Supporting Information for

Graphene Oxide: A Green Oxidant-Acid Bifunctional Carbon

Material for Synthesis of Functionalized Isoindolin-1-ones via Formal

Amide Insertion and Substitution

Xiangjun Peng,^b Dan Hu,^a Panpan Huang,^a Huiwu Liao,^a Yong Zeng,^b Qian, Liu*^b Liangxian

Liu*a

^a Department of Chemistry and Chemical Engineering, Gannan Normal University, Ganzhou,

Jiangxi 341000, P. R. China

^b School of Pharmaceutical Science, Gannan Medical University, Ganzhou, Jiangxi 341000, P. R.

China

E-mail: liuliangxian1962@163.com

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1. General Methods

¹H and ¹³C NMR spectra were recorded on a Bruker spectrometers at 400 and 100 MHz, respectively. Mass spectra were recorded with Bruker Dalton Esquire 3000 plus LC-MS apparatus. Elemental analysis were carried out on a Perkin-Elmer 240B instrument. HRFABMS spectra were recorded on a FTMS apparatus. Silica gel (300-400 mesh) was used for flash column chromatography, eluting (unless otherwise stated) with an ethyl acetate/petroleum ether (PE) (60-90 °C) mixture.

Raman spectra were collected with a Horiba Jobin Y von-Labram HR UV-Visible-NIR Raman Microscope Spectrometer, using a 632 nm laser. The spectra were the average of 10 scans at a resolution of 2 cm⁻¹ between 1000-2000 cm⁻¹ Raman Shift.

2. Characterization of GO

GO was prepared by graphite oxidation using the Hummers and Offeman method and subsequent exfoliation. Further details and GO characterization have been previously reported.



Figure S1. (A) SEM image of graphite. (B) SEM image of GO.



Figure S2. TEM image of graphite.



Figure S3. TEM image of GO.



Figure S4. AFM image of GO.



Figure S5. Raman image of GO.



Figure S6. XRD image of GO.

3. Experimental procedure for the ¹⁸O labeling experiment under ¹⁸O₂

To a solution of benzoisofuran (36 mg, 0.3 mmol) in acetonitrile (25 mg, 0.6 mmol) was added GO (54 mg, 150 wt%) under ${}^{18}O_2$ and the mixture was stirred at 80 °C for 6 h. The reaction mixture was concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (eluent: EtOAc/PE = 1:2) to yield the corresponding product **3da** (45 mg, 85%).



To a solution of **3da** (35 mg, 0.2 mmol) in MeOH was added LiOH (1 mg, 0.04 mmol) and the mixture was stirred at room temperature for 8 h. Reaction mixture was diluted with EtOAc (20 mL) and washed with saturated aqueous NH₄Cl solution (10 mL). Aqueous layer was extracted with EtOAc (10 mL). Combined organic layers were dried over anhydrous Na₂SO₄. Solvents were removed under reduced pressure and the residue was purified by flash chromatography on silica gel (eluent: EtOAc/PE = 2:1) to yield the corresponding product ¹⁸O-**12a** (21.6 mg, 80%).





5. Experimental procedure for the ¹⁸O labeling experiment in the present of H₂¹⁸O

To a solution of benzoisofuran (36 mg, 0.3 mmol) in acetonitrile (25 mg, 0.6 mmol) and H_2O (16 mg, 0.9 mmol) was added GO (54 mg, 150 wt%) under air and the mixture was stirred at 80 °C for

12 h. The reaction mixture was concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (eluent: EtOAc/PE = 1:2) to yield the corresponding product **3db** (38 mg, 71%).

To a solution of **3db** (35 mg, 0.2 mmol) in MeOH was added LiOH (1 mg, 0.04 mmol) and the mixture was stirred at room temperature for 8 h. Reaction mixture was diluted with EtOAc (20 mL) and washed with saturated aqueous NH₄Cl solution (10 mL). Aqueous layer was extracted with EtOAc (10 mL). Combined organic layers were dried over anhydrous Na₂SO₄. Solvents were removed under reduced pressure and the residue was purified by flash chromatography on silica gel (eluent: EtOAc/PE = 2:1) to yield the corresponding product ¹⁶O-**12b** (22.1 mg, 82%). **6. Copy of GC-MS Spectra for ¹⁶O-12b** (molecular weight: 133).



7. General Procedure and Spectroscopic Data of the Products 3

To a solution of benzoisofuran (36 mg, 0.3 mmol) and nitrile (0.6 mmol) was added GO (54 mg, 150 wt%) under an air atmosphere and the mixture was stirred at 80 °C for 12 h. The reaction mixture was concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (eluent: EtOAc/PE = 1:2) to yield the corresponding product **3**.

2-(2-Phenylacetyl)isoindolin-1-one (3a). White amorphous solid, 62 mg, 82% yield. ¹H NMR (400 MHz, Chloroform-d): δ 7.95 (dd, J = 7.2, 1.5 Hz, 1H, Ar-H), 7.69 (dt, J = 7.4, 1.5 Hz, 1H, Ar-H), 7.54 (d, J = 7.2 Hz, 1H, Ar-H), 7.53 (d, J = 7.4 Hz, 1H, Ar-H), 7.41(dt, J = 1.5, 8.1 Hz, 2H, Ar-H), 7.36 (dt, J = 1.5, 8.1 Hz, 2H, Ar-H), 7.29 (dt, J = 1.5, 9.5 Hz, 1H, Ar-H), 4.86 (s, 2H, NCH₂), 4.47 (s, 2H, CH₂). ¹³C NMR (101 MHz, Chloroform-d): δ 172.0, 167.6, 141.2, 134.2, 134.1, 131.3, 129.8, 128.7, 128.5, 127.0, 125.3, 123.4, 48.5, 42.9. MS (ESI): 252 (M+H⁺, 100). These assignments matched with those previously published.¹

2-(2-(*p*-tolyl)acetyl)isoindolin-1-one (**3b**). White amorphous solid, 67 mg, 84% yield. ¹H NMR (400 MHz, Chloroform-*d*): δ 7.94 (d, J = 7.4 Hz, 1H, Ar-H), 7.69 (dt, J = 7.5, 1.0 Hz, 1H, Ar-H), 7.53 (t, J = 7.4 Hz, 1H, Ar-H), 7.52 (d, J = 7.5 Hz, 1H, Ar-H), 7.29 (d, J = 7.9 Hz, 2H, Ar-H), 7.16 (d, J = 7.9 Hz, 2H, Ar-H), 4.85 (s, 2H, NCH₂), 4.45 (s, 2H, CH₂), 2.35 (s, 3H, CH₃). ¹³C NMR

(101 MHz, Chloroform-*d*): δ 172.2, 167.5, 141.2, 136.6, 134.1, 131.3, 131.0, 129.6, 129.2, 128.6, 125.3, 123.4, 48.5, 42.4, 21.1. HRESIMS calcd for $[C_{17}H_{15}NO_2 + H]^+$ 266.1181, found 266.1175. *2-(2-(4-Methoxyphenyl)acetyl)isoindolin-1-one (3c)*. White amorphous solid, 74 mg, 88% yield. ¹H NMR (400 MHz, Chloroform-*d*): δ 7.94 (d, *J* = 7.5 Hz, 1H, Ar-H), 7.68 (dt, *J* = 7.5, 1.1 Hz, 1H), 7.53 (t, *J* = 7.6 Hz, 1H, Ar-H), 7.52 (d, *J* = 7.6 Hz, 1H, Ar-H), 7.33 (dt, *J* = 2.4, 8.7 Hz, 2H, Ar-H), 6.90 (dt, *J* = 2.4, 8.7 Hz, 2H, Ar-H), 4.85 (s, 2H, NCH₂), 4.43 (s, 2H, CH₂), 3.81 (s, 3H, CH₃). ¹³C NMR (101 MHz, Chloroform-*d*): δ 172.4, 167.6, 158.7, 141.2, 134.1, 131.3, 130.8, 128.7, 126.1, 125.3, 123.4, 114.0, 55.3, 48.5, 42.0. HRESIMS calcd for $[C_{17}H_{16}NO_3 + H]^+$ 282.1130, found 282.1115.

2-Acetylisoindolin-1-one (3d). White amorphous solid, 47 mg, 89% yield. ¹H NMR (400 MHz, Chloroform-d): δ 7.94 (d, J = 8.0 Hz, 1H, Ar-H), 7.69 (dt, J = 7.6, 1.1 Hz, 1H, Ar-H), 7.54 (t, J = 7.4 Hz, 1H, Ar-H), 7.53 (d, J = 7.4 Hz, 1H, Ar-H), 4.84 (s, 2H, NCH₂), 2.71 (s, 3H, CH₃). ¹³C NMR (101 MHz, Chloroform-d): δ 171.2, 167.7, 141.1, 134.1, 131.3, 128.6, 125.2, 123.4, 48.1, 24.8. MS (ESI): 176 (M+H⁺, 100). These assignments matched with those previously published.²

2-Butyrylisoindolin-1-one (3e). White amorphous solid, 53 mg, 87% yield. ¹H NMR (400 MHz, Chloroform-*d*): δ 7.93 (d, J = 7.9 Hz, 1H, Ar-H), 7.68 (t, J = 7.5 Hz, 1H, Ar-H), 7.54 (d, J = 7.9 Hz, 1H, Ar-H), 7.53 (t, J = 7.5 Hz, 1H, Ar-H), 4.84 (s, 2H, NCH₂), 3.10 (t, J = 7.4 Hz, 2H), 1.80 (dt, J = 7.4, 14.8 Hz, 2H), 1.06 (t, J = 7.4 Hz, 3H, CH₃). ¹³C NMR (101 MHz, Chloroform-*d*): δ 174.3, 167.6, 141.2, 134.0, 131.5, 128.6, 125.2, 123.4, 48.2, 38.8, 17.8, 13.8. MS (ESI): 204 (M+H⁺, 100). Anal calcd for C₁₂H₁₃NO₂: C, 70.92; H, 6.45; N, 6.89. Found C, 70.65; H, 6.57; N, 6.63.

2-(2-Methoxyacetyl)isoindolin-1-one (**3f**). White amorphous solid, 56 mg, 92% yield. ¹H NMR (400 MHz, Chloroform-*d*): δ 7.92 (d, J = 7.9 Hz, 1H, Ar-H), 7.71 (t, J = 7.5 Hz, 1H, Ar-H), 7.55 (d, J = 7.9, Hz, 1H, Ar-H), 7.54 (d, J = 7.5, Hz, 1H, Ar-H), 4.87 (s, 2H, NCH₂), 4.81 (s, 2H, CH₂), 3.57 (s, 3H, CH₃). ¹³C NMR (101 MHz, Chloroform-*d*): δ 171.2, 167.9, 141.7, 134.3, 130.7, 128.8, 125.2, 123.6, 73.4, 59.5, 47.6. HRESIMS calcd for [C₁₁H₁₁NO₃ + Na]⁺ 228.0637, found 228.0625. 2-*Isobutyrylisoindolin-1-one* (**3g**). White amorphous solid, 52 mg, 85% yield. ¹H NMR (400 MHz, Chloroform-*d*): δ 7.93 (d, J = 8.0 Hz, 1H, Ar-H), 7.69 (dt, J = 7.5, 1.0 Hz, 1H, Ar-H), 7.54 (d, J = 7.0 Hz, 1H, Ar-H), 7.52 (t, J = 7.0 Hz, 1H, Ar-H), 4.84 (s, 2H, NCH₂), 3.98 (sep, J = 6.8 Hz, 1H, CH), 1.28 (d, J = 6.8 Hz, 6H, 2CH₃). ¹³C NMR (101 MHz, Chloroform-*d*): δ 178.7, 167.2, 141.2, 133.9, 131.6, 128.5, 125.2, 123.3, 48.6, 33.9, 18.8. MS (ESI): 204 (M+H⁺, 100). These assignments matched with those previously published.^{1a}

2-Hexanoylisoindolin-1-one (**3h**). White amorphous solid, 58 mg, 84% yield. ¹H NMR (400 MHz, Chloroform-*d*): δ 7.92 (d, J = 7.9 Hz, 1H, Ar-H), 7.68 (t, J = 7.4, 1H, Ar-H), 7.54 (d, J = 7.9 Hz, 1H, Ar-H), 7.52 (t, J = 7.4 Hz, 1H, Ar-H), 4.84 (s, 2H, NCH₂), 3.11 (t, J = 7.5 Hz, 2H), 1.76 (dt, J = 14.8, 7.5 Hz, 2H), 1.50-1.40 (m, 4H), 0.94 (t, J = 7.0 Hz, 3H, CH₃). ¹³C NMR (101 MHz, Chloroform-*d*): δ 174.5, 167.6, 141.2, 134.0, 131.5, 128.6, 125.1, 123.4, 48.2, 36.9, 31.4, 24.1, 22.5, 13.9. MS (ESI): 232 (M+H⁺, 100). These assignments matched with those previously published.¹

2-Octanoylisoindolin-1-one (3i). White amorphous solid, 61 mg, 79% yield. ¹H NMR (400 MHz, Chloroform-*d*): δ 7.93 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.68 (dt, *J* = 7.5, 1.2 Hz, 1H, Ar-H), 7.56-7.50 (m, 2H, Ar-H), 4.84 (s, 2H, NCH₂), 3.12 (t, *J* = 7.3 Hz, 2H), 1.76 (dt, *J* = 7.3, 14.8 Hz, 2H), 1.46-1.23 (m, 8H), 0.91 (t, *J* = 7.0 Hz, 3H, CH₃). ¹³C NMR (101 MHz, Chloroform-*d*): δ 174.5, 167.6, 141.2, 133.9, 131.5, 128.6, 125.2, 123.4, 48.2, 36.9, 31.7, 29.2, 29.1, 24.4, 22.6, 14.0. MS (ESI):

260 (M+H⁺, 100). Anal calcd for $C_{16}H_{21}NO_2$: C, 74.10; H, 8.16; N, 5.40. Found C, 73.87; H, 8.53; N, 5.09.

2-(5-Chloropentanoyl)isoindolin-1-one (**3j**). White amorphous solid, 57 mg, 75% yield. ¹H NMR (400 MHz, Chloroform-*d*): δ 7.93 (d, J = 8.0 Hz, 1H, Ar-H), 7.69 (t, J = 7.5 Hz, 1H, Ar-H), 7.55 (d, J = 7.5 Hz, 1H, Ar-H), 7.53 (d, J = 8.0 Hz, 1H, Ar-H), 4.84 (s, 2H, CH₂), 3.62 (t, J = 5.9 Hz, 2H, CH₂), 3.16 (t, J = 6.6 Hz, 2H, CH₂), 1.93 (m, 4H). ¹³C NMR (101 MHz, Chloroform-*d*): δ 173.7, 167.7, 141.2, 134.1, 131.3, 128.7, 125.2, 123.5, 48.2, 44.7, 36.1, 32.0, 21.6. HRESIMS calcd for [C₁₃H₁₄CINO₂ + H]⁺ 252.0791, found 252.0785.

2-(*Cyclohexanecarbonyl*)*isoindolin-1-one* (**3***k*). White amorphous solid, 55 mg, 76% yield. ¹H NMR (400 MHz, Chloroform-*d*): δ 7.92 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.68 (dt, *J* = 1.0, 7.5 Hz, 1H, Ar-H), 7.56-7.50 (m, 2H, Ar-H), 4.83 (s, 2H, NCH₂), 3.72 (tt, *J* = 14.3, 3.2 Hz, 1H), 2.00 (d, *J* = 11.9 Hz, 2H), 1.85 (dt, *J* = 12.5, 3.2 Hz, 2H), 1.80-1.73 (m, 1H), 1.59-1.40 (m, 5H). ¹³C NMR (101 MHz, Chloroform-*d*): δ 177.6, 167.3, 141.2, 133.9, 131.7, 128.6, 125.1, 123.4, 48.5, 43.7, 29.0, 26.0, 25.7. HRESIMS calcd for [C₁₅H₁₇NO₂ + H]⁺ 244.1338, found 244.1335.

2-(*Cyclopropanecarbonyl*)*isoindolin-1-one* (**3***I*). White amorphous solid, 54 mg, 89% yield. ¹H NMR (400 MHz, Chloroform-*d*): δ 7.95 (dd, J = 8.2, 1.0 Hz, 1H, Ar-H), 7.68 (td, J = 1.0, 8.2 Hz, 1H, Ar-H), 7.53 (t, J = 7.2, Hz, 1H, Ar-H), 7.52 (d, J = 7.2, Hz, 1H, Ar-H), 4.83 (s, 2H, NCH₂), 3.47 (dq, J = 4.0, 8.0 Hz, 1H), 1.23 (dt, J = 4.0, 8.0 Hz, 2H, CH₂), 1.07 (dt, J = 4.0, 8.0 Hz, 2H, CH₂). ¹³C NMR (101 MHz, Chloroform-*d*): δ 175.4, 168.1, 141.0, 134.0, 131.7, 128.6, 125.2, 123.3, 48.7, 13.6, 10.7. MS (ESI): 202 (M+H⁺, 100). Anal calcd for C₁₂H₁₁NO₂: C, 71.63; H, 5.51; N, 6.96. Found C, 71.75; H, 5.82; N, 6.68.

N-(2-Acetyl-1-oxoisoindolin-5-yl)pivalamide and *N*-(2-acetyl-3-oxoisoindolin-5-yl)pivalamide (4). White amorphous solid, 55 mg, 67% total yield, an inseperable mixture of two isomer in a ~2:1.5 ratio. ¹H NMR for major isomer (400 MHz, Chloroform-*d*): δ 9.49 (s, 1H, NH), 8.21 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.96 (t, *J* = 8.0 Hz, 1H, Ar-H), 7.59 (t, *J* = 8.0 Hz, 1H, Ar-H), 4.72 (s, 2H, NCH₂), 2.54 (s, 3H, CH₃), 1.25 (s, 9H, 3CH₃). ¹H NMR for minor isomer (400 MHz, Chloroform-*d*): δ 9.62 (s, 1H, NH), 8.21 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.96 (t, *J* = 8.0 Hz, 1H, Ar-H), 7.59 (t, *J* = 8.0 Hz, 1H, Ar-H), 7.59 (t, *J* = 8.0 Hz, 1H, Ar-H), 7.59 (t, *J* = 8.0 Hz, 1H, Ar-H), 4.74 (s, 2H, NCH₂), 2.53 (s, 3H, CH₃), 1.25 (s, 9H, 3CH₃). ¹³C NMR for major isomer (101 MHz, Chloroform-*d*): δ 172.5, 170.6, 167.7, 145.0, 140.1, 131.7, 125.4, 124.8, 114.1, 48.1, 25.0, 15.1, 7.9. ¹³C NMR for minor isomer (101 MHz, Chloroform-*d*): δ 172.5, 170.6, 167.7, 145.0, 140.1, 131.7, 125.4, 124.8, 114.1, 48.1, 25.0, 15.1, 7.9. ¹³C NMR for minor isomer (101 MHz, Chloroform-*d*): δ 172.5, 170.6, 167.7, 145.0, 140.1, 131.7, 125.4, 124.8, 114.1, 48.1, 25.0, 15.1, 7.9. ¹³C NMR for minor isomer (101 MHz, Chloroform-*d*): δ 172.9, 170.4, 167.2, 143.6, 136.3, 125.8, 125.3, 119.6, 113.4, 48.4, 24.9, 15.2, 8.2. MS (ESI): 275 (M+H⁺, 100). Anal calcd for C₁₅H₁₈N₂O₃: C, 65.68; H, 6.61; N, 10.21. Found C, 66.04; H, 6.89; N, 9.92.

N-(2-Acetyl-1-oxoisoindolin-5-yl)benzamide and *N*-(2-Acetyl-3-oxoisoindolin-5-yl)benzamide (5). White amorphous solid, 56 mg, 63% total yield, an inseperable mixture of two isomer in a ~2:1.6 ratio. ¹H NMR for major isomer (400 MHz, Chloroform-*d*): δ 10.66 (s, 1H, NH), 8.39 (d, *J* = 2.3 Hz, 1H, Ar-H), 8.12 (dd, *J* = 8.3, 2.3 Hz, 1H, Ar-H), 8.02 (t, *J* = 7.0 Hz, 2H, Ar-H), 7.81 (d, *J* = 8.3 Hz, 1H, Ar-H), 7.64 (d, *J* = 8.3 Hz, 1H, Ar-H), 7.54 (d, *J* = 7.0 Hz, 2H, Ar-H), 4.74 (s, 2H, NCH₂), 2.55 (s, 3H, CH₃). ¹H NMR for minor isomer (400 MHz, Chloroform-*d*): δ 10.80 (s, 1H, NH), 8.24 (s, 1H, Ar-H), 7.94 (d, *J* = 7.7 Hz, 1H, Ar-H), 8.02 (t, *J* = 7.0 Hz, 2H, Ar-H), 7.94 (d, *J* = 7.7 Hz, 1H, Ar-H), 7.54 (d, *J* = 7.7 Hz, 2H, Ar-H), 7.94 (d, *J* = 7.7 Hz, 1H, Ar-H), 7.54 (d, *J* = 7.7 Hz, 2H, Ar-H), 7.94 (d, *J* = 7.7 Hz, 1H, Ar-H), 7.54 (d, *J* = 7.7 Hz, 2H, Ar-H), 7.94 (d, *J* = 7.7 Hz, 1H, Ar-H), 7.54 (d, *J* = 7.7 Hz, 2H, Ar-H), 7.94 (d, *J* = 7.7 Hz, 1H, Ar-H), 7.54 (d, *J* = 7.7 Hz, 2H, Ar-H), 7.94 (d, *J* = 7.7 Hz, 1H, Ar-H), 7.54 (d, *J* = 7.7 Hz, 2H, Ar-H), 4.78 (s, 2H, NCH₂), 2.54 (s, 3H, CH₃). ¹³C NMR for major isomer (101 MHz, Chloroform-*d*): δ 170.6, 167.7, 166.3, 143.3, 137.0, 134.9, 132.4, 132.3, 131.6, 128.9, 128.3, 124.7, 115.6, 48.2, 25.0. ¹³C NMR for minor isomer (101 MHz, Chloroform-*d*): δ 170.6, 167.7, 132.3, 128.9, 128.4, 125.6, 121.0, 114.7, 48.4, 24.9. MS (ESI): 295 (M+H⁺, 100). Anal calcd for

C₁₇H₁₄N₂O₃: C, 69.38; H, 4.79; N, 9.52. Found C, 69.17; H, 5.06; N, 9.18.

N-(2-Acetyl-1-oxoisoindolin-5-yl)cyclopropanecarboxamide and *N*-(2-Acetyl-3-oxoisoindolin-5-yl)cyclopropanecarboxamide (6). White amorphous solid, 54 mg, 70% total yield, an inseperable mixture of two isomer in a ~2:1.26 ratio. ¹H NMR for major isomer (400 MHz, Chloroform-*d*): δ 10.50 (s, 1H, NH), 8.18 (d, J = 1.5 Hz, 1H, Ar-H), 7.79 (dd, J = 8.2, 1.5 Hz, 1H, Ar-H), 7.58 (d, J = 8.2 Hz, 1H, Ar-H), 4.70 (s, 2H, NCH₂), 2.52 (s, 3H, CH₃), 1.80-1.76 (m, 1H), 0.82 (d, J = 7.2 Hz, 4H, CH₂CH₂). ¹H NMR for minor isomer (400 MHz, Chloroform-*d*): δ 10.66 (s, 1H, NH), 8.00 (s, 1H, Ar-H), 7.75 (d, J = 8.3 Hz, 1H, Ar-H), 7.63 (d, J = 8.3 Hz, 1H, Ar-H), 4.73 (s, 2H, NCH₂), 2.51 (s, 3H, CH₃), 1.86-1.81 (m, 1H), 0.84 (d, J = 7.2 Hz, 4H, CH₂CH₂). ¹³C NMR for major isomer (101 MHz, Chloroform-*d*): δ 172.5, 170.6, 167.7, 140.1, 136.3, 131.7, 125.4, 124.8, 114.1, 48.1, 25.0, 15.1, 7.9. ¹³C NMR for minor isomer (101 MHz, Chloroform-*d*): δ 172.9, 170.4, 167.2, 145.0, 143.6, 125.8, 125.3, 119.6, 113.4, 48.4, 24.9, 15.2, 8.2. HRESIMS calcd for [C₁₄H₁₄NO₃ + Na]⁺ 281.0902, found 281.0895.

8. Copies of ¹H and ¹³C Spectra

¹H and ¹³C NMR Spectra for **3a**





























¹H and ¹³C NMR Spectra for 6



9. References

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