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SUPPORTING INFORMATION

A plant root-derived Ni-ecocatalyst for Suzuki cross coupling of aryl iodides

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I. Infrared spectra

1. *IR spectra of the biomaterials – Before and after functionalization*

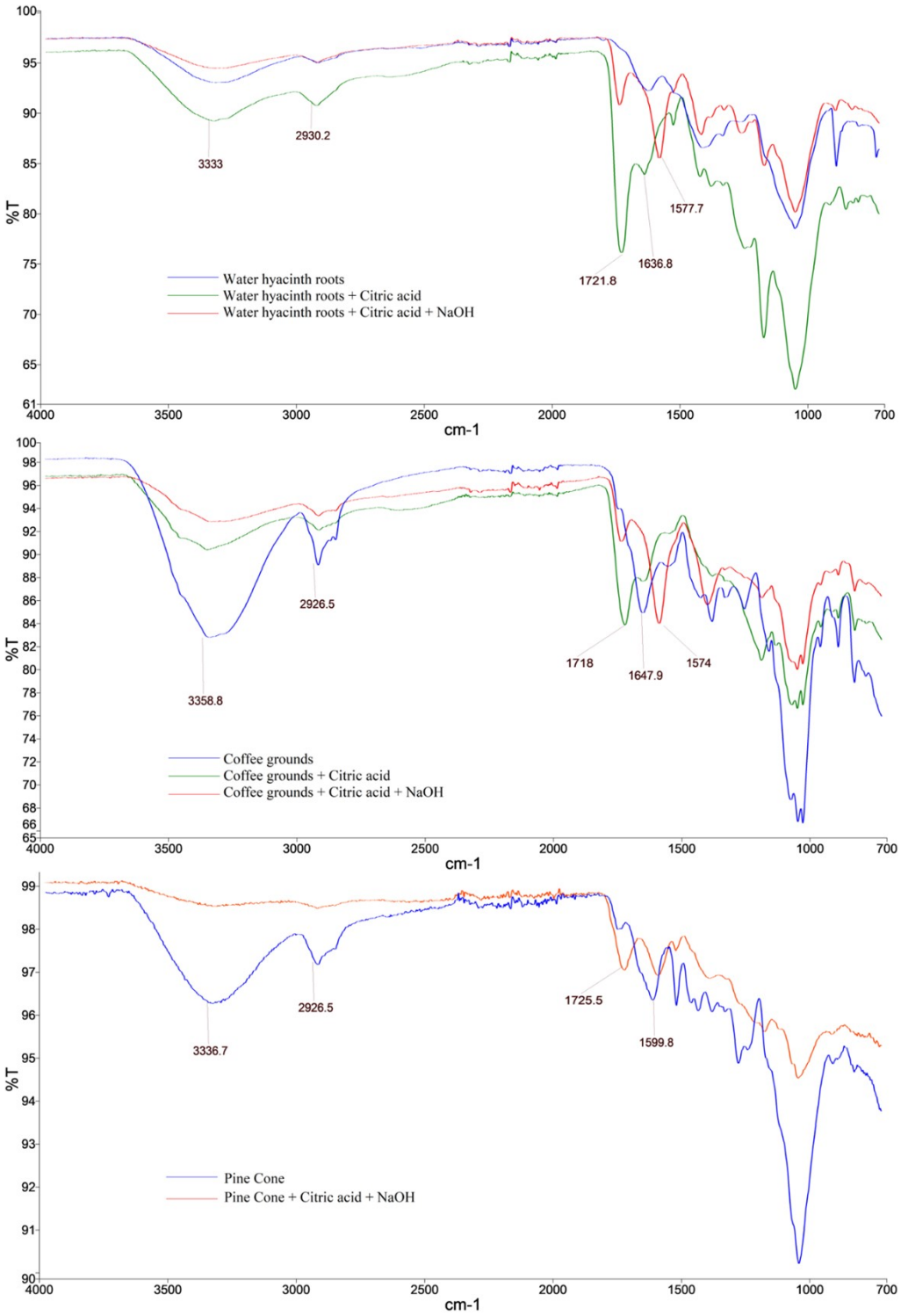


Figure 1. Infrared spectra of water hyacinth, coffee grounds and pinecone before (blue), after functionalization (green) and after titration with NaOH (red).

2. *Infrared spectrum of the Eco-Ni(HCOO)$_2$ ecocatalyst used for Suzuki coupling reaction*

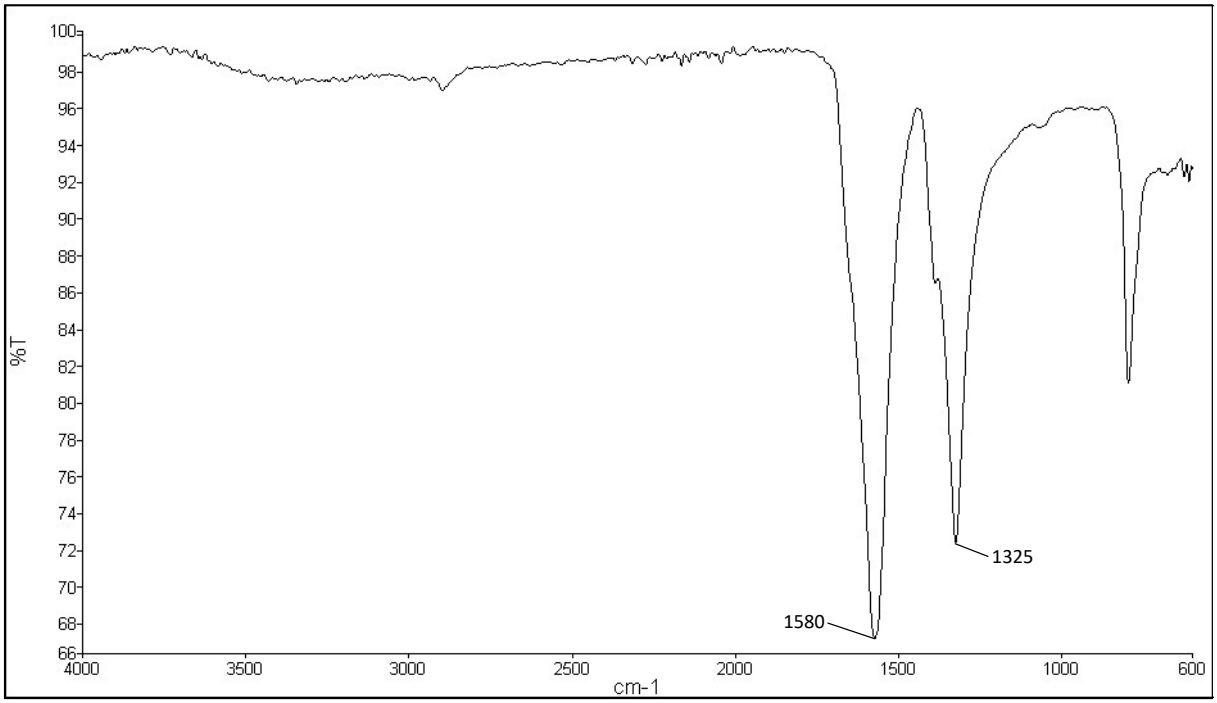
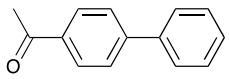


Figure 2. Infrared spectrum of Eco-Ni(HCOO)$_2$

II. Description of the products

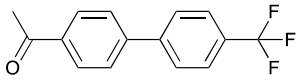
1. *NMR spectroscopic desciption*

1-(1,1'-biphenyl]-4-yl)ethan-1-one – [1]



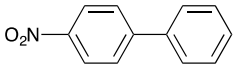
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 12 Hz, 2H), 7.69 (d, *J* = 8 Hz, 2H), 7.63 (d, *J* = 8Hz, 2H), 7.49-7.40 (m, 3H), 2.64 (s, 3H).

1-(4'-(trifluoromethyl)-[1,1'-biphenyl]-4-yl)ethan-1-one – [2]



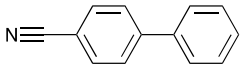
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.3 Hz, 1H), 7.72 (s, 2H), 7.68 (d, *J* = 8.3 Hz, 1H), 2.64 (s, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 197.63 (Ccarbonyle), 144.15 (Cq), 143.38 (Cq), 136.60 (Cq), 130.22 (q, *J* = 32.7 Hz, Cq), 129.05 (2C), 127.60 (2C), 127.45 (2C), 125.89 (q, *J* = 3.4 Hz, 2C), 124.14 (q, *J* = 272.2 Hz, CF_3), 26.65 (s).

4-nitrobiphenyl – [4]



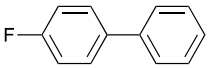
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 – 8.21 (m, 2H), 7.76 – 7.68 (m, 2H), 7.65 – 7.57 (m, 2H), 7.55 – 7.27 (m, 4H).

4-cyanobiphenyl – [5]



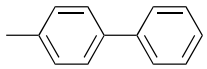
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 – 7.64 (m, 4H), 7.61 – 7.55 (m, 2H), 7.51 – 7.44 (m, 2H), 7.43 – 7.39 (m, 1H).

4-fluoro-1,1'-biphenyl – [6]



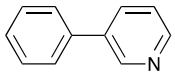
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 – 7.61 (m, 4H), 7.47 (t, *J* = 8 Hz, 2H), 7.37 (t, *J* = 8 Hz, 1H), 7.24 (d, *J* = 9 Hz, 2H).

4-methyl-1,1'-biphenyl – [7]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66-7.63 (m, 2H), 7.56 (d, *J* = 8 Hz, 2H), 7.45 (t, *J* = 8 Hz, 2H), 7.34 (t, *J* = 8 Hz, 1H), 7.24 (d, *J* = 8 Hz, 2H), 2.38 (s, 3H).

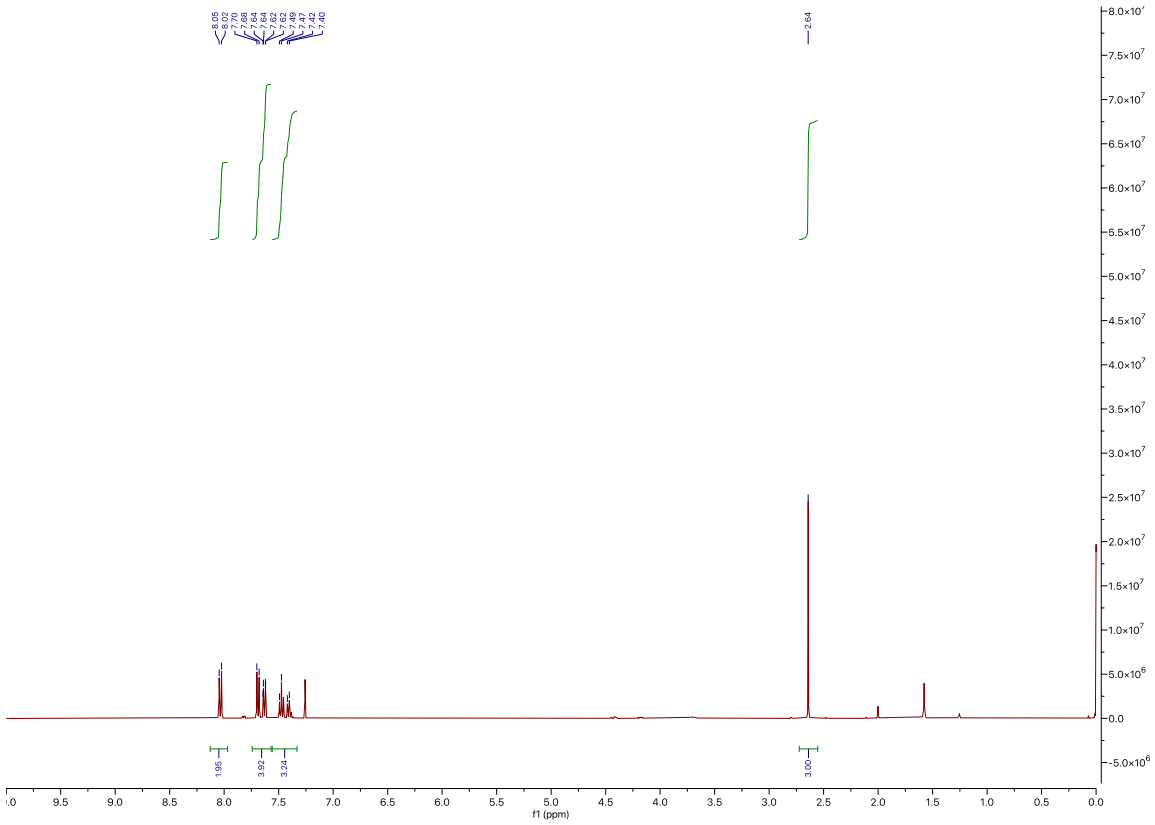
3-phenylpyridine – [8]



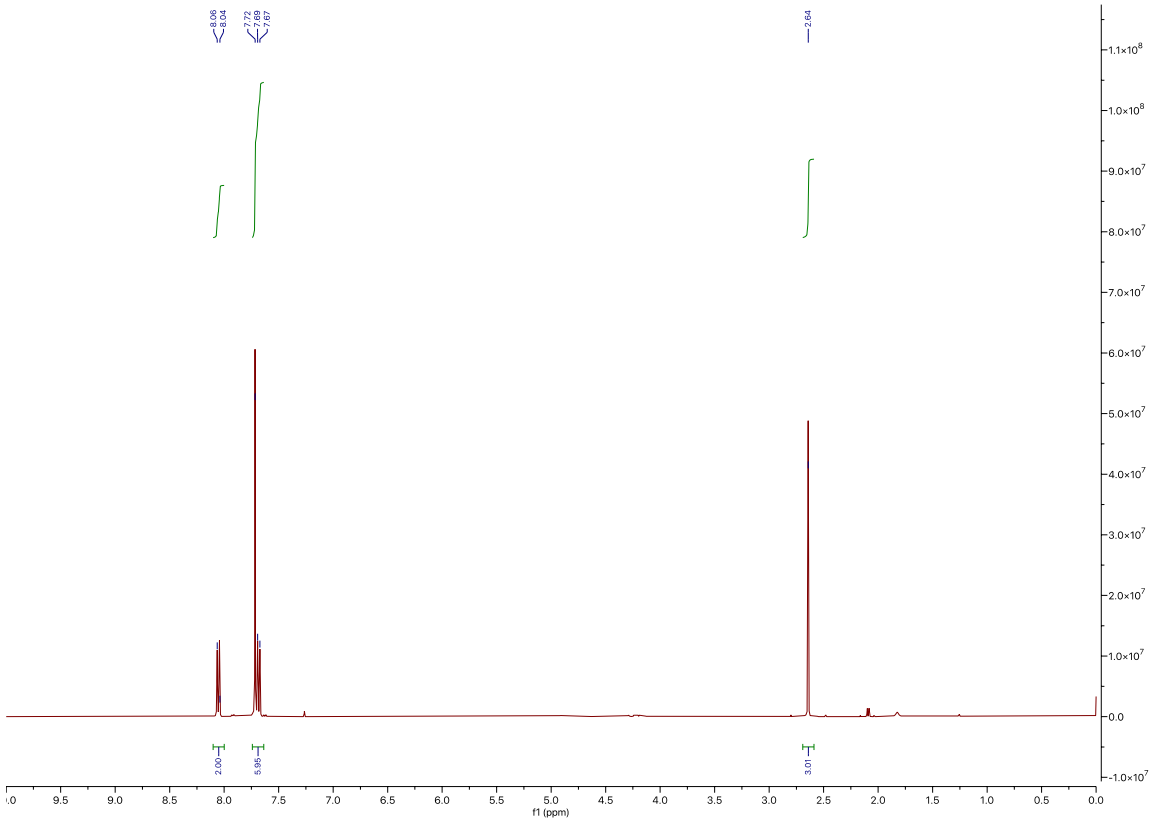
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.83 (d, J = 4 Hz, 2H), 8.57 (d, J = 4 Hz, 2H), 7.86 (d, J = 8 Hz, 1H), 7.89-7.83 (m, 1H), 7.57 (d, J = 8 Hz, 2H), 7.63 (d, J = 8Hz, 2H), 7.47 (t, J = 8Hz, 4Hz, 2H), 7.45-7.33 (m, 3H).

2. *NMR spectra*

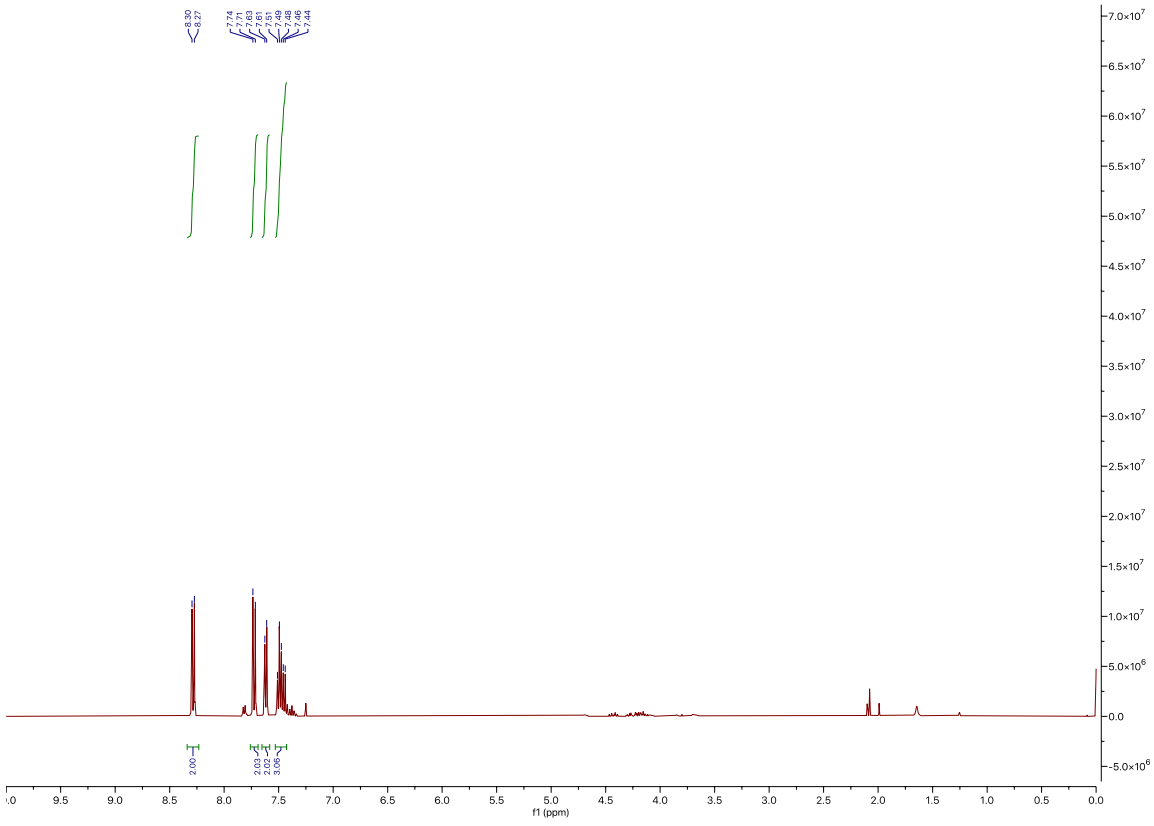
1-(1,1'-biphenyl]-4-yl)ethan-1-one – [1]



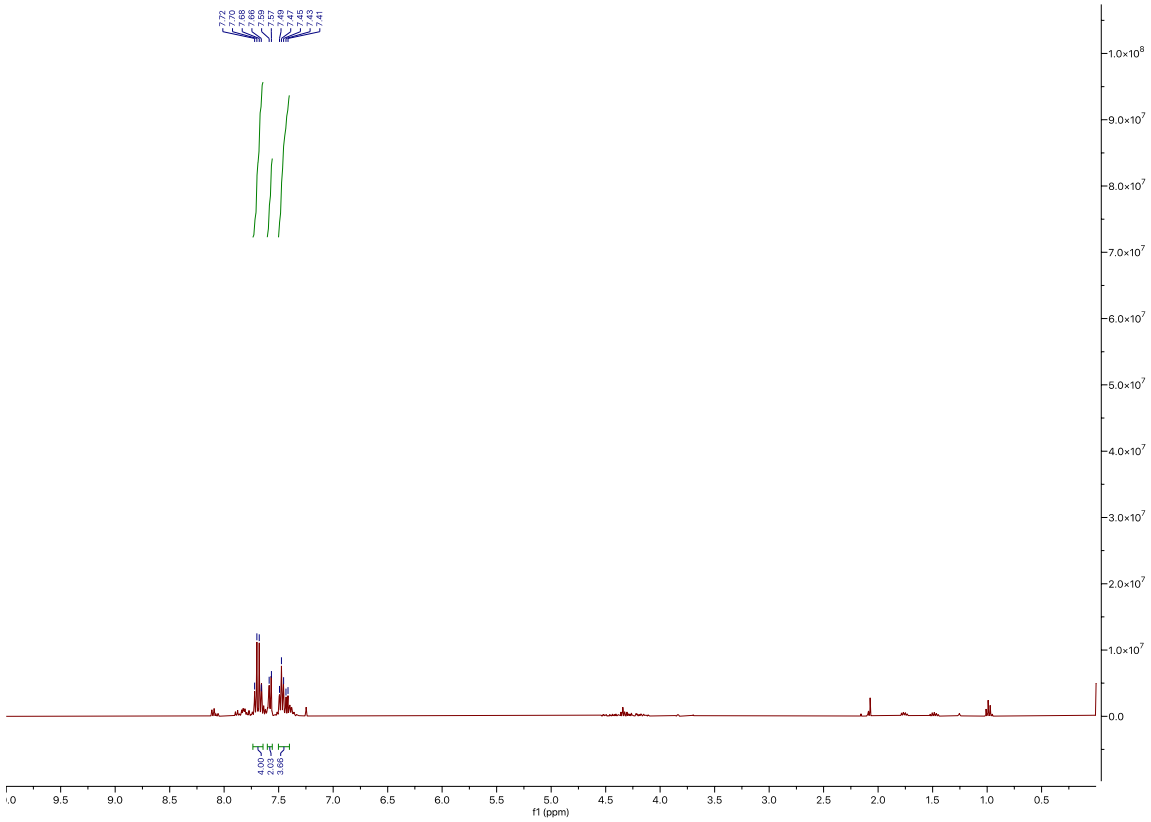
1-(4'-(trifluoromethyl)-[1,1'-biphenyl]-4-yl)ethan-1-one – [2]



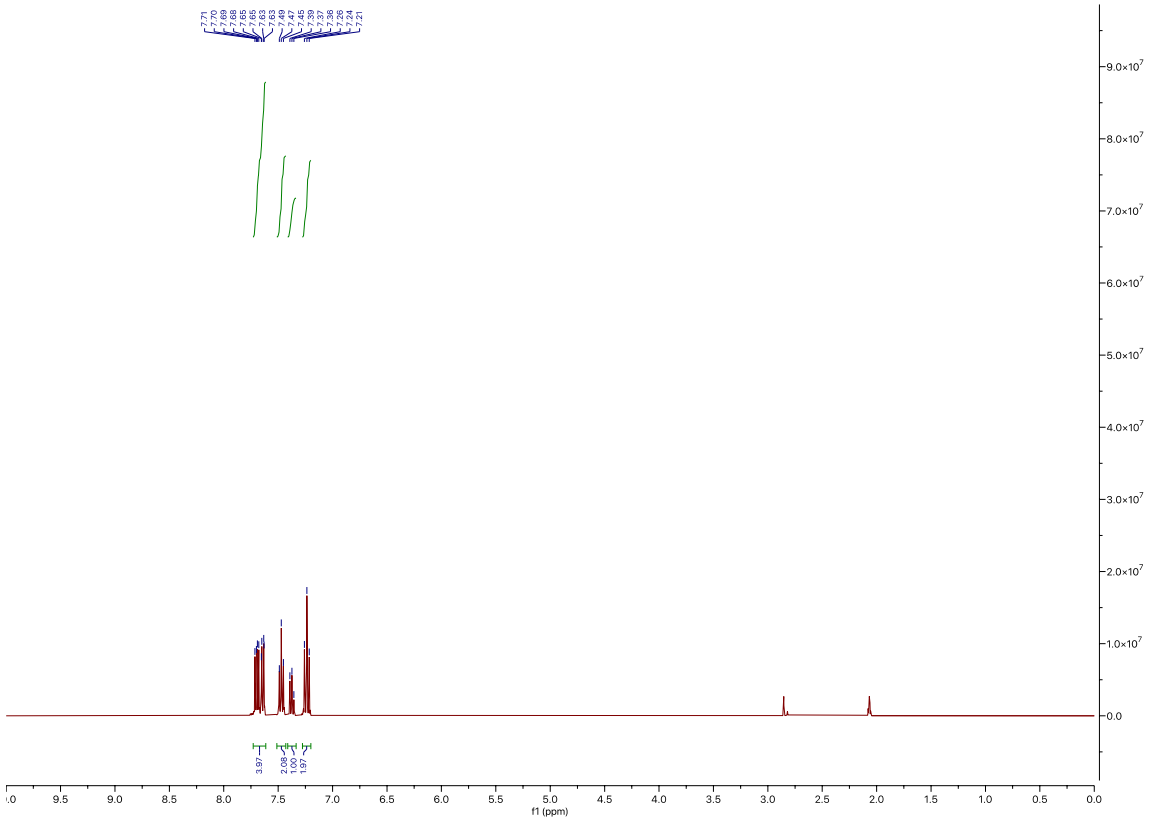
4-nitrobiphenyl – [4]



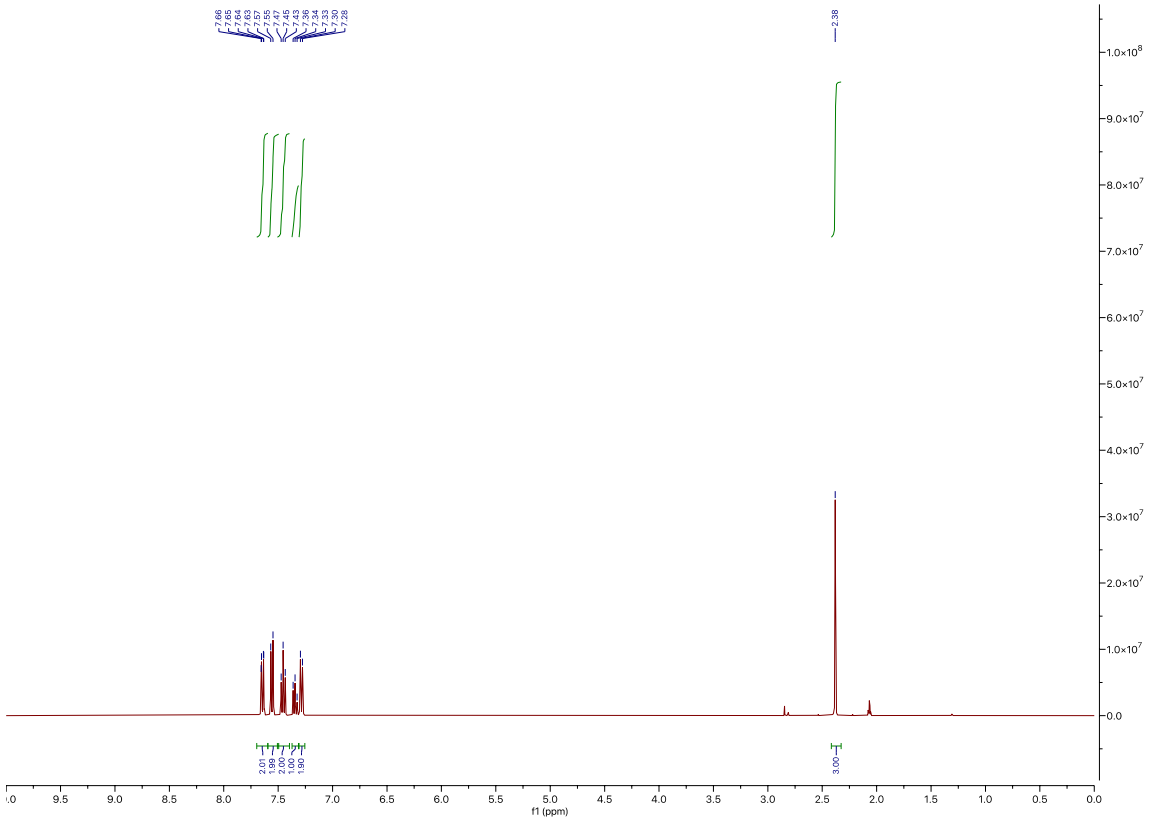
4-cyanobiphenyl – [5]



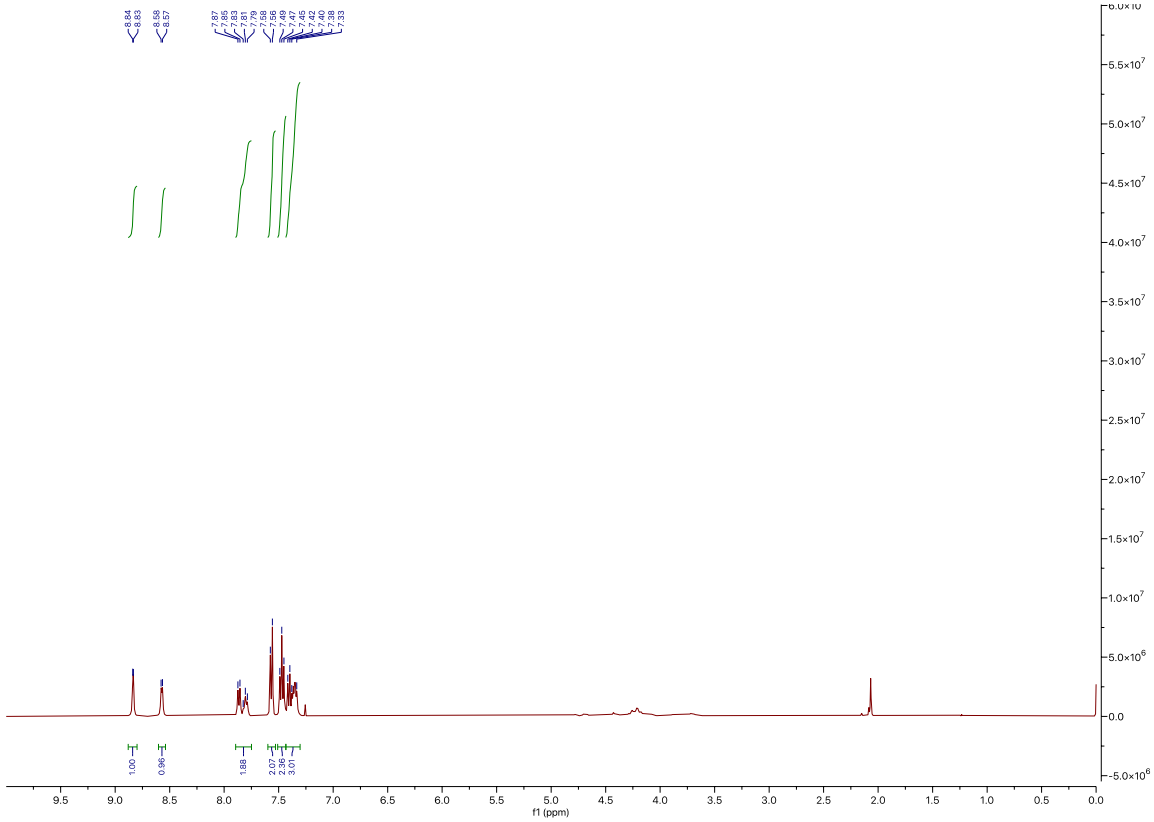
4-fluoro-1,1'-biphenyl – [6]



4-methyl-1,1'-biphenyl – [7]



3-phenylpyridine – [8]



3. GCMS and GCFID analyses of standards and synthesized products

1-(1,1'-biphenyl]-4-yl)ethan-1-one – [1] – expected mass: 196.09

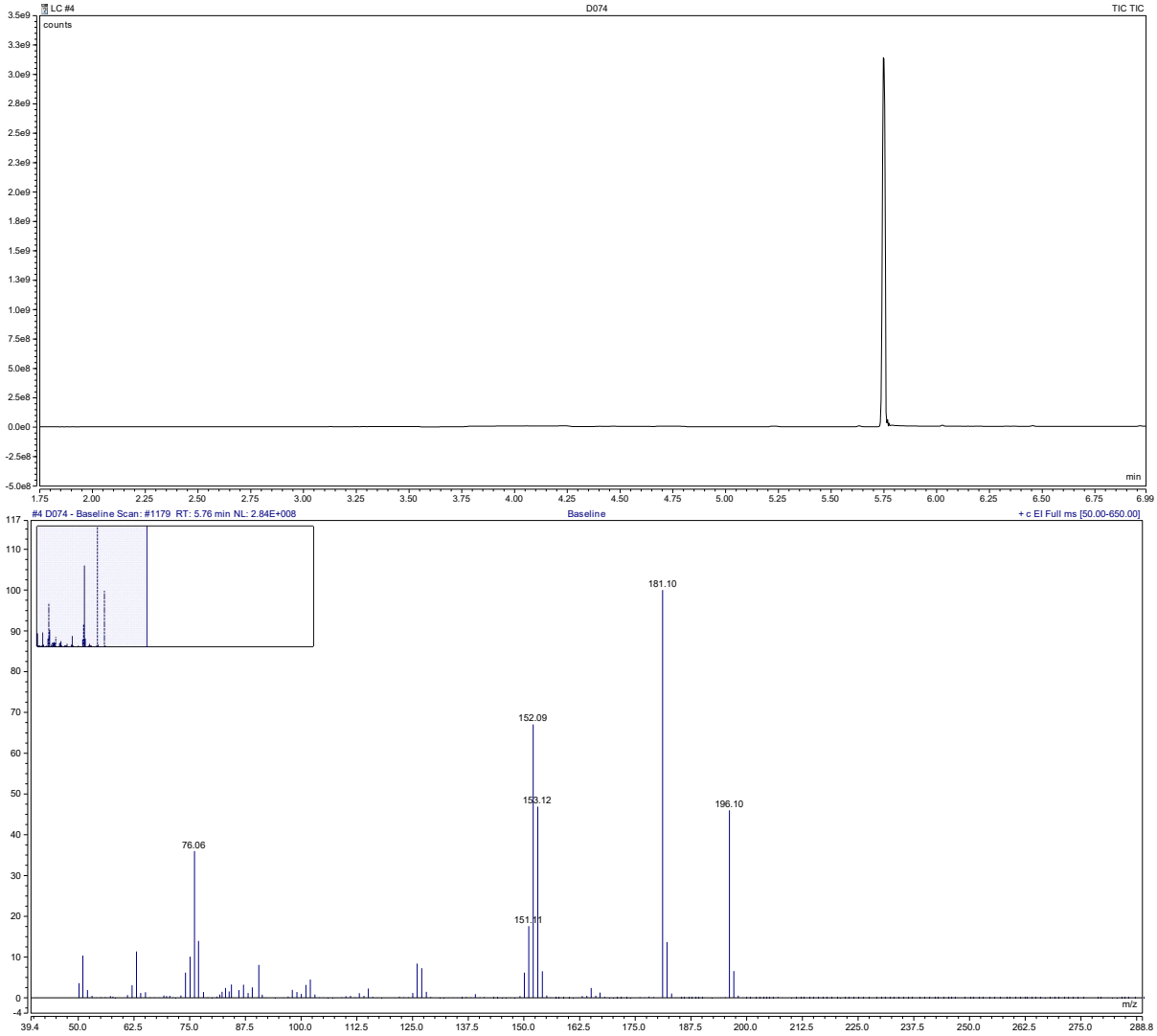


Figure 3. GCMS spectrum of synthesized product [1]

1-(4'-(trifluoromethyl)-[1,1'-biphenyl]-4-yl)ethan-1-one – [2] – expected mass: 264.04

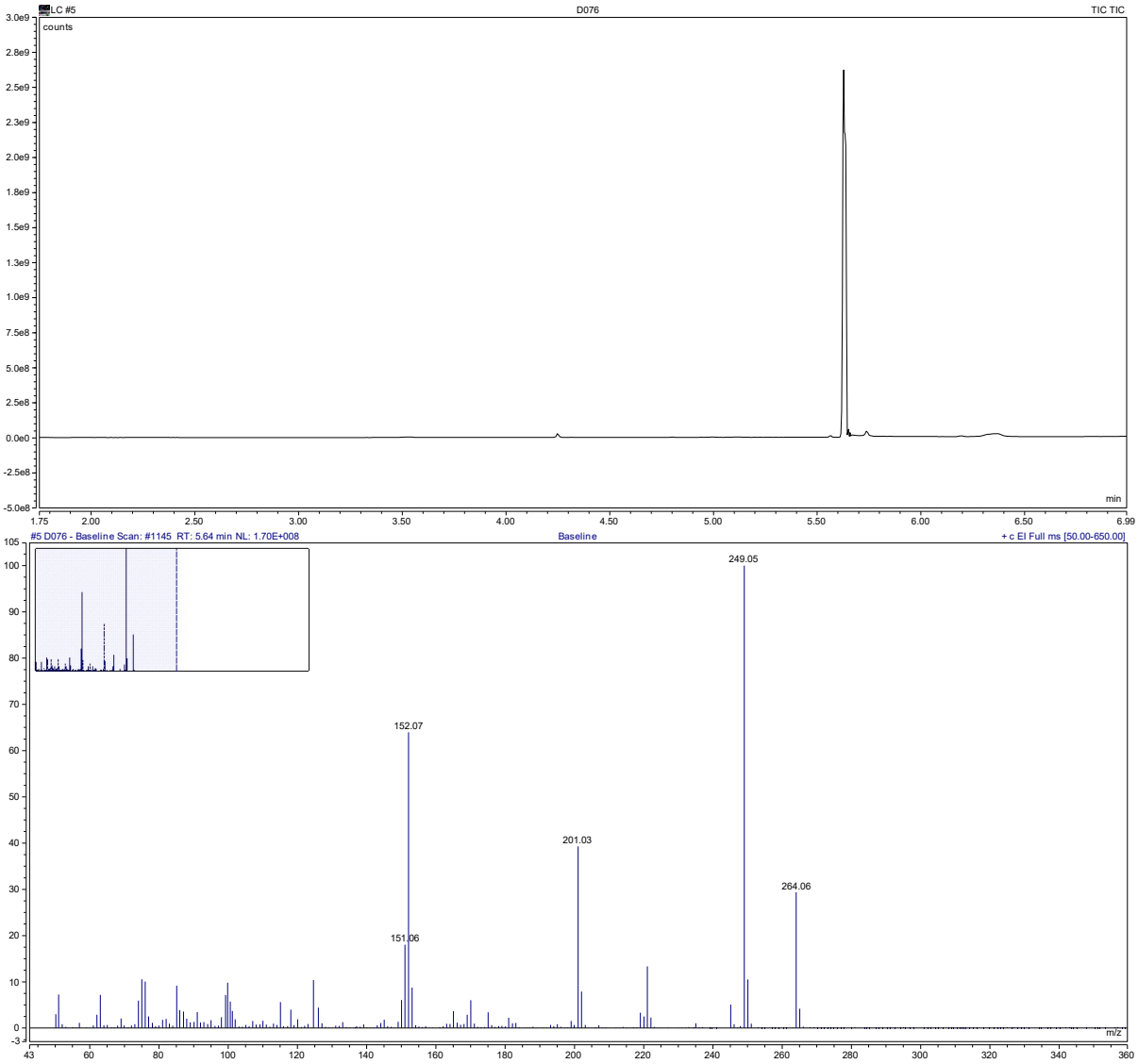


Figure 4. GCMS spectrum of synthesized product [2]

4-nitrobiphenyl – [4] - expected mass: 199.06 Da

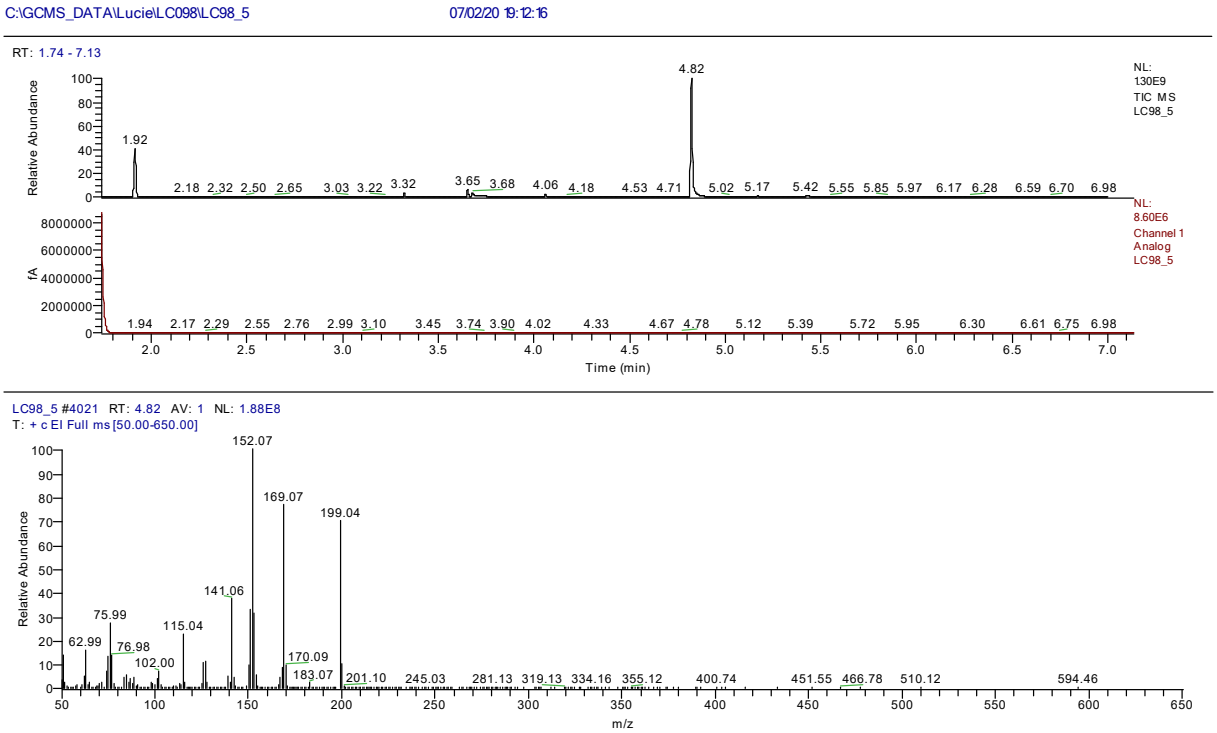


Figure 5. GCMS (black) & GCFID (red) spectra of synthesized product [4]

4-cyanobiphenyl – [5] - expected mass: 179.07 Da

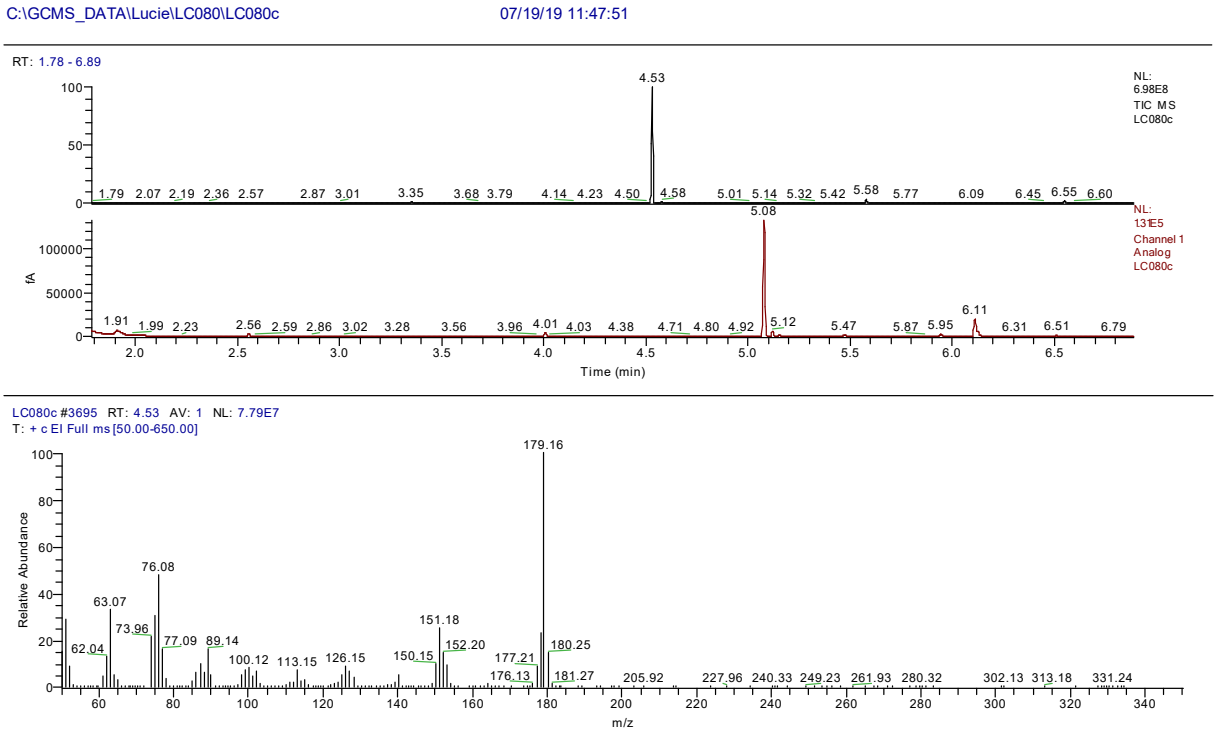


Figure 6.. GCMS (black) & GCFID (red) spectra of synthesized product [5]

4-fluoro-1,1'-biphenyl – [6] - expected mass: 172.07 Da

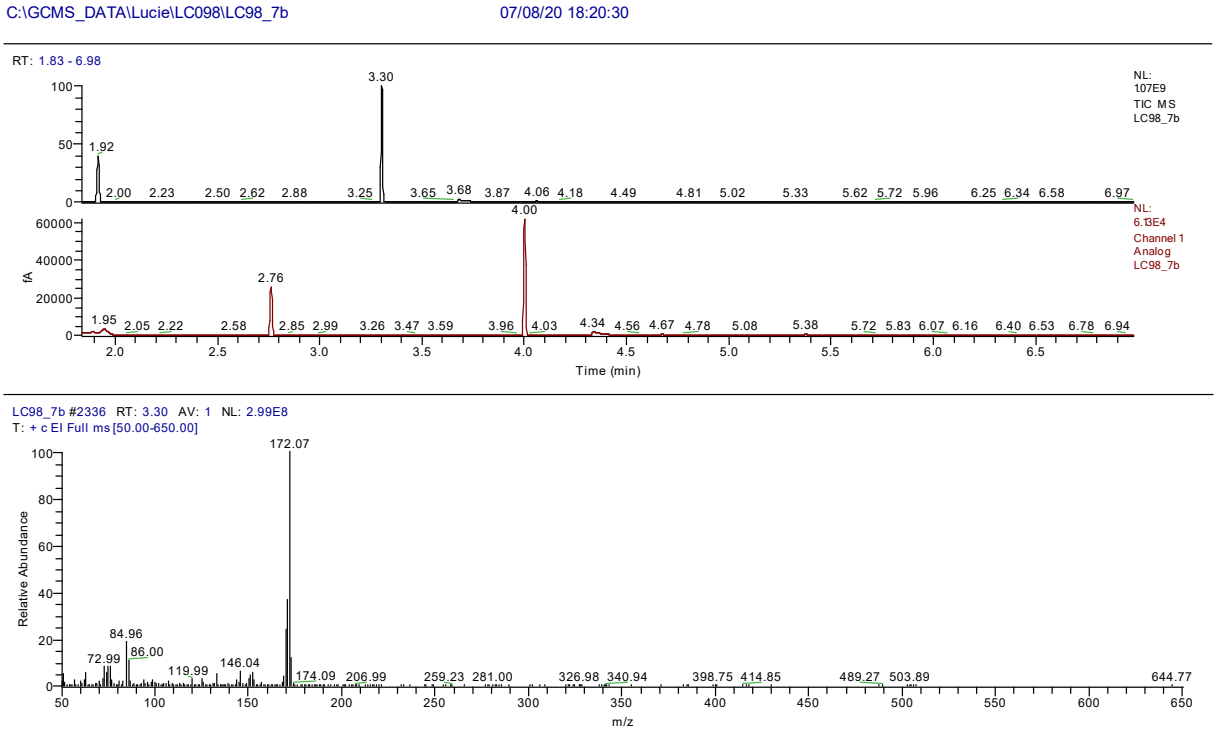


Figure 7. GCMS (black) & GCFID (red) spectra of synthesized product [6]

4-methyl-1,1'-biphenyl – [7] - expected mass: 168.09 Da

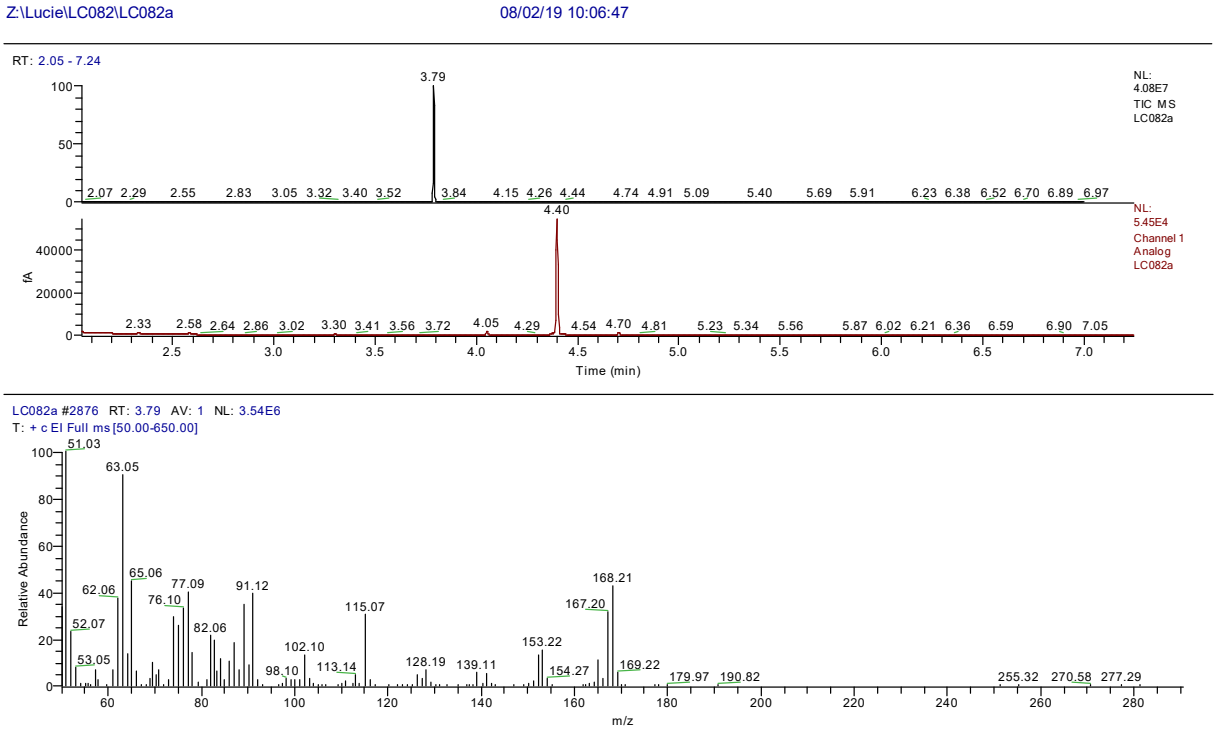


Figure 8. GCMS (black) & GCFID (red) spectra of synthesized product [7]

3-phenylpyridine – [8] – expected mass: 155.07 Da

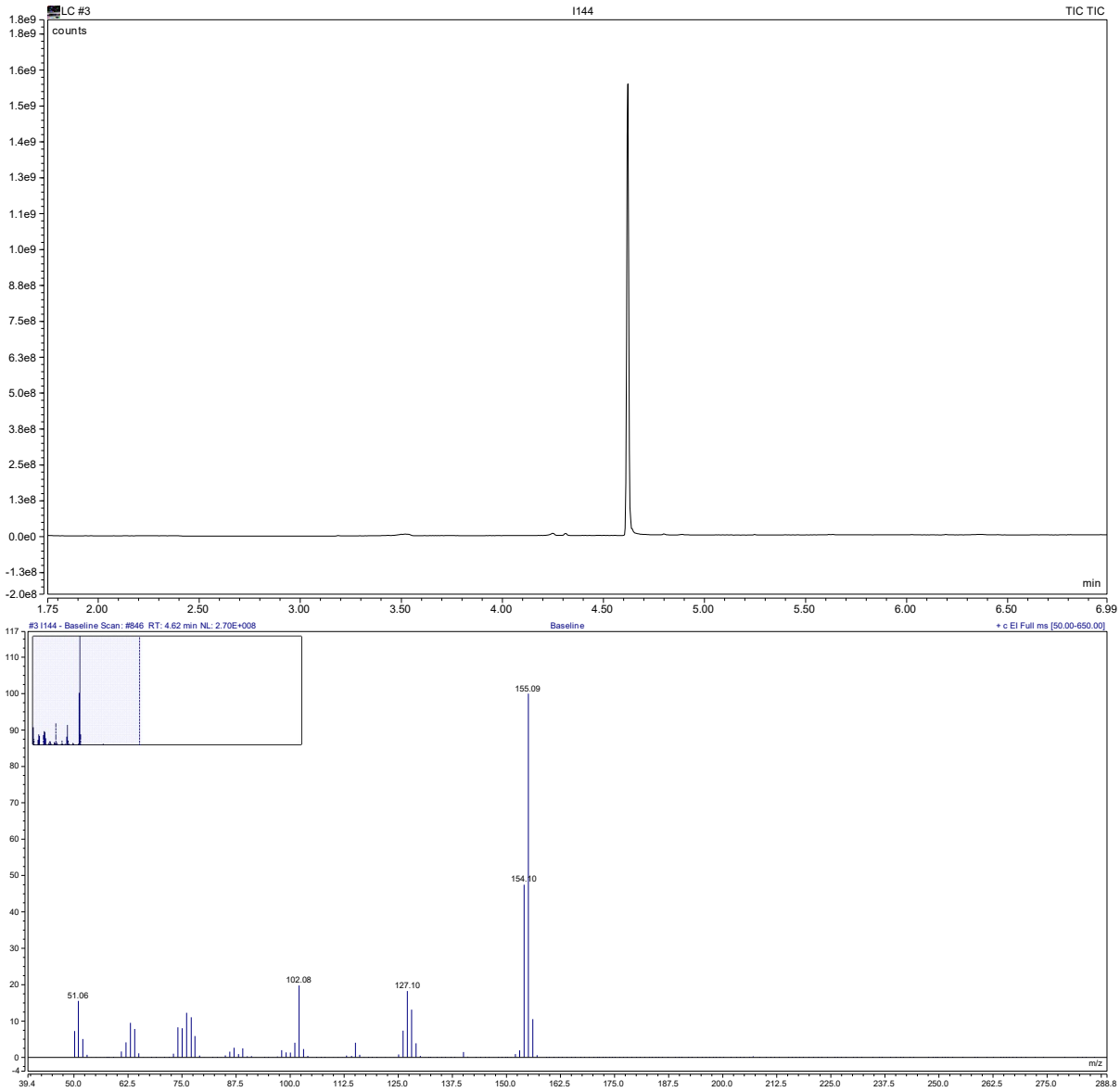
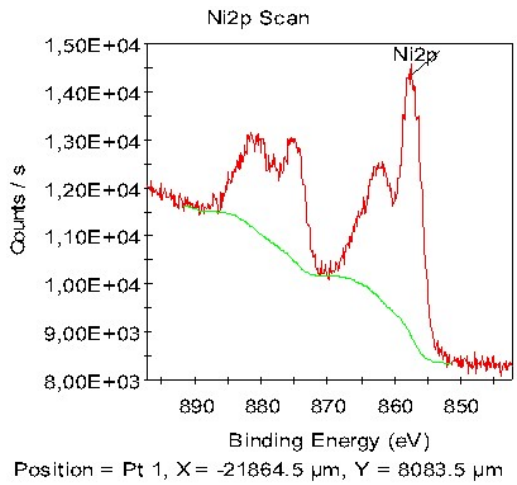


Figure 9. GCMS spectra of synthesized product [8]

III. XPS analyses of the Eco-Ni(HCOO)$_2$ ecocatalyst

Eco-Ni$(HCOO)_2$ before reaction



Eco-Ni$(HCOO)_2$ after reaction

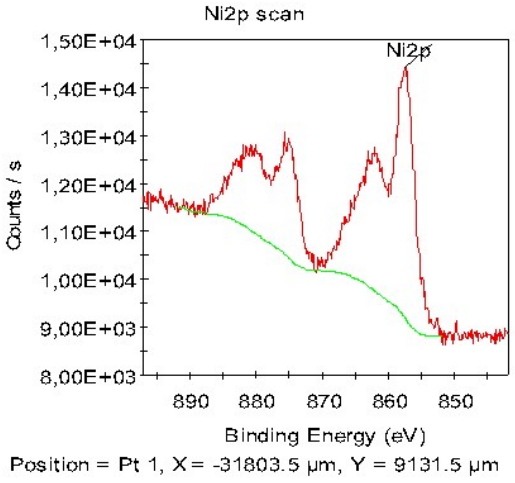


Figure 17. XPS analyses of the ecocatalyst before (left) and after the reaction (right)