

Supporting Information
for
Palladium NNC-pincer complex: an efficient catalyst for
Allylic Arylation at parts per billion levels

Go Hamasaka,^{a,b} Fumie Sakurai,^{a, b} and Yasuhiro Uozumi^{*a,b,c,d}

^aInstitute for Molecular Science, Okazaki 444-8787, Japan

^bThe Graduate School for Advanced Studies, Okazaki 444-8787, Japan

^cGreen Nanocatalysis Reserch Team, RIKEN Center for Sustainable Resource Science, Wako 351-0198,
Japan

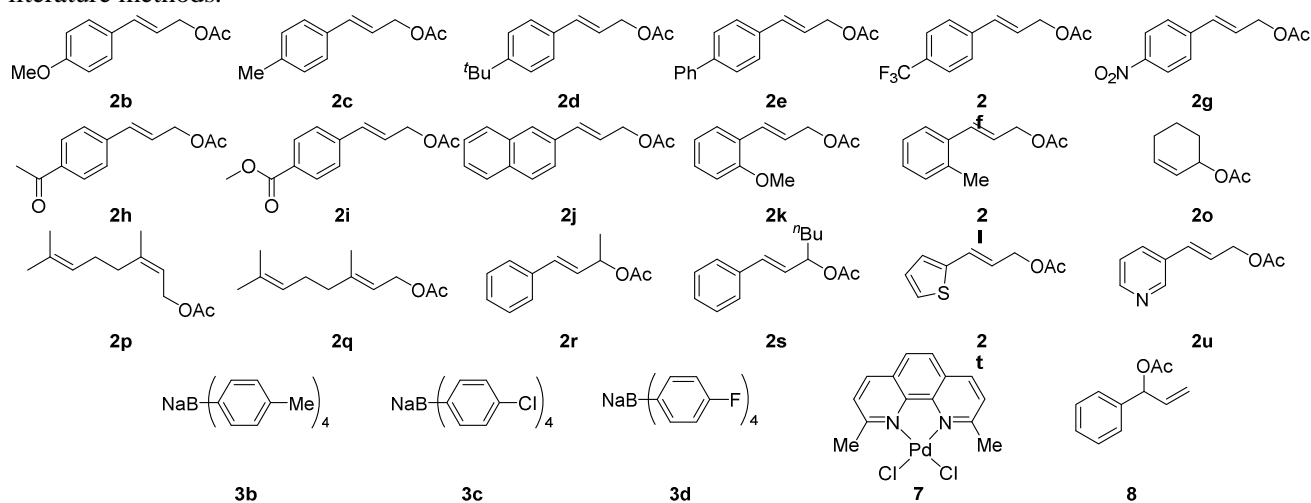
^dJST-CREST, Okazaki 444-8787, Japan

Table of Contents

General Information	S2
Synthesis of 1	S3
Typical procedure for the allylic arylation reaction	S3
Experimental procedure for Scheme 3	S9
References	S11
¹ H-NMR and ¹³ C-NMR Spectra	S12

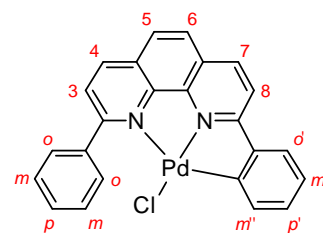
General Information

When manipulations were performed under a nitrogen atmosphere, nitrogen gas was dried by passage through P_2O_5 . Commercially available chemicals (purchased from Sigma-Aldrich, TCI, Kanto chemical, Wako Pure Chemical Industries, Nacalai tesque, and Merck) are used without further purification unless otherwise noted. Silica gel was purchased from Kanto chemical (Silica gel 60N, spherical neutral, particle size 40-50 μ m) or Yamazen corporation (Hi-FlashTM Column Silica gel 40 mm 60 \AA). TLC plates were purchased from Merck (TLC Silica gel 60 F₂₅₄). NMR spectra were recorded on a JEOL JNM A-500 spectrometer (500 MHz for 1H , 125 MHz for ^{13}C) or a JEOL JNM ECS-400 spectrometer (396 MHz for 1H , 100 MHz for ^{13}C). Chemical shifts are reported in δ (ppm) referenced to an internal tetramethylsilane standard for 1H NMR. Chemical shifts of ^{13}C NMR are given related to $CDCl_3$ as an internal standard (δ 77.0). 1H and ^{13}C NMR spectra were recorded in $CDCl_3$ at 25 $^\circ C$. GC-MS analyses were measured with an Agilent 6890 GC/5973N MS Detector. ESI mass spectra (LRMS and HRMS) were recorded on a JEOL JMS-T100LC spectrometer. Elemental analyses were performed on a J-SCIENCE LAB MICRO CORDER JM10. Melting points were determined using a Yanaco micro melting point apparatus MP-J3 and were uncorrected. IR spectra were obtained using a JASCO FT/IR-460plus spectrometer in ATR mode. Millipore water was obtained from a Millipore Milli-Q Academic A10 purification unit. (*E*)-3-(4-Methoxyphenyl)-2-propen-1-ol acetate (**2b**),¹ (*E*)-3-(4-methylphenyl)-2-propen-1-ol acetate (**2c**),¹ (*E*)-3-(4-*tert*-butylphenyl)-2-propen-1-ol acetate (**2d**),¹ (*E*)-3-(4-phenylphenyl)-2-propen-1-ol acetate (**2e**),¹ (*E*)-3-(4-trifluoromethylphenyl)-2-propen-1-ol acetate (**2f**),¹ (*E*)-3-(4-nitrophenyl)-2-propen-1-ol acetate (**2g**),¹ (*E*)-3-(4-acetylphenyl)-2-propen-1-ol acetate (**2h**),¹ (*E*)-3-((4-methoxycarbonyl)phenyl)-2-propen-1-ol acetate (**2i**),¹ (*E*)-(naphthalene-6-yl)allyl acetate (**2j**),² (*E*)-3-((2-methoxycarbonyl)phenyl)-2-propen-1-ol acetate (**2k**),¹ (*E*)-3-(2-methylphenyl)-2-propen-1-ol acetate (**2l**),¹ cyclohex-2-enyl acetate (**2o**),³ neryl acetate (**2p**),⁴ geranyl acetate (**2q**),⁴ (*IE*)-1-phenyl-1-buten-3-yl acetate (**2r**),¹³ (*IE*)-1-phenyl-1-hepten-3-yl acetate (**2s**),¹⁴ (*E*)-3-(2-thienyl)allyl acetate (**2t**),¹ (*E*)-3-(3-pyridyl)allyl acetate (**2u**),⁵ sodium tetraarylborates (**3b-3d**),⁶ complex **7**,¹⁷ 1-phenyl-2-propenyl acetate (**8**),⁴ 2-phenyl-1,10-phenanthroline,¹⁵ and 2,9-diphenyl-1,10-phenanthroline¹⁵ were prepared by literature methods.



Synthesis of Chloro-[2-(9-phenyl-1,10-phenanthrolin-2-yl)phenyl]palladium (1).

PdCl₂(MeCN)₂ (700.0 mg, 2.11 mmol) was added to a solution of 2,9-diphenyl-1,10-phenanthroline (546.1 mg, 2.11 mmol) in a benzene/methanol mixture (20 mL/25 mL). After being stirred for 6 h at 50 °C, a resulting insoluble material was collected by filtration. The obtained material was washed with dichloromethane, methanol, and diethyl ether, and dried in *vacuo* to give **1** (886.2 mg, 1.87 mmol, 89%) as yellow solids. Mp. >300 °C.



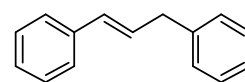
¹H-NMR (396 MHz, CD₂Cl₂) δ 8.44 (d, *J* = 8.6 Hz, 1H, phen 4-H), 8.43 (d, *J* = 8.6 Hz, 1H, phen 7-H), 7.95 (d, *J* = 8.6 Hz, 1H, phen 8-H), 7.93 (d, *J* = 8.6 Hz, 1H, phen 3-H), 7.87–7.90 (m, 4H, phen 5,6-H, *o*-H), 7.76–7.79 (m, 1H, *m*'-H), 7.53–7.59 (m, 4H, *m*-H, *p*-H, and *o*'-H), 7.15 (td, *J* = 2.0, 7.2 Hz, 1H, *p*'-H), 7.12 (td, *J* = 2.0, 7.2 Hz, 1H, *m*'-H). ¹³C-NMR (100 MHz, CD₂Cl₂) δ 163.64, 162.92, 151.79, 148.00, 138.20, 137.80, 137.33, 130.91, 130.28, 130.07, 129.15, 128.51, 128.21, 127.82, 126.68, 126.27, 125.26, 124.92, 118.98. IR (ATR): 3046, 2928, 1617, 1585, 1575, 1508, 1499, 1415, 1316, 1147, 1023, 856, 761, 733, 691 cm⁻¹. ESI-TOF-MS *m/z* 437 ([M-Cl]⁺), 469 ([M-Cl+MeOH]⁺), 911 ([2M-Cl]⁺). Anal. Calcd for C₂₄H₁₅ClN₂Pd·0.5H₂O: C, 59.77; H, 3.34; N, 5.81%. Found: C, 59.63; H, 3.26; N, 5.73%.

Typical procedure for the allylic arylation of allylic acetates with sodium tetraaryborates using **1**

The complex **1** (4.7 mg, 0.01 mmol) was dissolved in methanol (100 mL) to give a stock solution. Under a nitrogen atmosphere, the stock solution (0.1 mL, 1.00 × 10⁻⁵ mmol), methanol (9.9 mL), and NaBPh₄ (6.84 g, 20.0 mmol) were added to a reaction vessel. The resulting solution was degassed via three freeze-pump-thaw cycles. Cinnamyl acetate (1.76 g, 10.0 mmol) was added to the solution. The reaction mixture was stirred at 50 °C for 24 h and allowed to cool to 25 °C. After removal of the solvent, water (50 mL) was added to the residue. The resulting suspension was extracted with *tert*-butyl methyl ether (50 mL × 4). The combined organic layer was dried over Na₂SO₄. The resulting solution was concentrated under reduced pressure. The crude product was chromatographed on silica gel (eluent: hexane) to give 1,1'-[(*E*)-prop-1-ene-1,3-diyl]dibenzene (**4aa**) (1.69 g, 8.67 mmol, 87%) as colorless oil.

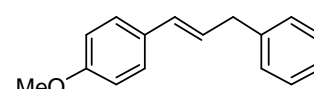
1,1'-[(*E*)-Prop-1-ene-1,3-diyl]dibenzene (4aa**)**⁷ [CAS: 3412-44-0] (1.69 g, 8.67 mmol, 87%)

¹H-NMR (396 MHz, CDCl₃) δ 7.37–7.18 (m, 10H, ArH), 6.46 (d, *J* = 15.8 Hz, 1H, -CH=CHCH₂-), 6.36 (dt, *J* = 15.8, 6.7 Hz, 1H, -CH=CHCH₂-), 3.55 (d, *J* = 6.7 Hz, 2H, -CH=CHCH₂-). ¹³C-NMR (100 MHz, CDCl₃) δ 140.19, 137.49, 131.09, 129.26, 128.72, 128.54, 127.15, 126.23, 126.17, 39.40. EI-MS *m/z* 194 (M⁺).



(*E*)-1-(4-Methoxyphenyl)-3-phenylpropene (4ba**)**⁷ [CAS: 35856-81-6] (1.79 g, 7.98 mmol, 80%)

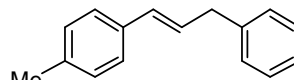
¹H-NMR (396 MHz, CDCl₃) δ 7.33–7.20 (m, 7H, ArH), 6.83 (d, *J* = 8.7 Hz, 2H, ArH), 6.40 (d, *J* = 15.7 Hz, 1H, -CH=CHCH₂-), 6.22 (dt, *J* = 15.7, 6.8 Hz, 1H, -CH=CHCH₂-), 3.80 (s, 3H, -OCH₃), 3.53 (d, *J* = 6.8 Hz, 2H, -CH=CHCH₂-). ¹³C-NMR (100 MHz, CDCl₃) δ



158.80, 140.43, 130.39, 130.27, 128.63, 128.44, 127.19, 127.03, 126.08, 113.88, 55.27, 39.32. EI-MS m/z 224 (M^+).

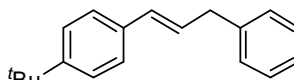
(E)-1-(4-Methylphenyl)-3-phenylpropene (4ca)⁷ [CAS: 134539-87-0] (1.68 g, 8.07 mmol, 81%)

¹H-NMR (396 MHz, CDCl₃) δ 7.35–7.19 (m, 7H, ArH), 7.10 (d, $J = 8.3$ Hz, 2H, ArH), 6.43 (d, $J = 15.4$ Hz, 1H, -CH=CHCH₂-), 6.30 (dt, $J = 15.4, 7.0$ Hz, 1H, -CH=CHCH₂-), 3.54 (d, $J = 7.0$ Hz, 2H, -CH=CHCH₂-), 2.31 (s, 3H, CH₃). ¹³C-NMR (100 MHz, CDCl₃) δ 140.32, 136.82, 134.65, 130.88, 129.17, 128.65, 128.44, 128.14, 126.11, 125.98, 39.33, 21.15. EI-MS m/z 208 (M^+).



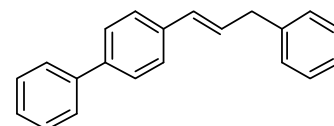
(E)-1-(4-Methylphenyl)-3-phenylpropene (4da)⁸ [CAS: 62056-41-1] (2.32 g, 9.27 mmol, 93%)

¹H-NMR (396 MHz, CDCl₃) δ 7.34–7.28 (m, 6H, ArH), 7.25–7.19 (m, 3H, ArH), 6.45 (d, $J = 15.4$ Hz, 1H, -CH=CHCH₂-), 6.32 (dt, $J = 15.4, 7.2$ Hz, 1H, -CH=CHCH₂-), 3.54 (d, $J = 7.2$ Hz, 2H, -CH=CHCH₂-), 1.31 (s, 3Hx3, -C(CH₃)₃). ¹³C-NMR (100 MHz, CDCl₃) δ 150.10, 140.30, 134.65, 130.80, 128.63, 128.42, 128.34, 126.09, 125.80, 125.39, 39.33, 34.48, 31.28. EI-MS m/z 250 (M^+).



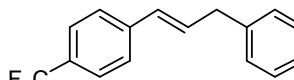
(E)-1-(4-Phenylphenyl)-3-phenylpropene (4ea) [CAS: none] (2.30 g, 8.51 mmol, 85%)

Mp. 90-91 °C. ¹H-NMR (396 MHz, CDCl₃) δ 7.60–7.52 (m, 4H, ArH), 7.45–7.41 (m, 4H, ArH), 7.35–7.31 (m, 2H, ArH), 7.27–7.21 (m, 4H, ArH), 6.50 (d, $J = 15.6$ Hz, 1H, -CH=CHCH₂-), 6.41 (dt, $J = 15.6, 6.5$ Hz, 1H, -CH=CHCH₂-), 3.58 (d, $J = 6.5$ Hz, 2H, -CH=CHCH₂-). ¹³C-NMR (100 MHz, CDCl₃) δ 140.72, 140.09, 139.79, 136.47, 130.56, 129.36, 128.72, 128.66, 128.48, 127.16, 126.86, 126.50, 126.18, 39.38. IR (ATR): 1600, 1487, 966, 836, 754, 700, 685, 588 cm⁻¹. EI-MS m/z 270 (M^+). Anal. Calcd for C₂₁H₁₈: C, 93.29; H, 6.71%. Found: C, 93.24; H, 6.71%.

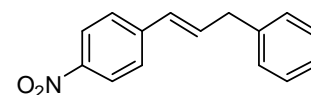


(E)-1-(4-trifluoromethylphenyl)-3-phenylpropene (4fa)⁹ [CAS: 62056-35-3] (2.50 g, 9.53 mmol, 95%)

¹H-NMR (396 MHz, CDCl₃) δ 7.53 (d, $J = 8.0$ Hz, 2H, ArH), 7.43 (d, $J = 8.0$ Hz, 2H, ArH), 7.35–7.23 (m, 5H, ArH), 6.48–6.46 (m, 2H, -CH=CHCH₂-), 3.57 (d, $J = 3.7$ Hz, 2H, -CH=CHCH₂-). ¹³C-NMR (100 MHz, CDCl₃) δ 140.93, 139.55, 132.13, 129.79, 128.90 (q, $J = 32.4$ Hz), 128.71, 128.63, 126.41, 126.26, 125.46 (q, $J_{C-F} = 3.8$ Hz), 124.30 (q, $J_{C-F} = 271.8$ Hz), 39.36. EI-MS m/z 262 (M^+).



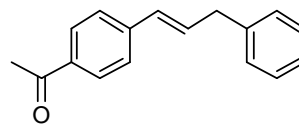
(E)-1-(4-Nitrophenyl)-3-phenylpropene (4ga)⁷ [CAS: 156904-24-4] (2.27 g, 9.49 mmol, 95%)



¹H-NMR (396 MHz, CDCl₃) δ 8.16 (d, *J* = 9.1 Hz, 2H, ArH), 7.47 (d, *J* = 9.1 Hz, 2H, ArH), 7.36–7.32 (m, 2H, ArH), 7.27–7.23 (m, 3H, ArH), 6.57 (dt, *J* = 15.8, 6.3 Hz, 1H, -CH=CHCH₂-), 6.50 (d, *J* = 15.8 Hz, 1H, -CH=CHCH₂-), 3.61 (brd, *J* = 6.3 Hz, 2H, -CH=CHCH₂-). ¹³C-NMR (100 MHz, CDCl₃) δ 146.42, 143.82, 138.91, 134.52, 129.00, 128.61, 128.56, 126.43, 126.42, 123.80, 39.32. EI-MS *m/z* 239 (M⁺).

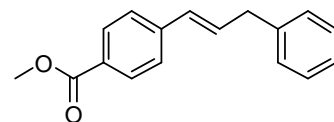
(*E*)-1-(4-Acetylphenyl)-3-phenylpropene (4ha) [CAS: none] (1.82 g, 7.72 mmol, 77%)

Mp. 37-39 °C. ¹H-NMR (396 MHz, CDCl₃) δ 7.89 (d, *J* = 7.9 Hz, 2H, ArH), 7.43 (d, *J* = 7.9 Hz, 2H, ArH), 7.35–7.31 (m, 2H, ArH), 7.26–7.22 (m, 3H, ArH), 6.56–6.45 (m, 2H, -CH=CHCH₂-), 3.58 (d, *J* = 5.5 Hz, 2H, -CH=CHCH₂-), 2.58 (s, 3H, C(O)CH₃). ¹³C-NMR (100 MHz, CDCl₃) δ 197.53, 142.07, 139.40, 135.53, 132.42, 130.03, 128.67, 128.62, 128.51, 126.30, 126.06, 39.35, 26.47. IR (ATR): 1676, 1598, 1492, 1450, 1409, 1356, 1265, 1181, 976, 957, 938, 808, 738, 696, 595 cm⁻¹. EI-MS *m/z* 236 (M⁺). Anal. Calcd for C₁₇H₁₆O: C, 86.40%; H, 6.82%. Found: C, 86.01%; H, 6.81%.



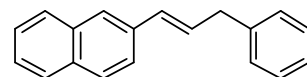
(*E*)-methyl 4-(3-phenylprop-1-enyl)benzoate (4ia)¹⁰ [CAS: 1012036-96-2] (2.32 g, 9.18 mmol, 92%)

¹H-NMR (396 MHz, CDCl₃) δ 7.96 (d, *J* = 8.3 Hz, 2H, ArH), 7.40 (d, *J* = 8.3 Hz, 2H, ArH), 7.34–7.31 (m, 2H, ArH), 7.24 (d, *J* = 7.1 Hz, 3H, ArH), 6.50–6.48 (m, 1H, -CH=CHCH₂-), 3.91 (s, 3H, -OCH₃), 3.58 (d, *J* = 5.1 Hz, 2H, -CH=CHCH₂-). ¹³C-NMR (100 MHz, CDCl₃) δ 166.82, 141.87, 139.46, 132.13, 130.10, 129.80, 128.61, 128.49, 128.45, 126.27, 125.89, 51.92, 39.33. EI-MS *m/z* 252 (M⁺).



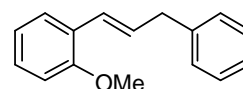
(*E*)-1-(2-Naphthyl)-3-phenylpropene (4ja)¹¹ [CAS: 5751-32-6] (2.41g, 9.87 mmol, 99%)

¹H-NMR (396 MHz, CDCl₃) δ 7.79–7.74 (m, 3H, ArH), 7.70 (s, 1H, ArH), 7.58 (dd, *J* = 8.3, 1.8 Hz, 1H, ArH), 7.46–7.39 (m, 2H, ArH), 7.29–7.22 (m, 5H, ArH), 6.62 (d, *J* = 15.7 Hz, 1H, -CH=CHCH₂-), 6.49 (dt, *J* = 15.7, 6.9 Hz, 1H, -CH=CHCH₂-), 3.61 (d, *J* = 6.9 Hz, 2H, -CH=CHCH₂-). ¹³C-NMR (100 MHz, CDCl₃) δ 140.08, 134.87, 133.60, 132.72, 131.09, 129.64, 128.69, 128.49, 128.05, 127.82, 127.59, 126.19, 126.12, 125.73, 125.54, 123.50, 39.42. EI-MS *m/z* 244 (M⁺).



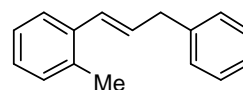
(*E*)-1-(2-Methoxyphenyl)-3-phenylpropene (4ka)¹⁰ [CAS: 1246889-00-6] (2.09 g, 9.33 mmol, 93%)

¹H-NMR (396 MHz, CDCl₃) δ 7.60 (d, *J* = 7.5 Hz, 1H, ArH), 7.46–7.41 (m, 2H, ArH), 7.37–7.16 (m, 4H, ArH), 6.92–6.85 (m, 2H, ArH), 6.82 (d, *J* = 15.8 Hz, 1H, -CH=CHCH₂-), 6.42 (dt, *J* = 15.8, 7.1 Hz, 1H, -CH=CHCH₂-), 3.85 (s, 3H, -OCH₃), 3.57 (d, *J* = 7.1 Hz, 2H, -CH=CHCH₂-). ¹³C-NMR (100 MHz, CDCl₃) δ 156.35, 140.46, 129.70, 128.57, 128.37, 128.05, 126.52, 126.39, 125.99, 125.68, 120.54, 110.69, 55.32, 39.80. EI-MS *m/z* 224 (M⁺).



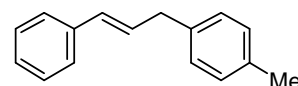
(E)-1-(2-Methylphenyl)-3-phenylpropene (4la)¹² [CAS: 83135-54-0] (1.73 g, 8.30 mmol, 83%)

¹H-NMR (396 MHz, CDCl₃) δ 7.43–7.41 (m, 1H, ArH), 7.33–7.20 (m, 5H, ArH), 7.15–7.13 (m, 3H, ArH), 6.67 (d, *J* = 15.4 Hz, 1H, -CH=CHCH₂-), 6.23 (dt, *J* = 15.4, 7.3 Hz, 1H, -CH=CHCH₂-), 3.59 (d, *J* = 7.3 Hz, 2H, -CH=CHCH₂-), 2.34 (s, 3H, CH₃). ¹³C-NMR (100 MHz, CDCl₃) δ 140.24, 136.54, 135.03, 130.45, 130.14, 128.94, 128.58, 128.44, 127.02, 126.11, 125.99, 125.52, 39.61, 19.83. EI-MS *m/z* 208 (M⁺).



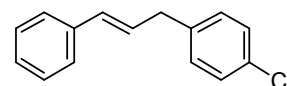
(E)-3-(4-Methylphenyl)-1-phenylpropene (4ab)⁷ [CAS: 134539-86-9] (1.75 g, 8.40 mmol, 84%)

¹H-NMR (396 MHz, CDCl₃) δ 7.35 (d, *J* = 7.5 Hz, 2H, ArH), 7.29 (d, *J* = 7.5 Hz, 2H, ArH), 7.21–7.18 (m, 1H, ArH), 7.15–7.10 (m, 4H, ArH), 6.45 (d, *J* = 15.6 Hz, 1H, -CH=CHCH₂-), 6.34 (dt, *J* = 15.6, 6.7 Hz, 1H, -CH=CHCH₂-), 3.51 (d, *J* = 6.7 Hz, 2H, -CH=CHCH₂-), 2.33 (s, 3H, CH₃). ¹³C-NMR (100 MHz, CDCl₃) δ 137.48, 137.01, 135.62, 130.78, 129.47, 129.14, 128.52, 128.45, 127.00, 126.07, 38.89, 20.99. EI-MS *m/z* 208 (M⁺).



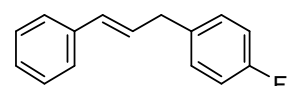
(E)-3-(4-Chlorophenyl)-1-phenylpropene (4ac)⁷ [CAS: 511234-96-1] (1.34 g, 5.86 mmol, 59%)

¹H-NMR (396 MHz, CDCl₃) δ 7.35 (d, *J* = 7.9 Hz, 2H, ArH), 7.31–7.25 (m, 4H, ArH), 7.24–7.19 (m, 1H, ArH), 7.17 (d, *J* = 7.9 Hz, 2H, ArH), 6.44 (d, *J* = 15.3 Hz, 1H, -CH=CHCH₂-), 6.31 (dt, *J* = 15.3, 6.7 Hz, 1H, -CH=CHCH₂-), 3.52 (d, *J* = 6.7 Hz, 2H, -CH=CHCH₂-). ¹³C-NMR (100 MHz, CDCl₃) δ 138.52, 137.17, 131.90, 131.42, 129.98, 128.52, 128.50, 128.49, 127.23, 126.09, 38.56. EI-MS *m/z* 228 (M⁺).



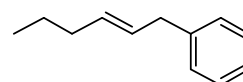
(E)-3-(4-Fluorophenyl)-1-phenylpropene (4ad)⁷ [CAS: 485844-19-7] (1.37 g, 6.45 mmol, 65%)

¹H-NMR (396 MHz, CDCl₃) δ 7.37–7.18 (m, 7H, ArH), 6.99 (t, *J* = 8.1 Hz, 2H, ArH), 6.44 (d, *J* = 15.0 Hz, 1H, -CH=CHCH₂-), 6.32 (dt, *J* = 15.0, 6.6 Hz, 1H, -CH=CHCH₂-), 3.52 (d, *J* = 6.6 Hz, 2H, -CH=CHCH₂-). ¹³C-NMR (100 MHz, CDCl₃) δ 161.45 (d, *J* = 243.3 Hz), 137.26, 135.68 (d, *J* = 3.9 Hz), 131.16, 129.99 (d, *J* = 7.7 Hz), 128.93, 128.49, 127.18, 126.09, 115.18 (d, *J* = 21.0 Hz), 38.43. EI-MS *m/z* 212 (M⁺).



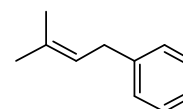
(E)-1-Phenyl-2-hexene (4ma)⁷ [CAS: 78633-31-5] (1.25 g, 7.80 mmol, 78%)

¹H-NMR (396 MHz, CDCl₃) δ 7.31–7.26 (m, 2H, ArH), 7.20–7.17 (m, 3H, ArH), 5.57 (dt, *J* = 15.0, 5.9 Hz, 1H, -CH=CHCH₂Ph), 5.50 (dt, *J* = 15.4, 5.9 Hz, 1H, -CH=CHCH₂Ph), 3.33 (d, *J* = 5.9 Hz, 2H, -CH=CHCH₂Ph), 2.00 (q, *J* = 6.7 Hz, 2H, -CH₂CH=CHCH₂Ph), 1.40 (sext, *J* = 7.4 Hz, 2H, -CH₂CH₂CH=CHCH₂Ph), 0.90 (t, 3H, *J* = 7.4 Hz, -CH₃). ¹³C-NMR (100 MHz, CDCl₃) δ 141.12, 131.90, 128.86, 128.46, 128.30, 125.82, 39.06, 34.60, 22.59, 13.69. EI-MS *m/z* 160 (M⁺).



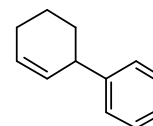
2-Methyl-4-phenyl-2-butene (4na)⁷ [CAS: 286376-80-5] (1.06 g, 7.25 mmol, 73%)

¹H-NMR (396 MHz, CDCl₃) δ 7.29–7.25 (m, 2H, ArH), 7.19–7.15 (m, 3H, ArH), 5.35–5.30 (m, 2H, (CH₃)₂C=CHCH₂Ph), 3.34 (d, *J* = 7.1 Hz, 2H, (CH₃)₂C=CHCH₂Ph), 1.74 (s, 3H, -CH₃), 1.72 (s, 3H, -CH₃). ¹³C-NMR (100 MHz, CDCl₃) δ 141.79, 132.46, 128.32, 128.28, 125.67, 123.18, 34.35, 25.74, 17.79. EI-MS *m/z* 146 (M⁺).



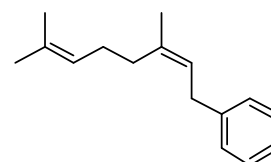
3-Phenylcyclohexene (4oa)⁷ [CAS: 15232-96-9] (1.12 g, 7.08 mmol, 71%)

¹H-NMR (396 MHz, CDCl₃) δ 7.32–7.28 (m, 2H, ArH), 7.23–7.18 (m, 3H, ArH), 5.91–5.88 (m, 1H, -CH=CH-CHPh-), 5.73–5.70 (m, 1H, -CH=CH-CHPh-), 3.43–3.38 (m, 1H, -CH=CH-CHPh-), 2.11–1.98 (m, 3H, -(CH₂)₃-CHPh-), 1.77–1.72 (m, 1H, -(CH₂)₃-CHPh-), 1.67–1.51 (m, 2H, -(CH₂)₃-CHPh-). ¹³C-NMR (100 MHz, CDCl₃) δ 140.60, 130.13, 128.31, 128.23, 127.69, 125.91, 41.82, 32.61, 24.98, 21.16. EI-MS *m/z* 158 (M⁺).



(Z)-3,7-Dimethyl-1-phenyl-2,6-octadiene (4pa)⁷ [CAS: 21488-83-5] (1.16 g, 5.39 mmol, 54%)

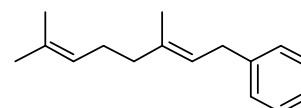
¹H-NMR (396 MHz, CDCl₃) δ 7.29–7.24 (m, 2H, ArH), 7.19–7.15 (m, 3H, ArH), 5.33 (t, *J* = 7.2 Hz, 1H, -(CH₃)C=CHCH₂Ph), 5.16–5.13 (m, 1H, (CH₃)₂C=CH-(CH₂)₂-), 3.35 (d, *J* = 7.2 Hz, 2H, -(CH₃)C=CHCH₂Ph), 2.17–2.10 (m, 4H, (CH₃)₂C=CH-(CH₂)₂-), 1.75 (s, 3H, -CH₃), 1.69 (s, 3H, -CH₃), 1.62 (s, 3H, -CH₃).



¹³C-NMR (100 MHz, CDCl₃) δ 141.80, 136.14, 131.72, 128.33, 128.31, 125.67, 124.15, 123.81, 34.08, 31.95, 26.56, 25.71, 17.65. EI-MS *m/z* 214 (M⁺).

(E)-3,7-Dimethyl-1-phenyl-2,6-octadiene (4qa)⁷ [CAS: 21488-84-6] (1.38 g, 6.44 mmol, 64%)

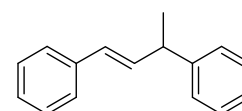
¹H-NMR (396 MHz, CDCl₃) δ 7.29–7.25 (m, 2H, ArH), 7.20–7.15 (m, 3H, ArH), 5.34 (t, *J* = 7.0 Hz, 1H, -(CH₃)C=CHCH₂Ph), 5.10 (t, *J* = 6.9 Hz, 1H, (CH₃)₂C=CH-(CH₂)₂-), 3.36 (d, *J* = 7.0 Hz, 2H, -(CH₃)C=CHCH₂Ph), 2.14–2.09 (m, 2H,



(CH₃)₂C=CH-(CH₂)₂-), 2.07–2.03 (m, 2H, (CH₃)₂C=CH-(CH₂)₂-), 1.71 (s, 3H, -CH₃), 1.68 (s, 3H, -CH₃), 1.60 (s, 3H, -CH₃). ¹³C-NMR (100 MHz, CDCl₃) δ 141.75, 136.16, 131.43, 128.33, 128.30, 125.64, 124.25, 123.01, 39.69, 34.16, 26.57, 25.71, 17.68, 16.08. EI-MS *m/z* 214 (M⁺).

(E)-1,3-Diphenyl-1-butene (4ra)⁷ [CAS: 7302-01-4] (1.53 g, 7.35 mmol, 74%)

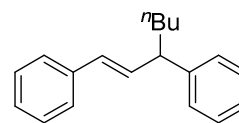
¹H-NMR (396 MHz, CDCl₃) δ 7.37–7.17 (m, 10H, ArH), 6.40–6.35 (m, 2H), 3.65–3.62 (m, 1H), 1.46 (d, *J* = 7.1 Hz, 3H, CH₃). ¹³C-NMR (100 MHz, CDCl₃) δ 145.60, 137.52, 135.19, 128.47, 127.29, 127.02, 126.20, 126.12, 42.54, 21.20. EI-MS *m/z* 208 (M⁺).



(E)-1,3-Diphenyl-1-heptene (4sa)¹⁶ [CAS: 485844-22-2] (1.45 g, 5.77 mmol, 58%)

¹H-NMR (396 MHz, CDCl₃) δ 7.35–7.16 (m, 10H, ArH), 6.41–6.29 (m, 2H), 3.39 (q, *J* = 7.1 Hz, 1H), 1.79 (q, *J* = 7.1 Hz, 2H), 1.36–1.22 (m, 4H) 1.0 (t, *J* = 7.1 Hz, 3H, CH₃).

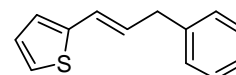
¹³C-NMR (100 MHz, CDCl₃) δ 144.73, 137.59, 134.48, 129.19, 128.46, 128.44, 127.62, 126.98, 126.14, 126.11, 49.18, 35.62, 29.85, 22.69, 14.05. EI-MS *m/z* 250 (M⁺).



(E)-1-(2-Thiophene)-3-phenylpropene (4ta)¹¹ [CAS: 1403462-93-0] (0.029 g, 0.14 mmol, 1%)

¹H-NMR (396 MHz, CDCl₃) δ 7.33–7.30 (m, 2H, ArH), 7.26–7.21 (m, 3H, ArH), 7.10 (d, *J* = 4.8 Hz, 1H, thiophene 5-H), 6.93 (dd, *J* = 4.8, 3.2 Hz, 1H, thiophene 4-H), 6.89 (d, *J* =

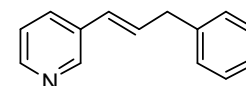
3.2 Hz, 1H, thiophene 3-H), 6.56 (d, *J* = 15.6 Hz, 1H, -CH=CHCH₂-), 6.21 (dt, *J* = 15.6, 6.7 Hz, 1H, -CH=CHCH₂-), 3.51 (d, *J* = 6.7 Hz, 2H, -CH=CHCH₂-). ¹³C-NMR (100 MHz, CDCl₃) δ 142.58, 139.76, 129.08, 128.67, 128.48, 127.19, 126.21, 124.75, 124.22, 123.46, 39.06. EI-MS *m/z* 200 (M⁺).



(E)-1-(3-Pyridine)-3-phenylpropene (4ua)¹⁰ [CAS: 1380310-78-0] (0.053 g, 0.27 mmol, 3%)

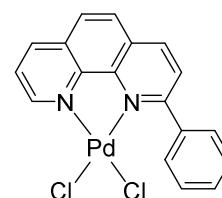
¹H-NMR (396 MHz, CDCl₃) δ 8.58 (d, *J* = 1.6 Hz, 1H, ArH), 8.44 (d, *J* = 4.8, 1.6 Hz, 1H, ArH), 7.67 (dt, *J* = 7.9, 1.6 Hz, 1H, ArH), 7.35–7.31 (m, 2H, ArH), 7.25–7.20 (m, 4H, ArH), 6.49–6.39 (m, 2H, -CH=CHCH₂-), 3.57 (d, *J* = 5.1 Hz, 2H, -CH=CHCH₂-). ¹³C-

NMR (100 MHz, CDCl₃) δ 147.97, 147.89, 139.43, 133.05, 132.64, 131.86, 128.64, 128.57, 127.35, 126.36, 123.40, 39.38. FAB-MS *m/z* 196 ([M+1]⁺).



Synthesis of Dichloro-(2-phenyl-1,10-phenanthroline)palladium (6).

PdCl₂(MeCN)₂ (25.9 mg, 0.100 mmol) was added to a solution of 2,9-diphenyl-1,10-phenanthroline (25.6 mg, 0.100 mmol) in CH₂Cl₂. After being stirred for 4 h at 40 °C, a resulting insoluble material was collected by filtration. The obtained material was washed with dichloromethane and hexane, and dried in *vacuo* to give **6** (29.1 mg, 0.067 mmol,



67%) as orange solids. ¹H-NMR (396 MHz, DMSO-d₆) δ 9.51 (dd, *J* = 1.2, 5.3 Hz, 1H), 8.71 (d, *J* = 8.1 Hz, 1H), 8.67 (dd, *J* = 1.2, 8.3 Hz, 2H), 8.17 (d, *J* = 8.9 Hz, 1H), 8.01 (d, *J* = 8.9 Hz, 1H), 7.90 (dd, *J* = 5.3, 8.3, 2H), 7.88 (d, *J* = 8.1, 2H), 7.42 (d, *J* = 7.9, 2H), 6.87 (t, *J* = 7.9, 1H), 6.66 (t, *J* = 7.9, 2H). ¹³C-NMR (100 MHz, DMSO-d₆) δ 158.90, 153.94, 145.26, 144.26, 140.22, 139.91, 138.75, 136.77, 130.65, 129.12, 129.02, 128.53, 127.51, 126.99, 125.62, 124.84. ESI-TOF-MS *m/z* 653 ([2M-PdCl₃]⁺).

Experimental Procedure for Scheme 3

The reaction of **8** with **3a** using **1** (Scheme 3a)

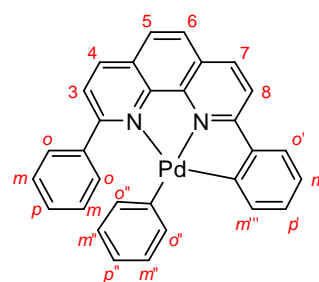
Complex **1** (4.7 mg, 0.01 mmol) was dissolved in methanol (100 mL) to give a stock solution. Under a nitrogen atmosphere, the stock solution (0.1 mL, 1.00×10^{-5} mmol), methanol (9.9 mL), and NaBPh₄ (**3a**, 6.84 g, 20.0 mmol) were added to a reaction vessel. The resulting solution was degassed via three freeze-pump-thaw cycles. 1-Phenyl-2-propenyl acetate (**8**, 1.76 g, 10.0 mmol) was added to the solution. The reaction mixture was stirred at 50 °C for 24 h and allowed to cool to 25 °C. After removal of the solvent, water (50 mL) was added to the residue. The resulting suspension was extracted with *tert*-butyl methyl ether (50 mL \times 4). The combined organic layer was dried over Na₂SO₄. The resulting solution was concentrated under reduced pressure. The crude product was chromatographed on silica gel (eluent: hexane) to give (*E*)-1,3-diphenylpropene (**4a**) (1.46 g, 7.52 mmol, 75%) as colorless oil.

The reaction of the complex **1** with sodium tetraphenylborate (**3a**) in a NMR tube (Scheme 3b)

In a glove box, the complex **1** (1.0 mg, 2.1×10^{-3} mmol), NaBPh₄ (0.7 mg, 2.1×10^{-3} mmol), hexamethylbenzene as an internal standard were placed in a valved NMR tube. THF-d₈ (0.75 mL) was added to the NMR tube. After closed the valve, the NMR tube was taken out from the glove box. The NMR tube was heated in an oil bath at 80 °C for 24 h. After being cooled to 25 °C, the yield of **9** was determined by the ¹H NMR analysis to be 96%.

Isolation of Phenyl-[2-(9-phenyl-1,10-phenanthrolin-2-yl)phenyl]palladium (**9**)

Under a nitrogen atmosphere, NaBPh₄ (36.0 mg, 0.106 mmol) was added to a degassed solution of phenyl-[2-(9-phenyl-1,10-phenanthrolin-2-yl)phenyl]palladium (50.0 mg, 0.106 mmol) in THF (35 mL). The reaction mixture was refluxed for 38 h and allowed to cool to 25 °C. After removal of the solvent, the residue was washed with THF (5 mL) and dried in *vacuo*. The crude product was dissolved in CH₂Cl₂ (10 mL) and filtered through Celite. After concentration of the filtrate, the resulting residue was washed with pentane (10 mL) to give phenyl-[2-(9-phenyl-1,10-phenanthrolin-2-yl)phenyl]palladium (32.7 mg, 0.063 mmol, 59%) as orange solids. Mp. 160-164 °C (decomp.). ¹H-NMR (396 MHz, CD₂Cl₂) δ 8.50 (d, $J = 8.7$ Hz, 1H, 4-H), 8.43 (d, $J = 8.7$ Hz, 1H, 7-H), 8.11 (d, $J = 8.3$ Hz, 1H, 8-H), 7.91 (d, $J = 8.7$ Hz, 1H, 5-H or 6-H), 7.88 (d, $J = 8.7$ Hz, 1H, 5-H or 6-H), 7.86 (d, $J = 8.3$ Hz, 1H, 3-H), 7.62 (dd, $J = 1.8, 7.6$ Hz, 1H, *o'*-H), 7.52–7.50 (m, 2H, *o*-H), 7.18–7.15 (m, 2H, *o''*-H), 6.98 (dd, $J = 1.8, 7.6$ Hz, 1H, *m'''*-H), 6.92–6.87 (m, 2H, *p*-H and *p'*-H), 6.84–6.80 (m, 3H, *m*-H and *m'*-H), 6.53–6.50 (m, 3H, *m''*-H and *p''*-H). ¹³C-NMR (100 MHz, CD₂Cl₂) δ 167.68, 161.24, 156.03, 152.58, 148.84, 139.41, 138.00, 137.75, 137.51, 137.22, 130.66, 130.28, 229.73, 129.28, 129.17, 128.51, 127.90, 127.76, 127.19, 126.31, 126.22, 126.18, 124.71, 123.93,



121.31, 118.74. IR (ATR): 3060, 3037, 1620, 1587, 1547, 1509, 1498, 1487, 1463, 1418, 1273, 1149, 1019, 850, 828, 774, 750, 724, 690, 656, 643, 596 cm^{-1} . MALDI-TOF-MS m/z 514 ($[\text{M}]^+$). Anal. Calcd for $\text{C}_{30}\text{H}_{20}\text{N}_2\text{Pd}\cdot 0.5\text{CH}_2\text{Cl}_2$: C, 68.19; H, 3.87; N, 5.27%. Found: C, 68.29; H, 3.98; N, 5.31%.

The reaction of the complex **9 with cinnamyl acetate (**2a**) in a NMR tube (Scheme 3c)**

In a glove box, complex **9** (1.1 mg, 2.1×10^{-3} mmol) and hexamethylbenzene as an internal standard were placed in a valved NMR tube. THF- d_8 (0.75 mL) and a solution of cinnamyl acetate in THF- d_8 (20 μL (concentration is 3.7 mg/200 μL), 2.1×10^{-3} mmol) were added to the NMR tube. After closed the valve, the NMR tube was taken out from the glove box. The NMR tube was heated in an oil bath at 80 $^\circ\text{C}$ for 24 h. After being cooled to 25 $^\circ\text{C}$, the yield of **4aa** was determined by the ^1H NMR analysis to be 57%.

The allylic arylation of cinnamyl acetate **2a with sodium tetraphenylborate **3a** using **9** (Scheme 3d)**

Complex **9** (5.2 mg, 0.01 mmol) was dissolved in methanol (100 mL) to give a stock solution. Under a nitrogen atmosphere, the stock solution (0.1 mL, 1.00×10^{-5} mmol), methanol (9.9 mL), and NaBPh_4 (6.84 g, 20.0 mmol) were added to a reaction vessel. The resulting solution was degassed via three freeze-pump-thaw cycles. Cinnamyl acetate (1.76 g, 10.0 mmol) was added to the solution. The reaction mixture was stirred at 50 $^\circ\text{C}$ for 24 h and allowed to cool to 25 $^\circ\text{C}$. After removal of the solvent, water (50 mL) was added to the residue. The resulting suspension was extracted with *tert*-butyl methyl ether (50 mL \times 4). The combined organic layer was dried over Na_2SO_4 . The resulting solution was concentrated under reduced pressure. The crude product was chromatographed on silica gel (eluent: hexane) to give (*E*)-1,3-diphenylpropene (**4aa**) (1.81 g, 9.32 mmol, 93%) as colorless oil.

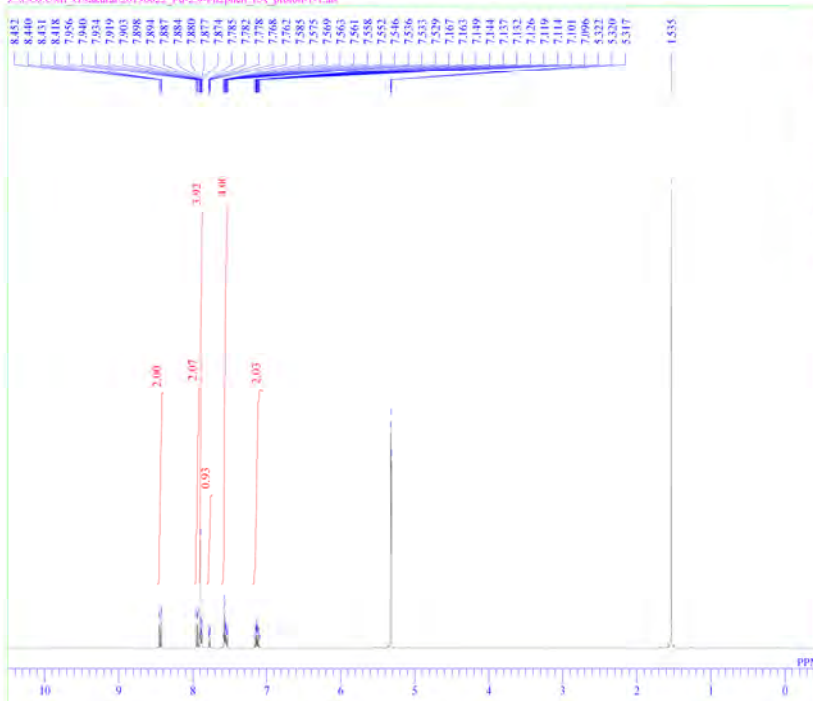
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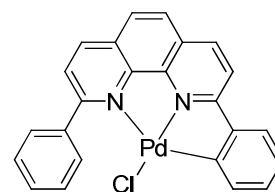
Chloro-[2-(9-phenyl-1,10-phenanthrolin-2-yl)phenyl]palladium (1).

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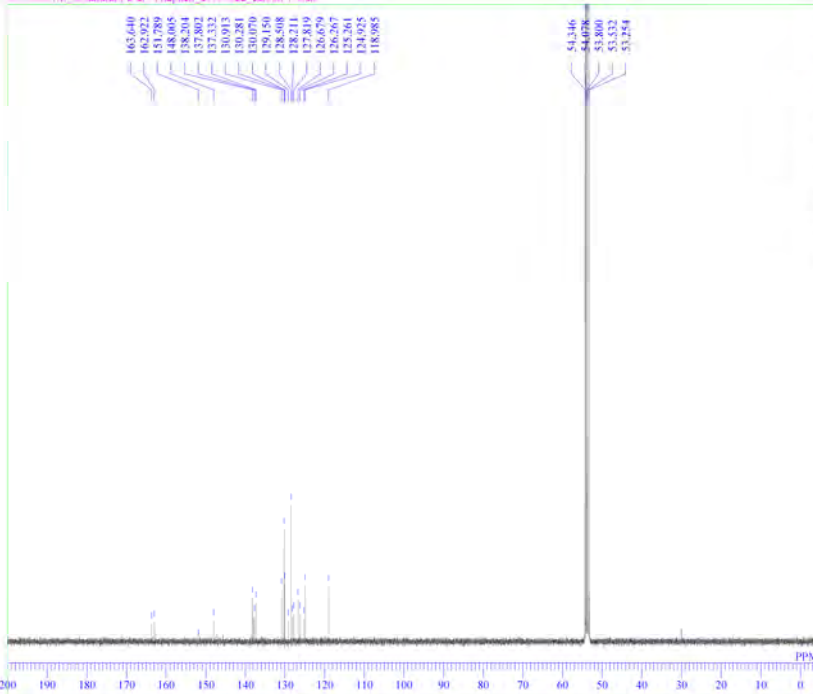


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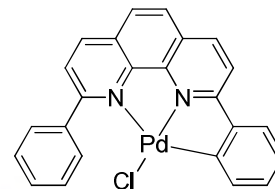


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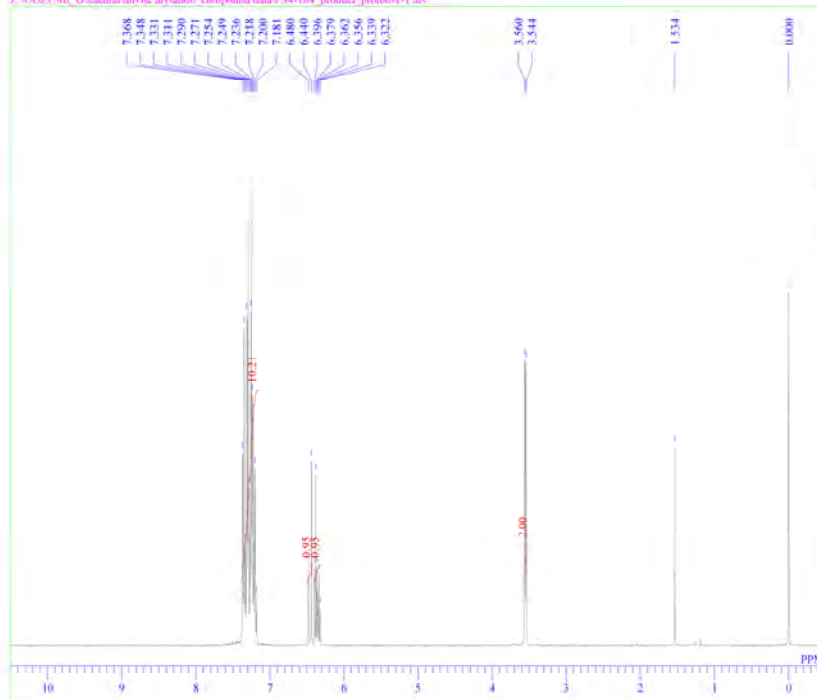
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 RGAIN 60



1,1'-[(1E)-prop-1-ene-1,3-diyl]dibenzene (4aa)

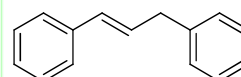
single_pulse

Z:\UOZUMI_G\sakurai\alylic arylation compound data\F84-184_product_proton-1-1.als



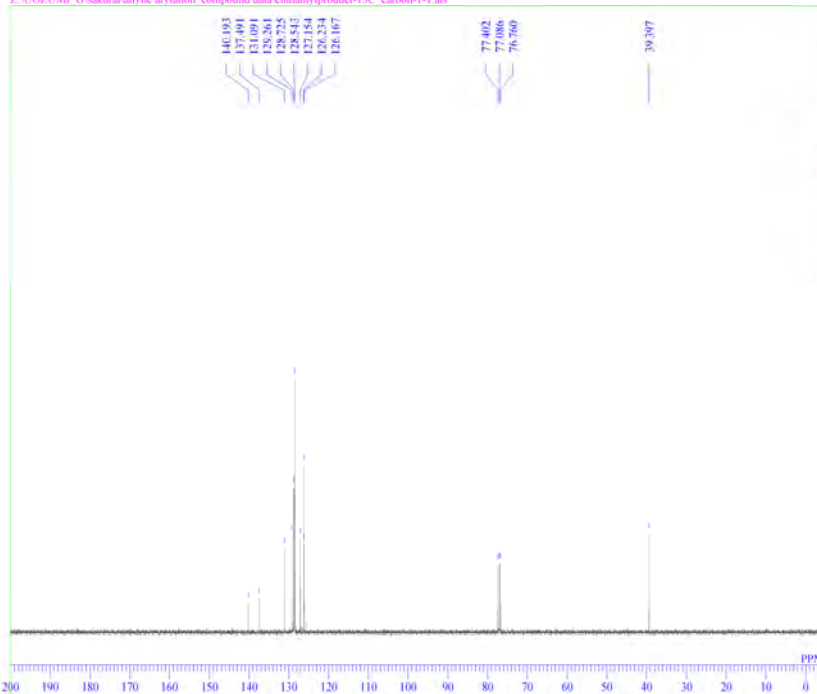
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D:\FILE F84-184_product_proton-1-1.als
COMNT single_pulse
DATIM 2013-10-30 18:20:56
OBNUC 1H
EXMOD proton_jsp
OBF1Q 395.88 MHz
OBSE1 6.28 KHz
OBF1N 0.87 Hz
POINT 13107
FREQU 5938.24 Hz
SCANS 8
ACQTM 2.2073 sec
PD 5.0000 sec
PW1 3.12 usec
IRNUC 1H
CTEMP 49.3 c
SLVNT CDCl3
XREF 0.00 ppm
BF 0.50 Hz
RGAIN 38
    
```



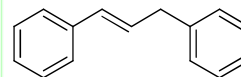
single pulse decoupled gated NOE

Z:\UOZUMI_G\sakurai\alylic arylation compound data\cinnamylproduct-13C_carbon-1-1.als



```

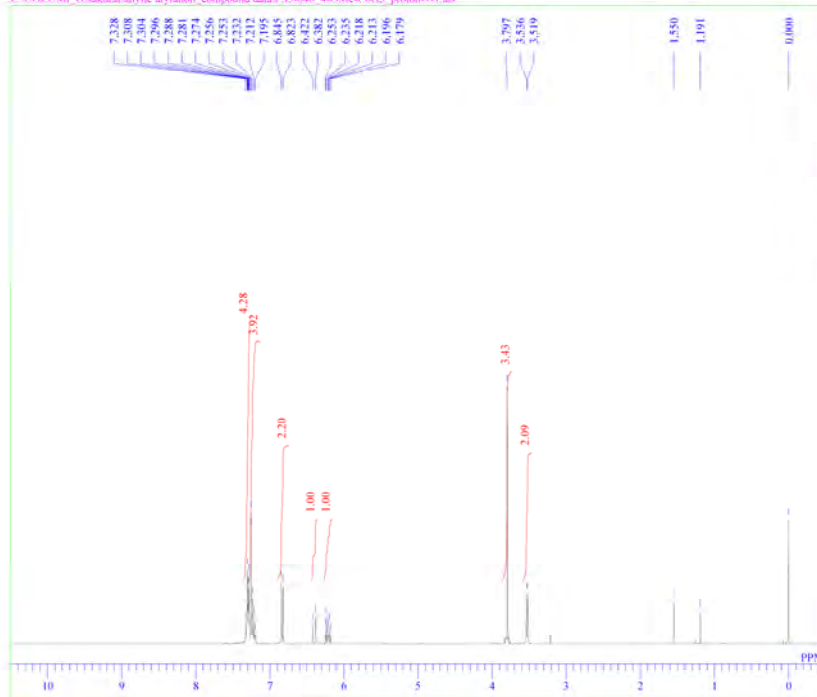
D:\FILE cinnamylproduct-13C_carbon-1-1.als
COMNT single pulse decoupled gated NOE
DATIM 2013-12-07 15:23:29
OBNUC 13C
EXMOD carbon_jsp
OBF1Q 99.55 MHz
OBSE1 5.13 KHz
OBF1N 0.98 Hz
POINT 26214
FREQU 25000.00 Hz
SCANS 64
ACQTM 1.0486 sec
PD 2.0000 sec
PW1 3.42 usec
IRNUC 13C
CTEMP 19.5 c
SLVNT CDCl3
XREF 77.00 ppm
BF 0.25 Hz
RGAIN 58
    
```



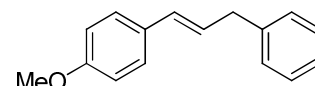
(E)-1-(4-Methoxyphenyl)-3-phenylpropene (4ba)

single_pulse

Z:\UOZUMI_G\sakurai\allylic arylation_compound data\FSS-040_4-OMe-C6H5_proton-1-1.als

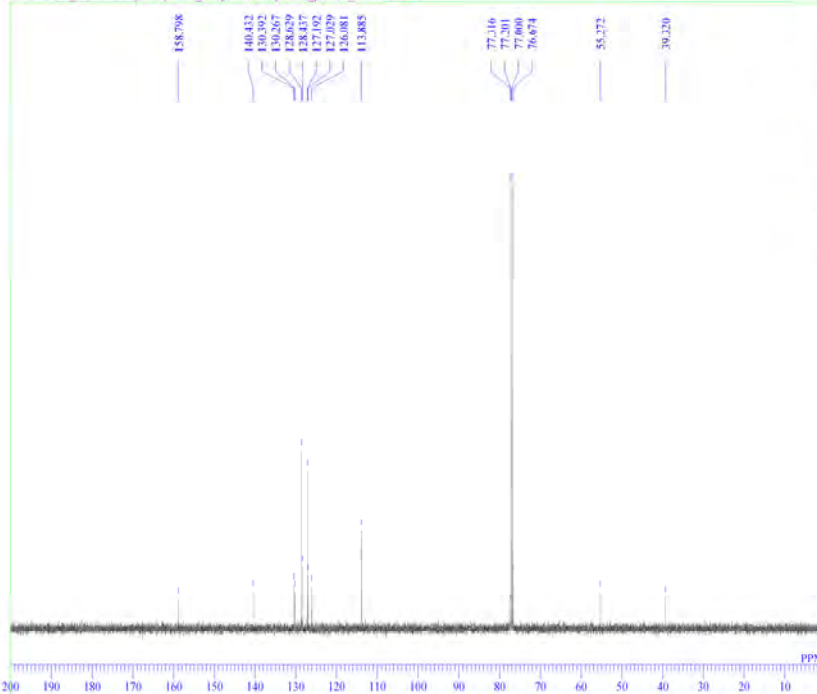


DFILE FSS-040_4-OMe-C6H5_proton-1-1.als
COMINT single_pulse
DATIM 2013-11-22 20:04:02
OBNUC 1H1
EXMOD proton_xsp
OBFREQ 395.88 MHz
OBSET 6.28 KHz
OBFIN 0.87 Hz
POINT 13107
FREQU 5938.24 Hz
SCANS 8
ACQTM 2.2073 sec
PD 5.0000 sec
PWT 3.12 usec
IRNUC 1H1
CTEMP 19.1 c
SLVNT CDCl3
EXREF 0.00 ppm
BF 0.00 Hz
RGAIN 40

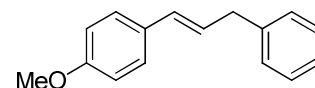


single pulse decoupled gated NOE

Z:\UOZUMI_G\sakurai\allylic arylation_compound data\p-OMe_product_carbon-1-1.als



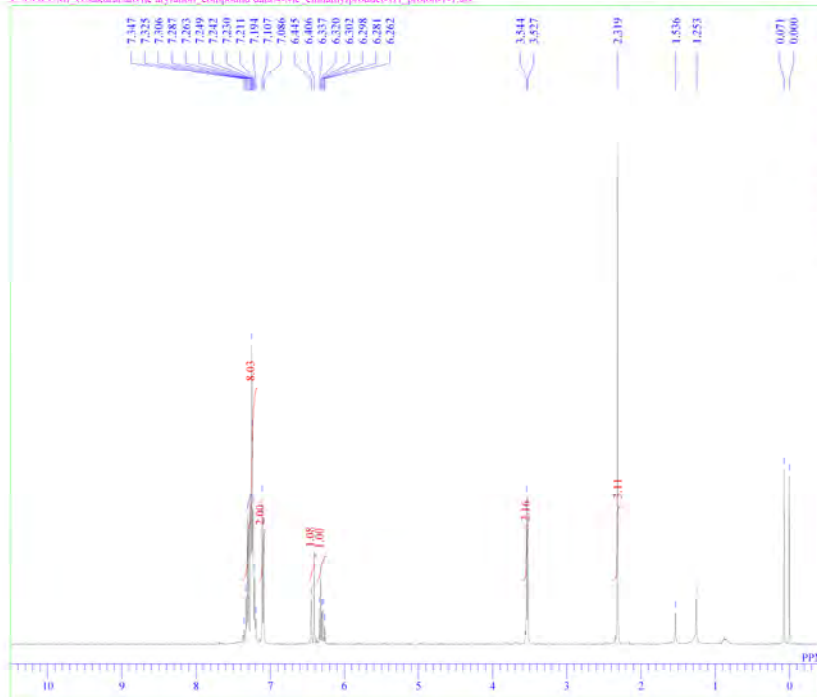
DFILE p-OMe_product_carbon-1-1.als
COMINT single_pulse decoupled gated NOE
DATIM 2014-12-16 21:33:16
OBNUC 13C
EXMOD carbon_xsp
OBFREQ 99.55 MHz
OBSET 5.13 KHz
OBFIN 0.98 Hz
POINT 26214
FREQU 25000.00 Hz
SCANS 512
ACQTM 1.0486 sec
PD 2.0000 sec
PWT 3.42 usec
IRNUC 13C
CTEMP 19.8 c
SLVNT CDCl3
EXREF 77.00 ppm
BF 0.00 Hz
RGAIN 60



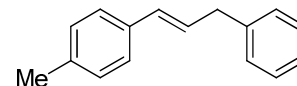
(E)-1-(4-Methylphenyl)-3-phenylpropene (4ca)

single_pulse

Z:\UOZUMI_Gisakurai\allylic arylation_compound data\4-Me_cinnamylproduct-1H_proton-1-1.als

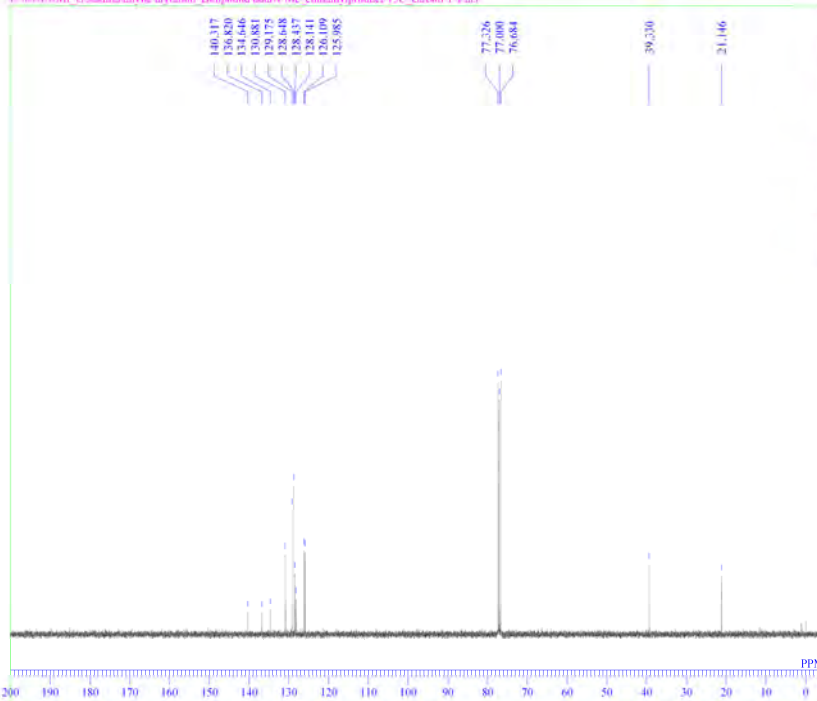


DFILE 4-Me_cinnamylproduct-1H_proton-1-1.als
COMNT single_pulse
DATIM 2013-12-07 15:01:17
ORNUC 1H
EXMOD proton_xsp
OBFREQ 395.88 MHz
OBSET 6.28 KHz
OBFIN 0.87 Hz
POINT 13107
FREQU 593.824 Hz
SCANS 8
ACQTM 2.2073 sec
PD 5.0000 sec
PWL 3.12 usec
IRNUC 1H
CTEMP 19.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.25 Hz
RGAIN 38

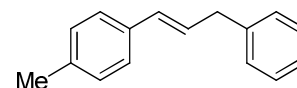


single_pulse decoupled gated NOE

Z:\UOZUMI_Gisakurai\allylic arylation_compound data\4-Me_cinnamylproduct-13C_carbon-1-1.als



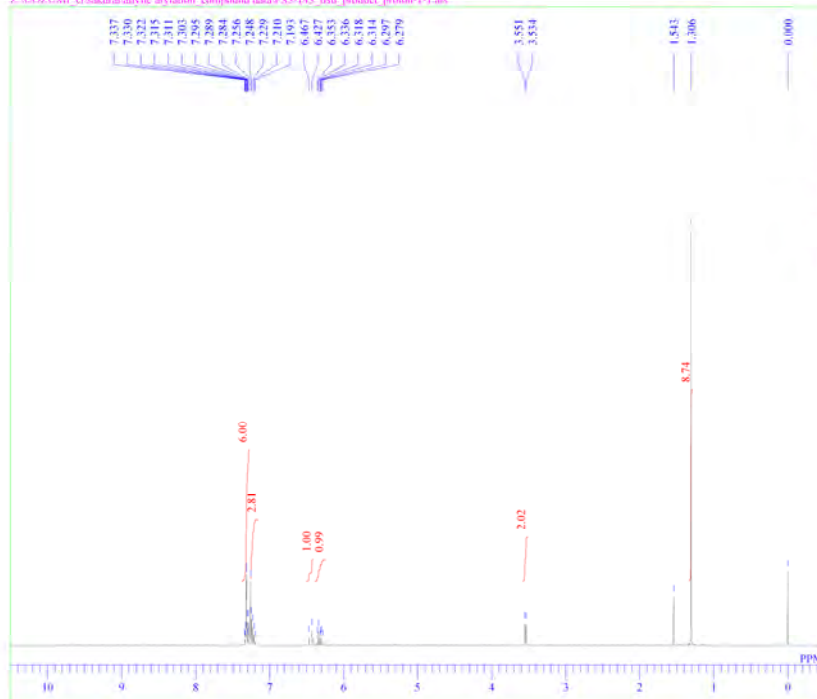
DFILE 4-Me_cinnamylproduct-13C_carbon-1-1.als
COMNT single_pulse decoupled gated NOE
DATIM 2013-12-07 15:02:43
ORNUC 13C
EXMOD carbon_xsp
OBFREQ 99.55 MHz
OBSET 5.13 KHz
OBFIN 0.98 Hz
POINT 26214
FREQU 25000.00 Hz
SCANS 257
ACQTM 1.0486 sec
PD 2.0000 sec
PWL 3.42 usec
IRNUC 13C
CTEMP 19.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.25 Hz
RGAIN 60



(E)-1-(4-Methylphenyl)-3-phenylpropene (4da)

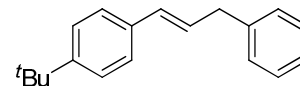
single_pulse

Z:\UOZUMI_Gisakura\allylic arylation_compound data\FSS-143_tBu_product_proton-1-1.als



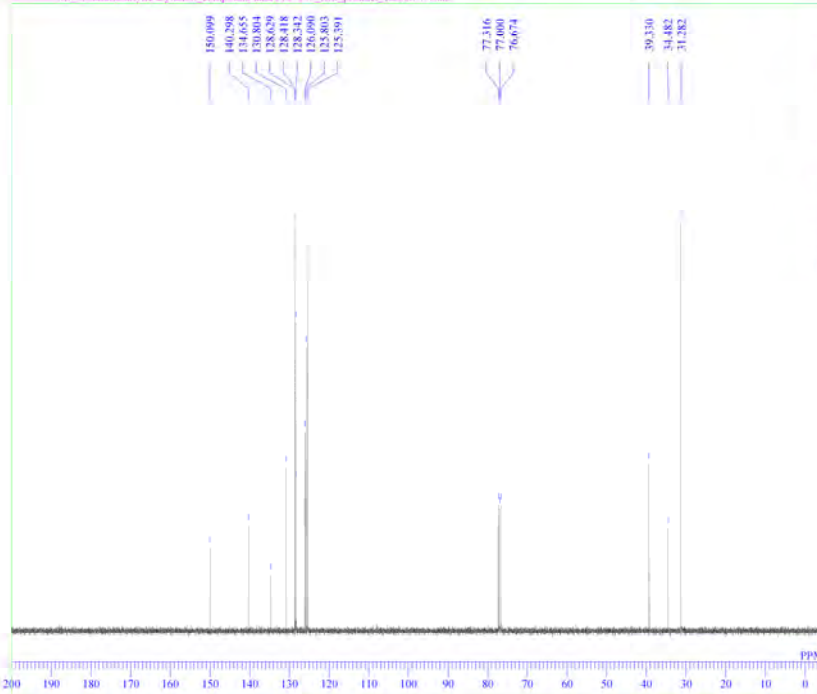
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D:\FILE FSS-143_tBu_product_proton-1-1.als
COMNT single_pulse
DATIM 2014-02-01 20:11:31
OBNUC 1H1
EXMOD proton_jxp
OBFREQ 395.88 MHz
OBSET 6.28 KHz
OBFIN 0.87 Hz
POINT 13107
FREQU 5938.24 Hz
SCANS 8
AQTM 2.2073 sec
PD 5.0000 sec
PW1 3.12 usec
IRNUC 1H1
CTEMP 20.1 c
SLVNT CDCl3
EXREF 0.00 ppm
BF 0.00 Hz
RGAIN 40
    
```



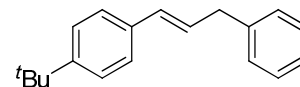
single_pulse decoupled gated NOE

Z:\UOZUMI_Gisakura\allylic arylation_compound data\FSS-143_tBu_product_carbon-1-1.als



```

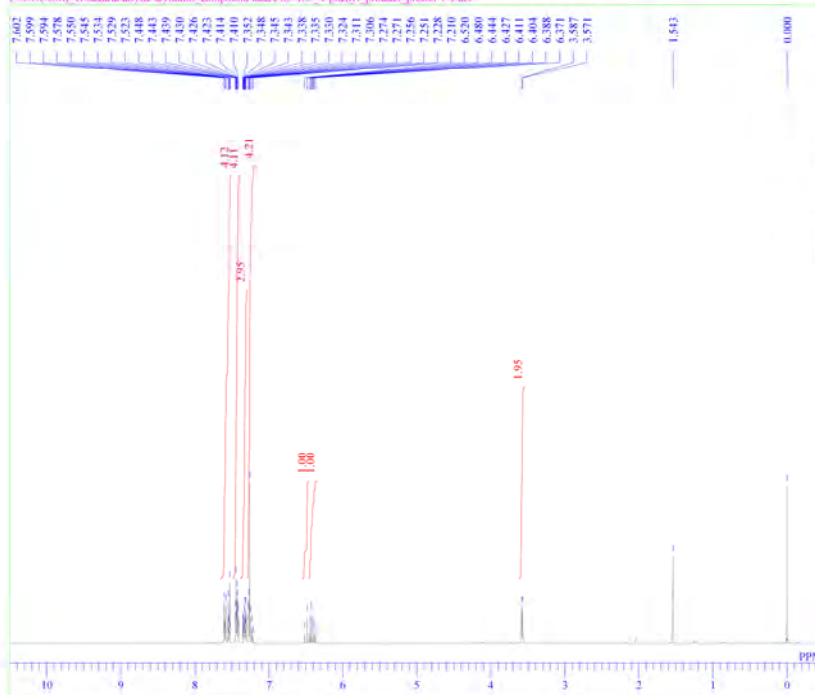
D:\FILE FSS-143_tBu_product_carbon-1-1.als
COMNT single_pulse decoupled gated NOE
DATIM 2014-02-01 20:36:13
OBNUC 13C
EXMOD carbon_jxp
OBFREQ 99.55 MHz
OBSET 5.13 KHz
OBFIN 0.98 Hz
POINT 26214
FREQU 25000.00 Hz
SCANS 111
AQTM 1.0486 sec
PD 2.0000 sec
PW1 3.42 usec
IRNUC 1H1
CTEMP 19.4 c
SLVNT CDCl3
EXREF 77.00 ppm
BF 0.00 Hz
RGAIN 60
    
```



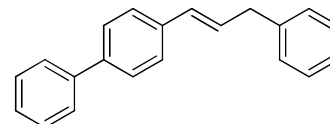
(E)-1-(4-Phenylphenyl)-3-phenylpropene (4ea)

single_pulse

Z:\UOZUMI_Gsokura\allylic arylation_compound data\F55-165_4-phenyl_product_proton-1-1.als

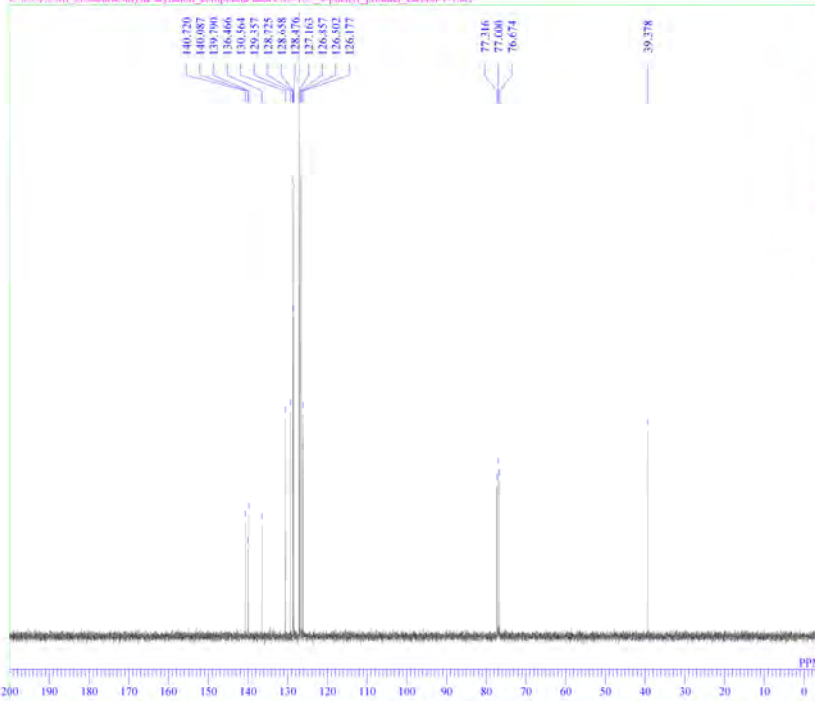


DFILE F55-165_4-phenyl_product_proton-1-1.als
COMNT single_pulse
DATIM 2014-02-19 17:17:54
ORNUC 1H
EXMOD proton_jsp
OBFREQ 395.88 MHz
OBSEI 6.28 KHz
OBFIN 0.87 Hz
POINT 13107
FREQU 593.824 MHz
SCANS 8
ACQTM 2.2073 sec
PD 5.0000 sec
PW1 3.12 usec
IRNUC 1H
CTEMP 20.1 c
SLVNT CDCl3
EXREF 0.00 ppm
BF 0.00 Hz
RGAIN 44

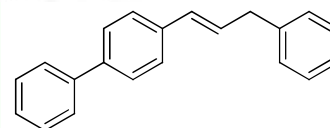


single_pulse decoupled gated NOE

Z:\UOZUMI_Gsokura\allylic arylation_compound data\F55-165_4-phenyl_product_carbon-1-1.als



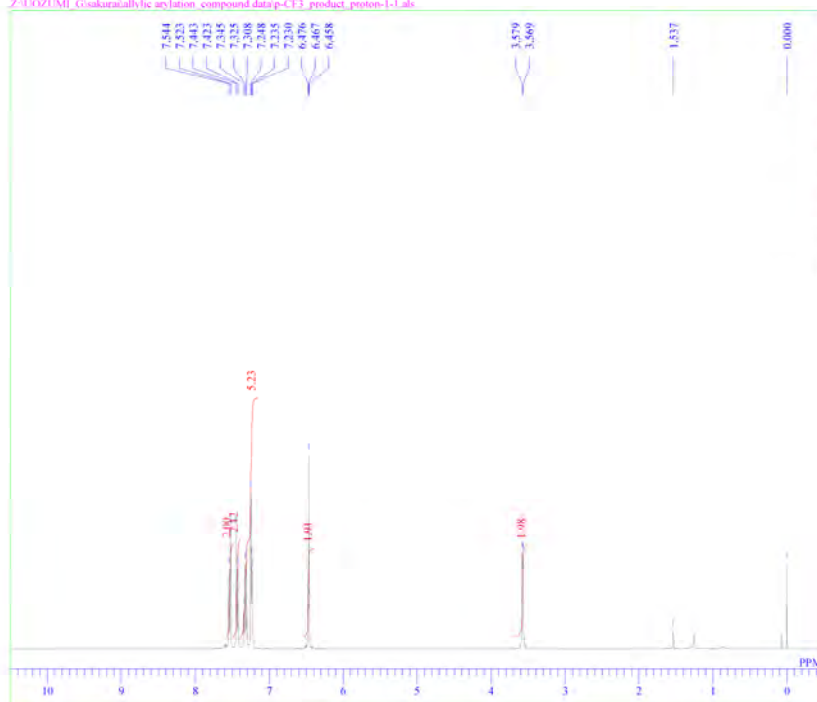
DFILE F55-165_4-phenyl_product_carbon-1-1.als
COMNT single_pulse decoupled gated NOE
DATIM 2014-02-19 17:25:06
ORNUC 13C
EXMOD carbon_jsp
OBFREQ 99.55 MHz
OBSEI 5.13 KHz
OBFIN 0.98 Hz
POINT 26214
FREQU 250.00 MHz
SCANS 132
ACQTM 1.0486 sec
PD 2.0000 sec
PW1 3.42 usec
IRNUC 13C
CTEMP 19.0 c
SLVNT CDCl3
EXREF 77.00 ppm
BF 0.00 Hz
RGAIN 60



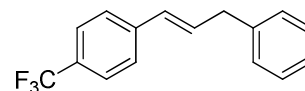
(E)-1-(4-Trifluoromethylphenyl)-3-phenylpropene (4fa)

single_pulse

Z:\UOZUMI_Gisakurai\allylic arylation_compound data\p-CF3_product_proton-1-1als

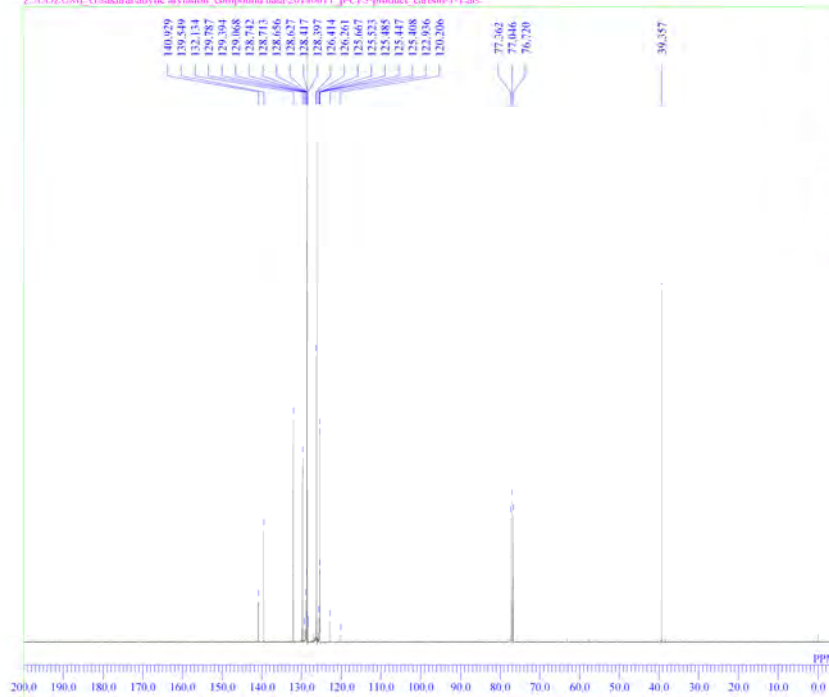


DFILE p-CF3_product_proton-1-1als
COMNT single_pulse
DATIM 2013-12-11 20:52:29
OBNUC 1H
EXMOD proton.jsp
OBFREQ 395.88 MHz
OBSET 8.28 kHz
OBFIN 0.87 Hz
POINT 13107
FREQU 5938.24 Hz
SCANS 8
ACQTM 2.2073 sec
PD 5.0000 sec
PWI 3.12 usec
IRNUC 1H
CTEMP 19.3 c
SLVNT CDCL3
XREF 0.00 ppm
BF 0.60 Hz
RGAIN 34

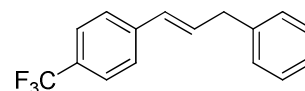


single pulse decoupled gated NOE

Z:\UOZUMI_Gisakurai\allylic arylation_compound data\20140611_p-CF3-product_carbon-1-1als



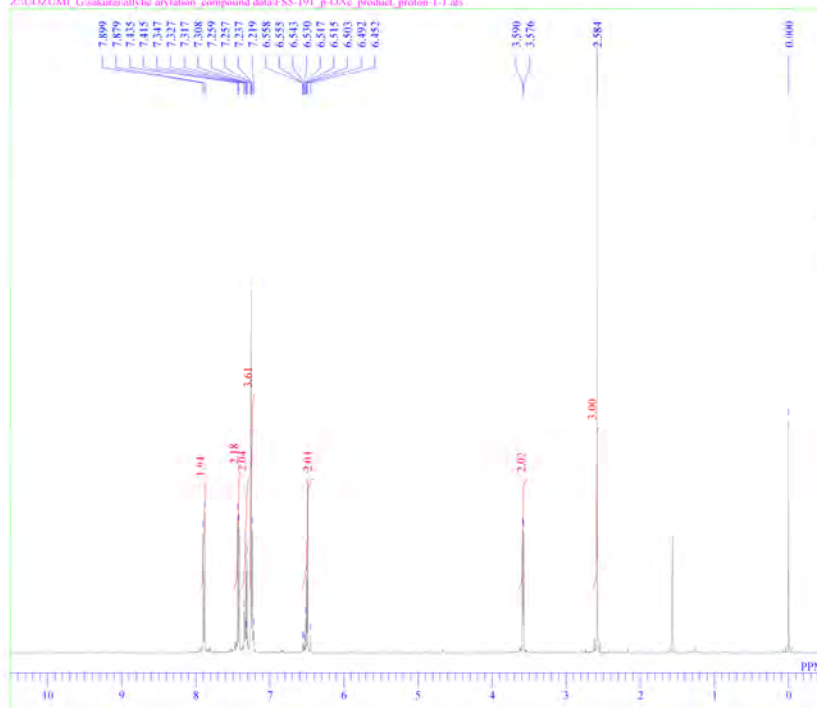
DFILE 20140611_p-CF3-product_carbon-1-1als
COMNT single pulse decoupled gated NOE
DATIM 2014-06-11 00:59:55
OBNUC 13C
EXMOD carbon.jsp
OBFREQ 99.55 MHz
OBSET 5.13 kHz
OBFIN 0.98 Hz
POINT 26214
FREQU 25000.00 Hz
SCANS 10000
ACQTM 1.0486 sec
PD 2.0000 sec
PWI 3.42 usec
IRNUC 13C
CTEMP 19.1 c
SLVNT CDCL3
XREF 0.00 ppm
BF 0.00 Hz
RGAIN 60



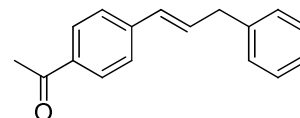
(E)-1-(4-Acetylphenyl)-3-phenylpropene (4ha)

single_pulse

Z:\UOZUMI_Gisakura\allylic arylation_compound data\F55-191_p-OAc_product_proton-1-1.als

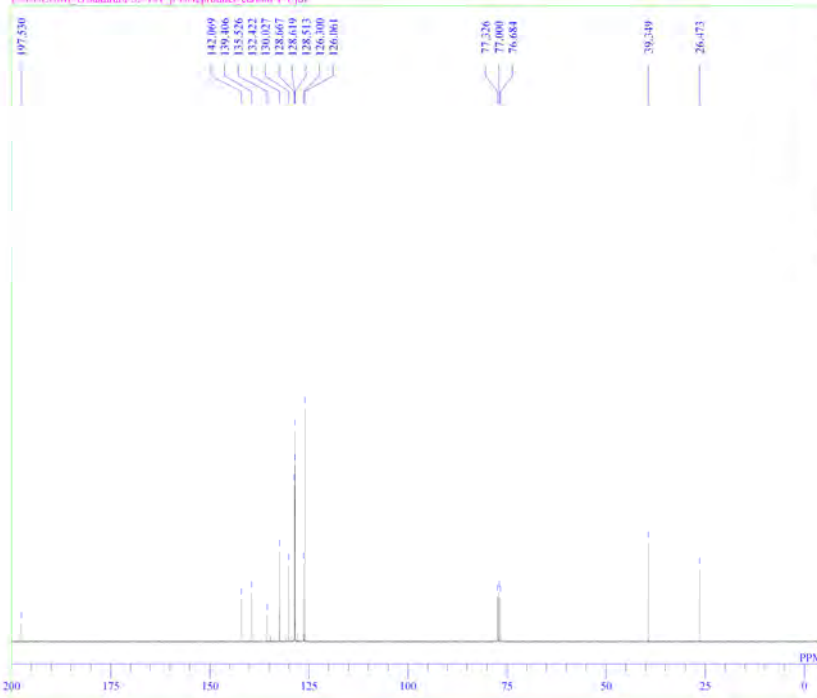


D\FILE F55-191_p-OAc_product_proton-1-1.als
 COMNT single_pulse
 DATIM 2014-03-10 19:41:00
 OBNUC 1H1
 EXMOD proton_xsp
 OBFREQ 395.88 MHz
 OBSETE 6.28 KHz
 OBFIN 0.87 Hz
 POINT 13107
 FREQU 593.824 Hz
 SCANS 8
 ACQTM 2.2073 sec
 PD 5.0000 sec
 PWI 3.12 usec
 IRNUC 1H1
 CTEMP 20.1 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.00 Hz
 RGAIN 42

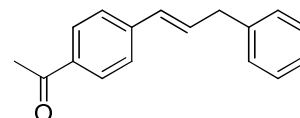


single pulse decoupled gated NOE

Z:\UOZUMI_Gisakura\F55-191_p-OAcproduct_carbon-1-1.jdf



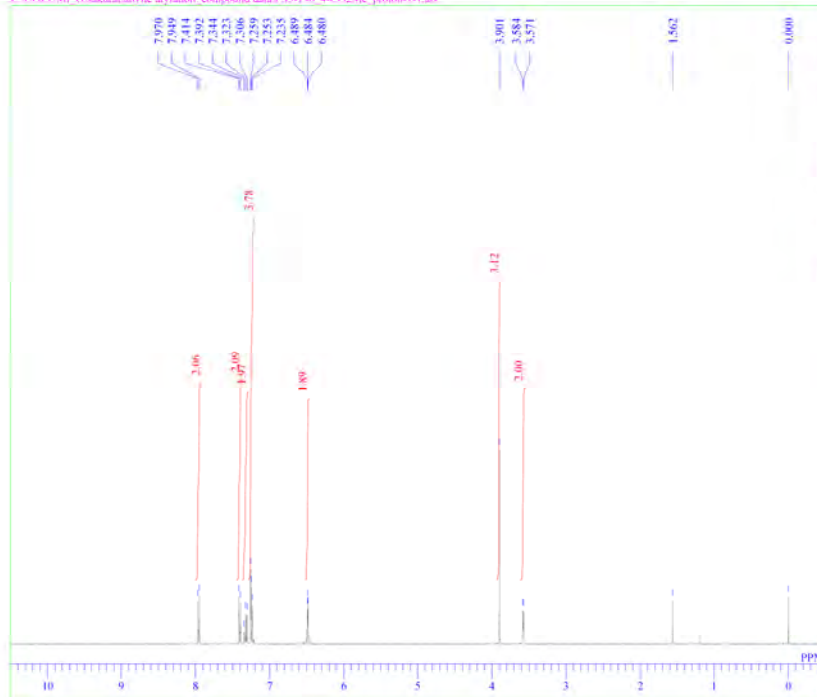
D\FILE F55-191_p-OAcproduct_carbon-1-1.jdf
 COMNT single pulse decoupled gated NOE
 DATIM 2014-03-10 20:07:10
 OBNUC 13C
 EXMOD carbon_xsp
 OBFREQ 99.55 MHz
 OBSETE 5.13 KHz
 OBFIN 0.98 Hz
 POINT 32767
 FREQU 51250.00 Hz
 SCANS 512
 ACQTM 1.0486 sec
 PD 2.0000 sec
 PWI 3.42 usec
 IRNUC 1H1
 CTEMP 19.7 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.50 Hz
 RGAIN 60



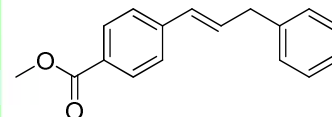
(E)-methyl 4-(3-phenylprop-1-enyl)benzoate (4ia)

single_pulse

Z:\UOZUMI_G\skuraj\allic arylatlon_compound data\FSS-196_4-CO2Me_proton-1-1.als

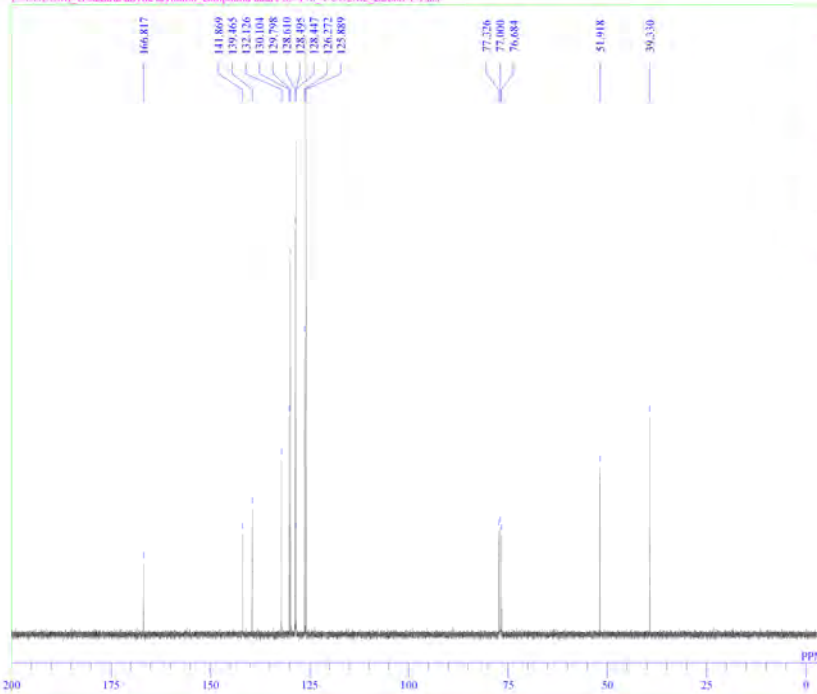


DFILE FSS-196_4-CO2Me_proton-1-1.als
COMNT single_pulse
DATIM 2014-03-14 19:17:48
OBNUC 1H
EXMOD proton_xp
OBFREQ 395.88 MHz
OBSET 6.28 KHz
OBFIN 0.87 Hz
POINT 13107
FREQU 5938.24 Hz
SCANS 8
ACQTM 2.2073 sec
PD 5.0000 sec
PWT 3.12 usec
IRNUC 1H
CTEMP 20.0 c
SLVNT CDCl3
EXREF 0.00 ppm
BF 0.00 Hz
RGAIN 40

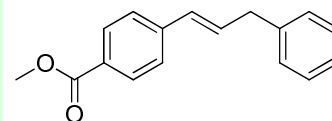


single_pulse decoupled gated NOE

Z:\UOZUMI_G\skuraj\allic arylatlon_compound data\FSS-196_4-CO2Me_carbon-1-1.als



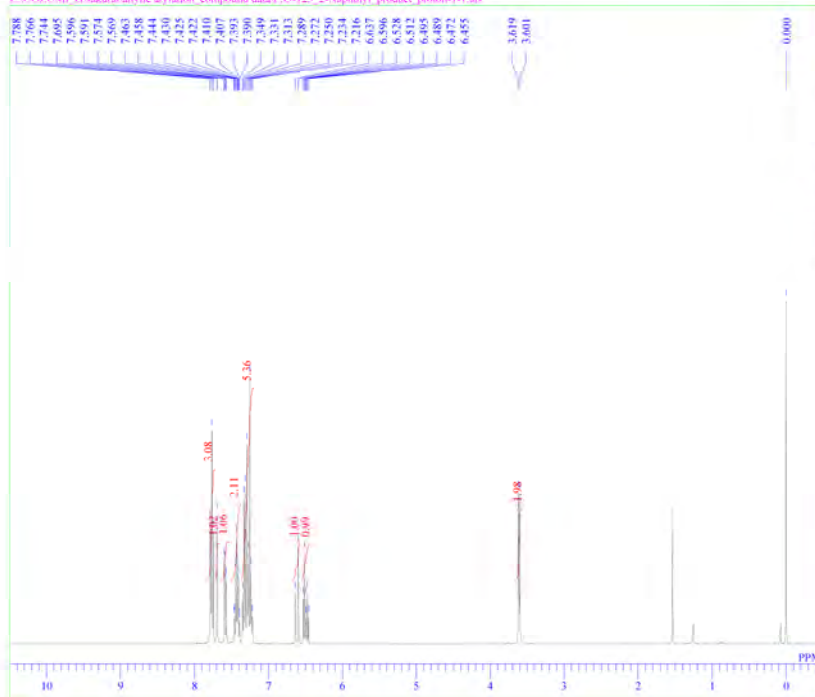
DFILE FSS-196_4-CO2Me_carbon-1-1.als
COMNT single_pulse decoupled gated NOE
DATIM 2014-03-14 19:31:29
OBNUC 13C
EXMOD carbon_xp
OBFREQ 99.55 MHz
OBSET 5.13 KHz
OBFIN 0.98 Hz
POINT 26214
FREQU 25000.00 Hz
SCANS 128
ACQTM 1.0486 sec
PD 2.0000 sec
PWT 3.42 usec
IRNUC 13C
CTEMP 19.6 c
SLVNT CDCl3
EXREF 77.00 ppm
BF 0.00 Hz
RGAIN 60



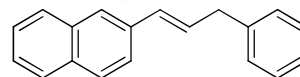
(E)-1-(2-Naphthyl)-3-phenylpropene (4ja)

single_pulse

Z:\UOZUMI_Gisakurai\allylic arylation_compound data\FSS-125_2-Naphthyl_product_proton-1-1.als

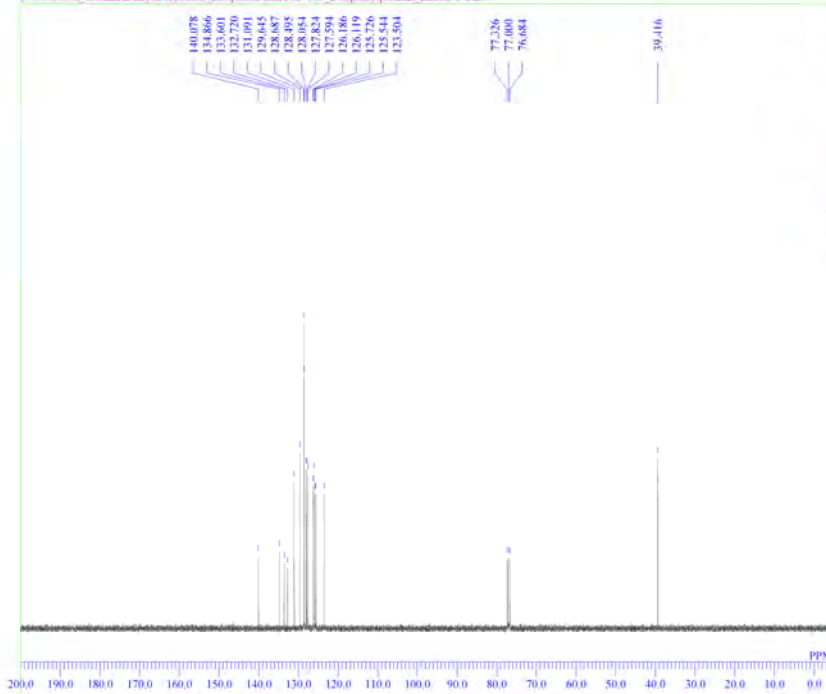


DFILE FSS-125_2-Naphthyl_product_proton-1-1.als
 COMNT single_pulse
 DATIM 2014-01-23 20:57:45
 OBNUC 1H1
 EXMOD proton_xyp
 OBFREQ 395.88 MHz
 OBSET 6.28 KHz
 OBFIN 0.87 Hz
 POINT 13107
 FREQU 5938.24 Hz
 SCANS 8
 ACQTM 2.2073 sec
 PD 5.0000 sec
 PWI 3.12 usec
 IRNUC 1H1
 CTEMP 19.9 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.50 Hz
 RGAIN 38

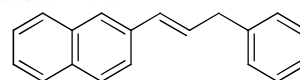


single_pulse decoupled gated NOE

Z:\UOZUMI_Gisakurai\allylic arylation_compound data\FSS-185_2-naphthylproduct_carbon-1-1.als



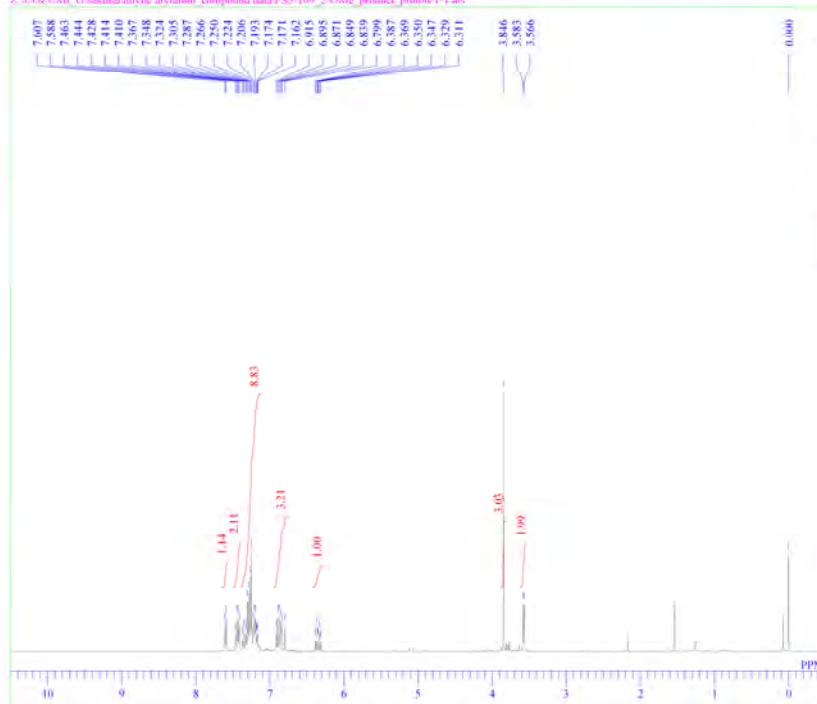
DFILE FSS-185_2-naphthylproduct_carbon-1-1.als
 COMNT single_pulse decoupled gated NOE
 DATIM 2014-05-09 18:24:28
 OBNUC 13C
 EXMOD carbon_xyp
 OBFREQ 99.55 MHz
 OBSET 5.13 KHz
 OBFIN 0.98 Hz
 POINT 26214
 FREQU 25000.00 Hz
 SCANS 128
 ACQTM 1.0486 sec
 PD 2.0600 sec
 PWI 3.42 usec
 IRNUC 13C
 CTEMP 19.1 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.00 Hz
 RGAIN 60



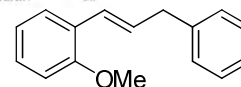
(E)-1-(2-Methoxyphenyl)-3-phenylpropene (4ka)

single_pulse

Z:\UOZUMI_G\sakurai\allylic arylation_compound data\FSS-109_2-OMe_product_proton-1-1.als

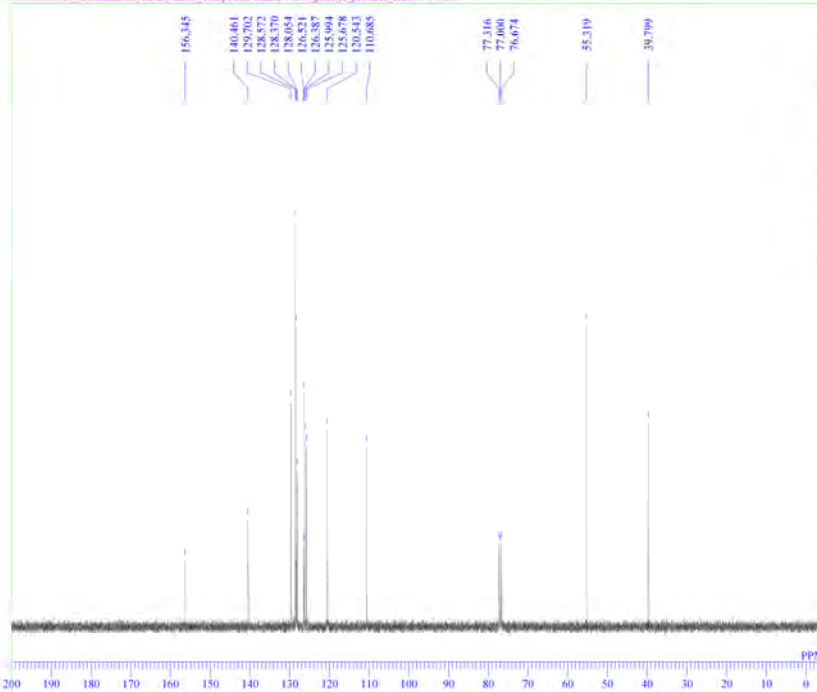


DFILE FSS-109_2-OMe_product_proton-1-1.als
COMNT single_pulse
DATIM 2014-01-23 20:49:51
ORNUC 1H
EXMOD proton.jsp
OBFRO 395.88 MHz
OBSET 6.28 kHz
OBFIN 9.87 Hz
POINT 13107
FREQU 593.824 Hz
SCANS 8
ACQTM 2.2073 sec
PD 5.0000 sec
PWI 3.12 usec
IRNUC 1H
CTEMP 19.3 c
SLVNT CDCl3
EXREF 0.00 ppm
BF 0.50 Hz
RGAIN 36

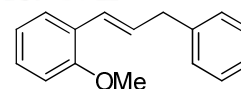


single_pulse decoupled gated NOE

Z:\UOZUMI_G\sakurai\allylic arylation_compound data\2-MeO_phenyl_product_carbon-1-1.als

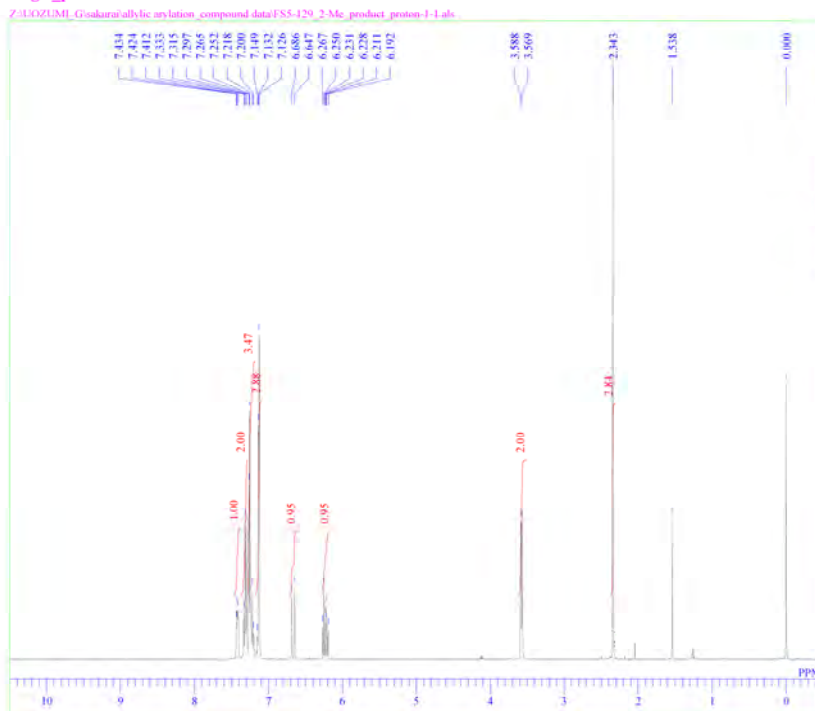


DFILE 2-MeO_phenyl_product_carbon-1-1.als
COMNT single_pulse decoupled gated NOE
DATIM 2014-03-14 19:45:01
ORNUC 13C
EXMOD carbon.jsp
OBFRO 99.55 MHz
OBSET 5.13 kHz
OBFIN 0.98 Hz
POINT 26214
FREQU 25000.00 Hz
SCANS 128
ACQTM 1.0486 sec
PD 2.0000 sec
PWI 3.42 usec
IRNUC 13C
CTEMP 20.0 c
SLVNT CDCl3
EXREF 77.00 ppm
BF 0.00 Hz
RGAIN 60

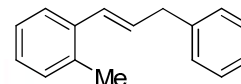


(E)-1-(2-Methylphenyl)-3-phenylpropene (4la)

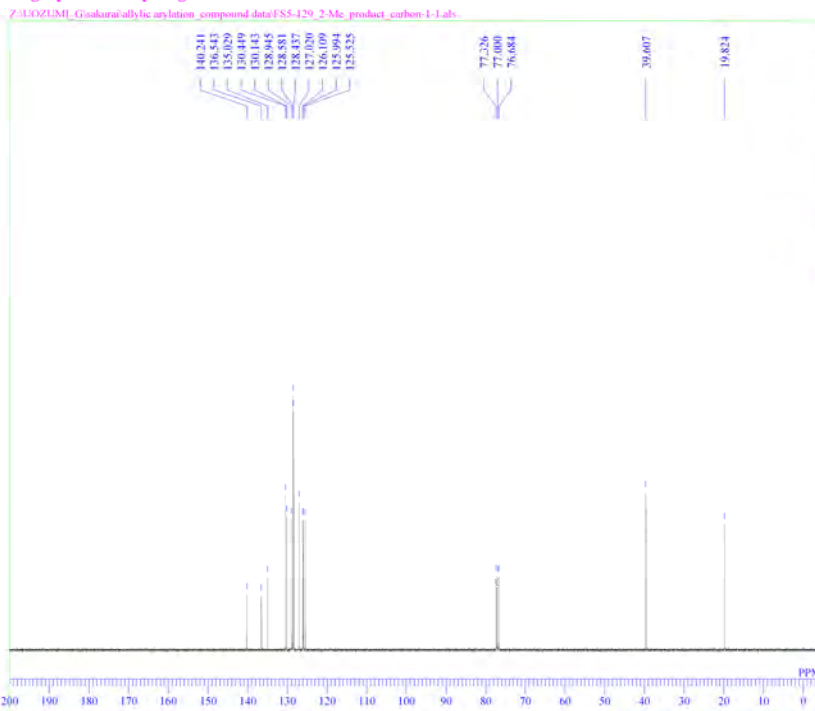
single_pulse



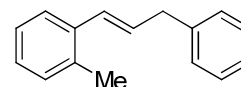
DFILE FSS-129_2-Me_product_proton-1-1.als
COMNT single_pulse
DATIM 2014-01-25 18:21:18
OBNUC 1H1
EXMOD proton_jsp
OBFRO 395.88 MHz
OBSET 6.28 KHz
OBFIN 0.87 Hz
POINT 13107
FREQU 593.824 Hz
SCANS 8
ACQTM 2.2073 sec
PD 5.0000 sec
PWI 3.12 usec
IRNUC 1H1
CTEMP 19.9 c
SLVNT CDCl3
EXREF 0.00 ppm
BF 0.25 Hz
RGAIN 38



single_pulse decoupled gated NOE



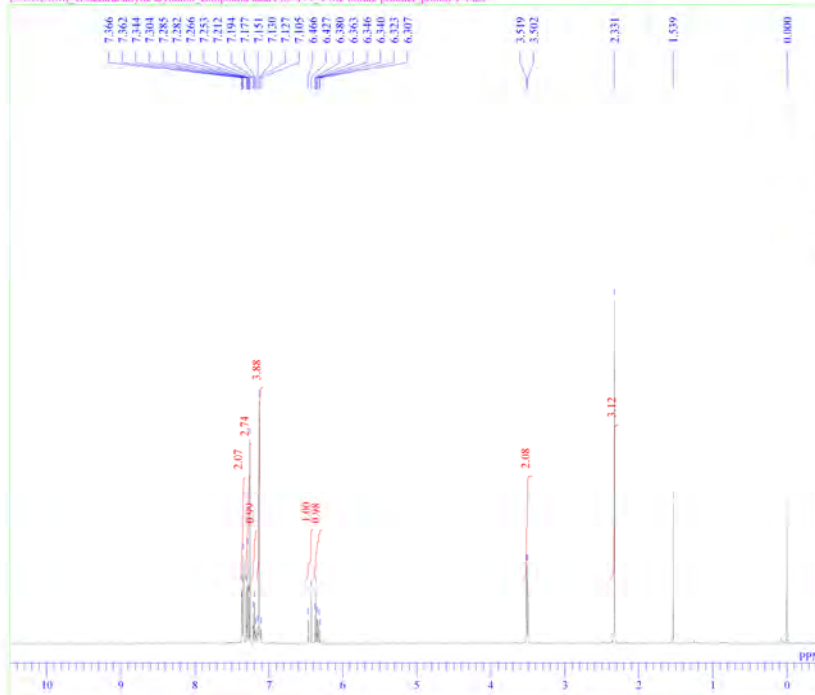
DFILE FSS-129_2-Me_product_carbon-1-1.als
COMNT single_pulse decoupled gated NOE
DATIM 2014-01-25 18:33:08
OBNUC 13C
EXMOD carbon_jsp
OBFRO 99.55 MHz
OBSET 5.13 KHz
OBFIN 0.98 Hz
POINT 26214
FREQU 25000.00 Hz
SCANS 187
ACQTM 1.0486 sec
PD 2.0600 sec
PWI 3.42 usec
IRNUC 13C
CTEMP 19.9 c
SLVNT CDCl3
EXREF 77.00 ppm
BF 0.25 Hz
RGAIN 60



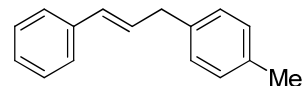
(E)-3-(4-Methylphenyl)-1-phenylpropene (4ab)

single_pulse

Z:\UOZUMI_Gsakurai\allylic arylation_compound data\FSS-199_4-Me-borate-product_proton-1-1.als

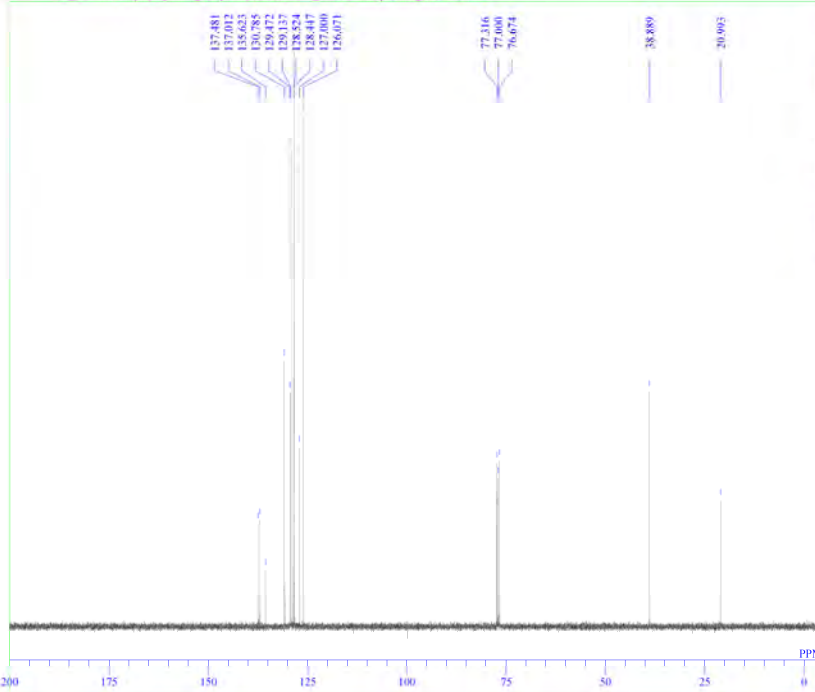


DFILE FSS-199_4-Me-borate-product_proton-1-1.als
COMNT single_pulse
DATIM 2014-03-15 19:35:19
ORNUC III
EXMOD proton.jsp
OBFREQ 395.88 MHz
OBSET 6.28 KHz
OBFIN 0.87 Hz
POINT 13107
FREQU 593.824 Hz
SCANS 8
ACQTM 2.2073 sec
PD 5.0000 sec
PWI 3.12 usec
IRNUC III
CTEMP 20.3 c
SLVNT CDCl3
EXREF 0.00 ppm
BF 0.00 Hz
RGAIN 40

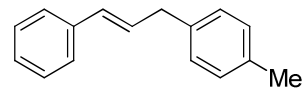


single_pulse decoupled gated NOE

Z:\UOZUMI_Gsakurai\allylic arylation_compound data\FSS-199_4-Me-borate-product_carbon-1-1.als



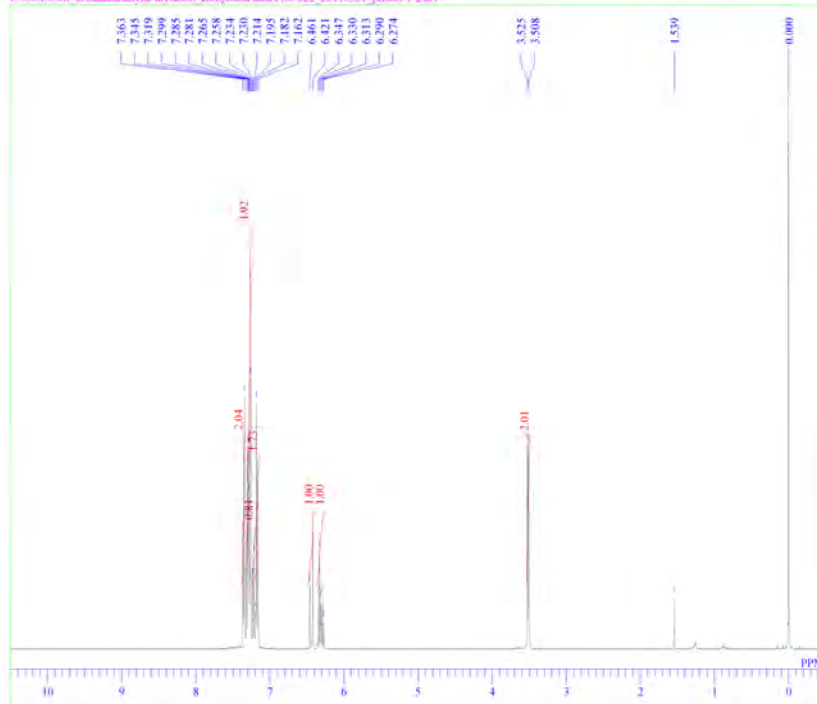
DFILE FSS-199_4-Me-borate-product_carbon-1-1.als
COMNT single_pulse decoupled gated NOE
DATIM 2014-03-15 19:43:38
ORNUC 13C
EXMOD carbon.jsp
OBFREQ 99.55 MHz
OBSET 5.13 KHz
OBFIN 0.98 Hz
POINT 26214
FREQU 25000.00 Hz
SCANS 218
ACQTM 1.0486 sec
PD 2.0000 sec
PWI 3.42 usec
IRNUC III
CTEMP 19.4 c
SLVNT CDCl3
EXREF 77.00 ppm
BF 0.00 Hz
RGAIN 60



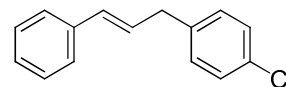
(E)-3-(4-Chlorophenyl)-1-phenylpropene (4ac)

single_pulse

Z:\UOZUMI_G\sakurai\allylic arylation_compound data\F6-022_20140331_proton-1-2.als

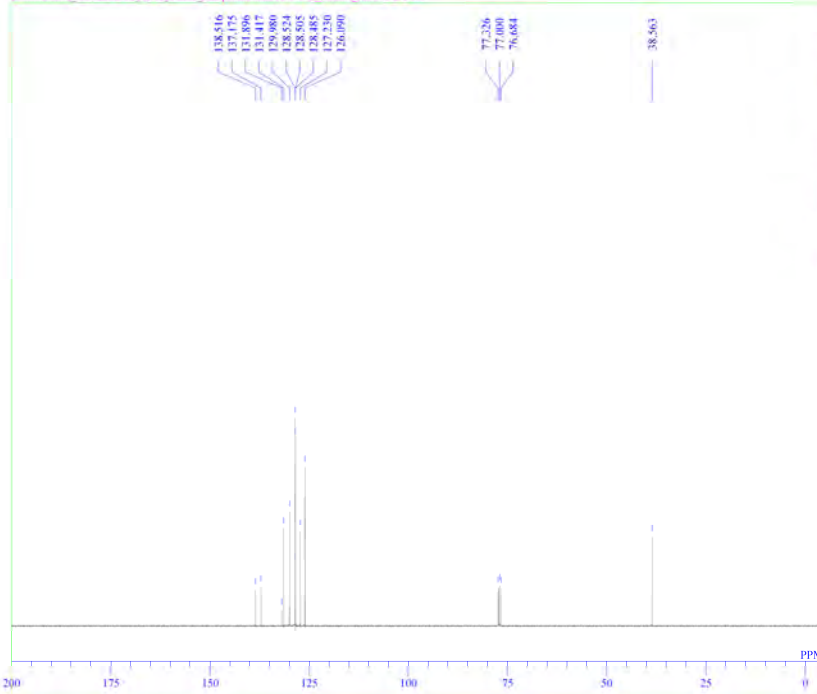


DFILE F6-022_20140331_proton-1-2.als
COMNT single_pulse
DATIM 2014-03-31 21:20:51
ORNUC 1H
EXMOD proton.jsp
OBFREQ 395.88 MHz
OBSET 6.28 KHz
OBFIN 9.87 Hz
POINT 13107
FREQU 593.24 Hz
SCANS 8
ACQTM 2.2073 sec
PD 5.0000 sec
PWI 3.12 usec
IRNUC 1H
CTEMP 20.0 c
SOLVT CDCl3
EXREF 0.00 ppm
BF 0.05 Hz
RGAIN 44

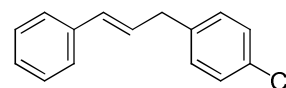


single_pulse decoupled gated NOE

Z:\UOZUMI_G\sakurai\allylic arylation_compound data\F6-022_carbon-carbon-1-1.als



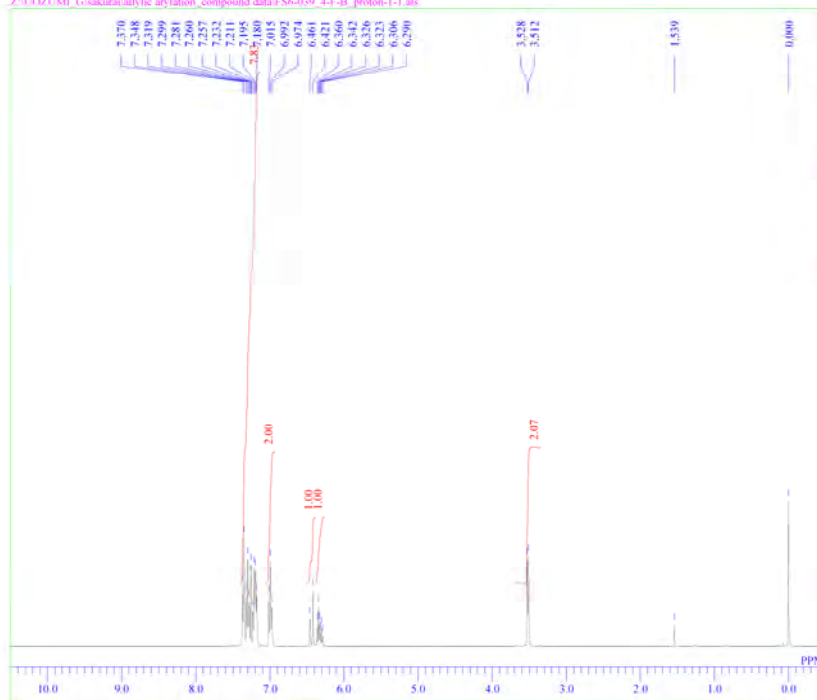
DFILE F6-022_carbon-carbon-1-1.als
COMNT single_pulse decoupled gated NOE
DATIM 2014-03-31 21:58:53
ORNUC 13C
EXMOD carbon.jsp
OBFREQ 99.55 MHz
OBSET 5.13 KHz
OBFIN 0.98 Hz
POINT 26214
FREQU 25000.00 Hz
SCANS 232
ACQTM 1.0486 sec
PD 2.0000 sec
PWI 3.42 usec
IRNUC 13C
CTEMP 18.9 c
SOLVT CDCl3
EXREF 77.00 ppm
BF 0.20 Hz
RGAIN 60



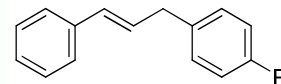
(E)-3-(4-Fluorophenyl)-1-phenylpropene (4ad)

single_pulse

Z:\UOZUMI_Gisakura\allylic arylation_compound data\F56-039_4-F-B_proton-1-1.als

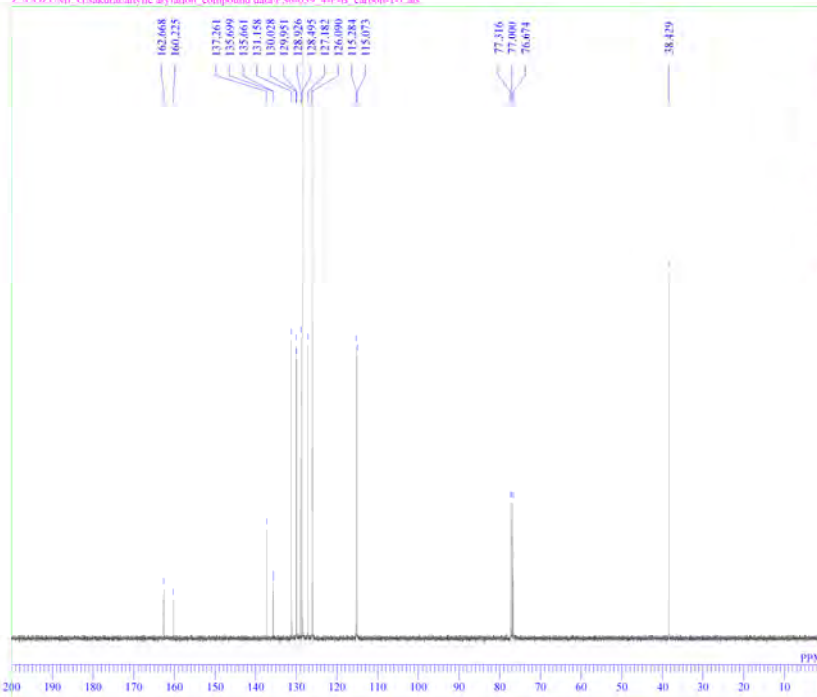


DFILE F56-039_4-F-B_proton-1-1.als
COMNT single_pulse
DATIM 2014-04-07 17:45:00
OBNUC 1H1
EXMOD proton_xsp
OBFREQ 595.88 MHz
OBSET 6.28 KHz
OBFIN 0.87 Hz
POINT 13107
FREQU 5938.24 Hz
SCANS 8
ACQTM 2.2073 sec
PD 5.0000 sec
PWI 3.12 usec
IRNUC 1H1
CTEMP 19.6 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.05 Hz
RGAIN 42

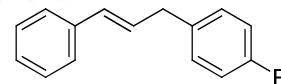


single_pulse decoupled gated NOE

Z:\UOZUMI_Gisakura\allylic arylation_compound data\F56-039_4-F-B_carbon-1-1.als



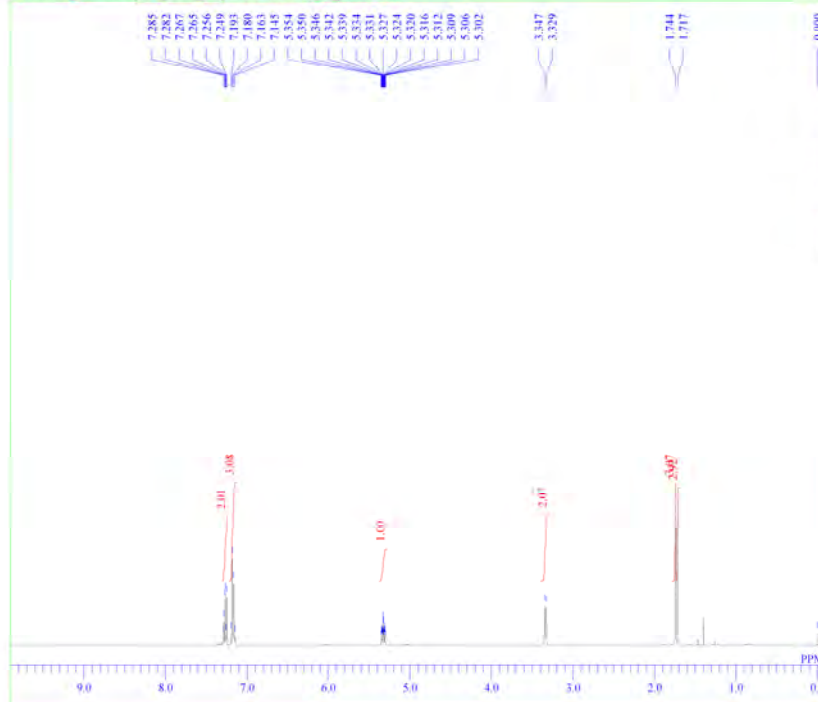
DFILE F56-039_4-F-B_carbon-1-1.als
COMNT single_pulse decoupled gated NOE
DATIM 2014-04-07 17:53:37
OBNUC 13C
EXMOD carbon_xsp
OBFREQ 99.55 MHz
OBSET 5.13 KHz
OBFIN 0.98 Hz
POINT 26214
FREQU 25000.00 Hz
SCANS 382
ACQTM 1.0486 sec
PD 2.0000 sec
PWI 3.42 usec
IRNUC 13C
CTEMP 19.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.20 Hz
RGAIN 60



2-Methyl-4-phenyl-2-butene (4na)

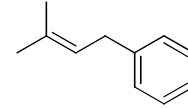
single pulse

Z:\UOZUMI_Gisakana\allylic arylation compound data\F86-133_1c_proton-1-1.als



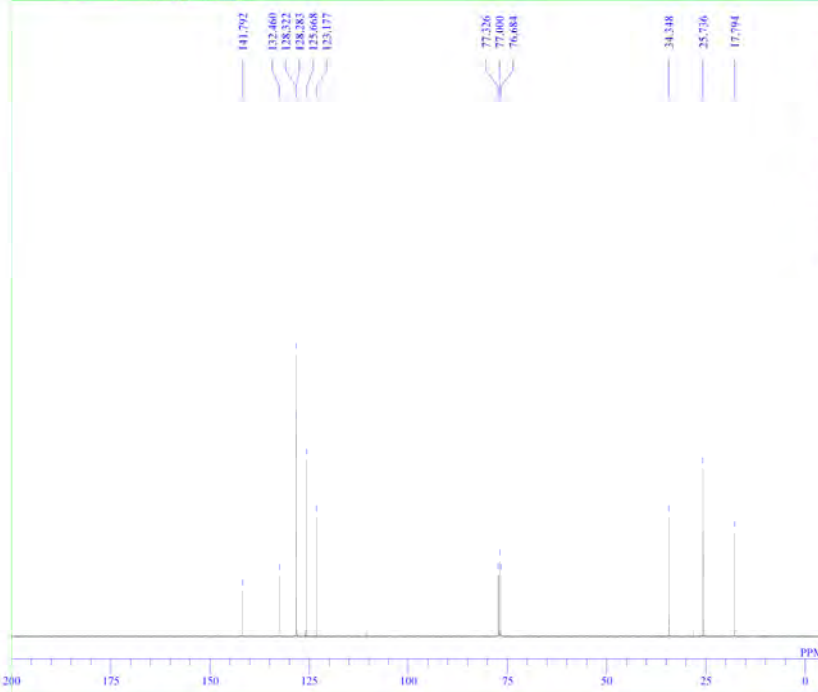
```

DFILE F86-133_1c_proton-1-1.als
COMNT single_pulse
DATIM 2014-07-11 17:31:14
ORNUC 1H
EXMOD proton.jsp
OBFRO 395.88 MHz
OBSET 6.28 KHz
OBFIN 9.87 Hz
POINT 13107
FREQU 593.24 Hz
SCANS 8
ACQTM 2.2073 sec
PD 5.0000 sec
PWI 3.12 usec
IRNUC 1H
CTEMP 20.0 c
SLVNT CDCl3
EXREF 0.00 ppm
BF 0.05 Hz
RGAIN 22
    
```



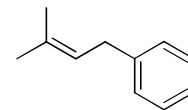
single pulse decoupled gated NOE

Z:\UOZUMI_Gisakana\F86-133_1c_carbon-1-1.jdf



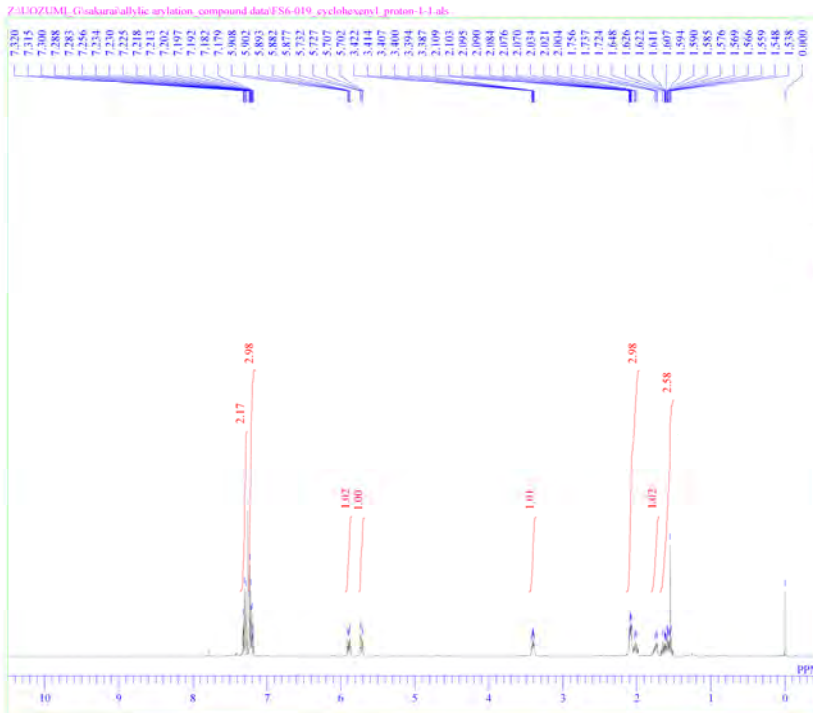
```

DFILE F86-133_1c_carbon-1-1.jdf
COMNT single pulse decoupled gated NOE
DATIM 2014-07-11 17:32:46
ORNUC 13C
EXMOD carbon.jsp
OBFRO 99.55 MHz
OBSET 5.13 KHz
OBFIN 0.98 Hz
POINT 32767
FREQU 31250.00 Hz
SCANS 512
ACQTM 1.0486 sec
PD 2.0000 sec
PWI 3.42 usec
IRNUC 13C
CTEMP 20.0 c
SLVNT CDCl3
EXREF 77.00 ppm
BF 0.45 Hz
RGAIN 60
    
```



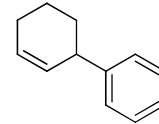
3-Phenylcyclohexene (40a)

single_pulse

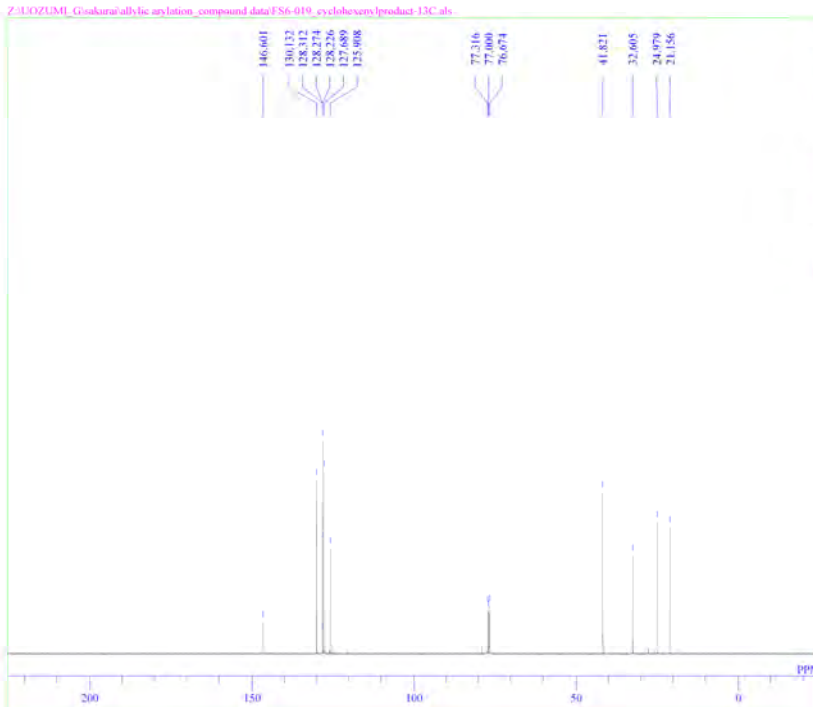


```

D1FILE  E6-019_cyclohexenyl_proton-1-1.als
COMNT   single_pulse
DATIM   2014-03-20 19:01:42
ORNUC   1H
EXMOD   proton_jsp
OBFREQ  395.88 MHz
OBSETE  6.28 kHz
OBFIN   0.87 Hz
POINT   13107
FREQU   593.824 MHz
SCANS   8
ACQTM   2.2073 sec
PD      5.0000 sec
PWI     3.12 usec
IRNUC   1H
CTEMP   19.8 c
SLVNT   CDCl3
EXREF   0.00 ppm
BF      0.00 Hz
RGAIN   38
    
```

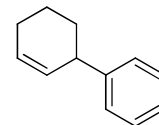


single_pulse decoupled gated NOE



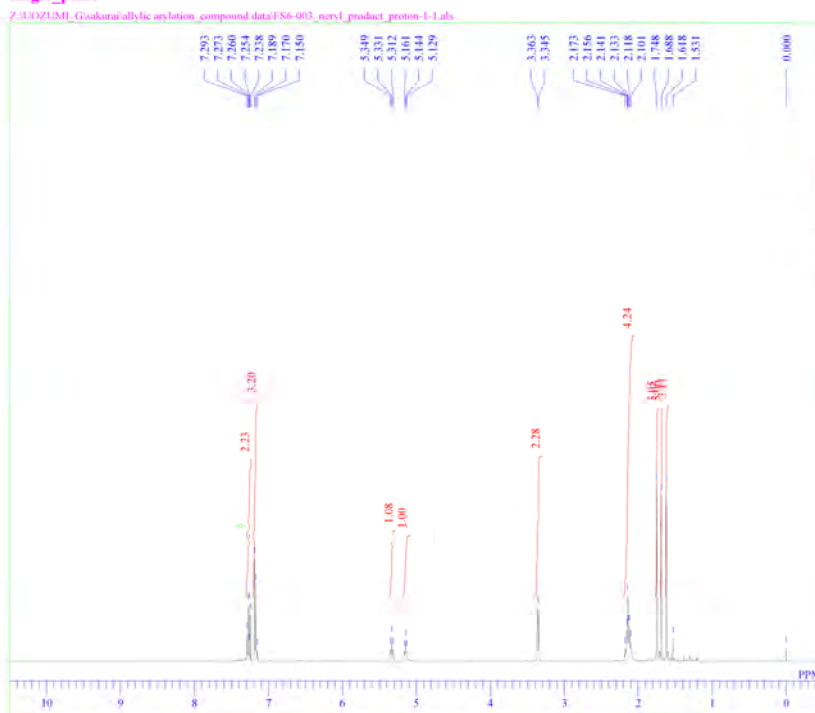
```

D1FILE  E6-019_cyclohexenyl/product-13C.als
COMNT   single_pulse decoupled gated NOE
DATIM   2014-03-20 19:39:52
ORNUC   13C
EXMOD   carbon_jsp
OBFREQ  99.55 MHz
OBSETE  5.13 kHz
OBFIN   0.98 Hz
POINT   32767
FREQU   31250.00 MHz
SCANS   512
ACQTM   1.0486 sec
PD      2.0000 sec
PWI     3.42 usec
IRNUC   13C
CTEMP   19.4 c
SLVNT   CDCl3
EXREF   77.00 ppm
BF      0.50 Hz
RGAIN   60
    
```

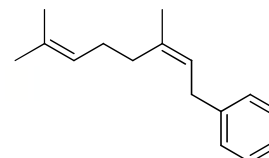


(Z)-3,7-Dimethyl-1-phenyl-2,6-octadiene (4pa)

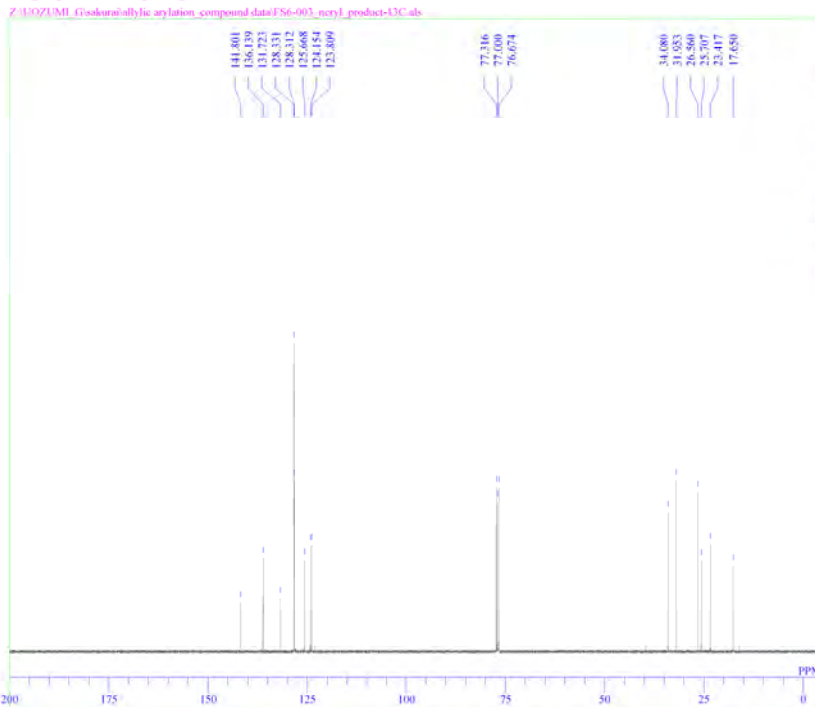
single_pulse



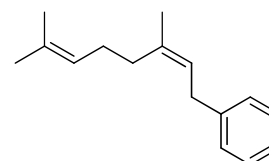
DFILE F56-003_neryl_product_proton-1-1.als
COMNT single_pulse
DATIM 2014-03-17 19:37:50
OBNUC 1H1
EXMOD proton_1vp
OBFREQ 395.88 MHz
OBSEI 6.28 KHz
ORFIN 0.87 Hz
POINT 13107
FREQU 593.824 Hz
SCANS 8
ACQTM 2.2073 sec
PD 5.0000 sec
PWI 3.12 usec
IRNUC 1H1
CTEMP 19.2 c
SLVNT CDCl3
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 24



single_pulse decoupled gated NOE



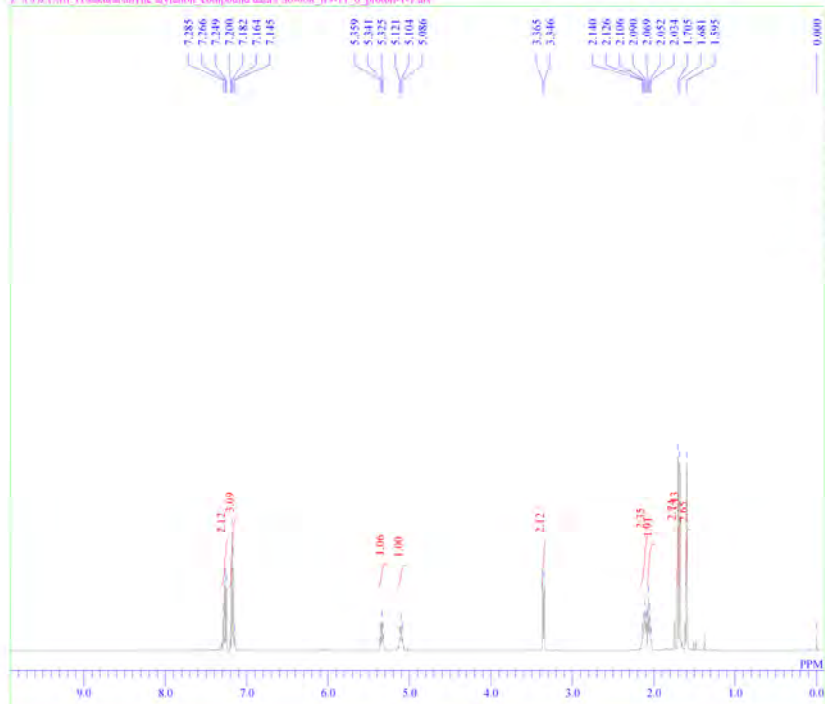
DFILE F56-003_neryl_product-13C-1.als
COMNT single_pulse decoupled gated NOE
DATIM 2014-03-17 19:39:16
OBNUC 13C
EXMOD carbon_1vp
OBFREQ 99.55 MHz
OBSEI 5.13 KHz
ORFIN 0.98 Hz
POINT 32767
FREQU 31250.00 Hz
SCANS 512
ACQTM 1.0486 sec
PD 2.0000 sec
PWI 3.42 usec
IRNUC 1H1
CTEMP 18.9 c
SLVNT CDCl3
EXREF 77.00 ppm
BF 0.50 Hz
RGAIN 60



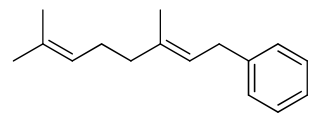
(E)-3,7-Dimethyl-1-phenyl-2,6-octadiene (4qa)

single_pulse

Z:\UOZ\1M1_G\skurui\allylic_arylation_compound data\F86-008_69-11_6_proton-1-1.als

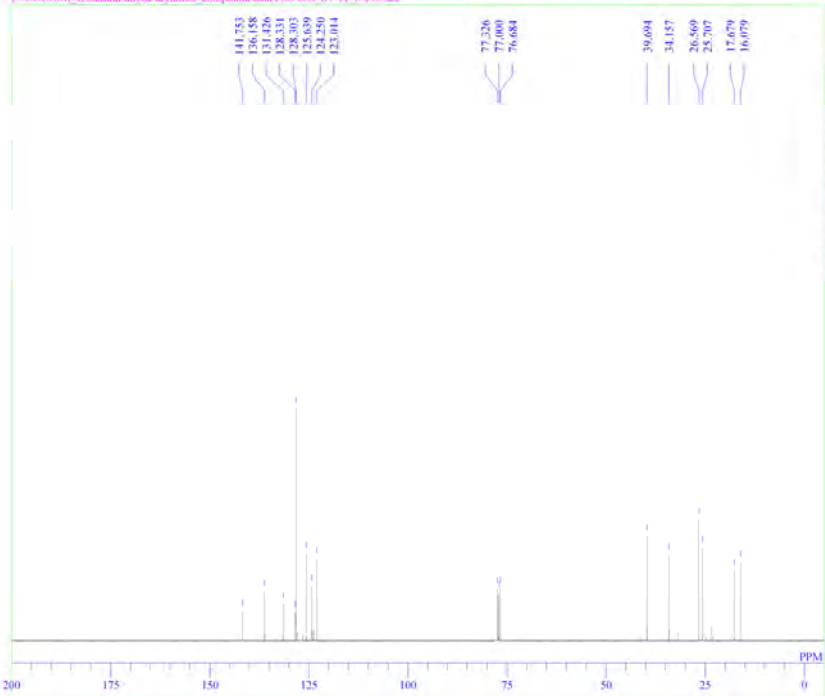


DFILE F86-008_69-11_6_proton-1-1.als
COMNT single_pulse
DATIM 2014-05-19 16:51:47
OBNUC 1H
EXMOD proton.jsp
OBFRQ 395.88 MHz
OBSET 6.28 kHz
OBFIN 0.87 Hz
POINT 13107
FREQU 593.824 Hz
SCANS 8
ACQTM 2.2073 sec
PD 5.0000 sec
PWI 3.12 usec
IRNUC 1H
CTEMP 19.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.00 Hz
RGAIN 20

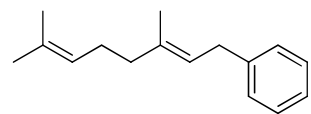


single pulse decoupled gated NOE

Z:\UOZ\1M1_G\skurui\allylic_arylation_compound data\F86-008_69-11_6-13C.als



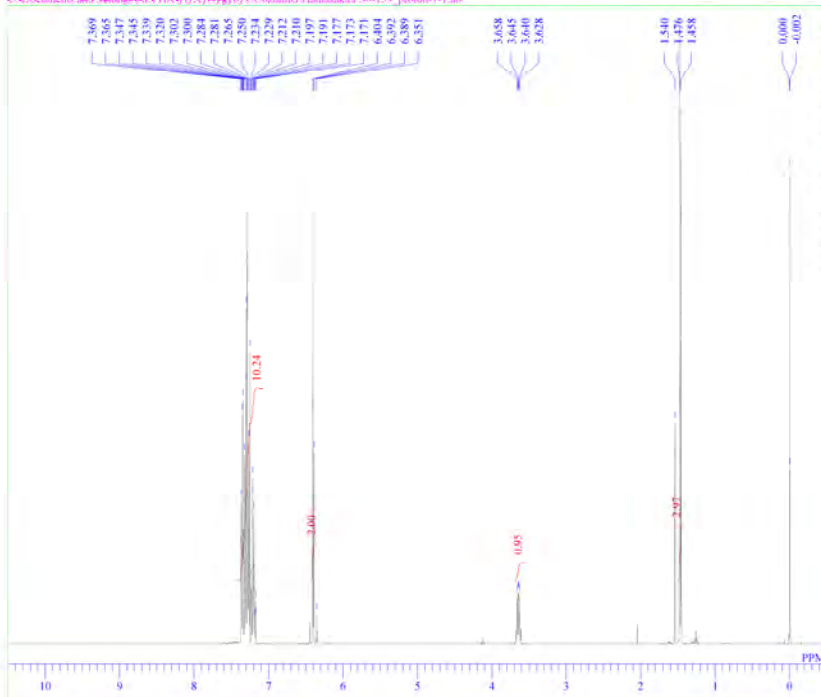
DFILE F86-008_69-11_6-13C.als
COMNT single pulse decoupled gated NOE
DATIM 2014-05-19 16:53:13
OBNUC 13C
EXMOD carbon.jsp
OBFRQ 99.55 MHz
OBSET 5.13 kHz
OBFIN 0.98 Hz
POINT 32767
FREQU 31250.00 Hz
SCANS 472
ACQTM 3.0486 sec
PD 2.0000 sec
PWI 3.42 usec
IRNUC 1H
CTEMP 19.7 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.40 Hz
RGAIN 60



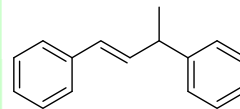
(E)-1,3-Diphenyl-1-butene (4ra)

FS6-159-11E

C:\Documents and Settings\ALPHA\1\1\N\1\g\h\vl\ozumiG\Hamasaki\FS6-159_proton-1-1.als

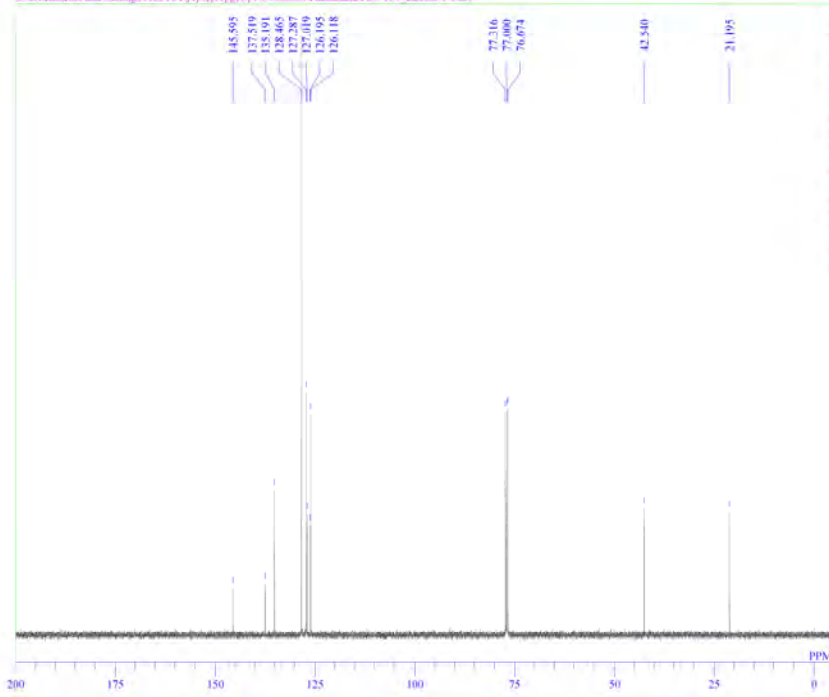


DFILE FS6-159_proton-1-1.als
COMNT FS6-159-11E
DATIM 2014-12-27 18:31:25
OBNUC 1H
EXMOD proton.jsp
OBFREQ 395.88 MHz
OBSET 6.28 KHz
OBFIN 0.87 Hz
POINT 16384
FREQU 7422.80 Hz
SCANS 8
ACQTM 2.2073 sec
PD 3.0000 sec
PWL 3.12 usec
IRNUC 1H
CTEMP 19.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.00 Hz
RGAIN 38

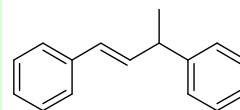


FS6-159-13C

C:\Documents and Settings\ALPHA\1\1\N\1\g\h\vl\ozumiG\Hamasaki\FS6-159_carbon-1-1.als



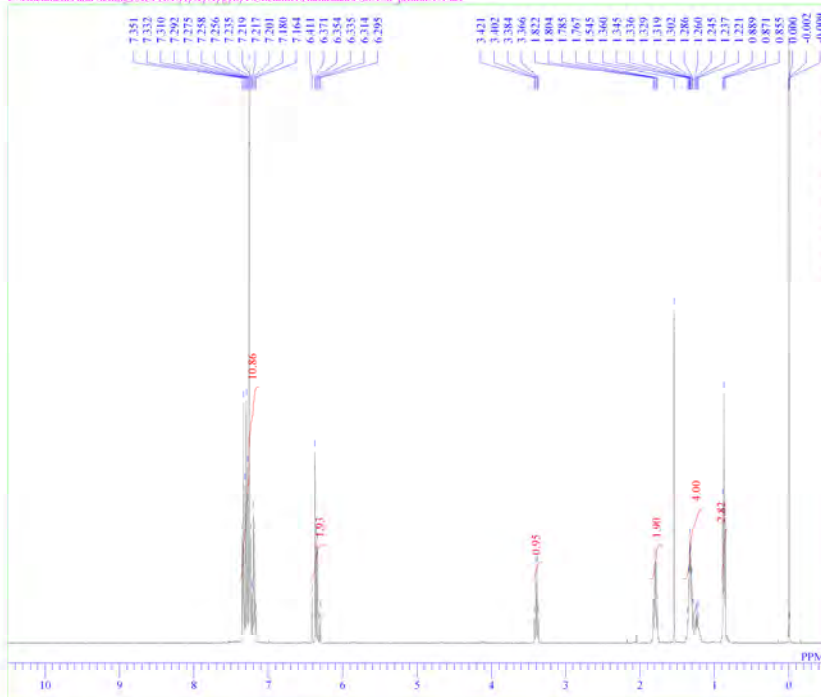
DFILE FS6-159_carbon-1-1.als
COMNT FS6-159-13C
DATIM 2014-12-27 18:51:06
OBNUC 13C
EXMOD carbon.jsp
OBFREQ 99.55 MHz
OBSET 5.13 KHz
OBFIN 0.98 Hz
POINT 32767
FREQU 31250.00 Hz
SCANS 257
ACQTM 1.0486 sec
PD 2.0000 sec
PWL 3.42 usec
IRNUC 13C
CTEMP 19.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF -0.50 Hz
RGAIN 60



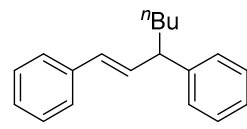
(E)-1,3-Diphenyl-1-heptene (4sa)

FS6-158-1H

C:\Documents and Settings\ALPHA\1\X\N\g\h\c\Uozumi\G\Hamaska\FS6-158_proton-1-1.als

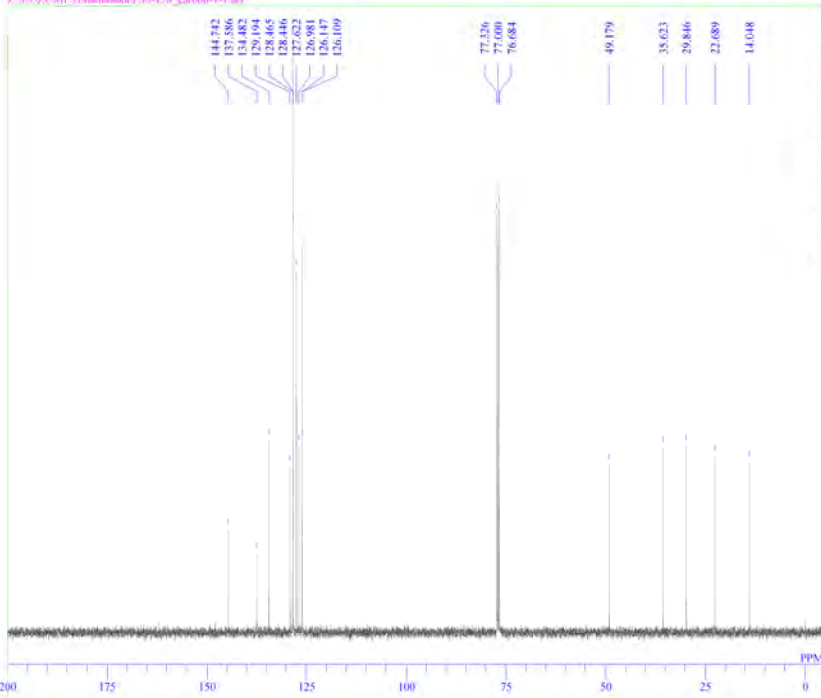


DFILE FS6-158_proton-1-1.als
COMNT FS6-158-1H
DATIM 2014-12-27 17:40:04
OBNUC 1H
EXMOD proton.jsp
OBFRQ 395.88 MHz
OBSET 6.28 kHz
OBFIN 0.87 Hz
POINT 16384
FREQU 7422.80 Hz
SCANS 8
ACQTM 2.2073 sec
PD 3.0000 sec
PWI 3.12 usec
JRNUC 1H
CTEMP 19.6 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.00 Hz
RGAIN 40

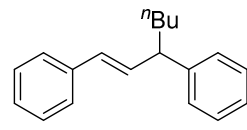


FS6-158-13C

Z:\UOZUMI_G\hamaska\FS6-158_carbon-1-1.als

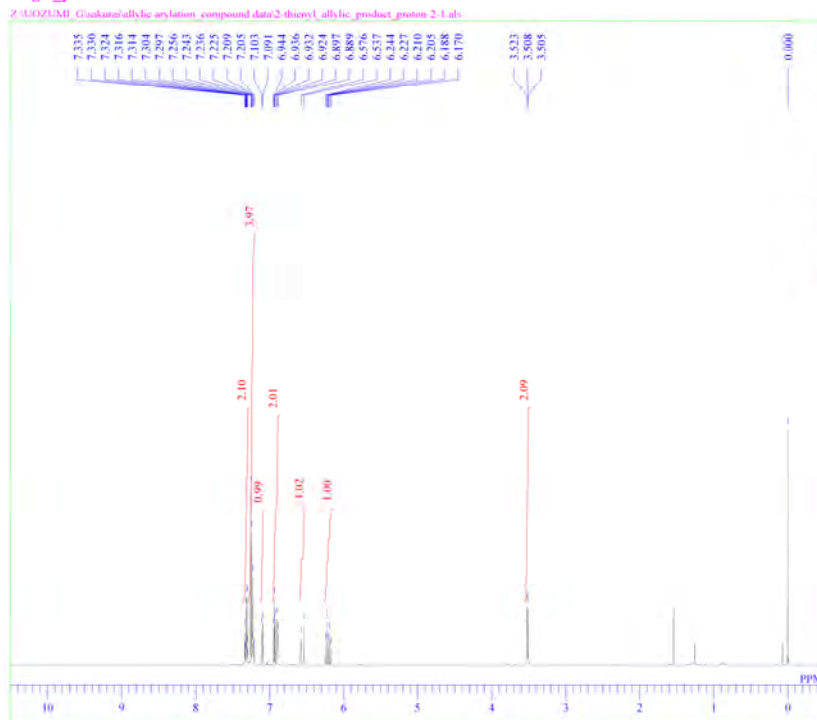


DFILE FS6-158_carbon-1-1.als
COMNT FS6-158-13C
DATIM 2014-12-27 17:51:29
OBNUC 13C
EXMOD carbon.jsp
OBFRQ 99.55 MHz
OBSET 5.13 kHz
OBFIN 0.98 Hz
POINT 32767
FREQU 31250.00 Hz
SCANS 652
ACQTM 3.0486 sec
PD 2.0000 sec
PWI 3.42 usec
JRNUC 13C
CTEMP 19.8 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.50 Hz
RGAIN 60

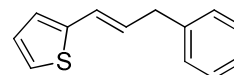


(E)-1-(2-Thiophene)-3-phenylpropene (4ta)

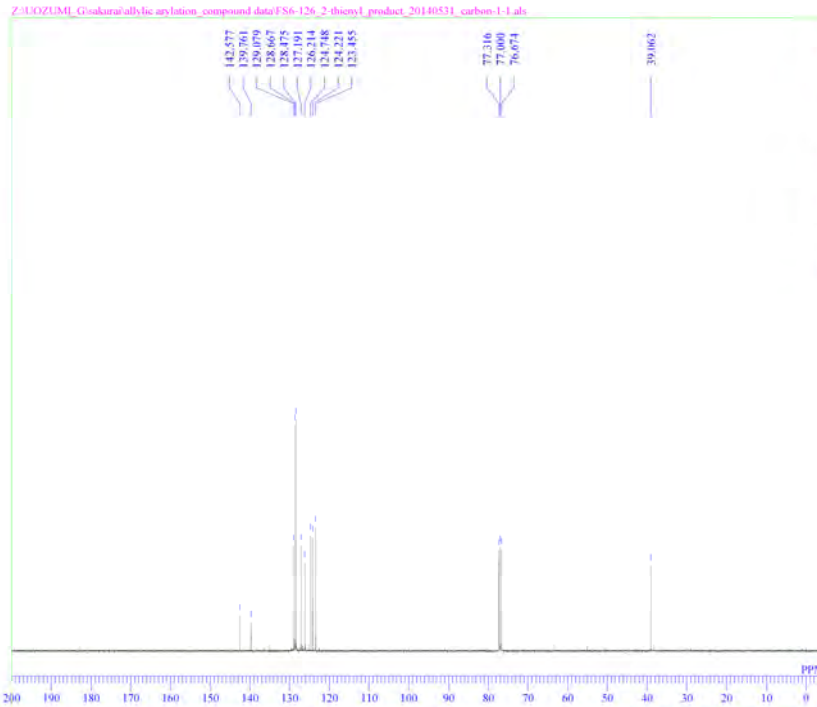
single pulse



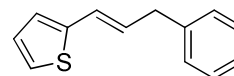
DFILE 2-thienyl allylic_product_proton_2-1_als
 COMNT single_pulse
 DATIM 2014-01-21 21:25:13
 OBNUC 1H1
 EXMOD proton_jvp
 OBFRO 395.88 MHz
 OBSET 6.28 KHz
 OBFIN 0.87 Hz
 POINT 13107
 FREQU 593.824 Uo
 SCANS 8
 ACQTM 2.2073 sec
 PD 5.0000 sec
 PW1 3.12 usec
 IRNUC 1H1
 CTEMP 19.9 c
 SLVNT CDCl3
 EXREF 0.00 ppm
 BF 0.00 Hz
 RGAIN 40



single pulse decoupled gated NOE



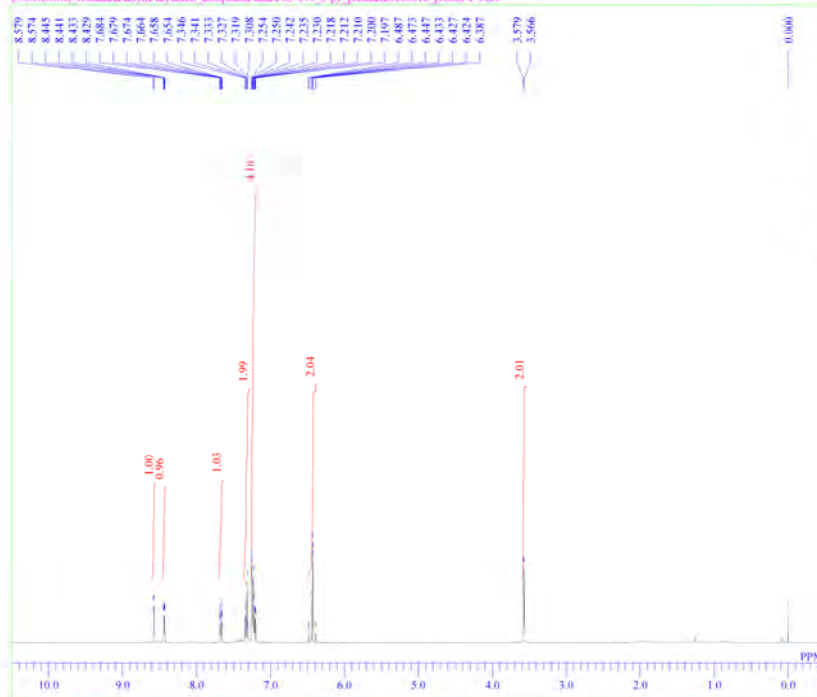
DFILE ES6-126_2-thienyl_product_20140531_carbon-1_als
 COMNT single pulse decoupled gated NOE
 DATIM 2014-05-31 20:54:05
 OBNUC 13C
 EXMOD carbon_jvp
 OBFRO 99.55 MHz
 OBSET 5.13 KHz
 OBFIN 0.98 Hz
 POINT 32767
 FREQU 31250.00 Hz
 SCANS 456
 ACQTM 1.0486 sec
 PD 2.0000 sec
 PW1 3.42 usec
 IRNUC 13C
 CTEMP 19.1 c
 SLVNT CDCl3
 EXREF 77.00 ppm
 BF 0.50 Hz
 RGAIN 60



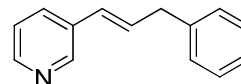
(E)-1-(3-Pyridine)-3-phenylpropene (4ua)

single_pulse

Z:\UOZ\ML_Gsakurai\allylic arylation_compound data\FSS-170_3-py_product20140610_proton-1-1.als

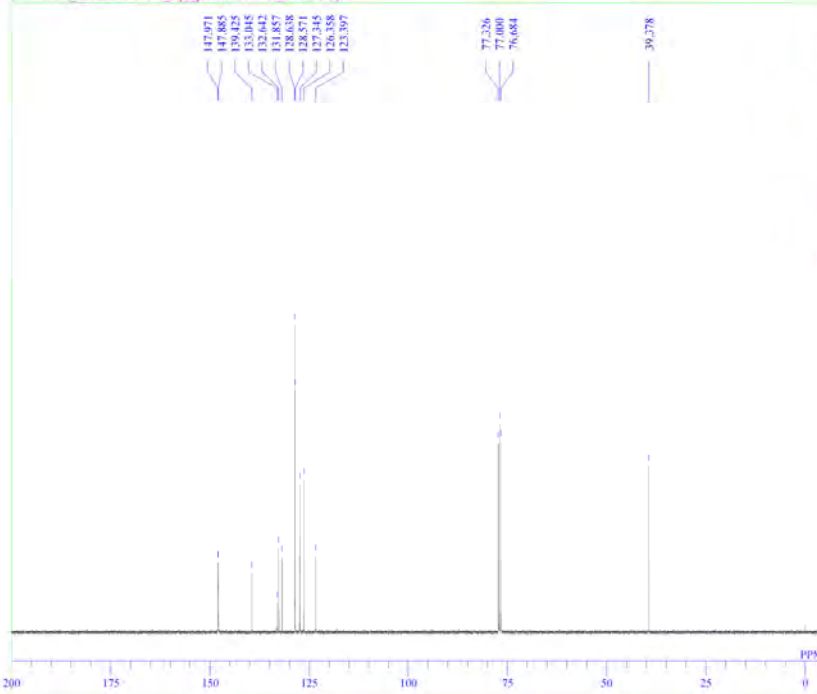


DFILE FSS-170_3-py_product20140610_proton-1-1.als
 COMMT single_pulse
 DATIM 2014-06-10 21:24:26
 OBNUC 1H
 EXMOD proton.jsp
 OBFQ 395.88 MHz
 OBSE1 8.28 KHz
 OBFIN 0.87 Hz
 POINT 13107
 FREQU 593.824 Hz
 SCANS 8
 ACQTM 2.2073 sec
 PD 5.0000 sec
 PW1 3.12 usec
 IRNUC 1H
 CTEMP 19.2 c
 SLVNT CDCl3
 EXREF 0.00 ppm
 BF 0.00 Hz
 RGAIN 30

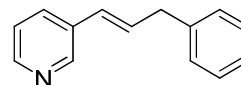


single_pulse decoupled gated NOE

Z:\UOZ\ML_Gsakurai\FSS-170_3-py_product20140610_carbon-1-1.jdf



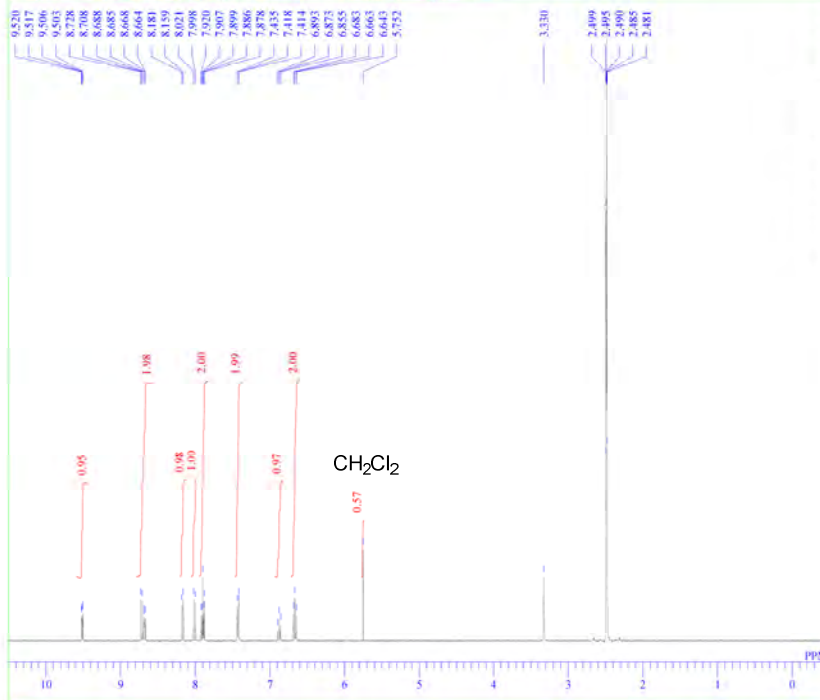
DFILE FSS-170_3-py_product20140610_carbon-1-1.jdf
 COMMT single_pulse decoupled gated NOE
 DATIM 2014-06-10 21:41:45
 OBNUC 13C
 EXMOD carbon.jsp
 OBFQ 99.55 MHz
 OBSE1 5.13 KHz
 OBFIN 0.98 Hz
 POINT 32767
 FREQU 31250.00 Hz
 SCANS 536
 ACQTM 1.0486 sec
 PD 2.0000 sec
 PW1 3.42 usec
 IRNUC 13C
 CTEMP 19.2 c
 SLVNT CDCl3
 EXREF 77.00 ppm
 BF 0.50 Hz
 RGAIN 60



Dichloro-(2-phenyl-1,10-phenanthroline)palladium (6)

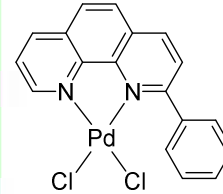
GH-1942-dmso-1H

C:\Documents and Settings\ALPHA\1\X\N\g\h\p\UozumiG\Hamasaki\GH-1942-dmso_proton-1-Lab



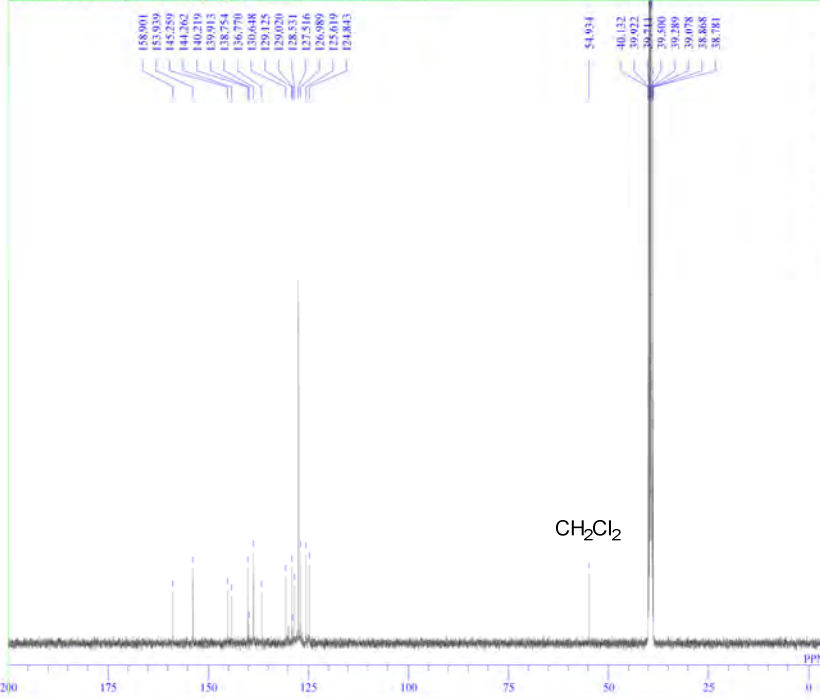
```

D1FILE GH-1942-dmso_proton-1-Lab
COMNT GH-1942-dmso-1H
DATIM 2014-12-25 18:55:05
OBNUC 1H
EXMOD proton 1xp
OBFREQ 395.88 MHz
OBSETE 6.28 KHz
OBFEN 0.87 Hz
POINT 13107
FREQU 5938.24 Hz
SCANS 8
ACQTM 2.2073 sec
PD 5.0000 sec
PWI 5.16 usec
IRNUC 1H
CTEMP 18.8 c
SLVNT DMSO
EXREF 2.49 ppm
BF 0.00 Hz
RGAIN 38
    
```



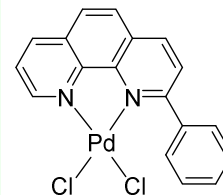
GH-1942-13C

C:\Documents and Settings\ALPHA\1\X\N\g\h\p\UozumiG\Hamasaki\GH-1942-13C-conc als



```

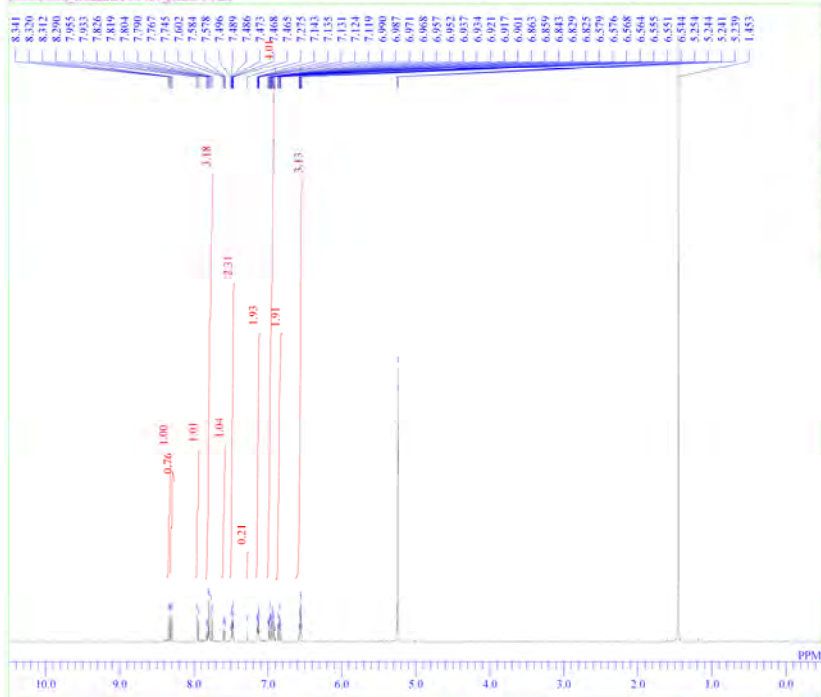
D1FILE GH-1942-13C-conc als
COMNT GH-1942-13C
DATIM 2014-12-26 15:41:23
OBNUC 13C
EXMOD carbon 1xp
OBFREQ 99.55 MHz
OBSETE 5.13 KHz
OBFEN 0.98 Hz
POINT 26214
FREQU 25000.00 Hz
SCANS 7342
ACQTM 1.0486 sec
PD 2.0000 sec
PWI 3.42 usec
IRNUC 1H
CTEMP 19.1 c
SLVNT DMSO
EXREF 39.50 ppm
BF 0.50 Hz
RGAIN 60
    
```



Phenyl-[2-(9-phenyl-1,10-phenanthrolin-2-yl)phenyl]palladium (9)

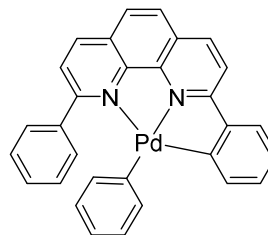
single_pulse

Z:\UOZUMI_Gisakura\F56-137_proton-1-1.als



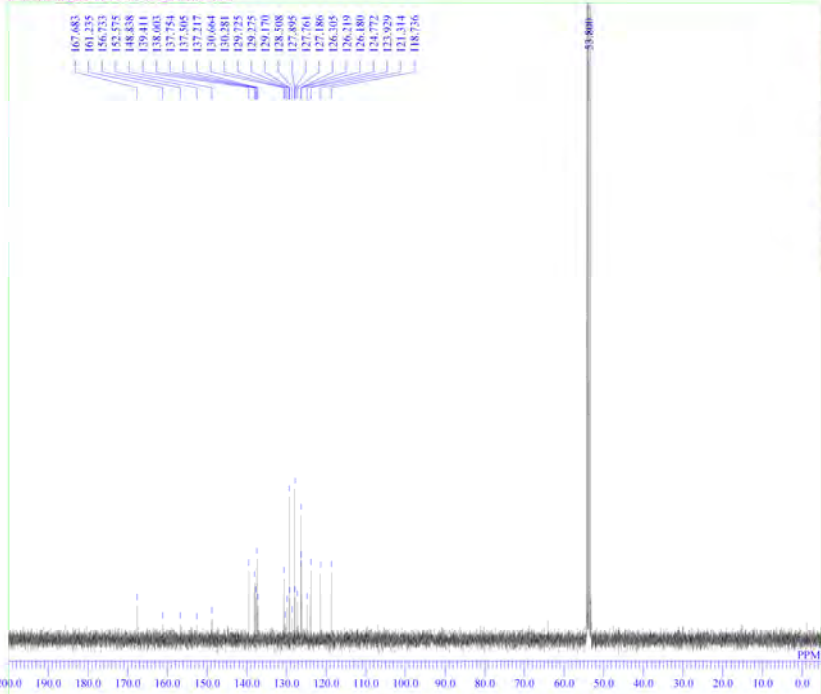
```

D:\FILE F56-137_proton-1-1.als
COMNT single_pulse
DATIM 2014-08-13 15:06:48
OBNUC 1H
EXMOD proton.jsp
OBFREQ 395.88 MHz
OBSETE 6.28 KHz
OBFIN 0.87 Hz
POINT 13107
FREQU 593.24 Hz
SCANS 16
ACQTM 2.2073 sec
PD 5.0000 sec
PWI 3.12 usec
IRNUC 1H
CTEMP 20.2 c
SLVNT CD2Cl2
EXREF 0.00 ppm
BF 0.50 Hz
RGAIN 50
    
```



single pulse decoupled gated NOE

Z:\UOZUMI_Gisakura\F56-137_carbon-2-1.als



```

D:\FILE F56-137_carbon-2-1.als
COMNT single pulse decoupled gated NOE
DATIM 2014-08-13 22:03:08
OBNUC 13C
EXMOD carbon.jsp
OBFREQ 99.55 MHz
OBSETE 5.13 KHz
OBFIN 0.98 Hz
POINT 26214
FREQU 25000.00 Hz
SCANS 12658
ACQTM 1.0486 sec
PD 2.0000 sec
PWI 3.42 usec
IRNUC 13C
CTEMP 19.4 c
SLVNT CD2Cl2
EXREF 53.80 ppm
BF 0.00 Hz
RGAIN 60
    
```

