Electronic Supplementary Information (ESI)

Simple and Efficient Nickel-Catalyzed Cross-Coupling Reaction of Alkynylalanes with Benzylic and Aryl Bromides

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I. Reagents and General Techniques

All solvents were dried by refluxing for at least 24 h over P_2O_5 (dichloromethane) or sodium-benzophenone and were freshly distilled prior to use. All synthesis and manipulations were carried out under a dry nitrogen atmosphere.

II. Physical measurements

¹H and ¹³C NMR spectra were obtained with a Varian Mercury-400 (¹H, 400 MHz; ¹³C, 100 MHz) spectrometer, and chemical shifts were measured relative to tetramethylsilane (0.00 ppm) as the internal reference. Mass spectroscopy were performed by using Finnigan MAT 95 XL ThermoQuest Mass Spectrometer.

III. General Procedures for the Preparation of the Alkynylalane Reagents

To a cooled (0 $^{\circ}$ C) solution of an alkyne (1.5 mmol) in hexane (3 mL) was added *n*-BuLi (1.5 mmol, 2.5 M in hexane) and stirred for 20 min, followed by an addition of AlEt₂Cl (1.5 mmol, 1 *M* in hexane). The mixture thus obtained had been stirred at 0 $^{\circ}$ C for 20 min and then at room temperature for 2 h. The resulted solution was filtered, followed by an evaporation of hexane under reduced pressures and then added 2 mL of dry diethyl ether to give a alkynylaluminum reagent which was used in the coupling reactions.

IV. General Procedures for the Coupling Reaction of Benzylic Halides with Alkynylalanes Catalyzed by NiCl₂(PPh₃)₂

Under a dry nitrogen atmosphere, NiCl₂(PPh₃)₂ (0.0262 g, 0.0400 mmol) and alkynylaluminum reagent (1.5 mmol) were mixed in 3 mL dry diethyl ether at room temperature and stirred the mixture for 15 min, followed by an addition of benzylic bromide (1.00 mmol). After stirring for 1 h, the reaction mixture was quenched by aqueous hydrochloric acid (3 M). The organic layer was separated, and the aqueous layer was extracted with hexane or ether. The combined organic phase was dried over MgSO₄, filtered, and concentrated. The residue was purified by column chromatography to give the products

V. General Procedures for the Coupling Reaction of Aryl Halides with Alkynylalanes Catalyzed by NiCl₂(PPh₃)₂

Under a dry nitrogen atmosphere, NiCl₂(PPh₃)₂ (0.0262 g, 0.0400 mmol) and alkynylaluminum reagent (1.5 mmol) were mixed in 3 mL dry DME at room temperature and stirred the mixture for 15 min, followed by an addition of Aryl bromide (1.00 mmol). After stirring for 4 h at 80 $^{\circ}$ C, the reaction mixture was allowed to cool down to room temperature and then quenched by aqueous hydrochloric acid (3 *M*). The organic layer was separated, and the aqueous layer was extracted with hexane or ether. The combined organic phase was dried over MgSO₄, filtered, and concentrated. The residue was purified by column chromatography

to give the products.

VI. ¹H and ¹³C NMR and High-resolution Mass Spectroscopic Data of Coupling Products

- Prop-1-yne-1,3-diyldibenzene (2a): ¹H NMR (400 MHz, CDCl₃): δ 7.47-7.41 (m, 4H), 7.37-7.23 (m, 6H), 3.84 (s, 2H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 136.8, 131.6, 128.5, 128.2, 128.0, 127.8, 126.6, 123.7, 87.5, 82.7, 25.7 ppm. HRMS calculated for C₁₅H₁₂ [M⁺]: 192.0939, found 192.0943.
- 2. 1-methyl-2-(3-phenylprop-2-ynyl)benzene (2b): ¹H NMR (400 MHz, CDCl₃): δ 7.51 (d, J = 6.4 Hz, 1H), 7.46-7.41 (m, 2H), 7.32-7.27 (m, 3H), 7.25-7.17 (m, 3H), 3.75 (s, 2H), 2.38 (s, 3H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 136.0, 135.0, 131.6, 130.1, 128.3, 128.2, 127.7, 126.9, 126.2, 123.7, 87.2, 82.7, 23.9, 19.3 ppm. HRMS calculated for C₁₆H₁₄ [M⁺]: 206.1096, found 206.1092.
- 3. 1-methyl-3-(3-phenylprop-2-ynyl)benzene (2c): ¹H NMR (400 MHz, CDCl₃): δ 7.47-7.43 (m, 2H), 7.32-7.28 (m, 3H), 7.26-7.21 (m, 3H), 7.09-7.05 (m, 1H), 3.80 (s, 2H), 2.36 (s, 3H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 138.2, 136.6, 131.6, 128.7, 128.4, 128.2, 127.8, 127.4, 125.0, 123.7, 87.7, 82.5, 25.6, 21.4 ppm. HRMS calculated for C₁₆H₁₄ [M⁺]: 206.1096, found 206.1088.
- **1-methyl-4-(3-phenylprop-2-ynyl)benzene (2d):** ¹H NMR (400 MHz, CDCl₃): δ
 7.46-7.42 (m, 2H), 7.32-7.26 (m, 5H), 7.14 (d, J = 7.6 Hz, 2H), 3.79 (s, 2H), 2.34 (s, 3H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 136.2, 133.7, 131.6, 129.2, 128.2, 127.8, 127.7, 123.8, 87.8, 82.4, 25.3, 21.0 ppm. HRMS calculated for C₁₆H₁₄ [M⁺]: 206.1096, found 206.1088.
- **1-methoxy-3-(3-phenylprop-2-ynyl)benzene** (2e): ¹H NMR (400 MHz, CDCl₃): δ
 7.46-7.44 (m, 2H), 7.31-7.25 (m, 4H), 7.01-6.98 (m, 2H), 6.81-6.77 (m, 1H), 3.81 (s, 5H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 159.8, 138.3, 131.6, 129.5, 128.2, 127.8, 123.6, 120.3, 113.7, 112.0, 87.3, 82.7, 55.2, 25.7 ppm. HRMS calculated for C₁₆H₁₄O [M⁺]: 222.1045, found 222.1051.
- 6. Methyl(4-(3-phenylprop-2-ynyl)phenyl)sulfane (2f): ¹H NMR (400 MHz, CDCl₃): δ 7.46-7.43 (m, 2H) 7.36-7.32 (m, 2H), 7.31-7.29 (m, 3H), 7.27-7.24 (m, 2H), 3.80 (s, 2H), 2.49 (s, 3H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 136.4, 133.7, 131.6, 128.4, 128.2, 127.8, 127.0, 123.5, 87.3, 82.6, 25.2, 16.1 ppm. HRMS calculated for C₁₆H₁₄S [M⁺]: 238.0816, found 238.0824.

- 7. 1-tert-butyl-4-(3-phenylprop-2-ynyl)benzene (2g): ¹H NMR (400 MHz, CDCl₃): δ
 7.46-7.43 (m, 2H), 7.39-7.33 (m, 4H), 7.31-7.27 (m, 3H), 3.81 (s, 2H) 1.32 (s, 9H) ppm.
 ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 149.5, 133.7, 131.6, 128.2, 127.7, 127.6, 125.5, 123.7, 87.8, 82.4, 34.4, 31.4, 25.2 ppm. HRMS calculated for C₁₉H₂₀ [M⁺]: 248.1565, found 248.1570.
- 8. 2-(3-phenylprop-2-ynyl)biphenyl (2h): ¹H NMR (400 MHz, CDCl₃): δ 7.71-7.68 (m, 1H), 7.46-7.25 (m, 13H), 3.72 (s, 2H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 141.5, 141.0, 134.3, 131.6, 130.0, 129.2, 129.0, 128.4, 128.24, 128.17, 127.7, 127.1, 126.7, 123.7, 88.2, 82.5, 24.1 ppm. HRMS calculated for C₂₁H₁₆ [M⁺]: 268.1252, found 268.1262.
- **9. 3-(3-phenylprop-2-ynyl)biphenyl (2i):** ¹H NMR (400 MHz, CDCl₃): δ 7.65-7.59 (m, 3H), 7.51-7.40 (m, 7H), 7.38-7.28 (m, 4H), 3.91 (s, 2H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 141.5, 141.0, 137.2, 131.6, 129.0, 128.7, 128.2, 127.8, 127.3, 127.2, 126.9, 126.8, 125.5, 123.6, 87.4, 82.8, 25.8 ppm. HRMS calculated for C₂₁H₁₆ [M⁺]: 268.1252, found 268.1261.
- **10. 1,3-dimethoxy-5-(3-phenylprop-2-ynyl)benzene (2j):** ¹H NMR (400 MHz, CDCl₃): δ 7.46-7.43 (m, 2H), 7.31-7.28 (m, 3H), 6.60-6.58 (m, 2H), 6.36 (t, *J* = 2.4 Hz, 1H), 3.80 (s, 6H), 3.78 (s, 2H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 160.8, 139.0, 131.6, 128.2, 127.8, 123.6, 106.0, 98.6, 87.2, 82.7, 55.2, 25.9 ppm. HRMS calculated for C₁₇H₁₆O₂ [M⁺]: 252.1150, found 252.1153.
- **11. 1-chloro-4-(3-phenylprop-2-ynyl)benzene (2k):** ¹H NMR (400 MHz, CDCl₃): δ 7.46-7.42 (m, 2H), 7.37-7.28 (m, 7H), 3.80 (s, 2H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 135.2, 132.4, 131.6, 129.3, 128.6, 128.3, 128.0, 123.4, 86.8, 83.0, 25.2 ppm. HRMS calculated for C₁₅H₁₁Cl [M⁺]: 226.0549, found 226.0557.
- 12. 4-(3-phenylprop-2-ynyl)benzonitrile (2l): ¹H NMR (400 MHz, CDCl₃): δ 7.66-7.63 (m, 2H), 7.56-7.52 (m, 2H), 7.47-7.43 (m, 2H), 7.34-7.30 (m, 3H), 3.90 (s, 2H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 142.3, 132.3, 131.6, 128.7, 128.3, 128.2, 123.0, 118.8, 110.7, 85.5, 83.7, 25.9 ppm. HRMS calculated for C₁₆H₁₁N [M⁺]: 217.0891, found 217.0886.
- 13. 1-(3-phenylprop-2-ynyl)-3,5-bis(trifluoromethyl)benzene (2m): ¹H NMR (400 MHz, CDCl₃): δ 7.89 (s, 2H), 7.79 (s, 1H), 7.48-7.43 (m, 2H), 7.35-7.32 (m, 3H), 3.97 (s, 3H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 139.3, 132.5, 132.0, 131.7, 128.3 (m), 128.2 (m), 123.3 (q, *J* = 270 Hz), 122.9, 120.8 (m), 84.9, 84.2, 25.5 ppm. HRMS calculated for

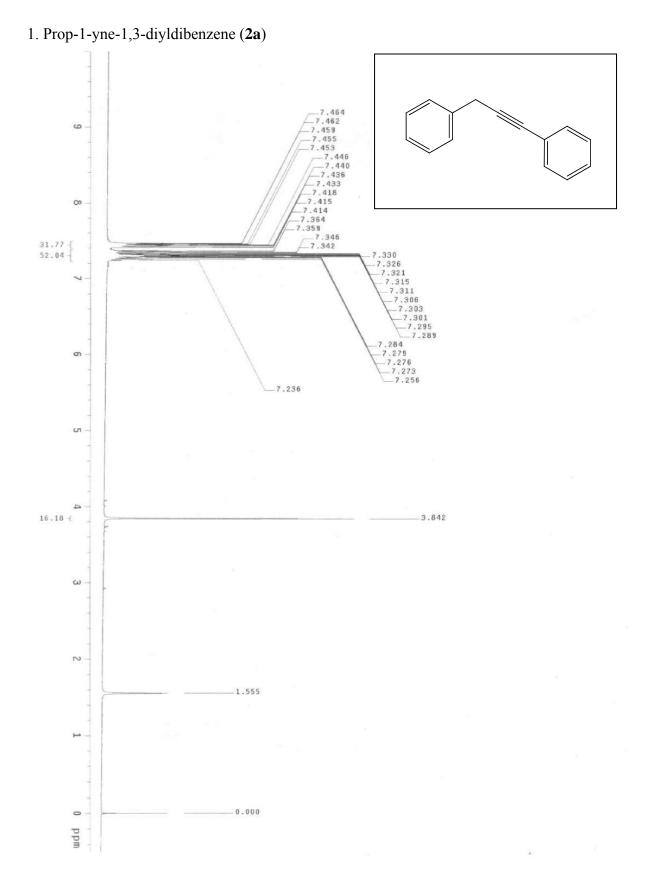
 $C_{17}H_{10}F_6$ [M⁺]: 328.0687, found 328.0681.

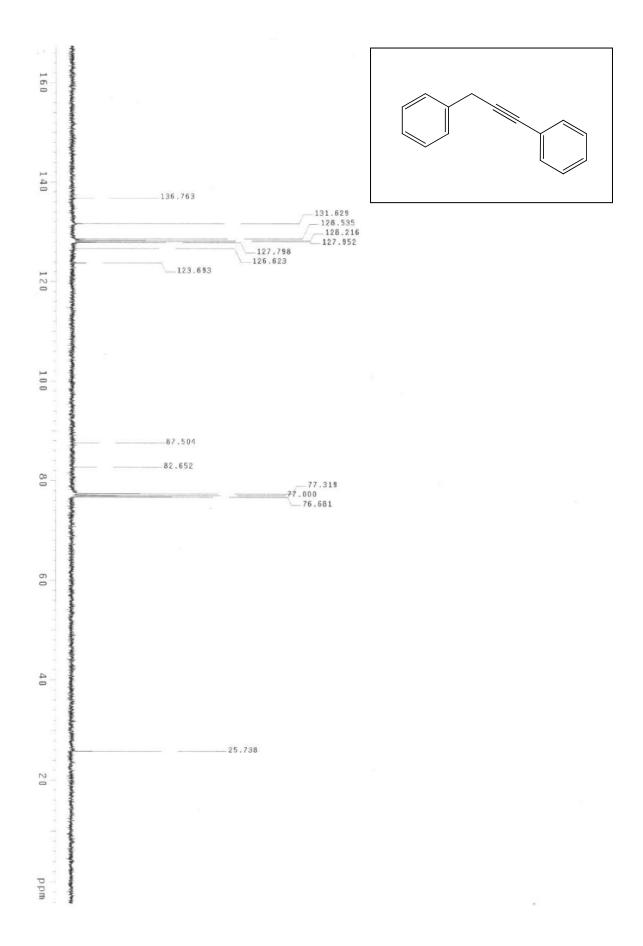
- 14. 2-(3-phenylprop-2-ynyl)thiophene (2n): ¹H NMR (400 MHz, CDCl₃): δ 7.47-7.43 (m, 2H), 7.32-7.28 (t, 3H), 7.21-7.18 (m, 1H), 7.04-7.01 (m, 1H), 6.98-6.95 (m, 1H), 3.99 (s, 2H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 139.5, 131.6, 128.2, 128.0, 126.8, 125.0, 124.1, 123.3, 86.7, 82.3, 20.6 ppm. HRMS calculated for C₁₃H₁₀S [M⁺]: 198.0503, found 198.0500.
- 15. Hept-2-ynylbenzene (20): ¹H NMR (400 MHz, CDCl₃): δ 7.37-7.28 (m, 4H), 7.27-7.19 (m, 1H), 3.58 (t,J = 2.0 Hz, 2H), 2.26-2.20 (m, 2H), 1.57-1.38 (m, 4H), 0.92 (t, J = 7.6 Hz, 3H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 137.6, 128.4, 127.8, 126.3, 82.6, 77.4, 31.1, 25.1, 22.0, 18.5, 13.6 ppm.
- 16. (7-chlorohept-2-ynyl)benzene (2p): ¹H NMR (400 MHz, CDCl₃): δ 7.35-7.19 (m, 5H), 3.57 (s, 2H), 3.57-3.53 (m, 2H), 2.30-2.23 (m, 2H), 1.94-1.86 (m, 2H), 1.71-1.63 (m, 2H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 137.3, 128.4, 127.8, 126.4, 81.6, 78.2, 44.6, 31.5, 26.1, 25.0, 18.1 ppm. HRMS calculated for C₁₃H₁₅Cl [M⁺]: 206.0862, found 206.0855.
- **17. 1,4-diphenylbut-2-yne (2q):** ¹H NMR (400 MHz, CDCl₃): δ 7.39-7.35 (m, 4H), 7.34-7.29 (m, 4H), 7.25-7.20 (m, 2H), 3.65 (s, 4H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 137.3, 128.4, 127.9, 126.5, 79.9, 25.2 ppm.
- **18. 4-(3-(trimethylsilyl)prop-2-ynyl)benzonitrile (2r):** ¹H NMR (400 MHz, CDCl₃): δ 7.62 (dt, *J* = 1.6, 8.4 Hz, 2H), 7.48-7.44 (m, 2H), 3.71 (s, 2H), 0.20 (s, 9H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 141.9, 132.3, 128.6, 118.8, 110.6, 102.1, 88.4, 26.3, -0.07 ppm. HRMS calculated for C₁₃H₁₅SiN [M⁺]: 213.0974, found 213.0983.
- **19. 2-methyl-6-(3-(trimethylsilyl)prop-2-ynyl)pyridine (2s):** ¹H NMR (400 MHz, CDCl₃): δ 7.58 (t, J = 8 .0 Hz, 1H), 7.37 (d, J = 7.6 Hz, 1H), 7.02 (d, J = 7.6 Hz, 1H), 3.81 (s, 2H), 2.53 (s, 3H), 0.20 (s, 9H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 157.8, 155.9, 137.0, 121.2, 118.7, 103.1, 87.8, 29.3, 24.4, 0.03 ppm. HRMS calculated for C₁₂H₁₇NSi [M⁺]: 203.1130, found 203.1127.
- **20. 1,2-diphenylethyne (2t):** ¹H NMR (400 MHz, CDCl₃): δ 7.55-7.50 (m, 4H), 7.36-7.30 (m, 6H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 131.6, 128.3, 128.2, 123.3, 89.4 ppm.
- **21. 1-methyl-4-(phenylethynyl)benzene (2u):** ¹Η NMR (400 MHz, CDCl₃): δ 7.54-7.50 (m,

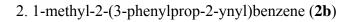
2H), 7.43 (d, J = 8.0 Hz, 2H), 7.37-7.30 (m, 3H), 7.16 (d, J = 8.0 Hz, 2H), 2.37 (s, 3H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 138.4, 131.54, 131.49, 129.1, 128.3, 128.1, 123.5, 120.2, 89.5, 88.7, 21.5 ppm.

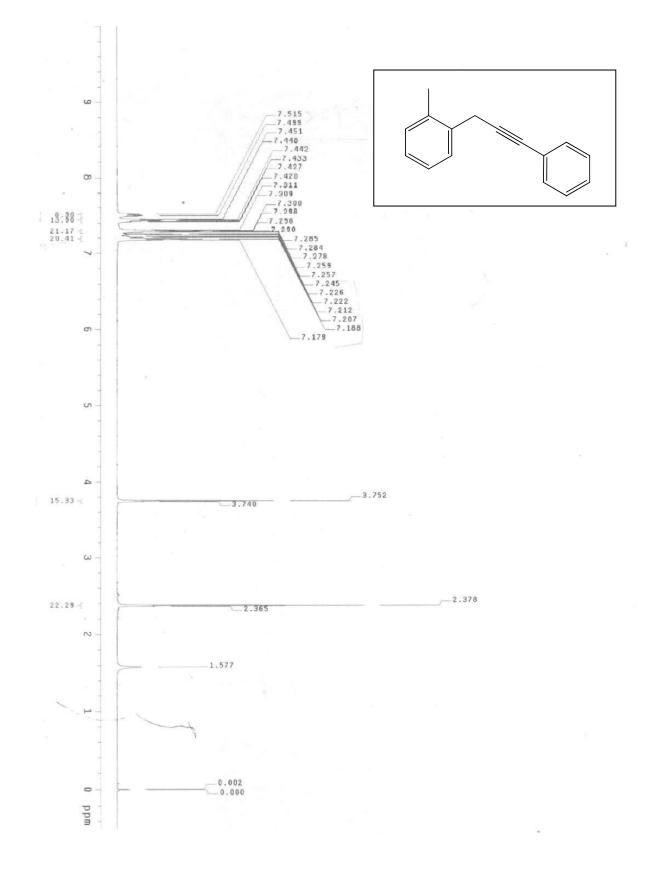
- **22. 1,3-dimethyl-5-(phenylethynyl)benzene (2v):** ¹H NMR (400 MHz, CDCl₃): δ 7.54-7.49 (m, 2H), 7.37-7.31 (m, 3H), 7.17 (m, 2H),) 6.97 (s, 1H), 2.31 (s, 6H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 137.9, 131.5, 130.2, 129.3, 128.3, 128.1, 123.4, 122.8, 89.7, 88.7, 21.1 ppm.
- **23. trimethyl(4-(phenylethynyl)phenyl)silane (2w):** ¹H NMR (400 MHz, CDCl₃): δ 7.55-7.52 (m, 2H), 7.50 (s, 4H), 7.37-7.33 (m, 3H), 0.28 (s, 9H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 141.0, 133.2, 131.6, 130.7, 128.3, 128.2, 123.6, 123.3, 89.8, 89.6, -1.2 ppm.
- 24. 1-fluoro-4-(phenylethynyl)benzene (2x): ¹H NMR (400 MHz, CDCl₃): δ 7.55-7.48 (m, 4H), 7.38-7.32 (m, 3H), 7.07-7.01 (m, 2H) ppm. ¹³C {¹H} NMR (100 MHz, CDCl₃): δ 162.4 (d, *J* = 248 Hz), 133.4 (d, *J* = 8.6 Hz), 131.5, 128.3 (d, *J* = 3.9 Hz), 123.0, 119.3 (d, *J* = 3.9 Hz), 115.7, 115.5, 89.0 (d, *J* = 1.6 Hz), 88.3 ppm.
- **25. 4-**(**phenylethynyl**)**benzonitrile** (**2y**): ¹H NMR (400 MHz, CDCl₃): δ 7.66-7.59 (m, 4H), 7.57-7.53 (m, 2H), 7.41-7.36 (m, 3H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 132.04, 132.02, 131.8, 129.1, 128.5, 128.2, 122.2, 118.5, 111.4, 93.7, 87.7 ppm.

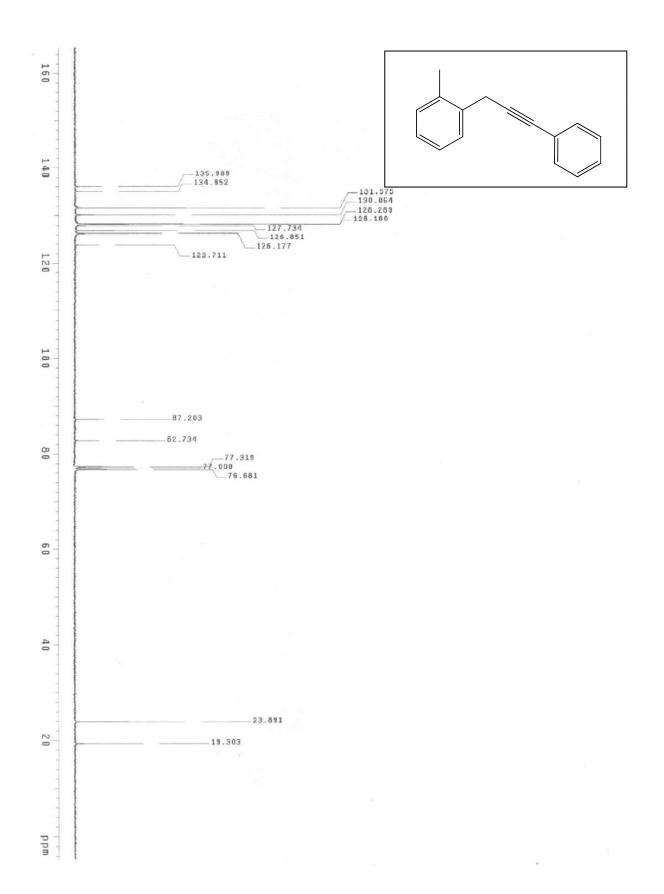
VII. ¹H and ¹³ C NMR Spectra of Coupling Products

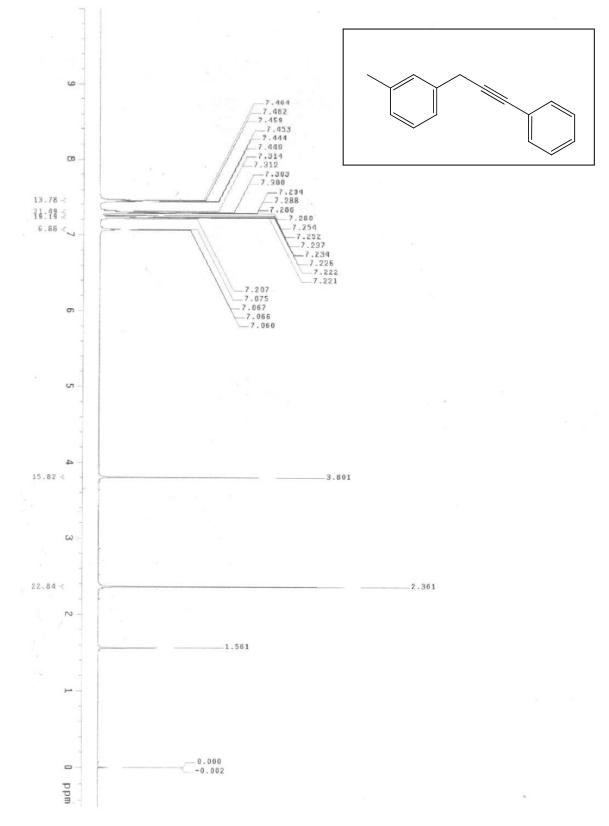




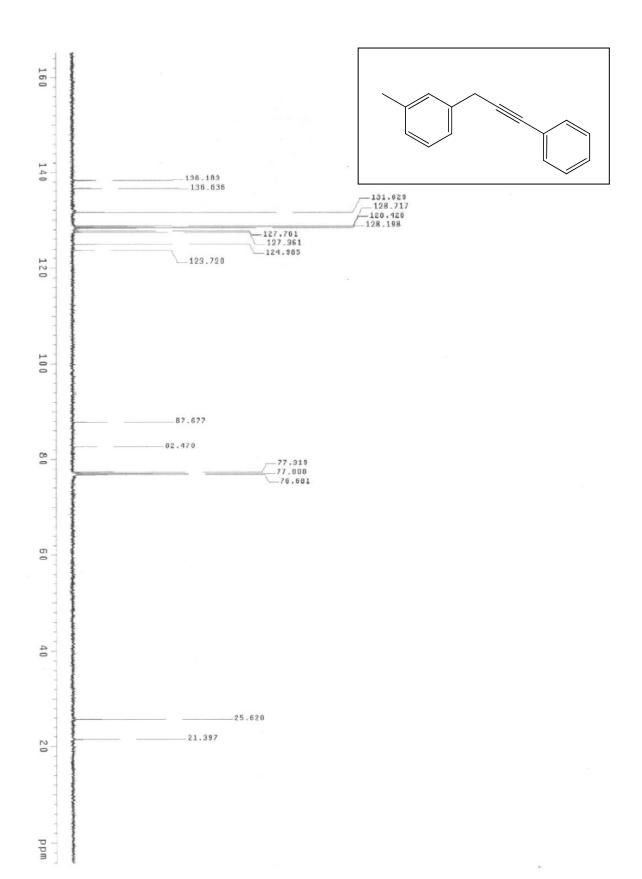




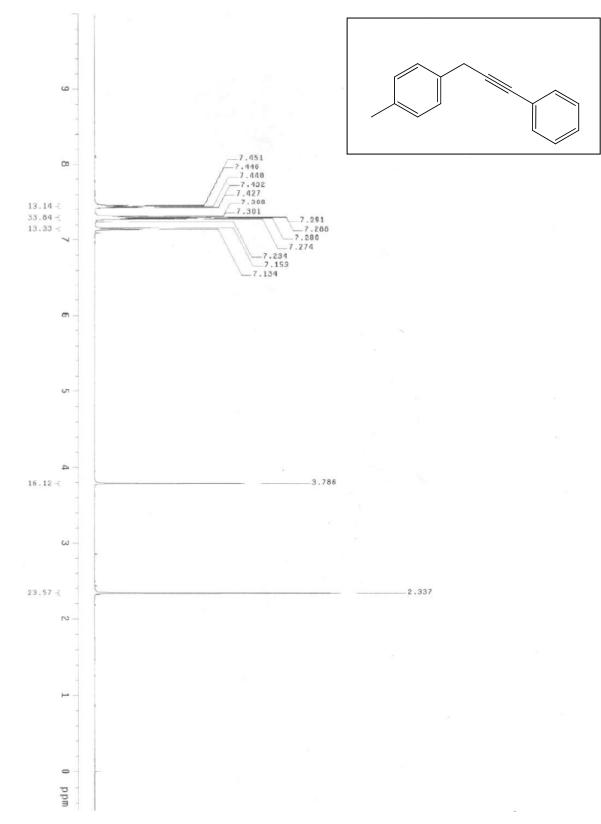




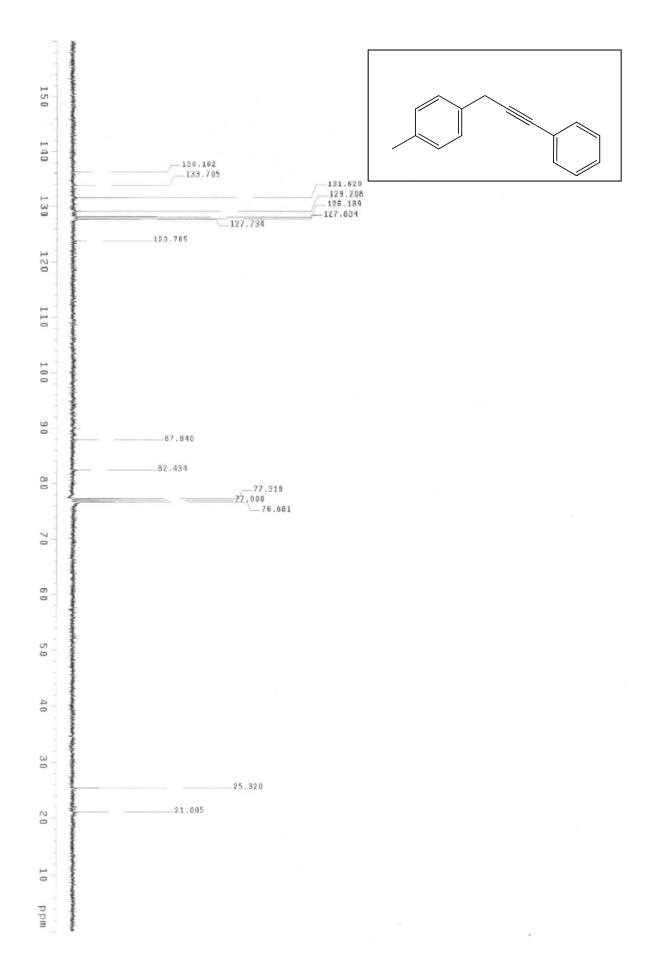
3. 1-methyl-3-(3-phenylprop-2-ynyl)benzene (2c)

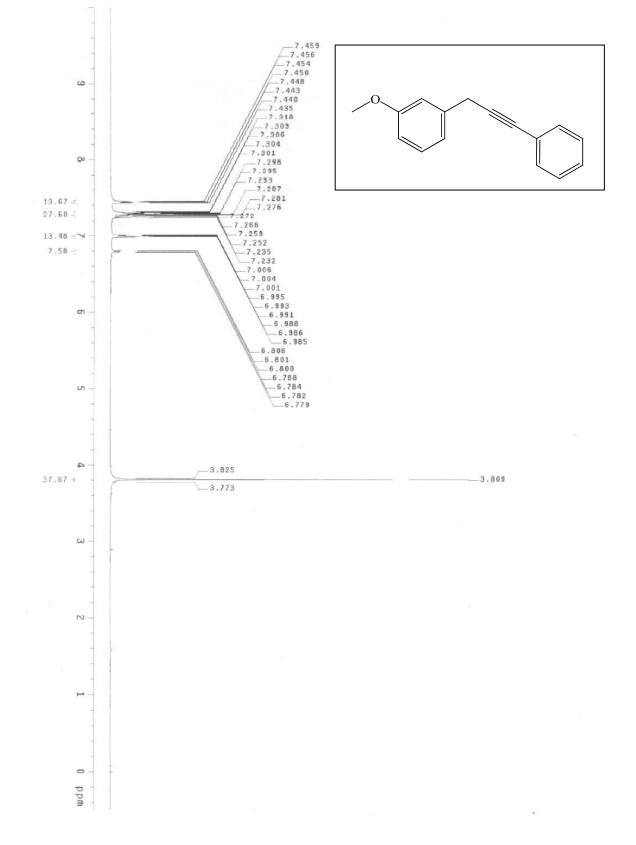


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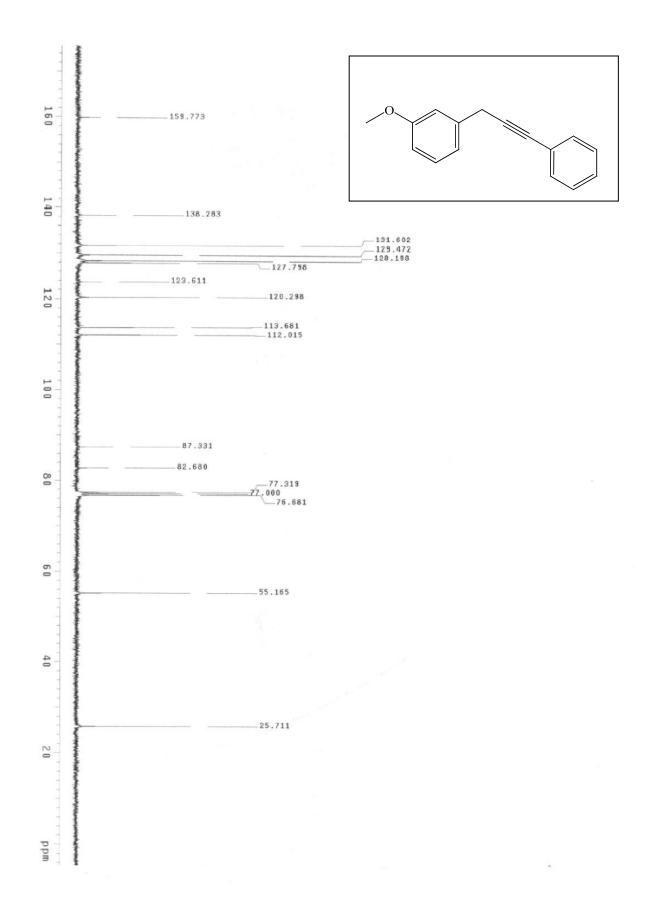


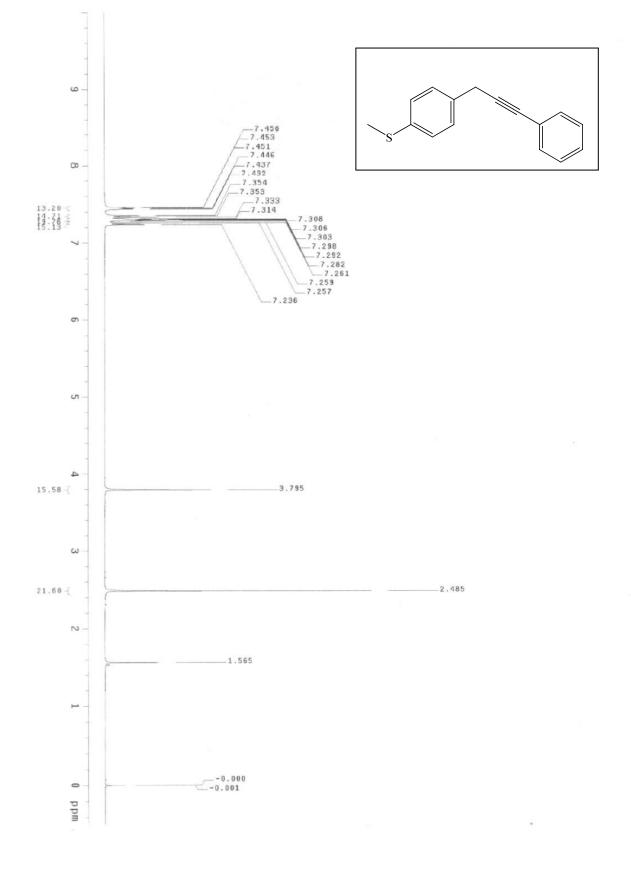
4. 1-methyl-4-(3-phenylprop-2-ynyl)benzene (2d)



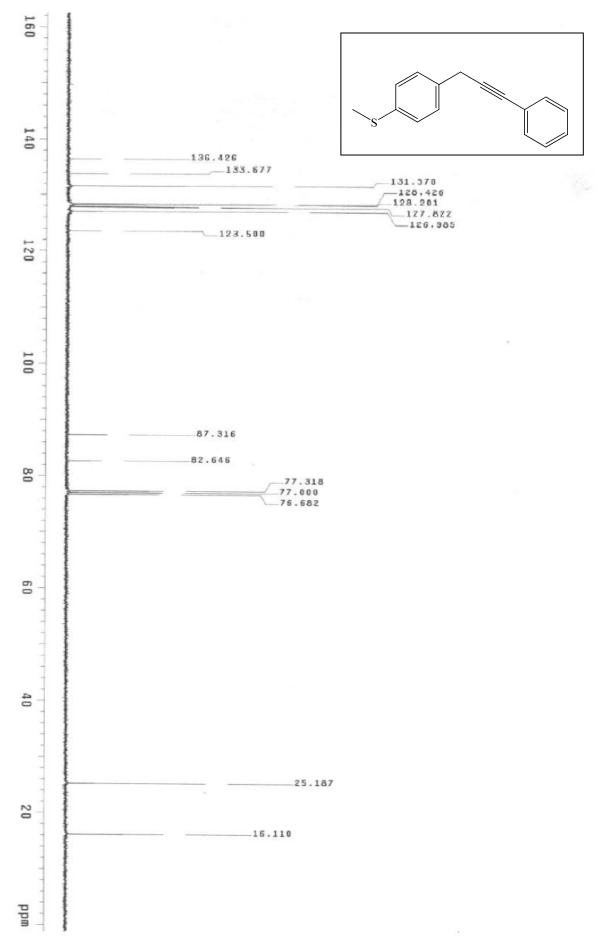


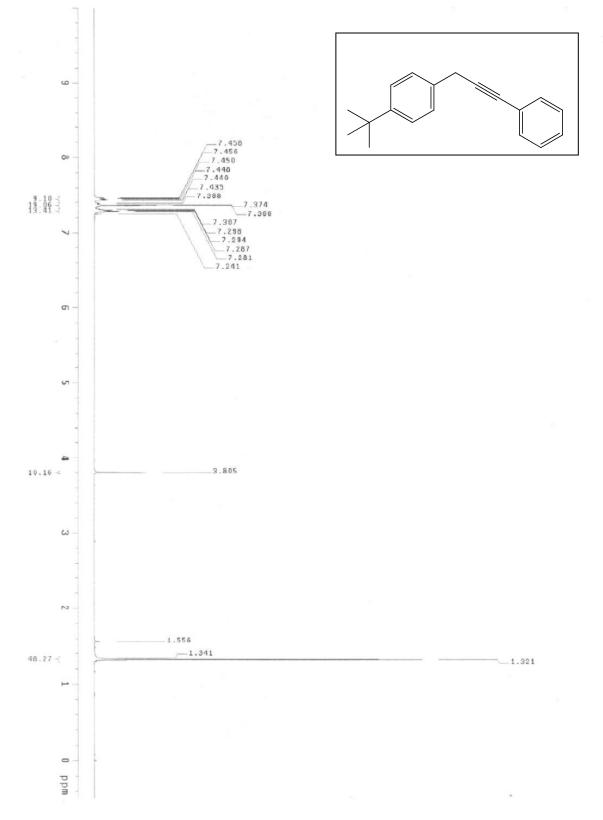
5. 1-methoxy-3-(3-phenylprop-2-ynyl)benzene (2e)



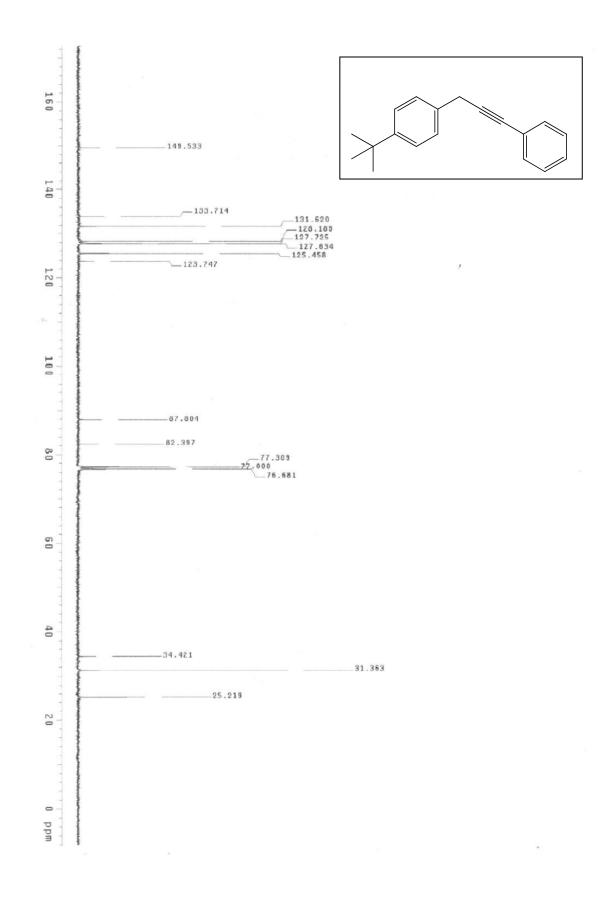


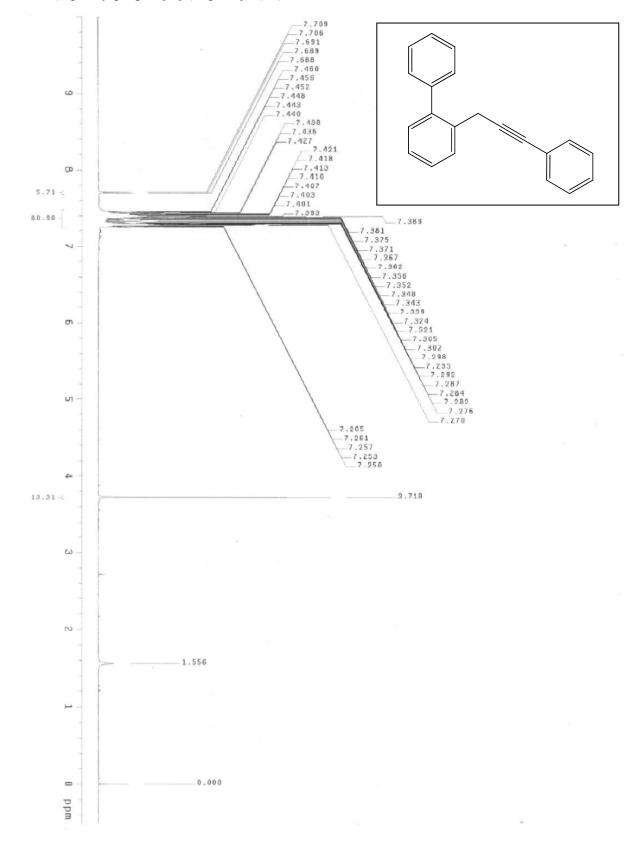
6. Methyl(4-(3-phenylprop-2-ynyl)phenyl)sulfane (2f)



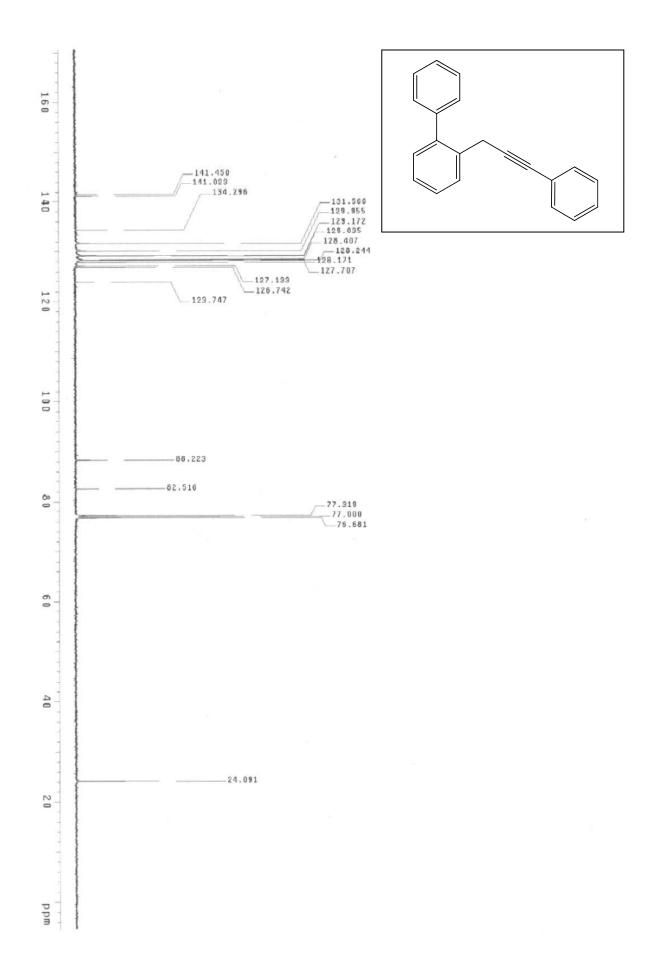


7. 1-tert-butyl-4-(3-phenylprop-2-ynyl)benzene (2g)

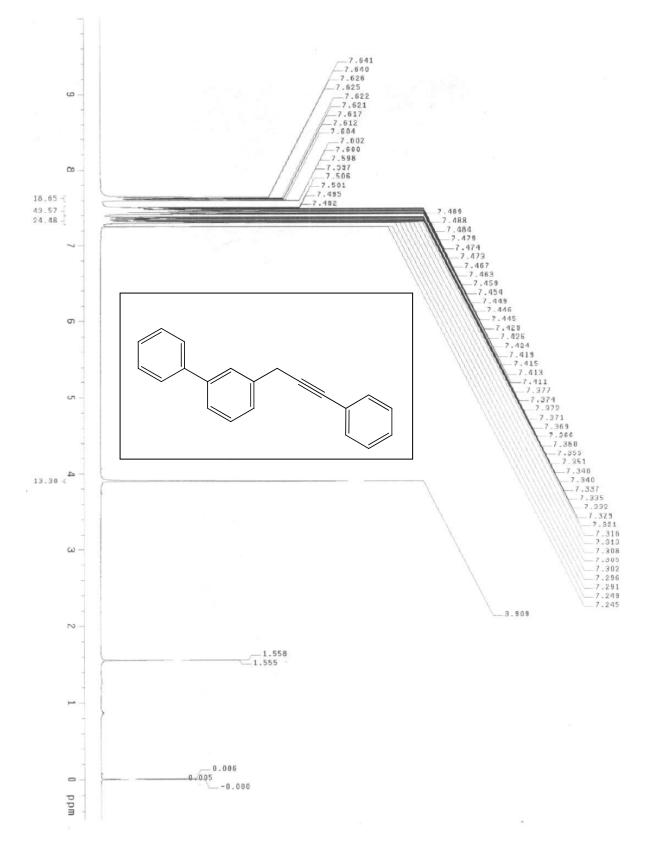


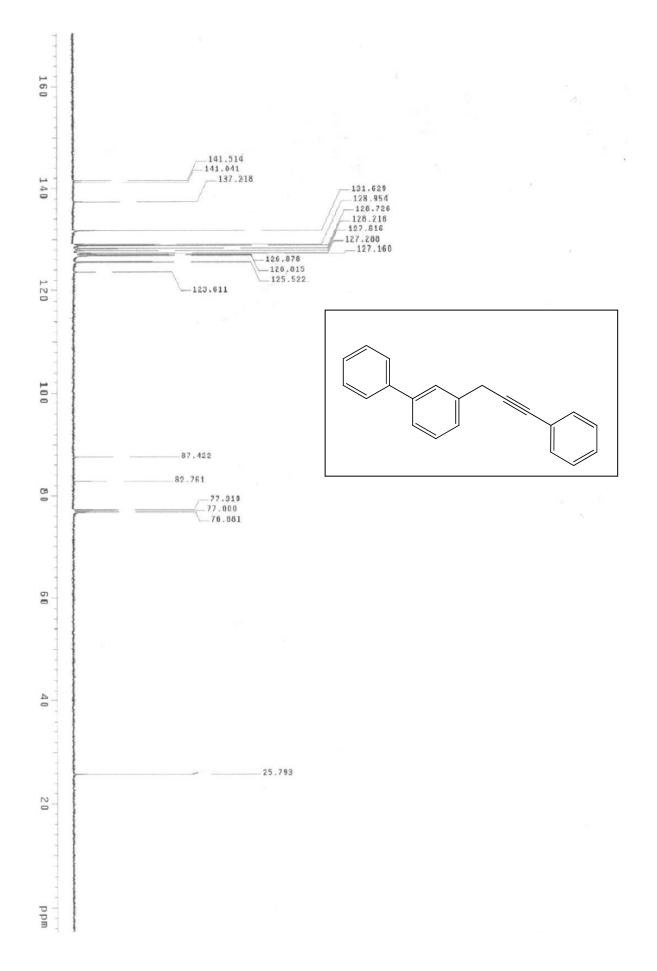


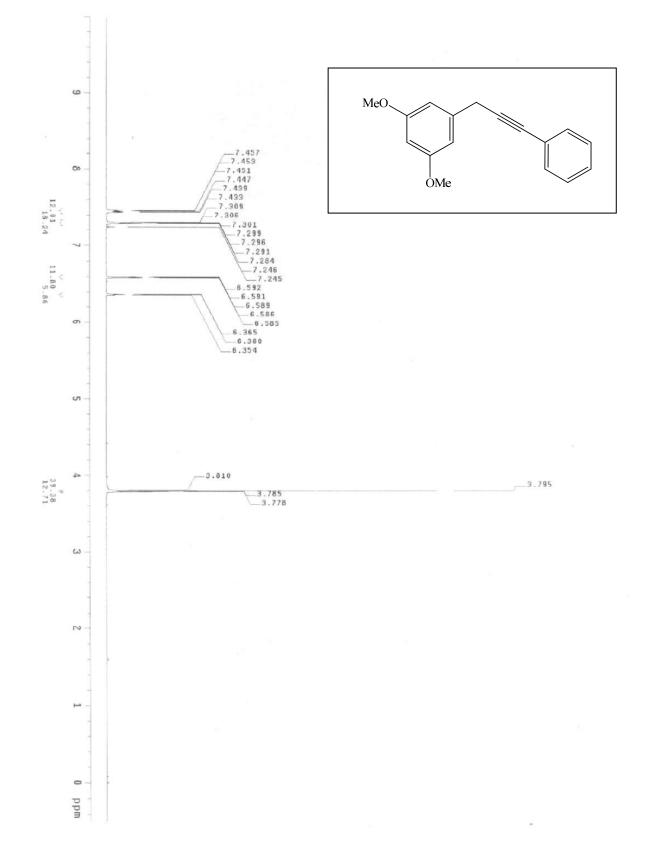
8. 2-(3-phenylprop-2-ynyl)biphenyl (2h)

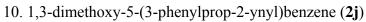


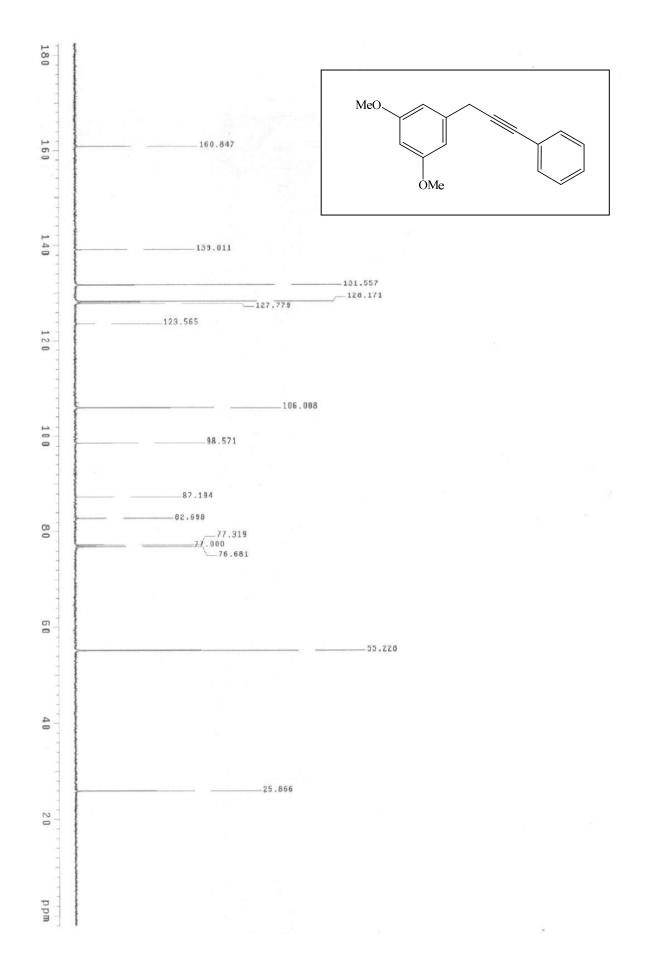
9. 3-(3-phenylprop-2-ynyl)biphenyl (2i)

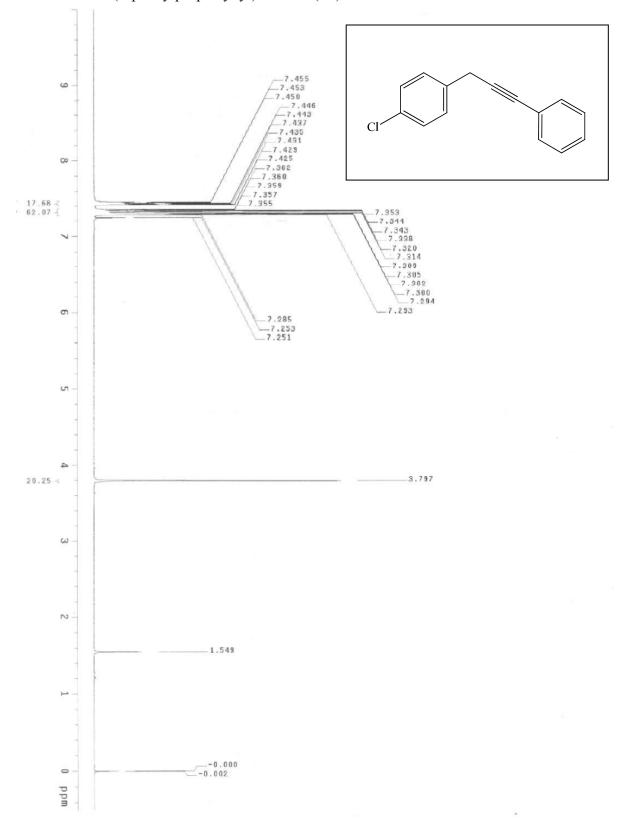




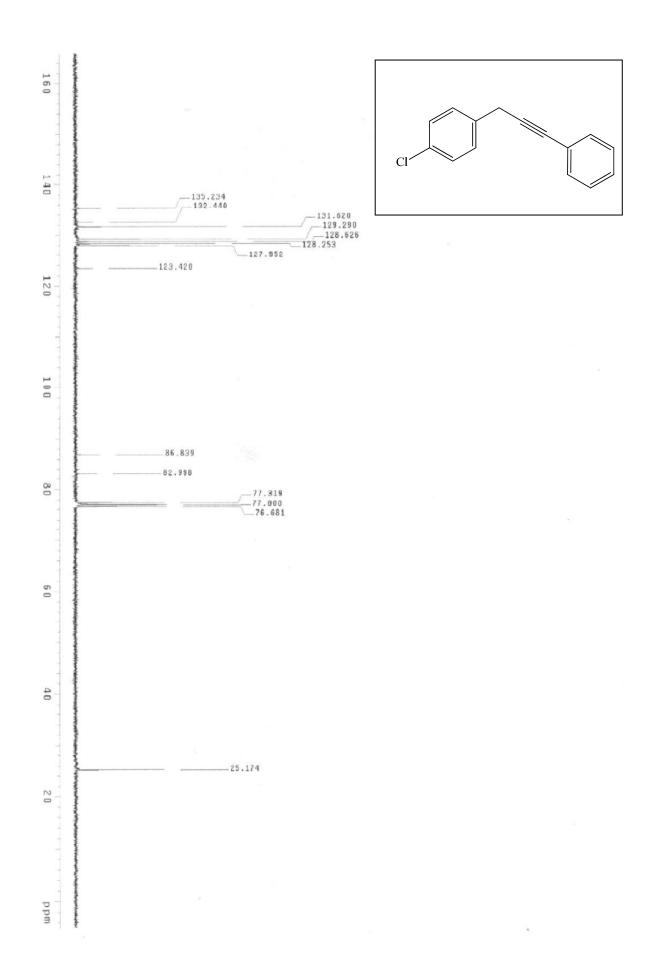




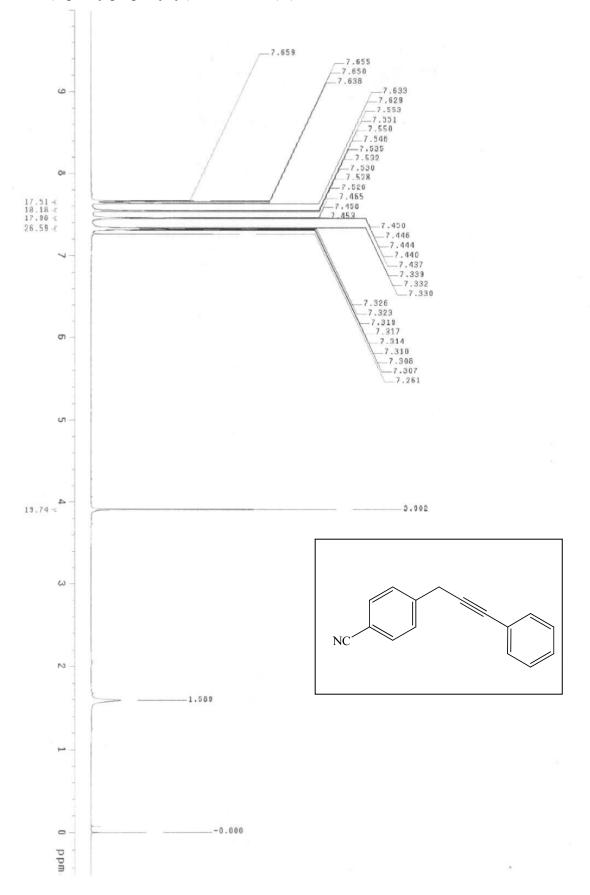


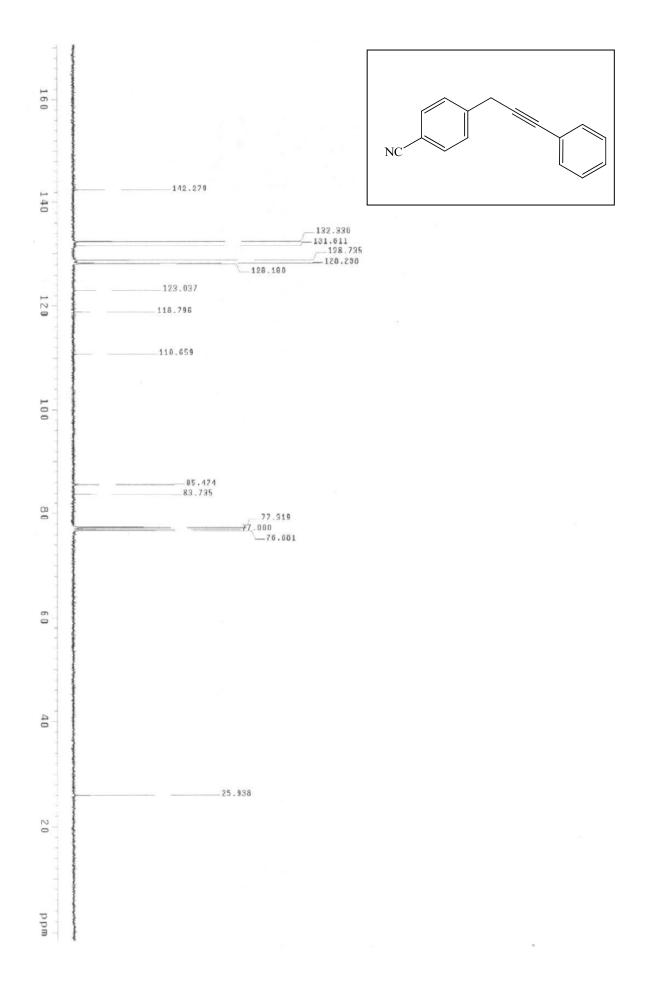


11. 1-chloro-4-(3-phenylprop-2-ynyl)benzene (2k)

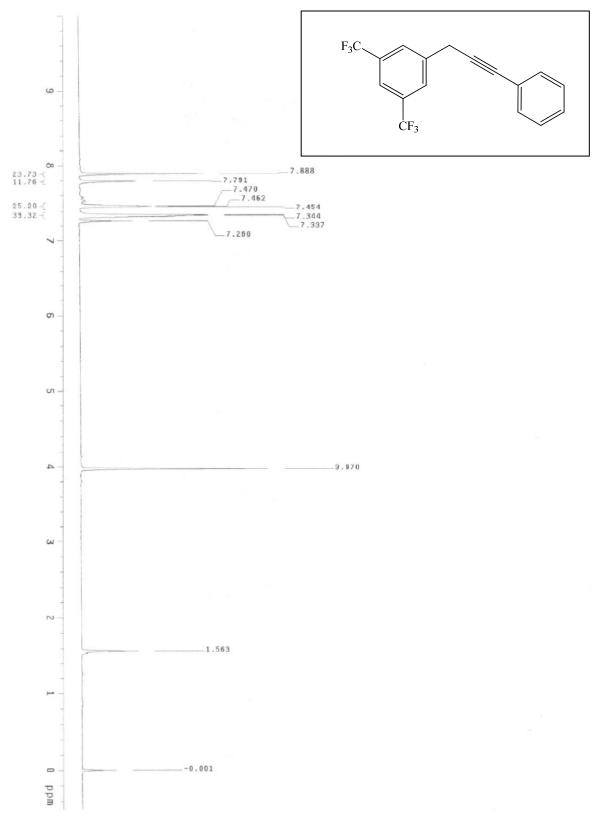


12. 4-(3-phenylprop-2-ynyl)benzonitrile (21)



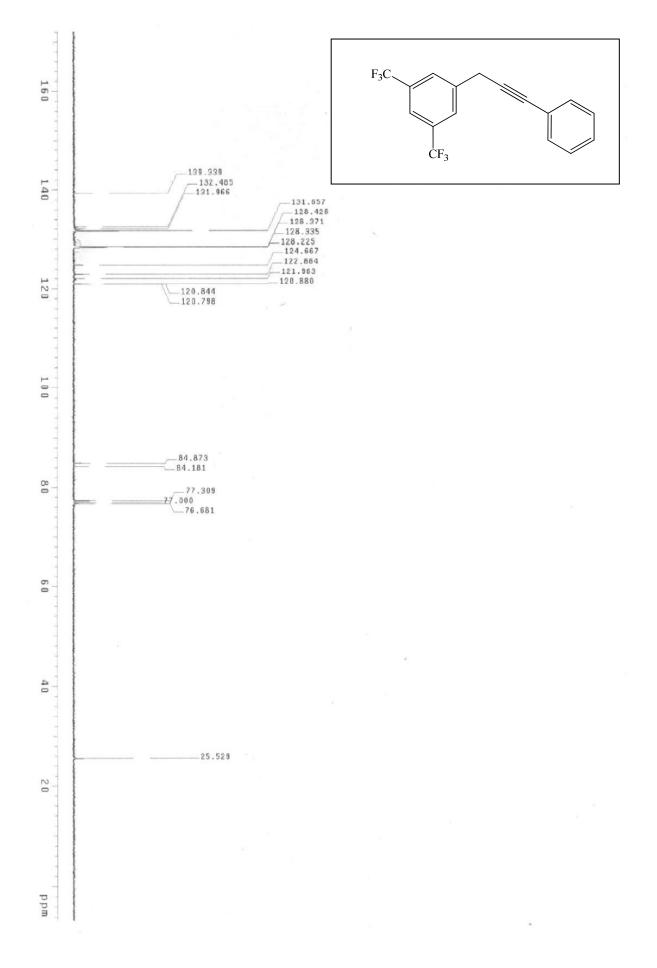


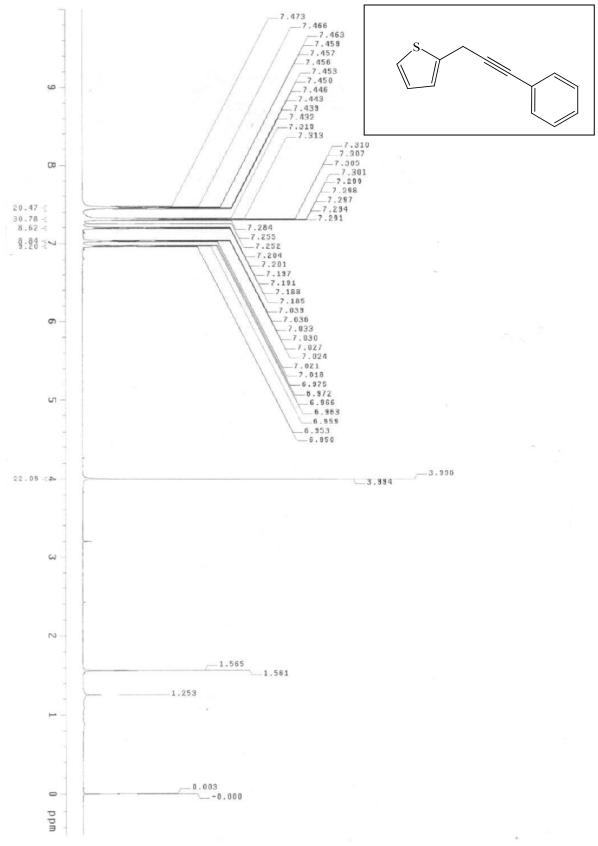
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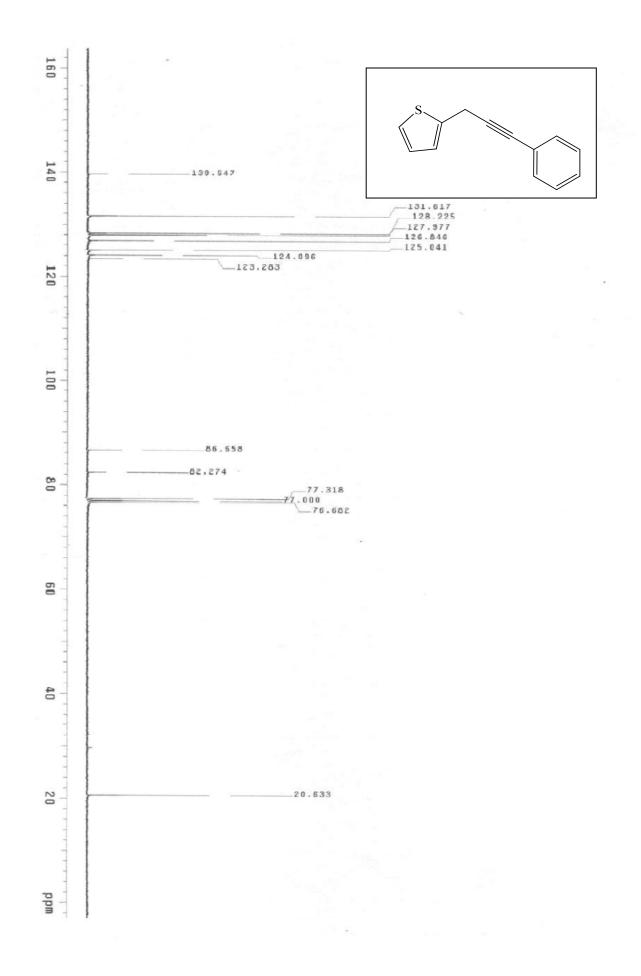
13. 1-(3-phenylprop-2-ynyl)-3,5-bis(trifluoromethyl)benzene (2m)

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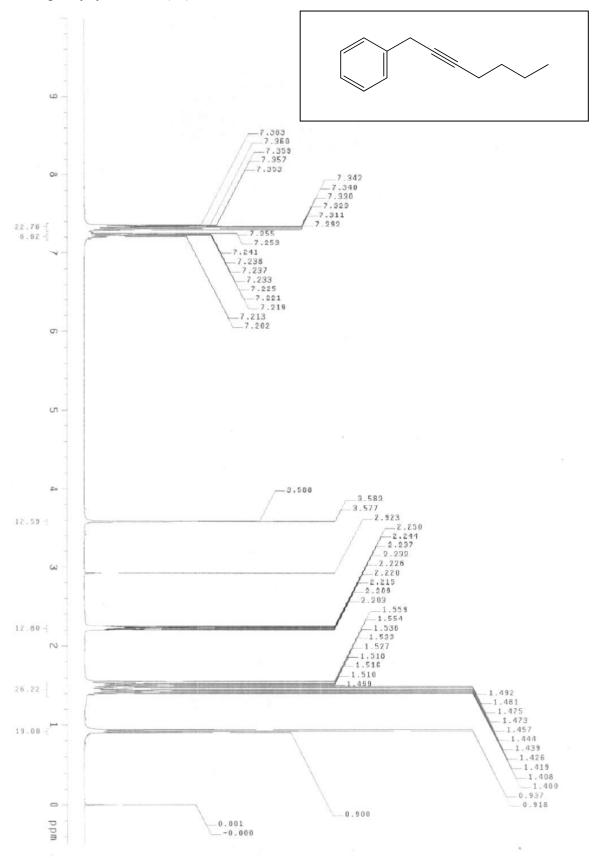


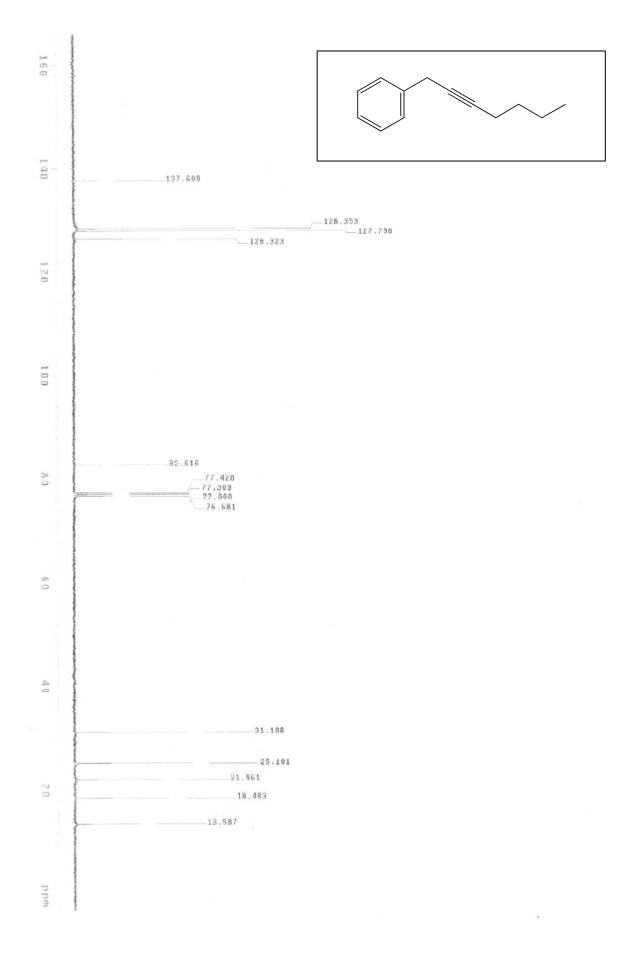


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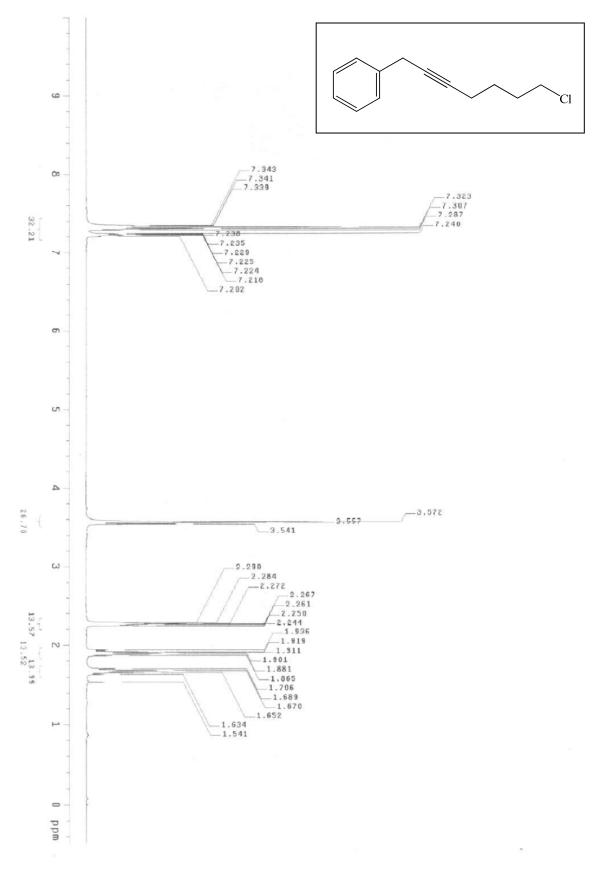


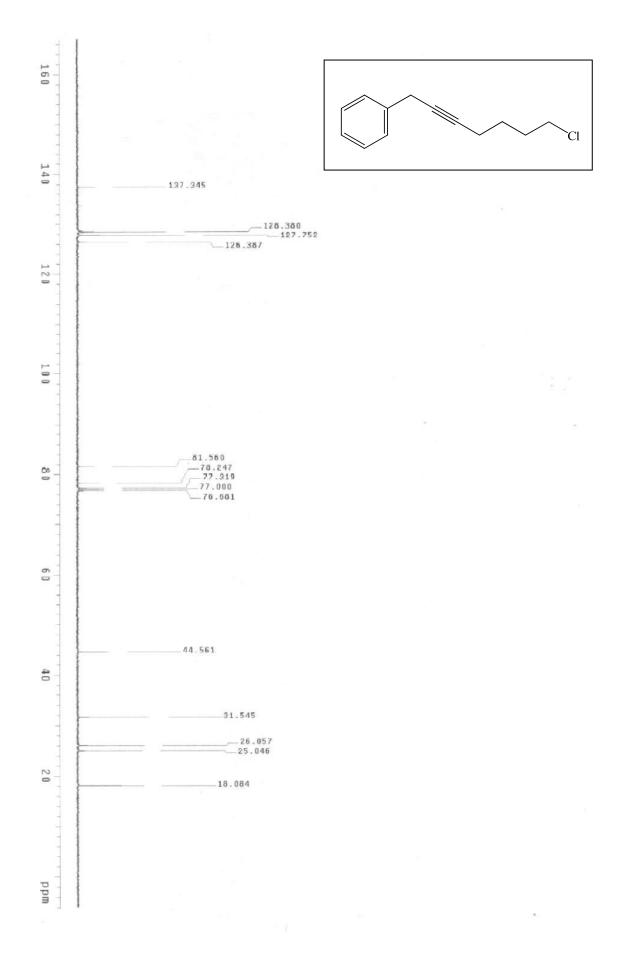
15. Hept-2-ynylbenzene (20)





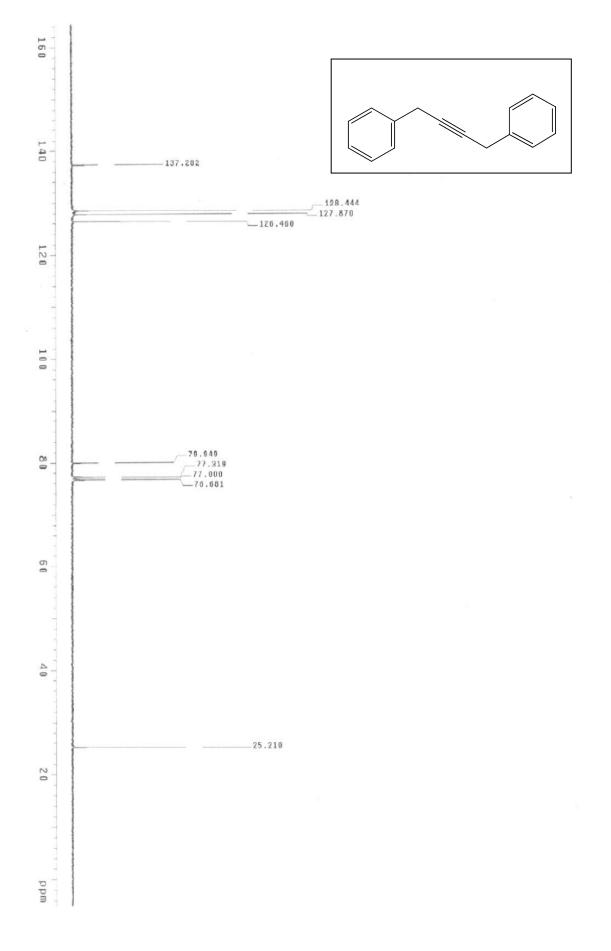
16. (7-chlorohept-2-ynyl)benzene (2p)



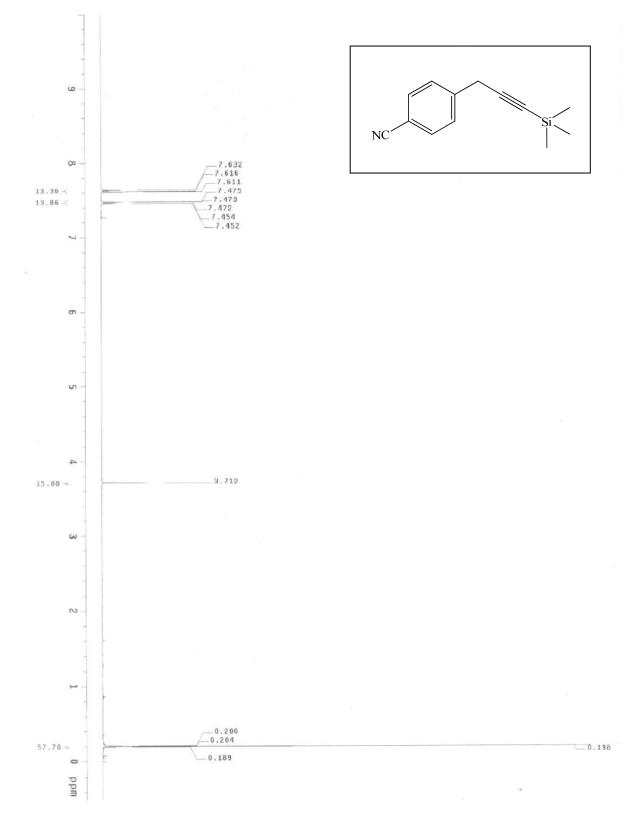


17. 1,4-diphenylbut-2-yne (2q)

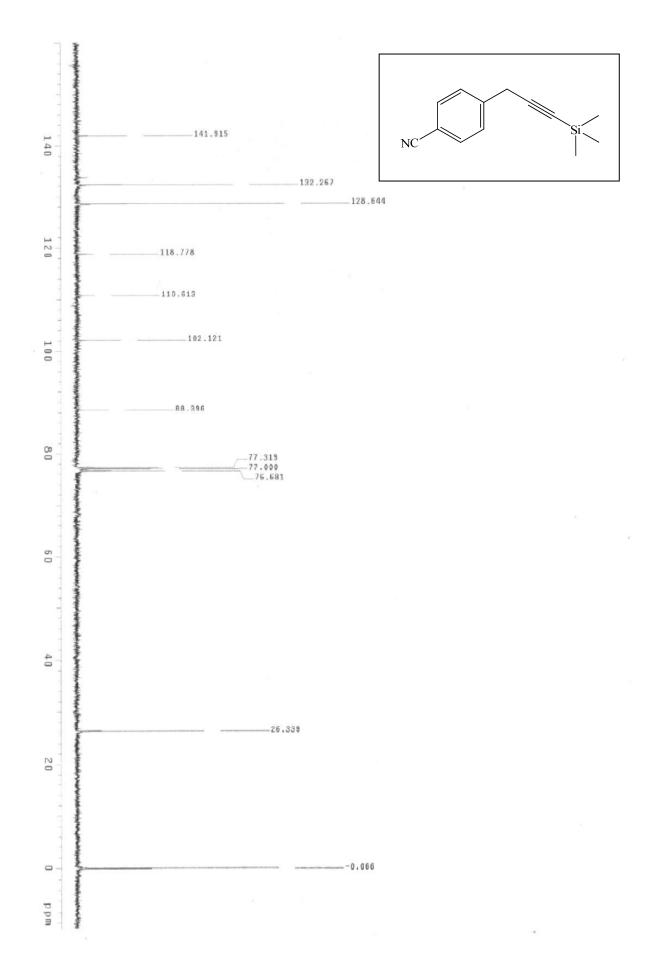
7.382 7.378 7.373 7.359 7.359 7.358 7.353 7.343 7.335 7.335 7.333 7.332 7.326 9 00 7.326 7.326 7.322 7.318 -7.316 25:56 F 27:42 14:31 F 7.3 -7.310 -7.299 -7.290 -7.246 -7.246 -7.230 -7.230 -7.230 -7.230 -7.225 -7.225 -7.210 -7.210 -7.207 -7.203 ____7.314 1 6 сл 4 _3.651 32.70 -ω N -0.000 0 ppm



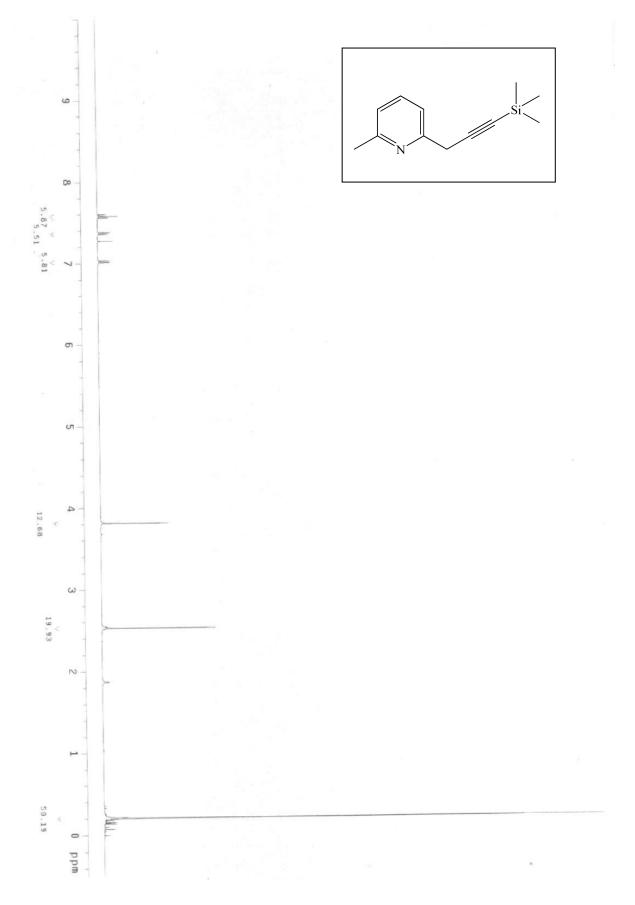
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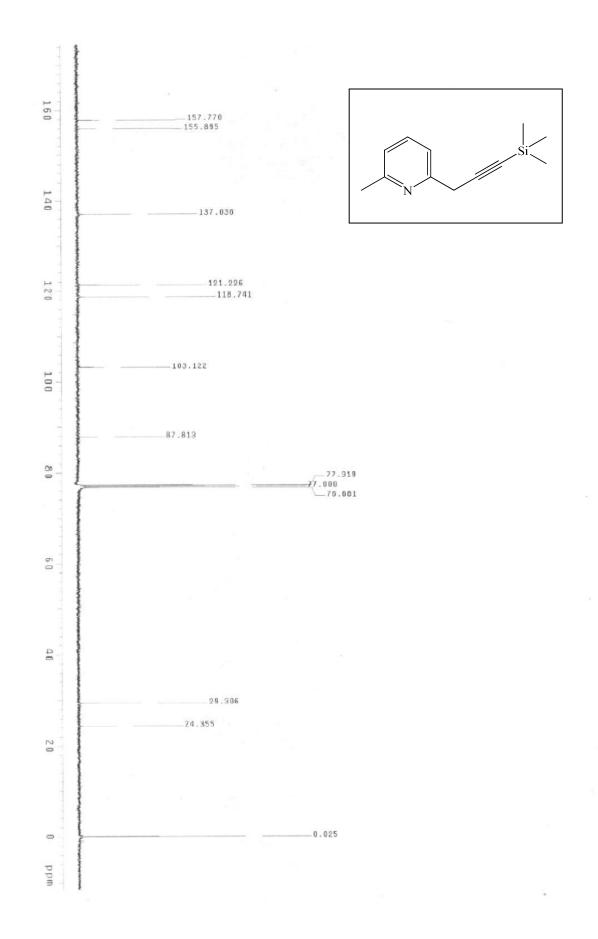


18. 4-(3-(trimethylsilyl)prop-2-ynyl)benzonitrile (2r)

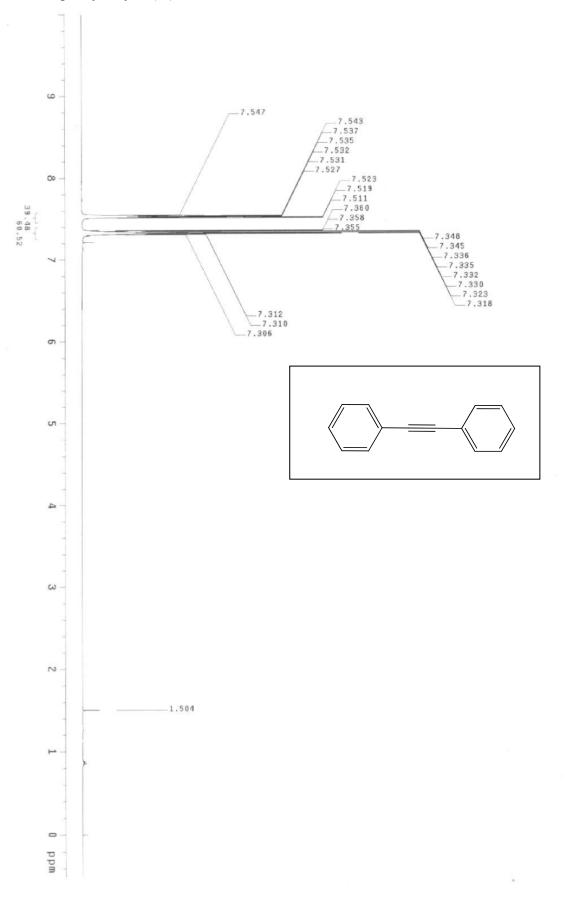


19. 2-methyl-6-(3-(trimethylsilyl)prop-2-ynyl)pyridine (2s)

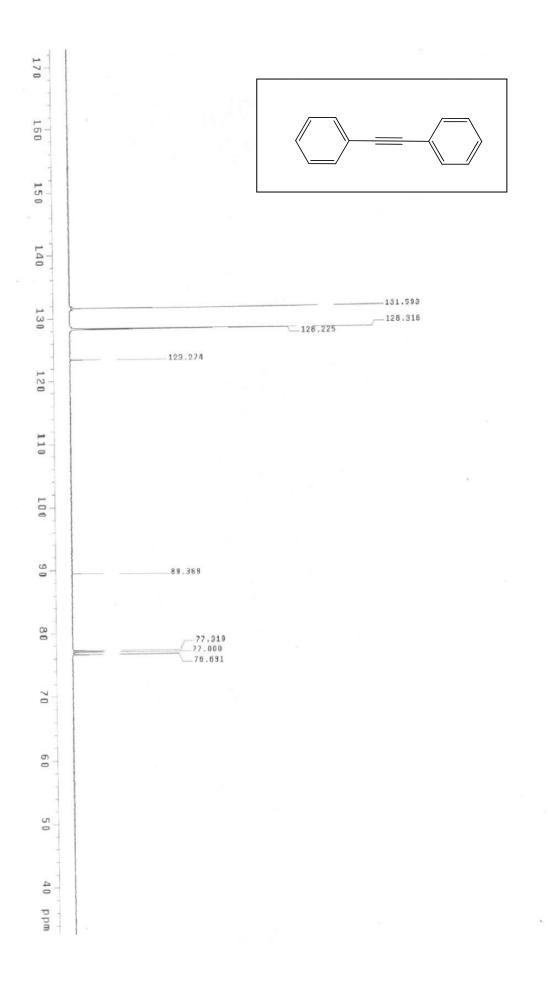


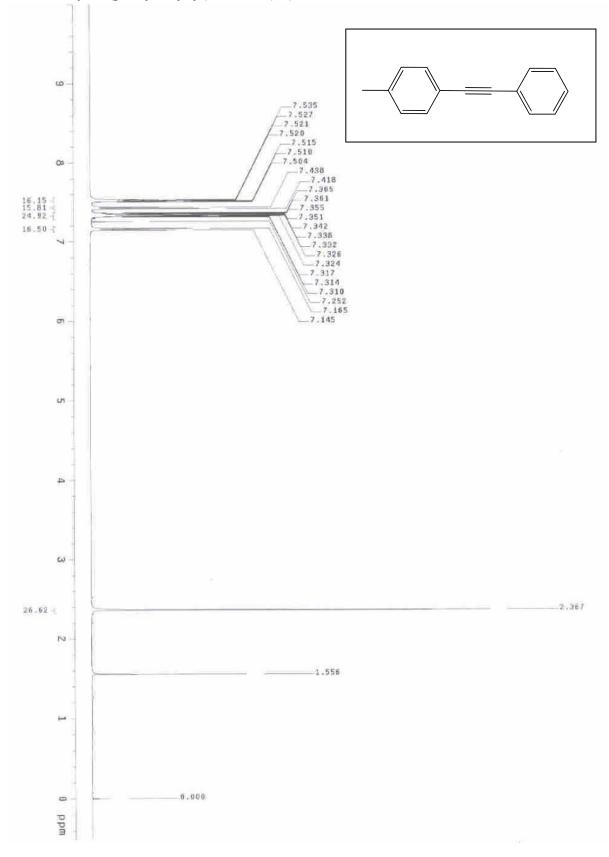


20. 1,2-diphenylethyne (2t)

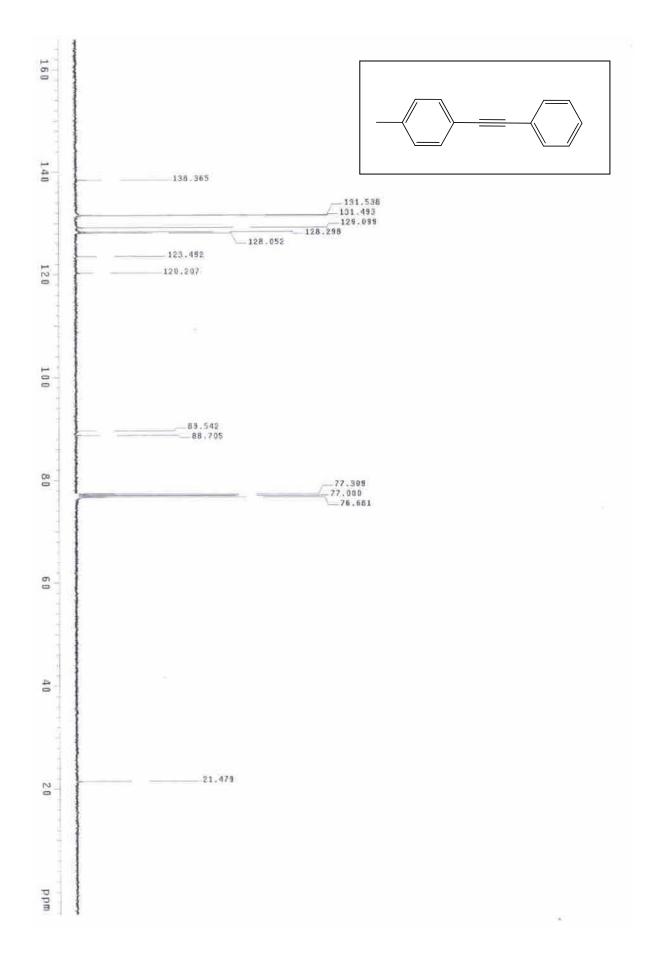


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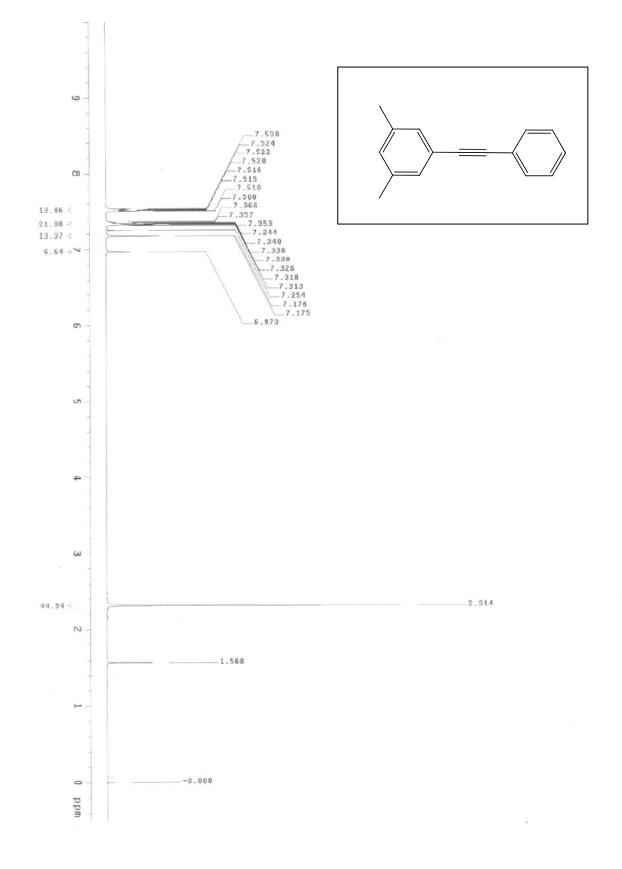




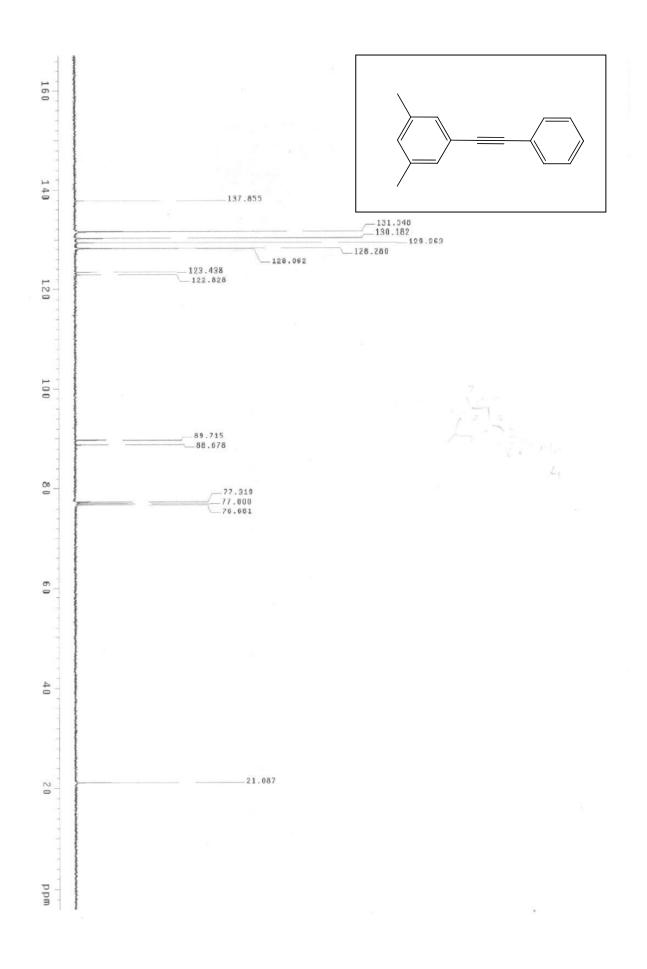
21. 1-methyl-4-(phenylethynyl)benzene (2u)

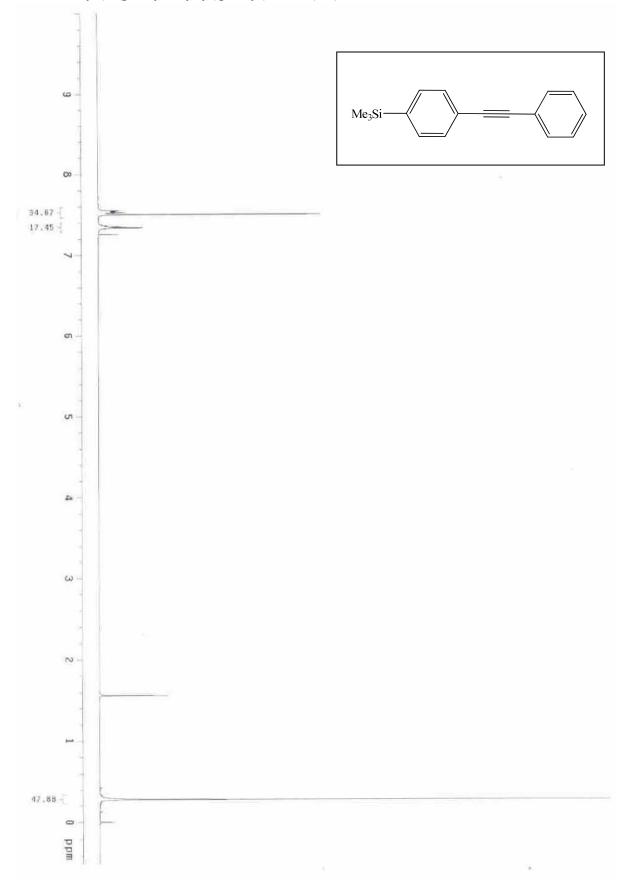


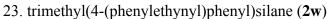
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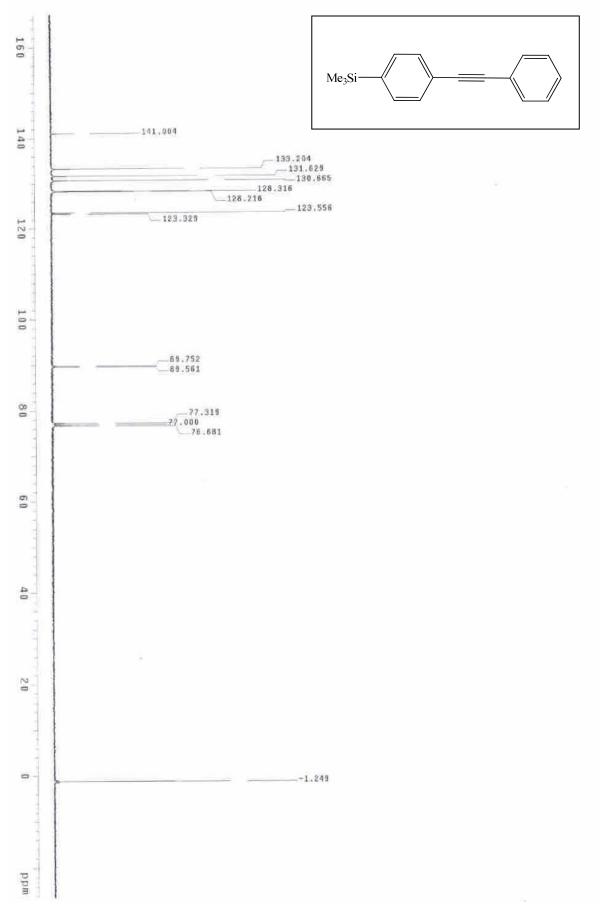


22. 1,3-dimethyl-5-(phenylethynyl)benzene (2v)









24. 1-fluoro-4-(phenylethynyl)benzene (2x)

