**Supporting Information**

# Anchored palladium nanoparticles onto single walled carbon nanotubes: Efficient recyclable catalyst to *N*-containing heterocycles

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## Contents

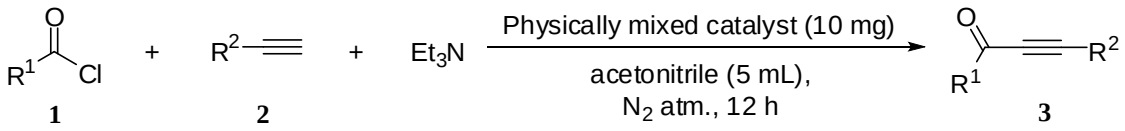
## Synthetic procedure for preparation of physically mixed catalyst

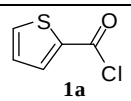
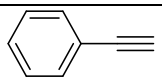
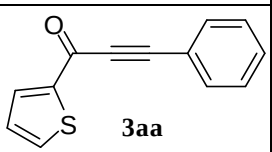
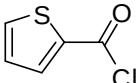
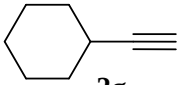
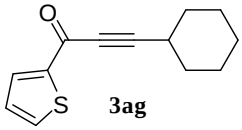
Palladium acetate (100 mg) was subjected to thermal treatment at 95 °C in DMF for 4 h fashion as reported in the manuscript but in the absence of SWNT. A black powder (28 mg) was isolated after stepwise treatment of the resulting reaction mixture such as, centrifugation (30 minutes at 8000 rpm, 8 °C), filtration (*via* Millipore membrane filter paper) followed by the sufficient washing with ethanol, acetone and finally with diethyl ether. It was then blended properly with SWNT (100 mg) in a mortar-pestle and then utilized for the subsequent catalytic reactions. The stoichiometry for physical mixing was kept unaltered to that used for preparation of anchored SWNT-PdNPs catalyst.

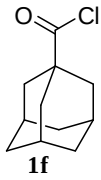
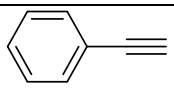
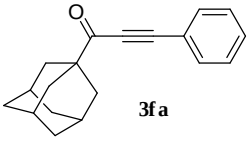
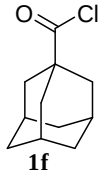
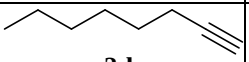
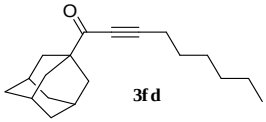
## Catalytic results with physically mixed catalyst

Table S1 lists the catalytic results using the physically mixed catalyst and the results are compared the result with that obtained using anchored SWNT-PdNPs catalysts under identical reaction condition.

**Table S1.** Acyl Sonogashira reaction catalyzed by physically mixed catalyst [a]




| Entry | Acid Chloride, **1** | Alkyne, **2** | Ynone, **3** | Temp. (° C) | Yield (%)[b] |
|---|---|---|---|---|---|
| 1 |  **1a** |  **2a** |  **3aa** | 25 | 92 (99) |
| 2 |  **1a** |  **2g** |  **3ag** | 50 | 11 (98) |

| | | | | | |
|---|---|---|---|---|---|
| 3 |  **1f** |  **2a** |  **3fa** | 50 | 80 (84) |
| 4 |  **1f** |  **2d** |  **3fd** | 50 | 58 (83) |

[a] Reaction condition: Physically mixed catalyst (10 mg) was used together with acid chlorides **1** (1 mmol), terminal acetylenes **2** (1 mmol) and dry triethylamine (1 mmol) in 5 mL dry acetonitrile. [b]Isolated yields of the products after purification through column chromatography and yields in the parenthesis represent that obtained utilizing the anchored SWNT-PdNPs (10 mg) catalysts under identical reaction condition.

**DFT calculation**

The DFT calculations have been performed using the Quantum-ESPRESSO software which is a plane wave based implementation of DFT. The Kohn-Sham equations are solved using ultrasoft pseudopotentials[1] and a plane-wave basis with a cut-off of 35 Ry for the wavefunction and 360 Ry for the augmentation charge density. The electron-electron exchange and correlation has been described using the Perdew-Burke-Ernzerhof (PBE) parametrization of the generalized gradient approximation (GGA).[2] In order to improve convergence, a Marzari-Vanderbilt smearing[3] with a width of 0.001 Ry was used. In order to study the anchoring of the PdNPs on SWNT-COOH, we have used infinitely long zigzag nanotubes with chirality (4,0) semi-conducting and (3,0) metallic SWNTs. Pd trimer ($Pd_3$) has been used to model the PdNPs. The semi-conducting SWNT-COOH-$Pd_3$ (box dimensions 14.55×21.82×12.62 $Å^3$) and metallic SWNT-COOH-$Pd_3$ (box dimensions 13.78×16.54×12.63 $Å^3$) systems have been placed in large hexagonal boxes so as to ensure

negligible interactions between the periodic images. Brillouin-zone integrations have been performed using (1x1x6) Monkhorst-Pack k-point mesh.

The calculations were performed using the Quantum-ESPRESSO software which is a plane wave based implementation of DFT.[4] Indeed, the calculation conveyed that the palladium metal trimer ($Pd_3$) binds with the –C=O oxygen of the carboxylic acid groups (Figure S1). The calculation employed infinitely long zigzag nanotubes with chirality (3,0) for metallic SWNTs (Figure S1A) and (4,0) for semi-conducting SWNTs (Figure S1B) and Pd trimer ($Pd_3$) has been considered as a replica model of PdNPs. The binding energies of the $Pd_3$ bound to SWNT–COOH are given by:

$$\Delta E = E_{\text{NT-Pd}_3} - E_{\text{NT}} - E_{\text{Pd}_3}$$

where $\Delta E$ is the binding energy of $Pd_3$ to SWNT-COOH, and $E_{\text{NT-Pd3}}$, $E_{\text{NT}}$ and $E_{\text{Pd3}}$ are the total energies of SWNT-COOH with $Pd_3$ attached to it , SWNT-COOH alone and $Pd_3$ in gas phase respectively. The binding energies of $Pd_3$ cluster on metallic SWNT and semiconducting SWNT were calculated as -0.66 eV and -0.95 eV respectively indicating a strong interaction of $Pd_3$ cluster through the carboxyl groups.

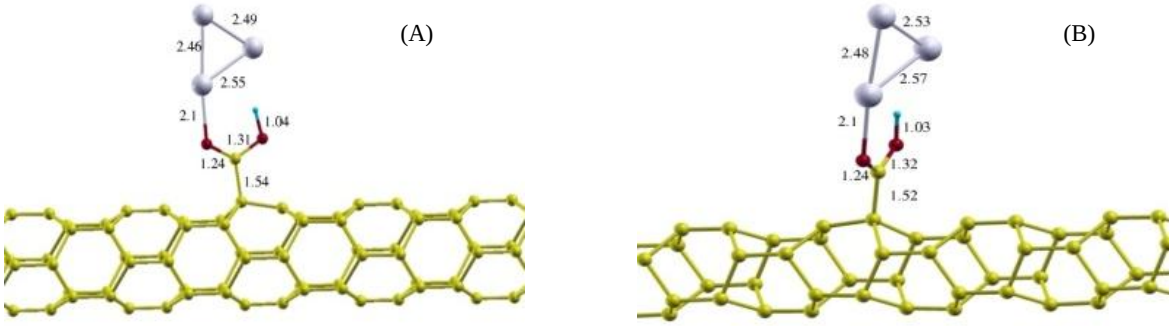
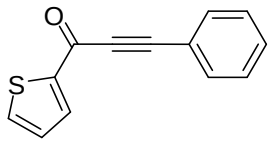



**Figure S1.** Optimized structure of (A) metallic SWNT-COOH-$Pd_3$ and (B) semi-conducting SWNT-COOH-$Pd_3$ revealing that the C=O oxygen of carboxylic acid group binds with the $Pd_3$ cluster. The bond lengths indicated in the figure are in Å.

## Characterization data

### 1. 3-phenyl-1-(thiophen-2-yl)prop-2-yn-1-one[5]

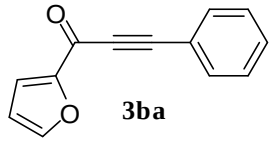



**Eluent:** Hexane:ethyl acetate (100:1)

**$^{1}$H NMR** ($CDCl_3$, 400 MHz): $\delta$ 7.89-7.89 (dd, $J$ = 3.7 Hz, 1H), 7.59-7.61 (dd, $J$ = 4.6 Hz, 1H), 7.51-7.53 (m, 2H), 7.32-7.34 (m, 1H), 7.26-7.29 (m, 2H), 7.06-7.08 (m, 1H) ppm.

**$^{13}$C NMR** ($CDCl_3$, 125 MHz): $\delta$ 169.3, 144.5, 135.1, 134.9, 132.7, 130.6, 128.4, 128.1, 119.5, 91.4, 86.2 ppm.

### 2. 1-(furan-2-yl)-3-phenylprop-2-yn-1-one[6]



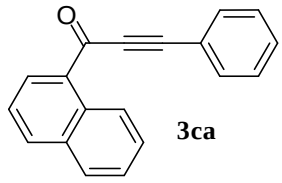

**3ba**

**Eluent:** Hexane:ethyl acetate (100:2)

**$^{1}$H NMR** ($CDCl_3$, 400 MHz): $\delta$ 7.67 (s, 1H), 7.61-7.63 (m, 2H), 7.37-7.46 (m, 4H), 7.58-7.59 (q, 1H) ppm.

**$^{13}$C NMR** ($CDCl_3$, 100 MHz): $\delta$ 164.6, 153.1, 147.9, 132.9, 130.8, 128.6, 120.9, 119.7, 112.6, 91.8, 86.1 ppm.

### 3. 1-(naphthalen-1-yl)-3-phenylprop-2-yn-1-one[5]



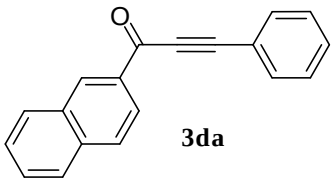

**3ca**

**Eluent:** Hexane:ethyl acetate (100:1.5)

**$^{1}$H NMR** ($CDCl_3$, 400 MHz): $\delta$ 9.30-9.32 (d, $J$ = 8.7 Hz, 1H), 8.62-8.66 (dd, $J$ = 6.9 Hz, 1H), 8.03-8.05 (d, $J$ = 8.2 Hz, 1H), 7.83-7.86 (d, $J$ = 14 Hz, 1H), 7.66-7.70 (m, 3H), 7.55-7.59 (m, 2H), 7.38-7.46 (m, 3H) ppm.

**$^{13}$C NMR** ($CDCl_3$, 100 MHz): $\delta$ 179.5, 134.9, 134.4, 133.6, 132.7, 132.6, 130.5, 130.4, 128.7, 128.4, 128.4, 126.5, 125.7, 124.3, 120.0, 91.5, 88.3 ppm.

**4. 1-(naphthalen-2-yl)-3-phenylprop-2-yn-1-one**[5]



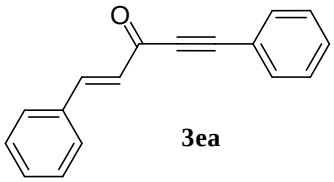
**3da**

**Eluent:** Hexane:ethyl acetate (100:1.5)

**$^{1}$H NMR** ($CDCl_3$, 500 MHz): $\delta$ 8.73 (s, 1H), 8.17-8.19 (dd, $J$ = 6.8 Hz, 1H), 7.96-7.98 (d, $J$ = 6.4 Hz, 1H), 7.83-7.87 (m, 2H), 7.69-7.72 (m, 2H), 7.51-7.59 (m, 2H), 7.39-7.48 (m, 3H) ppm.

**$^{13}$C NMR** ($CDCl_3$, 100 MHz): $\delta$ 177.6, 135.9, 134.1, 132.8, 132.4, 132.1, 130.6, 129.6, 128.8, 128.5, 128.3, 127.7, 126.7, 123.6, 119.9, 92.8, 86.9 ppm.

**5. (*E*)-1,5-diphenylpent-1-en-4-yn-3-one**[5]



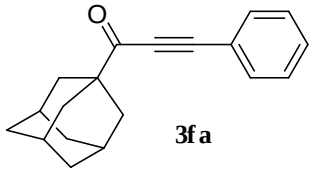
**3ea**

**Eluent:** Hexane:ethyl acetate (100:1.5)

**$^{1}$H NMR** ($CDCl_3$, 400 MHz): $\delta$ 7.86-7.90 (d, $J$ = 16 Hz, 1H), 7.53-7.63 (m, 4H), 7.36-7.44 (m, 6H), 6.81-6.85 (d, $J$ = 16 Hz, 1H) ppm.

**$^{13}$C NMR** ($CDCl_3$, 100 MHz): $\delta$ 177.8, 148.0, 133.7, 132.7, 130.9, 130.4, 128.8, 128.4, 128.4, 128.1, 119.8, 91.3, 86.4 ppm.

**6. 1-(1-Adamantyl)-3-phenylprop-2-yn-1-one**[7]



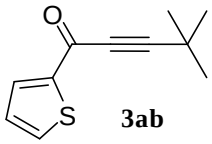
**3fa**

**Eluent:** Hexane:ethyl acetate (100:1)

**$^{1}$H NMR** ($CDCl_3$, 400 MHz): $\delta$ 7.58-7.61 (d, $J$ = 6.8 Hz, 2H), 7.43-7.48 (t, $J$ = 7.8 Hz, 1H), 7.36-7.40 (t, $J$ = 7.3 Hz, 2H), 2.09 (s, 3H), 1.94 (m, 6H), 1.71-1.79 (m, 6H) ppm.

**$^{13}$C NMR** ($CDCl_3$, 100 MHz): $\delta$ 193.9, 132.9, 130.4, 128.5, 120.2, 92.2, 85.9, 46.9, 38.0, 36.4, 27.8 ppm.

**7. 4,4-dimethyl-1-(thiophen-2-yl)pent-2-yn-1-one**



**3ab**

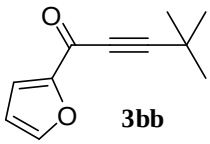
**Eluent:** Hexane:ethyl acetate (100:1.5)

**$^1$H NMR** ($CDCl_3$, 400 MHz): $\delta$ 7.64-7.67 (m, 1H), 7.11-7.13 (m, 1H), 6.76 (s, 1H), 1.29 (s, 9H) ppm.

**$^{13}$C NMR** ($CDCl_3$, 100 MHz): $\delta$ 182.7, 155.9, 144.9, 134.1, 132.4, 128.1, 118.4, 40.0, 28.6 ppm.

**HRMS (ESI)**: Calculated for $C_{11}H_{12}OS$ $[M+H]^+$: 193.0687; Found: 192.9775.

**8. 1-(furan-2-yl)-4,4-dimethylpent-2-yn-1-one**



**3bb**

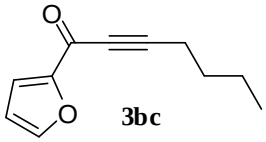
**Eluent:** Hexane:ethyl acetate (100:2)

**$^1$H NMR** ($CDCl_3$, 400 MHz): $\delta$ 7.59 (s, 1H), 7.24-7.25 (d, $J$ = 3.7 Hz, 1H), 6.50-6.51 (m, 1H), 1.29 (s, 9H) ppm.

**$^{13}$C NMR** ($CDCl_3$, 100 MHz): $\delta$ 177.6, 158.3, 153.5, 146.3, 117.6, 116.8, 112.5, 40.4, 28.7 ppm.

**HRMS (ESI)**: Calculated for $C_{11}H_{12}O_2$ $[M+H]^+$: 177.0915; Found: 177.0198.

**9. 1-(furan-2-yl)hept-2-yn-1-one**[8]



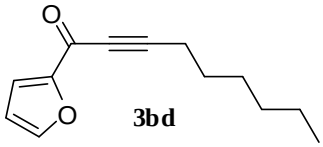
**3bc**

**Eluent:** Hexane:ethyl acetate (100:2)

**$^1$H NMR** ($CDCl_3$, 400 MHz): $\delta$ 7.62 (s, 1H), 7.28-7.29 (d, $J$ = 3.7 Hz, 1H), 6.53-6.54 (m, 1H), 2.42-2.46 (t, $J$ = 6.7 Hz, 2H), 1.57-1.63 (m, 2H), 1.44-1.49 (m, 2H), 0.91-0.95 (t, $J$ = 7.4 Hz, 3H) ppm.

**$^{13}$C NMR** ($CDCl_3$, 100 MHz): $\delta$ 164.9, 153.2, 147.7, 120.6, 112.4, 95.5, 78.9, 29.6, 21.9, 18.7, 13.4 ppm.

**10. 1-(furan-2-yl)non-2-yn-1-one**[9]



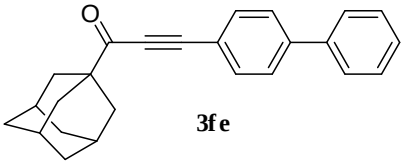
**3bd**

**Eluent:** Hexane:ethyl acetate (100:2)

**$^1$H NMR** ($CDCl_3$, 400 MHz): $\delta$ 7.62 (s, 1H), 7.28-7.29 (d, $J$ = 3.6 Hz, 1H), 6.53-6.54 (m, 1H), 2.41-2.45 (t, $J$ = 7.3 Hz, 2H), 1.58-1.66 (m, 2H), 1.39-1.47 (m, 2H), 1.27-1.33 (m, 4H), 0.86-0.89 (t, $J$ = 7.3 Hz, 3H) ppm.

**$^{13}$C NMR** ($CDCl_3$, 100 MHz): $\delta$ 164.9, 153.2, 147.7, 120.5, 112.4, 95.6, 78.9, 31.1, 28.5, 27.6, 22.4, 19.0, 13.9 ppm.

**11. 3-(Biphenyl-4-yl)-1-(1-adamantyl)prop-2-yn-1-one**



**3fe**

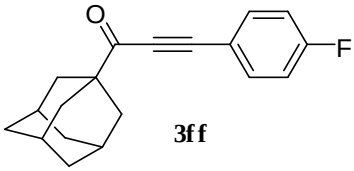
**Eluent:** Hexane:ethyl acetate (100:1)

**$^{1}$H NMR** ($CDCl_3$, 400 MHz): $\delta$ 7.66-7.68 (m, 2H), 7.59-7.63 (m, 4H), 7.44-7.49 (t, $J$ = 7.3 Hz, 2H), 7.37-7.41 (t, $J$ = 7.3 Hz, 1H), 2.12 (s, 3H), 1.97-1.98 (m, 6H), 1.73-1.82 (m, 6H) ppm.

**$^{13}$C NMR** ($CDCl_3$, 100 MHz): $\delta$ 193.9, 143.3, 139.8, 133.4, 128.9, 128.1, 127.2, 127.1, 119.0, 92.2, 86.7, 46.9, 38.1, 36.5, 27.9 ppm.

**HRMS (ESI)**: Calculated for $C_{25}H_{24}O$ $[M+H]^+$: 341.1905; Found: 341.1027.

**12. 3-(4-Fluorophenyl)-1-(1-adamantyl)prop-2-yn-1-one**



**3ff**

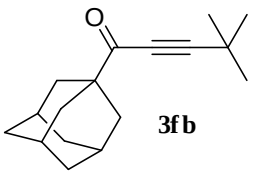
**Eluent:** Hexane:ethyl acetate (100:1)

**$^{1}$H NMR** ($CDCl_3$, 400 MHz): $\delta$ 7.55-7.58 (m, 2H), 7.04-7.08 (m, 2H), 2.07 (s, 3H), 1.91-1.92 (m, 6H), 1.69-1.78 (m, 6H) ppm.

**$^{13}$C NMR** ($CDCl_3$, 100 MHz): $\delta$ 193.7, 165.0, 162.5, 135.2, 135.1, 116.4, 116.3, 116.1, 115.9, 90.9, 85.9, 46.8, 38.0, 36.4, 27.8 ppm.

**HRMS (ESI)**: Calculated for $C_{19}H_{19}FO$ $[M+H]^+$: 283.3598; Found: 283.1346.

**13. 1-adamantyl-4,4-dimethylpent-2-yn-1-one**



**3fb**

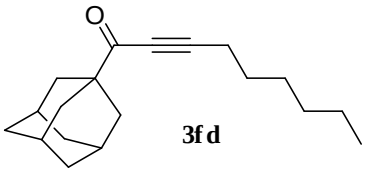
**Eluent:** Hexane:ethyl acetate (100:1)

**$^{1}$H NMR** ($CDCl_3$, 400 MHz): $\delta$ 2.03 (s, 3H), 1.81-1.82 (m, 6H), 1.64-1.74 (m, 6H), 1.28 (s, 9H) ppm.

**$^{13}$C NMR** ($CDCl_3$, 100 MHz): $\delta$ 194.3, 102.9, 77.06, 46.7, 38.1, 36.4, 30.1, 27.8, 27.7 ppm.

**HRMS (ESI)**: Calculated for $C_{17}H_{24}O$ $[M+H]^+$: 245.1905; Found: 245.1125.

**14. 1-(1-Adamantyl)non-2-yn-1-one**[7]



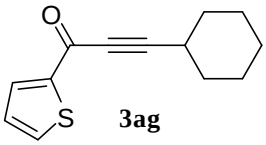
**3fd**

**Eluent:** Hexane:ethyl acetate (100:1)

**$^{1}$H NMR** ($CDCl_3$, 400 MHz): $\delta$ 2.33-2.37 (t, $J$ = 6.7 Hz, 2H), 2.02 (s, 3H), 1.81 (s, 6H), 1.63-1.73 (m, 6H), 1.52-1.58 (m, 2H), 1.39-1.42 (m, 2H), 1.26-1.29 (m, 4H), 0.84-0.88 (t, $J$ = 6.7 Hz, 3H) ppm.

**$^{13}$C NMR** ($CDCl_3$, 100 MHz): $\delta$ 194.2, 95.7, 78.7, 46.6, 37.9, 36.4, 31.1, 28.5, 27.8, 27.7, 22.4, 18.9, 13.9 ppm.

**15. 3-cyclohexyl-1-(thiophen-2-yl)prop-2-yn-1-one**



**3ag**

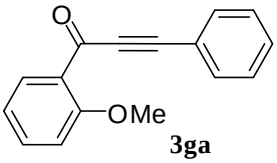
**Eluent:** Hexane:ethyl acetate (100:0.5)

**$^{1}$H NMR** ($CDCl_3$, 400 MHz): $\delta$ 7.87-7.88 (dd, 1H), 7.65-7.67 (dd, 1H), 7.12-7.14 (m, 1H), 2.64-2.69 (m, 1H), 1.87-1.90 (m, 2H), 1.73-1.77 (m, 2H), 1.53-1.62 (m, 3H), 1.35-1.42 (m, 3H) ppm.

**$^{13}$C NMR** ($CDCl_3$, 100 MHz): $\delta$ 170.1, 145.1, 134.7, 128.1, 98.9, 79.2, 31.5, 29.125.6, 24.6 ppm.

**HRMS (ESI)**: Calculated for $C_{13}H_{14}OS$ $[M+H]^+$: 219.0843; Found: 219.0467.

**16. 1-(2-methoxyphenyl)-3-phenylprop-2-yn-1-one**[5]



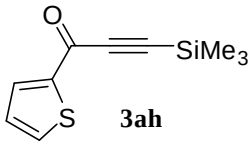
**3ga**

**Eluent:** Hexane:ethyl acetate (100:1.5)

**$^{1}$H NMR** ($CDCl_3$, 500 MHz): $\delta$ 8.05-8.07 (dd, $J$ = 7.5 Hz, 1H), 7.58-7.60 (m, 2H), 7.48-7.52 (m, 1H), 7.33-7.42 (m, 3H), 6.97-7.03 (m, 2H), 3.91 (s, 3H) ppm.

**$^{13}$C NMR** ($CDCl_3$, 125 MHz): $\delta$ 176.2, 159.4, 134.8, 132.5, 132.1, 130.2, 128.3, 126.2, 120.2, 119.9, 111.9, 91.2, 88.9, 55.5 ppm.

**17. 1-(thiophen-2-yl)-3-(trimethylsilyl)prop-2-yn-1-one**[5]



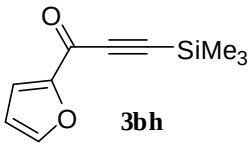

**3ah**

**Eluent:** Hexane:ethyl acetate (100:0.5)

**$^{1}$H NMR** ($CDCl_3$, 400 MHz): $\delta$ 7.89-7.90 (dd, $J$ = 4.1 Hz, 1H), 7.68-7.69 (dd, $J$ = 5 Hz, 1H), 7.12-7.14 (m, 1H), 0.27 (s, 9H) ppm.

**$^{13}$C NMR** ($CDCl_3$, 100 MHz): $\delta$ 169.3, 144.4, 135.5, 135.4, 128.2, 100.2, 99.0, -0.85 ppm.

**18. 1-(furan-2-yl)-3-(trimethylsilyl)prop-2-yn-1-one**[10]



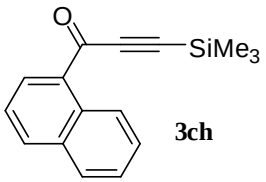

**3bh**

**Eluent:** Hexane:ethyl acetate (100:2)

**$^{1}$H NMR** ($CDCl_3$, 400 MHz): $\delta$ 7.65 (s, 1H), 7.34-7.35 (d, J = 3.7 Hz, 1H), 6.56-6.57 (m, 1H), 0.27 (s, 9H) ppm.

**$^{13}$C NMR** ($CDCl_3$, 100 MHz): $\delta$ 164.2, 152.9, 148.2, 121.6, 112.6, 100.1, 99.2, -0.8 ppm.

**19. 1-(naphthalen-1-yl)-3-(trimethylsilyl)prop-2-yn-1-one**




**3ch**

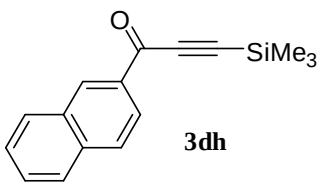
**Eluent:** Hexane:ethyl acetate (100:0.5)

**$^{1}$H NMR** ($CDCl_3$, 400 MHz): $\delta$ 9.19-9.22 (d, $J$ = 8.6 Hz, 1H), 8.58-8.59 (m, 1H), 8.05-8.08 (d, $J$ = 8.6 Hz, 1H), 7.87-7.89 (d, $J$ = 8.6 Hz, 1H), 7.64-7.66 (m, 1H), 7.55-7.59 (m, 2H), 0.35 (s, 9H) ppm.

**$^{13}$C NMR** ($CDCl_3$, 100 MHz): $\delta$ 179.2, 135.1, 134.9, 133.7, 132.3, 130.6, 128.9, 128.5, 126.7, 125.9, 124.4, 102.3, 98.7, -0.7 ppm.

**HRMS (ESI)**: Calculated for $C_{16}H_{16}OSi$ $[M+H]^+$: 253.1048; Found: 253.0907.

**20. 1-(naphthalen-2-yl)-3-(trimethylsilyl)prop-2-yn-1-one**




**3dh**

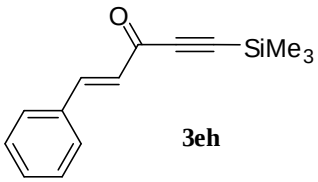
**Eluent:** Hexane:ethyl acetate (100:0.5)

**$^1$H NMR** ($CDCl_3$, 400 MHz): $\delta$ 8.71 (s, 1H), 8.12-8.15 (m, 1H), 7.99-8.01 (d, $J$ = 7.9 Hz, 1H), 7.87-7.89 (m, 2H), 7.55-7.64 (m, 2H), 0.37 (s, 9H) ppm.

**$^{13}$C NMR** ($CDCl_3$, 100 MHz): $\delta$ 177.6, 136.1, 133.9, 132.3, 129.9, 129.0, 128.4, 127.9, 126.9, 123.8, 100.9, 100.5, -0.6 ppm.

**HRMS (ESI)**: Calculated for $C_{16}H_{16}OSi$ $[M+H]^+$: 253.1048; Found: 253.0819.

**21. (*E*)-1-phenyl-5-(trimethylsilyl)pent-1-en-4-yn-3-one**[11]



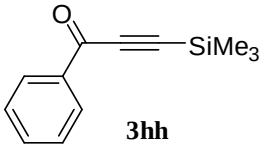

**3eh**

**Eluent:** Hexane:ethyl acetate (100:1.5)

**$^1$H NMR** ($CDCl_3$, 400 MHz): $\delta$ 7.82-7.86 (d, $J$ = 16.5 Hz, 1H), 7.56-7.58 (m, 2H), 7.42-7.43 (m, 3H), 6.76-6.80 (d, $J$ = 15.9 Hz, 1H), 0.31 (s, 9H) ppm.

**$^{13}$C NMR** ($CDCl_3$, 100 MHz): $\delta$ 177.9, 148.8, 133.9, 131.2, 129.0, 128.7, 128.2, 100.6, 98.7, -0.7 ppm.

**22. 1-phenyl-3-(trimethylsilyl)prop-2-yn-1-one**[12]



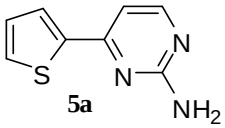

**3hh**

**Eluent:** Hexane:ethyl acetate (100:0.5)

**$^1$H NMR** ($CDCl_3$, 400 MHz): $\delta$ 8.12-8.14 (d, $J$ = 8 Hz, 2H), 7.57-7.61 (t, $J$ = 7.9 Hz, 1H), 7.45-7.49 (t, $J$ = 8 Hz, 2H), 0.31 (s, 9H) ppm.

**$^{13}$C NMR** ($CDCl_3$, 100 MHz): $\delta$ 177.6, 136.4, 134.1, 129.5, 128.5, 100.7, 100.4, -0.8 ppm.

**23. 4-(thiophen-2-yl)pyrimidin-2-amine**[5]



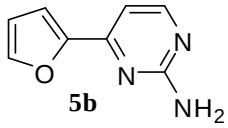

**5a**

**Eluent:** Hexane:ethyl acetate (1:1)

**$^1$H NMR** (DMSO-$d_6$, 400 MHz): $\delta$ 8.22-8.23 (d, $J$ = 4.9 Hz, 1H), 7.84-7.85 (d, $J$ = 3.6 Hz, 1H), 7.69-7.70 (d, $J$ = 4.9 Hz, 1H), 7.15-7.18 (t, $J$ = 4.3 Hz, 1H), 7.03-7.05 (d, $J$ = 4.9 Hz, 1H), 6.64 (s, 2H) ppm.

**$^{13}$C NMR** (DMSO-$d_6$, 100 MHz): $\delta$ 163.6, 159.1, 158.9, 142.9, 130.1, 128.6, 127.8, 104.5 ppm.

**24. 4-(furan-2-yl)pyrimidin-2-amine**[5]



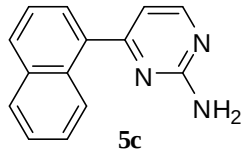

**5b**

**Eluent:** Hexane:ethyl acetate (1:1)

**$^1$H NMR** (DMSO-$d_6$, 400 MHz): $\delta$ 8.26-8.27 (d, $J$ = 4.9 Hz, 1H), 7.85 (s, 1H), 7.16-7.17 (d, $J$ = 3.6 Hz, 1H), 6.87-6.88 (d, $J$ = 4.9 Hz, 1H), 6.64-6.66 (m, 3H) ppm.

**$^{13}$C NMR** (DMSO-$d_6$, 100 MHz): $\delta$ 163.6, 159.2, 155.5, 151.8, 145.5, 112.6, 111.7, 104.1 ppm.

**25. 4-(naphthalen-1-yl)pyrimidin-2-amine**[5]



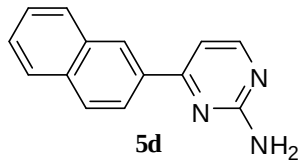

**5c**

**Eluent:** Hexane:ethyl acetate (1:1)

**$^1$H NMR** (DMSO-$d_6$, 400 MHz): $\delta$ 8.36-8.37 (d, $J$ = 5.5 Hz, 1H), 8.16-8.18 (m, 1H), 7.98-8.02 (m, 2H), 7.52-7.60 (m, 4H), 6.80-6.81 (d, $J$ = 4.9 Hz, 1H), 6.75 (s, 2H) ppm.

**$^{13}$C NMR** (DMSO-$d_6$, 100 MHz): $\delta$ 166.6, 163.6, 158.7, 136.6, 133.4, 130.1, 129.4, 128.4, 127.1, 126.7, 126.2, 125.4, 125.3, 110.8 ppm.

**26. 4-(naphthalen-2-yl)pyrimidin-2-amine**[5]



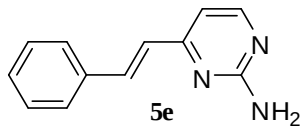

**5d**

**Eluent:** Hexane:ethyl acetate (1:1)

**$^1$H NMR** (DMSO-$d_6$, 400 MHz): $\delta$ 8.67 (s, 1H), 8.35-8.37 (d, $J$ = 4.9 Hz, 1H), 8.19-8.21 (q, 1H), 8.01-8.05 (t, $J$ = 7.3 Hz, 2H), 7.96-7.98 (m, 1H), 7.57-7.59 (m, 2H), 7.28-7.29 (d, $J$ = 5.5 Hz, 1H), 6.72 (s, 2H) ppm.

**$^{13}$C NMR** (DMSO-$d_6$, 100 MHz): $\delta$ 163.8, 163.4, 159.1, 134.4, 133.9, 132.7, 128.8, 128.2, 127.6, 127.2, 126.6, 126.5, 123.9, 106.1 ppm.

**27. (*E*)-4-styrylpyrimidin-2-amine**




**5e**

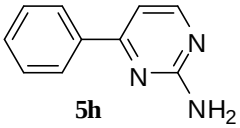
**Eluent:** Hexane:ethyl acetate (1:1)

**$^1$H NMR** (DMSO-$d_6$, 400 MHz): $\delta$ 8.21-8.23 (d, $J$ = 4.9 Hz, 1H), 7.69-7.73 (d, $J$ = 16.5 Hz, 1H), 7.62-7.64 (d, $J$ = 7.3 Hz, 2H), 7.32-7.42 (m, 3H), 7.02-7.06 (d, $J$ = 16.5 Hz, 1H), 6.72-6.73 (d, $J$ = 4.9 Hz, 1H), 6.52 (s, 2H) ppm.

**$^{13}$C NMR** (DMSO-$d_6$, 100 MHz): $\delta$ 163.6, 162.5, 158.9, 135.8, 135.1, 129.2, 129.1, 127.6, 126.9, 108.5 ppm.

**HRMS (ESI)**: Calculated for $C_{12}H_{11}N_3$ $[M+H]^+$: 198.1031; Found: 197.9872.

**28. 4-phenylpyrimidin-2-amine**[13]



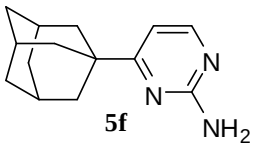

**5h**

**Eluent:** Hexane:ethyl acetate (100:35)

**$^1$H NMR** (DMSO-$d_6$, 400 MHz): $\delta$ 8.30-8.32 (d, $J$ = 5.5 Hz, 1H), 8.05-8.07 (m, 2H), 7.47-7.48 (t, $J$ = 3.1 Hz, 3H), 7.09-7.11 (d, $J$ = 4.9 Hz, 1H), 6.72 (s, 2H) ppm.

**$^{13}$C NMR** (DMSO-$d_6$, 100 MHz): $\delta$ 163.8, 163.6, 159.1, 137.0, 130.5, 128.7, 126.7, 105.8 ppm.

**29. 1-Adamantylpyrimidin-2-amine**[14]



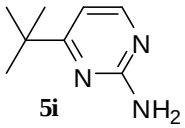

**5f**

**Eluent:** Hexane:ethyl acetate (100:35)

**$^1$H NMR** (DMSO-$d_6$, 400 MHz): $\delta$ 8.11-8.12 (d, J = 4.9 Hz, 1H), 6.49-6.51 (d, J = 4.9 Hz, 1H), 6.32 (s, 2H), 2.01 (s, 3H), 1.82-1.83 (s, 6H), 1.65-1.73 (m, 6H) ppm.

**$^{13}$C NMR** (DMSO-$d_6$, 100 MHz): $\delta$ 177.4, 163.4, 158.3, 105.3, 40.6, 38.4, 36.4, 28.0 ppm.

**30. 4-*tert*-butylpyrimidin-2-amine**




**5i**

**Eluent:** Hexane:ethyl acetate (100:25)

**$^1$H NMR** (DMSO-$d_6$, 400 MHz): $\delta$ 8.12-8.13 (d, $J$ = 5.5 Hz, 1H), 6.56-6.57 (d, $J$ = 4.9 Hz, 1H), 6.41 (s, 2H), 1.16 (s, 9H) ppm.

**$^{13}$C NMR** (DMSO-$d_6$, 100 MHz): $\delta$ 177.6, 163.2, 158.1, 105.3, 36.8, 29.1 ppm.

**HRMS (ESI)**: Calculated for $C_8H_{13}N_3$ $[M+H]^+$: 152.1187; Found: 152.0898.

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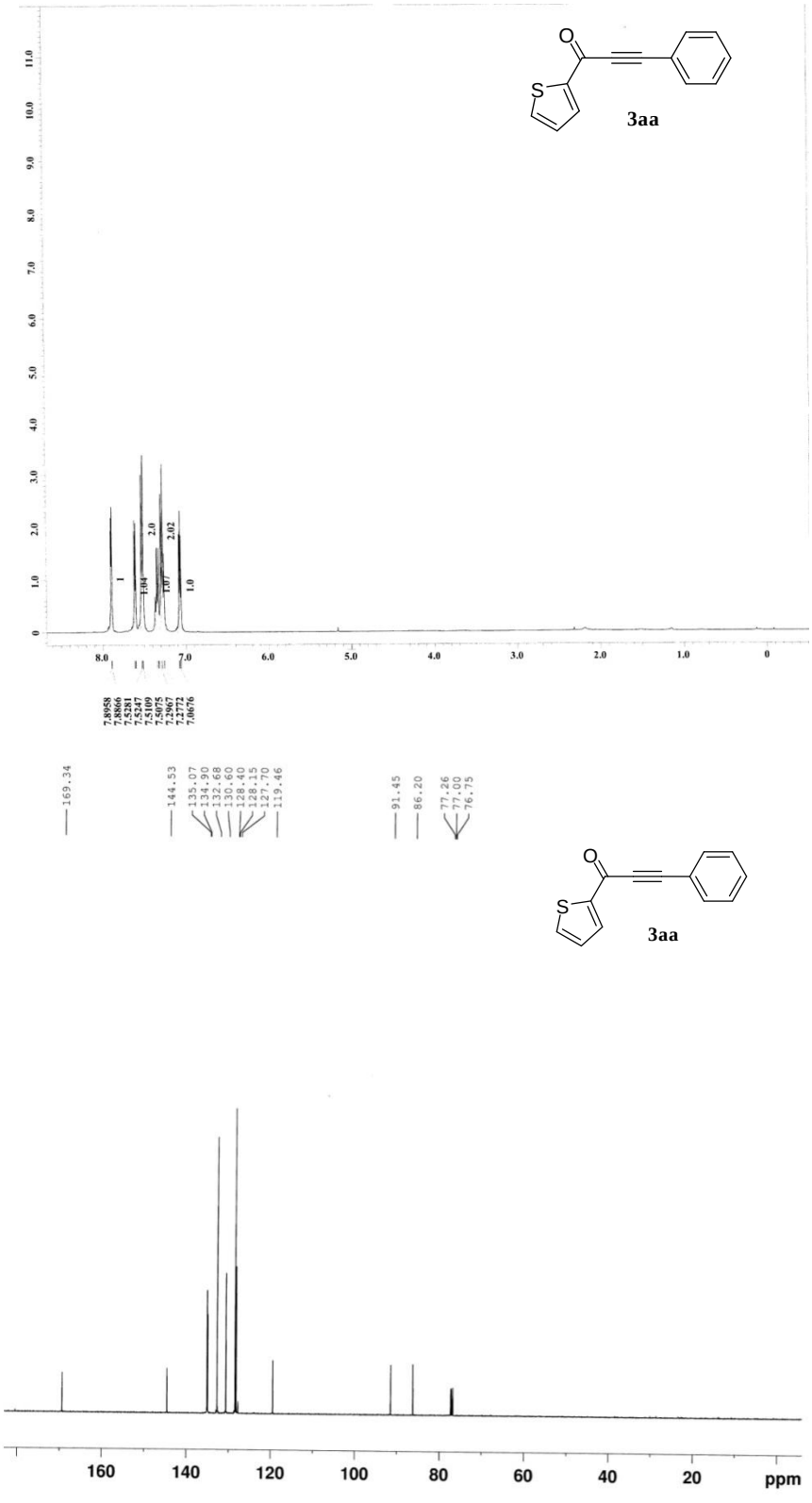



**Figure S2.** $^{1}H$ and $^{13}C$ NMR spectra of 3-phenyl-1-(thiophen-2-yl)prop-2-yn-1-one.

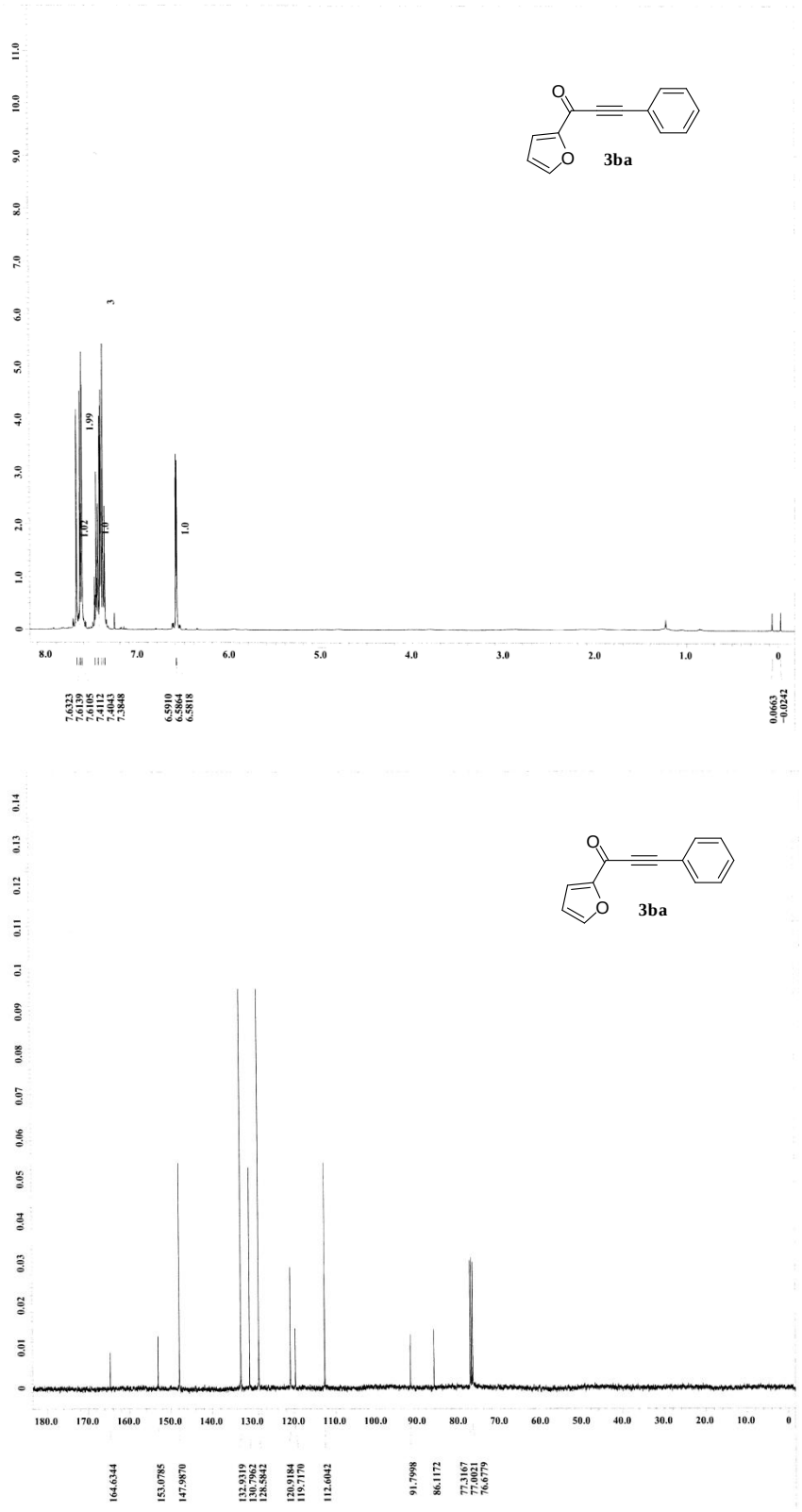



**Figure S3.** $^{1}H$ and $^{13}C$ NMR spectra of 1-(furan-2-yl)-3-phenylprop-2-yn-1-one.

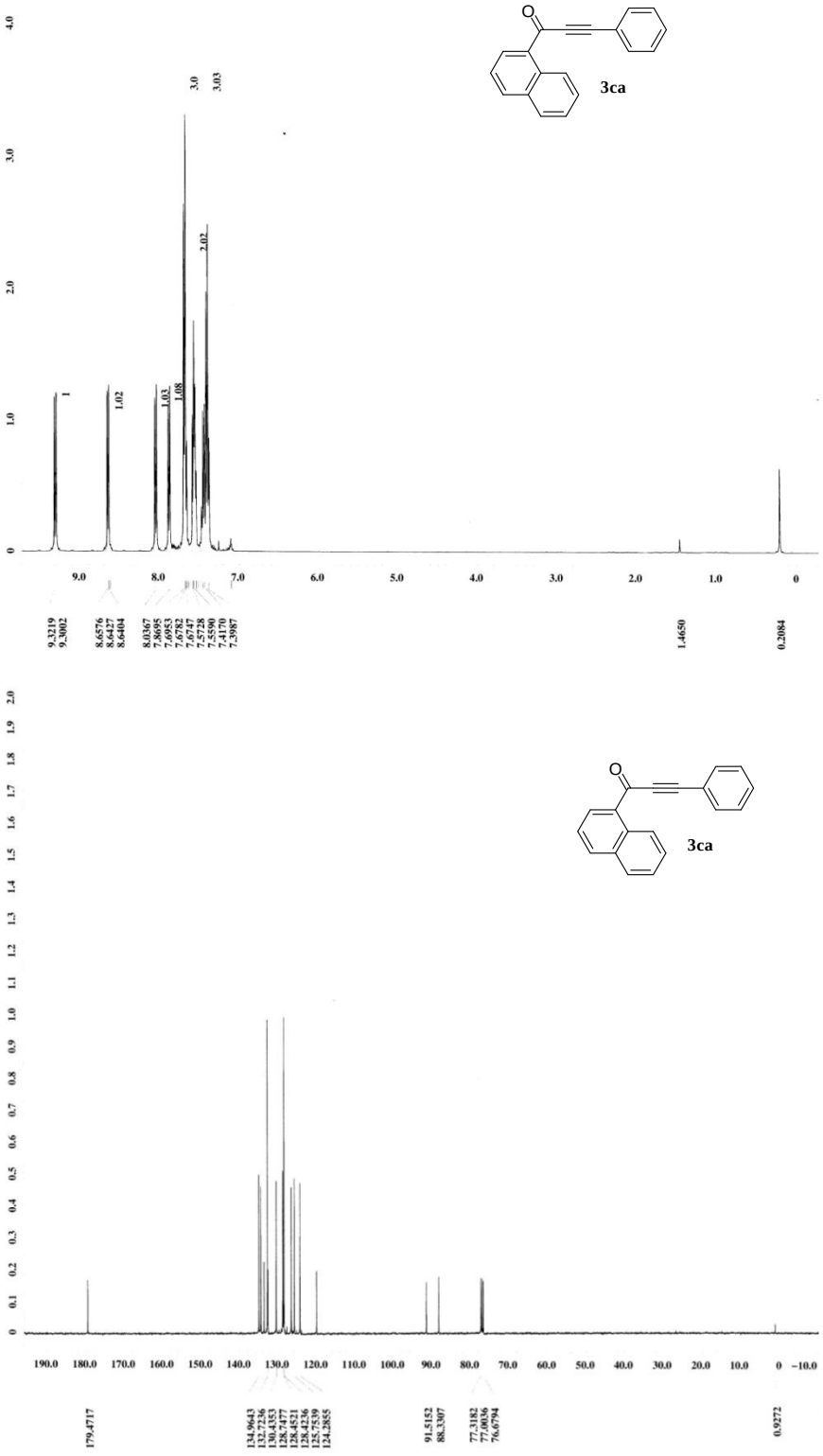



**Figure S4.** $^{1}H$ and $^{13}C$ NMR spectra of 1-(naphthalen-1-yl)-3-phenylprop-2-yn-1-one.

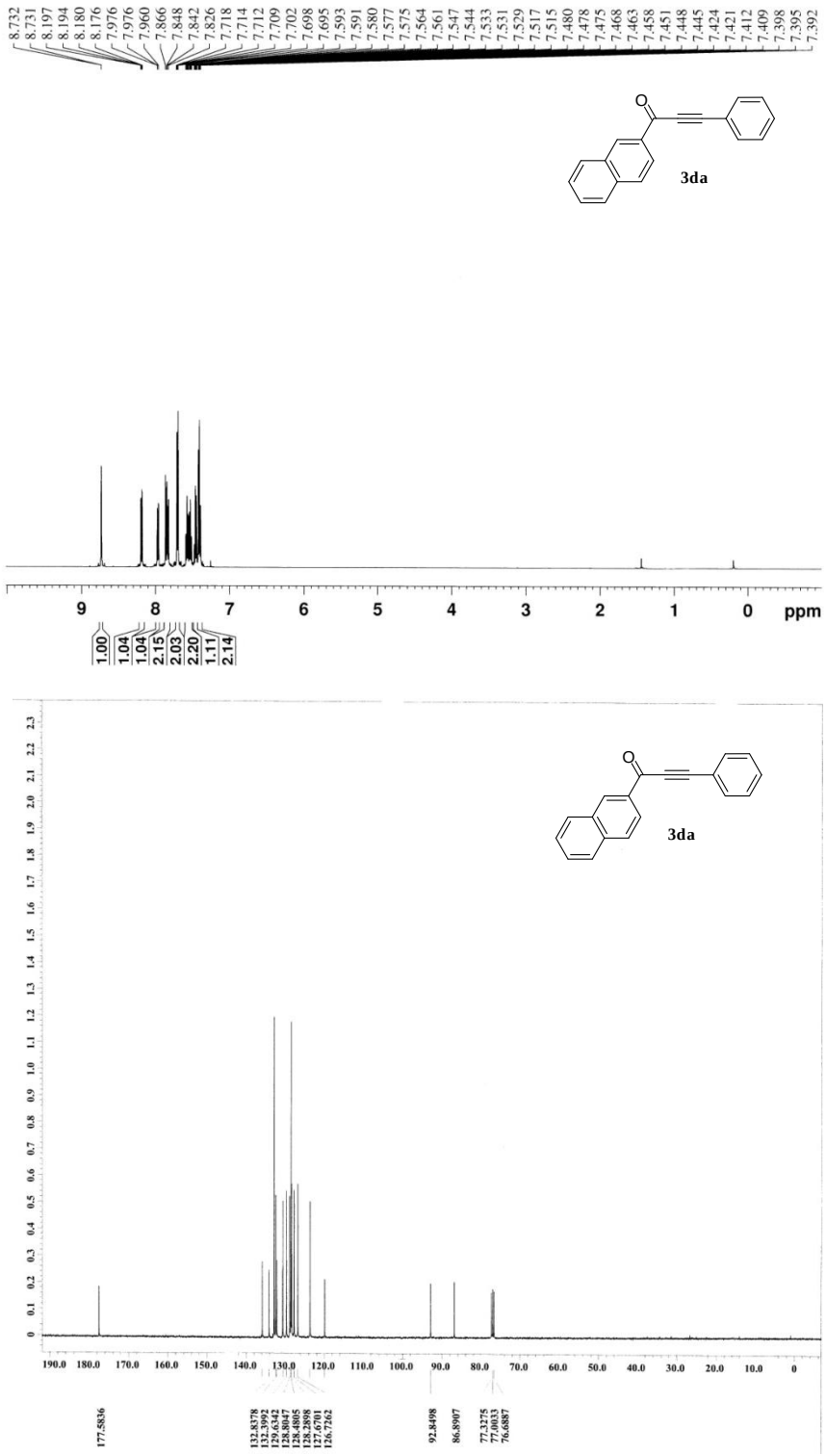



**Figure S5.** $^{1}H$ and $^{13}C$ NMR spectra of 1-(naphthalen-2-yl)-3-phenylprop-2-yn-1-one.

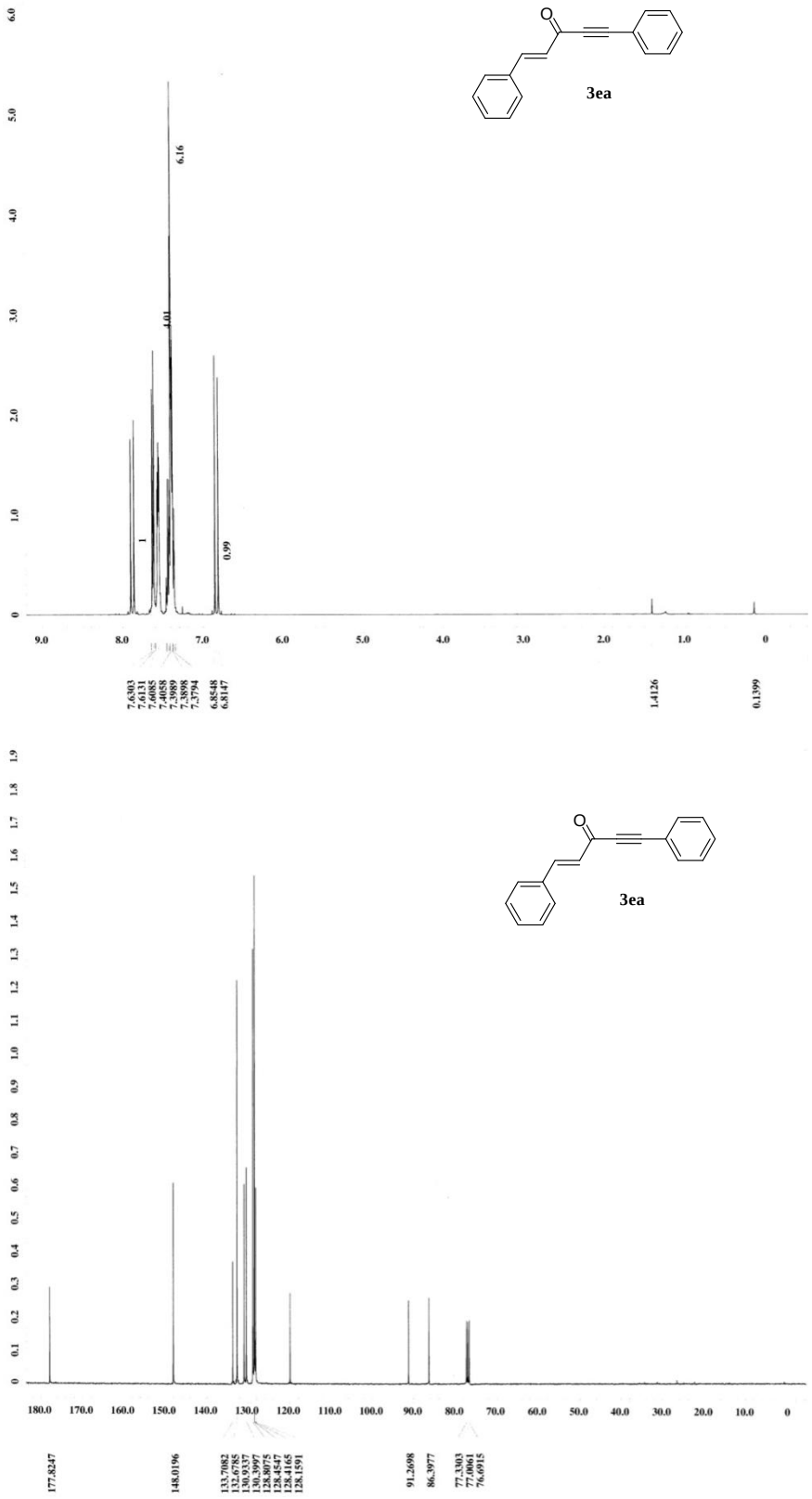



**Figure S6.** $^{1}H$ and $^{13}C$ NMR spectra of (*E*)-1,5-diphenylpent-1-en-4-yn-3-one.

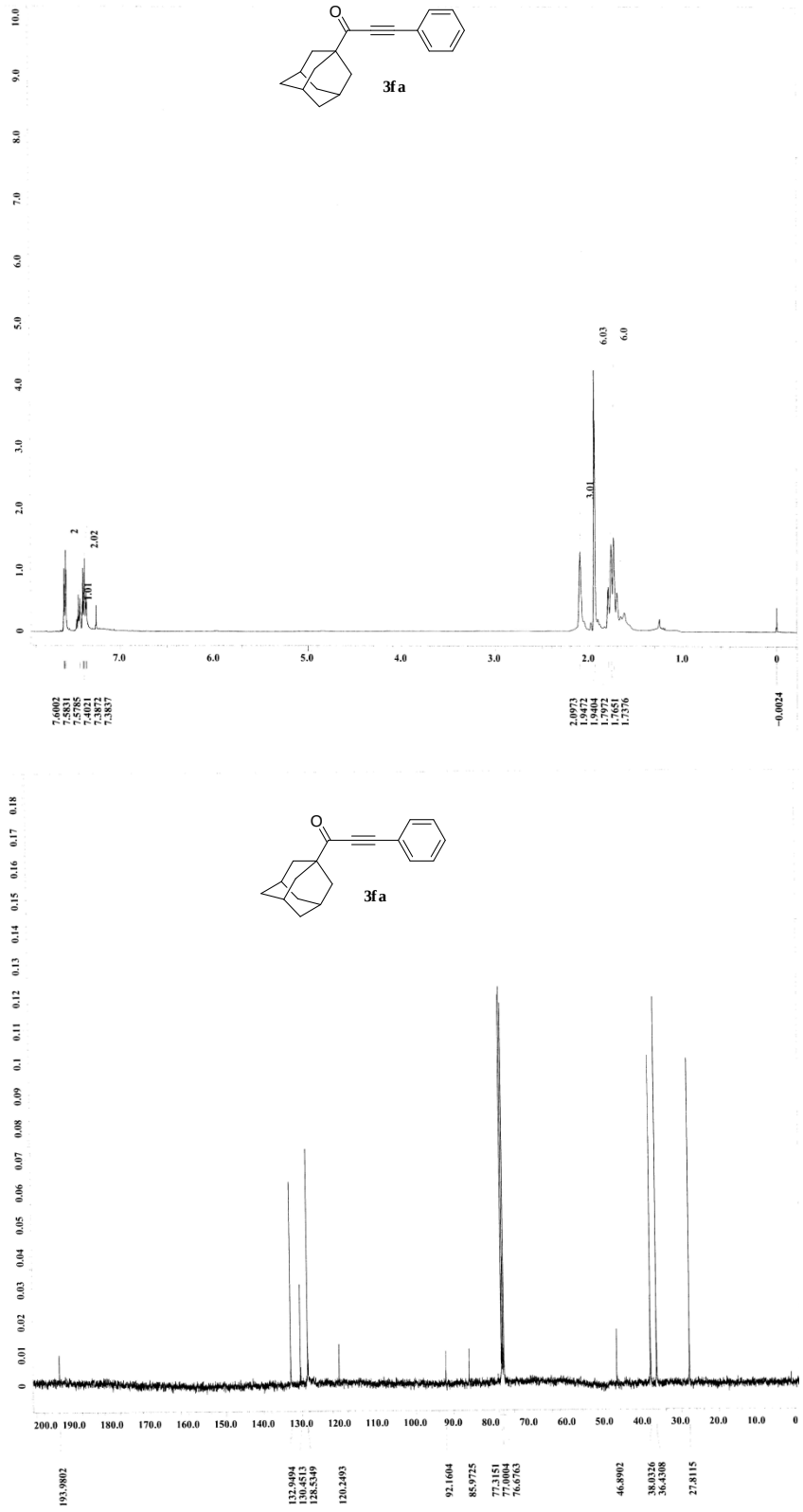



**Figure S7.** $^{1}H$ and $^{13}C$ NMR spectra of 1-(1-Adamantyl)-3-phenylprop-2-yn-1-one.

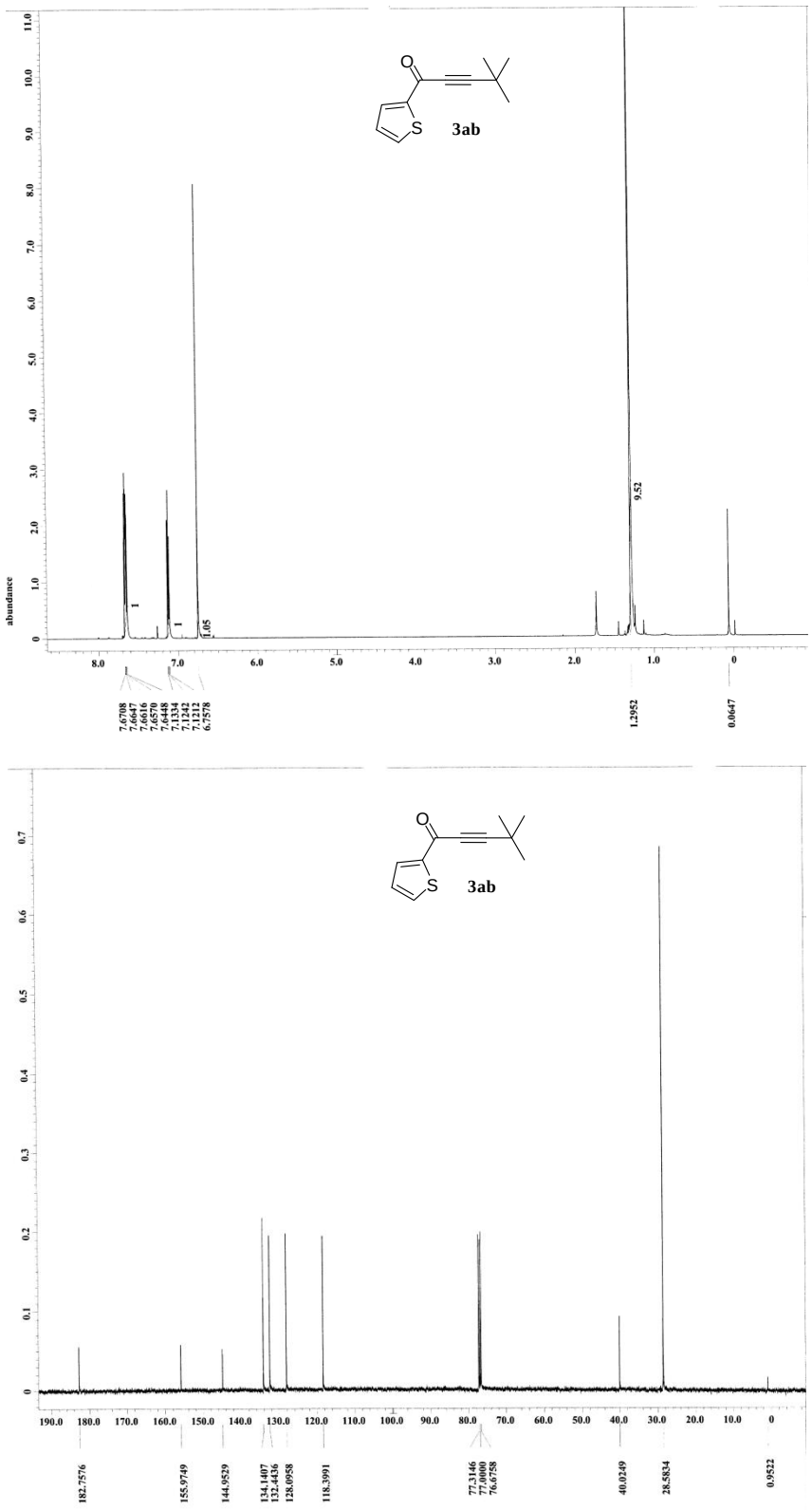



**Figure S8.** $^{1}H$ and $^{13}C$ NMR spectra of 4,4-dimethyl-1-(thiophen-2-yl)pent-2-yn-1-one.

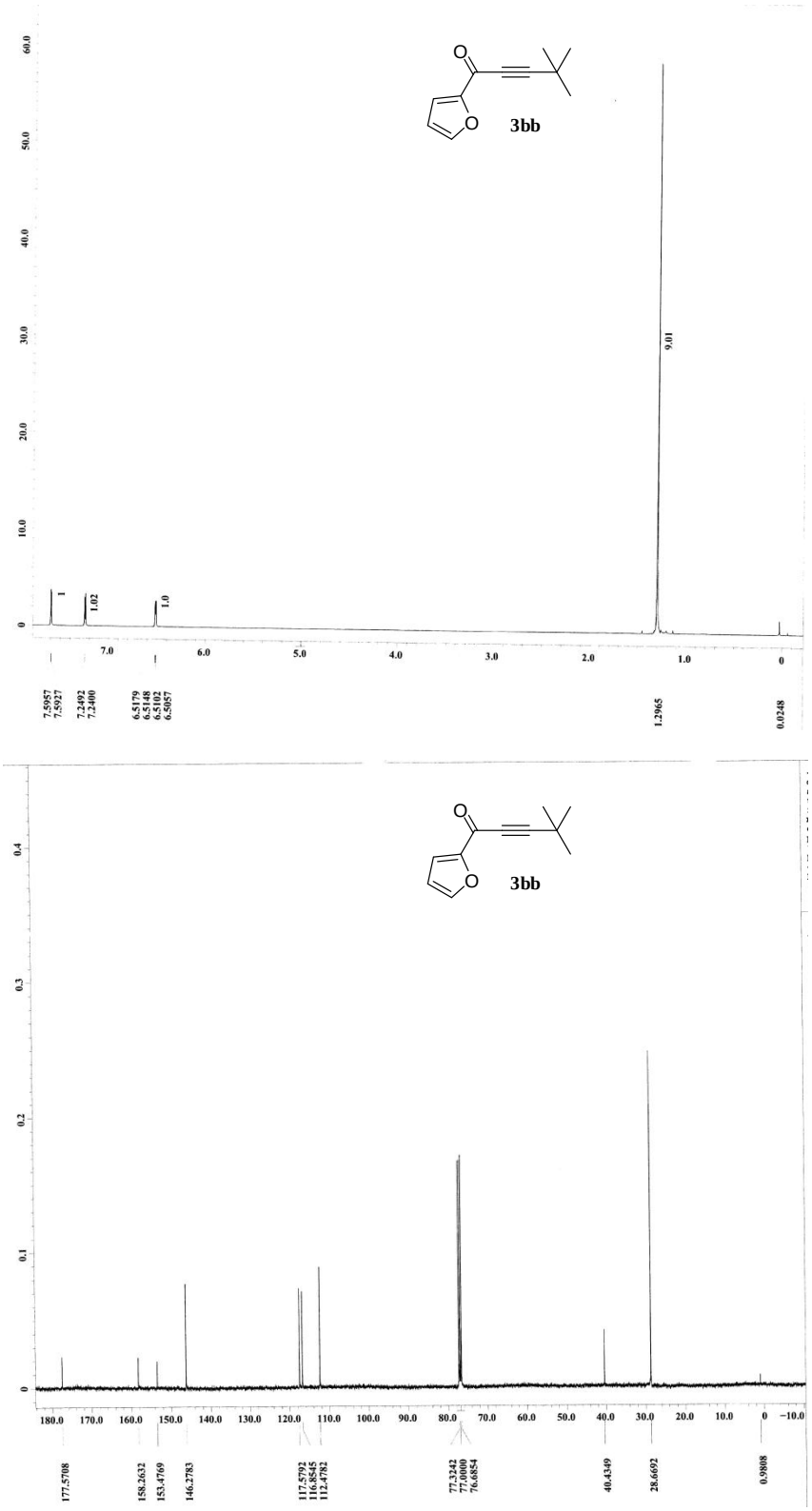



**Figure S9.** $^{1}H$ and $^{13}C$ NMR spectra of 1-(furan-2-yl)-4,4-dimethylpent-2-yn-1-one.

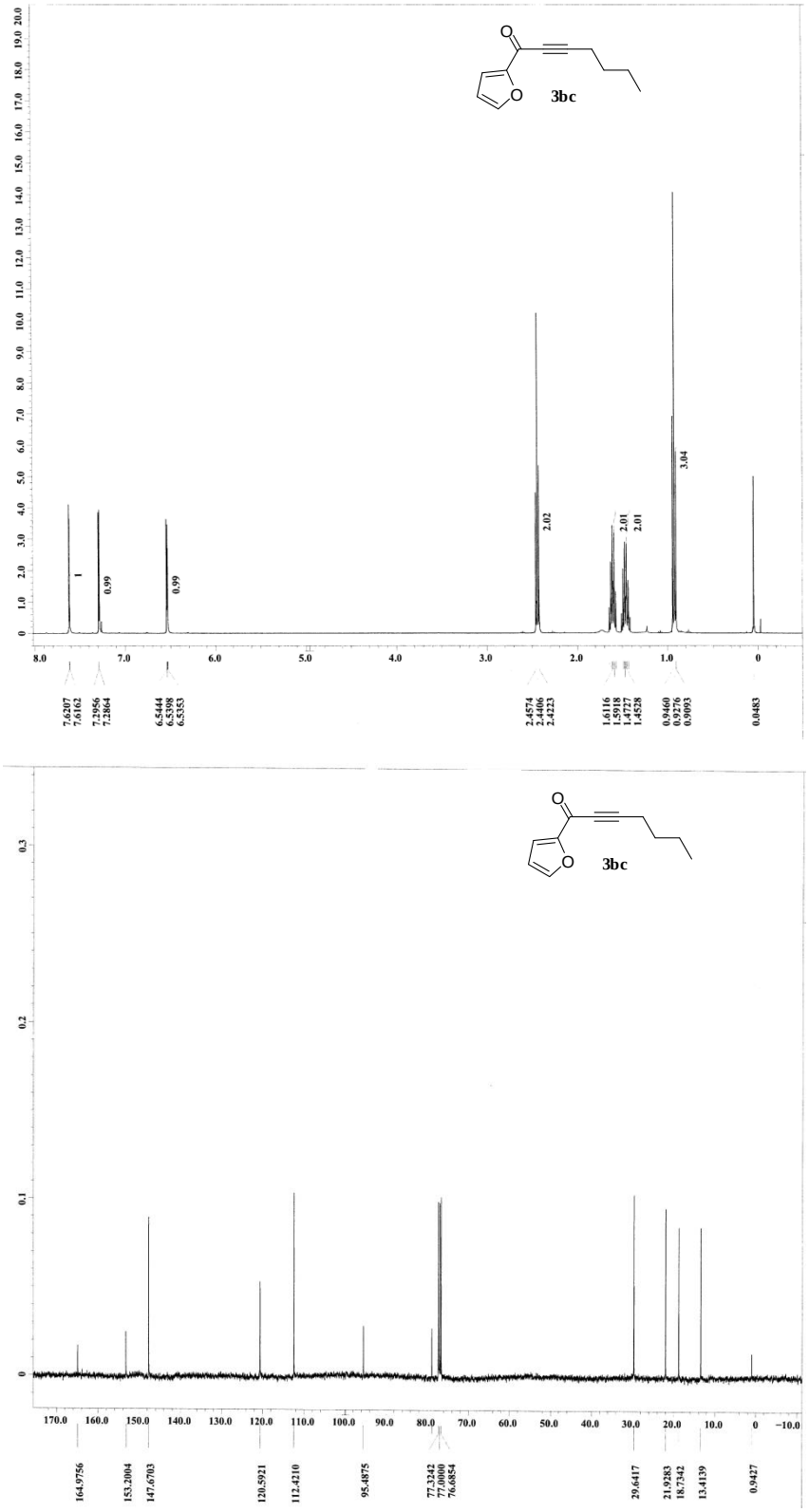



**Figure S10.** $^{1}H$ and $^{13}C$ NMR spectra of 1-(furan-2-yl)hept-2-yn-1-one.

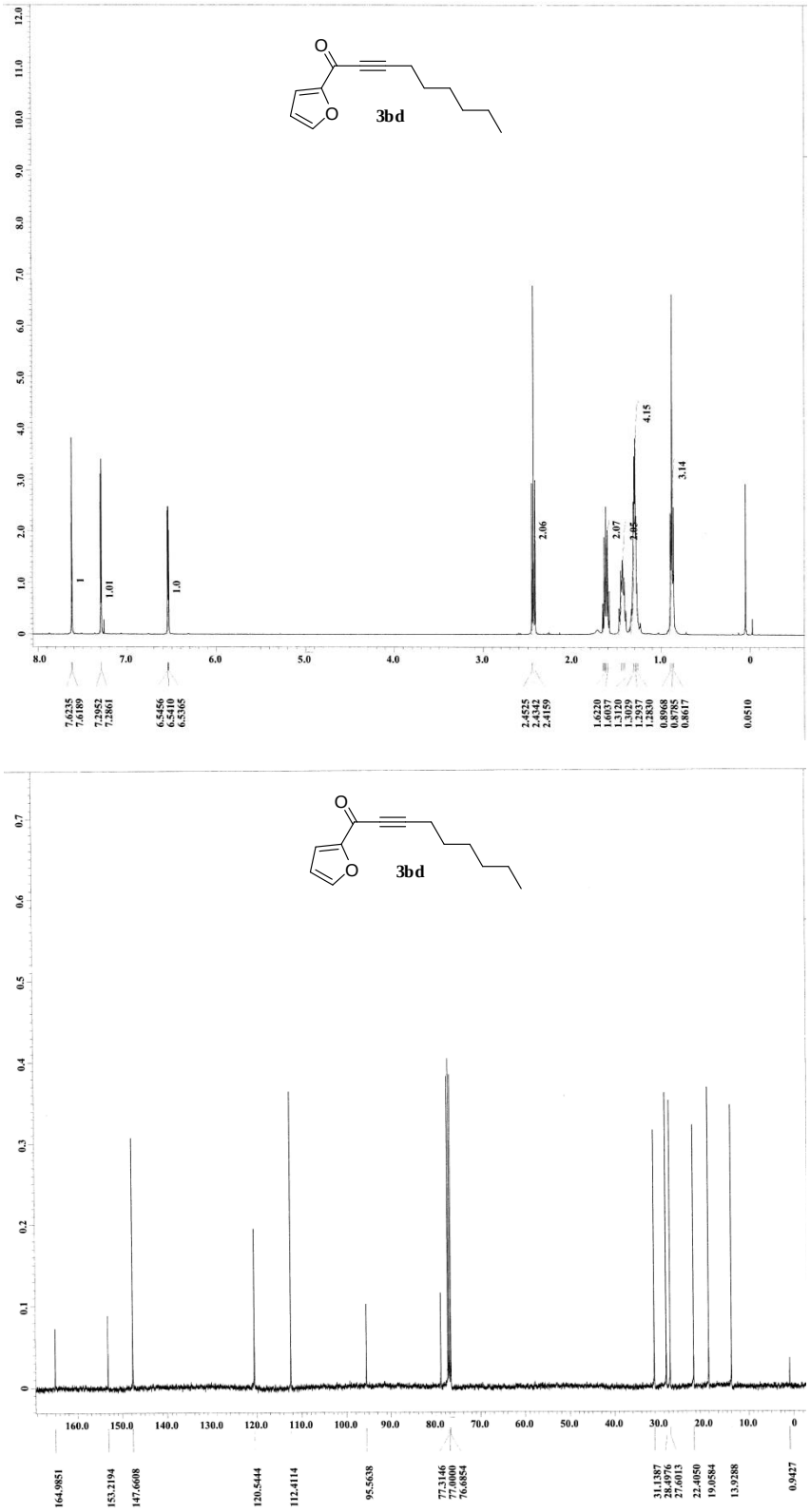



**Figure S11.** $^{1}H$ and $^{13}C$ NMR spectra of 1-(furan-2-yl)non-2-yn-1-one.

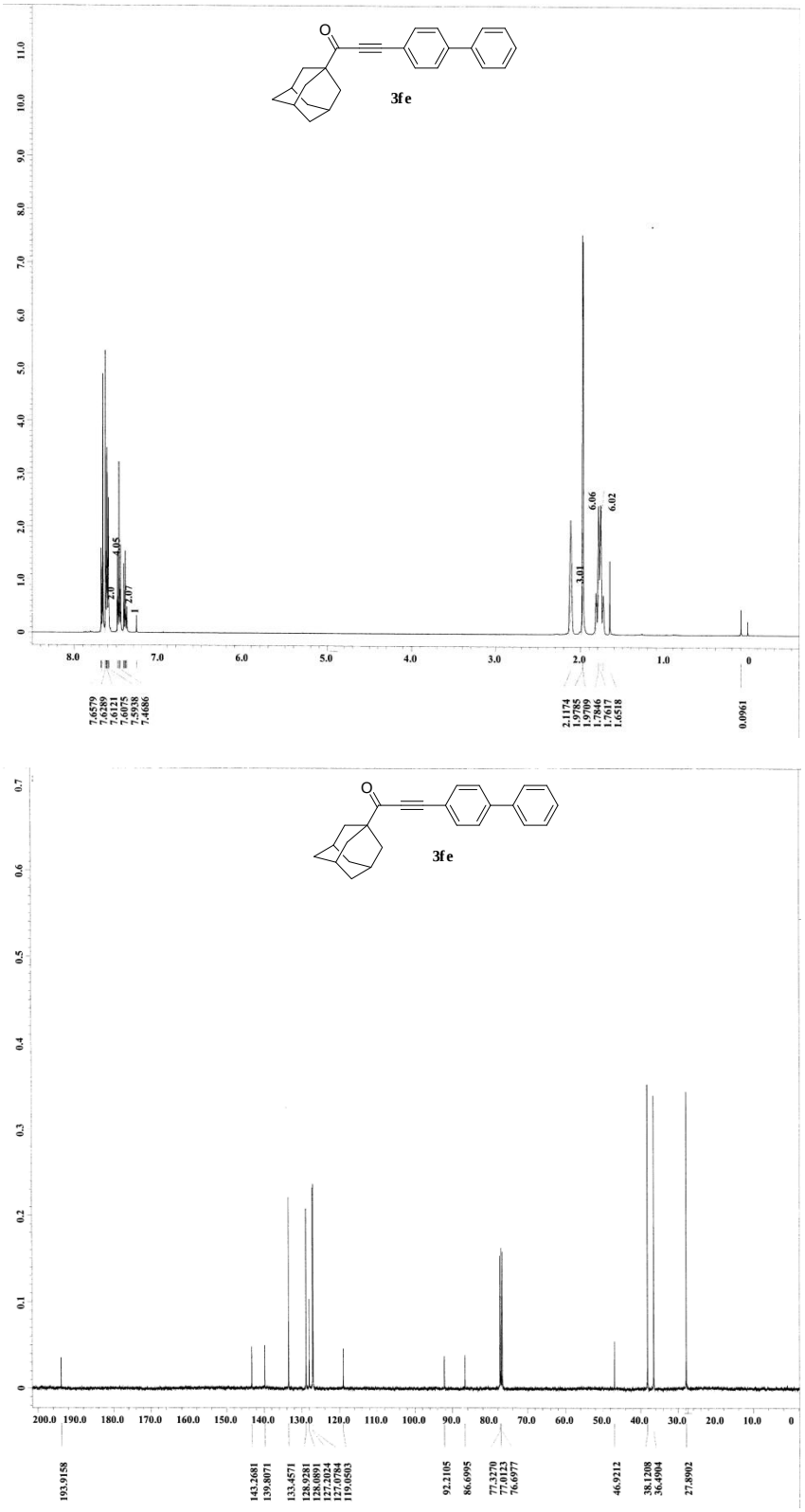



**Figure S12.** $^{1}H$ and $^{13}C$ NMR spectra of 3-(Biphenyl-4-yl)-1-(1-adamantyl)prop-2-yn-1-one.

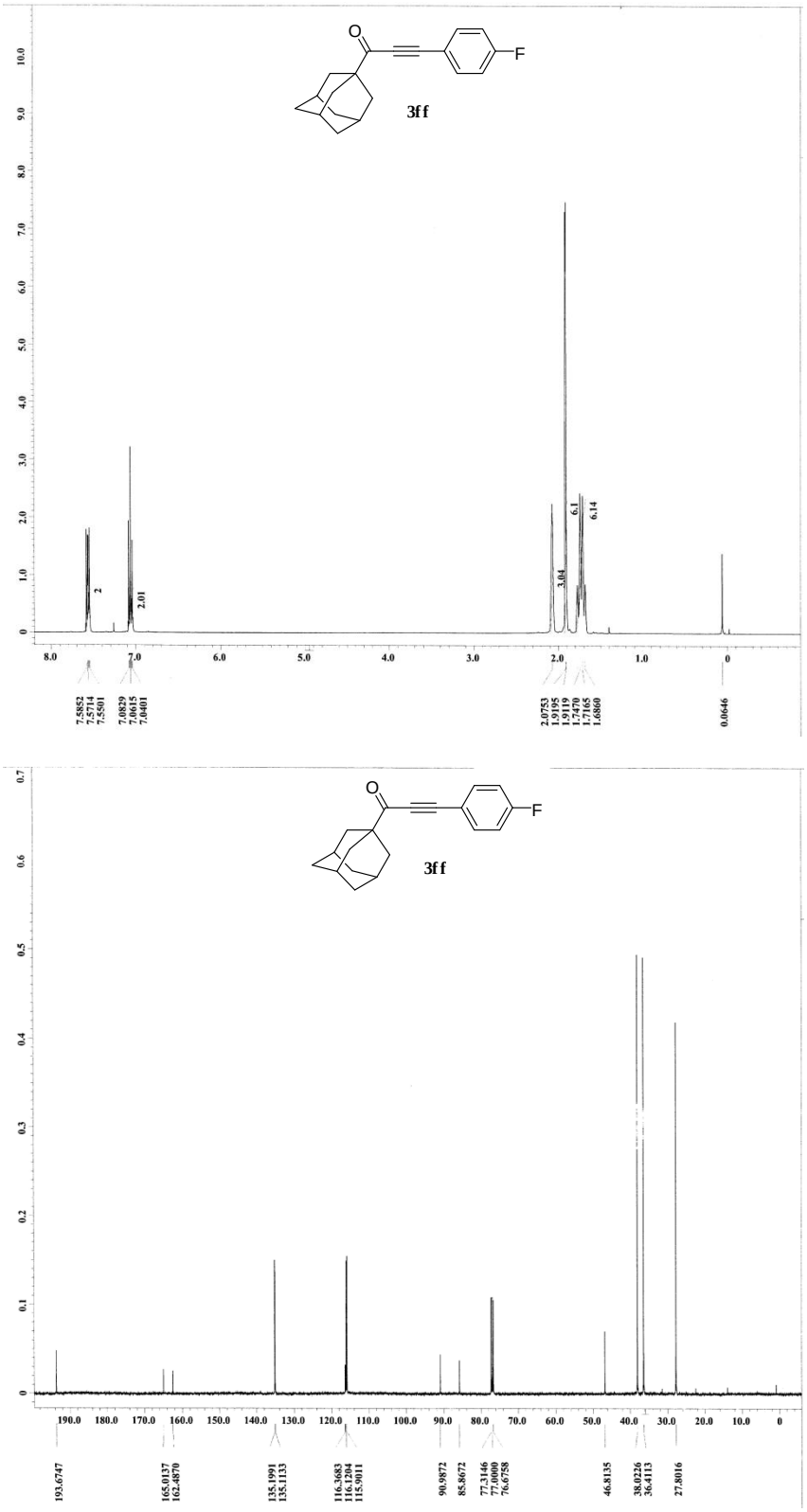



**Figure S13.** $^{1}H$ and $^{13}C$ NMR spectra of 3-(4-Fluorophenyl)-1-(1-adamantyl)prop-2-yn-1-one.

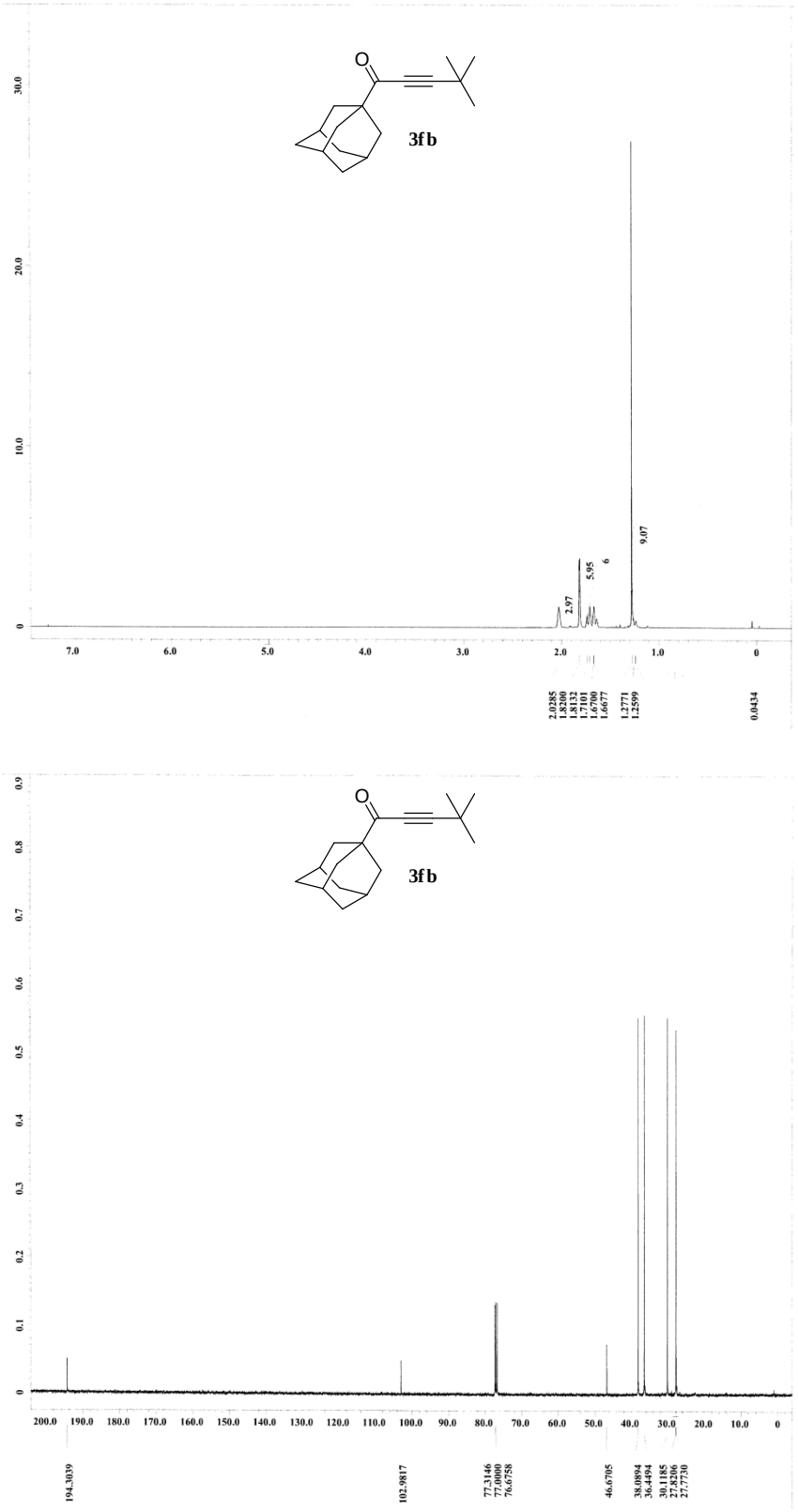



**Figure S14.** $^{1}H$ and $^{13}C$ NMR spectra of 1-adamantyl-4,4-dimethylpent-2-yn-1-one.

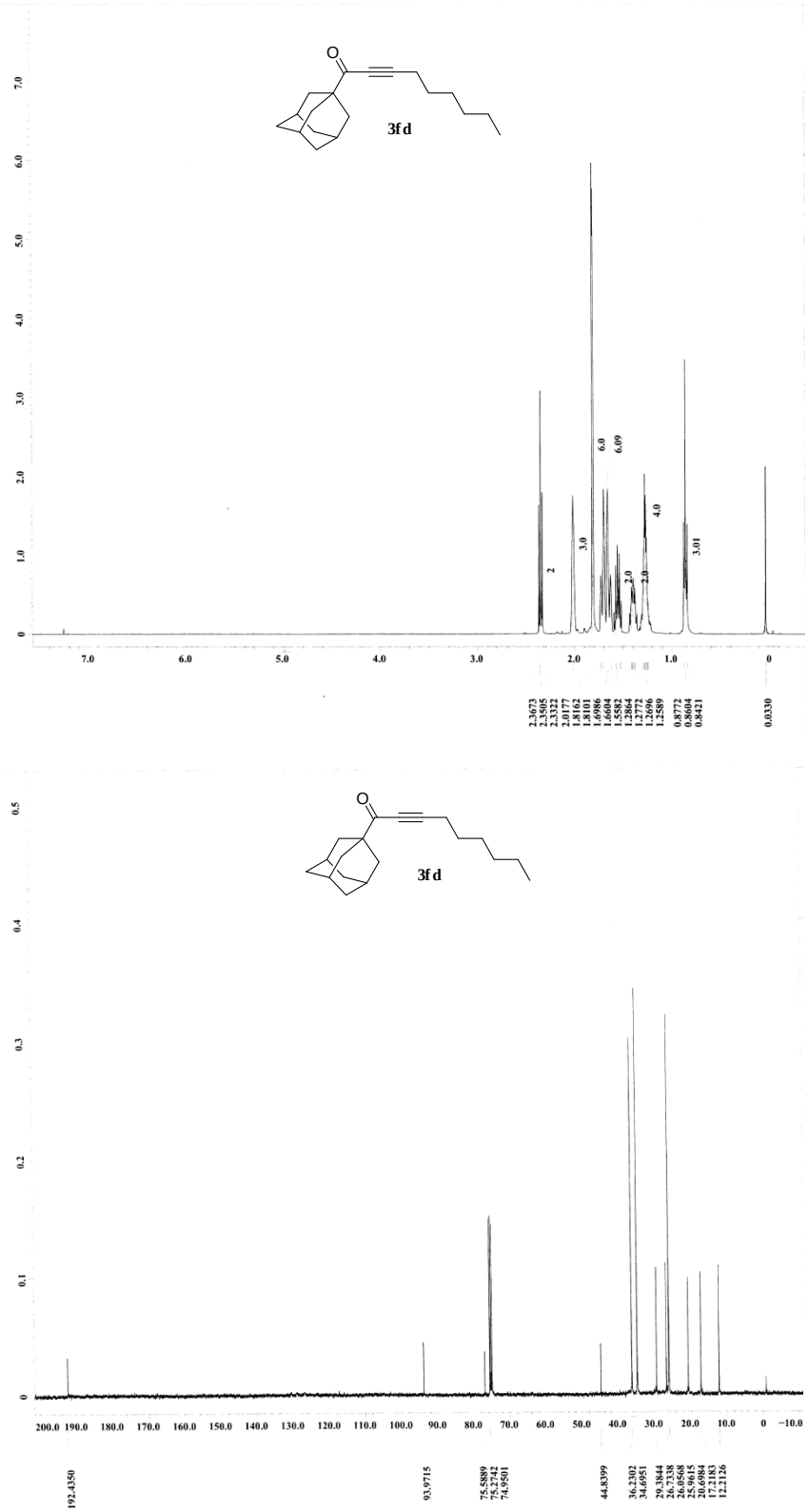



**Figure S15.** $^{1}H$ and $^{13}C$ NMR spectra of 1-(1-Adamantyl)non-2-yn-1-one.

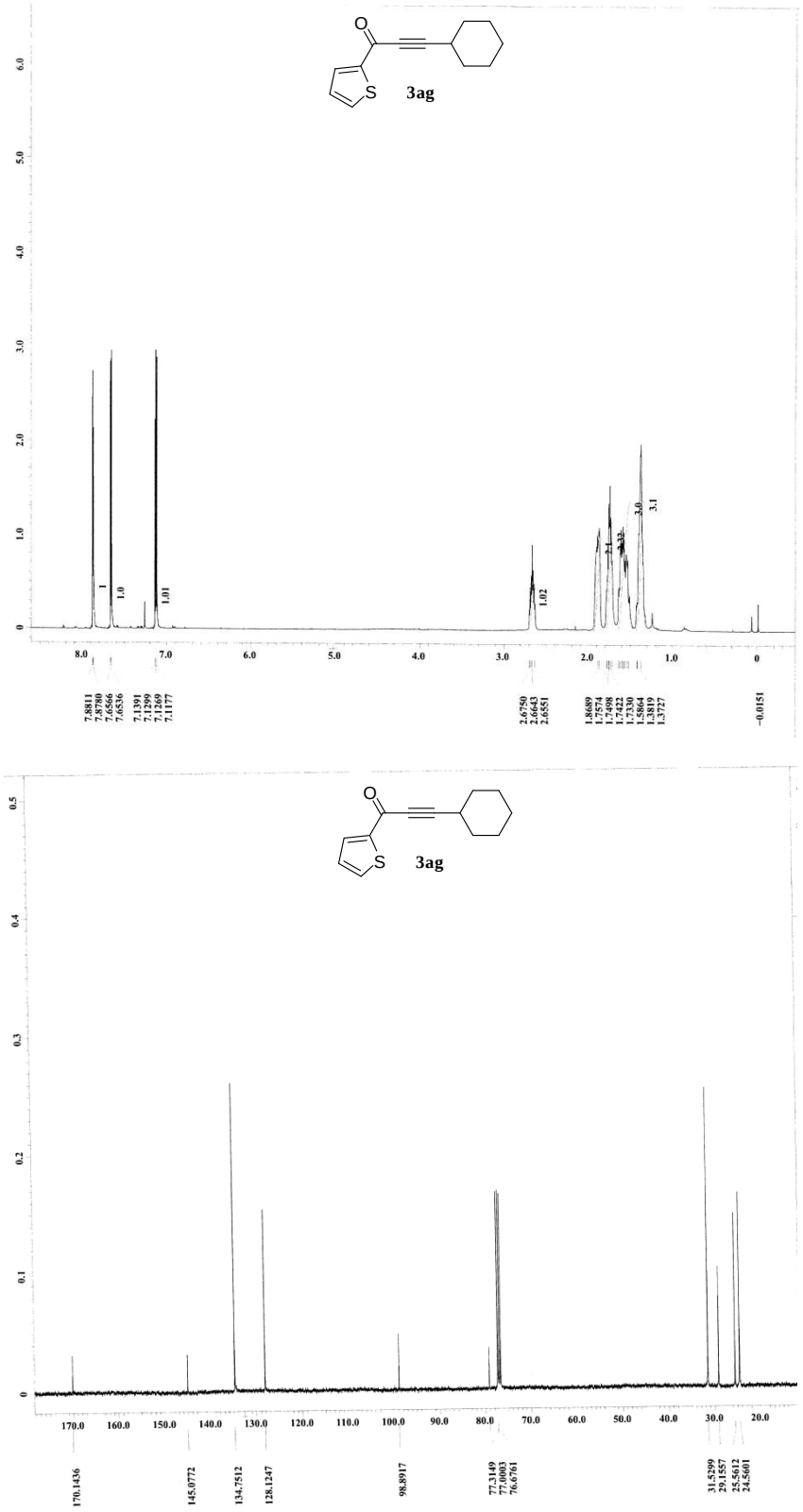



**Figure S16.** $^{1}H$ and $^{13}C$ NMR spectra of 3-cyclohexyl-1-(thiophen-2-yl)prop-2-yn-1-one.

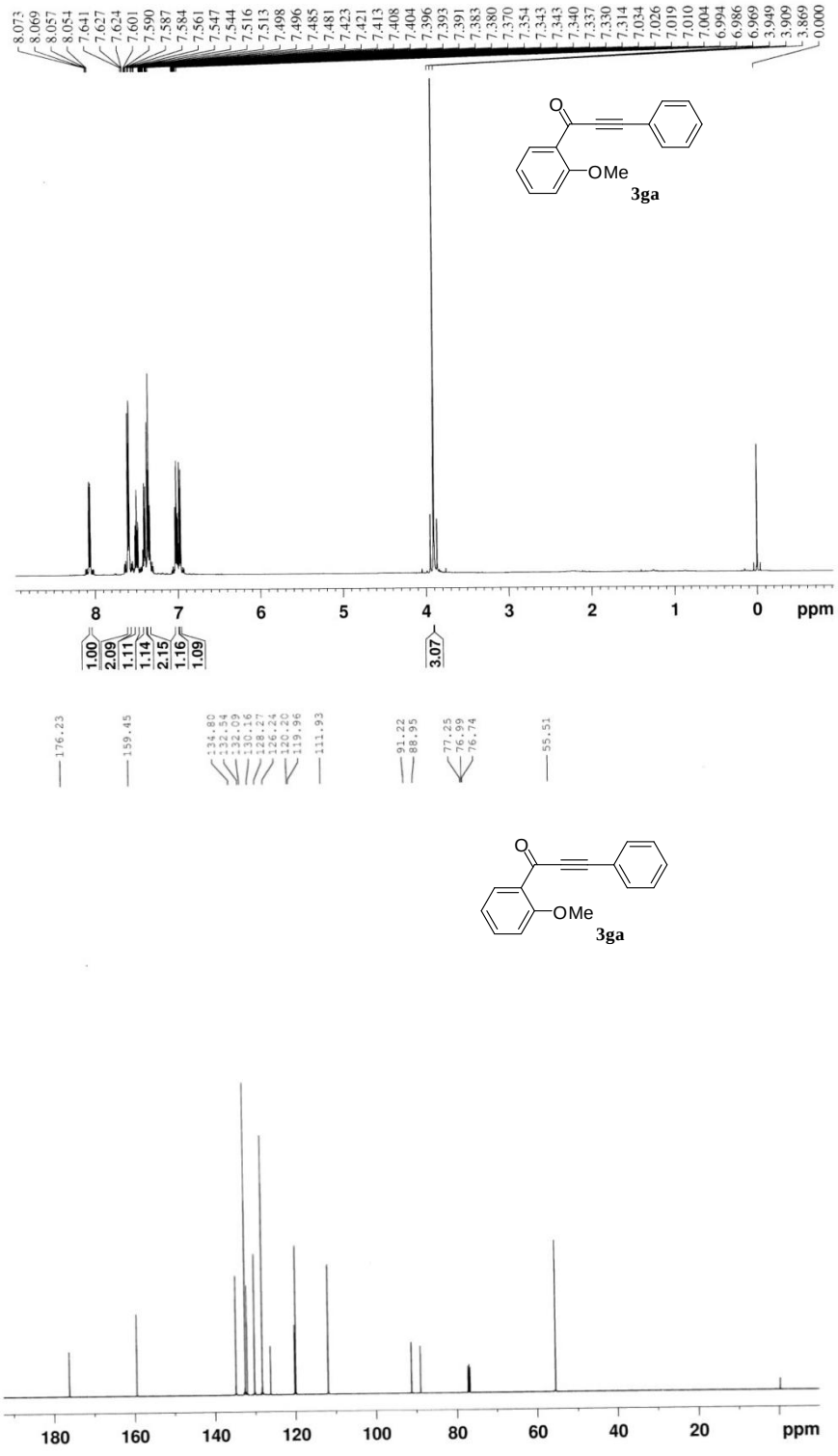



**Figure S17.** $^{1}H$ and $^{13}C$ NMR spectra of 1-(2-methoxyphenyl)-3-phenylprop-2-yn-1-one.

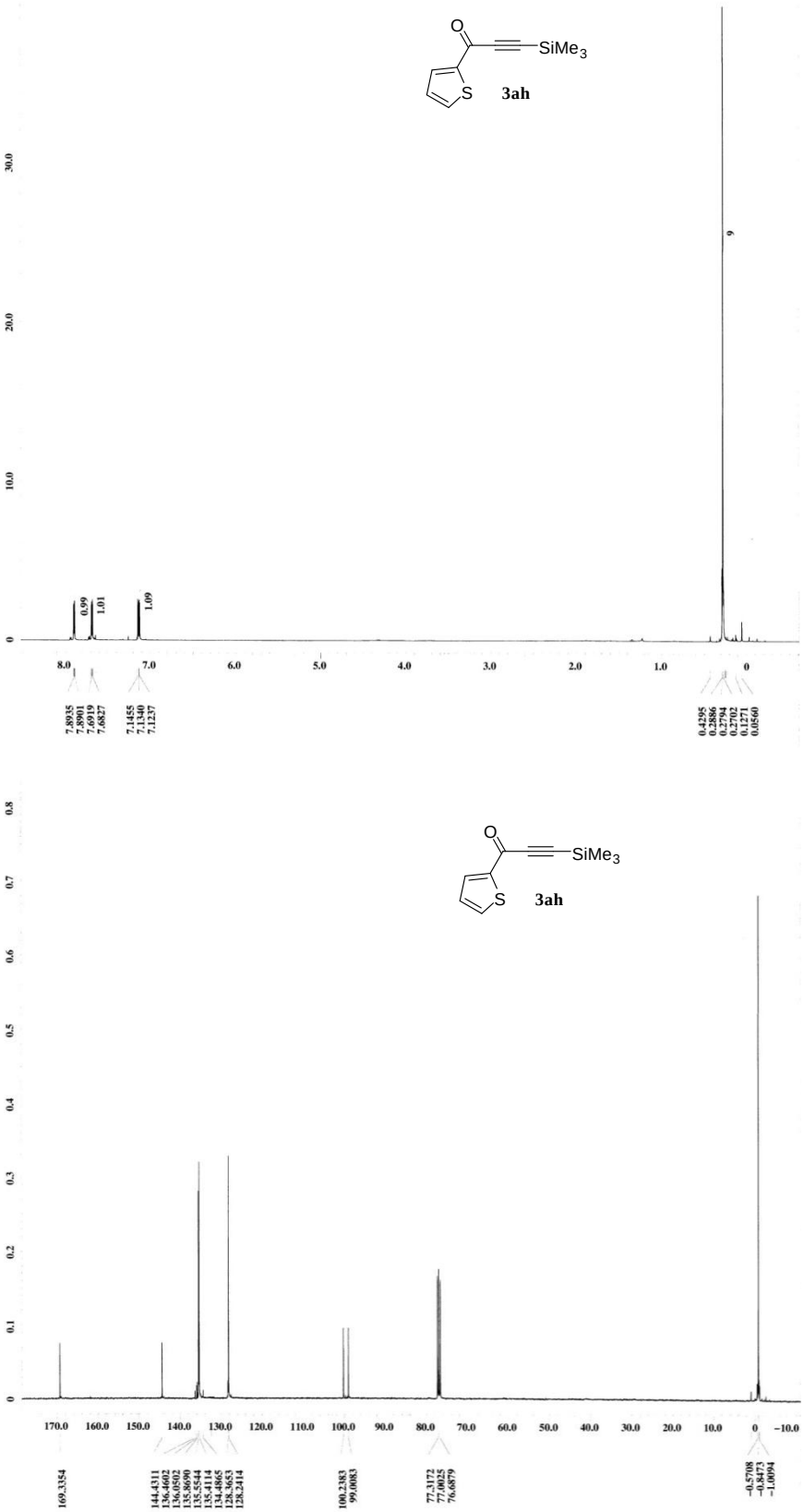



**Figure S18.** $^{1}H$ and $^{13}C$ NMR spectra of 1-(thiophen-2-yl)-3-(trimethylsilyl)prop-2-yn-1-one.

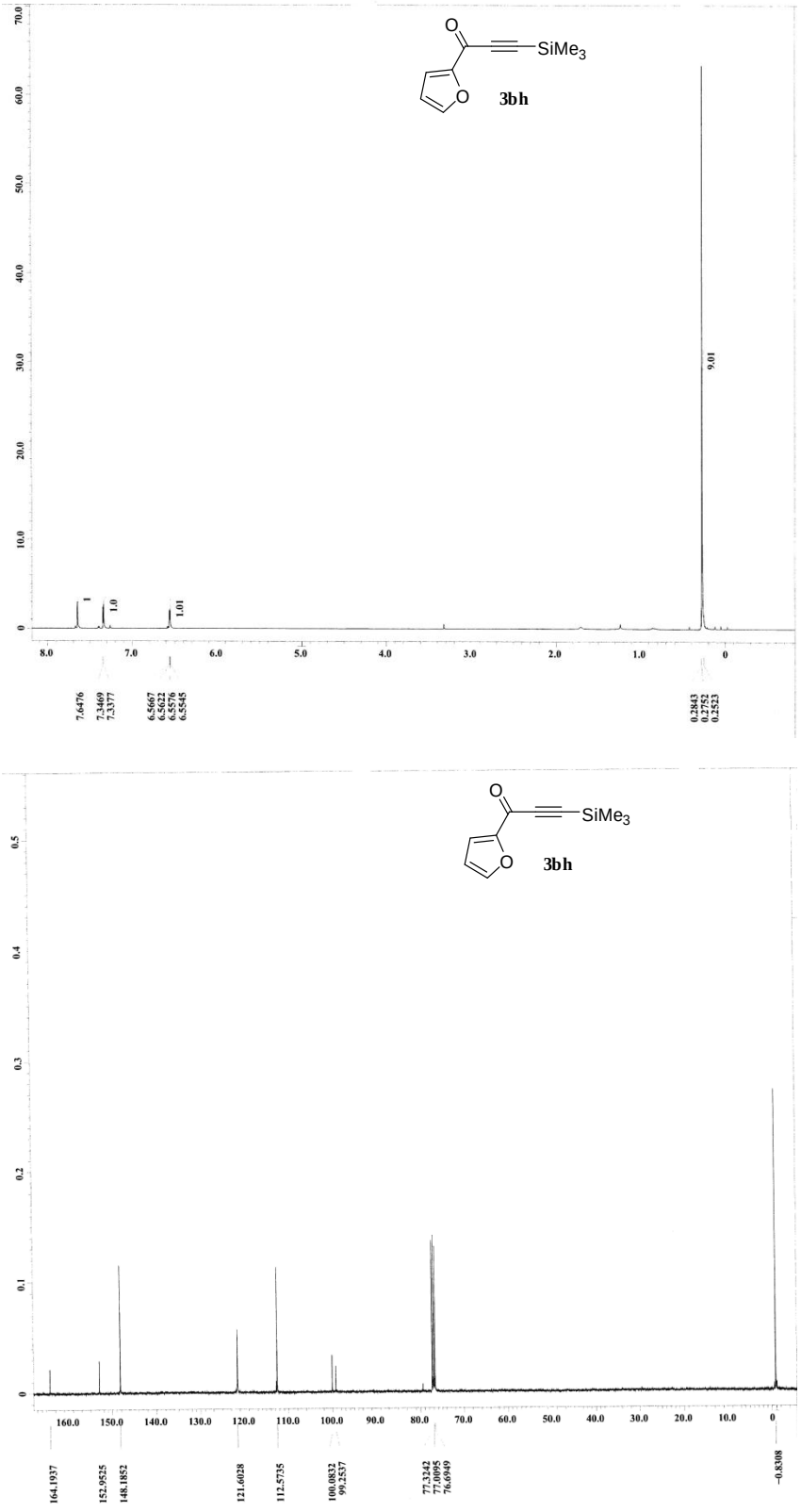



**Figure S19.** $^{1}H$ and $^{13}C$ NMR spectra of 1-(furan-2-yl)-3-(trimethylsilyl)prop-2-yn-1-one.

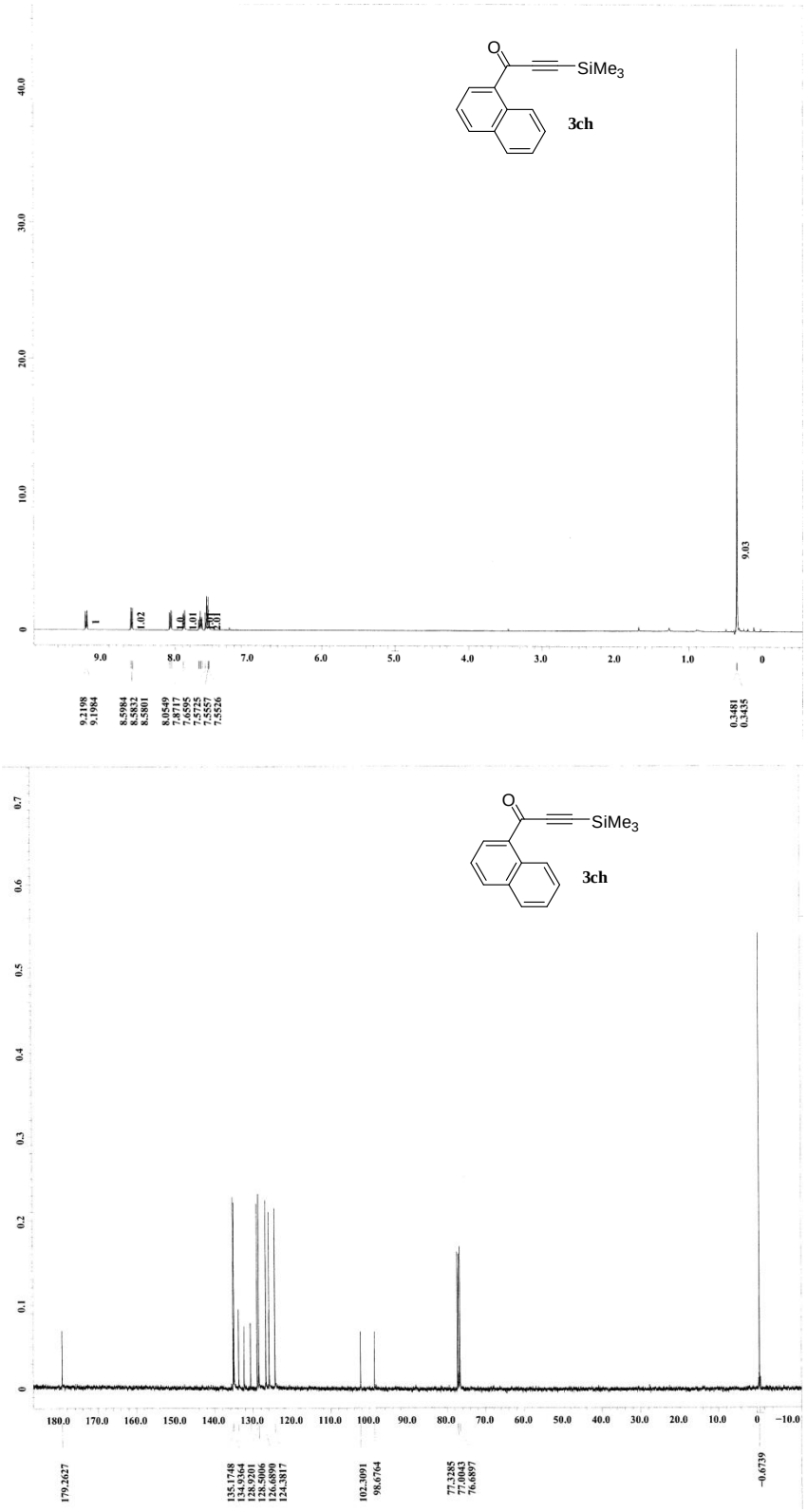



**Figure S20.** $^{1}H$ and $^{13}C$ NMR spectra of 1-(naphthalen-1-yl)-3-(trimethylsilyl)prop-2-yn-1-one.

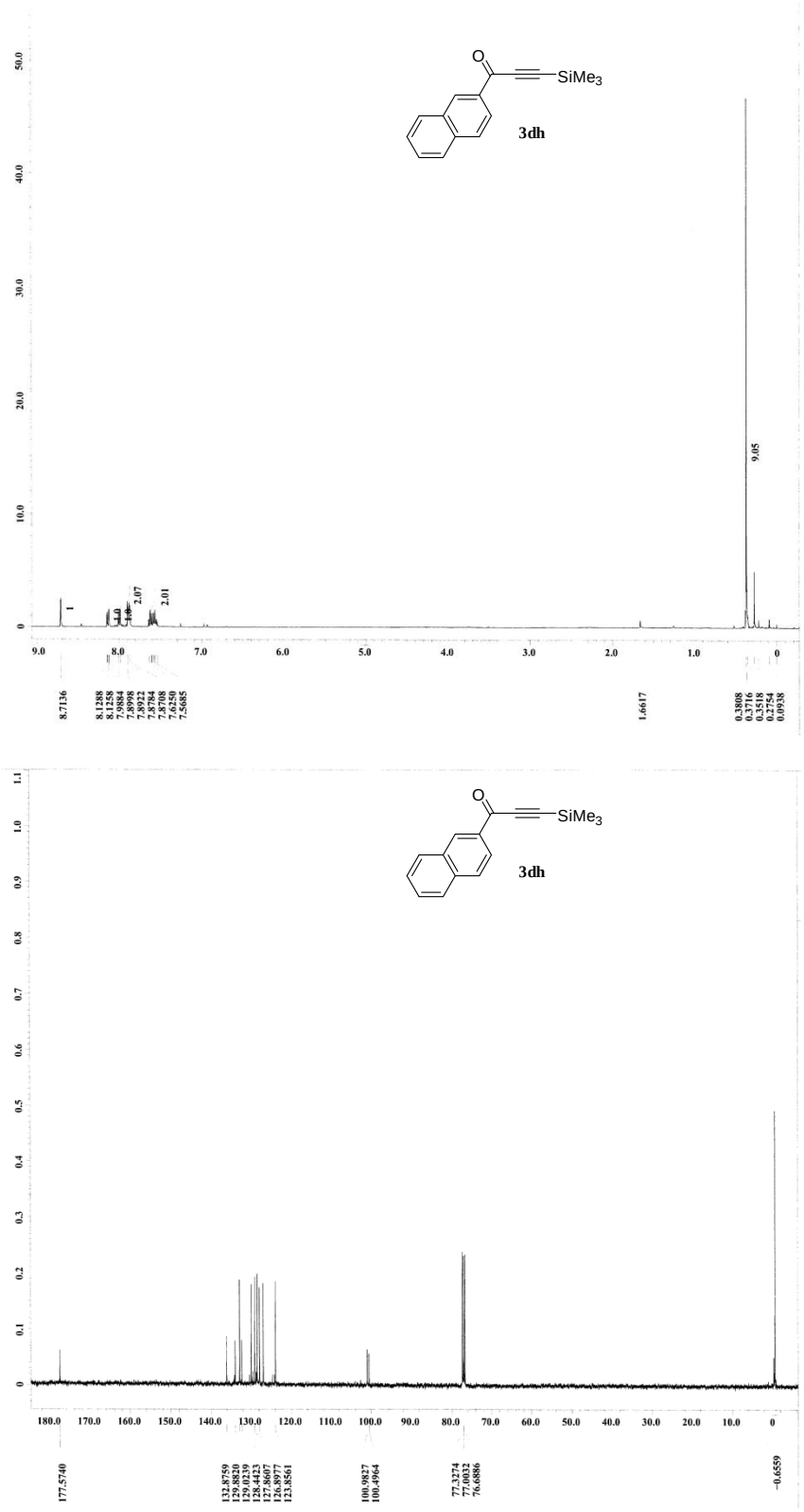



**Figure S21.** $^{1}H$ and $^{13}C$ NMR spectra of 1-(naphthalen-2-yl)-3-(trimethylsilyl)prop-2-yn-1-one.

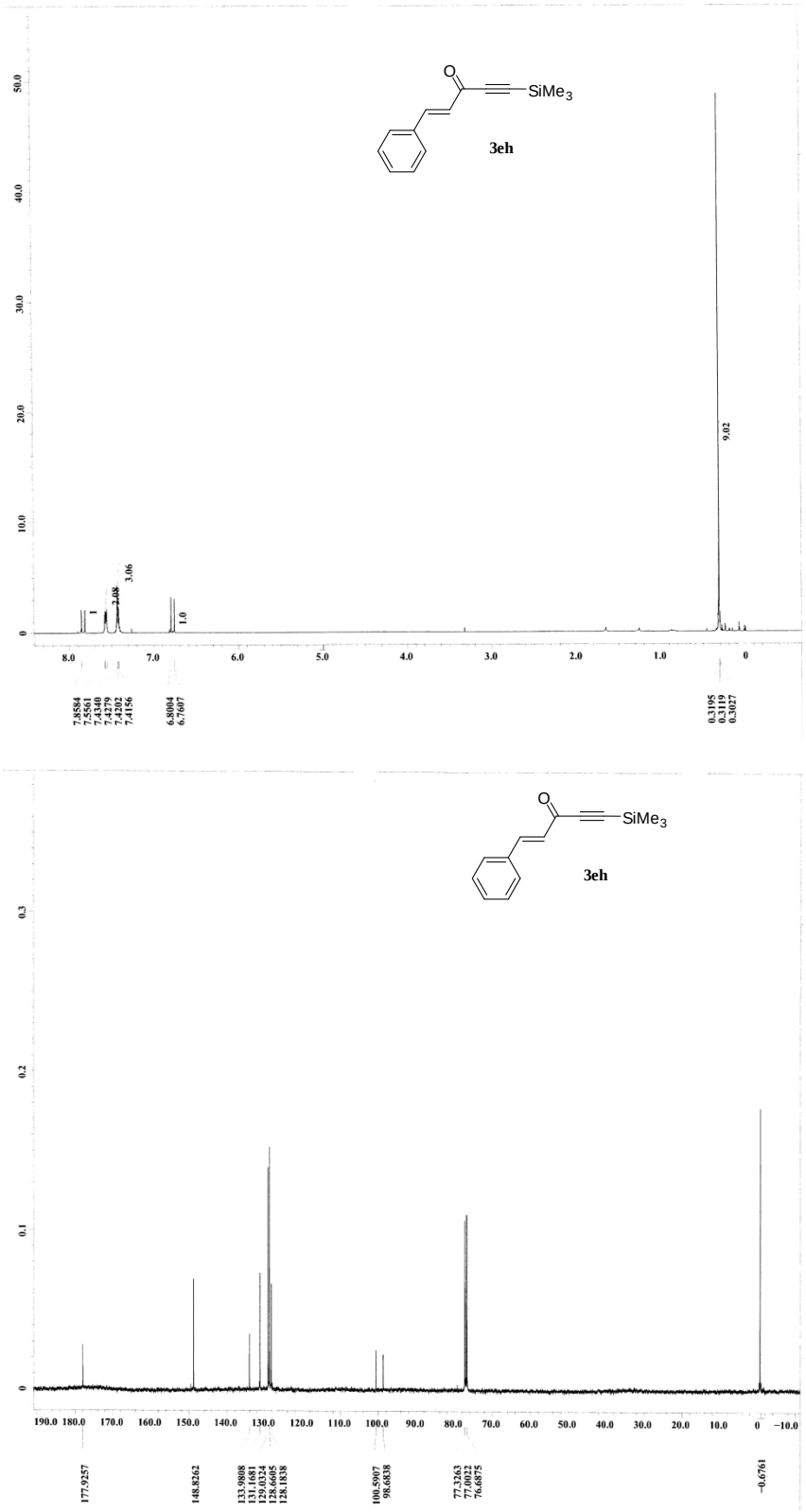



**Figure S22.** $^{1}$H and $^{13}$C NMR spectra of (*E*)-1-phenyl-5-(trimethylsilyl)pent-1-en-4-yn-3-one.

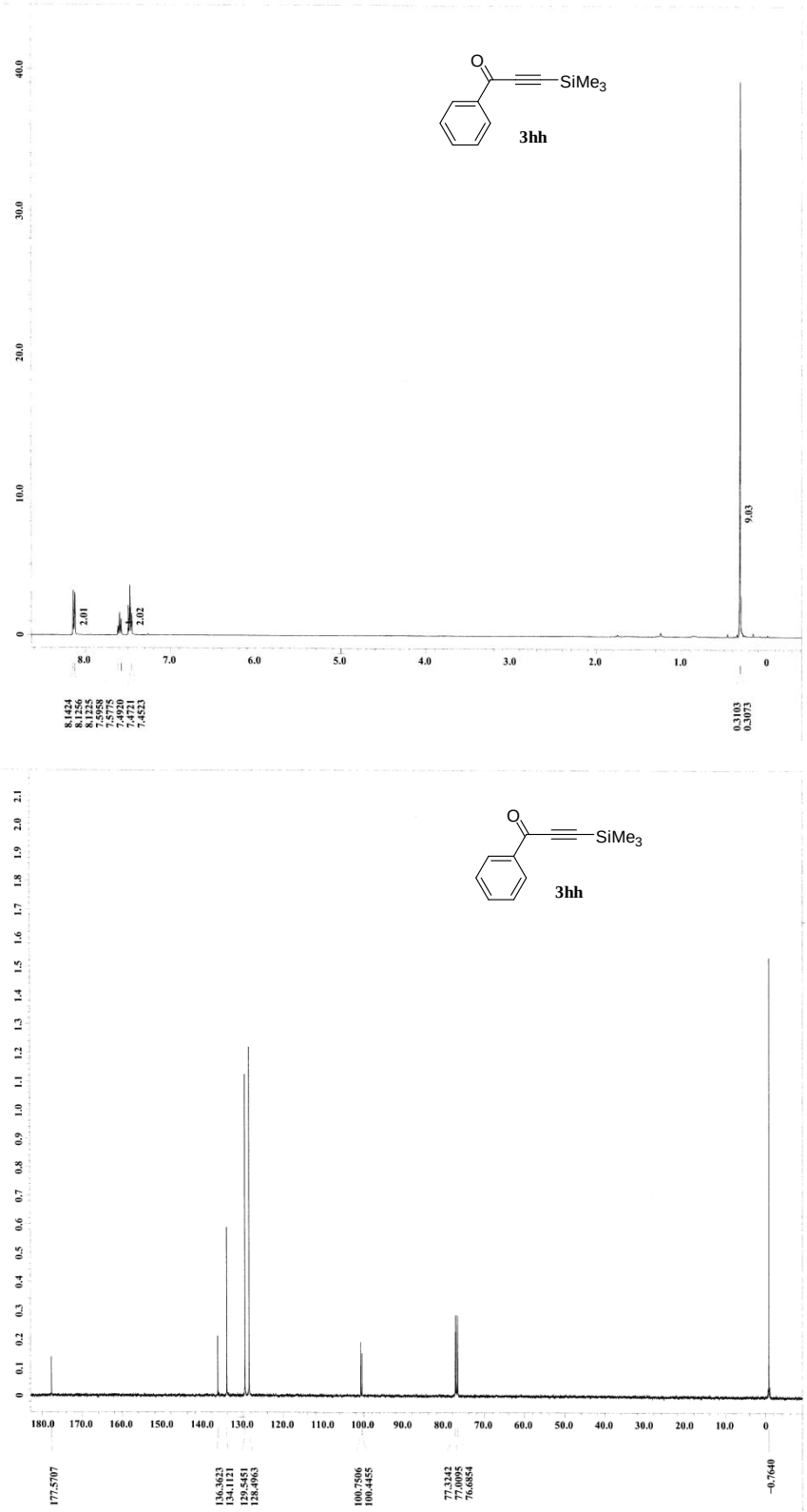



**Figure S23.** $^{1}H$ and $^{13}C$ NMR spectra of 1-phenyl-3-(trimethylsilyl)prop-2-yn-1-one.

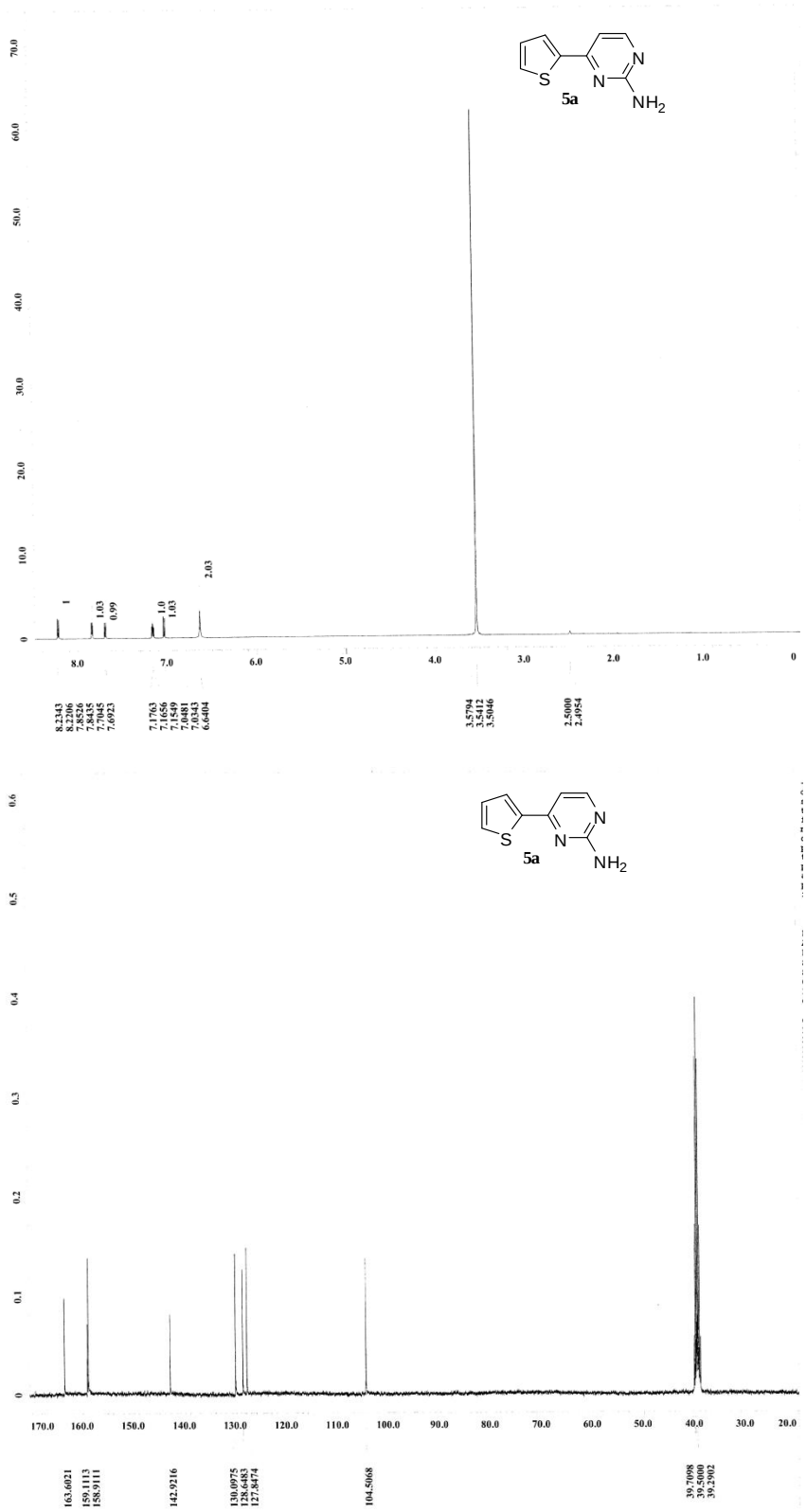



**Figure S24.** $^{1}H$ and $^{13}C$ NMR spectra of 4-(thiophen-2-yl)pyrimidin-2-amine.

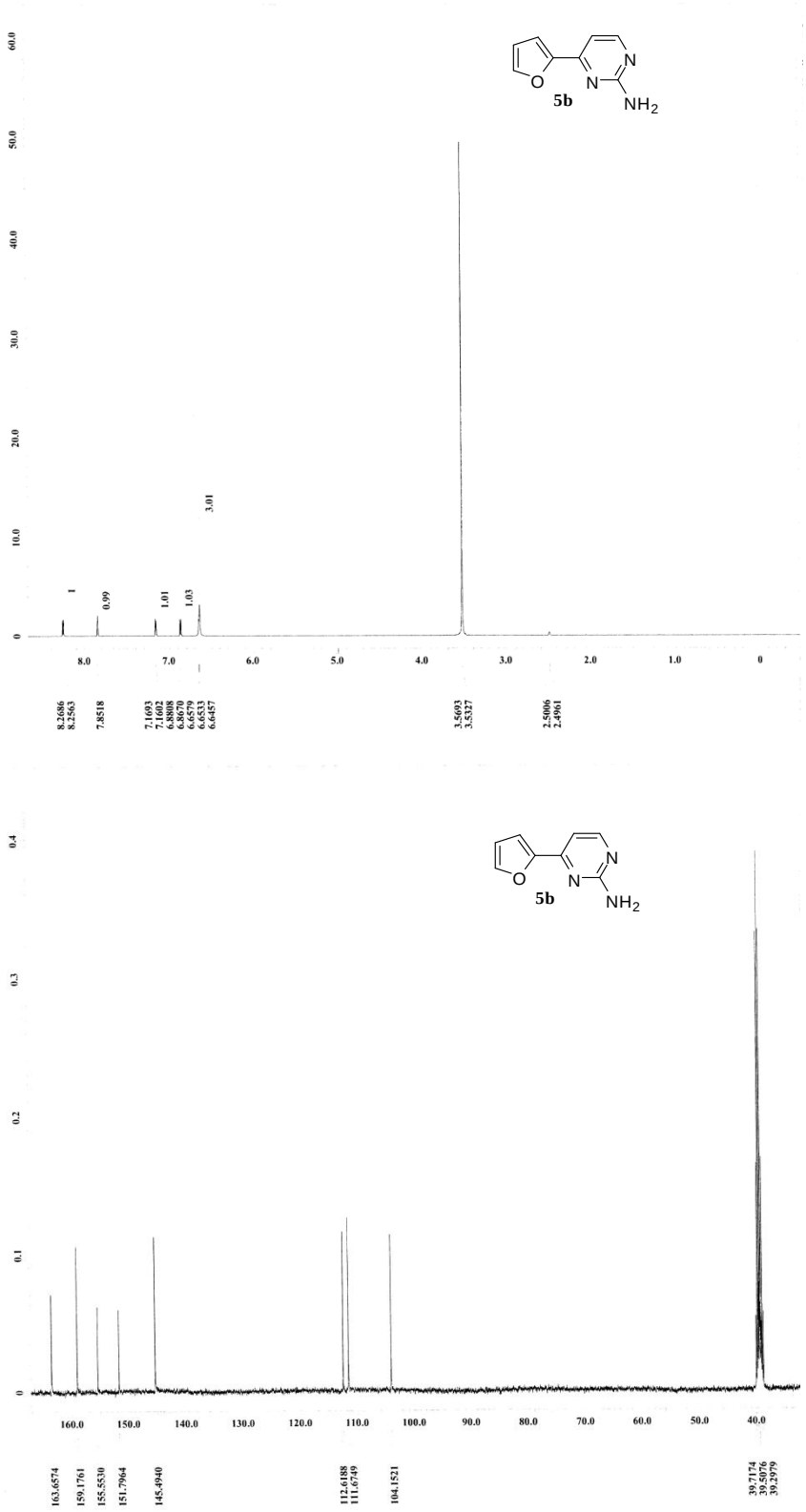



**Figure S25.** $^{1}H$ and $^{13}C$ NMR spectra of 4-(furan-2-yl)pyrimidin-2-amine.

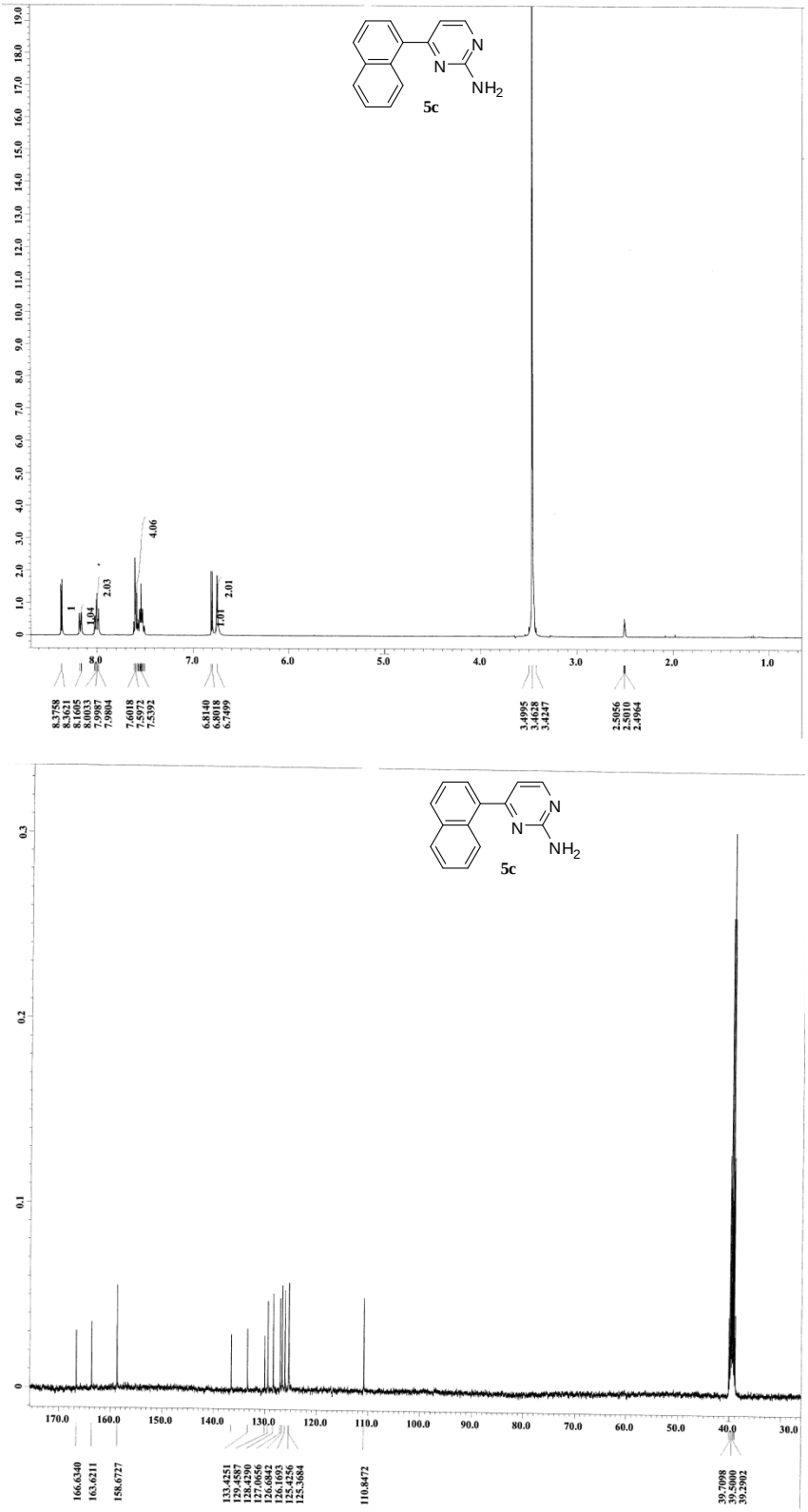



**Figure S26.** $^{1}H$ and $^{13}C$ NMR spectra of 4-(naphthalen-1-yl)pyrimidin-2-amine.

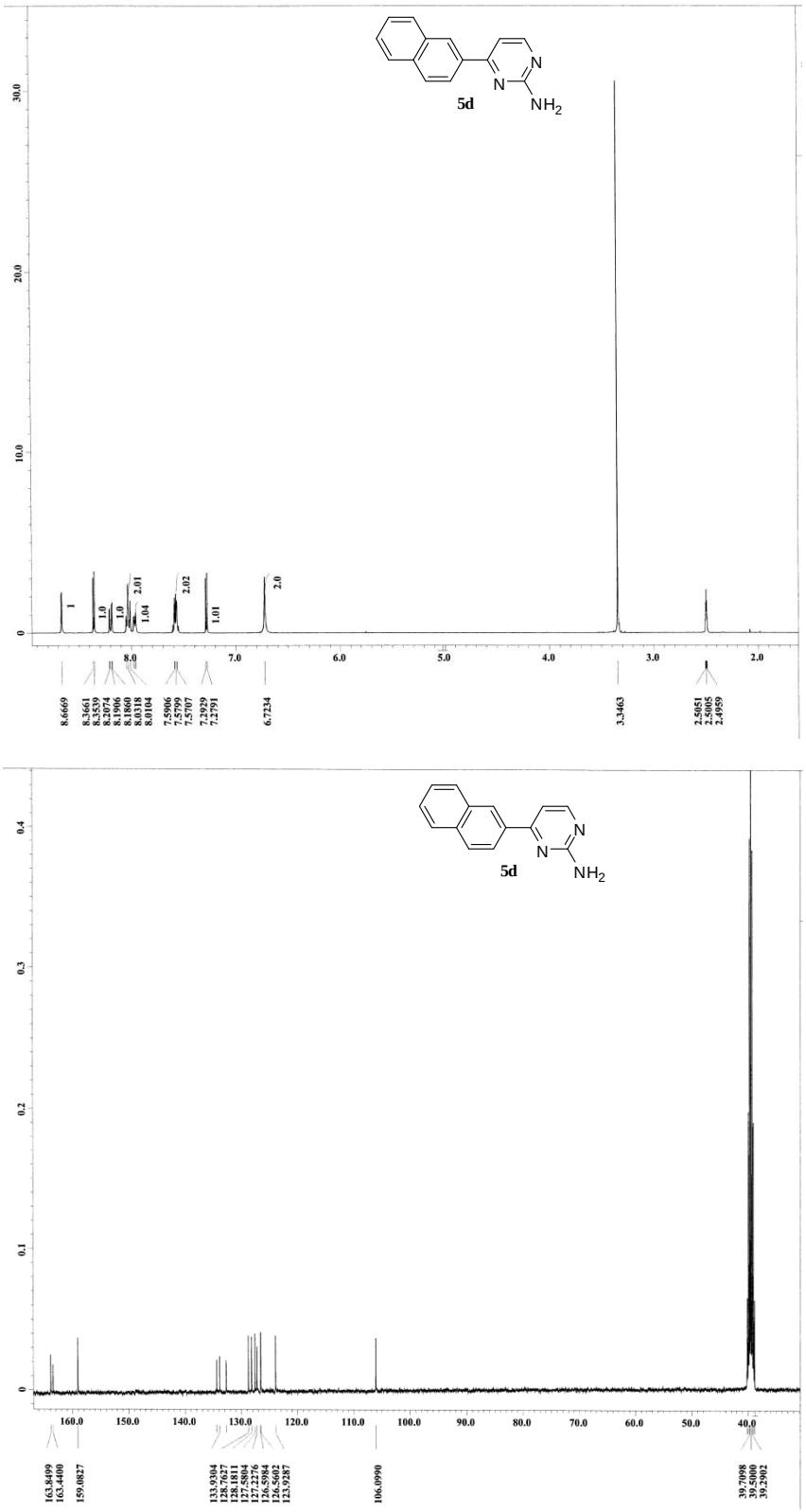



**Figure S27.** $^{1}H$ and $^{13}C$ NMR spectra of 4-(naphthalen-2-yl)pyrimidin-2-amine.

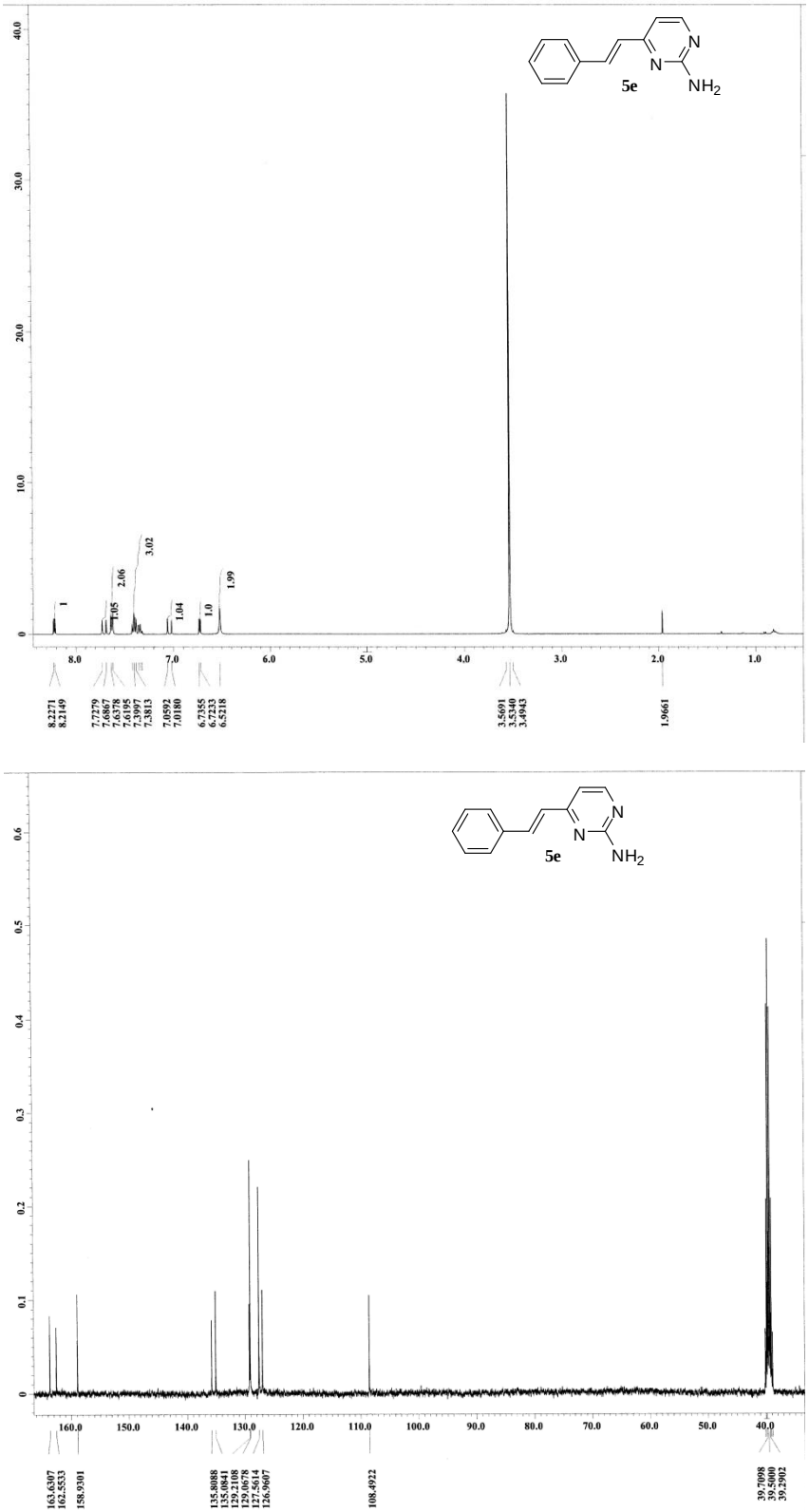



**Figure S28.** $^{1}$H and $^{13}$C NMR spectra of (*E*)-4-styrylpyrimidin-2-amine.

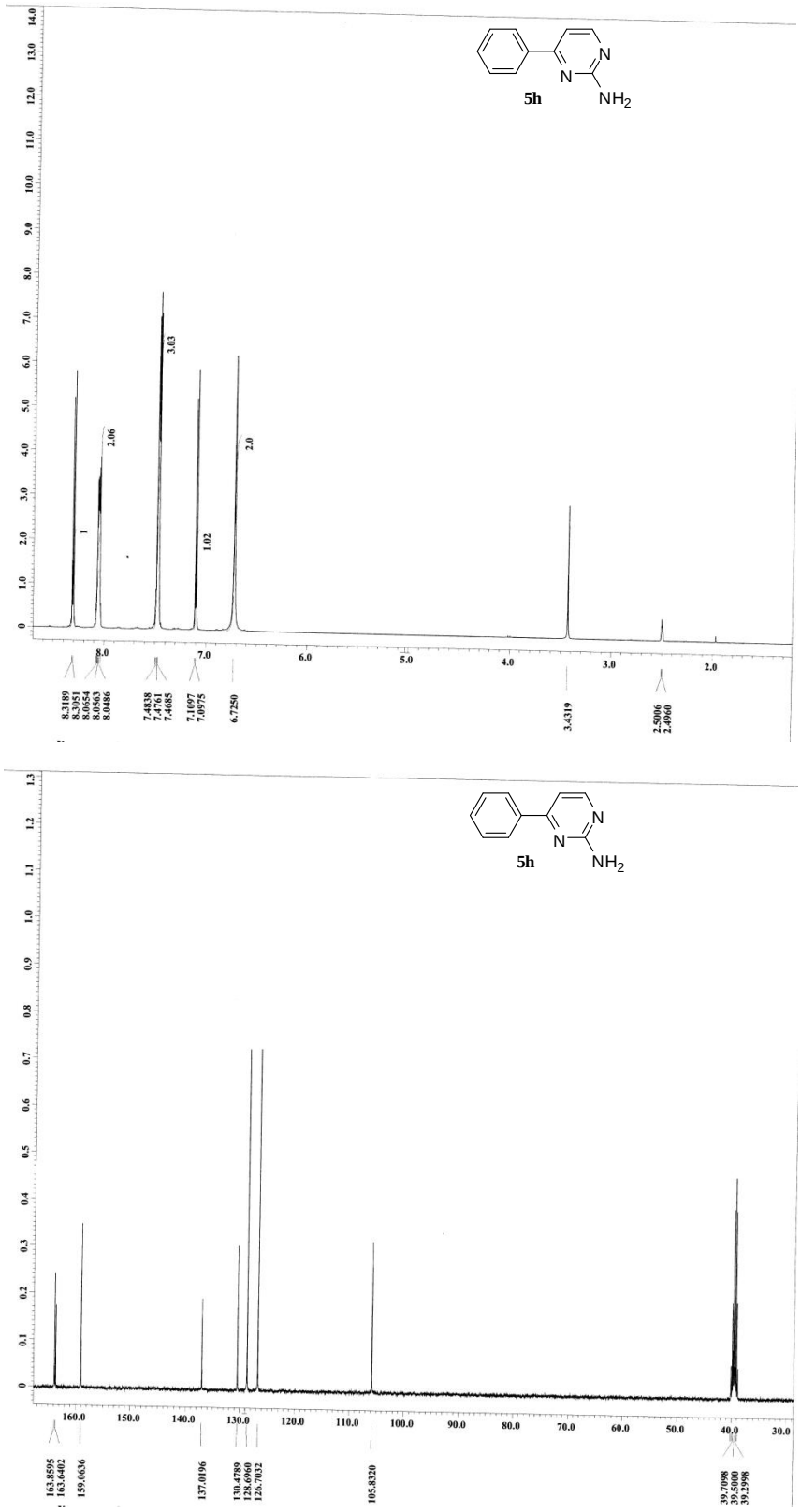



**Figure S29.** $^{1}H$ and $^{13}C$ NMR spectra of 4-phenylpyrimidin-2-amine.

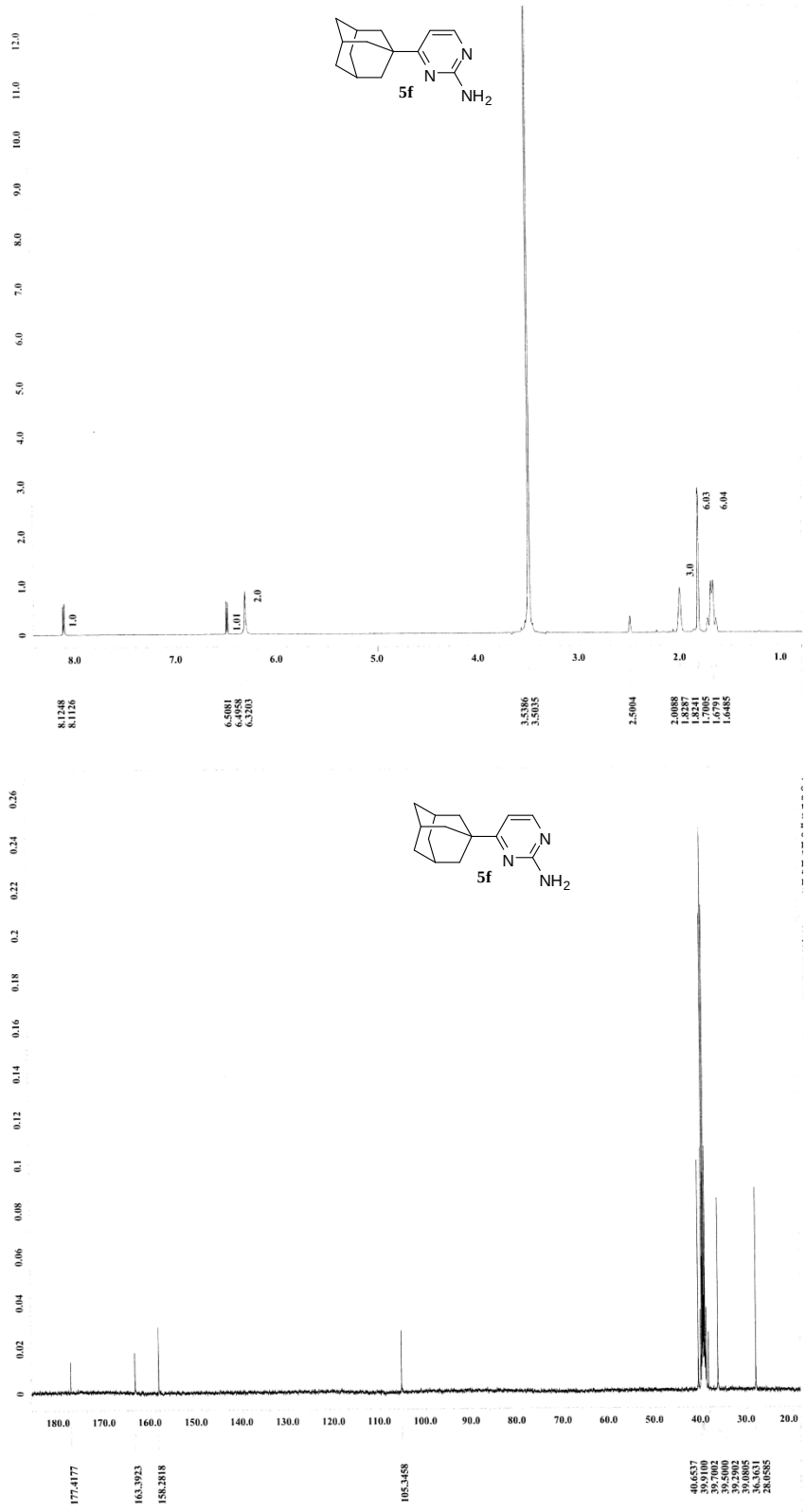



**Figure S30.** $^{1}H$ and $^{13}C$ NMR spectra of 1-Adamantylpyrimidin-2-amine.

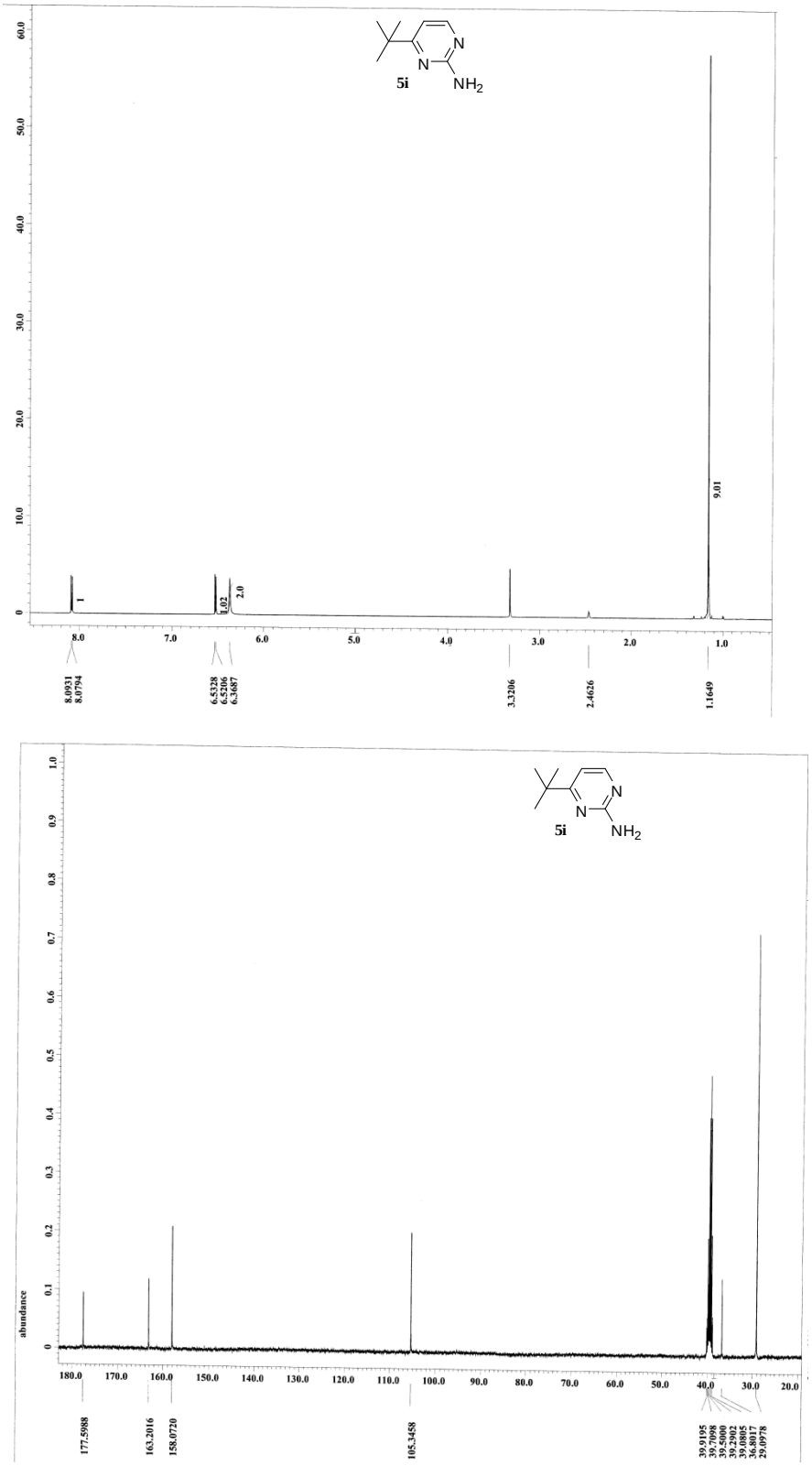



**Figure S31.** $^{1}H$ and $^{13}C$ NMR spectra of 4-*tert*-butylpyrimidin-2-amine.

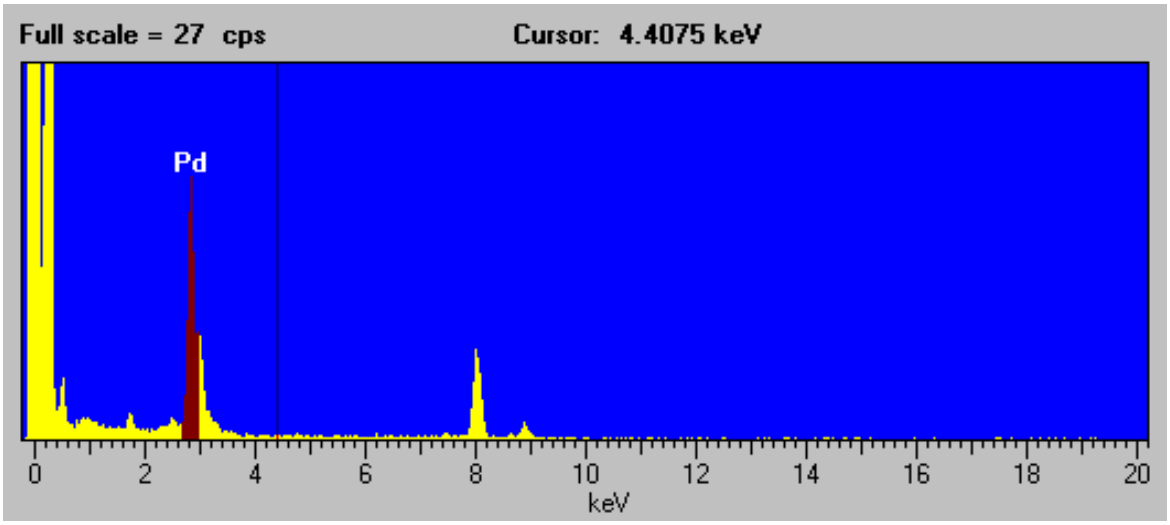
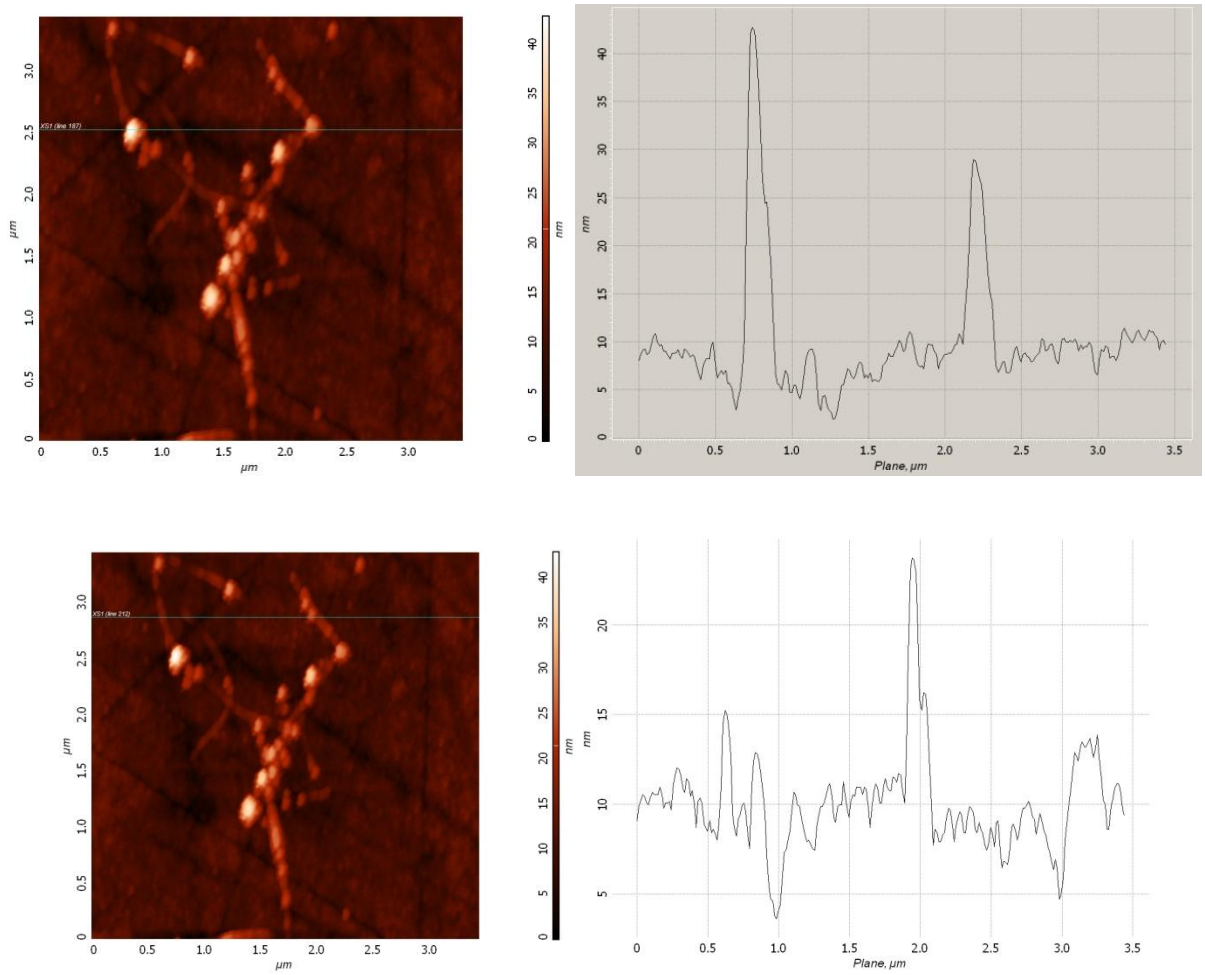



**Figure S32.** EDX spectrum of SWNT-PdNPs collected from TEM confirming the presence of palladium.



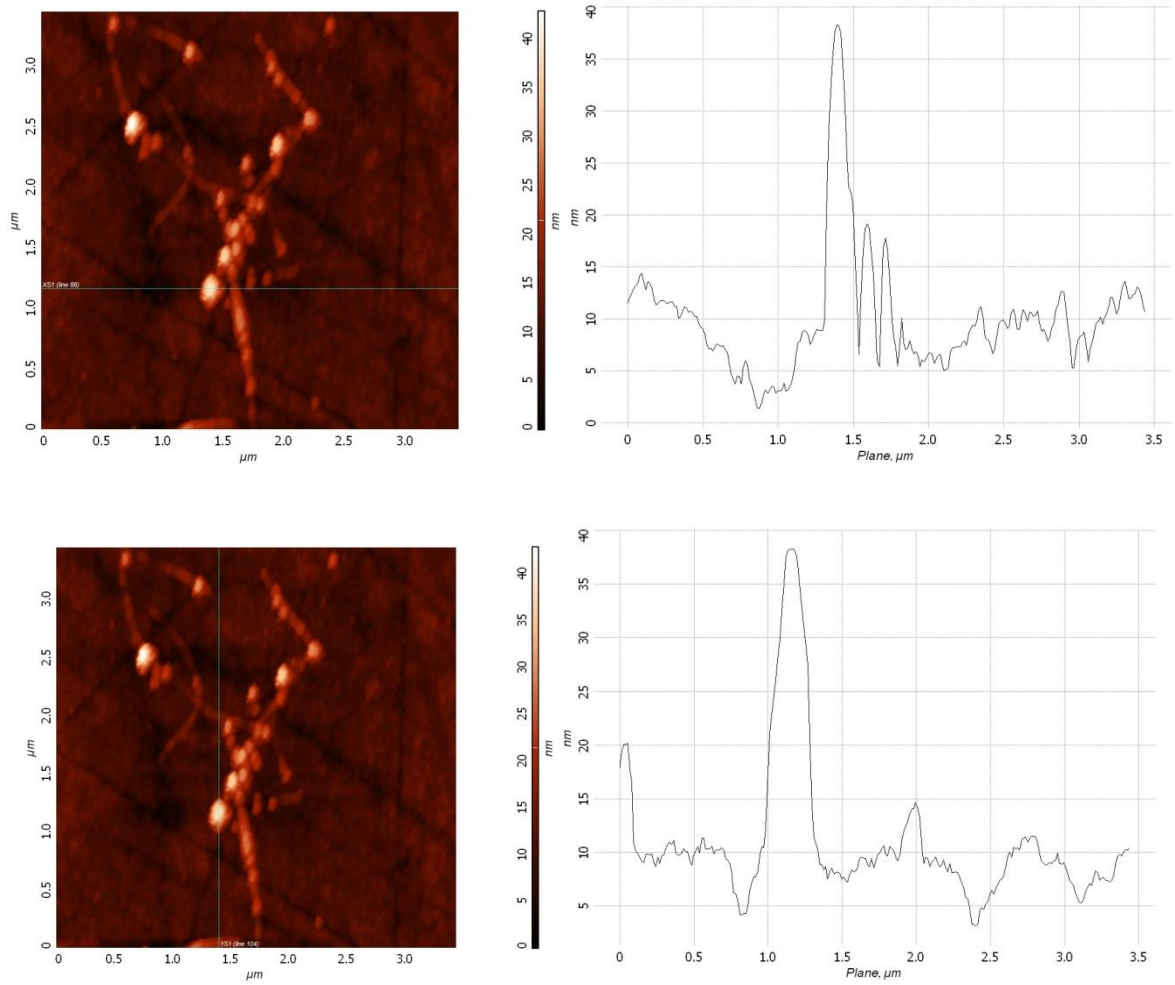



**Figure S33.** Images on the left hand side represent the AFM images of SWNT-PdNPs while the right hand side images represent corresponding height profile diagrams along the horizontal/vertical lines.

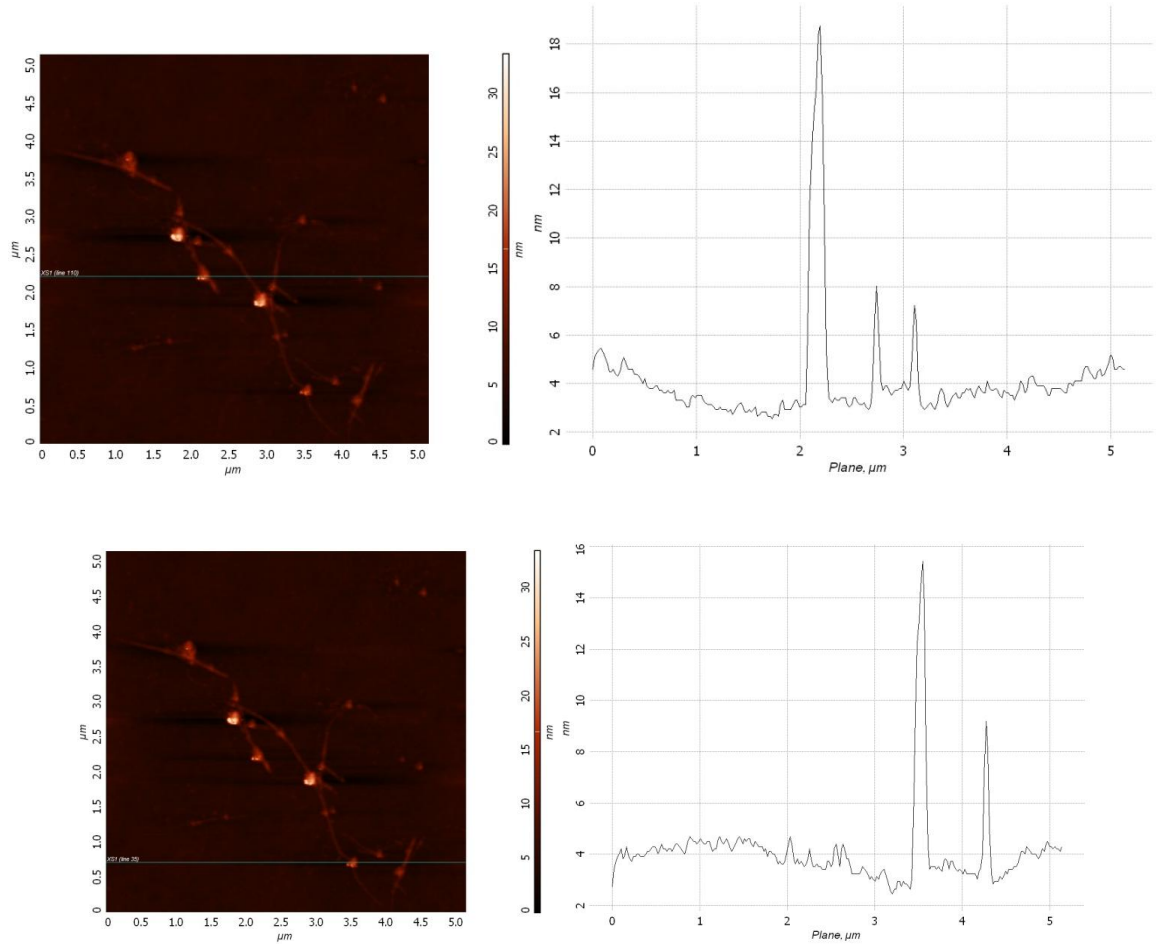



**Figure S34.** Images on the left hand side represent the AFM images of SWNT-PdNPs after 1st catalytic cycle while the right hand side images represent corresponding height profile diagrams along the horizontal lines.

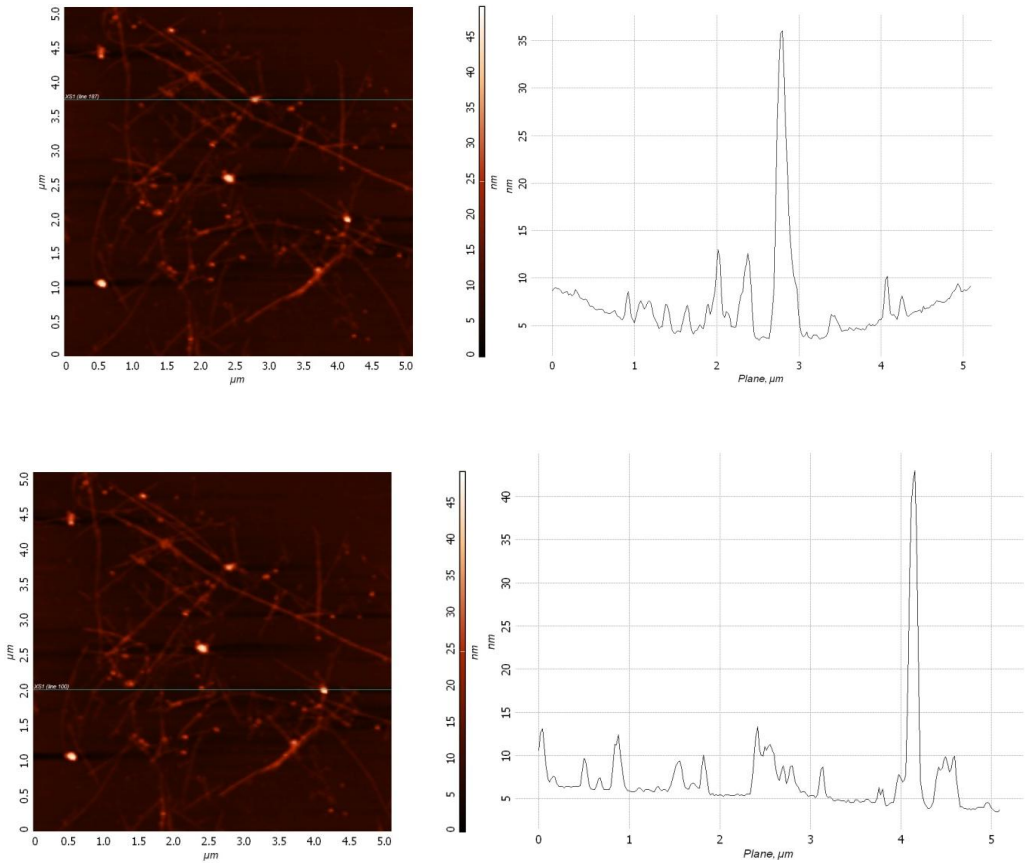



**Figure S35.** Images on the left hand side represent the AFM images of SWNT-PdNPs after 4$^{th}$ catalytic cycle while the right hand side images represent corresponding height profile diagrams along the horizontal lines.