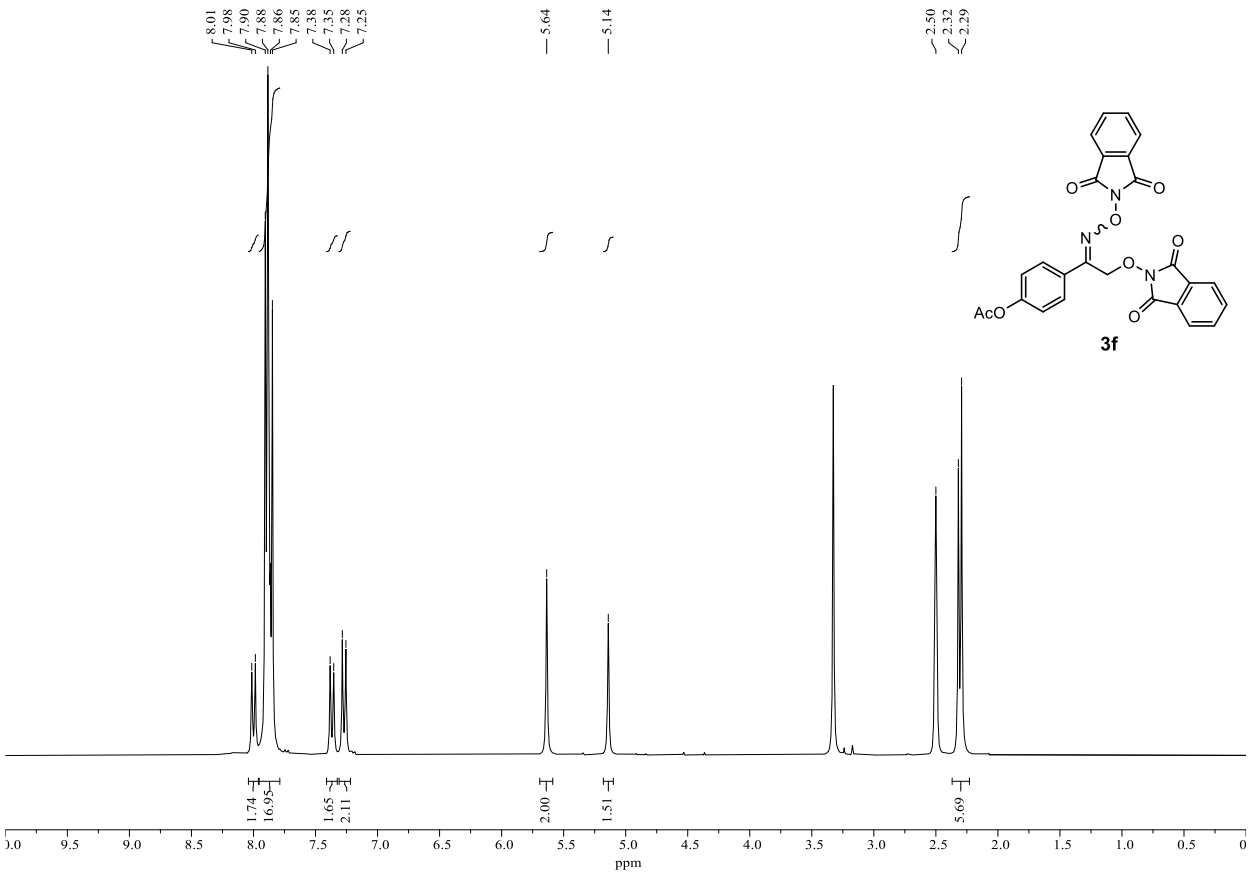
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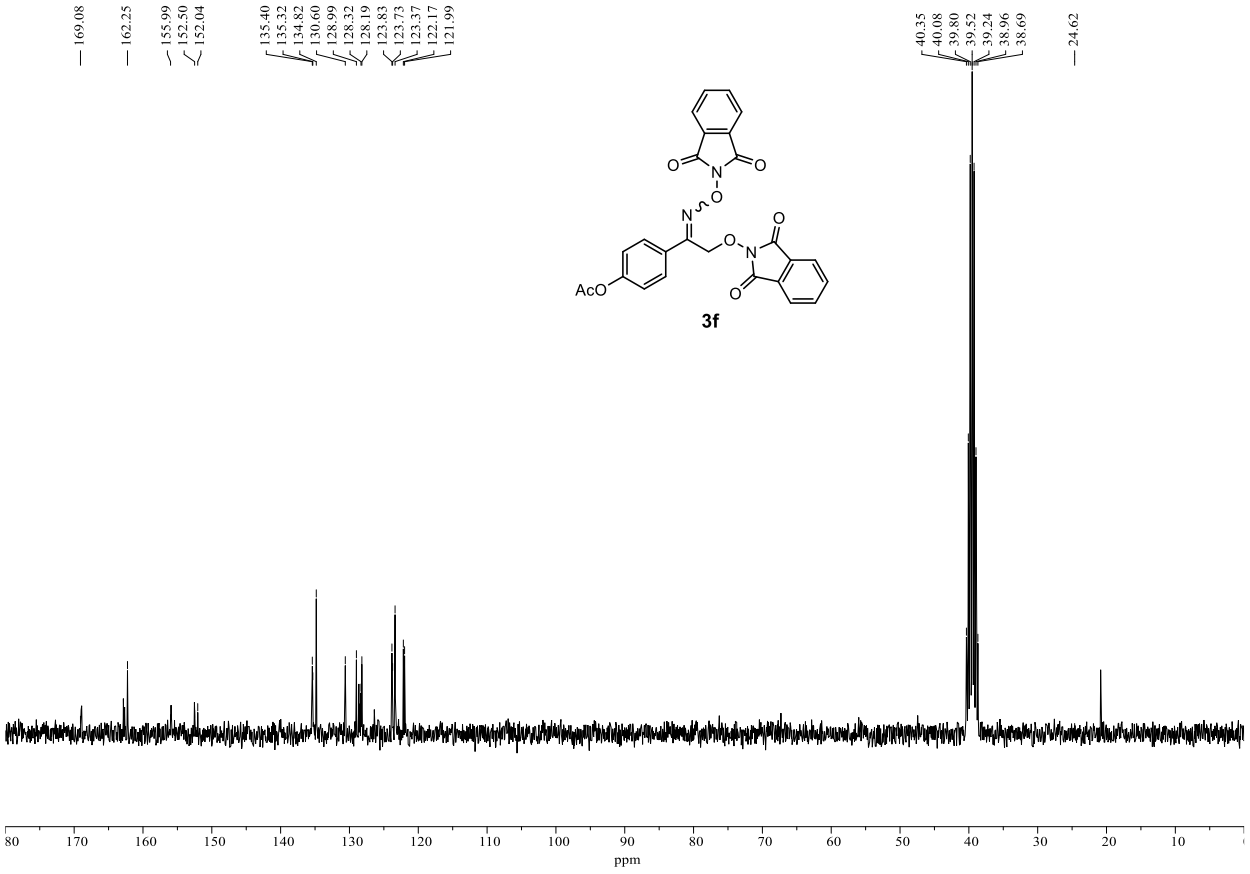
ppm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123.37
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AcO
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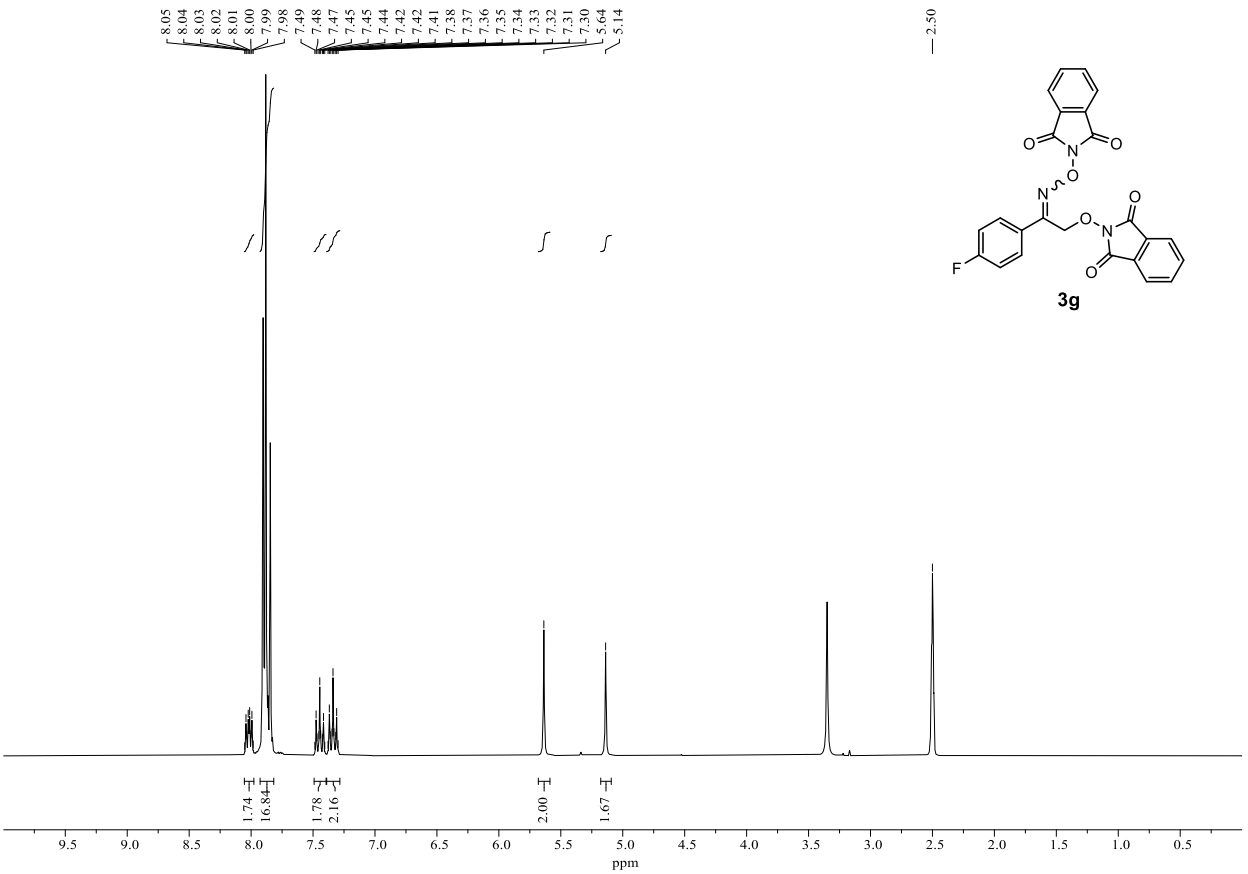
ppm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7.45
7.44
7.42
7.42
7.41
7.38
7.37
7.36
7.35
7.34
7.33
7.32
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7.30
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5.14
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1.74
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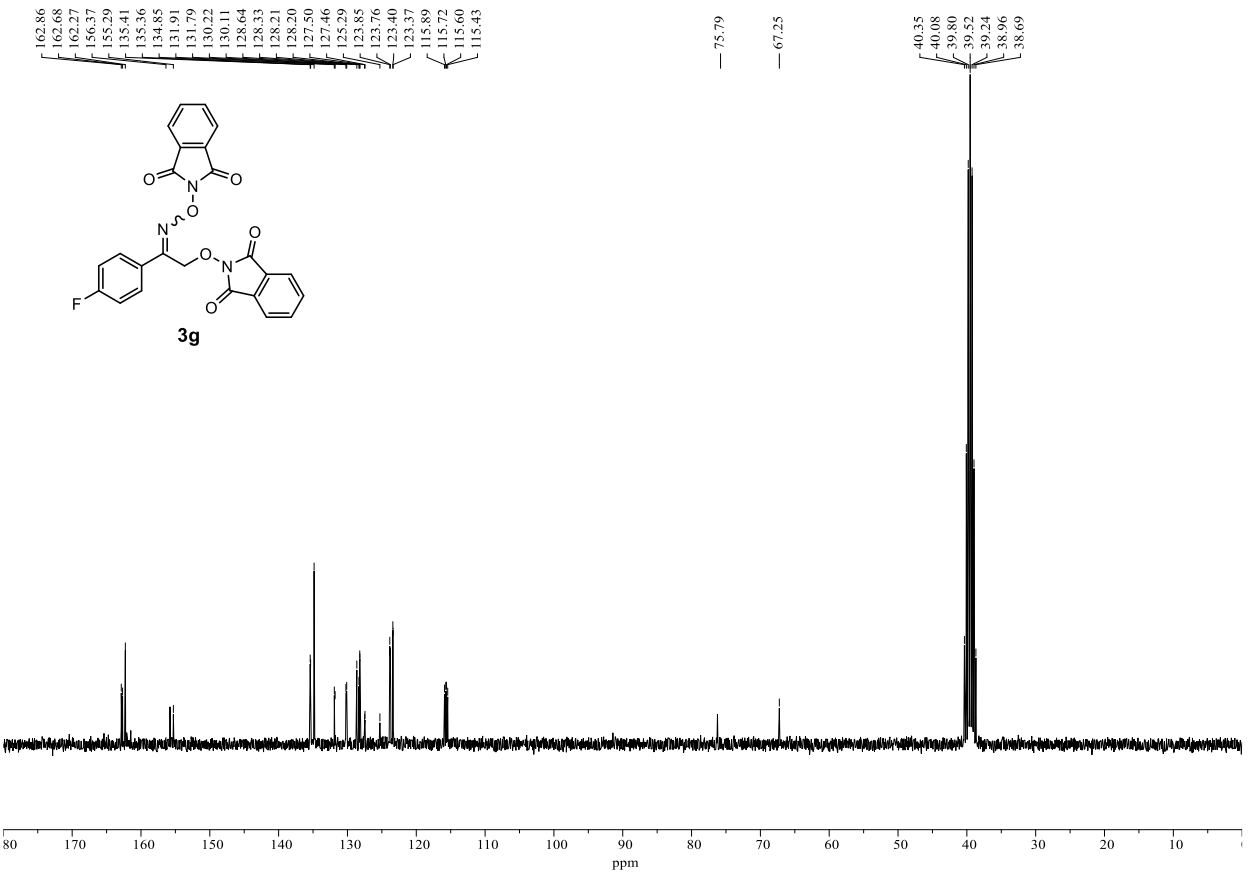
O
O
F

3g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128.21
128.20
127.50
127.46
125.29
123.85
123.76
123.40
123.37
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115.72
115.60
115.43
75.79
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40.35
40.08
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O
F

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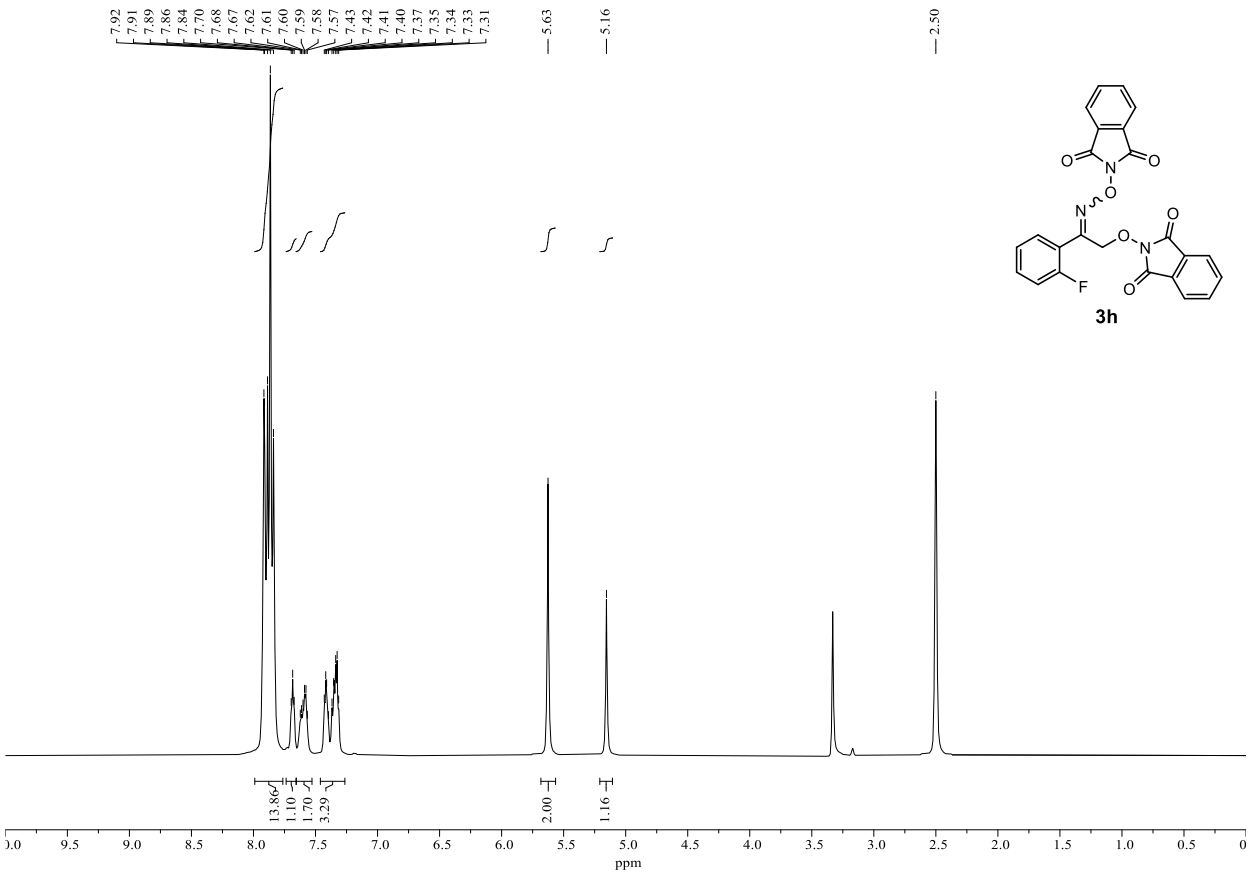
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7.57
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7.41
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7.35
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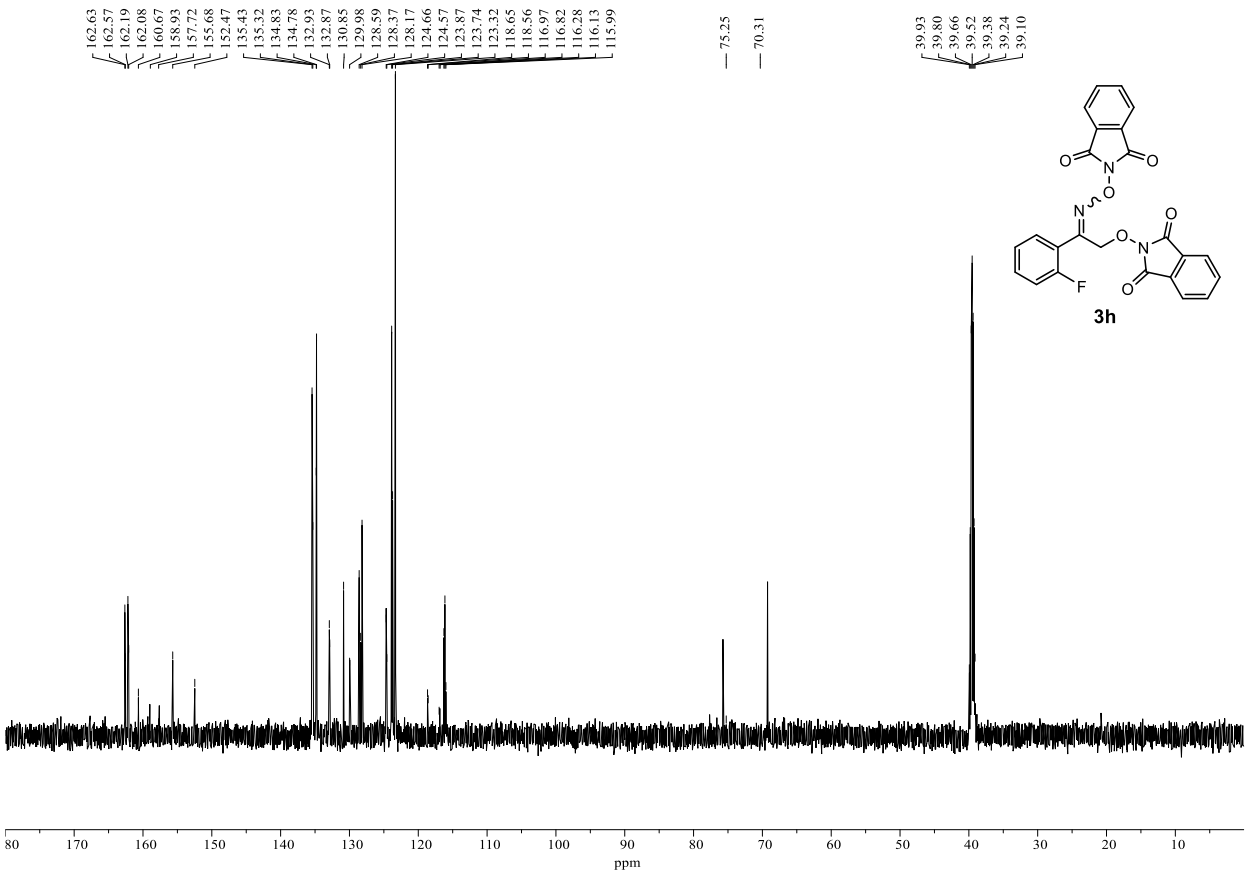
3h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129.98
128.59
128.37
128.17
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124.57
123.87
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116.97
116.82
116.28
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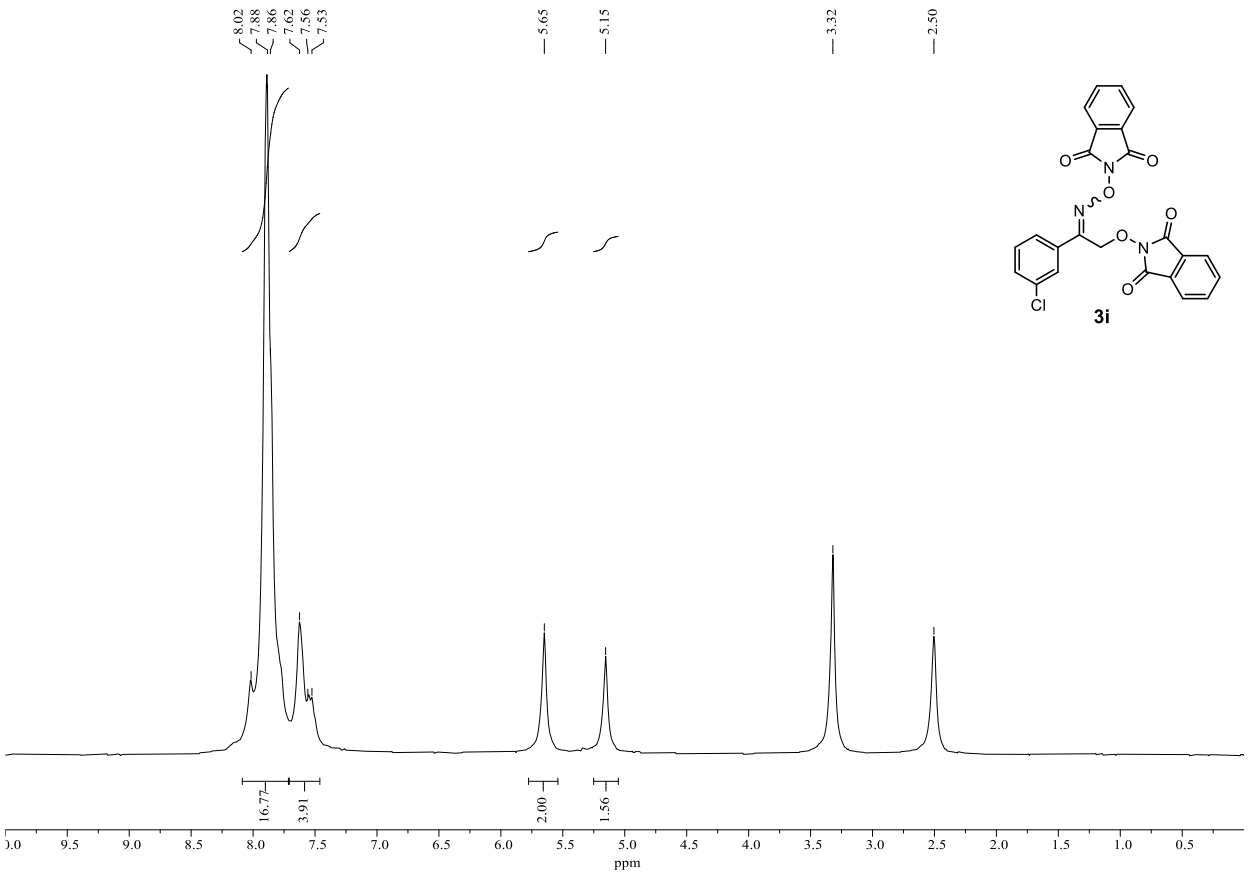
39.24
39.10
ppm

3h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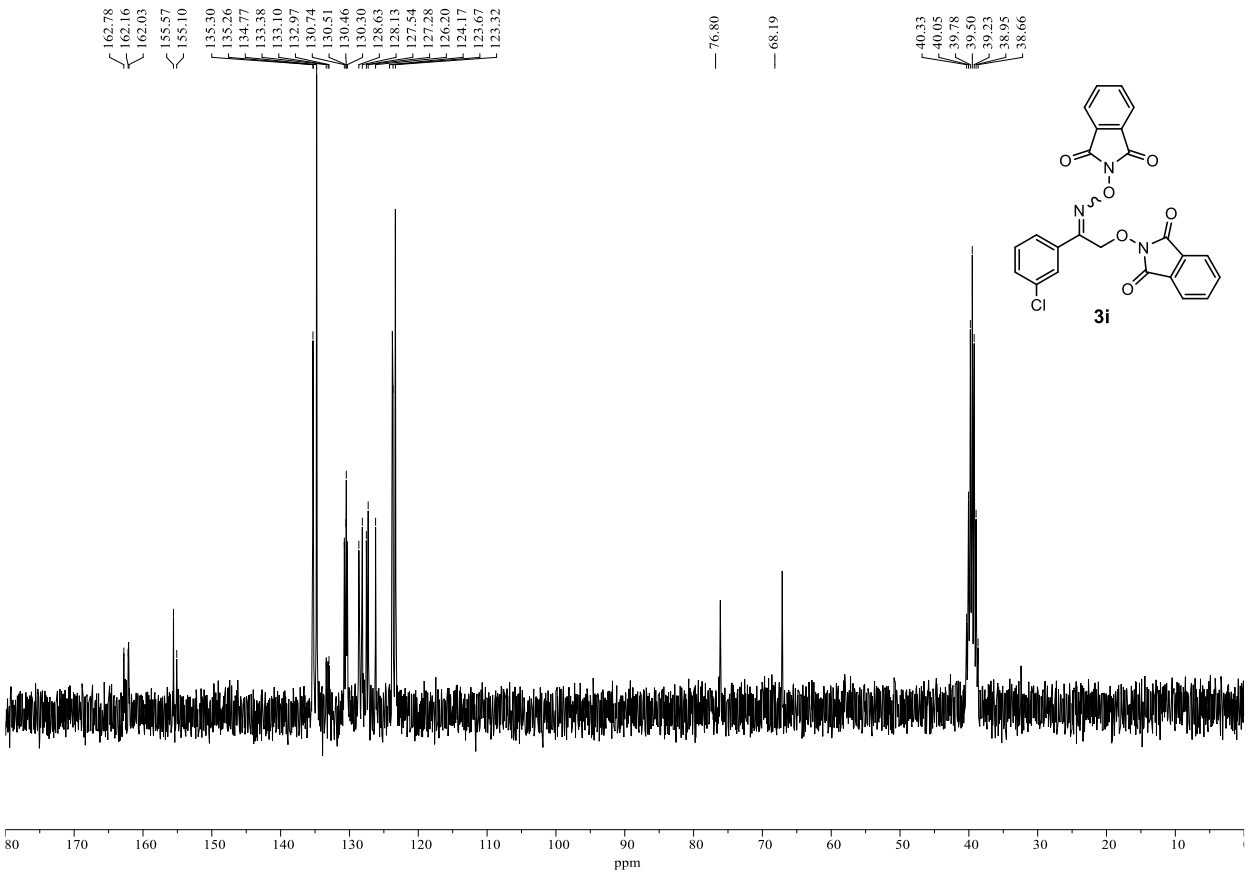
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127.54
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126.20
124.17
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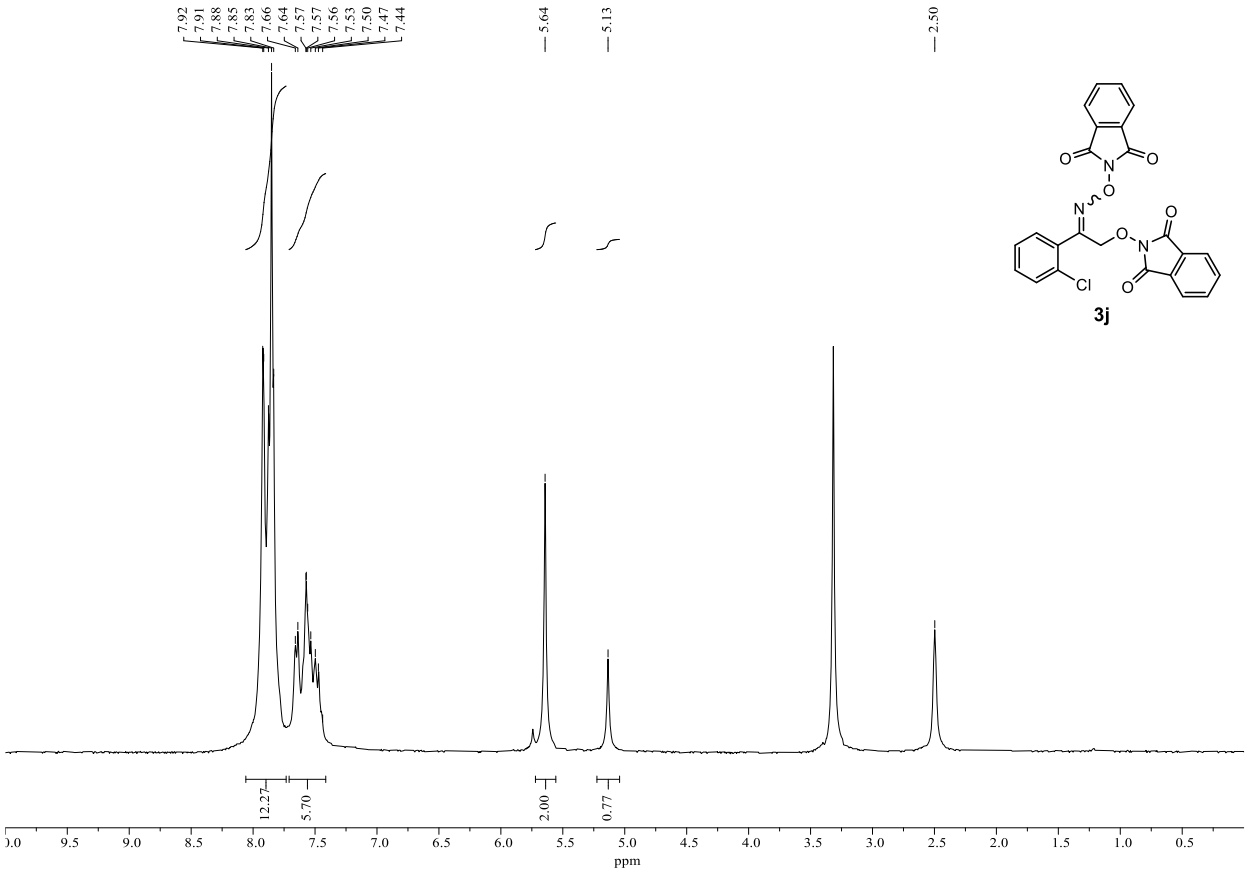
3i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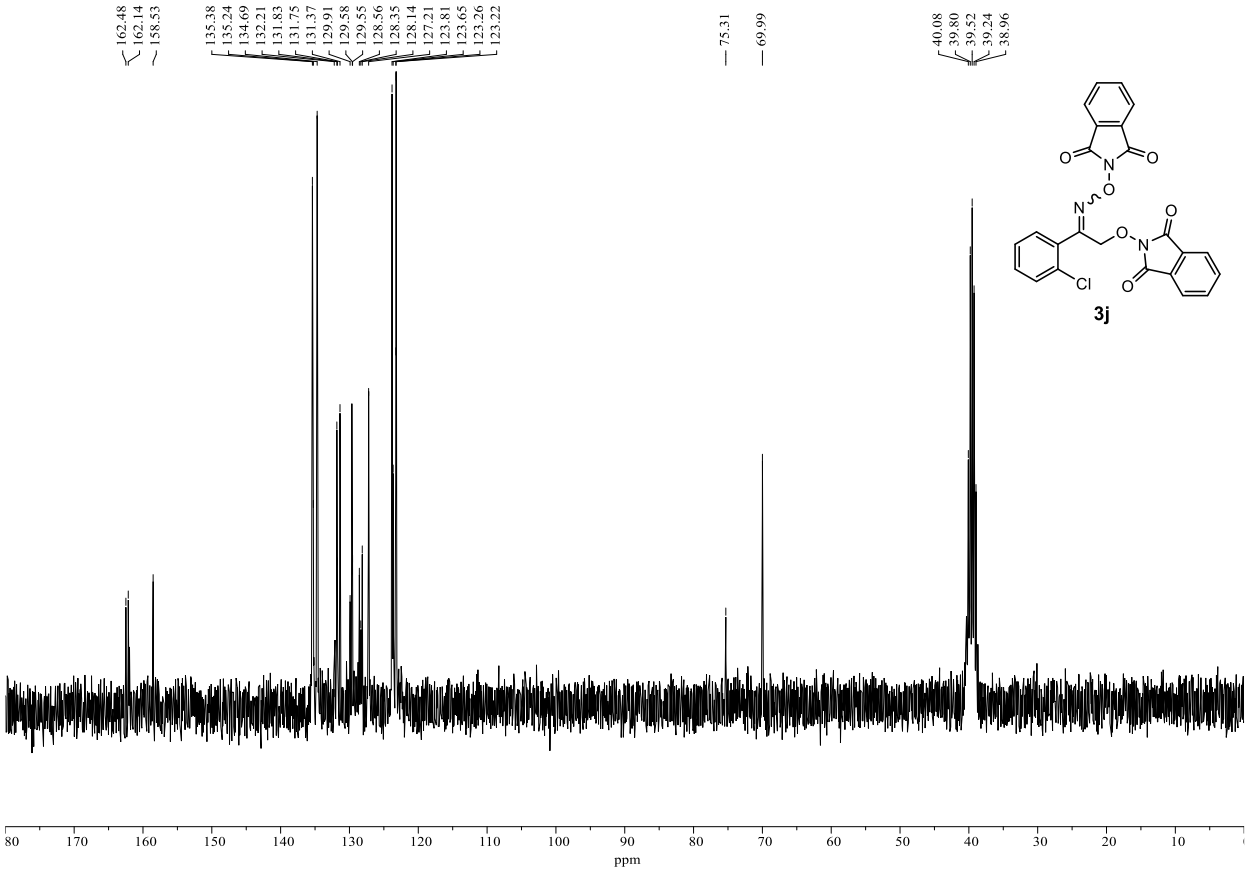
3j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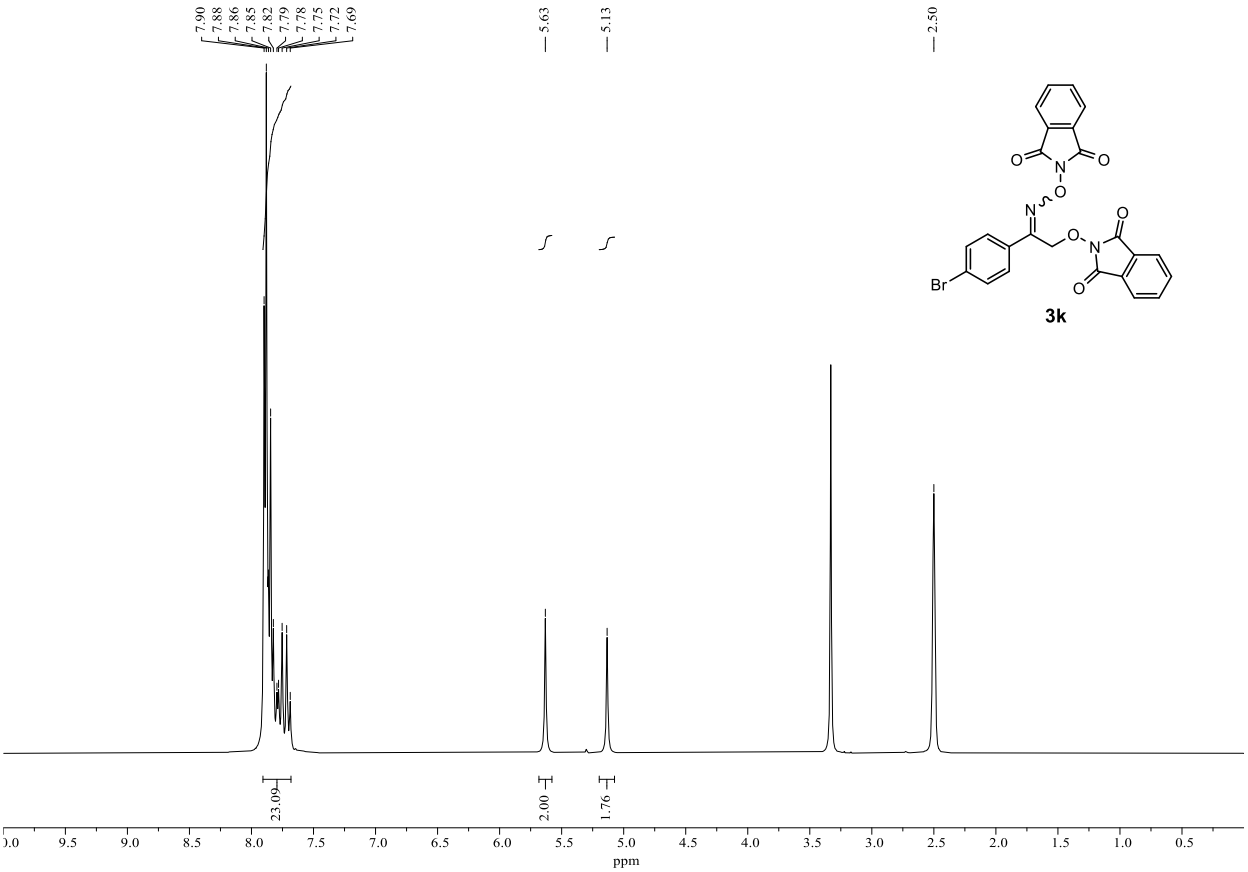
39.24
38.96
ppm

3j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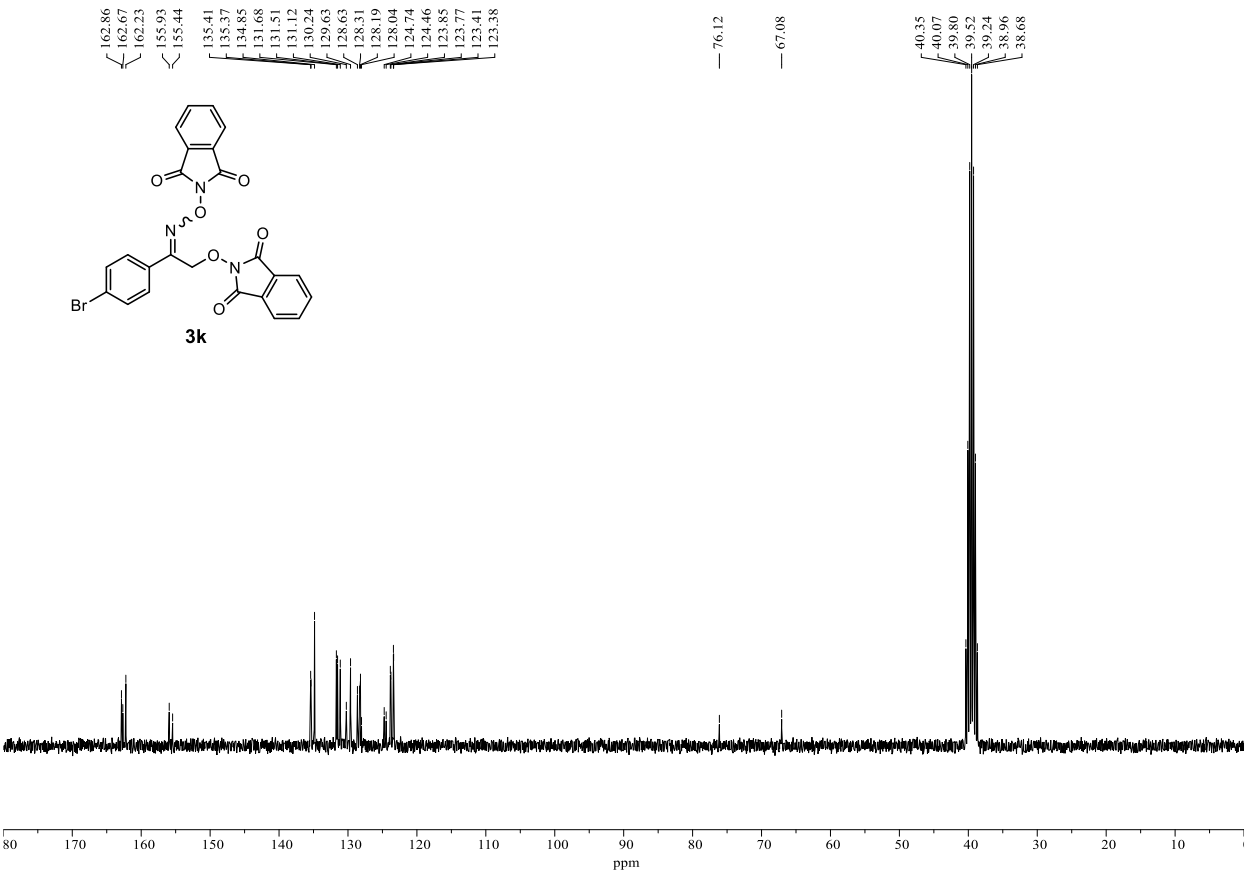
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123.77
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40.07
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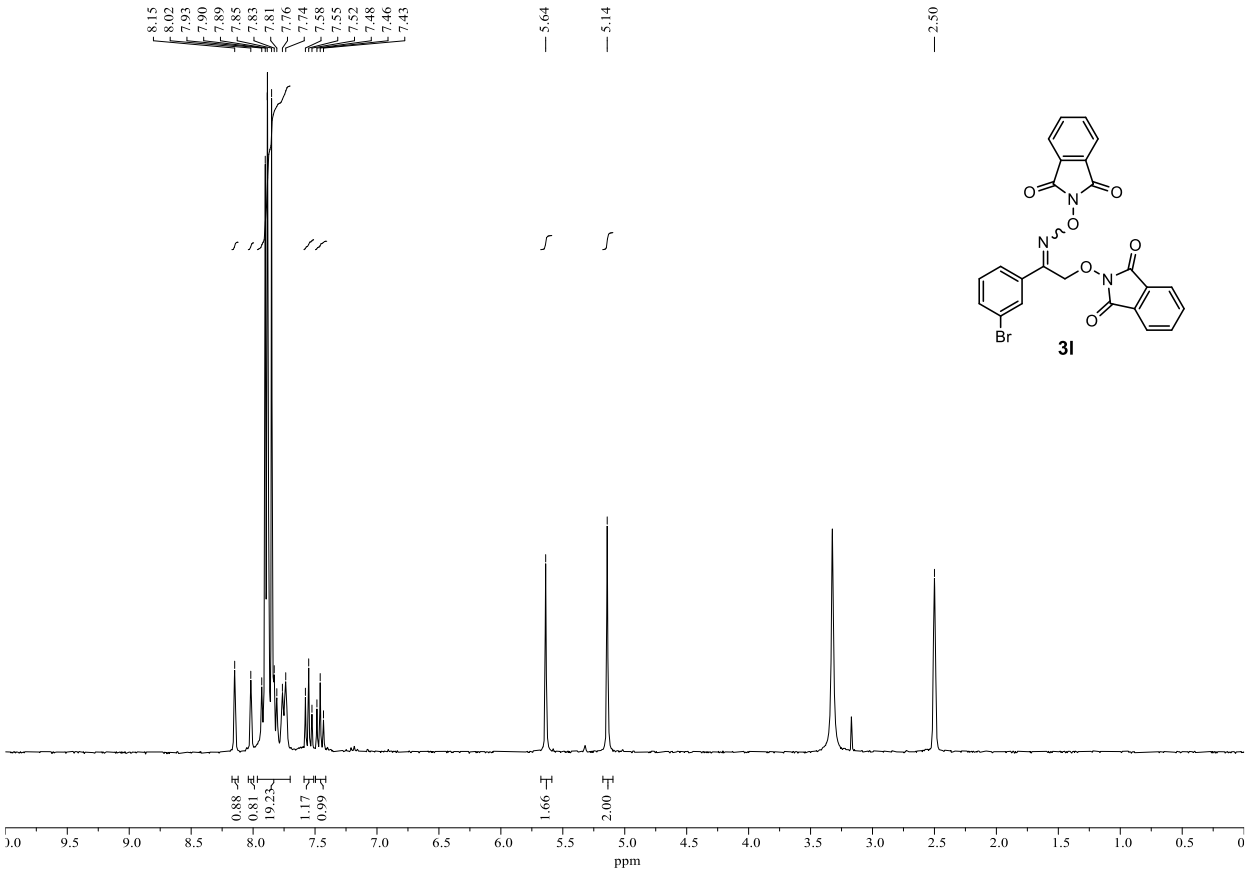
ppm
3k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7.46
7.43
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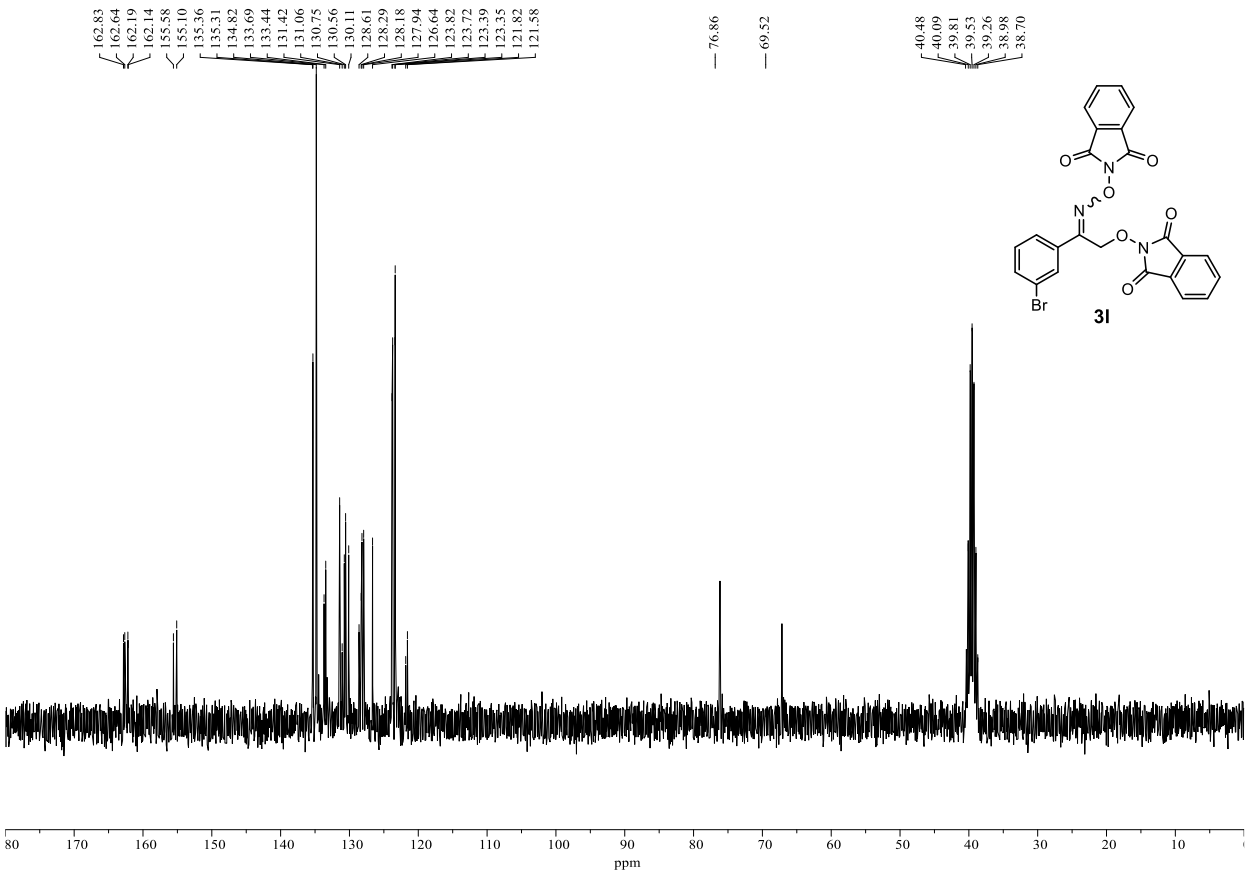
Br
3l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126.64
123.82
123.72
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121.82
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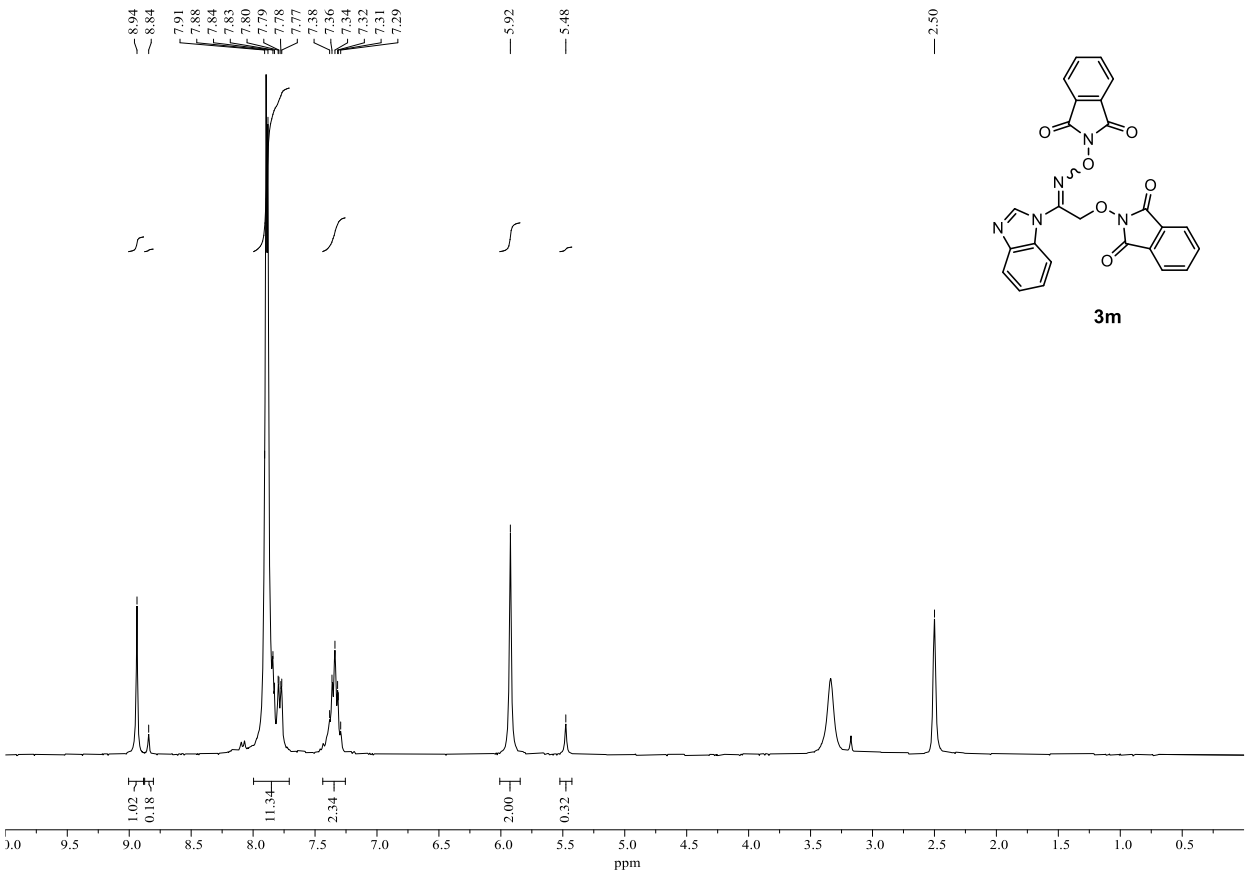
Br
3l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7.34
7.32
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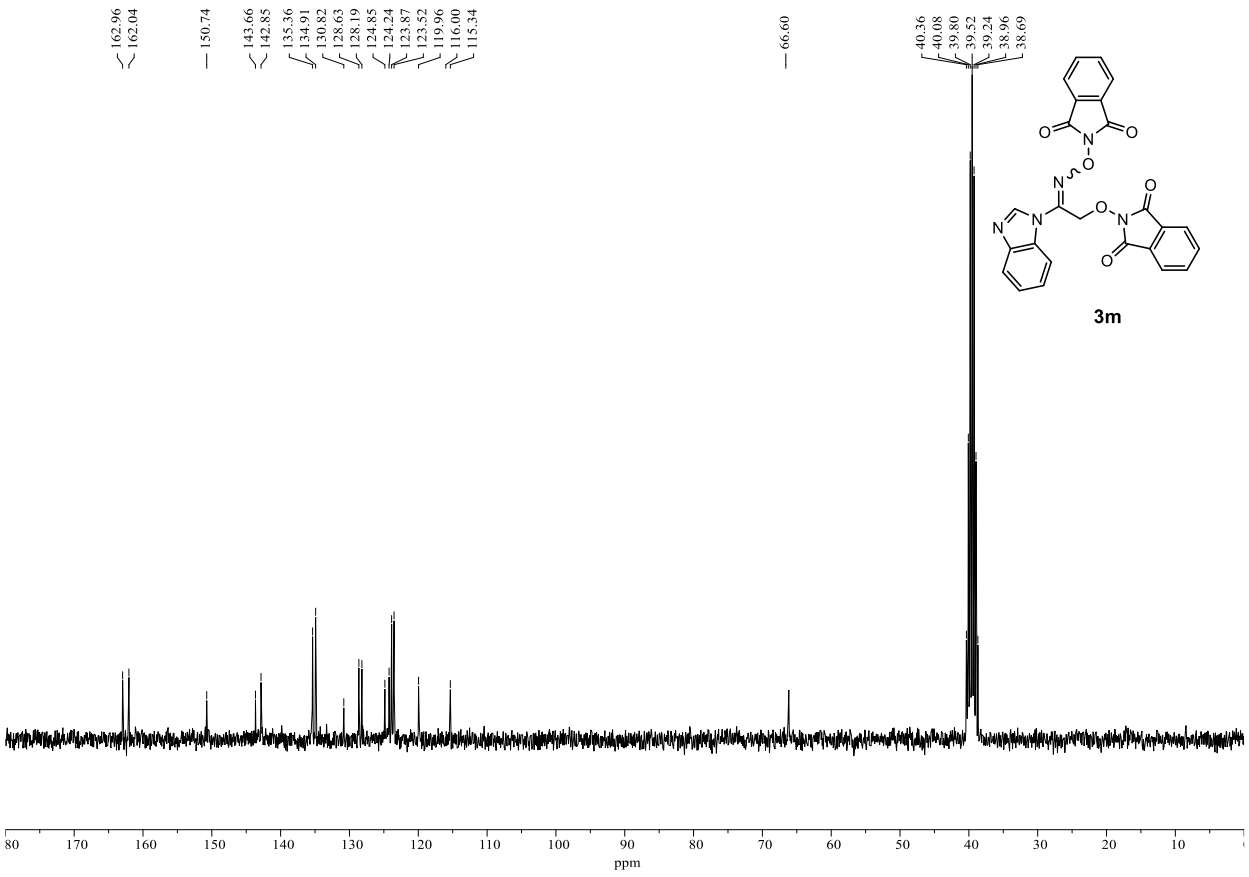
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123.52
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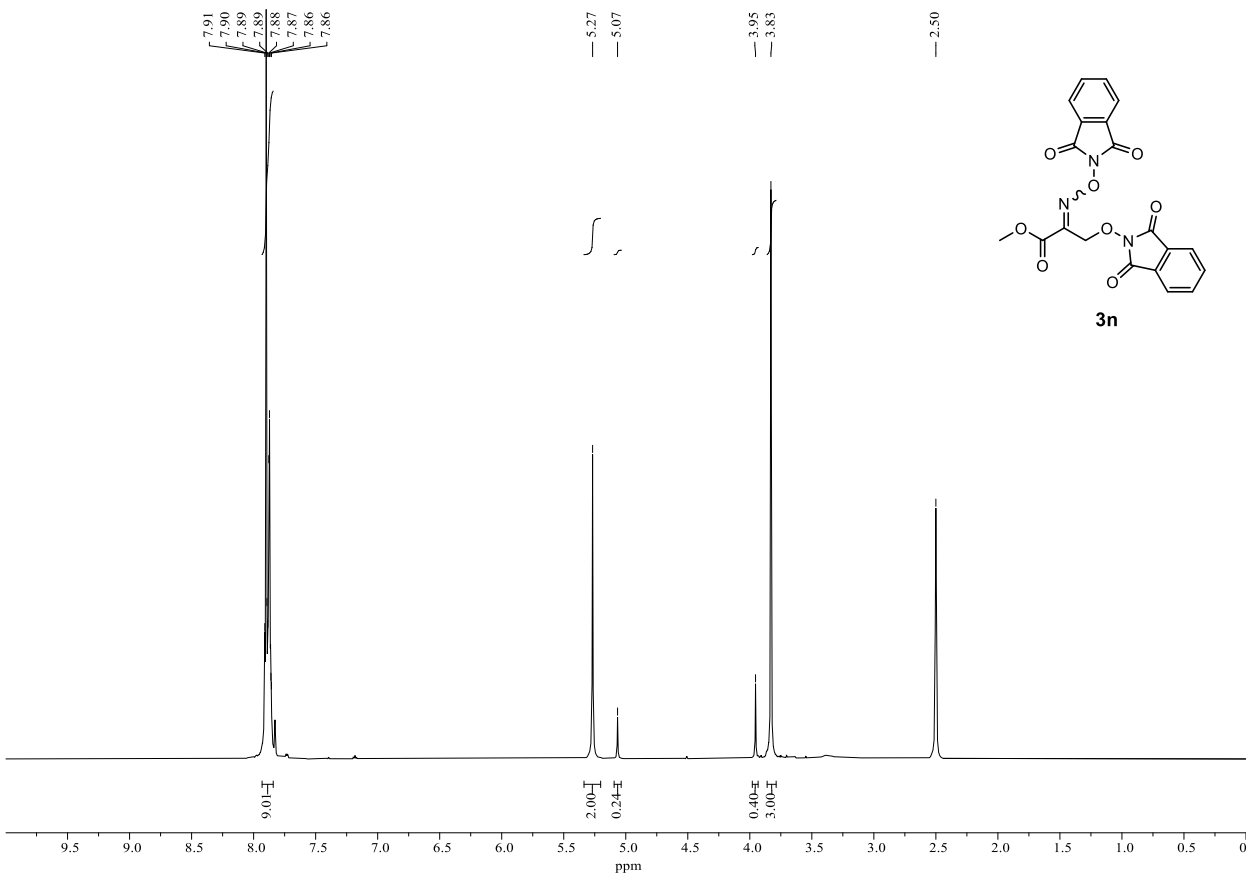
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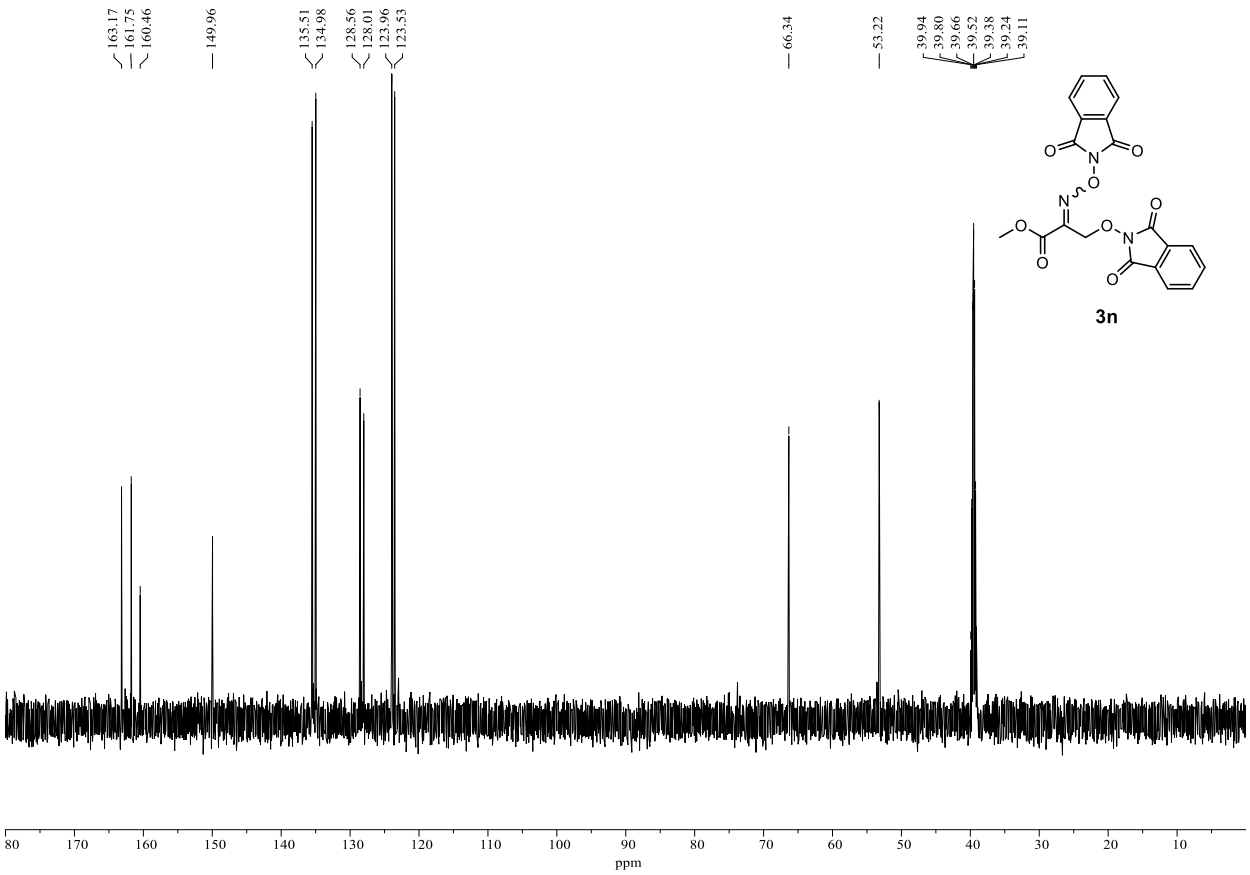
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39.66
39.52
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