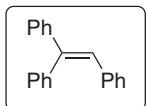


# Supplementary Information

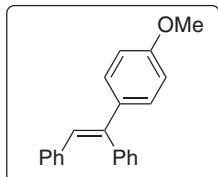
## Pd-Catalyzed Heck Reactions of Aryl Bromides with 1,2-Diarylethenes

**Jones Limberger, Silvia Poersch and Adriano L. Monteiro\***

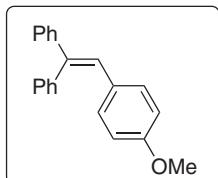
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*1,1,2-triphenylethene:* white solid, mp 70-73 °C (72-73 °C)<sup>7</sup>. <sup>1</sup>H NMR<sup>1,2</sup> (300 MHz, CDCl<sub>3</sub>) δ ppm 6.96 (s, 1H), 7.06-7.00 (m, 2H), 7.16-7.07 (m, 3H), 7.24-7.17 (m, 2H), 7.39-7.26 (m, 8H). <sup>13</sup>C NMR<sup>1,2</sup> (75 MHz, CDCl<sub>3</sub>) δ ppm 126.7, 127.4, 127.5, 127.6, 127.9, 128.1, 128.2, 128.6, 129.5, 130.4, 137.3, 140.3, 142.5, 143.4. GC-MS m/z (%): 257 (21), 256 (100, M<sup>+</sup>), 241 (21), 204 (9), 178 (53), 165 (21), 152 (13).

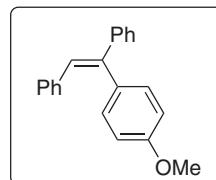


*1-methoxy-4-((E)-1,2-diphenylvinyl)benzene:* oil. <sup>1</sup>H NMR<sup>2,4</sup> (300 MHz, CDCl<sub>3</sub>) δ ppm 3.82 (s, 3H), 6.85 (d, 2H, J 8.93 Hz), 6.90 (s, 1H), 7.03-6.98 (m, 2H), 7.15-7.07 (m, 3H), 7.23-7.18 (m, 2H), 7.26 (d, 2H, J 8.92 Hz), 7.35-7.30 (m, 1H). <sup>13</sup>C-NMR<sup>4</sup> (75 MHz, CDCl<sub>3</sub>) δ ppm 55.1, 113.5, 126.3, 126.4, 127.3, 127.8, 128.5, 128.7, 129.3, 130.3, 135.9, 137.5, 140.4, 142.0, 159.1. GC-MS m/z (%): 287 (24), 286 (100, M<sup>+</sup>), 255 (12), 228 (11), 215 (9), 178 (16), 165 (26), 126 (12), 120 (21).

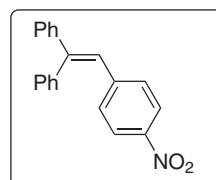


*1-methoxy-4-(2,2-diphenylvinyl)benzene:* white solid obtained with 80% of purity (20% of 4-methoxystilbene). <sup>1</sup>H NMR<sup>5,6</sup> (300 MHz, CDCl<sub>3</sub>) δ ppm

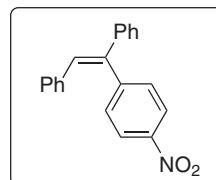
3.75 (s, 3H), 6.68 (d, 2H, J 8.80 Hz), 6.92 (s, 1H), 6.96 (d, 2H, J 8.88 Hz), 7.38-7.20 (m, 10H). GC-MS m/z (%): 287 (22), 286 (100, M<sup>+</sup>), 271 (7), 253 (7), 239 (8), 228 (9), 215 (6), 178 (8), 165 (38).



*1-((Z)-1-(4-methoxyphenyl)-2-phenylvinyl)benzene:* GC-MS m/z (%): 287 (24), 286 (100, M<sup>+</sup>), 253 (11), 228 (10), 215 (9), 178 (17), 165 (25), 126 (11), 119 (16).



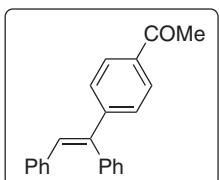
*1-(2-(4-nitrophenyl)-1-phenylvinyl)benzene:* yellow solid, mp 148-151 °C (148-150 °C)<sup>5</sup>. <sup>1</sup>H NMR<sup>1</sup> (300 MHz, CDCl<sub>3</sub>) δ ppm 7.00 (s, 1H), 7.14 (d, 2H, J 8.97 Hz), 7.21-7.16 (m, 2H), 7.49-7.30 (m, 8H), 7.98 (d, 2H, J 8.91 Hz). <sup>13</sup>C NMR<sup>1,5</sup> (75 MHz, CDCl<sub>3</sub>) δ ppm 123.2, 125.6, 127.8, 128.2, 128.3, 128.4, 128.9, 129.9, 130.1, 139.2, 142.3, 144.2, 145.8, 146.9. GC-MS m/z (%): 302 (22), 301 (100, M<sup>+</sup>), 254 (30), 253 (38), 239 (27), 178 (18), 165 (27), 126 (16), 113 (11).



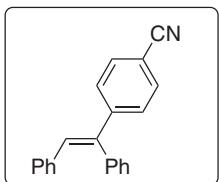
*1-((Z)-2-(4-nitrophenyl)-2-phenylvinyl)benzene:* yellow crystals, mp 160-163 °C. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ ppm 7.08-7.01 (m, 2H), 7.10 (s, 1H), 7.22-7.17 (m, 3H),

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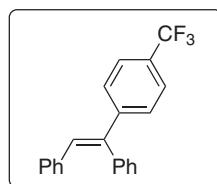
7.32-7.26 (m, 2H), 7.38-7.34 (m, 2H), 7.40 (dd, 2H, J 6.94, 1.86 Hz), 8.19 (dd, 2H, J 6.88, 1.88 Hz).  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm 123.7, 127.4, 127.5, 128.0, 128.2, 128.4, 129.4, 130.1, 131.4, 136.3, 140.4, 142.0, 146.9, 147.6. GC-MS (IE, 70 eV)  $m/z$  (%): 302 (24), 301 (100,  $\text{M}^+$ ), 253 (36), 239 (27), 215 (12), 179 (26), 165 (23), 126 (20), 113 (14).



*I*-(4-((E)-1,2-diphenylvinyl)phenyl)ethanone: GC-MS (IE, 70 eV)  $m/z$  (%):<sup>3</sup> 299 (22), 298 (100,  $\text{M}^+$ ), 283 (60), 255 (27), 253 (29), 239 (28), 207 (20), 178 (15), 152 (9), 120 (14).



4-((E)-1,2-diphenylvinyl)benzonitrile: GC-MS (IE, 70 eV)  $m/z$  (%):<sup>3</sup> 282 (23), 281 (100,  $\text{M}^+$ ), 266 (21), 253 (11), 203 (17), 179 (28), 165 (14), 126 (13).



*I*-(trifluoromethyl)-4-((E)-1,2-diphenylvinyl)benzene: GC-MS (IE, 70 eV)  $m/z$  (%):<sup>2,7</sup> 325 (22), 324 (100,  $\text{M}^+$ ), 309 (17), 283 (21), 253 (21), 246 (16), 178 (35), 165 (17), 126 (16).

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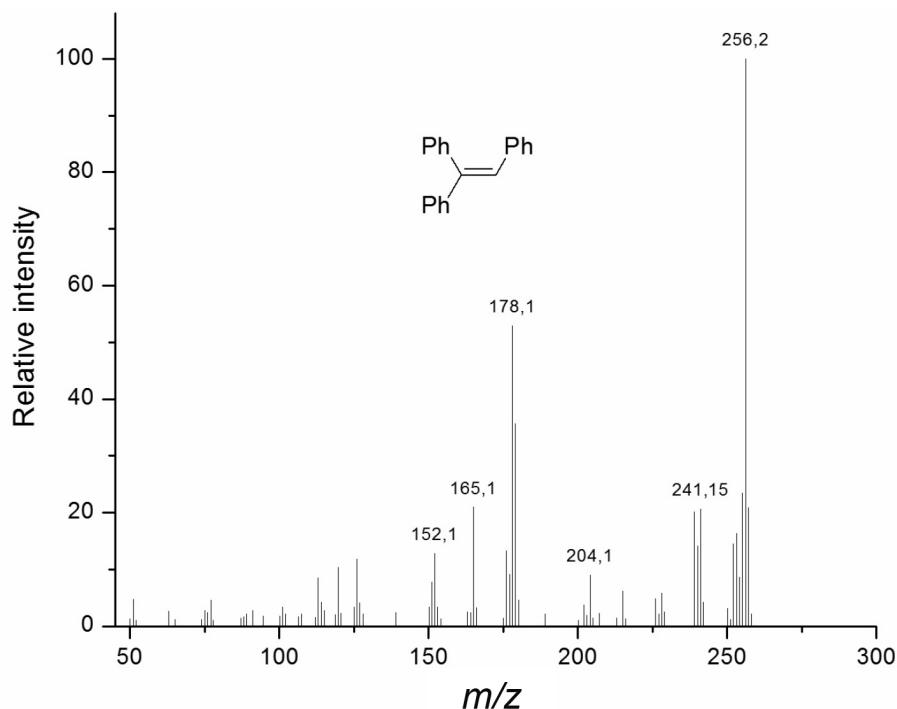
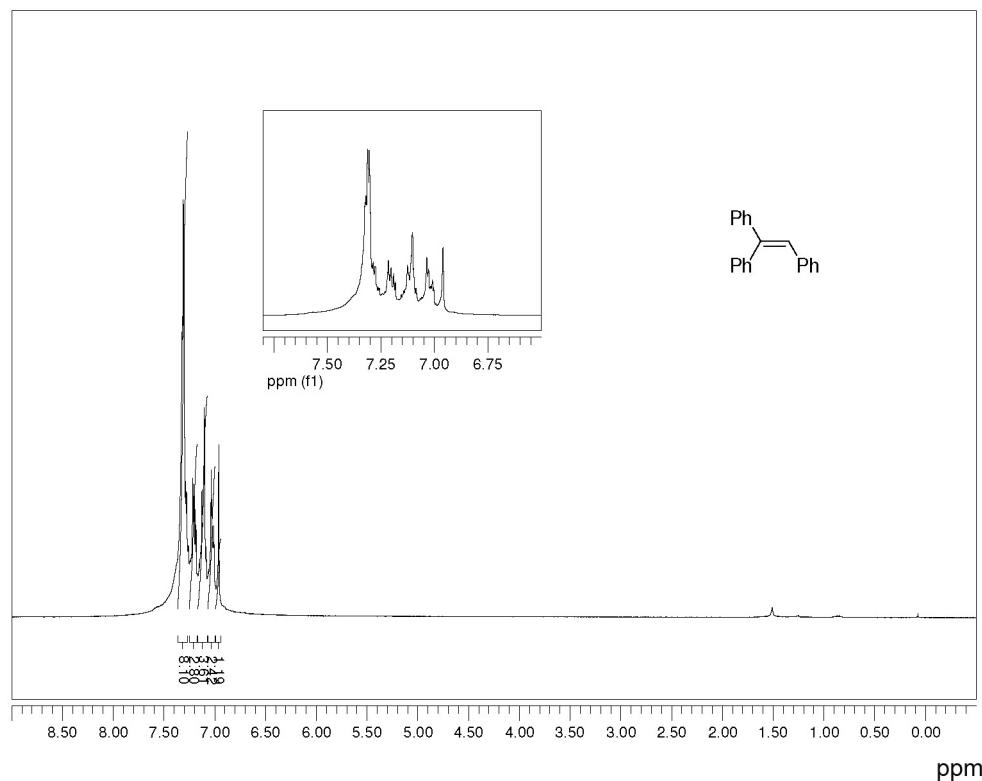
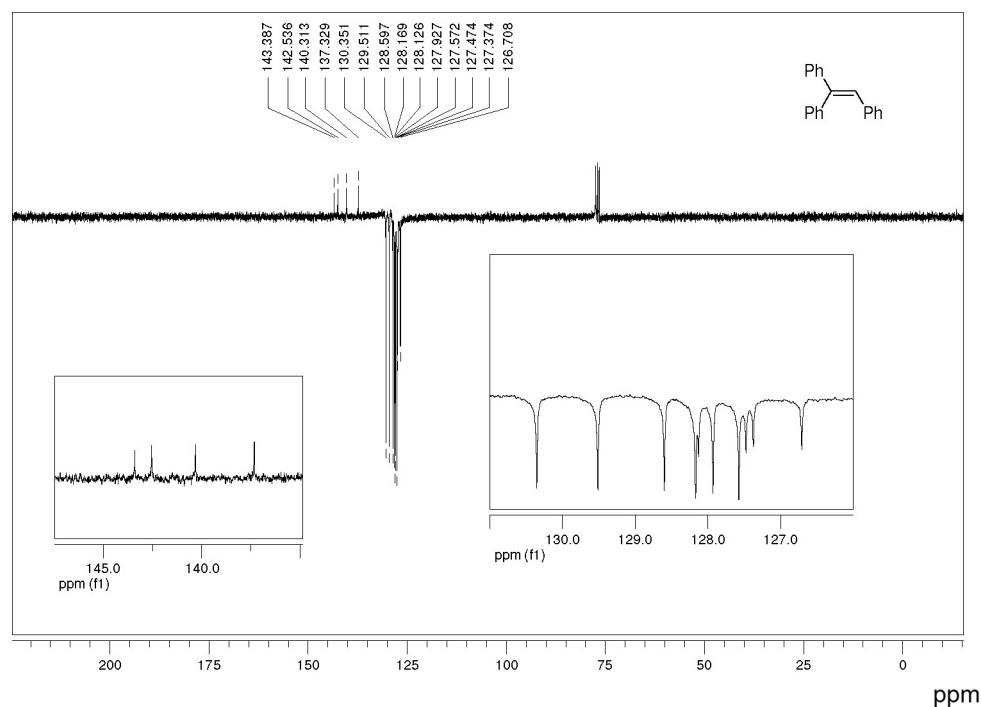


Figure S1. Mass spectrum of 1,1,2-triphenylethene.



**Figure S2.** <sup>1</sup>H NMR spectrum of 1,1,2-triphenylethene.



**Figure S3.** <sup>13</sup>C (APT) NMR spectrum of 1,1,2-triphenylethene.

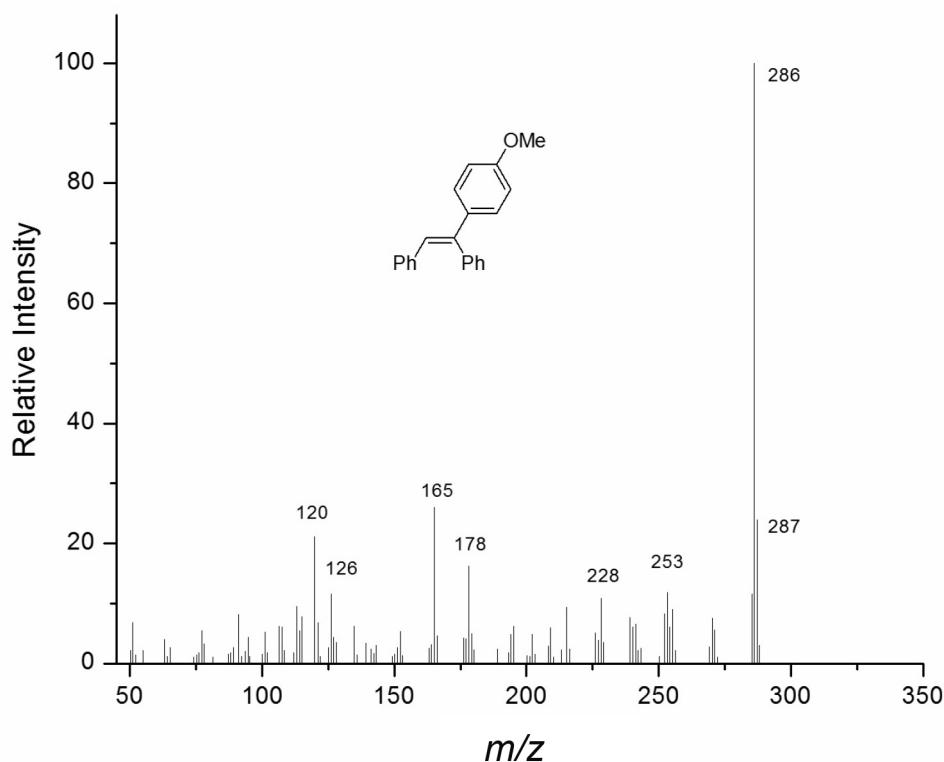


Figure S4. Mass spectrum of 1-methoxy-4-((E)-1,2-diphenylvinyl)benzene.

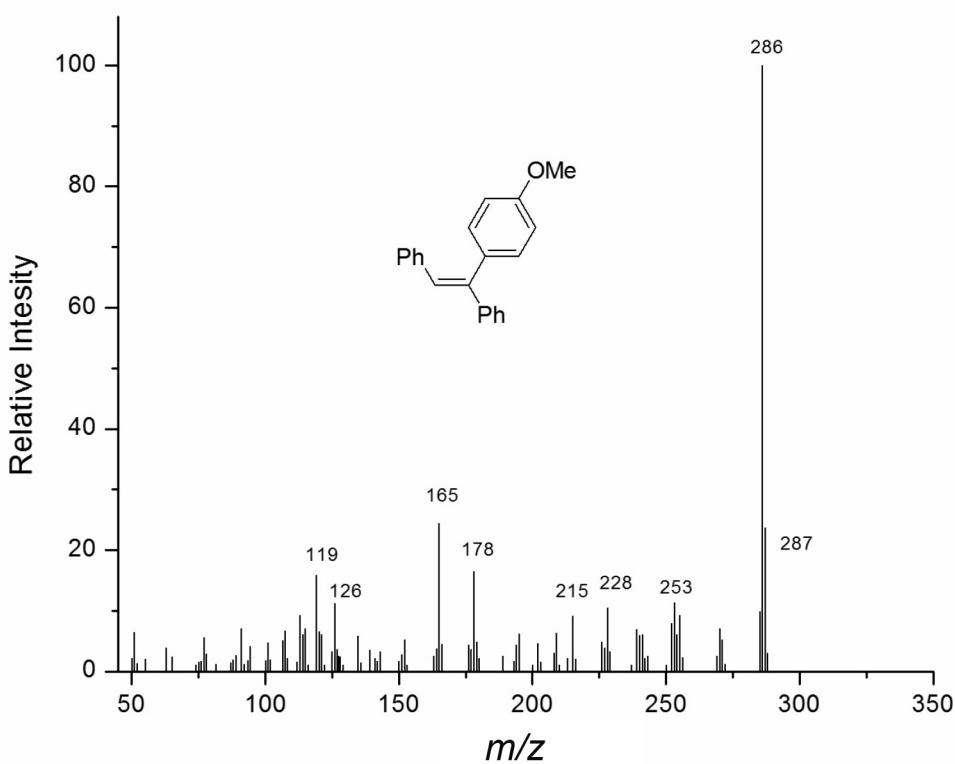
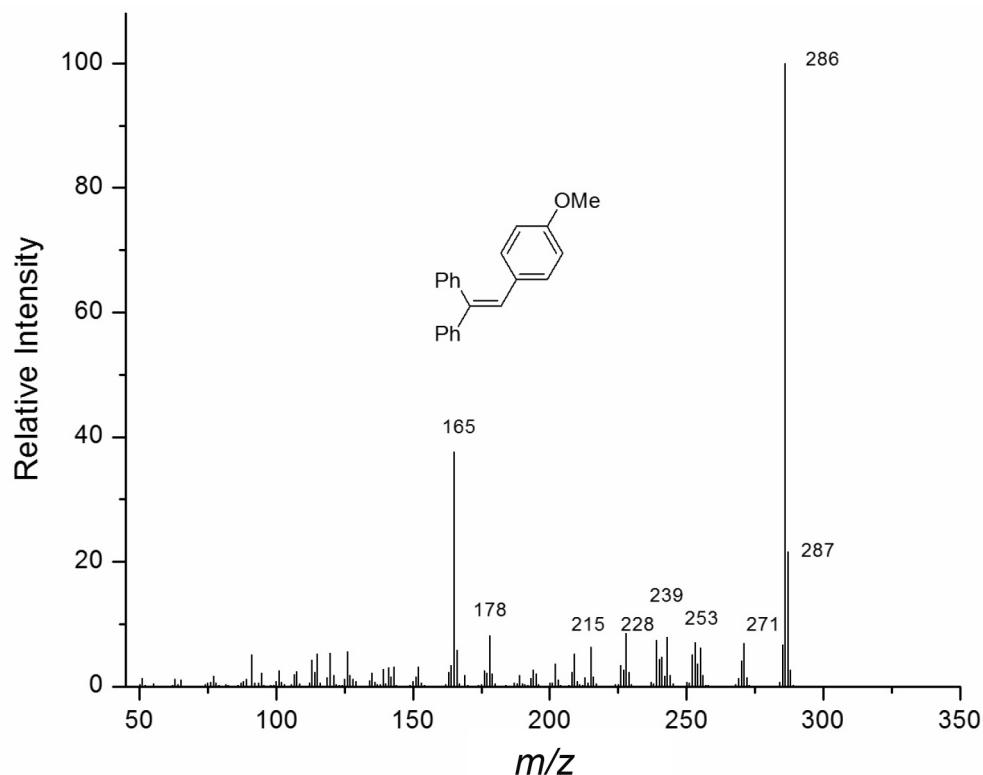
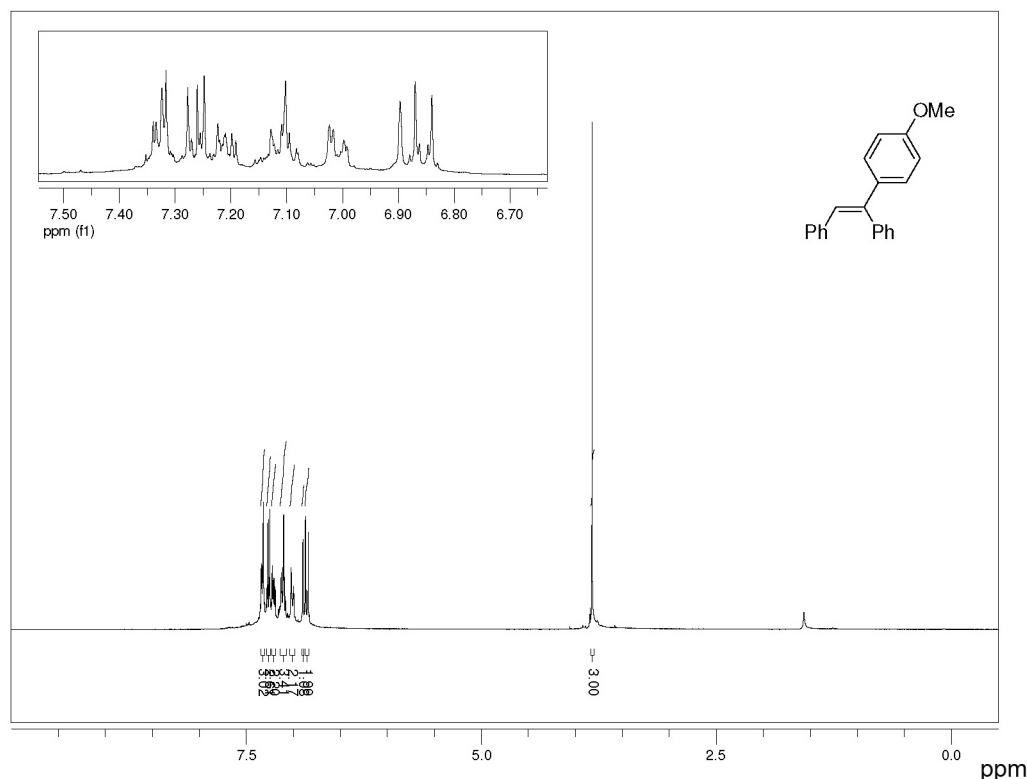


Figure S5. Mass spectrum of 1-((Z)-1-(4-methoxyphenyl)-2-phenylvinyl)benzene.



**Figure S6.** Mass spectrum of 1-methoxy-4-(2,2-diphenylvinyl)benzene.



**Figure S7.**  $^1\text{H}$  NMR spectrum of 1-methoxy-4-(*E*)-1,2-diphenylvinylbenzene.

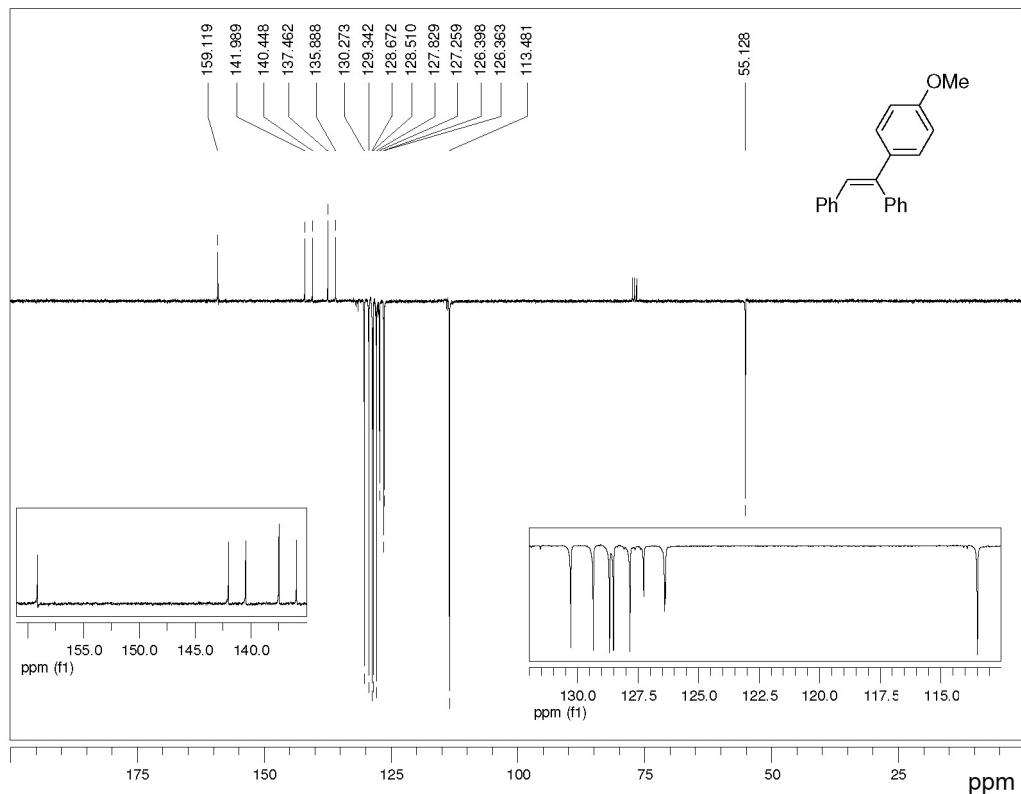


Figure S8.  $^{13}\text{C}$  (APT) NMR spectrum of 1-methoxy-4-((E)-1,2-diphenylvinyl)benzene.

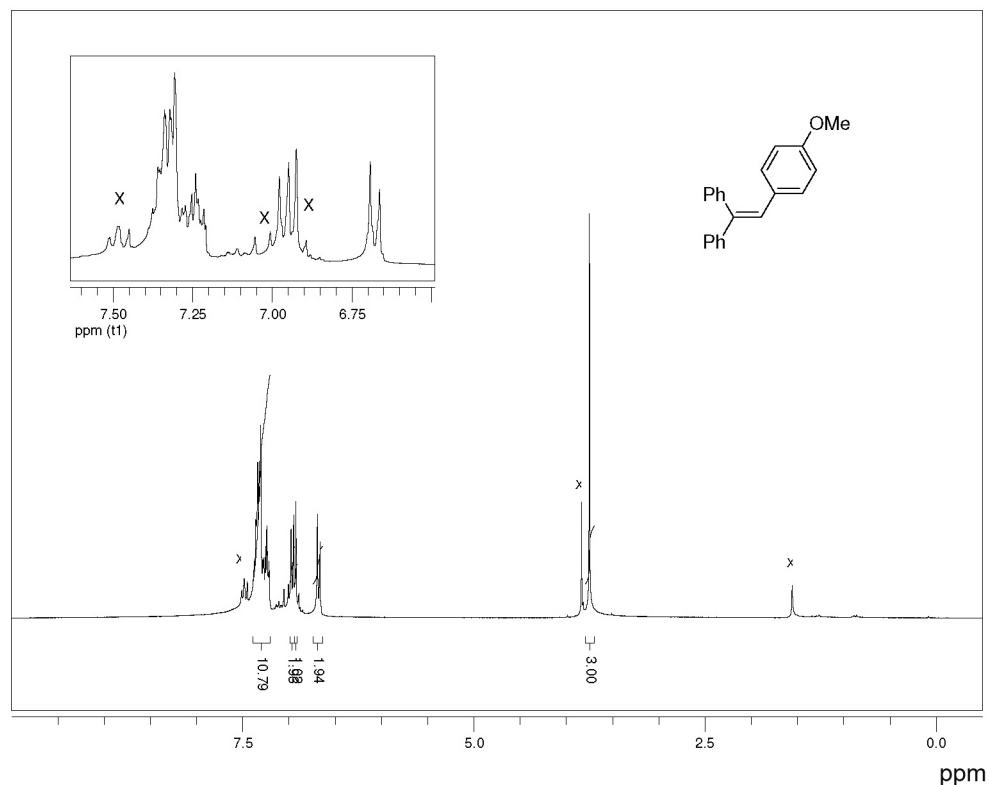
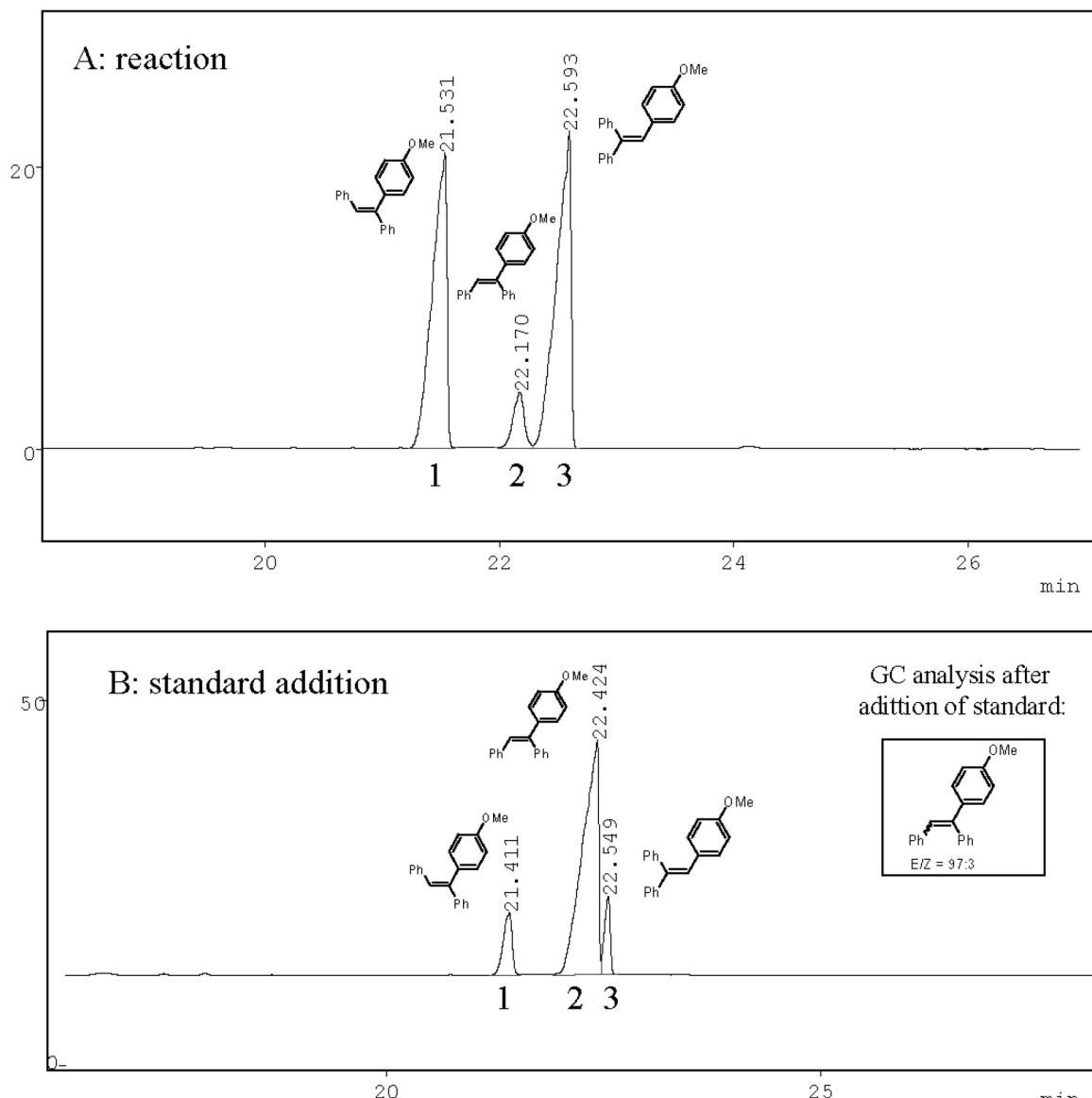
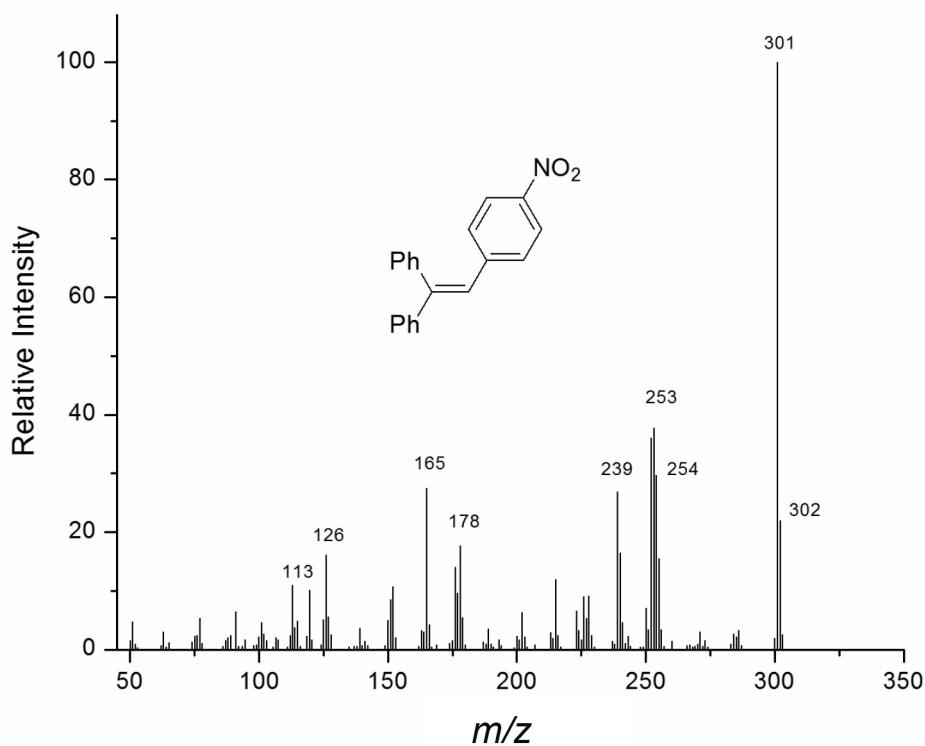


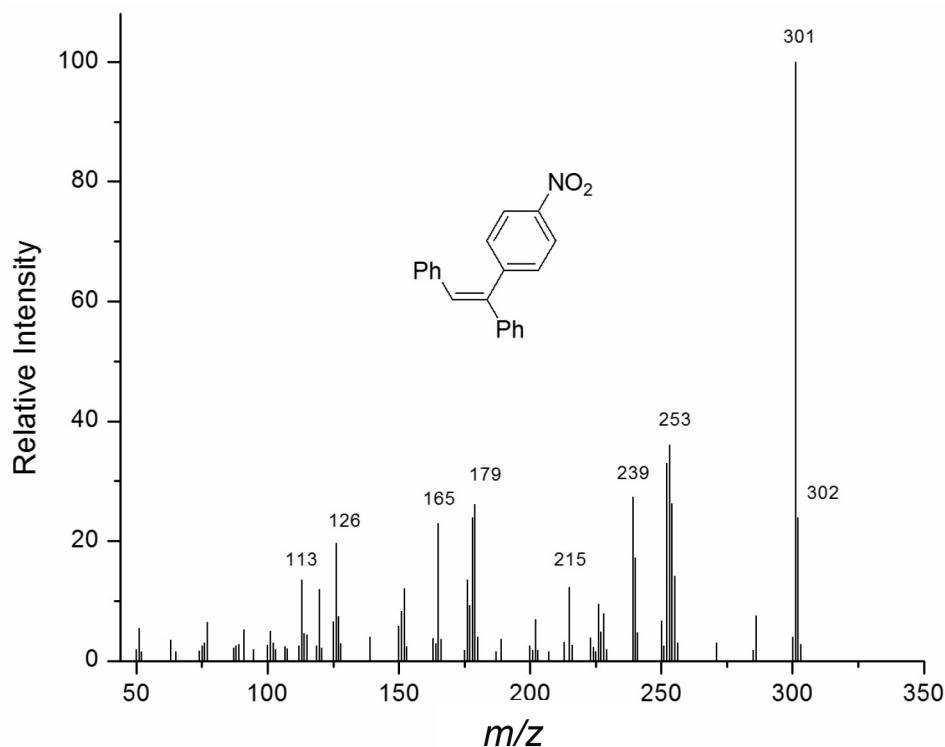
Figure S9.  $^1\text{H}$  NMR spectrum of 1-methoxy-4-(2,2-diphenylvinyl)benzene with 80% purity (20% of 4-methoxystilbene).



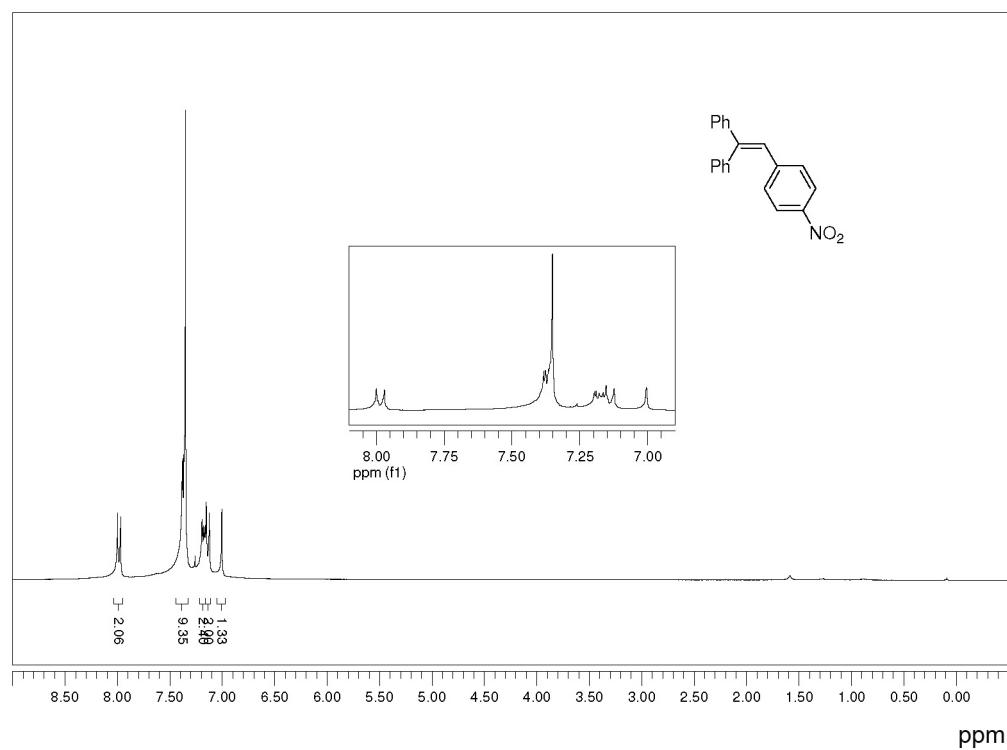
**Figure S10.** A: GC chromatogram with analysis of Heck reaction between 4-methoxy-stilbene and bromobenzene; B: GC chromatogram of the same sample after addition of 1-methoxy-4-((E)-1,2-diphenylvinyl)benzene (97%).



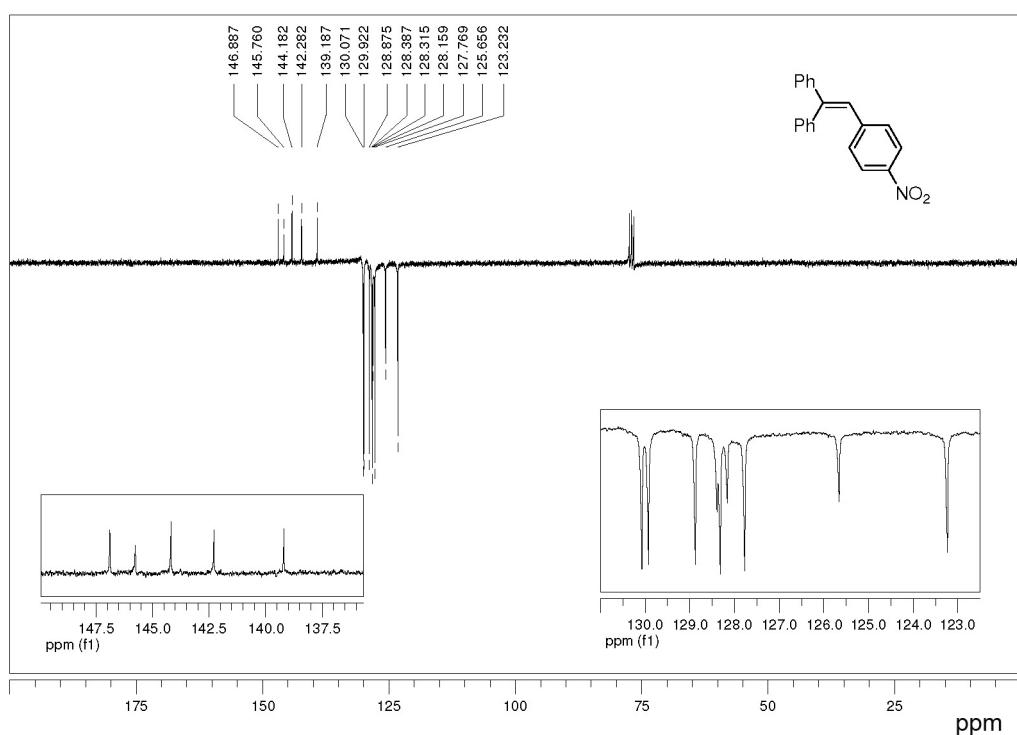
**Figure S11.** Mass spectrum of 1-(2-(4-nitrophenyl)-1-phenylvinyl)benzene.



**Figure S12.** Mass spectrum of 1-((Z)-2-(4-nitrophenyl)-2-phenylvinyl)benzene.



**Figure S13.** <sup>1</sup>H NMR spectrum of 1-(2-(4-nitrophenyl)-1-phenylvinyl)benzene.



**Figure S14.** <sup>13</sup>C (APT) NMR spectrum of 1-(2-(4-nitrophenyl)-1-phenylvinyl)benzene.

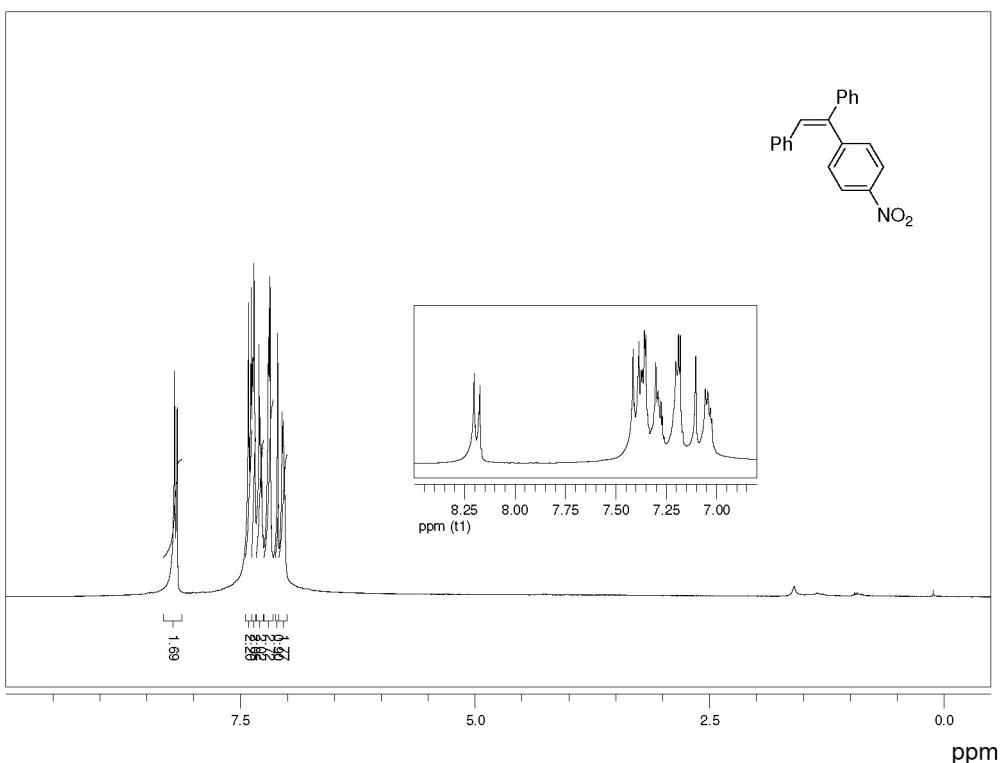


Figure S15.  $^1\text{H}$  NMR spectrum of 1-((Z)-2-(4-nitrophenyl)-2-phenylvinyl)benzene.

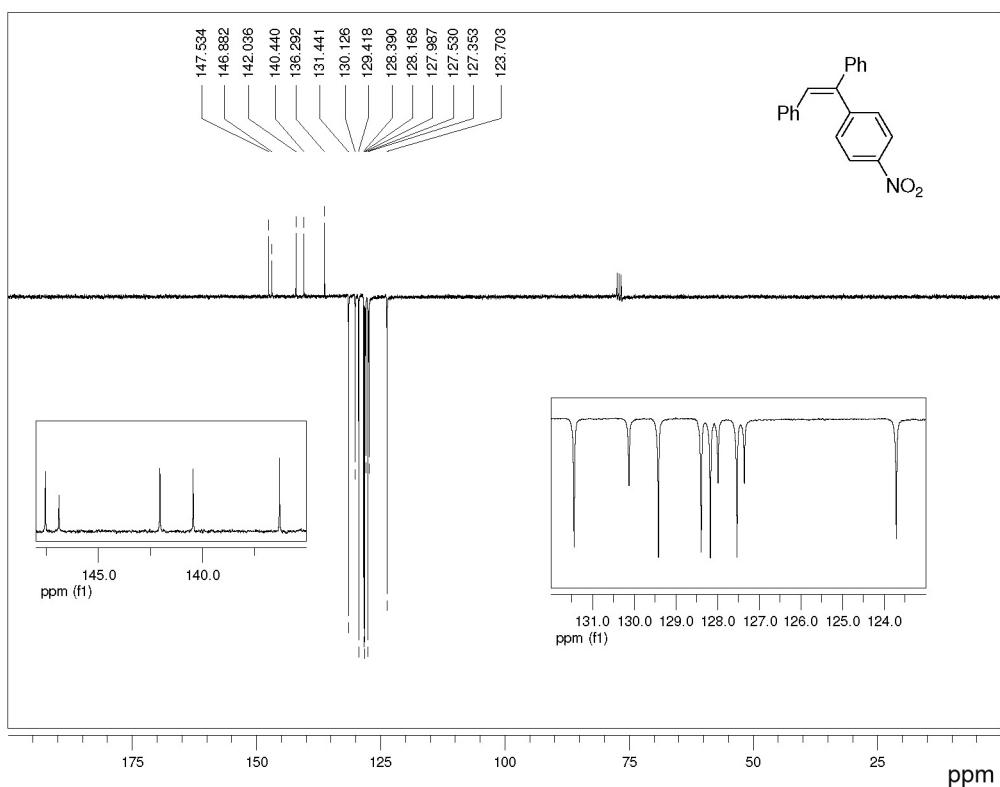
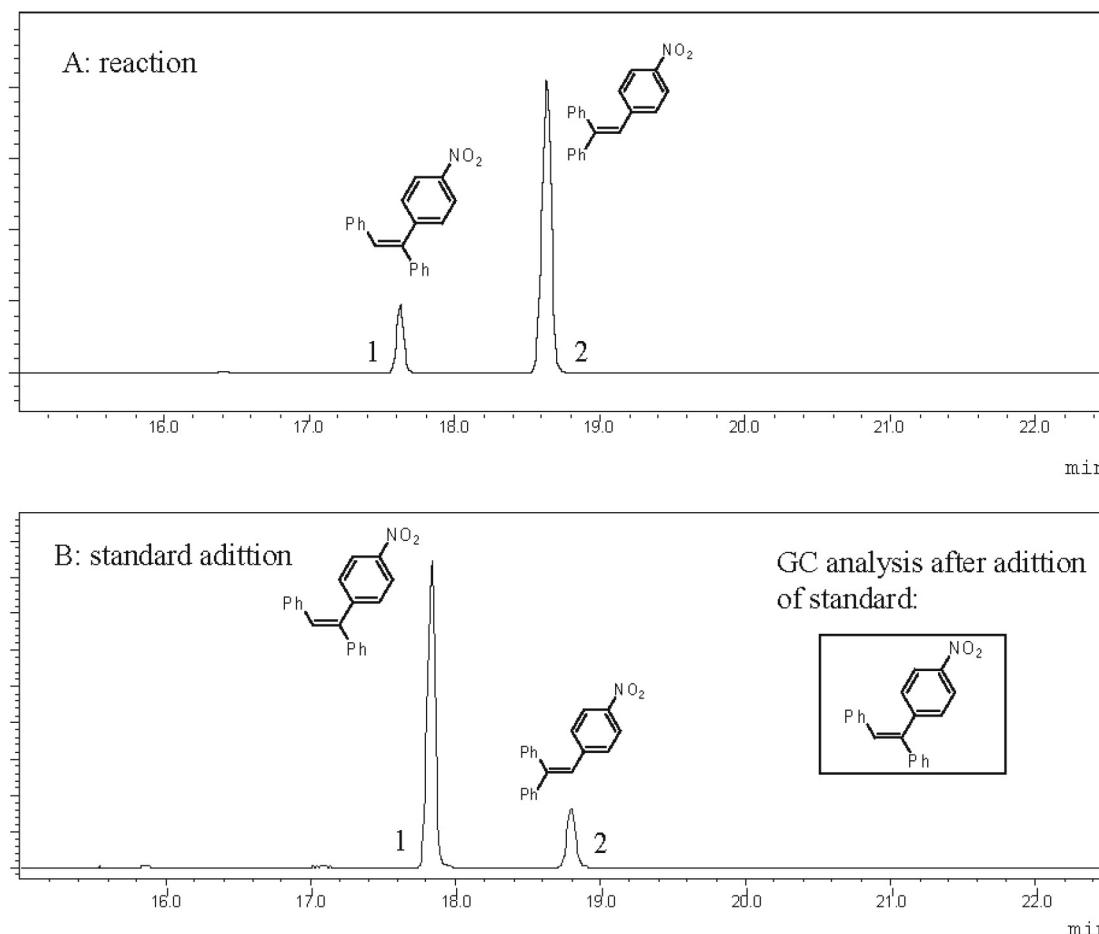
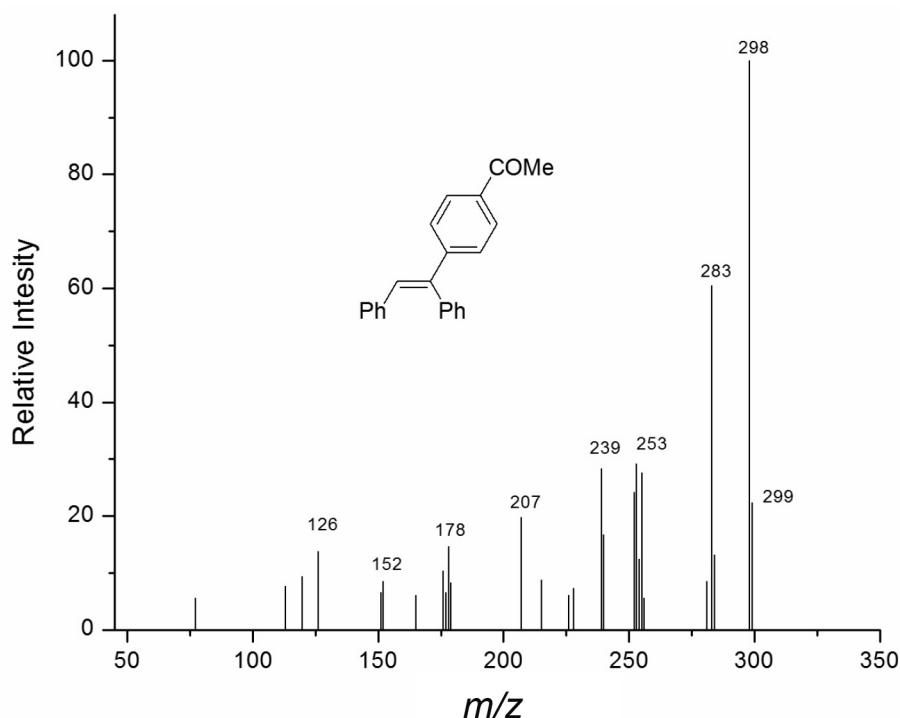


Figure S16.  $^{13}\text{C}$  (APT) NMR spectrum of 1-((Z)-2-(4-nitrophenyl)-2-phenylvinyl)benzene.



**Figure S17.** A: GC chromatogram with analysis of Heck reaction between 4-nitro-stilbene and bromobenzene; B: GC analysis of the same sample after addition of 1-((Z)-2-(4-nitrophenyl)-2-phenylvinyl)benzene.



**Figure S18.** Mass spectrum of 1-((E)-1,2-diphenylvinyl)phenyl)ethanone.

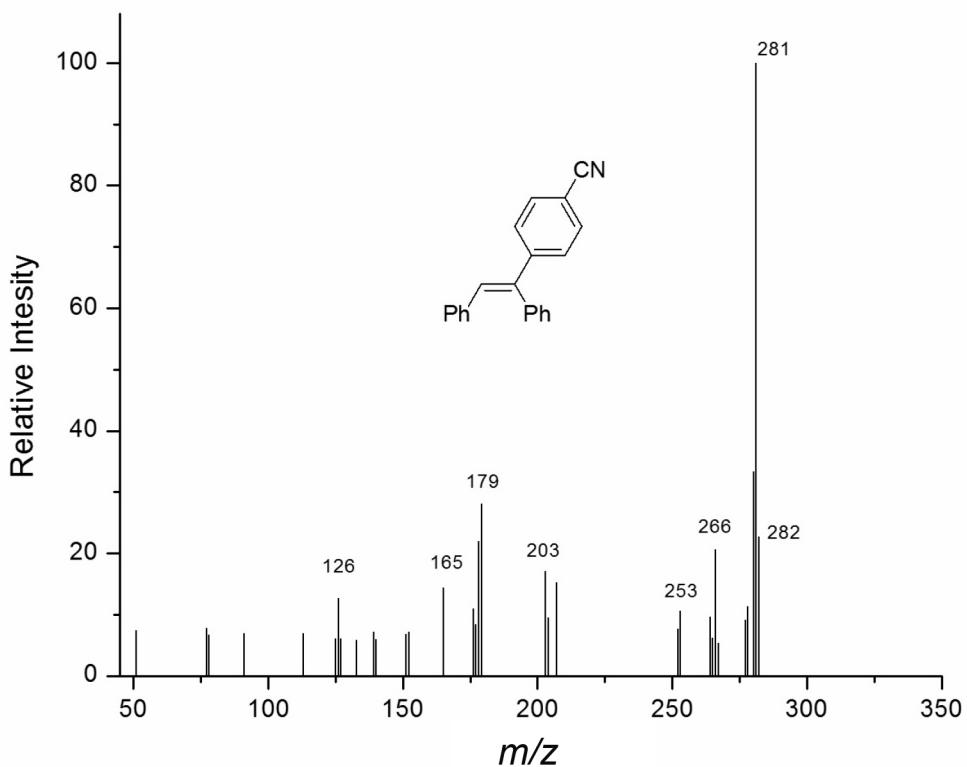


Figure S19. Mass spectrum of 4-((E)-1,2-diphenylvinyl)benzonitrile.

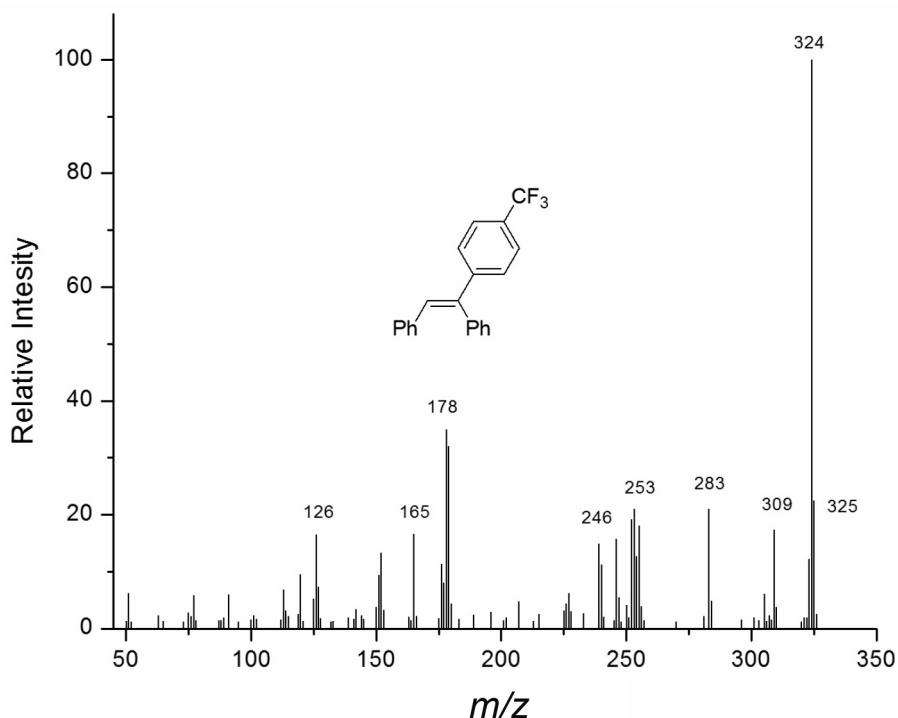


Figure S20. Mass spectrum of 1-(trifluoromethyl)-4-((E)-1,2-diphenylvinyl)benzene.