



SUPPLEMENTARY MATERIAL TO
**Palladium on carbon in PEG-400/cyclohexane: Recoverable and
recyclable catalytic system for efficient decarbonylation of
aldehydes**

NATAŠA TERZIĆ-JOVANOVIĆ¹ and VLADIMIR AJDAČIĆ^{2*}

¹University of Belgrade – Institute of Chemistry, Technology and Metallurgy, National
Institute of the Republic of Serbia, Njegoševa 12, 11000 Belgrade, Serbia and ²Innovative
Centre Ltd., Faculty of Chemistry, Studentski Trg 12–16, 11158 Belgrade, Serbia

J. Serb. Chem. Soc. 87 (6) (2022) 669–675

SPECTRAL DATA OF THE SYNTHESIZED COMPOUNDS

Biphenyl-4-carbaldehyde to biphenyl (2a). ¹H-NMR (500 MHz, CDCl₃, δ / ppm): 7.60–7.55 (m, 4H), 7.45–7.40 (m, 4H), 7.36–7.31 (m, 2H). ¹³C-NMR (125 MHz, CDCl₃, δ / ppm): 141.2, 128.7, 127.2, 127.2. EI-MS (m/z (%)): 154.1 [M]⁺ (100), 153.1 (38), 152.1 (26), 76.1 (7).

2-Naphthaldehyde to naphthalene (2b). ¹H-NMR (500 MHz, CDCl₃, δ / ppm): 7.89 (dd, J₁ = 8.0 Hz, J₂ = 4.0 Hz, 4H), 7.53 (dd, J₁ = 8.0 Hz, J₂ = 4.0 Hz, 4H). ¹³C-NMR (125 MHz, CDCl₃, δ / ppm): 133.6, 128.0, 126.0. EI-MS (m/z (%)): 128.2 [M]⁺ (100), 127.1 (16), 83.7 (11), 48.9 (16).

Anthracene-9-carbaldehyde to anthracene (2c). ¹H-NMR (500 MHz, CDCl₃, δ / ppm): 8.42 (s, 2 H), 8.05–7.95 (m, 4 H), 7.50–7.45 (m, 4 H). ¹³C-NMR (125 MHz, CDCl₃, δ / ppm): 131.7, 128.1, 126.2, 125.3. EI-MS (m/z (%)): 178.1 [M]⁺ (100), 176.0 (18), 152.0 (7), 89.2 (8).

4-Nitrobenzaldehyde to nitrobenzene (2d). EI-MS (m/z (%)): 123.0 [M]⁺ (66), 93.1 (13), 77.0 (100), 51.1 (39).

5-Fluoro-2-methoxybenzaldehyde to 4-fluoroanisole (2e). EI-MS (m/z (%)): 126.0 [M]⁺ (100), 96.0 (71), 83.1 (40), 57.1 (14).

Diphenylacetaldehyde to diphenylmethyl (2h). ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 7.33–7.23 (m, 4H), 7.30–7.20 (m, 6H), 3.97 (s, 2H). ¹³C-NMR (101 MHz, CDCl₃, δ / ppm): 140.9, 128.8, 128.3, 125.9, 41.8. EI-MS (m/z (%)): 168.1 [M]⁺ (100), 152.1 (30), 91.1 (20).

3-(1,3-Benzodioxol-5-yl)-2-methylpropanal to dihydrosafrole (2i). ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 6.79–6.56 (m, 3H), 5.90 (s, 2H), 2.50 (dd, J₁ = 8.5 Hz, J₂ = 6.7 Hz, 2H), 1.59 (d, J = 7.5 Hz, 2H), 1.26 (s, 2H), 0.92 (t, J = 7.3 Hz, 3H). ¹³C-NMR (101 MHz, CDCl₃, δ / ppm): 147.3, 145.2, 136.4, 120.9, 108.7, 107.8, 100.5, 37.6, 29.5, 24.6, 13.5. EI-MS (m/z (%)): 164.1 [M]⁺ (40), 135.1 (100), 105.1 (10), 77.1 (20).

* Corresponding author. E-mail: ajdacic@chem.bg.ac.rs

1-Adamantanecarboxaldehyde to adamantane (2j). $^1\text{H-NMR}$ (400 MHz, CDCl_3 , δ / ppm): 1.86 (*bs*, 4H), 1.74 (*bs*, 12H). $^{13}\text{C-NMR}$ (101 MHz, CDCl_3 , δ / ppm): 38.2, 28.8. EI-MS (m/z (%)): 136.1 $[\text{M}]^+$ (100), 121.1 (10), 107.1 (10), 93.1 (40), 79.1 (40).

1-Adamantaneacetaldehyde to 1-methyl adamantane (2k). $^1\text{H-NMR}$ (400 MHz, CDCl_3 , δ / ppm): 1.92 (*bs*, 3H), 1.56–1.72 (*m*, 6H), 1.45 (*d*, $J = 2.8$ Hz, 6H), 0.76 (*s*, 3H). $^{13}\text{C-NMR}$ (125 MHz, CDCl_3 , δ / ppm): 44.8, 37.1, 31.6, 29.0, 27.1. EI-MS (m/z (%)): 150.1 $[\text{M}]^+$ (20), 135.1 (100), 107.1 (10), 93.1 (30), 79.1 (20).

Benzo[b]thiophene-3-carboxaldehyde to benzo[b]thiophene (2l). $^1\text{H-NMR}$ (500 MHz, CDCl_3 , δ / ppm): 7.88 (*d*, $J = 8.0$ Hz, 1H), 7.80–7.84 (*m*, 1H), 7.43 (*d*, $J = 5.5$ Hz, 1H), 7.30–7.37 (*m*, 3H). $^{13}\text{C-NMR}$ (125 MHz, CDCl_3 , δ / ppm): 139.7, 139.6, 126.3, 124.2, 124.1, 123.8, 123.6, 122.5. EI-MS (m/z (%)): 134.0 $[\text{M}]^+$ (100), 128.1 (14), 89.1 (10).

1-Prop-2-yn-1-yl-1H-indole-3-carbaldehyde to 1-prop-2-yn-1-yl-1H-indole (2m). $^1\text{H-NMR}$ (400 MHz, CDCl_3 , δ / ppm): 7.68–7.60 (*m*, 1H), 7.29–7.06 (*m*, 9H), 6.54 (*dd*, $J_1 = 3.2$, Hz, $J_2 = 0.8$ Hz, 1H), 5.27 (*s*, 2H). $^{13}\text{C-NMR}$ (101 MHz, CDCl_3 , δ / ppm): 137.7, 136.4, 128.9, 128.8, 128.0, 127.7, 121.8, 121.1, 119.6, 109.8, 101.8, 50.2. EI-MS (m/z (%)): 207.1 $[\text{M}]^+$ (70), 91.1 (100), 65.1 (20).

1-Benzyl-1H-indole-3-carbaldehyde to 1-benzyl-1H-indole (2n). $^1\text{H-NMR}$ (400 MHz, CDCl_3 , δ / ppm): 7.62 (*dt*, $J_1 = 7.9$ Hz, $J_2 = 1.0$ Hz, 1H), 7.36 (*dd*, $J_1 = 8.2$ Hz, $J_2 = 0.9$ Hz, 1H), 7.23 (*d*, $J = 1.2$ Hz, 1H), 7.18–7.08 (*m*, 2H), 6.51 (*dd*, $J_1 = 3.2$ Hz, $J_2 = 0.9$ Hz, 2H), 4.79 (*d*, $J = 2.5$ Hz, 2H), 2.37 (*t*, $J = 2.6$ Hz, 1H). $^{13}\text{C-NMR}$ (125 MHz, CDCl_3 , δ / ppm): 135.6, 128.7, 127.0, 121.7, 121.0, 120.9; 119.7, 109.1, 101.9, 73.3, 35.5. EI-MS (m/z (%)): 154.1 $[\text{M}]^+$ (100), 127.1 (10), 116.1 (30), 89.1 (20).

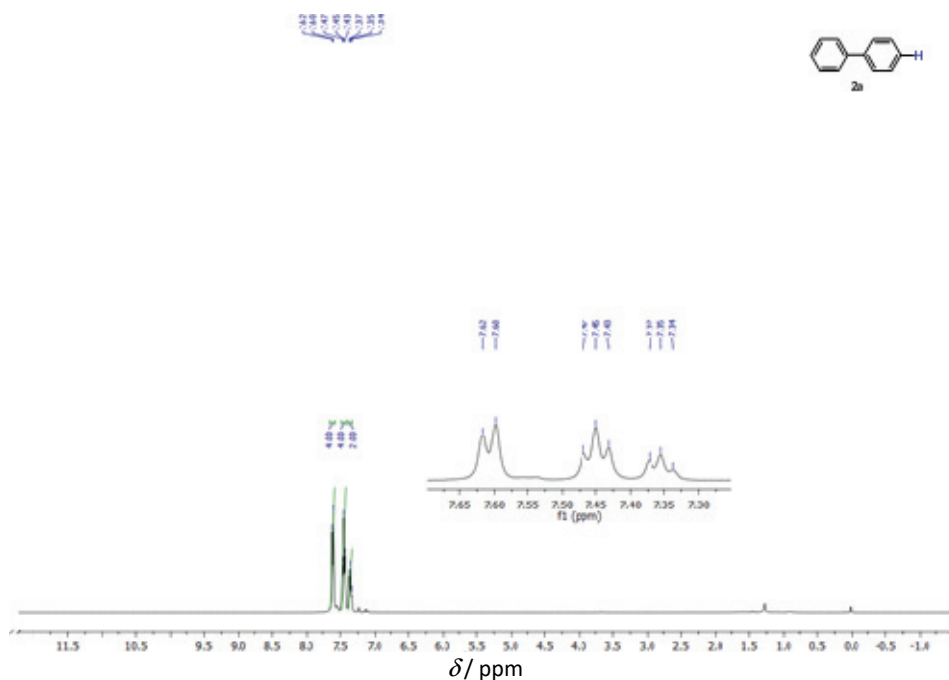
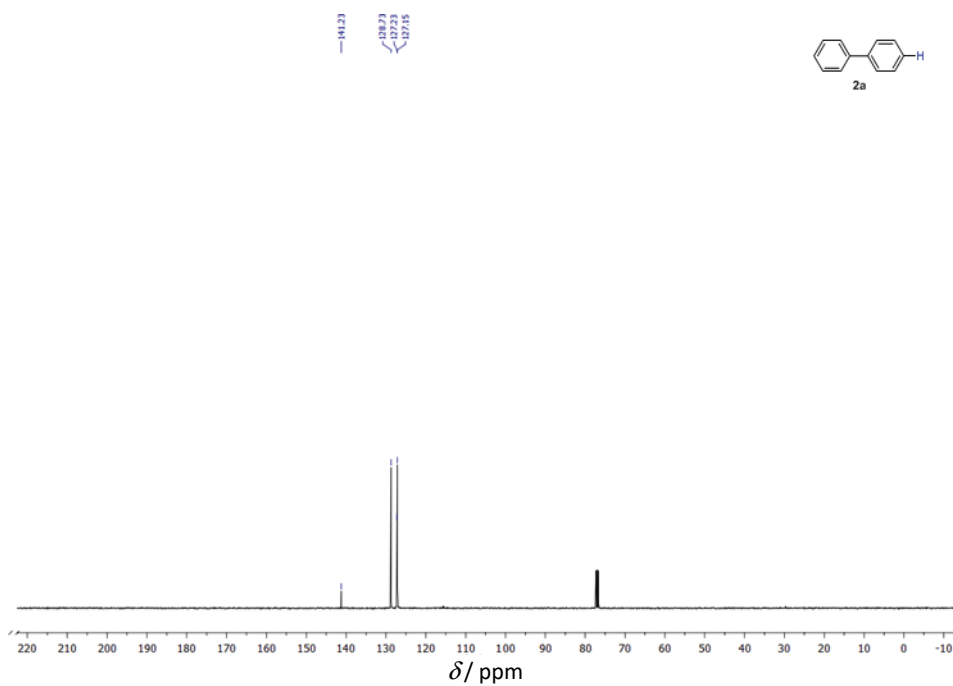
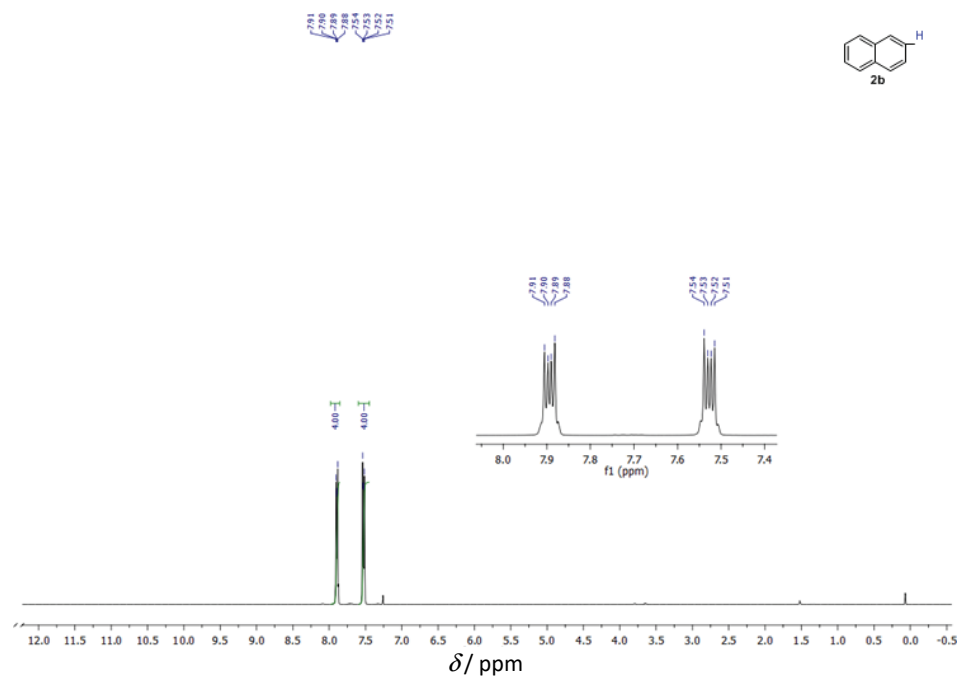


Fig. S-1. $^1\text{H-NMR}$ spectra of compound **2a**.

Fig. S-2. ¹³C-NMR spectra of compound **2a**.Fig. S-3. ¹H-NMR spectra of compound **2b**.

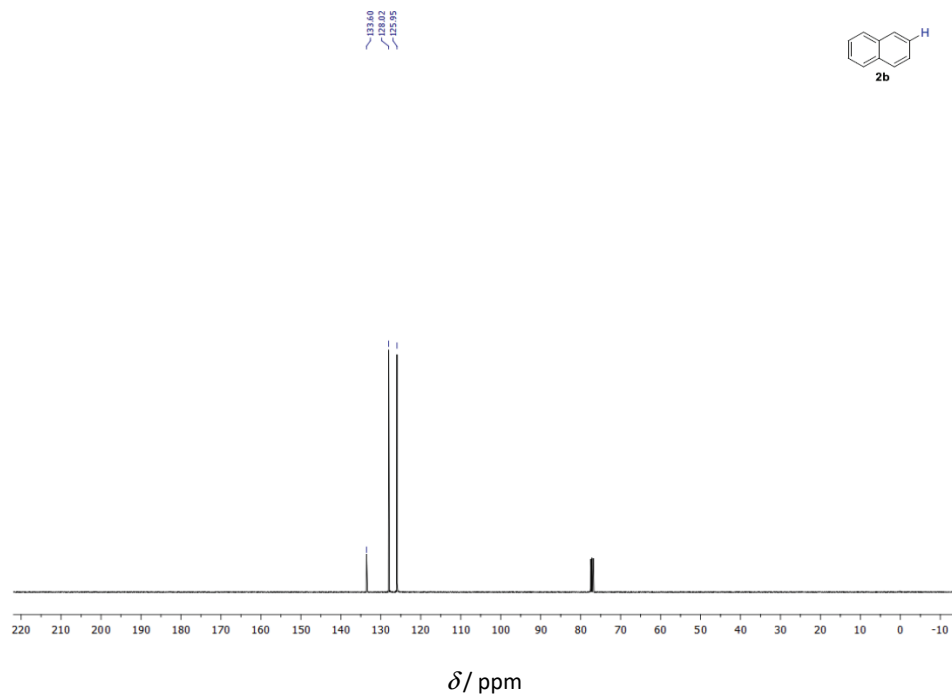
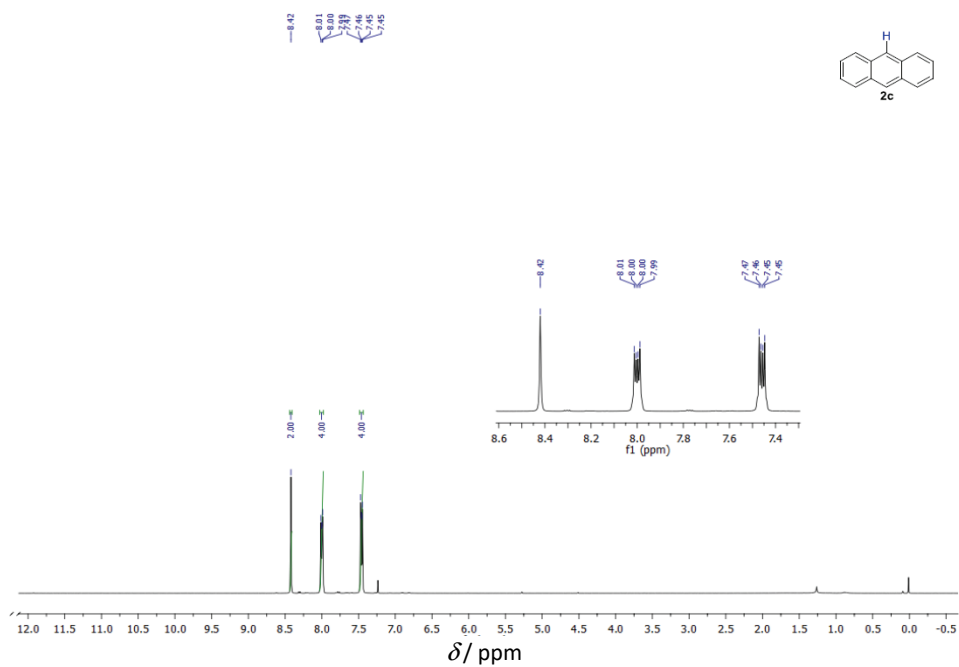
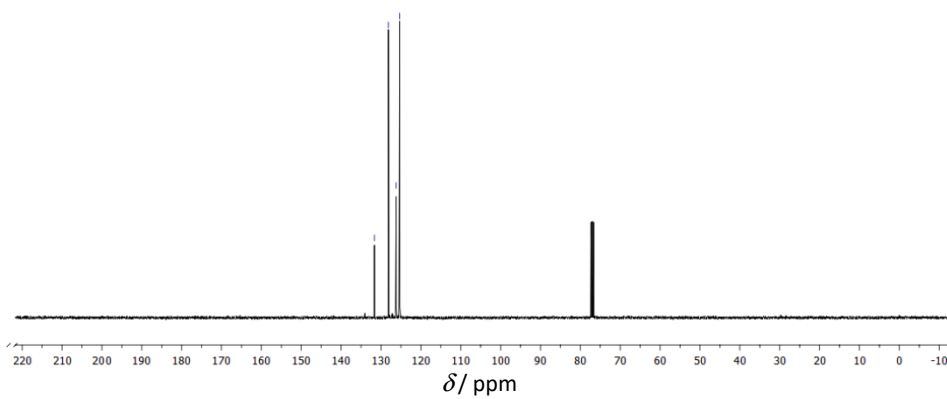
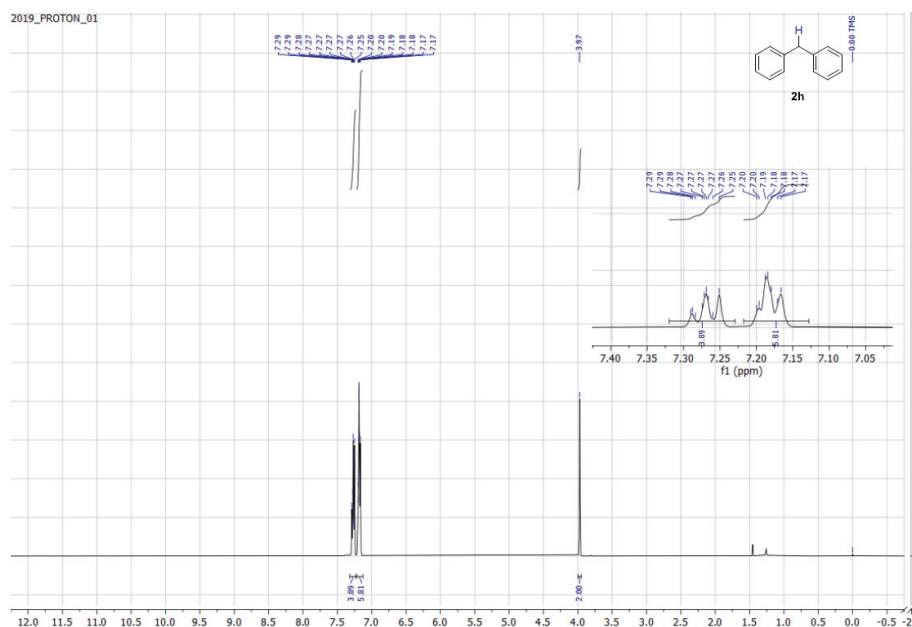
Fig. S-4. ^{13}C -NMR spectra of compound **2b**.

Fig. S-5. $^1\text{H-NMR}$ spectra of compound **2c**.131.46
128.19
126.18
125.31Fig. S-6. $^{13}\text{C-NMR}$ spectra of compound **2c**.

δ /ppm
Fig. S-7. ^1H -NMR spectra of compound **2h**.

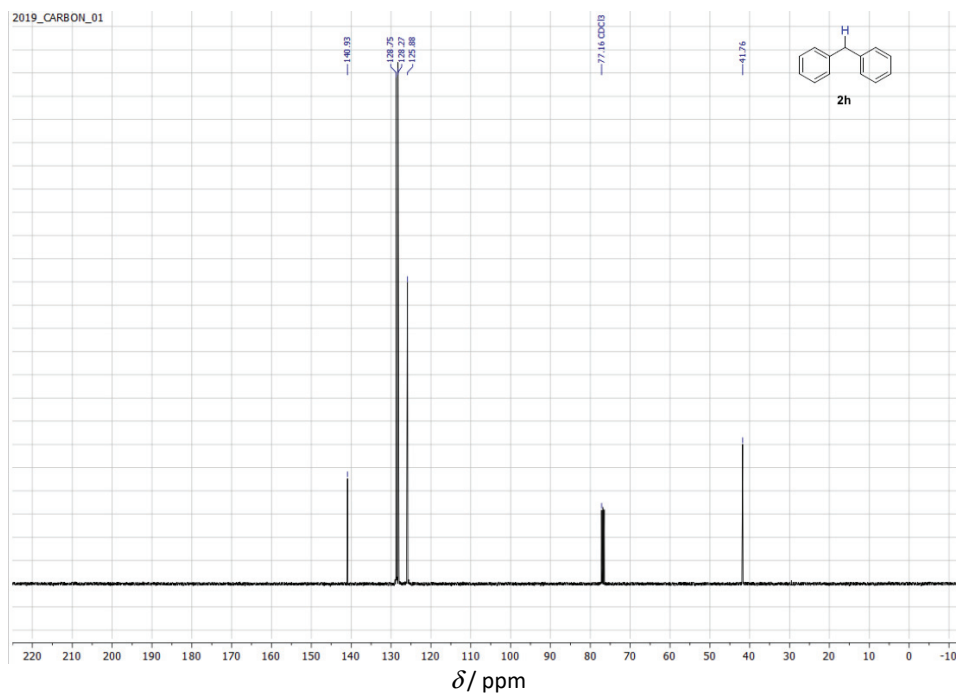


Fig. S-8. ^{13}C -NMR spectra of compound **2h**.

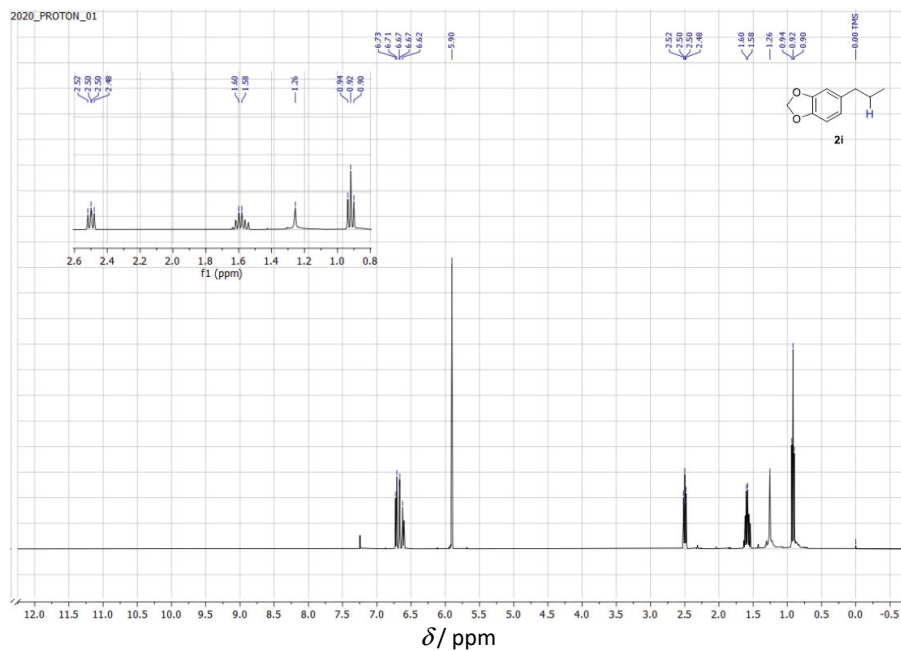


Fig. S-9. ¹H-NMR spectra of compound **2i**.

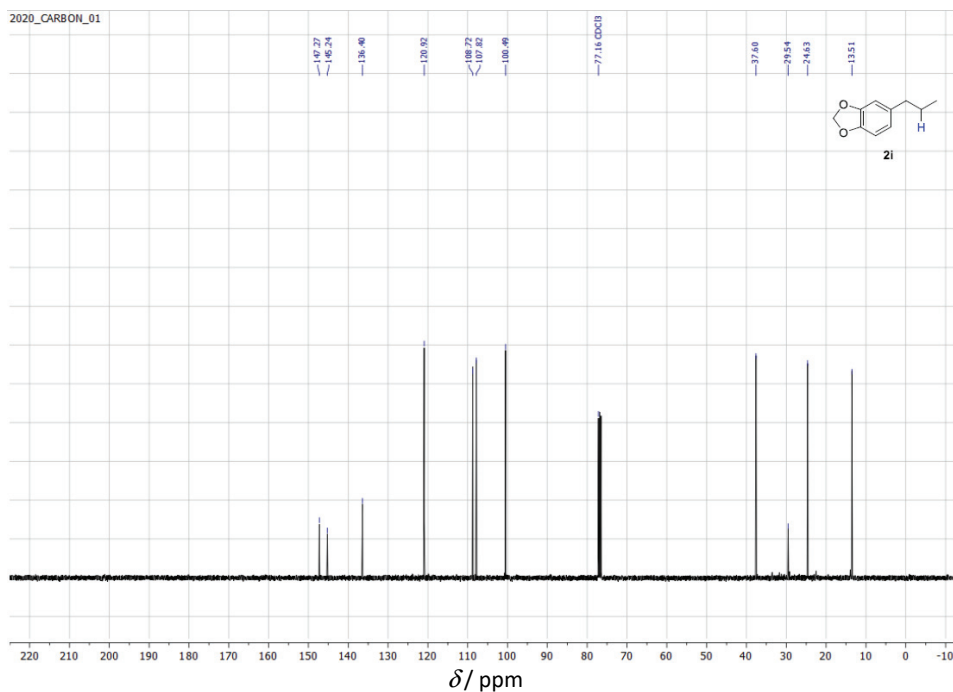
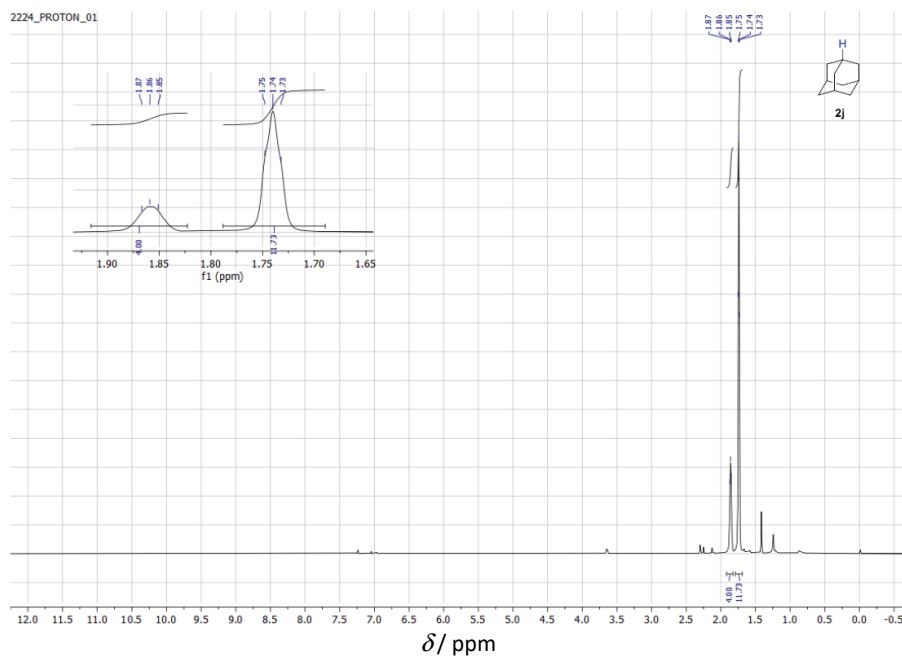
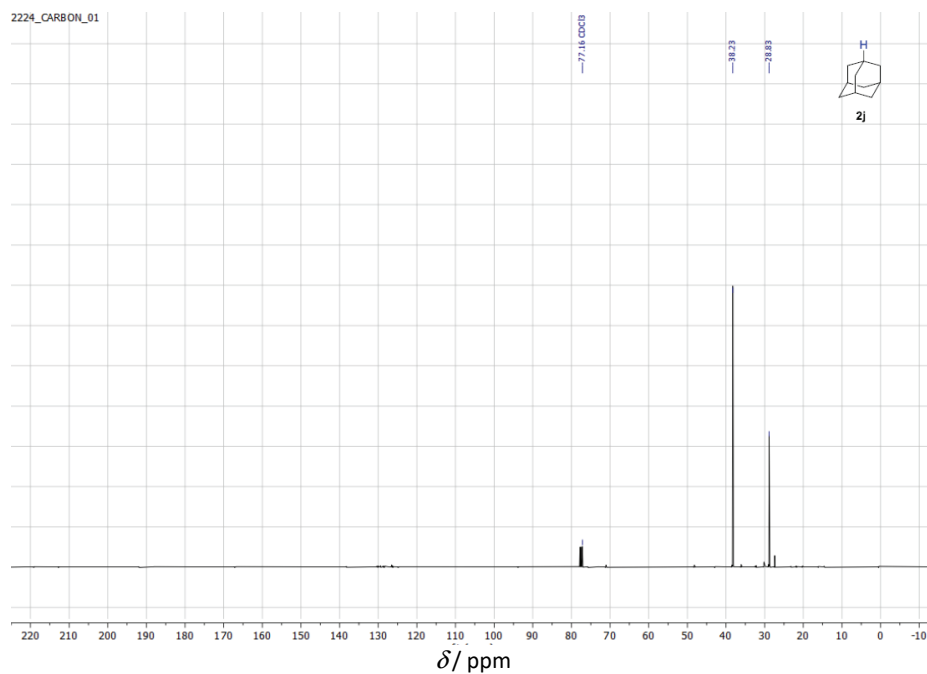


Fig. S-10. ¹³C-NMR spectra of compound **2i**.

Fig. S-11. $^1\text{H-NMR}$ spectra of compound **2j**.Fig. S-12. $^{13}\text{C-NMR}$ spectra of compound **2j**.

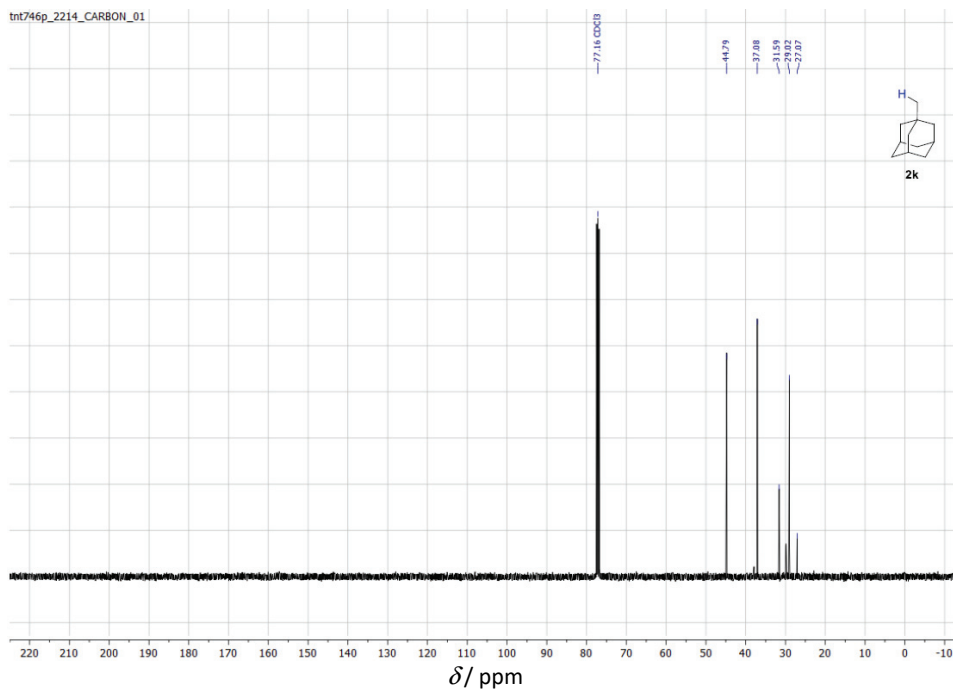
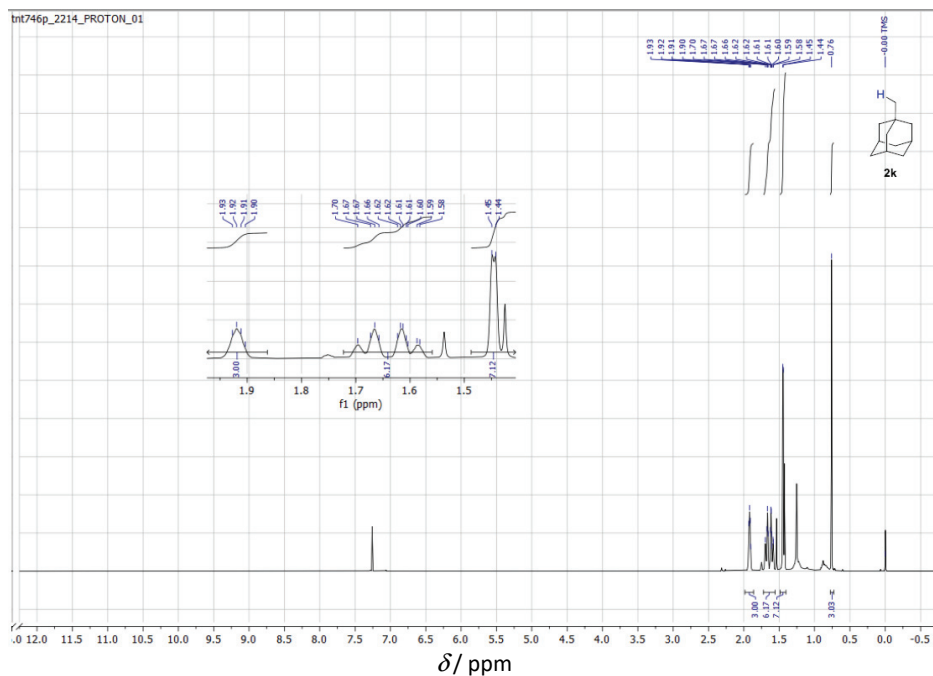
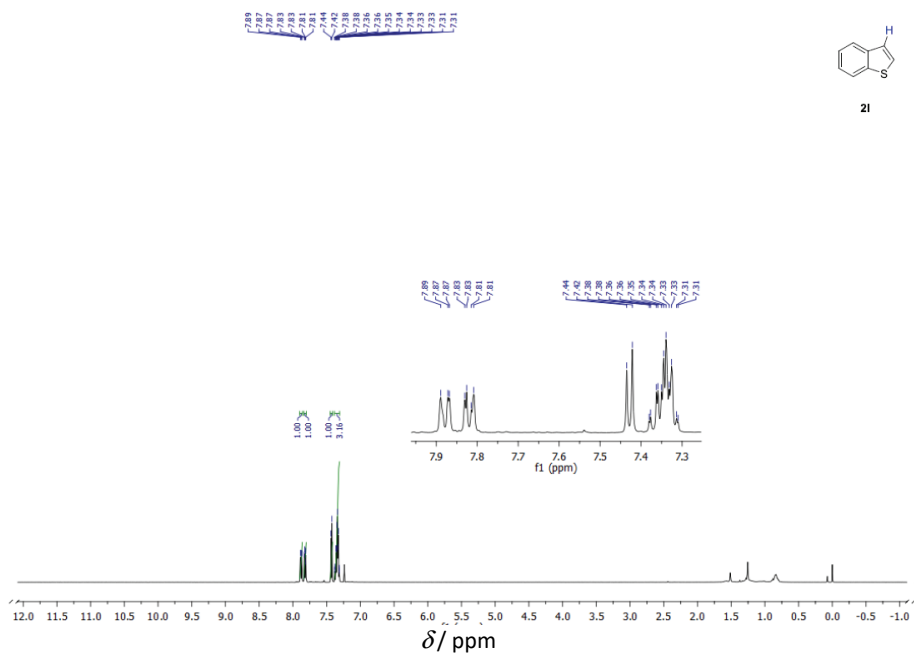
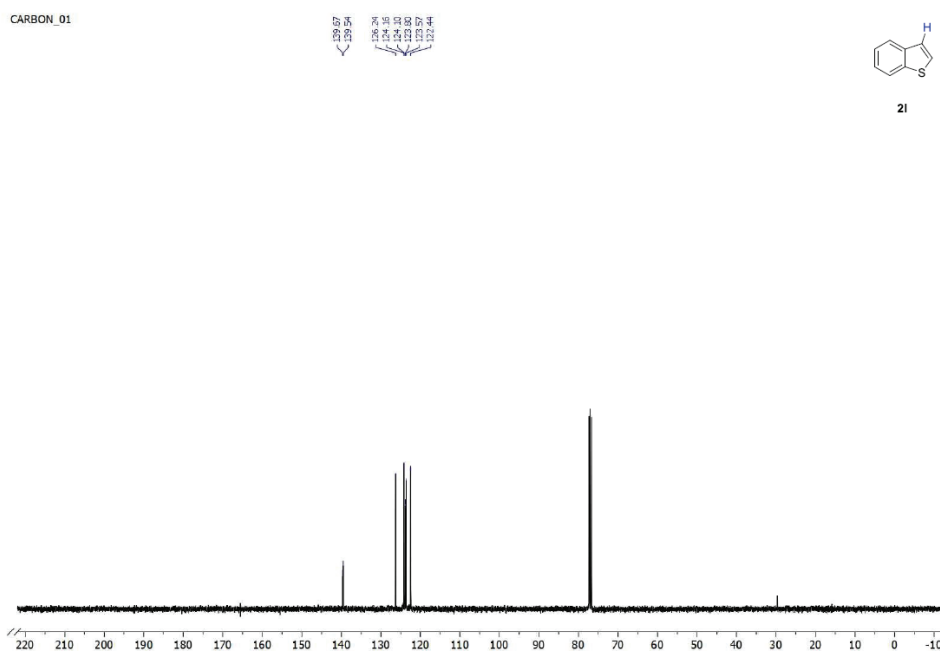


Fig. S-14. ^{13}C -NMR spectra of compound **2k**.Fig. S-15. ^1H -NMR spectra of compound **2l**.

δ / ppm
Fig. S-16. ^{13}C -NMR spectra of compound **2l**.

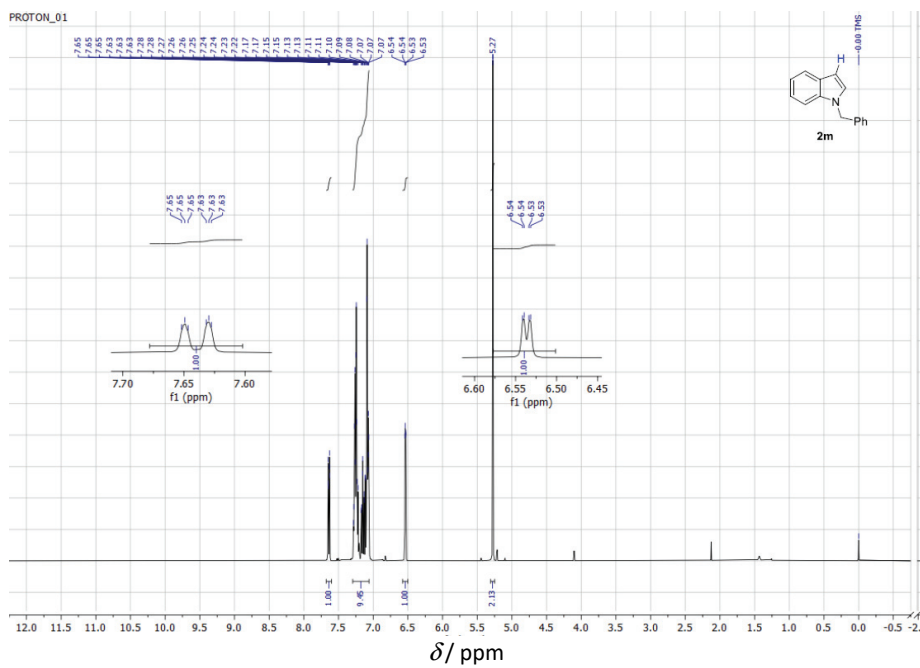
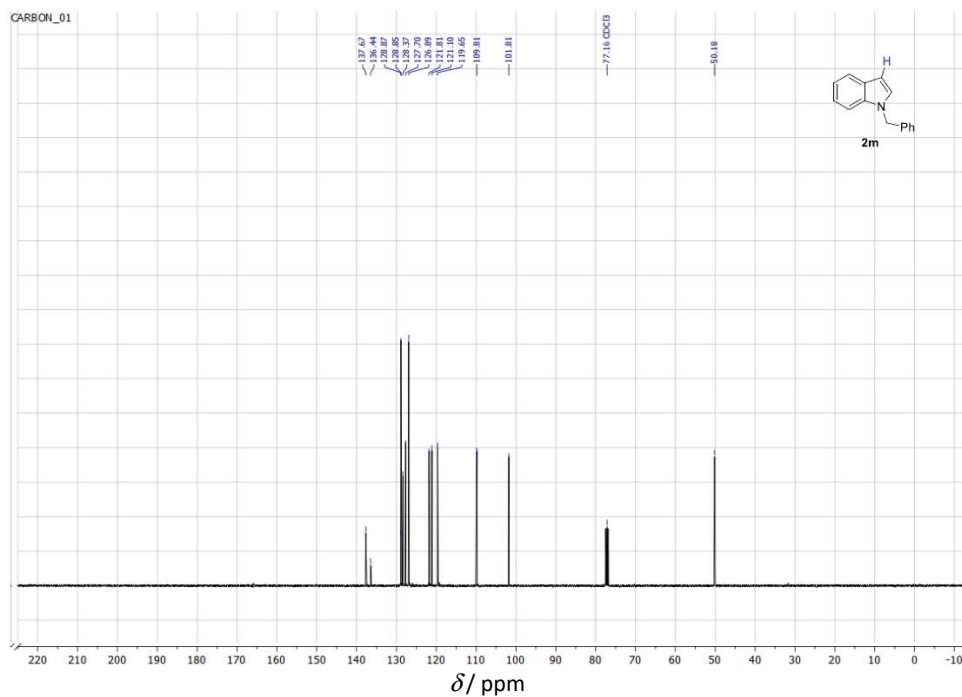
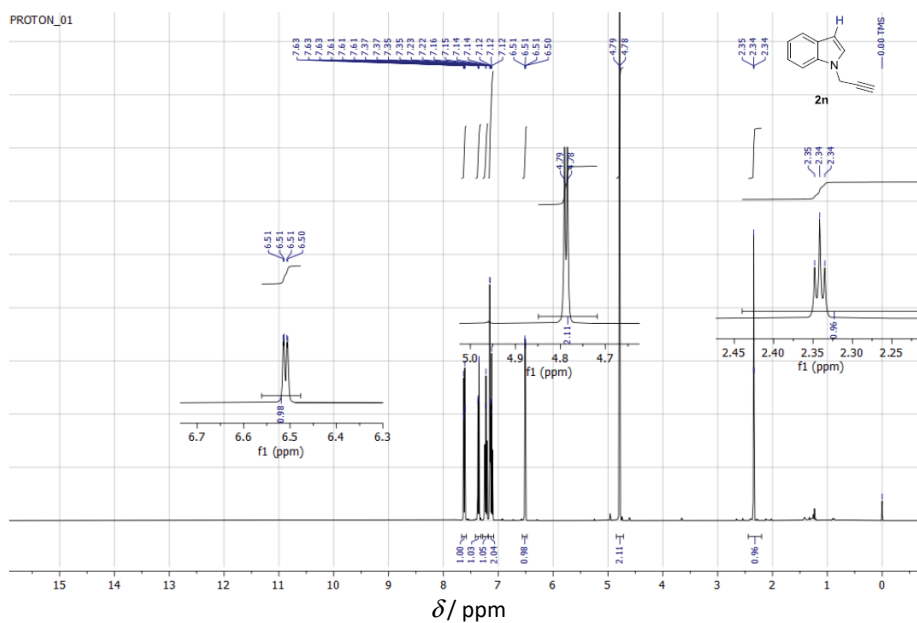


Fig. S-17. ^1H -NMR spectra of compound **2m**.

Fig. S-18. ¹³C-NMR spectra of compound **2m**.Fig. S-19. ¹H-NMR spectra of compound **2n**.

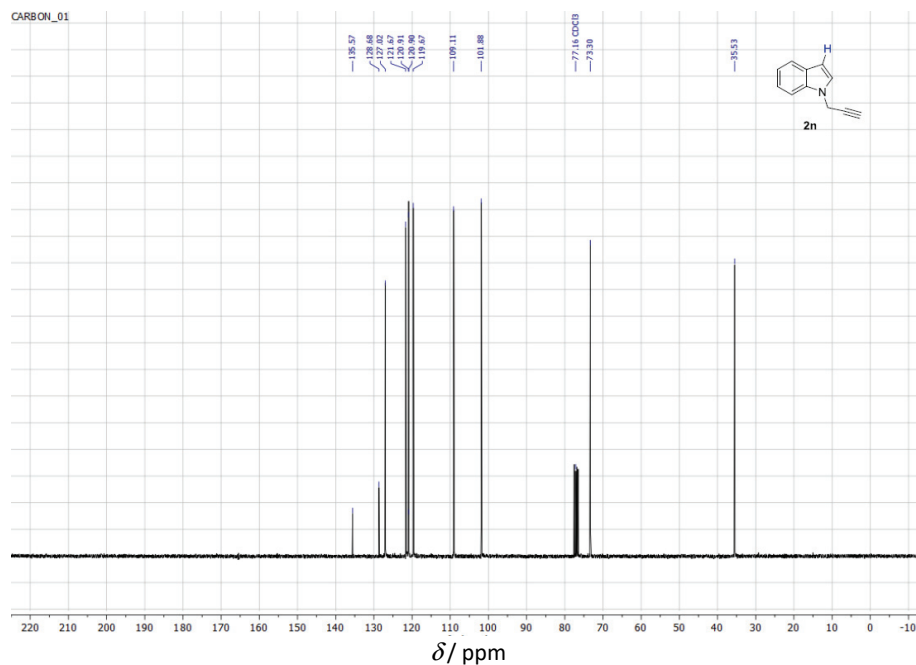
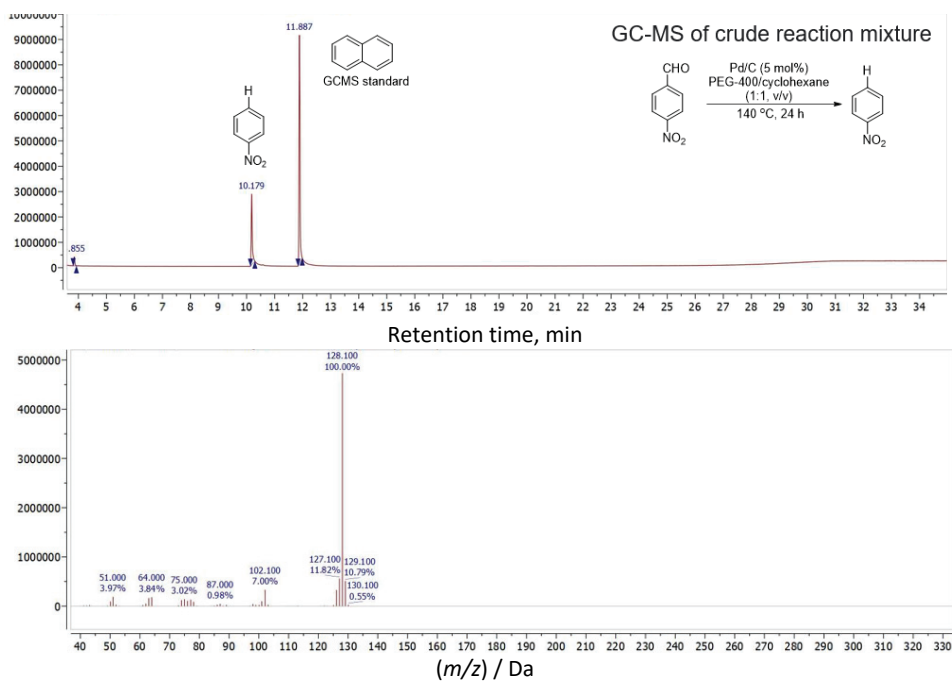
Fig. S-20. ¹³C-NMR spectra of compound **2m**.

Fig. S-21. GC-MS Analysis.