Electronic Supplementary Material (ESI) for Chemical Communications

Aryl-Aryl Interaction as Directing Motif in the Stereodivergent Iron-catalyzed Hydrosilylation of Internal Alkynes

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1 General remarks

All the reactions and manipulations which are sensitive to air or moisture were performed under dry nitrogen using standard Schlenk techniques. All solvents were purified prior to use. All chemicals were purchased from Acros Organics, Sigma Aldrich or Alfa Aesar. The employed alkynes were synthesized according to a slightly modified literature known procedure.[1] The catalyst $FeH(CO)(NO)(PPh_3)_2$ (**1**) was prepared according to slightly improved previously published procedures from commercial iron pentacarbonyl in a one-pot procedure.[2] NMR spectra were recorded on a Bruker AV 300 spectrometer at 300 MHz (^{1}H-NMR), 75 MHz (^{13}C-NMR), a Bruker AV 500 spectrometer at 500 MHz (^{1}H-NMR), 125.6 MHz (^{13}C-NMR) or a Bruker AV 250 spectrometer at 250 MHz (^{1}H-NMR), 62.5 MHz (^{13}C-NMR). Chemical shifts were reported in ppm down field using tetramethylsilane as an internal standard. IR spectra were measured on a Bruker Vector 22 FT-IR spectrometer in an ATR mode. Mass spectra were measured using electrospray ionization on a Bruker Micro-TOF-Q. All microwave manipulations were carried out on a CEM Discovery 300 watt microwave.

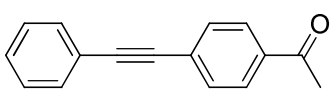
2 Preparation of starting materials

2.1 Preparation of alkynes

2.1.1 General procedure for the preparation of alkynes, GP-I[1]

The corresponding p-iodo or p-bromo benzene (1 equiv), $PdCl_2(PPh_3)_2$ (1 mol-%), CuI (4 mol-%) and phenylacetylene (1 equiv) were added to a 50 mL Schlenk flask with a stir bar under an atmosphere of nitrogen. To this was added tetrahydrofuran (1 M) and triethylamine (1 M). The reaction mixture was then stirred at room temperature over night. Thereafter 25 mL of water were added and the reaction mixture was extracted with 4×25 mL diethylether. The combined organic fractions were washed with brine and dried over Na_2SO_4. After filtration, the solvent was removed under reduced pressure. The crude product was purified by means of silica gel chromotagraphy using petroleum ether and ethylacetate as the eluent. The yields were not optimized for the synthesis of alkynes.

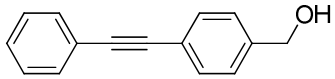
2.1.2 1-(4-(2-Phenylethynyl)phenyl)ethanone[3]



The product was obtained according to GP-I starting from p-iodo-acetophenone (2.46 g, 10.0 mmol) and phenylacetylene (1.1 mL, 10.0 mmol) after silica gel chromatography (10:1 petroleum ether / ethyl acetate) as a pale yellow solid (1.70 g, 7.7 mmol, 77%).

R_f = 0.3 (petroleum ether / ethyl acetate 10:1); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.98-7.91 (m, 2H), 7.64-7.59 (m, 2H), 7.58-7.52 (m, 2H), 7.40-7.34 (m, 3H), 2.62 (s, 3H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 197.3, 136.2, 131.8, 131.7, 128.8, 128.5, 128.3, 128.2, 122.6, 92.8, 88.7, 26.6 ppm; **IR** (film) 3338 (w), 3063 (w), 2998 (w), 2218 (w), 1676 (s), 1601 (m), 1403 (m), 1358 (m), 1261 (s), 1176 (m), 1070 (m), 957 (m), 832 (s), 758 (s), 690 (s), 640 (s) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 220 (52), 205 (100), 176 (48), 151 (16), 88 (5).

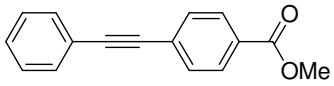
2.1.3 (4-(2-Phenylethynyl)phenyl)methanol[4]



The product was obtained according to GP-I starting from (4-iodophenyl)methanol (2.34 g, 10.0 mmol) and phenylacetylene (1.1 mL, 10.0 mmol) heated to 60 °C overnight after silica gel chromatography (3:1 petroleum ether / ethyl acetate) as a pale yellow solid (1.79 g, 8.6 mmol, 86%).

R_f = 0.4 (petroleum ether / ethyl acetate 3:1); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.58-7.48 (m, 4H), 7.40-7.30 (m, 5H), 4.70 (s, 2H), 1.8 (bs, 1H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 141.0, 131.8, 131.6, 128.4, 128.3, 126.9, 123.2, 122.5, 89.5, 89.2, 65.0 ppm; **IR** (film) 3341 (bm), 3049 (w), 2924 (w), 1596 (w), 1510 (m), 1487 (m), 1006 (s), 832 (s), 750 (s), 684 (s), 571 (m) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 208 (100), 191 (20), 178 (84), 165 (15), 151 (15), 102 (10), 77 (10), 63 (7), 51 (8).

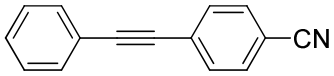
2.1.4 Methyl 4-(2-phenylethynyl)benzoate[5]



The product was obtained according to GP-I starting from methyl 4-iodobenzoate (2.62 g, 10.0 mmol) and phenylacetylene (1.1 mL, 10.0 mmol) after silica gel chromatography (10:1 petroleum ether / ethyl acetate) as a pale orange solid (1.94 g, 8.2 mmol, 82%).

R_f = 0.7 (petroleum ether / ethyl acetate 10:1); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 8.10-7.96 (m, 2H), 7.63-7.50 (m, 4H), 7.41-7.32 (m, 3H), 3.92 (s, 3H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 166.7, 131.7, 131.5, 129.5, 129.4, 128.8, 128.4, 128.0, 122.7, 92.4, 88.7, 52.4 ppm; **IR** (film) 2947 (w), 2849 (w), 2216 (w), 1709 (s), 1604 (m), 1436 (m), 1405 (w), 1309 (w), 1275 (s), 1174 (m), 1105 (s), 959 (m), 855 (m), 762 (s), 691 (s), 645 (m), 614 (m) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 236 (86), 205 (100), 176 (57), 151 (23), 126 (5), 102 (5), 88 (13), 75 (6), 51 (4).

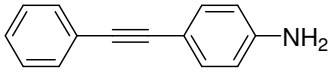
2.1.5 4-(2-Phenylethynyl)benzonitrile[6]



The product was obtained according to GP-I starting from 4-iodobenzonitrile (2.29 g, 10.0 mmol) and phenylacetylene (1.1 mL, 10.0 mmol) heated to 60 °C overnight after silica gel chromatography (10:1 petroleum ether / ethyl acetate) as a yellow solid (1.71 g, 8.4 mmol, 84%).

R_f = 0.50 (petroleum ether / ethyl acetate 10:1); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.72-7.49 (m, 6H), 7.42-7.33 (m, 3H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 132.1, 132.0, 131.8, 129.2, 128.5, 128.3, 122.3, 118.6, 111.5, 93.8, 87.8 ppm; **IR** (film) 3087 (w), 2226 (m), 2213 (m), 1602 (m), 1502 (m), 1442 (m), 1272 (w), 1175 (w), 1070 (w), 841 (s), 759 (s), 690 (s), 651 (m) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 203 (100), 176 (8), 151 (5), 98 (5), 74 (6), 63 (4), 51 (4).

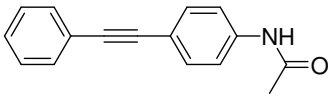
2.1.6 4-(2-Phenylethynyl)benzenamine[7]



The product was obtained according to GP-I starting from 4-iodobenzenamine (2.19 g, 10.0 mmol) and phenylacetylene (1.1 mL, 10.0 mmol) heated to 60 °C overnight after silica gel chromatography (4:1 petroleum ether / ethyl acetate) as a brown solid (1.45 g, 7.5 mmol, 75%).

R_f = 0.15 (petroleum ether / ethyl acetate 4:1); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.52-7.46 (m, 2H), 7.38-7.27 (m, 5H), 6.66-6.58 (m, 2H), 3.77 (bs, 2H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 146.7, 133.0, 131.4, 128.3, 127.7, 123.9, 114.8, 112.6, 90.2, 87.4 ppm; **IR** (film) 3475 (w), 3379 (m), 3036 (w), 2210 (m), 1614 (m), 1589 (m), 1513 (m), 1289 (m), 1177 (w), 1136 (w), 825 (s), 755 (s), 688 (s), 649 (s) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 193 (100), 165 (18), 139 (5), 89 (4), 63 (4).

2.1.7 N-(4-(2-phenylethynyl)phenyl)acetamide[8]

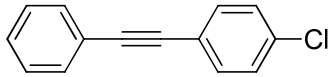


The product was obtained according to the following literature described procedure.[9] To a solution of 4-(2-phenylethynyl)benzenamine (773.0 mg, 4.0 mmol) and NEt_3 (1.1 mL, 8.0 mmol) in 25 mL dichloromethane at 0 °C was added dropwise a solution of acetyl chloride (428 µL, 6.0 mmol) in 10 mL dichloromethane. The reaction mixture was stirred overnight and allowed to warm to room temperature. The solvent was removed under reduced

pressure and the product was obtained after silica gel chromatography (3:1 petroleum ether / ethyl acetate) as a yellow solid (872.3 mg, 3.7 mmol, 93%).

R_f = 0.10 (petroleum ether / ethyl acetate 3:1); **^{1}H-NMR** (300 MHz, DMSO-d6) δ 10.10 (bs, 1H), 7.68-7.55 (m, 2H), 7.53-7.29 (m, 7H), 2.03 (s, 3H) ppm; **^{13}C-NMR** (125 MHz, DMSO-d6) δ 168.6, 139.8, 132.0, 131.2, 128.7, 128.5, 122.5, 118.8, 116.3, 89.5, 88.4, 24.1 ppm; **IR** (film) 3301 (m), 3183 (w), 3114 (w), 1664 (m), 1591 (s), 1526 (s), 1509 (s), 1369 (m), 1322 (s), 1257 (m), 1011 (m), 832 (s), 745 (s), 688 (s), 605 (m) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 235 (40), 207 (46), 193 (100), 165 (12).

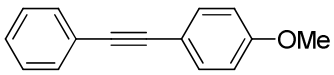
2.1.8 1-Chloro-4-(2-phenylethynyl)benzene[10]



The product was obtained according to GP-I starting from 1-chloro-4-iodobenzene (2.38 g, 10.0 mmol) and phenylacetylene (1.1 mL, 10.0 mmol) after silica gel chromatography (petroleum ether) as a white solid (1.85 g, 8.7 mmol, 87%).

R_f = 0.45 (petroleum); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.56-7.42 (m, 4H), 7.40-7.28 (m, 5H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 134.3, 132.8, 131.6, 128.7, 128.5, 128.4, 122.9, 121.8, 90.4, 88.3 ppm; **IR** (film) 3048 (w), 2215 (w), 1911 (w), 1586 (m), 1493 (s), 1480 (m), 1398 (m), 1088 (s), 1009 (m), 829 (s), 750 (s), 730 (m), 684 (s) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 212 (100), 176 (35), 151 (17), 106 (8), 88 (11), 75 (9), 51 (4).

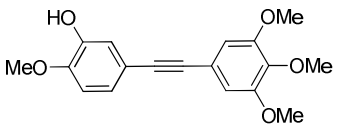
2.1.9 1-(2-(4-Methoxyphenyl)ethynyl)benzene[11]



The product was obtained according to GP-I starting from 1-iodo-4-methoxybenzene (2.34 g, 10.0 mmol) and phenylacetylene (1.1 mL, 10.0 mmol) after silica gel chromatography (10:1 petroleum ether / ethyl acetate) as a pale yellow solid (1.92 g, 9.2 mmol, 92%).

R_f = 0.5 (petroleum ether / ethyl acetate 10:1); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.57-7.46 (m, 4H), 7.40-7.28 (m, 3H), 6.93-6.86 (m, 2H), 3.83 (s, 3H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 159.7, 133.1, 131.5, 128.4, 128.0, 123.6, 115.4, 114.0, 89.4, 88.1, 55.3 ppm; **IR** (film) 3011 (w), 2838 (w), 2213 (w), 1604 (m), 1592 (m), 1507 (s), 1457 (m), 1439 (m), 1246 (s), 1173 (m), 1025 (s), 835 (s), 752 (s), 688 (s), 519 (m) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 208 (100), 193 (52), 165 (45), 139 (17), 115 (6), 88 (5), 63 (5).

2.1.10 2-Methoxy-5-(2-(3,4,5-trimethoxyphenyl)ethynyl)phenol (26)[12]



The product was obtained according to a literature described procedure[12] starting from 5-iodo-2-methoxyphenol (1.25 g, 5.0 mmol) and 3,4,5-Trimethoxyphenylethyne (0.96 g, 5.0 mmol) after silica gel chromatography (3:1 petroleum ether / ethyl acetate) as an pale orange oil (0.91 g, 2.9 mmol, 58%).

$\mathbf{R_f}$ = 0.20 (petroleum ether / ethyl acetate 3:1); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.09 (d, *J* = 2.0 Hz, 1H), 7.06 (dd, *J* = 8.3, 2.0 Hz, 1H), 6.82 (d, *J* = 8.3 Hz, 1H), 6.75 (s, 2H), 5.62 (s, 1H), 3.92 (s, 3H), 3.88 (s, 6H), 3.87 (s, 3H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 153.1, 147.0, 145.3, 138.6, 124.2, 118.5, 117.5, 116.0, 110.5, 108.7, 88.4, 87.9, 61.0, 56.1, 55.9 ppm; **IR** (film) 3421 (w), 2939 (w), 2252 (w), 1576 (m), 1510 (m), 1356 (m), 1247 (m), 1128 (m), 903 (s), 725 (s), 649 (m) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 314 (100), 299 (63), 271 (16), 241 (16), 157 (22), 142 (15), 99 (16), 69 (11).

2.2 Preparation $FeH(CO)(NO)(PPh_3)_2$ (1)[2,3]

In a 500 mL two necked flask $NaNO_2$ (2.6 g, 37.7 mmol) and NaOMe (4.7 g, 87.0) were suspended in 200 mL methanol. $Fe(CO)_5$ (5.03 mL, 37.2 mmol) was added and the reaction mixture refluxed for 3 hours. The solvent was removed under reduced pressure at room temperature while the mixture was protected from direct light. The remaining solid was dissolved in 500 mL of non-dried diethylether and filtered. (1st)

In a 1000 mL three necked flask the diethylether solution obtained in (1st) was placed and PPh_3 (39.0 g, 148.8 mmol) was added. After cooling to 0 °C TFA (4.3 mL, 55.8 mmol) was added dropwise and the reaction mixture stirred for 2 hours at room temperature. The orange precipitate was filtered over a syntered funnel under nitrogen, washed with 50 mL diethylether and dried while the filtrate was discarded. Subsequently the precipitate was washed with non-dried xylene until the filtrate remained colourless, the filtrate was then concentrated under reduced pressure and dried. Finally the orange solid is washed with 125 mL petroleum ether/ethyl acetate 40:1 and dried in vacuo to yield $FeH(CO)(NO)(PPh_3)_2$ (**1**) (6.66 g, 10.4 mmol, 28%) as an orange solid.

Crystals of $FeH(CO)(NO)(PPh_3)_2$ (**1**) were obtained by solubilizing the orange solid in xylene, addition of half the volume of pentane and slow evaporation of the solvents under nitrogen at room temperature affording dark orange crystals.

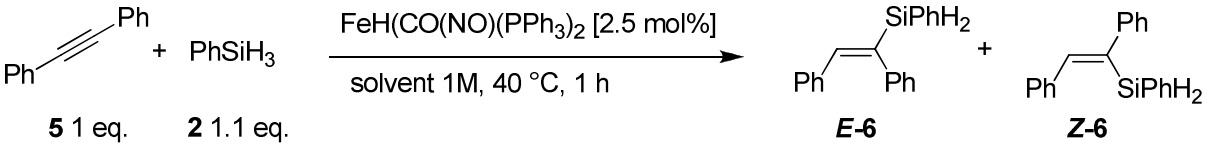
^{1}H-NMR (300 MHz, C_6D_6) δ 7.84-7.66 (m, 12H), 7.08-6.93 (m, 18H), -4.61 (t, *J* = 78.1 Hz, 1H) ppm; **^{13}C-NMR** (125 MHz, THF-d8) δ 221.3 (t, *J* = 21.7 Hz), 138.0 (t, *J* = 23.8 Hz), 133.1 (t, *J* = 5.8 Hz), 129.5, 128.1, 127.9 (t, *J* = 5.1 Hz); **^{31}P-NMR** (125 MHz, THF-d8) δ 91.3 (d, *J* = 77.4 Hz); **IR** (film) 1894 (s), 1682 (s), 1432 (m), 1090 (m), 743 (m), 690 (s); **MS** (EI, 70 eV):

m/z (%) 662 (1; M+Na), 608 (4), 580 (28), 318 (21), 262 (100), 183 (49), 108 (15); **HRMS** (EI$^+$HR): calcl. for $C_{37}H_{31}FeNO_2P_2$+Na: calcl. 662.1072, found: 662.1061.

3 Iron-catalyzed hydrosilylation

3.1 Optimization of the iron catalyzed hydrosilylation

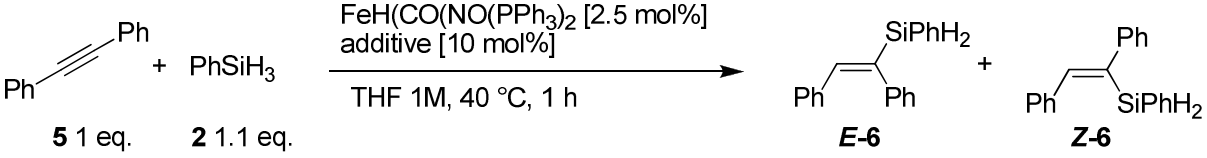
3.1.1 Solvent screening



5 1 eq. **2** 1.1 eq. ***E*-6** ***Z*-6**

Solvent	GC-yield [%]
EtOAc	xxx
DMF	17
DMA	27
Toluene	xxx
DCM	xxx
Acetonitrile	49
MTBE	xxx
1,4-Dioxane	xxx
DME	<10
Diethylether	xxx
THF	52

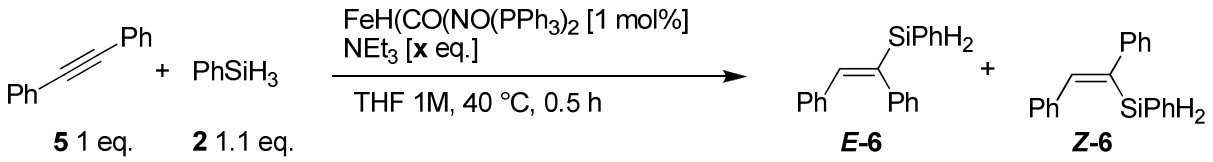
3.1.2 Additive screening



5 1 eq. **2** 1.1 eq. ***E*-6** ***Z*-6**

Additive	GC-yield [%]
DMAP	70
CuI	xxx
Me_3NO	<10
NEt_3	100
N-methyl-morpholine	78
Pyridine	100
Piperidine	39

3.1.3 Amount of additive screening



5 1 eq. **2** 1.1 eq. ***E*-6** ***Z*-6**

Amount of NEt_3	GC-yield [%]
NEt_3 [0.25 eq.]	44
NEt_3 [0.5 eq.]	81
NEt_3 [0.75 eq.]	62
NEt_3 [5 eq.]	65
NEt_3 as solvent	38

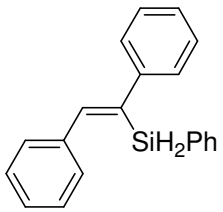
3.2 General Procedure for the Iron-catalyzed hydrosilylation (GP-II):

A 10 mL-Schlenk tube was charged with alkyne (if solid) (1.0 mmol), $FeH(CO)(NO)(PPh_3)_2$ (**1**) (0.01-0.05 mmol) and THF (1 mL). Subsequently alkyne (if liquid) (1.0 mmol), triethylamine (0.5 mmol, 138.8 µL) and the silane (1.1-2.1 mmol) were added and the reaction mixture was stirred for 12 hours at 40-60 °C. Unpolar products were isolated by filtration over a silica plug using pentane. All other products were purified by column chromatography on silica gel.

3.2.1 Hydrosilylation of diphenylacetylene (5) with phenylsilane (2)

The product was obtained according to GP-II starting from diphenylacetylene (**5**) (178.2 mg, 1.0 mmol) and phenylsilane (**2**) (135.6 µL, 1.1 mmol) using 1 mol% $FeH(CO)(NO)(PPh_3)_2$ (**1**) (6.4 mg, 0.01 mmol) at 40 °C as a mixture of isomers 20:1. The isomers were isolated by filtration over a silica plug (petroleum ether) as a colorless oil (280.7 mg, 0.98 mmol, 98%).

major isomer: phenyl((Z)-1,2-diphenylvinyl)silane (*Z*-6)

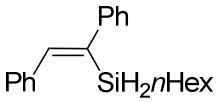


R_f = 0.3 (petroleum ether); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.61 (s, 1H), 7.54-7.48 (m, 2H), 7.43-7.19 (m, 13H), 4.81 (s, 2H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 147.7, 145.5, 138.7, 137.5, 135.5, 131.7, 129.7, 128.9, 128.5, 128.1, 128.0, 127.9, 127.5, 126.8 ppm; **IR** (film) 3053 (w), 3020 (w), 2143 (m), 1588 (w), 1490 (w), 1112 (w), 953 (w), 938 (w), 835 (w), 694 (w) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 286 (100) [M^{+}], 208 (58), 182 (73), 165 (11), 130 (28), 105 (23), 77(3), 53 (4); **HRMS** (EI^{+}HR): calcl. for $C_{20}H_{18}Si$: 286.1178, found: 286.1182.

3.2.2 Hydrosilylation of diphenylacetylene (5) with *n*-hexylsilane

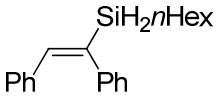
The product was obtained according to GP-II starting from diphenylacetylene (**5**) (178.2 mg, 1.0 mmol) and *n*-hexylsilane (161.7 µL, 1.1 mmol) using 1 mol% $FeH(CO)(NO)(PPh_3)_2$ (**1**) (6.4 mg, 0.01 mmol) at 40 °C as a mixture of isomers 5:1. The isomers were isolated by filtration over a silica plug (petroleum ether) as a colorless oil (276.8 mg, 0.94 mmol, 94%) and separated by semipreparative HPLC.

Major isomer: hexyl((Z)-1,2-diphenylvinyl)silane (*Z*-7)



$\mathbf{R_f}$ = 0.75 (petroleum ether); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.44-7.25 (m, 11H), 4.22 (t, *J* = 3.9 Hz, 2H), 1.28-1.07 (m, 8H), 0.83 (t, *J* = 6.8 Hz, 3H), 0.70-0.60 (m, 2H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 146.3, 145.9, 139.4, 139.0, 128.8, 128.4, 128.0, 127.6, 127.3, 126.5, 32.3, 31.4, 25.2, 22.5, 14.1, 9.8 ppm; **IR** (film) 2955 (w), 2922 (m), 2853 (w), 2135 (m), 1595 (w), 1490 (w), 1443 (w), 955 (m), 937 (m), 834 (s), 763 (s), 694 (s) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 294 (100), 210 (82), 180 (39), 165 (16), 132 (87), 105 (47), 97 (7), 84 (14), 77 (7), 43 (5); **HRMS** (EI^+HR): calcl. for $C_{20}H_{26}Si$: 294.1804, found: 294.1811.

Minor isomer: hexyl((E)-1,2-diphenylvinyl)silane (*E*-7)



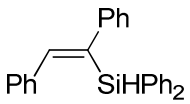
Could not be separated from hexyl((Z)-1,2-diphenylvinyl)silane (***Z*-7**)

$\mathbf{R_f}$ = 0.75 (petroleum ether); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 4.18 (t, *J* = 3.6 Hz, 2H) ppm;**^{13}C-NMR** (125 MHz, $CDCl_3$) δ 142.0, 140.8, 139.8, 137.0, 129.5, 128.8, 128.0, 127.6, 127.4, 126.2, 32.4, 31.5, 24.9, 22.5, 14.1, 9.3 ppm; **IR** (film) 3023 (w), 2956 (w), 2923 (w), 2853 (w), 2133 (m), 1491 (w), 957 (m), 937 (m), 835 (s), 764 (m), 696 (s) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 294 (100), 210 (79), 178 (23), 132 (80), 105 (30), 97 (5), 84 (14); **HRMS** (EI^+HR): calcl. for $C_{20}H_{26}Si$: 294.1804, found: 294.1813.

3.2.3 Hydrosilylation of diphenylacetylene (5) with diphenylsilane

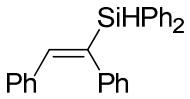
The product was obtained according to GP-II starting from diphenylacetylene (**5**) (178.2 mg, 1.0 mmol) and diphenylsilane (185.6 µL, 1.1 mmol) using 2.5 mol% $FeH(CO)(NO)(PPh_3)_2$ (**1**) (16.0 mg, 0.025 mmol) at 60 °C as a mixture of isomers 2:1. The isomers were isolated by filtration over a silica plug (petroleum ether) as a colorless oil (333.5 mg, 0.92 mmol, 92%) and separated by semipreparative HPLC.

Major isomer: diphenyl((Z)-1,2-diphenylvinyl)silane (*Z*-8)



R_f = 0.75 (petroleum ether / ethyl acetate 10:1); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.63 (s, 1H), 7.51-7.45 (m, 4H), 7.39-7.27 (m, 8H), 7.25-7.20 (m, 3H), 7.19-7.12 (m, 5H), 5.32 (s, 1H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 148.4, 145.3, 139.4, 138.3, 135.9, 133.5, 129.6, 129.0, 128.0, 127.9, 127.6, 126.3 ppm; **IR** (film) 3052 (w), 3021 (w), 2148 (m), 1587 (w), 1489 (w), 1428 (m), 1114 (m), 789 (m), 731 (m), 696 (s), 557 (w) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 362 (100), 284 (90), 259 (22), 207 (27), 181 (65), 155 (5), 105 (24); **HRMS** (EI^+HR): calcl. for $C_{26}H_{22}Si$: 362.1491, found: 362.1489.

Minor isomer: diphenyl((E)-1,2-diphenylvinyl)silane (*E*-8)[13]

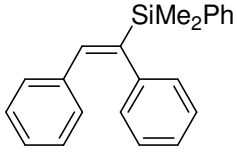


R_f = 0.75 (petroleum ether / ethyl acetate 10:1); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.61-7.53 (m, 4H), 7.45-7.31 (m, 6H), 7.23-7.06 (m, 6H), 7.04-6.96 (m, 5H), 5.28 (s, 1H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 142.9, 141.6, 140.2, 136.9, 135.9, 133.0, 129.8, 129.7, 128.6, 128.2, 128.0, 127.9, 127.5, 126.2 ppm; **IR** (film) 3055 (w), 3016 (w), 2122 (m), 1597 (w), 1487 (m), 1427 (m), 1117 (m), 1106 (m), 955 (m), 920 (w), 791 (s), 730 (s), 690 (s), 593 (s) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 362 (32) [M^+], 284 (57), 259 (19), 207 (33), 181 (100), 105 (63), 79 (9), 53 (10).

3.2.4 Hydrosilylation of diphenylacetylene (5) with dimethylphenylsilane

The product was obtained according to GP-II starting from diphenylacetylene (**5**) (178.2 mg, 1.0 mmol) and dimethylphenylsilane (153.3 µL, 1.1 mmol) using 2.5 mol% $FeH(CO)(NO)(PPh_3)_2$ (**1**) (16.0 mg, 0.025 mmol) at 60 °C as a mixture of isomers 20:1. The isomers were isolated by filtration over a silica plug (petroleum ether) as a colorless oil (305.1 mg, 0.97 mmol, 97%).

Major isomer: dimethyl(phenyl)((E)-1,2-diphenylvinyl)silane (*E*-10)[14]



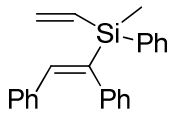
R_f = 0.4 (petroleum ether); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.58-7.51 (m, 2H), 7.39-7.31 (m, 3H), 7.27-7.16 (m, 3H), 7.10-7.04 (m, 3H), 6.97-6.86 (m, 4H), 6.82 (s, 1H), 0.39 (s, 6H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 144.0, 141.3, 138.1, 136.7, 136.2, 133.3, 128.5, 128.1, 127.5, 126.9, 126.7, 126.6, 126.1, 124.7, -4.1 ppm; **IR** (film) 3052 (w), 3021 (w), 2956 (w), 1597 (w),

1489 (m), 1247 (m), 1111 (m), 952 (m), 821 (s), 774 (s), 730 (s), 692 (s), 652 (m) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 314 (100), 299 (49), 271 (12), 236 (17), 221 (60), 197 (26), 178 (22), 135 (97), 121 (17), 105 (12), 43 (7); **HRMS** (EI^+HR): calcl. for $C_{22}H_{22}Si$: 314.1491, found: 314.1486.

3.2.5 Hydrosilylation of diphenylacetylene (5) with methylphenylvinylsilane (3)

The product was obtained according to GP-II starting from diphenylacetylene (**5**) (178.2 mg, 1.0 mmol) and methylphenylvinylsilane (166.6 µL, 1.1 mmol) using 2.5 mol% $FeH(CO)(NO)(PPh_3)_2$ (**1**) (16.0 mg, 0.025 mmol) at 60 °C as a mixture of isomers 20:1. The isomers were isolated by filtration over a silica plug (petroleum ether) as a colorless oil (316.7 mg, 0.97 mmol, 97%).

Major isomer: methyl(phenyl)((E)-1,2-diphenylvinyl)(vinyl)silane (*E*-11)

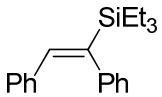


R_f = 0.20 (petroleum ether); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.62-7.53 (m, 2H), 7.42-7.31 (m, 3H), 7.25-7.12 (m, 3H), 7.11-7.04 (m, 3H), 6.99-6.90 (m, 4H), 6.88 (s, 1H), 6.38 (dd, *J* = 20.0, 14.7 Hz, 1H), 6.16 (dd, *J* = 14.7, 3.8 Hz, 1H), 5.78 (dd, *J* = 20.0, 3.8 Hz, 1H), 0.42 (s, 3H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 143.1, 142.1, 140.7, 137.2, 136.0, 135.5, 134.9, 129.6, 129.3, 128.5, 127.9, 127.8, 127.8, 127.3, 125.8, -4.9 ppm; **IR** (film) 3050 (w), 3020 (w), 2962 (w), 1489 (m), 1427 (m), 1250 (m), 1109 (m), 952 (s), 784 (s), 728 (s), 692 (s) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 326 (100), 311 (18), 248 (35), 233 (25), 222 (16), 207 (21), 197 (30), 178 (13), 147 (59), 121 (70), 105 (12), 43 (5); **HRMS** (EI^+HR): calcl. for $C_{23}H_{22}Si$: 326.1491, found: 326.1493.

3.2.6 Hydrosilylation of diphenylacetylene (5) with triethylsilane

The product was obtained according to GP-II starting from diphenylacetylene (**5**) (178.2 mg, 1.0 mmol) and triethylsilane (159.7 µL, 1.1 mmol) using 5 mol% $FeH(CO)(NO)(PPh_3)_2$ (**1**) (32.0 mg, 0.05 mmol) at 60 °C as a mixture of isomers 4:1. The isomers were isolated by filtration over a silica plug (petroleum ether) as a colorless oil (265.1 mg, 0.90 mmol, 90%) and separated by semipreparative HPLC.

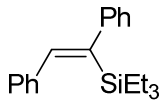
Major isomer: triethyl((E)-1,2-diphenylvinyl)silane (*E*-12)[15]



R_f = 0.4 (petroleum ether); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.33-7.15 (m, 3H), 7.13-7.05 (m, 3H), 7.02-6.91 (m, 4H), 6.77 (s, 1H), 0.95 (t, *J* = 7.9 Hz, 9H), 0.64 (q, *J* = 15.5, 7.9 Hz, 6H)

ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 144.1, 143.2, 138.8, 137.4, 129.5, 128.6, 127.9, 127.3, 127.0, 125.5, 7.3, 2.8 ppm; **IR** (film) 2951 (m), 2908 (w), 2873 (m), 1598 (w), 1490 (w), 1236 (w), 1004 (m), 964 (w), 946 (w), 765 (m), 717 (s), 690 (s) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 294 (25), 265 (100), 237 (32), 207 (25), 178 (17), 163 (16), 135 (32), 107 (33), 87 (23), 59 (53).

Minor isomer: triethyl((Z)-1,2-diphenylvinyl)silane (*Z*-12)[16]

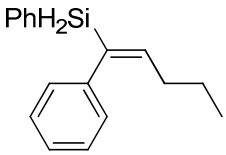


Could not be isolated. Comparison of raw ^{1}H-spectra with literature[15] indicated the mixture to be 4:1. **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 0.80 (t, *J* = 7.9 Hz, 9H), 0.40 (q, *J* = 7.9 Hz, 6H) ppm.

3.2.7 Hydrosilylation of 1-phenyl-1-pentyne with phenylsilane (2)

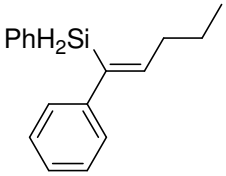
The product was obtained according to GP-II starting from 1-phenyl-1-pentyne (158.5 µL, 1.0 mmol) and phenylsilane (**2**) (135.6 µL, 1.1 mmol) using 1 mol% $FeH(CO)(NO)(PPh_3)_2$ (**1**) (6.4 mg, 0.01 mmol) at 40 °C as a mixture of isomers 4:1. The isomers were isolated by filtration over a silica plug (petroleum ether) as a colorless oil (224.7 mg, 0.89 mmol, 89%) and separated by semipreparative HPLC.

Major isomer: phenyl((E)-1-phenylpent-1-enyl)silane (*regio-E* 13)



R_f = 0.60 (petroleum ether); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.55-7.47 (m, 2H), 7.42-7.26 (m, 5H), 7.21-7.13 (1H), 7.07-6.98 (m, 2H), 6.25 (t, *J* = 7.2 Hz, 1H), 4.67 (s, 2H), 2.07 (q, *J* = 7.2 Hz, 2H), 1.47-1.32 (m, 2H), 0.85 (t, *J* = 7.2 Hz, 3H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 147.4, 141.2, 136.3, 135.6, 132.0, 129.6, 128.2, 128.1, 127.9, 125.9, 32.3, 22.6, 13.8 ppm; **IR** (film) 2958 (w), 2926 (w), 2134 (m), 1115 (w), 947 (m), 930 (m), 844 (s), 698 (s) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 252 (100) [$M^{+\cdot}$], 209 (37), 196 (25), 183 (56), 174 (24), 145 (51), 132 (44), 105 (54), 91 (14), 81 (5), 53 (7); **HRMS** (EI^+HR): calcl. for $C_{17}H_{20}Si$: 252.1334, found: 252.1341.

Minor isomer: phenyl((Z)-1-phenylpent-1-enyl)silane (*regio-Z* 13)



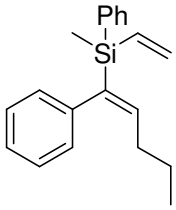
R_f = 0.60 (petroleum ether); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.60-7.53 (m, 2H), 7.41-7.26 (m, 5H), 7.25-7.15 (m, 3H), 6.56 (t, *J* = 7.5 Hz, 1H), 4.83 (s, 2H), 2.34 (q, *J* = 7.4 Hz, 2H), 1.49-

1.38 (m, 2H), 0.92 (t, *J* = 7.4 Hz, 3H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 149.7, 145.2, 135.3, 134.3, 131.8, 129.6, 128.3, 128.1, 127.2, 126.2, 35.1, 22.8, 13.8; **IR** (film) 2958 (w), 2927 (w), 2133 (m), 1595 (w), 1428 (w), 1115 (m), 1071 (m), 947 (m), 931 (m), 840 (s), 697 (s) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 252 (100) [M^{+}], 209 (35), 196 (24), 183 (57), 174 (26), 145 (48), 132 (40), 105 (49), 91 (11), 81 (5), 53 (5); **HRMS** (EI^{+}HR): calcl. for $C_{17}H_{20}Si$: 252.1334, found: 252.1339.

3.2.8 Hydrosilylation of 1-phenyl-1-pentyne with methylphenylvinylsilane (3)

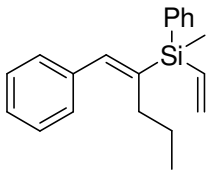
The product was obtained according to GP-II starting from 1-phenyl-1-pentyne (158.5 µL, 1.0 mmol) and methylphenylvinylsilane (**3**) (166.6 µL, 1.1 mmol) using 5 mol% $FeH(CO)(NO)(PPh_3)_2$ (**1**) (32.0 mg, 0.05 mmol) at 60 °C for 36 hours as a mixture of isomers 2:1. The isomers were isolated by filtration over a silica plug (petroleum ether) as a yellow oil (251.5 mg, 0.86 mmol, 86%) and separated by semipreparative HPLC.

Major isomer: methyl(phenyl)((E)-1-phenylpent-1-enyl)(vinyl)silan (*regio-E* 14)



R_f = 0.40 (petroleum ether); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.54-7.48 (m, 2H), 7.37-7.29 (m, 3H), 7.23-7.05 (m, 3H), 6.92-6.86 (m, 2H), 6.31 (dd, *J* = 19.7, 14.4 Hz, 1H), 6.13-6.07 (m, 1H), 6.06 (t, *J* = 7.1 Hz, 1H), 7.72 (dd, *J* = 19.7, 4.0 Hz, 1H), 1.97 (dt, *J* = 7.4, 7.2 Hz, 2H), 1.36 (tq, *J* = 14.4, 7.4, 7.2 Hz, 2H), 0.82 (t, *J* = 7.4 Hz, 3H), 0.35 (s, 3H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 145.3, 141.9, 140.8, 136.6, 136.1, 134.8, 134.3, 129.1, 128.3, 127.8, 127.7, 125.4, 32.2, 22.6, 13.8, -4.7 ppm; **IR** (film) 3050 (w), 2957 (m), 1593 (m), 1488 (m), 1428 (m), 1249 (m), 1110 (m), 945 (m), 786 (s), 700 (s), 632 (s) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 292 (63), 277 (21), 249 (20), 235 (30), 214 (22), 197 (17), 147 (100), 121 (90), 105 (15), 91 (4), 43 (6); **HRMS** (EI^{+}HR): calcl. for $C_{20}H_{24}Si$: 292.1647, found: 292.1647.

Minor isomer: methyl(phenyl)((E)-1-phenylpent-1-en-2-yl)(vinyl)silane (*E* 14)



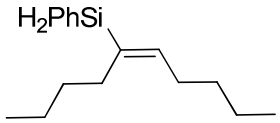
R_f = 0.40 (petroleum ether); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.61-7.55 (m, 2H), 7.40-7.27 (m, 7H), 7.25-7.18 (m, 1H), 6.83 (s, 1H), 6.43 (dd, *J* = 20.2, 14.5 Hz, 1H), 6.16 (dd, *J* = 14.5, 3.8 Hz, 1H), 5.80 (dd, *J* = 20.3, 3.8 Hz, 1H), 2.39-2.31 (m, 2H), 1.45-1.30 (m, 2H), 0.82 (t, *J* = 7.2

Hz, 3H), 0.53 (s, 3H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 141.8, 141.0, 138.3, 136.8, 136.3, 134.7, 134.3, 129.1, 128.7, 128.1, 127.8, 126.7, 33.2, 23.3, 14.5, -4.2 ppm; **IR** (film) 3050 (w), 2957 (m), 2870 (w), 1591 (w), 1427 (w), 1249 (m), 1109 (m), 1008 (m), 787 (s), 728 (s), 695 (s), 640 (w) cm^{-1}; **GC-MS** (EI, 70 eV): *m/z* (%) 292 (46), 277 (12), 249 (15), 214 (9), 147 (100), 121 (57), 105 (9), 43 (4); **HRMS** (EI$^+$HR): calcl. for $C_{20}H_{24}Si$: 292.1647, found: 292.1648.

3.2.9 Hydrosilylation of 5-decyne with phenylsilane (2)

The product was obtained according to GP-II starting from 5-decyne (179.8 µL, 1.0 mmol) and phenylsilane (**2**) (135.6 µL, 1.1 mmol) using 1 mol% $FeH(CO)(NO)(PPh_3)_2$ (**1**) (6.4 mg, 0.01 mmol) at 40 °C as a mixture of isomers 14:1. The isomers were isolated by filtration over a silica plug (petroleum ether) as a colorless oil (219.3 mg, 0.89 mmol, 89%).

Major isomer: ((E)-dec-5-en-5-yl)phenylsilane (*E*-15)

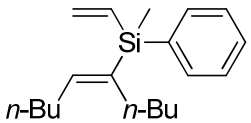


R_f = 0.90 (petroleum ether); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.59-7.54 (m, 2H), 7.41-7.31 (m, 3H), 6.00 (t, *J* = 6.9 Hz, 1H), 4.53 (s, 2H), 2.22-2.09 (m, 4H), 1.40-1-18 (m, 8H), 0.90 (t, *J* = 6.9 Hz, 3H), 0.84 (t, *J* = 6.9 Hz, 3H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 146.3, 135.6, 134.0, 132.8, 129.5, 128.0, 31.8, 30.1, 28.6, 22.7, 22.5, 14.0, 13.9 ppm; **IR** (film) 2955 (m), 2925 (m), 2857 (w), 2128 (m), 1428 (w), 1114 (m), 937 (m), 838 (s), 731 (m), 696 (s), 607 (m) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 246 (13), 203 (17), 189 (28), 175 (13), 168 (17), 161 (21), 147 (17), 133 (25), 107 (100), 98 (19), 83 (14), 55 (17); **HRMS** (EI$^+$HR): calcl. for $C_{16}H_{26}Si$: 246.1804, found: 246.1799.

3.2.10 Hydrosilylation of 5-decyne with methylphenylvinylsilane (3)

The product was obtained according to GP-II starting from 5-decyne (179.8 µL, 1.0 mmol) and methylphenylvinylsilane (**3**) (166.6 µL, 1.1 mmol) using 2.5 mol% $FeH(CO)(NO)(PPh_3)_2$ (**1**) (16.0 mg, 0.025 mmol) at 60 °C as a mixture of isomers 15:1. The isomers were isolated by filtration over a silica plug (petroleum ether) as a colorless oil (260.7 mg, 0.91 mmol, 91%).

Major isomer: ((E)-dec-5-en-5-yl)(methyl)(phenyl)(vinyl)silane (*E*-16)



R_f = 0.90 (petroleum ether); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.54-7.47 (m, 2H), 7.38-7.30 (m, 3H), 6.34 (dd, *J* = 20.0, 14.5 Hz, 1H), 6.09 (dd, *J* = 14.5, 3.7 Hz, 1H), 5.82 (t, *J* = 6.9 Hz, 1H),

5.72 (dd, *J* = 20.0, 3.7 Hz, 1H), 2.18-2.05 (m, 4H), 1.41-1.11 (m, 8H), 0.90 (t, *J* = 6.9 Hz, 3H), 0.81 (t, *J* = 6.9 Hz, 3H), 0.41 (s, 3H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 144.3, 137.4, 137.1, 136.8, 134.6, 133.7, 128.9, 127.6, 32.3, 31.8, 29.7, 28.5, 23.0, 22.5, 14.1, 13.9, -4.4 ppm; **IR** (film) 2956 (m), 2926 (m), 2858 (w), 1464 (w), 1249 (m), 1108 (m), 1007 (w), 953 (w), 785 (s), 724 (s), 697 (s) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 286 (30), 271 (39), 215 (19), 147 (100), 121 (95), 107 (19), 71 (7), 43 (8); **HRMS** (EI$^+$HR): calcl. for $C_{19}H_{30}Si$: 286.2117, found: 286.2115.

4 Hydrosilylation-Desilylation-Sequences (HS-DS-sequences)

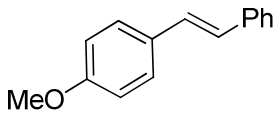
4.1 Desilylation using TBAF solution (GP-III)

After the required reaction time the reaction mixture of GP-II was transferred to a 25 mL two necked flask under nitrogen without further purification. Another 7.5 mL of THF were added and the reaction mixture cooled to 0 °C. At this point 1.5 mL TBAF-solution (1M in THF) was added and the reaction mixture stirred for 2 hours at 0 °C. Unpolar products were isolated by filtration over a plug of silica using pentane as the eluent. All other products were filtrated over a plug of silica using ethylacetate and after evaporation of the solvent purified by column chromatography on silica gel.

4.1.1 *E*-selective HS-DS-sequence starting from 1-(2-(4-methoxyphenyl)ethynyl) benzene

The product was obtained according to GP-III starting from 1-(2-(4-methoxyphenyl)ethynyl)benzene (208.3 mg, 1.0 mmol) and phenylsilane (**2**) (135.6 µL, 1.1 mmol) using 1 mol% $FeH(CO)(NO)(PPh_3)_2$ (**1**) (6.4 mg, 0.01 mmol) at 40 °C as a mixture of isomers 17:1 after silica gel chromatography (petroleum ether/ethyl acetate 10:1) as a white solid (201.9 mg, 0.96 mmol, 96%).

Major isomer: 1-(4-methoxystyryl)benzene (*E*-17)[17]

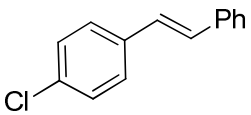


R_f = 0.75 (petroleum ether / ethyl acetate 10:1); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.52-7.42 (m, 4H), 7.38-7.30 (m, 2H), 7.25-7.18 (m, 1H), 7.07 (d, *J* = 16.7 Hz, 1H), 6.97 (d, *J* = 16.7 Hz, 1H), 6.90 (d, *J* = 8.9 Hz, 2H), 3.83 (s, 3H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 159.3, 137.7, 130.2, 128.7, 128.2, 127.7, 127.2, 126.6, 126.3, 114.1, 55.4 ppm; **IR** (film) 3019 (w), 2931 (w), 2837 (w), 1661 (m), 1489 (m), 1449 (m), 1248 (m), 1175 (m), 1087 (m), 1032 (m), 1000 (m), 963 (s), 862 (m), 815 (s), 749 (s), 688 (s) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 210 (100), 195 (17), 178 (35), 165 (49), 152 (32), 139 (7), 115 (9), 89 (11), 76 (9), 63 (10), 51 (9).

4.1.2 *E*-selective HS-DS-sequence starting from 1-(2-(4-chlorophenyl)ethynyl)benzene

The product was obtained according to GP-III starting from 1-(2-(4-chlorophenyl)ethynyl)benzene (212.7 mg, 1.0 mmol) and phenylsilane (**2**) (135.6 µL, 1.1 mmol) using 1 mol% $FeH(CO)(NO)(PPh_3)_2$ (**1**) (6.4 mg, 0.01 mmol) at 40 °C as a mixture of isomers 7:1 after silica gel chromatography (petroleum ether) as a white solid (199.7 mg, 0.93 mmol, 93%).

Major isomer: 1-(4-chlorostyryl)benzene (*E*-18)[18]

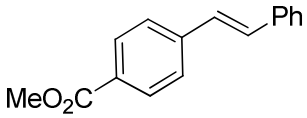


R_f = 0.50 (petroleum ether); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.54-7.48 (m, 2H), 7.46-7.41 (m, 2H), 7.39-7.24 (m, 5H), 7.06 (d, *J* = 1.6 Hz, 2H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 137.0, 135.9, 133.2, 129.3, 128.9, 128.8, 127.9, 127.7, 127.4, 126.6 ppm; **IR** (film) 3021 (w), 1587 (m), 1488 (m), 1448 (m), 1114 (m), 1085 (s), 1009 (m), 966 (s), 816 (s), 751 (s), 705 (s), 688 (s), 617 (m), 525 (s) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 214 (69), 178 (100), 152 (13), 102 (6), 89 (15), 76 (17), 63 (10), 51 (12).

4.1.3 *E*-selective HS-DS-sequence starting from 4-(2-phenylethynyl)benzoate xx

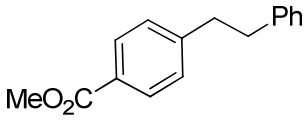
The product was obtained according to GP-III starting from methyl 4-(2-phenylethynyl)benzoate (236.3 mg, 1.0 mmol) and phenylsilane (**2**) (135.6 µL, 1.1 mmol) using 1 mol% $FeH(CO)(NO)(PPh_3)_2$ (**1**) (6.4 mg, 0.01 mmol) at 40 °C as a mixture of isomers 1:1 after silica gel chromatography (petroleum ether/ethyl acetate 10:1) as a white solid (119.1 mg, 0.50 mmol, 50%).

Major isomer: methyl 4-styrylbenzoate (*E*-19)[19]



R_f = 0.40 (petroleum ether / ethyl acetate 10:1); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 8.05-8.00 (m, 2H), 7.59-7.50 (m, 4H), 7.42-7.27 (m, 3H), 7.22 (d, *J* = 16.5 Hz, 1H), 7.12 (d, *J* = 16.5 Hz, 1H), 3.92 (s, 3H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 166.9, 141.8, 136.8, 131.2, 130.0, 128.9, 128.8, 128.3, 127.6, 126.8, 126.3, 52.1 ppm; **IR** (film) 3024 (w), 3001 (w), 2945 (w), 1708 (s), 1602 (w), 1434 (m), 1412 (m), 1277 (s), 1179 (m), 1105 (s), 963 (s), 835 (m), 771 (s), 698 (s), 670 (m), 579 (m) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 238 (88), 207 (55), 178 (100), 152 (18), 103 (15), 89 (37), 76 (23), 51 (8).

Byproduct methyl 4-phenethylbenzoate (alk-19):[20]



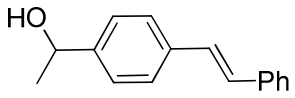
An additional 10 % of (**alk-19**) (26.4 mg, 0.1 mmol, 11%)

R_f = 0.40 (petroleum ether / ethyl acetate 10:1); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.4 Hz, 2H), 7.31-7.12 (m, 7H), 3.90 (s, 3H), 3.02-2.88 (m, 4H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 167.1, 147.2, 141.2, 129.7, 128.5, 128.4, 128.3, 127.9, 126.1, 52.1, 37.9, 37.5 ppm; **IR** (film) 3027 (w), 2948 (w), 2859 (w), 1716 (s), 1609 (m), 1434 (m), 1275 (s), 1178 (m), 1108 (m), 1020 (w), 841 (m), 767 (m), 745 (m), 699 (s), 632 (s), 528 (m) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 240 (21), 209 (5), 149 (19), 121 (11), 91 (100), 65 (11), 51 (4).

4.1.4 *E*-selective HS-DS-sequence starting from 1-(4-(2-phenylethynyl)phenyl)ethanol

The product was obtained according to GP-III starting from 1-(4-(2-phenylethynyl)phenyl)ethanol (222.3 mg, 1.0 mmol) and phenylsilane (**2**) (258.9 µL, 2.1 mmol) using 1 mol% $FeH(CO)(NO)(PPh_3)_2$ (**1**) (6.4 mg, 0.01 mmol) at 40 °C as a mixture of isomers 3:1 after silica gel chromatography (petroleum ether/ethyl acetate 3:1) as a white solid (56.1 mg, 0.25 mmol, 25%).

Major isomer: 1-(4-styrylphenyl)ethanol (*E*-20)[21]

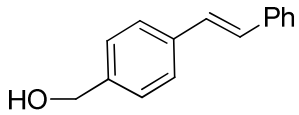


R_f = 0.3 (petroleum ether / ethyl acetate 3:1); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.55-7.48 (m, 4H), 7.41-7.27 (m, 5H), 7.16-7.08 (m, 2H), 4.92 (q, *J* = 6.4 Hz, 1H), 1.77 (bs, 1H), 1.52 (d, *J* = 6.4 Hz, 3H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 145.3, 137.3, 136.7, 128.7, 128.6, 128.3, 127.6, 126.7, 126.5, 125.8, 70.3, 25.2 ppm; **IR** (film) 3299 (bm), 3026 (w), 2972 (w), 2925 (w), 1447 (m), 1407 (m), 1177 (w), 1071 (s), 1018 (m), 962 (s), 895 (m), 817 (s), 750 (m), 687 (s), 550 (s) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 224 (75), 207 (100), 178 (96), 165 (43), 152 (24), 115 (12), 103 (45), 89 (12), 77 (35), 63 (12), 51 (15).

4.1.5 *E*-selective HS-DS-sequence starting from (4-(2-phenylethynyl)phenyl)methanol

The product was obtained according to GP-III starting from (4-(2-phenylethynyl)phenyl)methanol (208.3 mg, 1.0 mmol) and phenylsilane (**2**) (258.9 µL, 2.1 mmol) using 1 mol% $FeH(CO)(NO)(PPh_3)_2$ (**1**) (6.4 mg, 0.01 mmol) at 40 °C as a mixture of isomers 9:1 after silica gel chromatography (petroleum ether/ethyl acetate 3:1) as a white solid (159.8 mg, 0.76 mmol, 76%).

Major isomer: (4-styrylphenyl)methanol (*E*-22)[22]

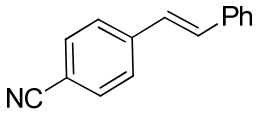


R_f = 0.25 (petroleum ether / ethyl acetate 3:1); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.56-7.48 (m, 4H), 7.41-7.32 (m, 4H), 7.29-7.23 (m, 1H), 7.11 (s, 2H), 1.65 (bs, 1H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 140.2, 137.3, 136.8, 128.8, 128.7, 128.2, 127.7, 127.4, 126.7, 126.5, 65.2 ppm; **IR** (film) 3285 (bm), 3022 (w), 2922 (w), 2867 (w), 14446 (m), 1418 (w), 1033 (m), 1012 (w), 970 (s), 956 (s), 812 (s), 687 (s) cm^{-1}; **GC-MS** (EI, 70 eV): *m/z* (%) 210 (100), 179 (80), 165 (28), 152 (15), 115 (15), 103 (23), 91 (10), 77 (26), 63 (7), 51 (9).

4.1.6 *E*-selective HS-DS-sequence starting from 4-(2-phenylethynyl)benzonitrile

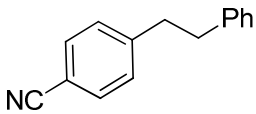
The product was obtained according to GP-III starting from 4-(2-phenylethynyl)benzonitrile (203.2 mg, 1.0 mmol) and phenylsilane (**2**) (135.6 µL, 1.1 mmol) using 1 mol% $FeH(CO)(NO)(PPh_3)_2$ (**1**) (6.4 mg, 0.01 mmol) at 40 °C as a mixture of isomers 3:1 after silica gel chromatography (petroleum ether/ethyl acetate 10:1) as a white solid (145.7 mg, 0.71 mmol, 71%).

Major isomer: 4-styrylbenzonitrile (*E*-23)[23]



R_f = 0.30 (petroleum ether / ethyl acetate 10:1); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.61-7.51 (m, 6H), 7.43-7.29 (m, 3H), 7.22 (d, *J* = 16.3 Hz, 1H), 7.09 (d, *J* = 16.3 Hz, 1H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 141.9, 136.3, 132.5, 132.4, 128.9, 128.7, 126.9, 126.8, 126.7, 119.1, 110.6 ppm; **IR** (film) 3024 (w), 2224 (m), 1600 (m), 1503 (m), 1412 (w), 1174 (w), 971 (m), 871 (w), 823 (s), 757 (s), 718 (s), 690 (s), 647 (s) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 205 (100), 190 (41), 176 (15), 165 (14), 151 (8), 102 (8), 89 (9), 76 (11), 63 (9), 51 (10).

Byproduct methyl 4-phenethylbenzonitrile (*alk*-23):[24]



An additional 10 % of (**alk-23**) (20.7 mg, 0.1 mmol, 10%)

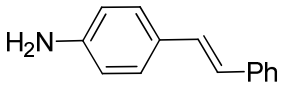
R_f = 0.30 (petroleum ether / ethyl acetate 10:1); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.58-7.52 (m, 2H), 7.32-7.17 (m, 5H), 7.15-7.09 (m, 2H), 3.03-2.88 (m, 4H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 147.3, 140.6, 132.1, 129.3, 128.4, 126.3, 119.1, 109.9, 37.9, 37.2 ppm; **IR** (film) 3023 (w), 2925 (w), 2860 (w), 2225 (s), 1600 (m), 1500 (w), 1490 (m), 1451 (w), 1176 (m),

1071 (m), 863 (m), 822 (s), 751 (s), 703 (s) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 207 (18), 91 (100), 65 (15).

4.1.7 *E*-selective HS-DS-sequence starting from 4-(2-phenylethynyl)benzenamine

The product was obtained according to GP-III starting from 4-(2-phenylethynyl)benzenamine (193.2 mg, 1.0 mmol) and phenylsilane (**2**) (258.9 µL, 2.1 mmol) using 1 mol% $FeH(CO)(NO)(PPh_3)_2$ (**1**) (6.4 mg, 0.01 mmol) at 40 °C as a mixture of isomers 20:1 after silica gel chromatography (petroleum ether/ethyl acetate 3:1) as a pale brown solid (179.6 mg, 0.92 mmol, 92%).

Major isomer: 4-styrylbenzenamine (*E*-24)[25]

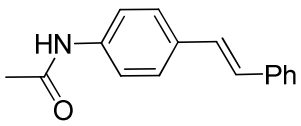


R_f = 0.25 (petroleum ether / ethyl acetate 3:1); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.50-7.44 (m, 2H), 7.37-7.29 (m, 4H), 7.24-7.17 (m, 1H), 7.03 (d, *J* = 16.3 Hz, 1H), 6.91 (d, *J* = 16.3 Hz, 1H), 6.71.6.65 (m, 2H), 3.74 (bs, 2H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 146.2, 137.9, 128.7, 128.6, 128.0, 127.8, 126.9, 126.1, 125.1, 115.2 ppm; **IR** (film) 3444 (w), 3358 (m), 3027 (w), 1613 (s), 1588 (s), 1513 (s), 1282 (m), 1268 (m), 1177 (m), 966 (s), 817 (s), 753 (m), 689 (s), 592 (m) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 195 (100), 180 (12), 165 (12), 152 (7), 117 (5), 89 (5), 77 (4), 63 (5), 51 (5).

4.1.8 *E*-selective HS-DS-sequence starting from N-(4-(2-phenylethynyl)phenyl) acetamide

The product was obtained according to GP-III starting from N-(4-(2-phenylethynyl)phenyl)acetamide (235.3 mg, 1.0 mmol) and phenylsilane (**2**) (258.9 µL, 2.1 mmol) using 1 mol% $FeH(CO)(NO)(PPh_3)_2$ (**1**) (6.4 mg, 0.01 mmol) at 40 °C as a mixture of isomers 14:1 after silica gel chromatography (petroleum ether/ethyl acetate 1:1) as a yellow solid (213.6 mg, 0.90 mmol, 90%).

Major isomer: N-(4-styrylphenyl)acetamide (*E*-25)[26]

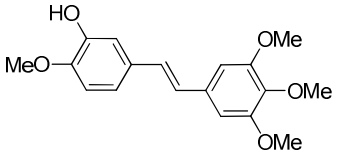


R_f = 0.20 (petroleum ether / ethyl acetate 1:1); **^{1}H-NMR** (300 MHz, DMSO-d6) δ 10.07 (s, 1H), 7.68-7.55 (m, 6H), 7.43-7.36 (m, 2H), 7.31-7.24 (m, 1H), 7.22-7.13 (m, 2H), 2.10 (s, 3H) ppm; **^{13}C-NMR** (125 MHz, DMSO-d6) δ 168.3, 138.9, 137.2, 131.8, 128.6, 128.0, 127.3, 126.9, 126.8, 126.2, 119.0, 24.0; **IR** (film) 3297 (m), 3180 (w), 3112 (w), 1661 (s), 1592 (s), 1511 (s), 1408 (m), 1320 (m), 968 (s), 823 (s), 756 (s), 715 (s), 691 (s) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 237 (77), 207 (32), 195 (100), 180 (13), 165 (25), 152 (14), 89 (6), 51 (5);

4.1.9 ***E*-selective HS-DS-sequence starting from 2-methoxy-5-(2-(3,4,5-trimethoxy phenyl)ethynyl)phenol (26)**

The product was obtained according to GP-III starting from 2-methoxy-5-(2-(3,4,5-trimethoxyphenyl)ethynyl)phenol (**26**) (157.2 mg, 0.5 mmol) and phenylsilane (**2**) (135.6 µL, 1.1 mmol) using 2.5 mol% $FeH(CO)(NO)(PPh_3)_2$ (**1**) (8.0 mg, 0.0125 mmol) at 60 °C as a mixture of isomers 3:1 after silica gel chromatography (petroleum ether/ethyl acetate 3:1) as an orange oil (112.3 mg, 0.36 mmol, 71%).

Major isomer: 5-(3,4,5-trimethoxystyryl)-2-methoxyphenol (*E*-27)[27]



R_f = 0.2 (petroleum ether / ethyl acetate 3:1); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.14 (d, *J* = 2.1 Hz, 1H), 6.97 (dd, *J* = 8.5, 2.1 Hz, 1H), 6.90 (d, *J* = 3.9 Hz, 2H), 6.84 (d, *J* = 8.5 Hz, 1H), 6.71 (s, 2H), 5.60 (bs, 1H), 3.92 (s, 9H), 3.86 (s, 3H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 153.5, 146.5, 145.9, 137.7, 133.3, 131.0, 127.8, 127.1, 119.2, 111.8, 110.7, 103.4, 61.0, 56.2, 56.0 ppm; **IR** (film) 3381 (bm), 2935 (m), 2836 (w), 1731 (w), 1685 (w), 1578 (s), 1505 (s), 1458 (s), 1417 (s), 1327 (s), 1119 (s), 1000 (m), 850 (m), 820 (m), 658 (s) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 316 (57), 301 (39), 207 (100), 115 (5), 105 (4), 77 (4).

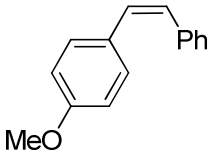
4.2 Desilylation using NaOH/MeOH (GP-IV)

After the required reaction time the reaction mixture of GP-II was transferred to a 10 mL microwave flask under nitrogen without further purification. After the addition of 1.5 mL THF, 1 mL MeOH and 1 mL 2 N NaOH the vial was transferred to the microwave and kept at 130 °C for 10 minutes. Unpolar products were isolated by filtration over a plug of silica using pentane as the eluent. All other products were filtrated over a plug of silica using ethylacetate and after evaporation of the solvent purified by column chromatography on silica gel.

4.2.1 ***Z*-selective HS-DS-sequence starting from 1-(2-(4-methoxyphenyl)ethynyl) benzene**

The product was obtained according to GP-IV starting from 1-(2-(4-methoxyphenyl)ethynyl)benzene (208.3 mg, 1.0 mmol) and methylphenylvinylsilane (**3**) (183.3 µL, 1.1 mmol) using 2.5 mol% $FeH(CO)(NO)(PPh_3)_2$ (**1**) (16.0 mg, 0.025 mmol) at 60 °C as a mixture of isomers 20:1 after silica gel chromatography (petroleum ether/ethyl acetate 10:1) as a colourless oil (195.6 mg, 0.93 mmol, 93%).

Major isomer: 1-(4-methoxystyryl)benzene (*Z*-17)[28]

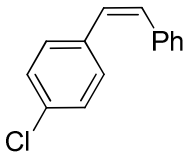


$\mathbf{R_f}$ = 0.75 (petroleum ether / ethyl acetate 10:1); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.31-7.13 (m, 7H), 6.80-6.71 (m, 2H), 6.56-6.47 (m, 2H), 3.78 (s, 3H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 158.7, 137.6, 130.1, 129.8, 129.7, 128.8, 128.7, 128.2, 126.9, 112.6, 55.2 ppm; **IR** (flüssigfilm) 3006 (w), 2953 (w), 2834 (w), 1605 (m), 1508 (s), 1460 (m), 1443 (m), 1247 (s), 1175 (m), 1032 (m), 829 (m), 770 (m), 695 (s), 635 (m) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 210 (100), 195 (19), 179 (15), 165 (47), 152 (34), 139 (8), 128 (6), 115 (10), 89 (12), 63 (9), 51 (7).

4.2.2 *Z*-selective HS-DS-sequence starting from 1-(2-(4-chlorophenyl)ethynyl)benzene

The product was obtained according to GP-IV starting from 1-(2-(4-chlorophenyl)ethynyl)benzene (212.7 mg, 1.0 mmol) and methylphenylvinylsilane (**3**) (183.3 µL, 1.1 mmol) using 2.5 mol% $FeH(CO)(NO)(PPh_3)_2$ (**1**) (16.0 mg, 0.025 mmol) at 60 °C as a mixture of isomers 10:1 after silica gel chromatography (petroleum ether) as a colourless oil (204.0 mg, 0.95 mmol, 95%).

Major isomer: 1-(4-chlorostyryl)benzene (*Z*-18)[26]

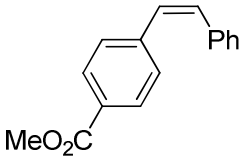


$\mathbf{R_f}$ = 0.50 (petroleum ether); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.27-7.21 (m, 7H), 6.62 (d, *J* = 12.3 Hz, 1H), 6.52 (d, *J* = 12.3 Hz, 1H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 136.9, 135.6, 132.7, 130.9, 130.2, 128.9, 128.8, 128.4, 128.3, 127.3 ppm; **IR** (film) 3013 (w), 1487 (s), 1446 (w), 1089 (s), 1013 (m), 919 (m), 872 (m), 822 (s), 726 (m), 695 (s), 599 (m) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 214 (60), 178 (100), 152 (13), 89 (26), 76 (27), 63 (11), 51 (12).

4.2.3 *Z*-selective HS-DS-sequence starting from methyl 4-(2-phenylethynyl)benzoate

The product was obtained according to GP-IV starting from methyl 4-(2-phenylethynyl)benzoate (236.3 mg, 1.0 mmol) and methylphenylvinylsilane (**3**) (183.3 µL, 1.1 mmol) using 2.5 mol% $FeH(CO)(NO)(PPh_3)_2$ (**1**) (16.0 mg, 0.025 mmol) at 60 °C as a mixture of isomers 10:1 after silica gel chromatography (petroleum ether/ethyl acetate 10:1) as a colourless oil (181.1 mg, 0.76 mmol, 76%).

Major isomer: methyl 4-styrylbenzoate (*Z*-19)[23]

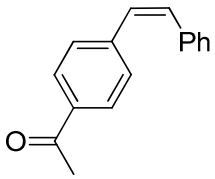


R_f = 0.4 (petroleum ether / ethyl acetate 10:1); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.1 Hz, 2H), 7.30 (d, *J* = 8.1 Hz, 2H), 7.24-7.18 (m, 5H), 6.71 (d, *J* = 12.4 Hz, 1H), 6.61 (d, *J* = 12.4 Hz, 1H), 3.90 (s, 3H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 167.1, 142.4, 136.7, 132.3, 129.6, 129.3, 128.9, 128.6, 128.4, 127.6, 52.1 ppm; **IR** (film) 3022 (w), 2949 (w), 1717 (s), 1607 (m), 1434 (m), 1311 (w), 1275 (s), 1179 (m), 1105 (m), 1018 (w), 781 (w), 713 (m), 699 (m), 633 (m) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 238 (81), 207 (52), 178 (100), 152 (20), 89 (18), 76 (16), 63 (8), 51 (10).

4.2.4 *Z*-selective HS-DS-sequence starting from 1-(4-(2-phenylethynyl)phenyl) ethanone

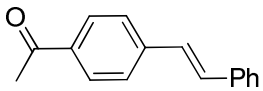
The product was obtained according to GP-IV starting from 1-(4-(2-phenylethynyl)phenyl)ethanone (220.3 mg, 1.0 mmol) and methylphenylvinylsilane (**3**) (349.9 µL, 2.1 mmol) using 2.5 mol% $FeH(CO)(NO)(PPh_3)_2$ (**1**) (16.0 mg, 0.025 mmol) at 60 °C as a mixture of isomers 10:1 after silica gel chromatography (petroleum ether/ethyl acetate 3:1) as a white solid (204.5 mg, 0.92 mmol, 92%).

Major isomer: 1-(4-styrylphenyl)ethanone (*Z*-21)[29]



R_f = 0.65 (petroleum ether / ethyl acetate 3:1); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.84-7.78 (m, 2H), 7.35-7.30 (m, 2H), 7.25-7.15 (m, 5H), 6.73 (d, *J* = 12.3 Hz, 1H), 6.60 (d, *J* = 12.3 Hz, 1H), 2.57 (s, 3H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 197.6, 142.3, 136.7, 135.6, 132.5, 129.1, 129.0, 128.8, 128.4, 128.3, 127.6, 26.6 ppm; **IR** (film) 3020 (w), 1675 (s), 1599 (m), 1409 (m), 1356 (m), 1262 (s), 1178 (m), 1103 (w), 963 (s), 867 (m), 819 (s), 723 (m), 689 (s), 591 (s) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 222 (60), 207 (100), 178 (66), 152 (15), 89 (10), 76 (8), 63 (7), 51 (8).

Minor isomer: 1-(4-styrylphenyl)ethanone (*E*-21)[30]

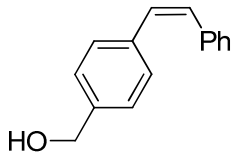


R_f = 0.65 (petroleum ether / ethyl acetate 3:1); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 8.00-7.93 (m, 2H), 7.63-7.51 (m, 4H), 7.43-7.29 (m, 3H), 7.24 (d, *J* = 16.5 Hz, 1H), 7.13 (d, *J* = 16.5 Hz, 1H), 2.61 (s, 3H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 197.5, 142.0, 136.7, 136.0, 131.5, 128.9, 128.8, 128.3, 127.5, 126.8, 126.5, 26.6 ppm; **IR** (film) 3020 (w), 2921 (w), 1675 (s), 1599 (m), 1491 (m), 1449 (m), 1410 (m), 1262 (s), 1178 (m), 1074 (m), 963 (s), 820 (s), 754 (m), 689 (m) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 222 (47), 207 (100), 178 (56), 152 (13), 89 (5), 76 (4), 63 (4), 51 (5).

4.2.5 *Z*-selective HS-DS-sequence starting from methyl (4-(2-phenylethynyl)phenyl) methanol

The product was obtained according to GP-IV starting from (4-(2-phenylethynyl)phenyl)methanol (208.3 mg, 1.0 mmol) and methylphenylvinylsilane (**3**) (349.9 µL, 2.1 mmol) using 2.5 mol% $FeH(CO)(NO)(PPh_3)_2$ (**1**) (16.0 mg, 0.025 mmol) at 60 °C as a mixture of isomers 9:1 after silica gel chromatography (petroleum ether/ethyl acetate 3:1) as a pale yellow oil (199.8 mg, 0.95 mmol, 95%).

Major isomer: (4-styrylphenyl)methanol (*Z*-22)[31]

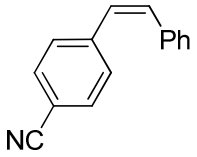


R_f = 0.3 (petroleum ether / ethyl acetate 3:1); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.28-7.16 (m, 9H), 6.63-6.55 (m, 2H), 4.64 (s, 2H), 1.67 (bs, 1H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 139.6, 137.2, 136.6, 130.4, 129.8, 129.1, 128.8, 128.3, 127.1, 126.9, 65.2 ppm; **IR** (film) 3319 (bm), 3021 (w), 2871 (w), 1491 (m), 1446 (w), 1418 (m), 1211 (w), 1028 (m), 1014 (m), 820 (m), 773 (m), 732 (m), 696 (s) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 210 (100), 179 (69), 165 (28), 152 (15), 115 (14), 103 (25), 77 (26), 63 (8), 51 (10).

4.2.6 *Z*-selective HS-DS-sequence starting from 4-(2-phenylethynyl)benzonitrile

The product was obtained according to GP-IV starting from 4-(2-phenylethynyl)benzonitrile (203.2 mg, 1.0 mmol) and methylphenylvinylsilane (**3**) (183.3 µL, 1.1 mmol) using 2.5 mol% $FeH(CO)(NO)(PPh_3)_2$ (**1**) (16.0 mg, 0.025 mmol) at 60 °C as a mixture of isomers 12:1 after silica gel chromatography (petroleum ether/ethyl acetate 10:1) as a colourless oil (149.8 mg, 0.73 mmol, 73%).

Major isomer: 4-styrylbenzonitrile (*Z*-23)[24]

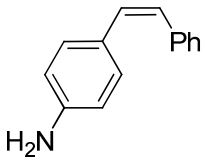


R_f = 0.30 (petroleum ether / ethyl acetate 10:1); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.52-7.46 (m, 2H), 7.35-7.29 (m, 2H), 7.28-7.13 (m, 5H), 6.77 (d, *J* = 12.3 Hz, 1H), 6.57 (d, *J* = 12.3 Hz, 1H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 142.1, 136.2, 133.3, 132.0, 129.5, 128.8, 128.5, 128.4, 127.8, 119.0, 110.5 ppm; **IR** (film) 3023 (w), 2224 (s), 1601 (s), 1503 (s), 1447 (m), 1413 (m), 1175 (m), 966 (s), 957 (m), 873 (s), 824 (s), 756 (s), 690 (s), 600 (m) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 205 (100), 190 (44), 176 (16), 165 (14), 152 (9), 102 (7), 89 (9), 76 (11), 63 (11), 51 (12).

4.2.7 *Z*-selective HS-DS-sequence starting from 4-(2-phenylethynyl)benzenamine

The product was obtained according to GP-IV starting from 4-(2-phenylethynyl)benzenamine (193.2 mg, 1.0 mmol) and methylphenylvinylsilane (**3**) (349.9 µL, 2.1 mmol) using 2.5 mol% $FeH(CO)(NO)(PPh_3)_2$ (**1**) (16.0 mg, 0.025 mmol) at 60 °C as a mixture of isomers 20:1 after silica gel chromatography (petroleum ether/ethyl acetate 3:1) as an orange solid (173.8 mg, 0.89 mmol, 89%).

Major isomer: 4-styrylbenzenamine (*Z*-24)[32]

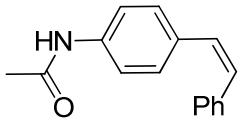


R_f = 0.25 (petroleum ether / ethyl acetate 3:1); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 7.38-7.13 (m, 5H), 7.10-7.04 (m, 2H), 6.57-6.51 (m, 2H), 6.48 (d, *J* = 12.3 Hz, 1H), 6.43 (d, *J* = 12.3 Hz, 1H), 3.72 (bs, 2H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 145.3, 138.0, 130.2, 130.1, 128.8, 128.2, 127.6, 127.5, 126.7, 114.8 ppm; **IR** (film) 3446 (m), 3360 (w), 3021 (w), 1615 (s), 1513 (s), 1282 (m), 1177 (m), 966 (m), 819 (s), 692 (s), 593 (m) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 195 (100), 180 (12), 165 (12), 152 (9), 89 (5), 77 (4), 63 (5), 51 (5).

4.2.8 *Z*-selective HS-DS-sequence starting from N-(4-(2-phenylethynyl)phenyl) acetamide

The product was obtained according to GP-IV starting from N-(4-(2-phenylethynyl)phenyl)acetamide (235.3 mg, 1.0 mmol) and methylphenylvinylsilane (**3**) (349.9 µL, 2.1 mmol) using 2.5 mol% $FeH(CO)(NO)(PPh_3)_2$ (**1**) (16.0 mg, 0.025 mmol) at 60 °C as a mixture of isomers 20:1 after silica gel chromatography (petroleum ether/ethyl acetate 1:1) as a white solid (194.6 mg, 0.82 mmol, 82%).

Major isomer: 4-styrylbenzenamine (*Z*-25)[33]

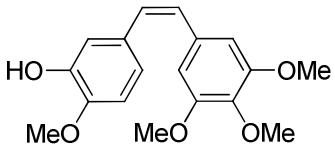


R_f = 0.20 (petroleum ether / ethyl acetate 1:1); **^{1}H-NMR** (300 MHz, DMSO-d6) δ 10.02 (s, 1H), 7.47 (d, *J* = 8.7 Hz, 2H), 7.33-7.22 (m, 5H), 7.20-7.13 (m, 2H), 6.59 (s, 2H), 2.05 (s, 3H) ppm;
^{13}C-NMR (125 MHz, DMSO-d6) δ 168.2, 138.4, 137.0, 131.3, 129.7, 129.0, 128.9, 128.4, 128.3, 127.1, 118.6, 24.0; **IR** (flüssig) 3436 (m), 1680 (m), 1531 (m), 1051 (s), 1023 (s), 821 (m), 758 (m) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 237 (82), 195 (100), 180 (14), 165 (27), 152 (16), 115 (4), 89 (4).

4.2.9 *Z*-selective HS-DS-sequence starting from 2-methoxy-5-(2-(3,4,5-trimethoxy phenyl)ethynyl)phenol (26)

The product was obtained according to GP-IV starting from 2-methoxy-5-(2-(3,4,5-trimethoxyphenyl)ethynyl)phenol (**26**) (157.2 mg, 0.5 mmol) and methylphenylvinylsilane (**3**) (183.3 µL, 1.1 mmol) using 5 mol% FeH(CO)(NO)(PPh_3)$_2$ (**1**) (16.0 mg, 0.025 mmol) at 80 °C as a mixture of isomers 8:1 after silica gel chromatography (petroleum ether/ethyl acetate 3:1) as an orange oil (120.2 mg, 0.76 mmol, 76%).

Major isomer: 5-(3,4,5-trimethoxystyryl)-2-methoxyphenol (*Z*-27)[21]



R_f = 0.2 (petroleum ether / ethyl acetate 3:1); **^{1}H-NMR** (300 MHz, $CDCl_3$) δ 6.92 (d, *J* = 2.1 Hz, 1H), 6.80 (dd, *J* = 8.3, 2.1 Hz, 1H), 6.73 (d, *J* = 8.3 Hz, 1H), 6.53 (s, 2H), 6.47 (d, *J* = 12.3 Hz, 1H), 6.41 (d, *J* = 12.3 Hz, 1H), 5.51 (s, 1H), 3.87 (s, 3H), 3.84 (s, 3H), 3.70 (s, 6H) ppm; **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 152.9, 145.8, 145.2, 137.1, 132.7, 130.6, 129.5, 129.0, 121.1, 115.0, 110.3, 106.1, 60.9, 56.0, 55.9 ppm; **IR** (film) 3428 (bm), 2938 (w), 2836 (w), 1736 (m), 1578 (m), 1507 (m), 1269 (m), 1234 (s), 1122 (s), 1042 (m), 880 (w), 852 (m) cm^{-1}; **MS** (EI, 70 eV): *m/z* (%) 316 (100), 301 (75), 241 (8), 226 (8), 183 (7), 155 (7), 115 (12), 77 (6), 63 (6), 51 (5).

5 References

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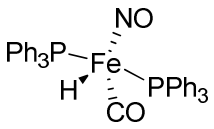
6 X-Ray structures

6.1 $FeH(CO)(NO)(PPh_3)_2$ [2] (1)



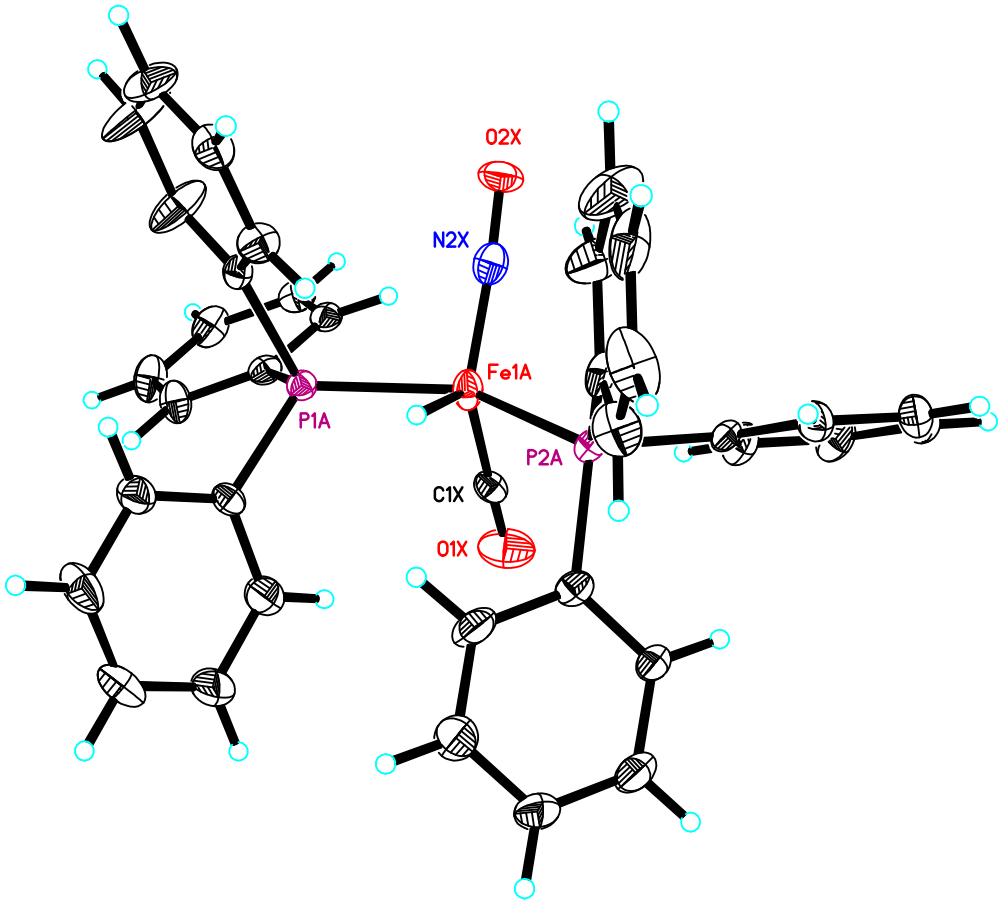


Table 1. Crystal data and structure refinement for s1797lm.

Identification code	s1797lm
Empirical formula	C37 H31 Fe N O2 P2
Formula weight	639.42
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	orthorhombic, Pca2(1)
Unit cell dimensions	a = 23.0443(6) A alpha = 90 deg. b = 13.4466(4) A beta = 90 deg. c = 20.2095(6) A gamma = 90 deg.
Volume	6262.3(3) A^3
Z, Calculated density	8, 1.356 Mg/m^3
Absorption coefficient	0.618 mm^-1
F(000)	2656
Crystal size	0.27 x 0.25 x 0.13 mm
Theta range for data collection	1.75 to 26.38 deg.
Limiting indices	-17<=h<=28, -16<=k<=16, -24<=l<=25
Reflections collected / unique	43410 / 12626 [R(int) = 0.0344]
Completeness to theta = 26.38	99.9 %
Max. and min. transmission	0.9239 and 0.8508
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12626 / 1 / 783
Goodness-of-fit on F^2	1.026
Final R indices [I>2sigma(I)]	R1 = 0.0324, wR2 = 0.0689
R indices (all data)	R1 = 0.0429, wR2 = 0.0718
Absolute structure parameter	0.032(9)
Largest diff. peak and hole	0.377 and -0.372 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for s1797lm.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1A)	2143(1)	4499(1)	4517(1)	21(1)
P(1A)	1320(1)	5286(1)	4487(1)	16(1)
P(2A)	3028(1)	4599(1)	4145(1)	17(1)
C(1X)	2347(1)	4866(2)	5308(1)	19(1)
O(1X)	2489(1)	5102(2)	5830(1)	41(1)
N(2X)	1893(1)	3371(2)	4293(1)	25(1)
O(2X)	1685(1)	2600(1)	4153(1)	31(1)
C(1A)	1363(1)	6638(2)	4488(1)	18(1)
C(2A)	1072(1)	7228(2)	4031(1)	27(1)
C(3A)	1137(1)	8255(2)	4034(1)	36(1)
C(4A)	1488(1)	8707(2)	4498(2)	33(1)
C(5A)	1775(1)	8134(2)	4957(2)	38(1)
C(6A)	1714(1)	7109(2)	4947(2)	33(1)
C(7A)	877(1)	4954(2)	3765(1)	19(1)
C(8A)	1126(1)	4933(2)	3142(1)	26(1)
C(9A)	810(1)	4626(2)	2595(1)	29(1)
C(10A)	250(1)	4307(2)	2670(2)	37(1)
C(11A)	5(1)	4291(3)	3286(2)	59(1)
C(12A)	315(1)	4627(3)	3834(2)	43(1)
C(13A)	825(1)	5007(2)	5170(1)	18(1)
C(14A)	842(1)	4059(2)	5444(1)	19(1)
C(15A)	431(1)	3768(2)	5906(1)	23(1)
C(16A)	6(1)	4436(2)	6101(1)	28(1)
C(17A)	-9(1)	5376(2)	5847(1)	30(1)
C(18A)	401(1)	5666(2)	5379(1)	25(1)
C(19A)	3357(1)	5803(2)	4325(1)	20(1)
C(20A)	3057(1)	6669(2)	4162(2)	37(1)
C(21A)	3276(1)	7591(2)	4316(2)	41(1)
C(22A)	3790(1)	7684(2)	4652(2)	34(1)
C(23A)	4086(1)	6836(2)	4829(2)	35(1)
C(24A)	3872(1)	5903(2)	4672(1)	26(1)
C(25A)	3103(1)	4429(2)	3250(1)	22(1)
C(26A)	2811(1)	3643(3)	2965(2)	42(1)
C(27A)	2878(1)	3440(3)	2292(2)	55(1)
C(28A)	3230(1)	4025(3)	1914(2)	44(1)
C(29A)	3518(1)	4813(2)	2194(2)	45(1)
C(30A)	3453(1)	5022(2)	2861(1)	33(1)
C(31A)	3555(1)	3693(2)	4470(1)	19(1)
C(32A)	3495(1)	3333(2)	5113(1)	27(1)
C(33A)	3891(1)	2667(2)	5372(2)	31(1)
C(34A)	4353(1)	2346(2)	4988(2)	30(1)
C(35A)	4416(1)	2692(2)	4353(1)	30(1)
C(36A)	4016(1)	3362(2)	4096(1)	26(1)
Fe(1B)	1250(1)	678(1)	2160(1)	21(1)
P(1B)	377(1)	450(1)	2561(1)	16(1)
P(2B)	2123(1)	40(1)	2187(1)	15(1)
N(2Y)	1372(1)	1896(2)	2259(1)	28(1)
O(2Y)	1472(1)	2752(2)	2268(1)	53(1)
C(1Y)	1098(1)	193(2)	1381(1)	20(1)
O(1Y)	1006(1)	-91(2)	845(1)	38(1)
C(1B)	81(1)	-803(2)	2461(1)	19(1)
C(2B)	-518(1)	-967(2)	2440(1)	29(1)

C(3B)	-732(1)	-1932(2)	2435(1)	37(1)
C(4B)	-357(1)	-2730(2)	2449(1)	35(1)
C(5B)	233(1)	-2578(2)	2444(1)	33(1)
C(6B)	452(1)	-1616(2)	2445(1)	24(1)
C(7B)	-196(1)	1250(2)	2210(1)	20(1)
C(8B)	-599(1)	1751(2)	2605(1)	24(1)
C(9B)	-1032(1)	2331(2)	2313(2)	30(1)
C(10B)	-1063(1)	2419(2)	1638(2)	33(1)
C(11B)	-663(1)	1928(2)	1249(2)	35(1)
C(12B)	-234(1)	1349(2)	1532(1)	28(1)
C(13B)	293(1)	680(2)	3451(1)	18(1)
C(14B)	5(1)	30(2)	3872(1)	22(1)
C(15B)	-60(1)	264(2)	4540(1)	26(1)
C(16B)	152(1)	1147(2)	4787(1)	26(1)
C(17B)	433(1)	1803(2)	4364(1)	27(1)
C(18B)	509(1)	1572(2)	3705(1)	25(1)
C(19B)	2543(1)	257(2)	2941(1)	18(1)
C(20B)	3092(1)	-178(2)	3030(1)	31(1)
C(21B)	3414(1)	-4(2)	3594(1)	31(1)
C(22B)	3193(1)	602(2)	4083(2)	39(1)
C(23B)	2664(2)	1016(3)	4007(2)	64(1)
C(24B)	2340(1)	845(3)	3438(2)	48(1)
C(25B)	2612(1)	493(2)	1536(1)	17(1)
C(26B)	2473(1)	1365(2)	1202(1)	22(1)
C(27B)	2849(1)	1764(2)	731(1)	27(1)
C(28B)	3366(1)	1290(2)	592(1)	28(1)
C(29B)	3506(1)	420(2)	913(1)	26(1)
C(30B)	3132(1)	10(2)	1379(1)	22(1)
C(31B)	2143(1)	-1309(2)	2085(1)	18(1)
C(32B)	2170(1)	-1936(2)	2626(1)	28(1)
C(33B)	2139(1)	-2965(2)	2542(2)	39(1)
C(34B)	2083(1)	-3366(2)	1918(1)	33(1)
C(35B)	2046(1)	-2745(2)	1379(1)	30(1)
C(36B)	2074(1)	-1725(2)	1457(1)	23(1)

Table 3. Bond lengths [A] and angles [deg] for s1797lm.

Fe(1A)-N(2X)	1.685(2)
Fe(1A)-C(1X)	1.738(3)
Fe(1A)-P(1A)	2.1722(7)
Fe(1A)-P(2A)	2.1779(7)
Fe(1A)-H(1A)	1.52(3)
P(1A)-C(1A)	1.821(2)
P(1A)-C(13A)	1.829(2)
P(1A)-C(7A)	1.836(3)
P(2A)-C(19A)	1.826(3)
P(2A)-C(25A)	1.830(3)
P(2A)-C(31A)	1.842(2)
C(1X)-O(1X)	1.148(3)
N(2X)-O(2X)	1.177(3)
C(1A)-C(6A)	1.385(4)
C(1A)-C(2A)	1.390(3)
C(2A)-C(3A)	1.390(4)
C(2A)-H(2A)	0.9500
C(3A)-C(4A)	1.379(4)
C(3A)-H(3A)	0.9500
C(4A)-C(5A)	1.376(4)
C(4A)-H(4A)	0.9500
C(5A)-C(6A)	1.386(4)

C(5A)-H(5A)	0.9500
C(6A)-H(6A)	0.9500
C(7A)-C(12A)	1.377(4)
C(7A)-C(8A)	1.383(4)
C(8A)-C(9A)	1.388(4)
C(8A)-H(8A)	0.9500
C(9A)-C(10A)	1.368(4)
C(9A)-H(9A)	0.9500
C(10A)-C(11A)	1.367(4)
C(10A)-H(10A)	0.9500
C(11A)-C(12A)	1.392(4)
C(11A)-H(11A)	0.9500
C(12A)-H(12A)	0.9500
C(13A)-C(18A)	1.385(3)
C(13A)-C(14A)	1.391(3)
C(14A)-C(15A)	1.387(3)
C(14A)-H(14A)	0.9500
C(15A)-C(16A)	1.385(4)
C(15A)-H(15A)	0.9500
C(16A)-C(17A)	1.365(4)
C(16A)-H(16A)	0.9500
C(17A)-C(18A)	1.393(4)
C(17A)-H(17A)	0.9500
C(18A)-H(18A)	0.9500
C(19A)-C(24A)	1.385(3)
C(19A)-C(20A)	1.393(4)
C(20A)-C(21A)	1.375(4)
C(20A)-H(20A)	0.9500
C(21A)-C(22A)	1.370(4)
C(21A)-H(21A)	0.9500
C(22A)-C(23A)	1.376(4)
C(22A)-H(22A)	0.9500
C(23A)-C(24A)	1.385(4)
C(23A)-H(23A)	0.9500
C(24A)-H(24A)	0.9500
C(25A)-C(26A)	1.379(4)
C(25A)-C(30A)	1.381(4)
C(26A)-C(27A)	1.395(4)
C(26A)-H(26A)	0.9500
C(27A)-C(28A)	1.364(5)
C(27A)-H(27A)	0.9500
C(28A)-C(29A)	1.372(5)
C(28A)-H(28A)	0.9500
C(29A)-C(30A)	1.385(4)
C(29A)-H(29A)	0.9500
C(30A)-H(30A)	0.9500
C(31A)-C(36A)	1.378(3)
C(31A)-C(32A)	1.393(4)
C(32A)-C(33A)	1.380(4)
C(32A)-H(32A)	0.9500
C(33A)-C(34A)	1.387(4)
C(33A)-H(33A)	0.9500
C(34A)-C(35A)	1.373(4)
C(34A)-H(34A)	0.9500
C(35A)-C(36A)	1.389(4)
C(35A)-H(35A)	0.9500
C(36A)-H(36A)	0.9500
Fe(1B)-N(2Y)	1.672(2)
Fe(1B)-C(1Y)	1.740(3)
Fe(1B)-P(2B)	2.1877(6)
Fe(1B)-P(1B)	2.1907(7)
Fe(1B)-H(1B)	1.44(3)
P(1B)-C(1B)	1.828(2)

P(1B)-C(13B)	1.835(3)
P(1B)-C(7B)	1.846(2)
P(2B)-C(31B)	1.826(2)
P(2B)-C(19B)	1.828(2)
P(2B)-C(25B)	1.835(2)
N(2Y)-O(2Y)	1.175(3)
C(1Y)-O(1Y)	1.168(3)
C(1B)-C(6B)	1.388(4)
C(1B)-C(2B)	1.398(3)
C(2B)-C(3B)	1.388(4)
C(2B)-H(2B)	0.9500
C(3B)-C(4B)	1.377(4)
C(3B)-H(3B)	0.9500
C(4B)-C(5B)	1.376(4)
C(4B)-H(4B)	0.9500
C(5B)-C(6B)	1.389(4)
C(5B)-H(5B)	0.9500
C(6B)-H(6B)	0.9500
C(7B)-C(12B)	1.379(4)
C(7B)-C(8B)	1.398(3)
C(8B)-C(9B)	1.396(4)
C(8B)-H(8B)	0.9500
C(9B)-C(10B)	1.372(4)
C(9B)-H(9B)	0.9500
C(10B)-C(11B)	1.379(4)
C(10B)-H(10B)	0.9500
C(11B)-C(12B)	1.383(4)
C(11B)-H(11B)	0.9500
C(12B)-H(12B)	0.9500
C(13B)-C(14B)	1.390(4)
C(13B)-C(18B)	1.396(3)
C(14B)-C(15B)	1.394(4)
C(14B)-H(14B)	0.9500
C(15B)-C(16B)	1.378(4)
C(15B)-H(15B)	0.9500
C(16B)-C(17B)	1.388(4)
C(16B)-H(16B)	0.9500
C(17B)-C(18B)	1.380(4)
C(17B)-H(17B)	0.9500
C(18B)-H(18B)	0.9500
C(19B)-C(24B)	1.362(4)
C(19B)-C(20B)	1.405(4)
C(20B)-C(21B)	1.381(4)
C(20B)-H(20B)	0.9500
C(21B)-C(22B)	1.379(4)
C(21B)-H(21B)	0.9500
C(22B)-C(23B)	1.349(4)
C(22B)-H(22B)	0.9500
C(23B)-C(24B)	1.390(4)
C(23B)-H(23B)	0.9500
C(24B)-H(24B)	0.9500
C(25B)-C(26B)	1.392(3)
C(25B)-C(30B)	1.400(3)
C(26B)-C(27B)	1.394(3)
C(26B)-H(26B)	0.9500
C(27B)-C(28B)	1.379(4)
C(27B)-H(27B)	0.9500
C(28B)-C(29B)	1.376(4)
C(28B)-H(28B)	0.9500
C(29B)-C(30B)	1.389(4)
C(29B)-H(29B)	0.9500
C(30B)-H(30B)	0.9500
C(31B)-C(32B)	1.382(4)

C(31B)-C(36B)	1.398(3)
C(32B)-C(33B)	1.397(4)
C(32B)-H(32B)	0.9500
C(33B)-C(34B)	1.378(4)
C(33B)-H(33B)	0.9500
C(34B)-C(35B)	1.374(4)
C(34B)-H(34B)	0.9500
C(35B)-C(36B)	1.381(4)
C(35B)-H(35B)	0.9500
C(36B)-H(36B)	0.9500
N(2X)-Fe(1A)-C(1X)	126.60(11)
N(2X)-Fe(1A)-P(1A)	97.60(7)
C(1X)-Fe(1A)-P(1A)	97.13(8)
N(2X)-Fe(1A)-P(2A)	106.41(7)
C(1X)-Fe(1A)-P(2A)	92.68(8)
P(1A)-Fe(1A)-P(2A)	141.04(3)
N(2X)-Fe(1A)-H(1A)	114.1(11)
C(1X)-Fe(1A)-H(1A)	119.3(11)
P(1A)-Fe(1A)-H(1A)	71.4(10)
P(2A)-Fe(1A)-H(1A)	70.9(10)
C(1A)-P(1A)-C(13A)	103.76(11)
C(1A)-P(1A)-C(7A)	105.91(11)
C(13A)-P(1A)-C(7A)	101.75(10)
C(1A)-P(1A)-Fe(1A)	116.04(8)
C(13A)-P(1A)-Fe(1A)	115.03(8)
C(7A)-P(1A)-Fe(1A)	112.87(8)
C(19A)-P(2A)-C(25A)	105.57(12)
C(19A)-P(2A)-C(31A)	103.90(11)
C(25A)-P(2A)-C(31A)	102.03(12)
C(19A)-P(2A)-Fe(1A)	112.01(8)
C(25A)-P(2A)-Fe(1A)	115.00(8)
C(31A)-P(2A)-Fe(1A)	116.98(8)
O(1X)-C(1X)-Fe(1A)	179.1(3)
O(2X)-N(2X)-Fe(1A)	175.8(2)
C(6A)-C(1A)-C(2A)	117.9(2)
C(6A)-C(1A)-P(1A)	119.3(2)
C(2A)-C(1A)-P(1A)	122.82(19)
C(3A)-C(2A)-C(1A)	120.8(2)
C(3A)-C(2A)-H(2A)	119.6
C(1A)-C(2A)-H(2A)	119.6
C(4A)-C(3A)-C(2A)	120.3(3)
C(4A)-C(3A)-H(3A)	119.8
C(2A)-C(3A)-H(3A)	119.8
C(5A)-C(4A)-C(3A)	119.5(3)
C(5A)-C(4A)-H(4A)	120.2
C(3A)-C(4A)-H(4A)	120.2
C(4A)-C(5A)-C(6A)	120.0(3)
C(4A)-C(5A)-H(5A)	120.0
C(6A)-C(5A)-H(5A)	120.0
C(1A)-C(6A)-C(5A)	121.5(3)
C(1A)-C(6A)-H(6A)	119.2
C(5A)-C(6A)-H(6A)	119.2
C(12A)-C(7A)-C(8A)	118.4(2)
C(12A)-C(7A)-P(1A)	121.4(2)
C(8A)-C(7A)-P(1A)	119.88(19)
C(7A)-C(8A)-C(9A)	120.9(2)
C(7A)-C(8A)-H(8A)	119.6
C(9A)-C(8A)-H(8A)	119.6
C(10A)-C(9A)-C(8A)	120.0(3)
C(10A)-C(9A)-H(9A)	120.0
C(8A)-C(9A)-H(9A)	120.0

C(11A)-C(10A)-C(9A)	119.7(3)
C(11A)-C(10A)-H(10A)	120.1
C(9A)-C(10A)-H(10A)	120.1
C(10A)-C(11A)-C(12A)	120.5(3)
C(10A)-C(11A)-H(11A)	119.8
C(12A)-C(11A)-H(11A)	119.8
C(7A)-C(12A)-C(11A)	120.5(3)
C(7A)-C(12A)-H(12A)	119.8
C(11A)-C(12A)-H(12A)	119.8
C(18A)-C(13A)-C(14A)	119.0(2)
C(18A)-C(13A)-P(1A)	122.6(2)
C(14A)-C(13A)-P(1A)	118.13(18)
C(15A)-C(14A)-C(13A)	120.5(2)
C(15A)-C(14A)-H(14A)	119.7
C(13A)-C(14A)-H(14A)	119.7
C(16A)-C(15A)-C(14A)	119.4(2)
C(16A)-C(15A)-H(15A)	120.3
C(14A)-C(15A)-H(15A)	120.3
C(17A)-C(16A)-C(15A)	120.8(2)
C(17A)-C(16A)-H(16A)	119.6
C(15A)-C(16A)-H(16A)	119.6
C(16A)-C(17A)-C(18A)	119.8(2)
C(16A)-C(17A)-H(17A)	120.1
C(18A)-C(17A)-H(17A)	120.1
C(13A)-C(18A)-C(17A)	120.4(2)
C(13A)-C(18A)-H(18A)	119.8
C(17A)-C(18A)-H(18A)	119.8
C(24A)-C(19A)-C(20A)	117.7(2)
C(24A)-C(19A)-P(2A)	122.9(2)
C(20A)-C(19A)-P(2A)	119.13(19)
C(21A)-C(20A)-C(19A)	121.2(2)
C(21A)-C(20A)-H(20A)	119.4
C(19A)-C(20A)-H(20A)	119.4
C(22A)-C(21A)-C(20A)	120.7(3)
C(22A)-C(21A)-H(21A)	119.6
C(20A)-C(21A)-H(21A)	119.6
C(21A)-C(22A)-C(23A)	118.9(3)
C(21A)-C(22A)-H(22A)	120.6
C(23A)-C(22A)-H(22A)	120.6
C(22A)-C(23A)-C(24A)	121.0(2)
C(22A)-C(23A)-H(23A)	119.5
C(24A)-C(23A)-H(23A)	119.5
C(23A)-C(24A)-C(19A)	120.5(2)
C(23A)-C(24A)-H(24A)	119.7
C(19A)-C(24A)-H(24A)	119.7
C(26A)-C(25A)-C(30A)	119.2(3)
C(26A)-C(25A)-P(2A)	117.6(2)
C(30A)-C(25A)-P(2A)	123.1(2)
C(25A)-C(26A)-C(27A)	120.3(3)
C(25A)-C(26A)-H(26A)	119.9
C(27A)-C(26A)-H(26A)	119.9
C(28A)-C(27A)-C(26A)	119.9(3)
C(28A)-C(27A)-H(27A)	120.1
C(26A)-C(27A)-H(27A)	120.1
C(27A)-C(28A)-C(29A)	120.2(3)
C(27A)-C(28A)-H(28A)	119.9
C(29A)-C(28A)-H(28A)	119.9
C(28A)-C(29A)-C(30A)	120.4(3)
C(28A)-C(29A)-H(29A)	119.8
C(30A)-C(29A)-H(29A)	119.8
C(25A)-C(30A)-C(29A)	120.0(3)
C(25A)-C(30A)-H(30A)	120.0
C(29A)-C(30A)-H(30A)	120.0

C(36A)-C(31A)-C(32A)	118.4(2)
C(36A)-C(31A)-P(2A)	121.8(2)
C(32A)-C(31A)-P(2A)	119.84(19)
C(33A)-C(32A)-C(31A)	120.9(3)
C(33A)-C(32A)-H(32A)	119.6
C(31A)-C(32A)-H(32A)	119.6
C(32A)-C(33A)-C(34A)	119.8(3)
C(32A)-C(33A)-H(33A)	120.1
C(34A)-C(33A)-H(33A)	120.1
C(35A)-C(34A)-C(33A)	120.0(3)
C(35A)-C(34A)-H(34A)	120.0
C(33A)-C(34A)-H(34A)	120.0
C(34A)-C(35A)-C(36A)	119.8(3)
C(34A)-C(35A)-H(35A)	120.1
C(36A)-C(35A)-H(35A)	120.1
C(31A)-C(36A)-C(35A)	121.1(3)
C(31A)-C(36A)-H(36A)	119.4
C(35A)-C(36A)-H(36A)	119.4
N(2Y)-Fe(1B)-C(1Y)	120.54(12)
N(2Y)-Fe(1B)-P(2B)	103.11(7)
C(1Y)-Fe(1B)-P(2B)	93.44(8)
N(2Y)-Fe(1B)-P(1B)	104.33(7)
C(1Y)-Fe(1B)-P(1B)	95.57(8)
P(2B)-Fe(1B)-P(1B)	141.31(3)
N(2Y)-Fe(1B)-H(1B)	118.4(11)
C(1Y)-Fe(1B)-H(1B)	121.0(11)
P(2B)-Fe(1B)-H(1B)	71.1(10)
P(1B)-Fe(1B)-H(1B)	72.1(10)
C(1B)-P(1B)-C(13B)	103.02(11)
C(1B)-P(1B)-C(7B)	103.11(11)
C(13B)-P(1B)-C(7B)	101.69(12)
C(1B)-P(1B)-Fe(1B)	115.55(8)
C(13B)-P(1B)-Fe(1B)	115.79(8)
C(7B)-P(1B)-Fe(1B)	115.70(8)
C(31B)-P(2B)-C(19B)	103.79(11)
C(31B)-P(2B)-C(25B)	103.49(11)
C(19B)-P(2B)-C(25B)	102.66(11)
C(31B)-P(2B)-Fe(1B)	114.22(7)
C(19B)-P(2B)-Fe(1B)	116.41(8)
C(25B)-P(2B)-Fe(1B)	114.65(8)
O(2Y)-N(2Y)-Fe(1B)	173.9(2)
O(1Y)-C(1Y)-Fe(1B)	176.8(3)
C(6B)-C(1B)-C(2B)	118.8(2)
C(6B)-C(1B)-P(1B)	119.89(18)
C(2B)-C(1B)-P(1B)	121.1(2)
C(3B)-C(2B)-C(1B)	119.8(3)
C(3B)-C(2B)-H(2B)	120.1
C(1B)-C(2B)-H(2B)	120.1
C(4B)-C(3B)-C(2B)	120.4(3)
C(4B)-C(3B)-H(3B)	119.8
C(2B)-C(3B)-H(3B)	119.8
C(5B)-C(4B)-C(3B)	120.3(3)
C(5B)-C(4B)-H(4B)	119.9
C(3B)-C(4B)-H(4B)	119.9
C(4B)-C(5B)-C(6B)	119.8(3)
C(4B)-C(5B)-H(5B)	120.1
C(6B)-C(5B)-H(5B)	120.1
C(1B)-C(6B)-C(5B)	120.7(2)
C(1B)-C(6B)-H(6B)	119.6
C(5B)-C(6B)-H(6B)	119.6
C(12B)-C(7B)-C(8B)	118.7(2)
C(12B)-C(7B)-P(1B)	118.86(19)
C(8B)-C(7B)-P(1B)	122.5(2)

C(9B)-C(8B)-C(7B)	120.1(3)
C(9B)-C(8B)-H(8B)	120.0
C(7B)-C(8B)-H(8B)	120.0
C(10B)-C(9B)-C(8B)	120.4(3)
C(10B)-C(9B)-H(9B)	119.8
C(8B)-C(9B)-H(9B)	119.8
C(9B)-C(10B)-C(11B)	119.4(3)
C(9B)-C(10B)-H(10B)	120.3
C(11B)-C(10B)-H(10B)	120.3
C(10B)-C(11B)-C(12B)	120.7(3)
C(10B)-C(11B)-H(11B)	119.6
C(12B)-C(11B)-H(11B)	119.6
C(7B)-C(12B)-C(11B)	120.7(3)
C(7B)-C(12B)-H(12B)	119.7
C(11B)-C(12B)-H(12B)	119.7
C(14B)-C(13B)-C(18B)	119.1(2)
C(14B)-C(13B)-P(1B)	122.95(19)
C(18B)-C(13B)-P(1B)	117.93(19)
C(13B)-C(14B)-C(15B)	120.1(2)
C(13B)-C(14B)-H(14B)	119.9
C(15B)-C(14B)-H(14B)	119.9
C(16B)-C(15B)-C(14B)	120.5(2)
C(16B)-C(15B)-H(15B)	119.7
C(14B)-C(15B)-H(15B)	119.7
C(15B)-C(16B)-C(17B)	119.4(2)
C(15B)-C(16B)-H(16B)	120.3
C(17B)-C(16B)-H(16B)	120.3
C(18B)-C(17B)-C(16B)	120.7(3)
C(18B)-C(17B)-H(17B)	119.7
C(16B)-C(17B)-H(17B)	119.7
C(17B)-C(18B)-C(13B)	120.2(2)
C(17B)-C(18B)-H(18B)	119.9
C(13B)-C(18B)-H(18B)	119.9
C(24B)-C(19B)-C(20B)	117.2(2)
C(24B)-C(19B)-P(2B)	121.7(2)
C(20B)-C(19B)-P(2B)	121.1(2)
C(21B)-C(20B)-C(19B)	121.3(3)
C(21B)-C(20B)-H(20B)	119.4
C(19B)-C(20B)-H(20B)	119.4
C(22B)-C(21B)-C(20B)	119.6(3)
C(22B)-C(21B)-H(21B)	120.2
C(20B)-C(21B)-H(21B)	120.2
C(23B)-C(22B)-C(21B)	119.7(3)
C(23B)-C(22B)-H(22B)	120.1
C(21B)-C(22B)-H(22B)	120.1
C(22B)-C(23B)-C(24B)	120.8(3)
C(22B)-C(23B)-H(23B)	119.6
C(24B)-C(23B)-H(23B)	119.6
C(19B)-C(24B)-C(23B)	121.4(3)
C(19B)-C(24B)-H(24B)	119.3
C(23B)-C(24B)-H(24B)	119.3
C(26B)-C(25B)-C(30B)	118.6(2)
C(26B)-C(25B)-P(2B)	119.06(18)
C(30B)-C(25B)-P(2B)	122.32(19)
C(25B)-C(26B)-C(27B)	120.8(2)
C(25B)-C(26B)-H(26B)	119.6
C(27B)-C(26B)-H(26B)	119.6
C(28B)-C(27B)-C(26B)	119.9(2)
C(28B)-C(27B)-H(27B)	120.1
C(26B)-C(27B)-H(27B)	120.1
C(29B)-C(28B)-C(27B)	120.0(2)
C(29B)-C(28B)-H(28B)	120.0
C(27B)-C(28B)-H(28B)	120.0

C(28B)-C(29B)-C(30B)	120.7(2)
C(28B)-C(29B)-H(29B)	119.6
C(30B)-C(29B)-H(29B)	119.6
C(29B)-C(30B)-C(25B)	120.0(2)
C(29B)-C(30B)-H(30B)	120.0
C(25B)-C(30B)-H(30B)	120.0
C(32B)-C(31B)-C(36B)	118.7(2)
C(32B)-C(31B)-P(2B)	121.22(19)
C(36B)-C(31B)-P(2B)	119.80(19)
C(31B)-C(32B)-C(33B)	120.4(3)
C(31B)-C(32B)-H(32B)	119.8
C(33B)-C(32B)-H(32B)	119.8
C(34B)-C(33B)-C(32B)	120.2(3)
C(34B)-C(33B)-H(33B)	119.9
C(32B)-C(33B)-H(33B)	119.9
C(35B)-C(34B)-C(33B)	119.5(3)
C(35B)-C(34B)-H(34B)	120.2
C(33B)-C(34B)-H(34B)	120.2
C(34B)-C(35B)-C(36B)	120.7(3)
C(34B)-C(35B)-H(35B)	119.6
C(36B)-C(35B)-H(35B)	119.6
C(35B)-C(36B)-C(31B)	120.4(2)
C(35B)-C(36B)-H(36B)	119.8
C(31B)-C(36B)-H(36B)	119.8

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for s1797lm.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Fe(1A)	16(1)	21(1)	28(1)	7(1)	4(1)	2(1)
P(1A)	15(1)	17(1)	16(1)	0(1)	0(1)	0(1)
P(2A)	14(1)	20(1)	18(1)	2(1)	-2(1)	-1(1)
C(1X)	22(1)	16(1)	20(1)	1(1)	4(1)	0(1)
O(1X)	57(1)	37(1)	28(1)	-2(1)	0(1)	-12(1)
N(2X)	20(1)	31(1)	25(1)	2(1)	3(1)	2(1)
O(2X)	30(1)	23(1)	39(1)	-11(1)	3(1)	-8(1)
C(1A)	21(1)	17(1)	17(1)	-3(1)	3(1)	2(1)
C(2A)	34(2)	22(1)	24(2)	-1(1)	-6(1)	3(1)
C(3A)	58(2)	26(2)	25(2)	1(1)	-5(1)	14(1)
C(4A)	47(2)	17(1)	37(2)	-2(1)	8(2)	2(1)
C(5A)	44(2)	28(2)	43(2)	-13(1)	-14(1)	4(1)
C(6A)	39(2)	26(2)	36(2)	-5(1)	-12(1)	5(1)
C(7A)	19(1)	18(1)	19(1)	2(1)	-3(1)	3(1)
C(8A)	26(1)	30(2)	21(1)	-2(1)	3(1)	-1(1)
C(9A)	39(2)	29(2)	18(1)	-1(1)	0(1)	8(1)
C(10A)	41(2)	44(2)	26(2)	0(1)	-16(1)	-11(1)
C(11A)	31(2)	108(3)	37(2)	4(2)	-13(2)	-32(2)
C(12A)	25(2)	87(3)	18(2)	-1(2)	-3(1)	-13(2)
C(13A)	19(1)	22(1)	13(1)	-3(1)	-1(1)	-2(1)
C(14A)	19(1)	23(1)	15(1)	-5(1)	-2(1)	1(1)
C(15A)	27(1)	25(1)	17(1)	4(1)	-2(1)	-5(1)
C(16A)	22(1)	43(2)	19(1)	2(1)	5(1)	-1(1)
C(17A)	24(1)	43(2)	23(2)	5(1)	5(1)	8(1)
C(18A)	27(1)	26(2)	21(1)	6(1)	3(1)	7(1)
C(19A)	19(1)	21(1)	20(1)	5(1)	1(1)	-5(1)
C(20A)	28(2)	28(2)	55(2)	13(2)	-22(1)	-10(1)
C(21A)	34(2)	24(2)	66(2)	15(2)	-12(2)	-4(1)
C(22A)	27(1)	25(1)	49(2)	3(1)	-4(1)	-9(1)
C(23A)	22(1)	34(2)	50(2)	3(1)	-12(1)	-5(1)
C(24A)	19(1)	23(1)	36(2)	1(1)	-7(1)	-1(1)
C(25A)	15(1)	33(2)	18(1)	3(1)	-2(1)	6(1)
C(26A)	28(2)	72(2)	28(2)	-18(2)	12(1)	-18(2)
C(27A)	30(2)	97(3)	36(2)	-31(2)	2(1)	-8(2)
C(28A)	33(2)	80(3)	19(2)	-5(2)	-1(1)	26(2)
C(29A)	58(2)	47(2)	30(2)	16(2)	19(2)	20(2)
C(30A)	40(2)	33(2)	25(2)	10(1)	3(1)	4(1)
C(31A)	13(1)	19(1)	25(1)	0(1)	-4(1)	-2(1)
C(32A)	21(1)	32(2)	29(2)	9(1)	-3(1)	-1(1)
C(33A)	26(1)	35(2)	33(2)	14(1)	-8(1)	-2(1)
C(34A)	24(1)	20(1)	46(2)	4(1)	-13(1)	2(1)
C(35A)	25(1)	29(2)	35(2)	-4(1)	-2(1)	8(1)
C(36A)	27(1)	24(2)	27(2)	1(1)	-4(1)	4(1)
Fe(1B)	14(1)	27(1)	21(1)	5(1)	3(1)	2(1)
P(1B)	14(1)	17(1)	16(1)	-1(1)	0(1)	-1(1)
P(2B)	14(1)	17(1)	15(1)	-2(1)	2(1)	-1(1)
N(2Y)	17(1)	34(1)	35(1)	-4(1)	8(1)	4(1)
O(2Y)	45(1)	22(1)	92(2)	-18(1)	21(1)	-5(1)
C(1Y)	14(1)	23(1)	24(2)	-2(1)	0(1)	5(1)
O(1Y)	31(1)	52(1)	32(1)	-11(1)	-7(1)	9(1)
C(1B)	24(1)	22(1)	13(1)	-3(1)	0(1)	-7(1)
C(2B)	26(1)	30(2)	31(2)	-9(1)	10(1)	-8(1)
C(3B)	39(2)	38(2)	34(2)	-10(1)	7(1)	-20(1)

C(4B)	58(2)	24(2)	22(1)	-5(1)	5(1)	-18(2)
C(5B)	54(2)	20(1)	24(2)	-2(1)	-9(1)	-2(1)
C(6B)	30(1)	23(1)	19(1)	-3(1)	-6(1)	-2(1)
C(7B)	15(1)	16(1)	28(1)	1(1)	-3(1)	-2(1)
C(8B)	19(1)	25(1)	27(1)	-4(1)	0(1)	-1(1)
C(9B)	20(1)	25(1)	45(2)	-8(1)	0(1)	3(1)
C(10B)	19(1)	24(2)	56(2)	8(1)	-8(1)	2(1)
C(11B)	25(1)	44(2)	35(2)	14(1)	0(1)	5(1)
C(12B)	18(1)	35(2)	31(2)	5(1)	3(1)	6(1)
C(13B)	11(1)	23(1)	20(1)	-3(1)	1(1)	3(1)
C(14B)	25(1)	20(1)	21(1)	1(1)	0(1)	0(1)
C(15B)	27(1)	28(1)	23(1)	3(1)	3(1)	4(1)
C(16B)	22(1)	37(2)	20(1)	-8(1)	-2(1)	6(1)
C(17B)	19(1)	34(2)	27(2)	-13(1)	1(1)	-4(1)
C(18B)	20(1)	28(2)	25(1)	-5(1)	3(1)	-7(1)
C(19B)	19(1)	17(1)	18(1)	2(1)	-2(1)	-4(1)
C(20B)	23(1)	44(2)	26(2)	-4(1)	2(1)	3(1)
C(21B)	20(1)	41(2)	33(2)	4(1)	-2(1)	-6(1)
C(22B)	42(2)	37(2)	37(2)	-3(1)	-21(2)	-4(1)
C(23B)	72(2)	80(3)	40(2)	-36(2)	-28(2)	46(2)
C(24B)	41(2)	63(2)	39(2)	-21(2)	-16(2)	30(2)
C(25B)	14(1)	22(1)	15(1)	-2(1)	2(1)	-3(1)
C(26B)	20(1)	24(1)	22(1)	1(1)	5(1)	2(1)
C(27B)	35(2)	21(1)	26(1)	5(1)	6(1)	1(1)
C(28B)	28(1)	32(2)	23(1)	-1(1)	10(1)	-5(1)
C(29B)	20(1)	29(2)	31(2)	-3(1)	9(1)	3(1)
C(30B)	19(1)	26(2)	23(1)	1(1)	2(1)	5(1)
C(31B)	14(1)	20(1)	20(1)	-2(1)	5(1)	-1(1)
C(32B)	43(2)	23(1)	20(1)	-4(1)	3(1)	-7(1)
C(33B)	69(2)	23(2)	24(2)	5(1)	5(2)	-8(2)
C(34B)	51(2)	19(1)	30(2)	-4(1)	7(1)	-8(1)
C(35B)	38(2)	27(2)	24(2)	-10(1)	1(1)	-1(1)
C(36B)	24(1)	21(1)	23(1)	-1(1)	3(1)	5(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for s1797lm.

	x	y	z	U(eq)
H(1A)	2162(11)	5250(20)	3958(14)	41(9)
H(2A)	826	6924	3712	32
H(3A)	938	8648	3716	43
H(4A)	1531	9410	4499	40
H(5A)	2014	8441	5281	46
H(6A)	1919	6720	5263	40
H(8A)	1519	5132	3088	31
H(9A)	982	4637	2168	34
H(10A)	32	4097	2296	44
H(11A)	-380	4050	3341	71
H(12A)	136	4630	4257	52
H(14A)	1137	3606	5313	23
H(15A)	440	3116	6088	28
H(16A)	-278	4237	6415	33
H(17A)	-299	5831	5989	36
H(18A)	390	6320	5202	29
H(20A)	2695	6620	3940	44
H(21A)	3069	8171	4187	50
H(22A)	3939	8322	4760	40

H(23A)	4443	6892	5062	42
H(24A)	4081	5326	4804	31
H(26A)	2564	3237	3227	51
H(27A)	2678	2895	2097	65
H(28A)	3276	3886	1456	53
H(29A)	3764	5217	1929	54
H(30A)	3649	5574	3050	39
H(32A)	3178	3548	5377	33
H(33A)	3847	2431	5812	38
H(34A)	4625	1885	5163	36
H(35A)	4733	2475	4089	35
H(36A)	4061	3595	3656	31
H(1B)	1299(11)	40(20)	2730(14)	36(8)
H(2B)	-778	-419	2429	35
H(3B)	-1139	-2043	2422	45
H(4B)	-507	-3387	2463	42
H(5B)	490	-3130	2439	39
H(6B)	859	-1513	2435	29
H(8B)	-578	1698	3074	28
H(9B)	-1306	2666	2583	36
H(10B)	-1356	2815	1440	40
H(11B)	-683	1987	781	42
H(12B)	38	1016	1257	34
H(14B)	-149	-575	3704	27
H(15B)	-251	-189	4827	31
H(16B)	107	1306	5242	32
H(17B)	573	2419	4531	32
H(18B)	710	2020	3423	29
H(20B)	3244	-600	2695	37
H(21B)	3786	-299	3645	38
H(22B)	3412	728	4473	46
H(23B)	2511	1430	4346	77
H(24B)	1968	1145	3395	57
H(26B)	2117	1694	1295	26
H(27B)	2749	2360	505	33
H(28B)	3625	1565	276	34
H(29B)	3861	95	815	32
H(30B)	3230	-597	1591	27
H(32B)	2209	-1665	3058	34
H(33B)	2158	-3391	2917	47
H(34B)	2069	-4067	1860	40
H(35B)	2001	-3019	949	35
H(36B)	2046	-1305	1080	27

Table 6. Torsion angles [deg] for s1797lm.

N(2X)-Fe(1A)-P(1A)-C(1A)	-164.88(12)
C(1X)-Fe(1A)-P(1A)-C(1A)	66.60(13)
P(2A)-Fe(1A)-P(1A)-C(1A)	-36.68(11)
N(2X)-Fe(1A)-P(1A)-C(13A)	73.77(12)
C(1X)-Fe(1A)-P(1A)-C(13A)	-54.75(12)
P(2A)-Fe(1A)-P(1A)-C(13A)	-158.03(9)
N(2X)-Fe(1A)-P(1A)-C(7A)	-42.39(12)
C(1X)-Fe(1A)-P(1A)-C(7A)	-170.92(12)
P(2A)-Fe(1A)-P(1A)-C(7A)	85.80(10)
N(2X)-Fe(1A)-P(2A)-C(19A)	178.21(12)
C(1X)-Fe(1A)-P(2A)-C(19A)	-52.30(12)
P(1A)-Fe(1A)-P(2A)-C(19A)	52.51(10)
N(2X)-Fe(1A)-P(2A)-C(25A)	57.68(12)

C(1X)-Fe(1A)-P(2A)-C(25A)	-172.83(13)
P(1A)-Fe(1A)-P(2A)-C(25A)	-68.02(11)
N(2X)-Fe(1A)-P(2A)-C(31A)	-62.01(12)
C(1X)-Fe(1A)-P(2A)-C(31A)	67.48(12)
P(1A)-Fe(1A)-P(2A)-C(31A)	172.29(9)
N(2X)-Fe(1A)-C(1X)-O(1X)	74(19)
P(1A)-Fe(1A)-C(1X)-O(1X)	179(100)
P(2A)-Fe(1A)-C(1X)-O(1X)	-39(19)
C(1X)-Fe(1A)-N(2X)-O(2X)	77(3)
P(1A)-Fe(1A)-N(2X)-O(2X)	-28(3)
P(2A)-Fe(1A)-N(2X)-O(2X)	-177(100)
C(13A)-P(1A)-C(1A)-C(6A)	78.9(2)
C(7A)-P(1A)-C(1A)-C(6A)	-174.4(2)
Fe(1A)-P(1A)-C(1A)-C(6A)	-48.3(2)
C(13A)-P(1A)-C(1A)-C(2A)	-103.4(2)
C(7A)-P(1A)-C(1A)-C(2A)	3.3(2)
Fe(1A)-P(1A)-C(1A)-C(2A)	129.4(2)
C(6A)-C(1A)-C(2A)-C(3A)	0.4(4)
P(1A)-C(1A)-C(2A)-C(3A)	-177.3(2)
C(1A)-C(2A)-C(3A)-C(4A)	-0.6(4)
C(2A)-C(3A)-C(4A)-C(5A)	0.0(4)
C(3A)-C(4A)-C(5A)-C(6A)	0.7(5)
C(2A)-C(1A)-C(6A)-C(5A)	0.4(4)
P(1A)-C(1A)-C(6A)-C(5A)	178.2(2)
C(4A)-C(5A)-C(6A)-C(1A)	-0.9(5)
C(1A)-P(1A)-C(7A)-C(12A)	-106.1(3)
C(13A)-P(1A)-C(7A)-C(12A)	2.1(3)
Fe(1A)-P(1A)-C(7A)-C(12A)	125.9(2)
C(1A)-P(1A)-C(7A)-C(8A)	80.5(2)
C(13A)-P(1A)-C(7A)-C(8A)	-171.4(2)
Fe(1A)-P(1A)-C(7A)-C(8A)	-47.5(2)
C(12A)-C(7A)-C(8A)-C(9A)	2.4(4)
P(1A)-C(7A)-C(8A)-C(9A)	176.0(2)
C(7A)-C(8A)-C(9A)-C(10A)	-2.2(4)
C(8A)-C(9A)-C(10A)-C(11A)	-0.1(5)
C(9A)-C(10A)-C(11A)-C(12A)	2.0(6)
C(8A)-C(7A)-C(12A)-C(11A)	-0.5(5)
P(1A)-C(7A)-C(12A)-C(11A)	-174.0(3)
C(10A)-C(11A)-C(12A)-C(7A)	-1.7(6)
C(1A)-P(1A)-C(13A)-C(18A)	27.1(2)
C(7A)-P(1A)-C(13A)-C(18A)	-82.8(2)
Fe(1A)-P(1A)-C(13A)-C(18A)	154.88(19)
C(1A)-P(1A)-C(13A)-C(14A)	-159.36(19)
C(7A)-P(1A)-C(13A)-C(14A)	90.8(2)
Fe(1A)-P(1A)-C(13A)-C(14A)	-31.5(2)
C(18A)-C(13A)-C(14A)-C(15A)	1.6(4)
P(1A)-C(13A)-C(14A)-C(15A)	-172.18(18)
C(13A)-C(14A)-C(15A)-C(16A)	-0.8(4)
C(14A)-C(15A)-C(16A)-C(17A)	-0.5(4)
C(15A)-C(16A)-C(17A)-C(18A)	0.9(4)
C(14A)-C(13A)-C(18A)-C(17A)	-1.2(4)
P(1A)-C(13A)-C(18A)-C(17A)	172.3(2)
C(16A)-C(17A)-C(18A)-C(13A)	-0.1(4)
C(25A)-P(2A)-C(19A)-C(24A)	-110.7(2)
C(31A)-P(2A)-C(19A)-C(24A)	-3.7(2)
Fe(1A)-P(2A)-C(19A)-C(24A)	123.5(2)
C(25A)-P(2A)-C(19A)-C(20A)	75.3(2)
C(31A)-P(2A)-C(19A)-C(20A)	-177.8(2)
Fe(1A)-P(2A)-C(19A)-C(20A)	-50.6(2)
C(24A)-C(19A)-C(20A)-C(21A)	2.6(4)
P(2A)-C(19A)-C(20A)-C(21A)	177.0(3)
C(19A)-C(20A)-C(21A)-C(22A)	-1.9(5)
C(20A)-C(21A)-C(22A)-C(23A)	0.5(5)

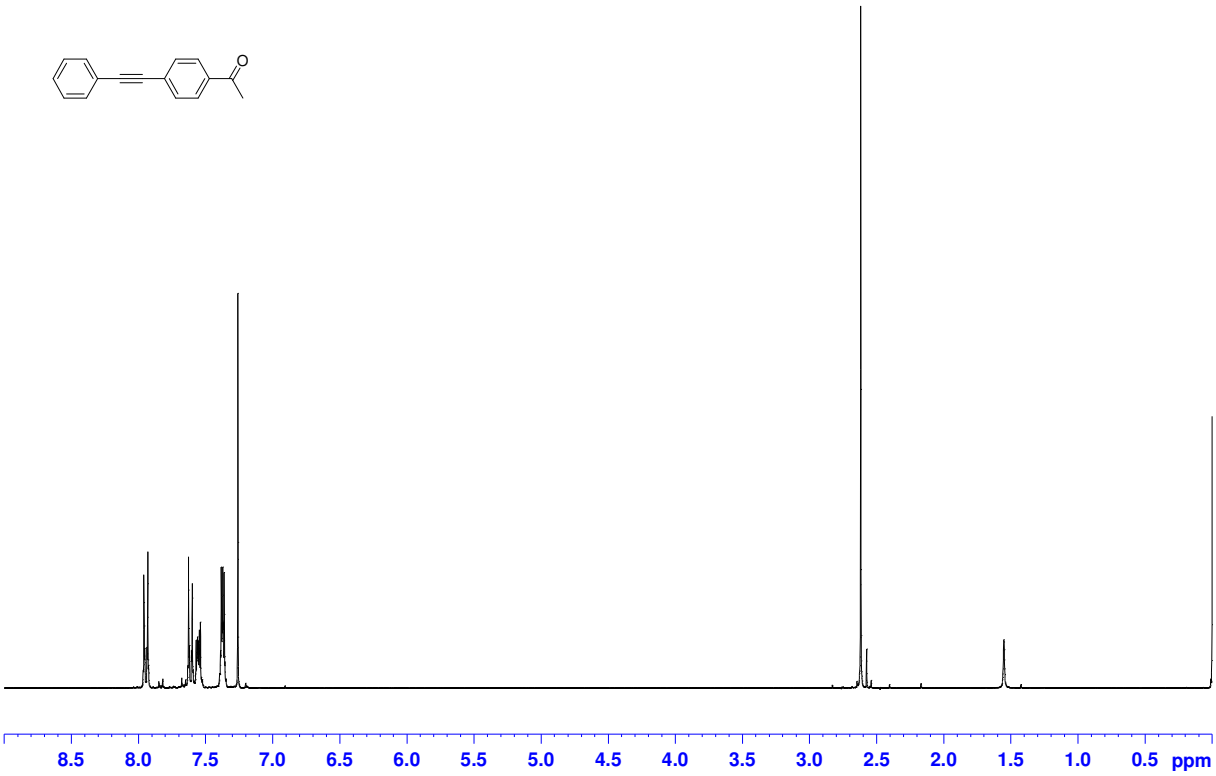
C(21A)-C(22A)-C(23A)-C(24A)	0.0(5)
C(22A)-C(23A)-C(24A)-C(19A)	0.8(4)
C(20A)-C(19A)-C(24A)-C(23A)	-2.1(4)
P(2A)-C(19A)-C(24A)-C(23A)	-176.2(2)
C(19A)-P(2A)-C(25A)-C(26A)	-170.5(2)
C(31A)-P(2A)-C(25A)-C(26A)	81.2(2)
Fe(1A)-P(2A)-C(25A)-C(26A)	-46.5(2)
C(19A)-P(2A)-C(25A)-C(30A)	12.3(3)
C(31A)-P(2A)-C(25A)-C(30A)	-96.0(2)
Fe(1A)-P(2A)-C(25A)-C(30A)	136.3(2)
C(30A)-C(25A)-C(26A)-C(27A)	1.0(5)
P(2A)-C(25A)-C(26A)-C(27A)	-176.3(3)
C(25A)-C(26A)-C(27A)-C(28A)	-0.3(5)
C(26A)-C(27A)-C(28A)-C(29A)	-0.1(5)
C(27A)-C(28A)-C(29A)-C(30A)	-0.1(5)
C(26A)-C(25A)-C(30A)-C(29A)	-1.3(4)
P(2A)-C(25A)-C(30A)-C(29A)	175.8(2)
C(28A)-C(29A)-C(30A)-C(25A)	0.9(4)
C(19A)-P(2A)-C(31A)-C(36A)	-86.5(2)
C(25A)-P(2A)-C(31A)-C(36A)	23.2(2)
Fe(1A)-P(2A)-C(31A)-C(36A)	149.54(18)
C(19A)-P(2A)-C(31A)-C(32A)	93.0(2)
C(25A)-P(2A)-C(31A)-C(32A)	-157.4(2)
Fe(1A)-P(2A)-C(31A)-C(32A)	-31.0(2)
C(36A)-C(31A)-C(32A)-C(33A)	0.6(4)
P(2A)-C(31A)-C(32A)-C(33A)	-178.8(2)
C(31A)-C(32A)-C(33A)-C(34A)	-0.4(4)
C(32A)-C(33A)-C(34A)-C(35A)	0.3(4)
C(33A)-C(34A)-C(35A)-C(36A)	-0.3(4)
C(32A)-C(31A)-C(36A)-C(35A)	-0.6(4)
P(2A)-C(31A)-C(36A)-C(35A)	178.8(2)
C(34A)-C(35A)-C(36A)-C(31A)	0.4(4)
N(2Y)-Fe(1B)-P(1B)-C(1B)	174.68(12)
C(1Y)-Fe(1B)-P(1B)-C(1B)	51.19(12)
P(2B)-Fe(1B)-P(1B)-C(1B)	-51.41(10)
N(2Y)-Fe(1B)-P(1B)-C(13B)	-64.76(12)
C(1Y)-Fe(1B)-P(1B)-C(13B)	171.74(12)
P(2B)-Fe(1B)-P(1B)-C(13B)	69.15(10)
N(2Y)-Fe(1B)-P(1B)-C(7B)	54.08(13)
C(1Y)-Fe(1B)-P(1B)-C(7B)	-69.42(13)
P(2B)-Fe(1B)-P(1B)-C(7B)	-172.02(9)
N(2Y)-Fe(1B)-P(2B)-C(31B)	-179.63(12)
C(1Y)-Fe(1B)-P(2B)-C(31B)	-57.17(13)
P(1B)-Fe(1B)-P(2B)-C(31B)	46.16(11)
N(2Y)-Fe(1B)-P(2B)-C(19B)	59.37(12)
C(1Y)-Fe(1B)-P(2B)-C(19B)	-178.17(12)
P(1B)-Fe(1B)-P(2B)-C(19B)	-74.84(10)
N(2Y)-Fe(1B)-P(2B)-C(25B)	-60.44(12)
C(1Y)-Fe(1B)-P(2B)-C(25B)	62.03(12)
P(1B)-Fe(1B)-P(2B)-C(25B)	165.35(9)
C(1Y)-Fe(1B)-N(2Y)-O(2Y)	-25(2)
P(2B)-Fe(1B)-N(2Y)-O(2Y)	77(2)
P(1B)-Fe(1B)-N(2Y)-O(2Y)	-130.2(19)
N(2Y)-Fe(1B)-C(1Y)-O(1Y)	15(4)
P(2B)-Fe(1B)-C(1Y)-O(1Y)	-92(4)
P(1B)-Fe(1B)-C(1Y)-O(1Y)	126(4)
C(13B)-P(1B)-C(1B)-C(6B)	-97.4(2)
C(7B)-P(1B)-C(1B)-C(6B)	157.1(2)
Fe(1B)-P(1B)-C(1B)-C(6B)	29.9(2)
C(13B)-P(1B)-C(1B)-C(2B)	78.6(2)
C(7B)-P(1B)-C(1B)-C(2B)	-26.9(2)
Fe(1B)-P(1B)-C(1B)-C(2B)	-154.08(19)
C(6B)-C(1B)-C(2B)-C(3B)	3.0(4)

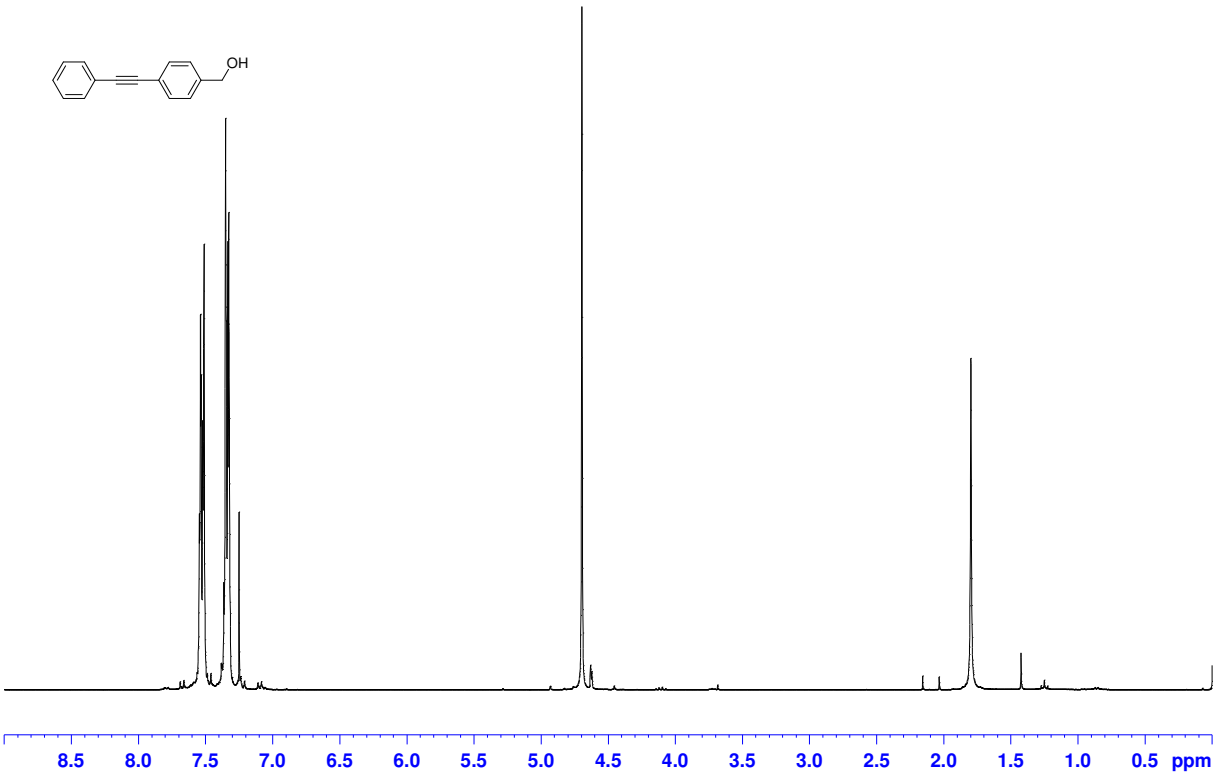
P(1B)-C(1B)-C(2B)-C(3B)	-173.1(2)
C(1B)-C(2B)-C(3B)-C(4B)	-0.2(4)
C(2B)-C(3B)-C(4B)-C(5B)	-2.4(4)
C(3B)-C(4B)-C(5B)-C(6B)	2.0(4)
C(2B)-C(1B)-C(6B)-C(5B)	-3.3(4)
P(1B)-C(1B)-C(6B)-C(5B)	172.8(2)
C(4B)-C(5B)-C(6B)-C(1B)	0.8(4)
C(1B)-P(1B)-C(7B)-C(12B)	-79.6(2)
C(13B)-P(1B)-C(7B)-C(12B)	173.9(2)
Fe(1B)-P(1B)-C(7B)-C(12B)	47.5(2)
C(1B)-P(1B)-C(7B)-C(8B)	99.7(2)
C(13B)-P(1B)-C(7B)-C(8B)	-6.8(2)
Fe(1B)-P(1B)-C(7B)-C(8B)	-133.16(18)
C(12B)-C(7B)-C(8B)-C(9B)	0.7(4)
P(1B)-C(7B)-C(8B)-C(9B)	-178.65(19)
C(7B)-C(8B)-C(9B)-C(10B)	-0.6(4)
C(8B)-C(9B)-C(10B)-C(11B)	0.2(4)
C(9B)-C(10B)-C(11B)-C(12B)	0.0(4)
C(8B)-C(7B)-C(12B)-C(11B)	-0.4(4)
P(1B)-C(7B)-C(12B)-C(11B)	178.9(2)
C(10B)-C(11B)-C(12B)-C(7B)	0.1(4)
C(1B)-P(1B)-C(13B)-C(14B)	-6.1(2)
C(7B)-P(1B)-C(13B)-C(14B)	100.4(2)
Fe(1B)-P(1B)-C(13B)-C(14B)	-133.27(18)
C(1B)-P(1B)-C(13B)-C(18B)	176.67(19)
C(7B)-P(1B)-C(13B)-C(18B)	-76.7(2)
Fe(1B)-P(1B)-C(13B)-C(18B)	49.6(2)
C(18B)-C(13B)-C(14B)-C(15B)	-0.9(4)
P(1B)-C(13B)-C(14B)-C(15B)	-178.00(18)
C(13B)-C(14B)-C(15B)-C(16B)	1.2(4)
C(14B)-C(15B)-C(16B)-C(17B)	-0.2(4)
C(15B)-C(16B)-C(17B)-C(18B)	-1.1(4)
C(16B)-C(17B)-C(18B)-C(13B)	1.4(4)
C(14B)-C(13B)-C(18B)-C(17B)	-0.4(4)
P(1B)-C(13B)-C(18B)-C(17B)	176.85(19)
C(31B)-P(2B)-C(19B)-C(24B)	-131.1(3)
C(25B)-P(2B)-C(19B)-C(24B)	121.4(3)
Fe(1B)-P(2B)-C(19B)-C(24B)	-4.7(3)
C(31B)-P(2B)-C(19B)-C(20B)	49.0(2)
C(25B)-P(2B)-C(19B)-C(20B)	-58.5(2)
Fe(1B)-P(2B)-C(19B)-C(20B)	175.42(18)
C(24B)-C(19B)-C(20B)-C(21B)	-0.9(4)
P(2B)-C(19B)-C(20B)-C(21B)	179.0(2)
C(19B)-C(20B)-C(21B)-C(22B)	0.5(4)
C(20B)-C(21B)-C(22B)-C(23B)	0.2(5)
C(21B)-C(22B)-C(23B)-C(24B)	-0.4(6)
C(20B)-C(19B)-C(24B)-C(23B)	0.6(5)
P(2B)-C(19B)-C(24B)-C(23B)	-179.3(3)
C(22B)-C(23B)-C(24B)-C(19B)	0.0(6)
C(31B)-P(2B)-C(25B)-C(26B)	142.6(2)
C(19B)-P(2B)-C(25B)-C(26B)	-109.6(2)
Fe(1B)-P(2B)-C(25B)-C(26B)	17.6(2)
C(31B)-P(2B)-C(25B)-C(30B)	-39.7(2)
C(19B)-P(2B)-C(25B)-C(30B)	68.1(2)
Fe(1B)-P(2B)-C(25B)-C(30B)	-164.74(18)
C(30B)-C(25B)-C(26B)-C(27B)	-1.4(4)
P(2B)-C(25B)-C(26B)-C(27B)	176.3(2)
C(25B)-C(26B)-C(27B)-C(28B)	0.0(4)
C(26B)-C(27B)-C(28B)-C(29B)	0.8(4)
C(27B)-C(28B)-C(29B)-C(30B)	-0.3(4)
C(28B)-C(29B)-C(30B)-C(25B)	-1.2(4)
C(26B)-C(25B)-C(30B)-C(29B)	2.0(4)
P(2B)-C(25B)-C(30B)-C(29B)	-175.7(2)

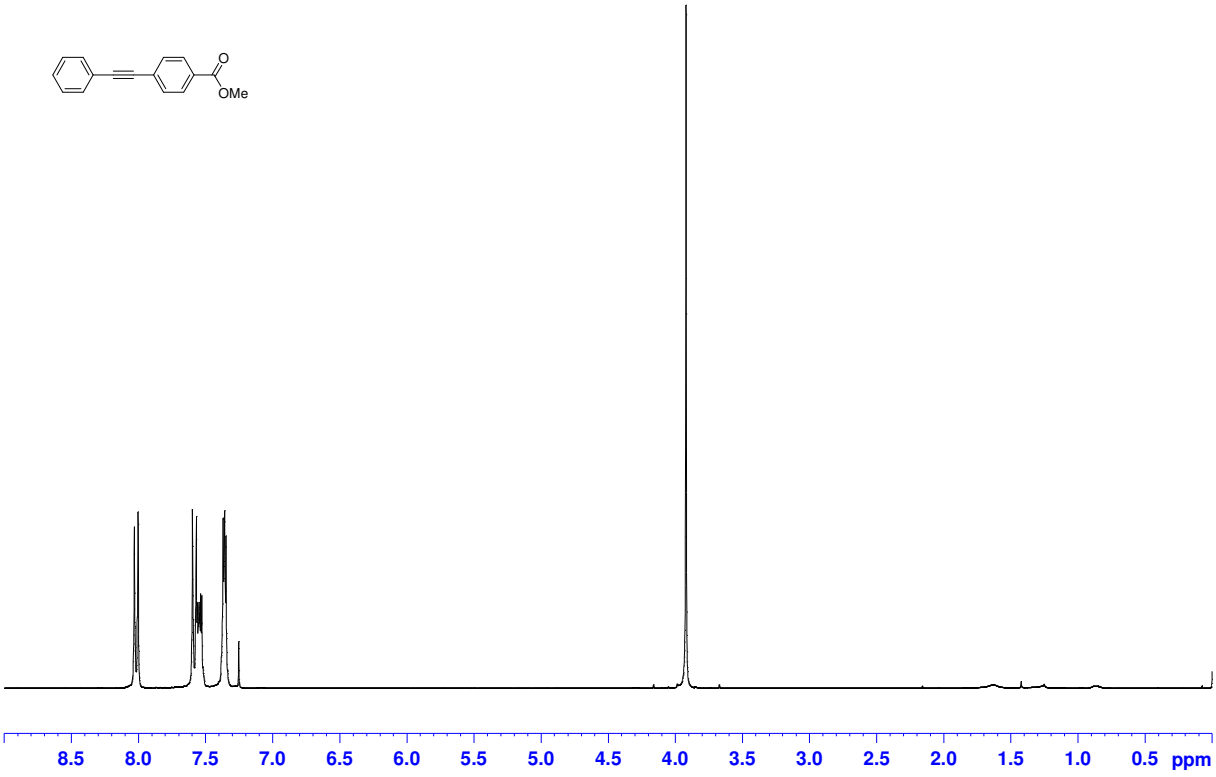
C(19B)-P(2B)-C(31B)-C(32B)	31.4(2)
C(25B)-P(2B)-C(31B)-C(32B)	138.3(2)
Fe(1B)-P(2B)-C(31B)-C(32B)	-96.4(2)
C(19B)-P(2B)-C(31B)-C(36B)	-154.92(18)
C(25B)-P(2B)-C(31B)-C(36B)	-48.0(2)
Fe(1B)-P(2B)-C(31B)-C(36B)	77.31(19)
C(36B)-C(31B)-C(32B)-C(33B)	1.2(4)
P(2B)-C(31B)-C(32B)-C(33B)	175.0(2)
C(31B)-C(32B)-C(33B)-C(34B)	0.0(4)
C(32B)-C(33B)-C(34B)-C(35B)	-1.1(5)
C(33B)-C(34B)-C(35B)-C(36B)	0.9(4)
C(34B)-C(35B)-C(36B)-C(31B)	0.4(4)
C(32B)-C(31B)-C(36B)-C(35B)	-1.4(3)
P(2B)-C(31B)-C(36B)-C(35B)	-175.28(19)

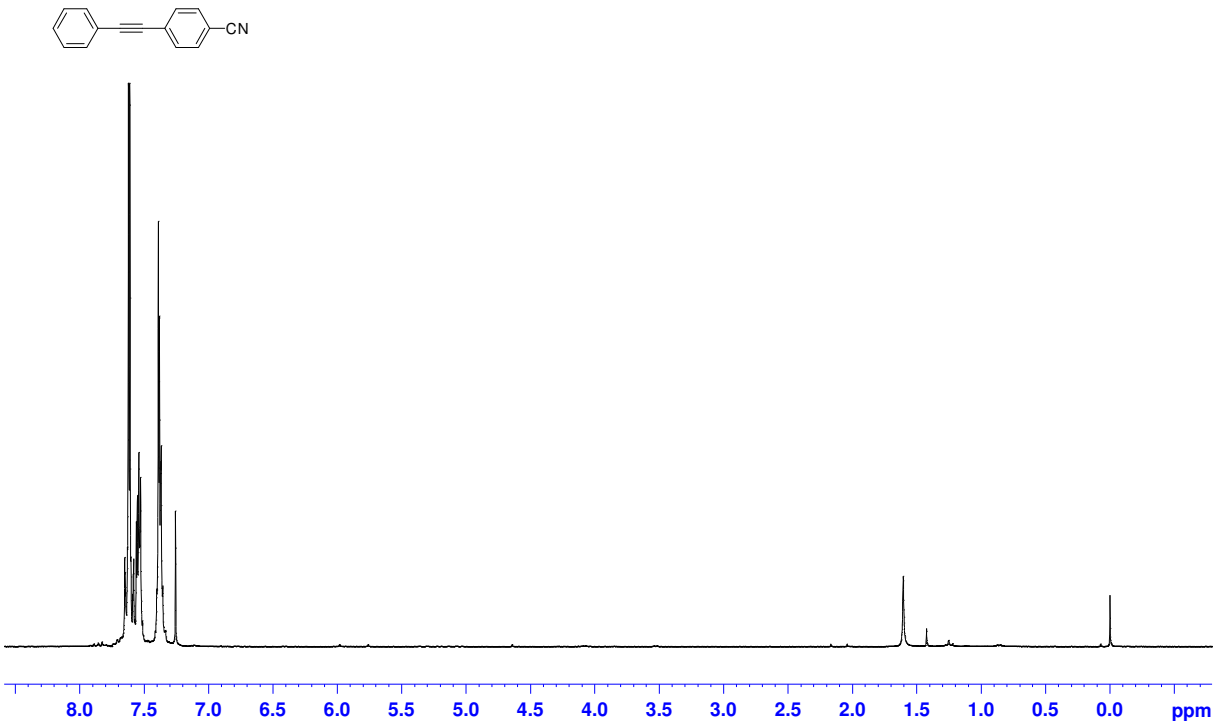
Symmetry transformations used to generate equivalent atoms:

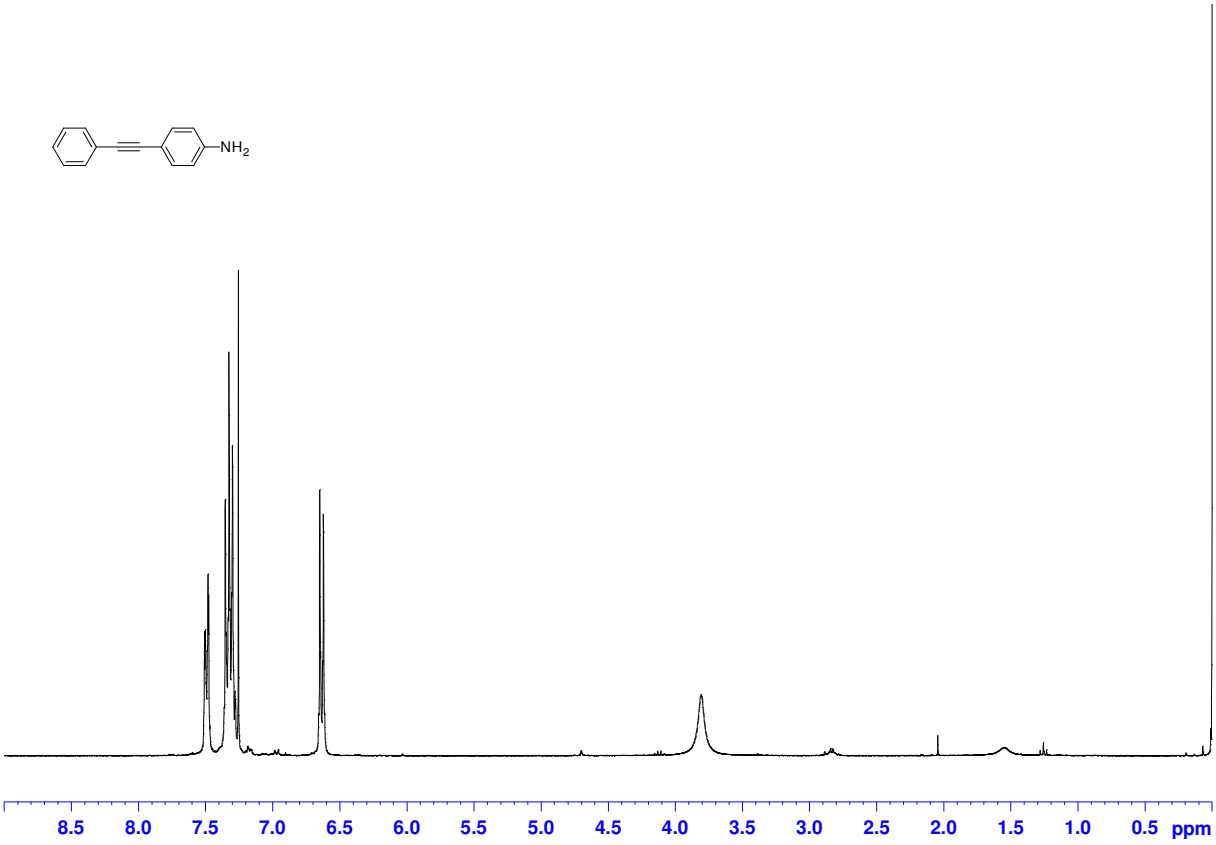
7 Spectra

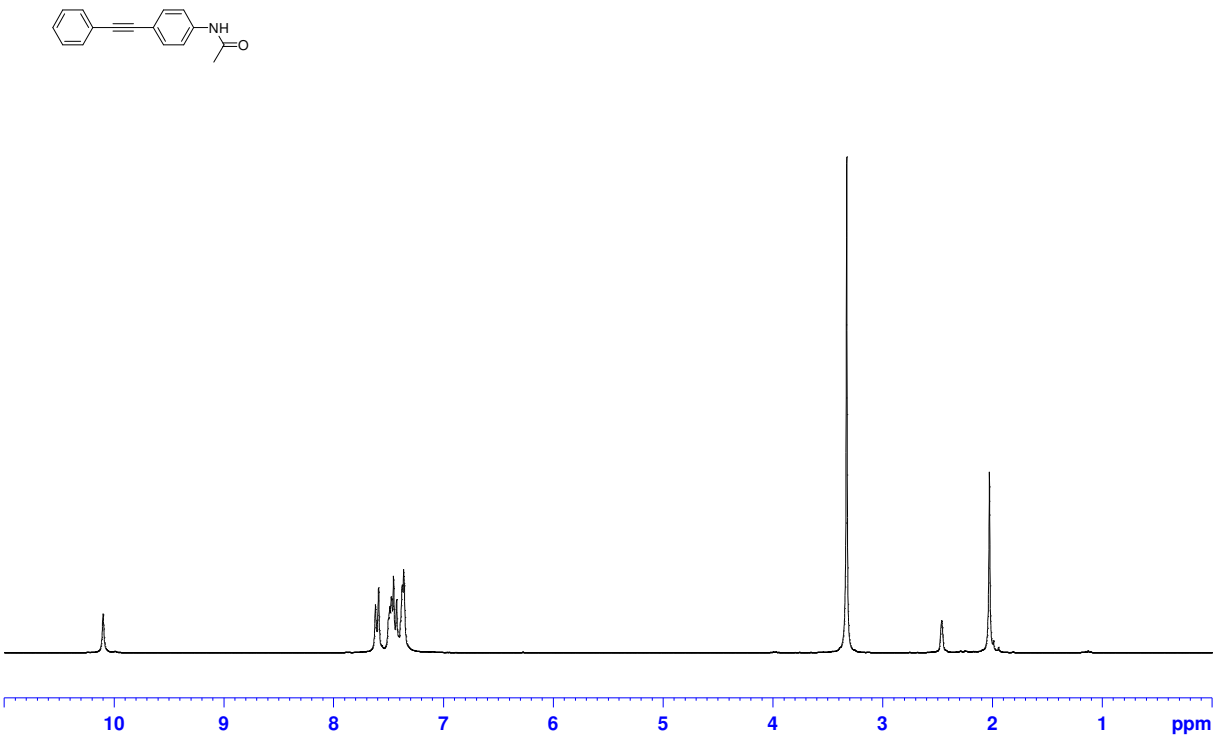


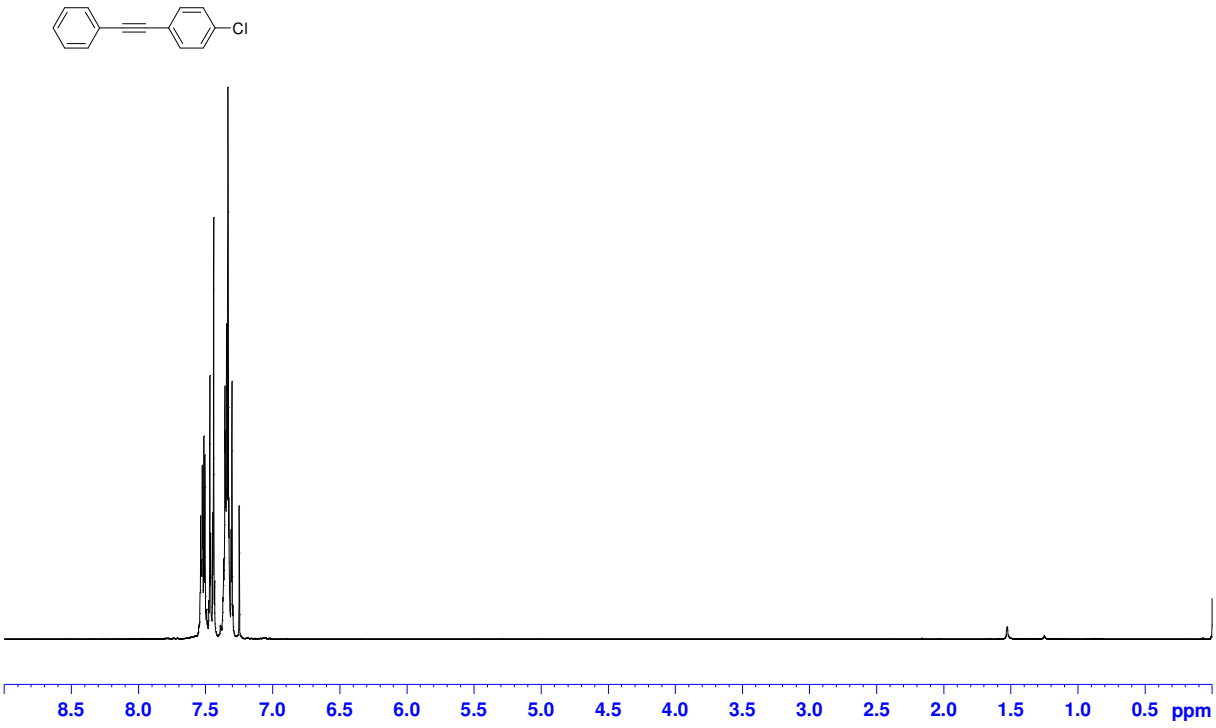








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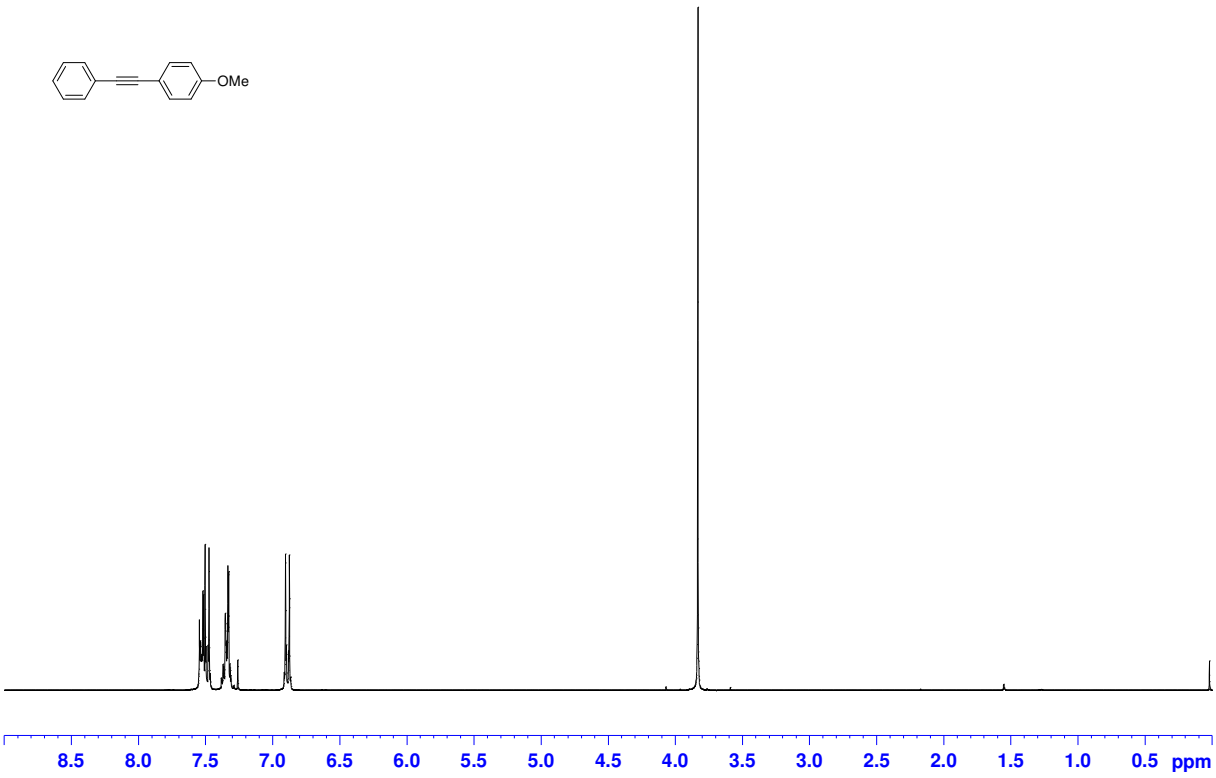
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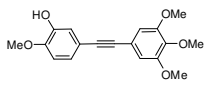

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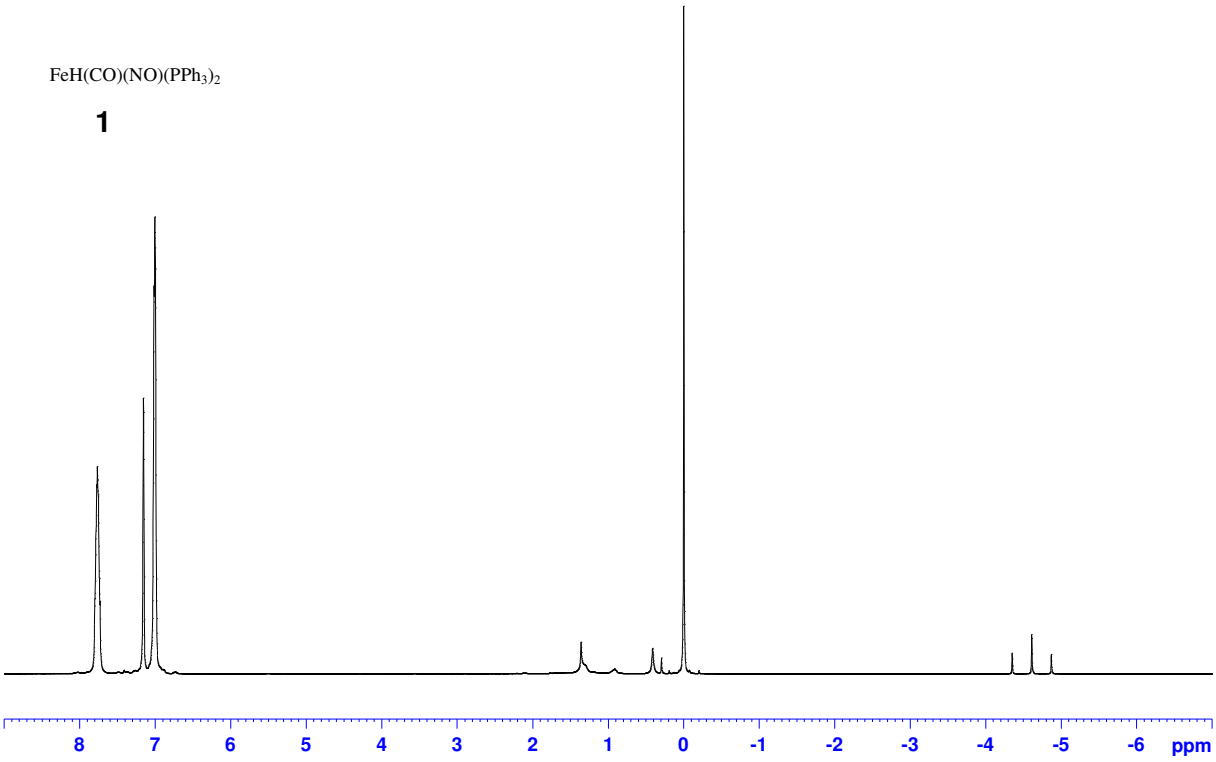
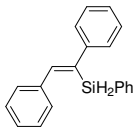
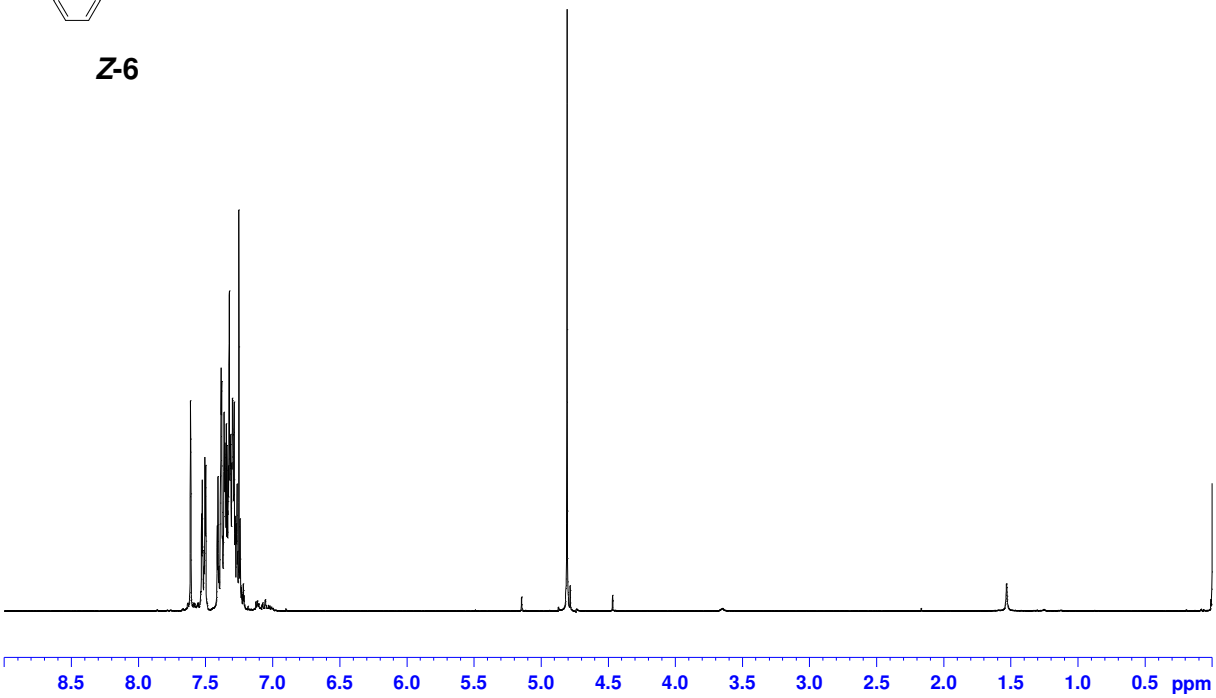
$FeH(CO)(NO)(PPh_3)_2$

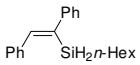
1



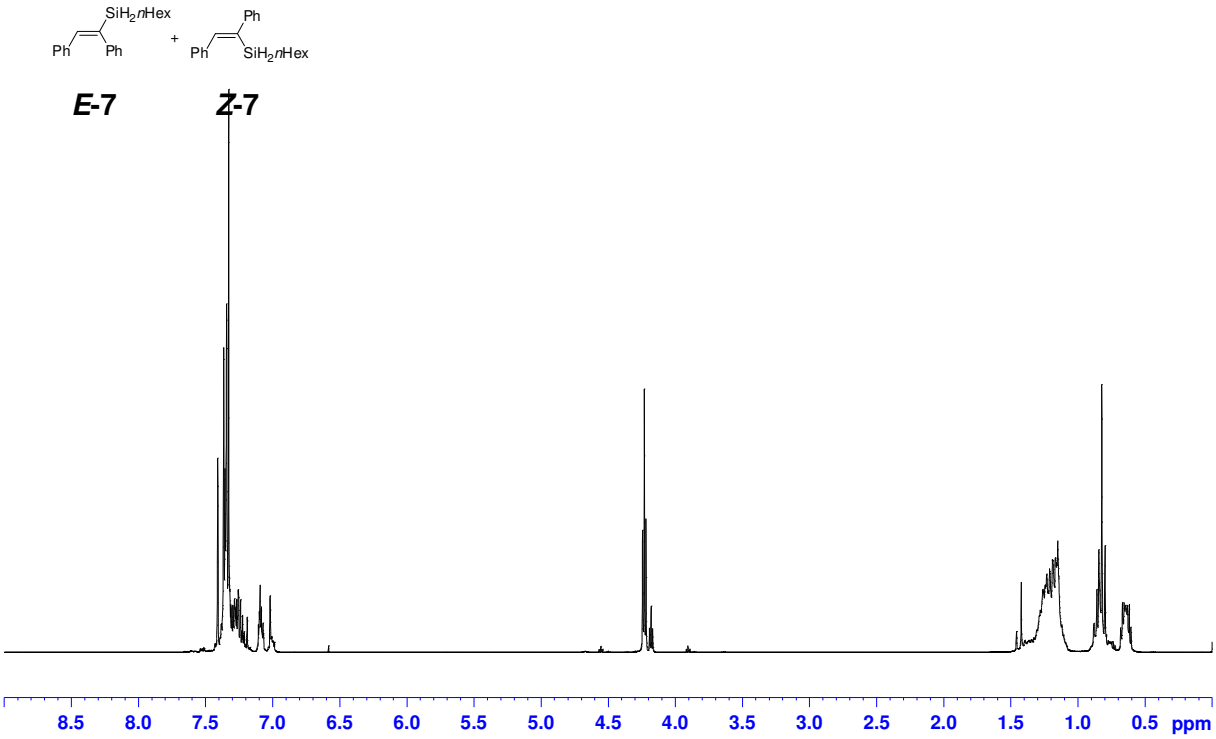


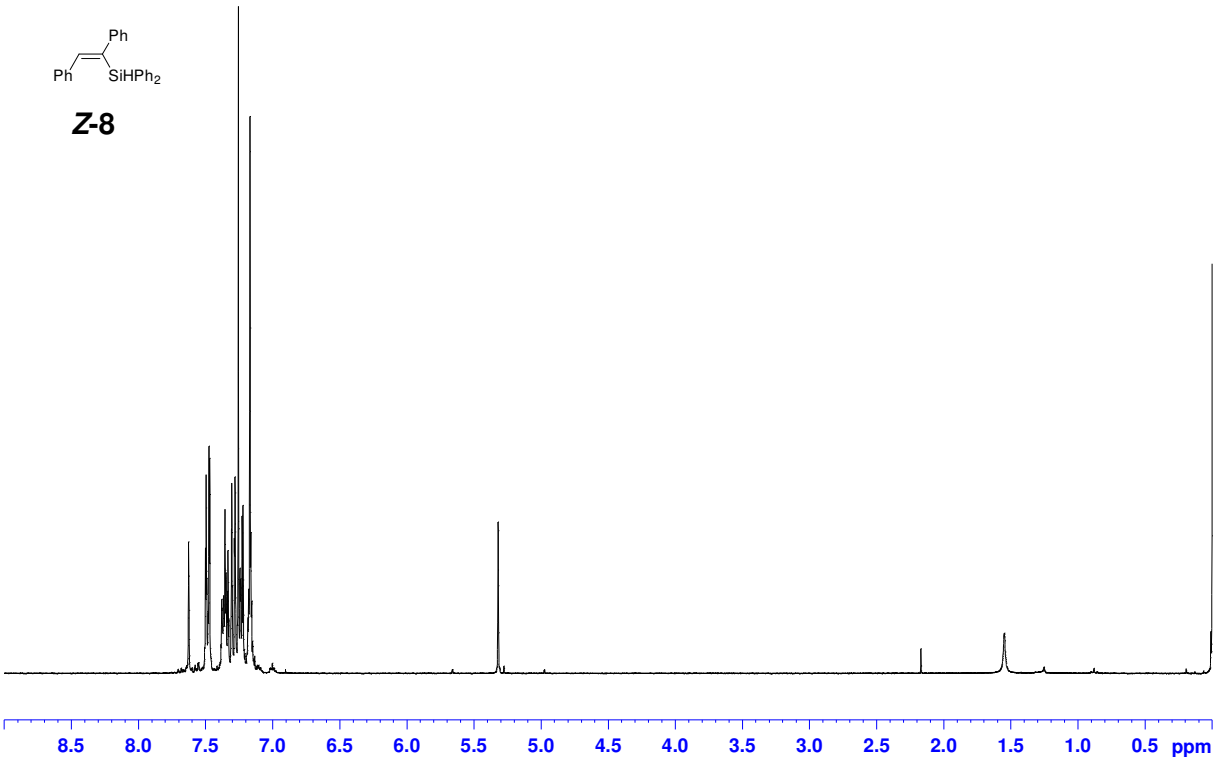
***Z*-6**

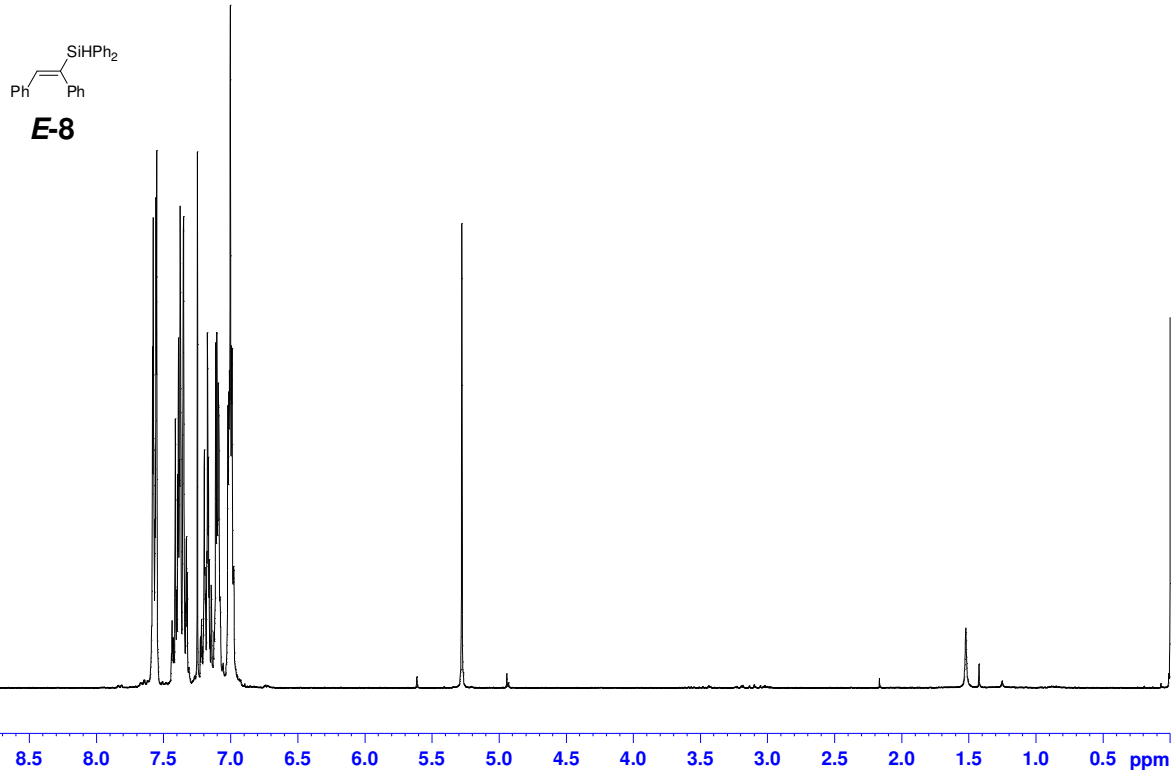




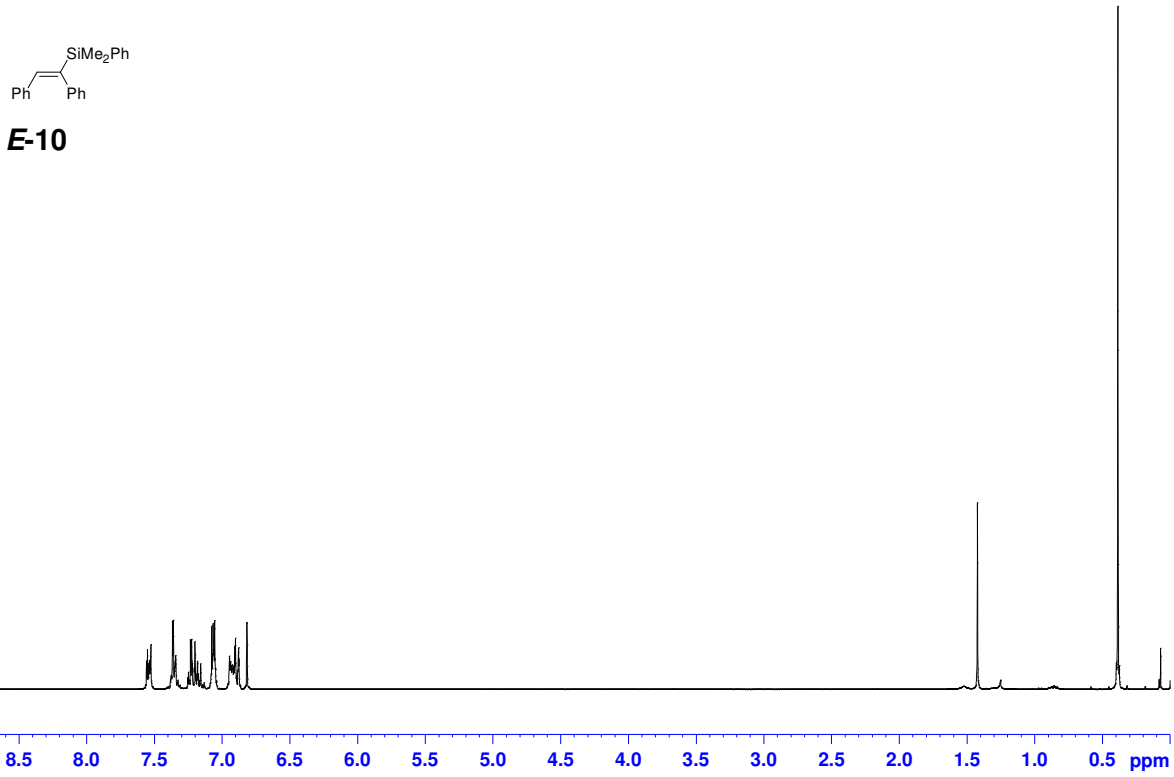
***Z*-7**


SiH2nHex
Ph
Ph
+
Ph
Ph
SiH2nHex
E-7
Z-7
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

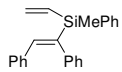

Ph
Ph
SiHPh2
Z-8
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm


SiHPh2
Ph
Ph
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

***E*-8**

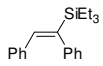

SiMe2Ph
Ph
Ph
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

***E*-10**


SiMePh
Ph
Ph

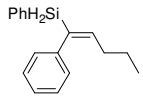
***E*-11**

9
8
7
6
5
4
3
2
1
0
-1
ppm

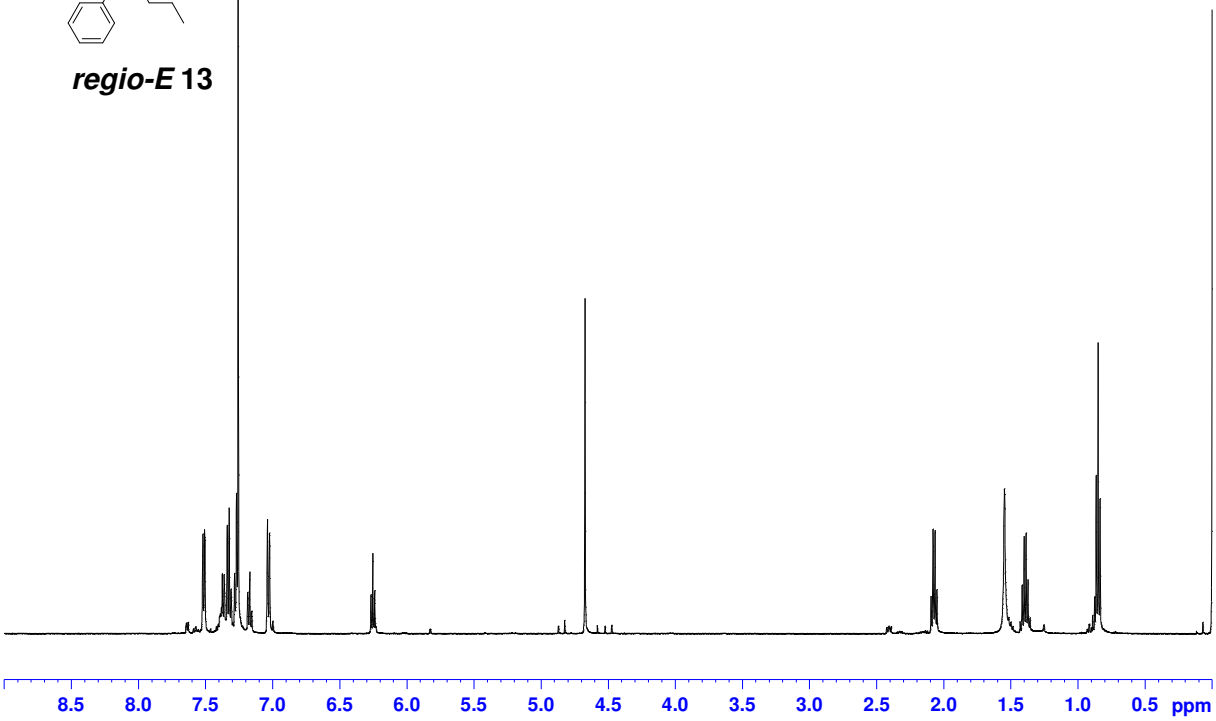

SiEt3
Ph
Ph

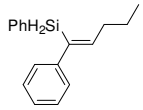
***E*-12**

8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

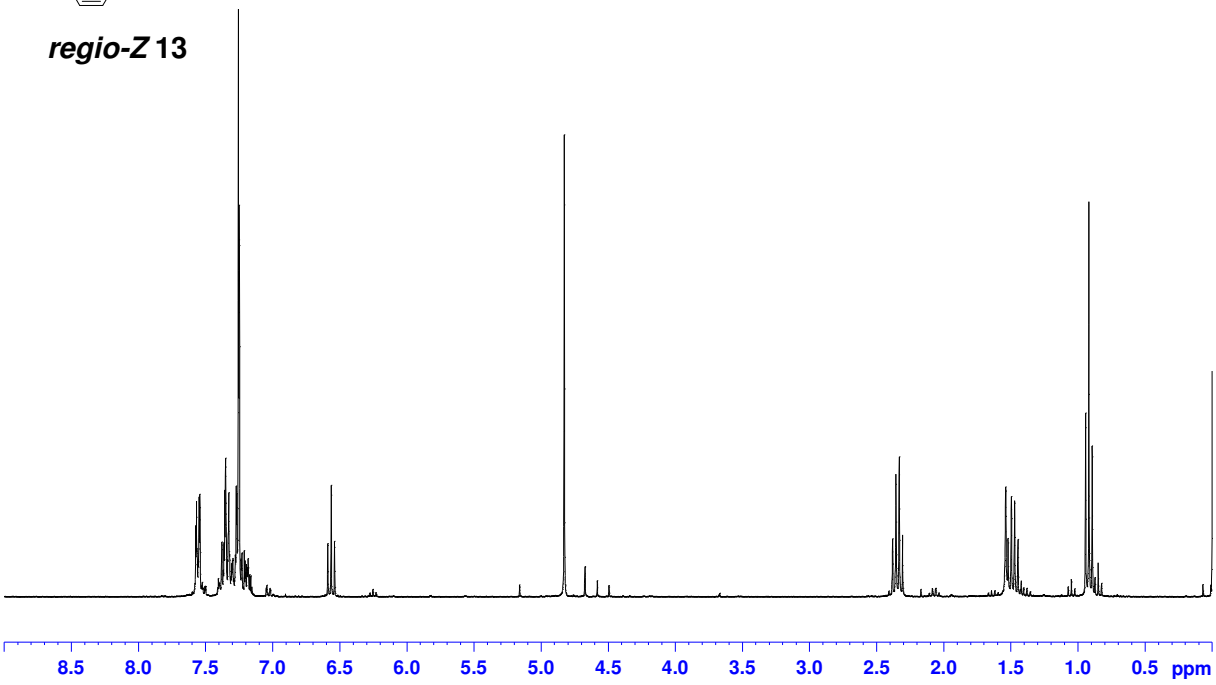


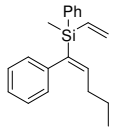
***regio-E* 13**



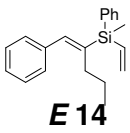


***regio-Z* 13**

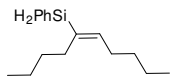




***regio-E* 14**

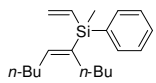


***E* 14**


H2PhSi

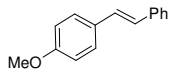
***E*-15**

8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm


Si
n-Bu
n-Bu

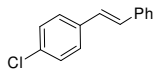
***E*-16**

8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm


Ph
MeO

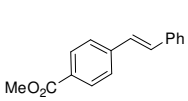
***E* 17**

8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

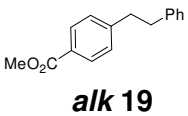

Ph
Cl

***E* 18**

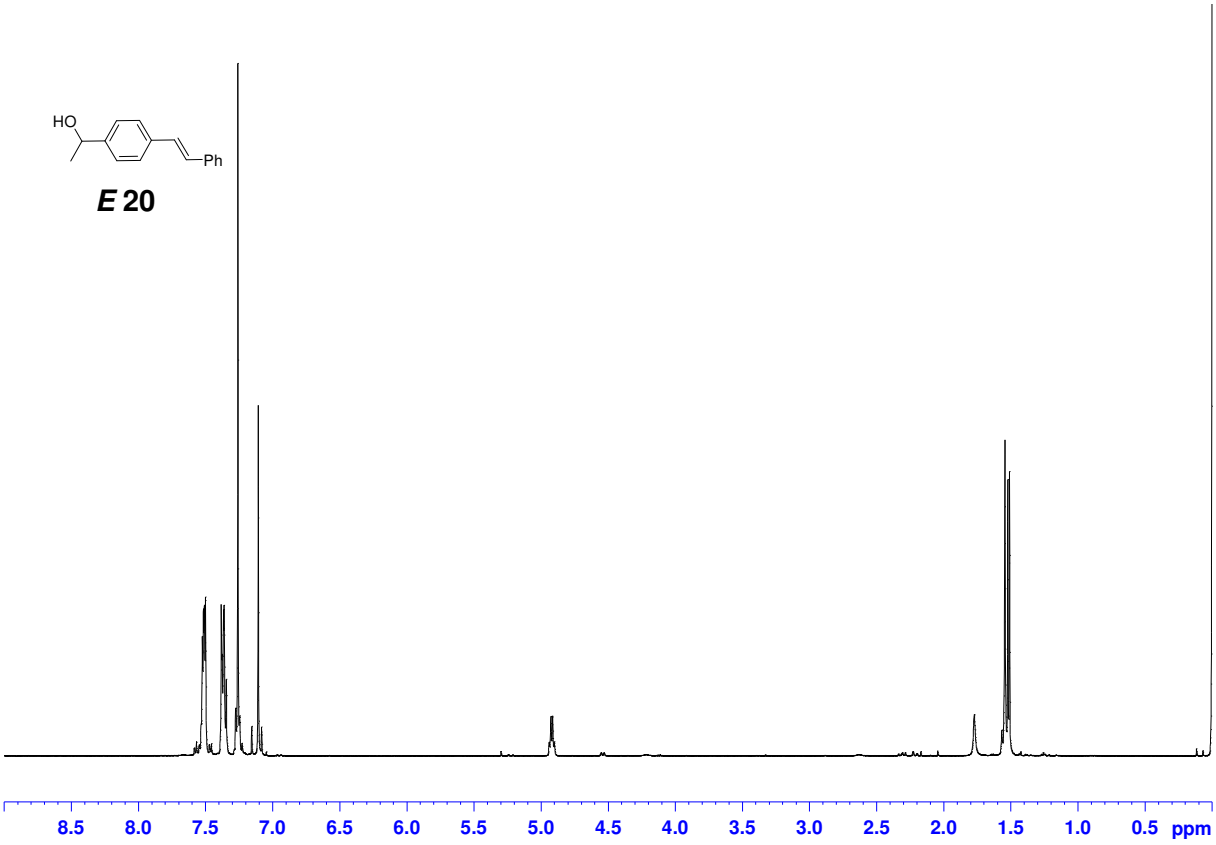
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm



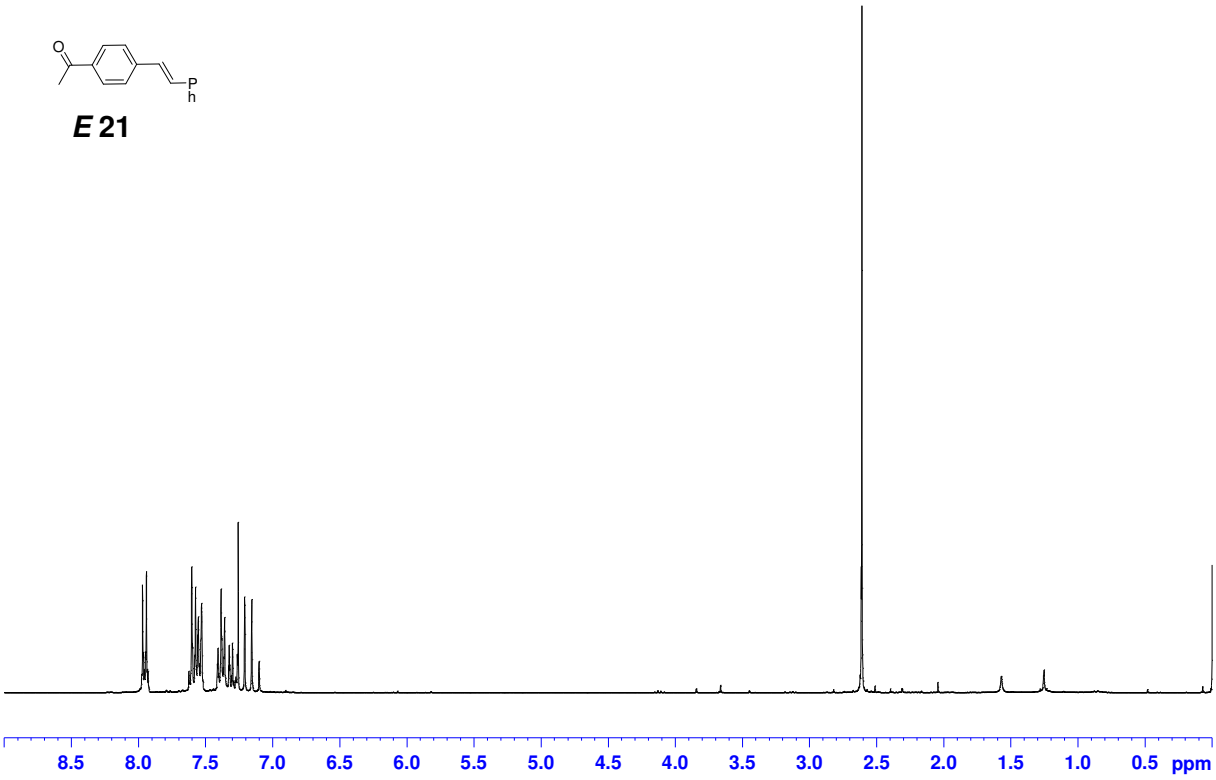
***E* 19**



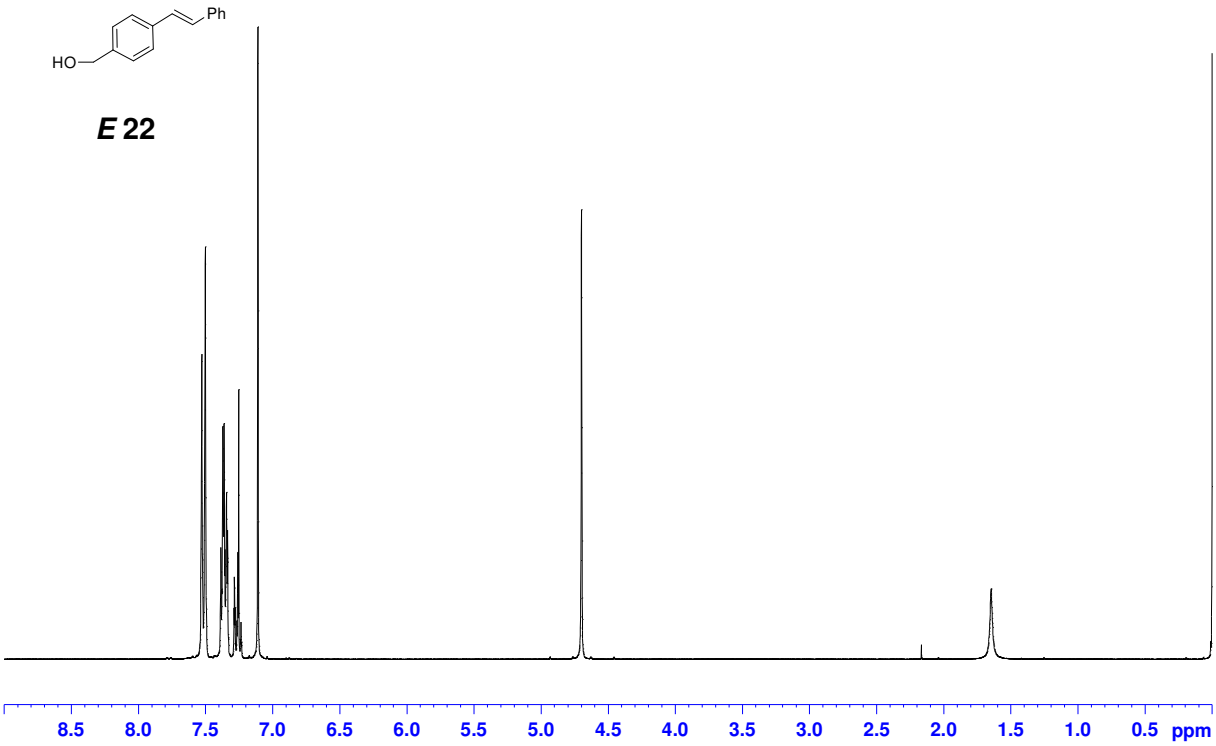
***alk* 19**



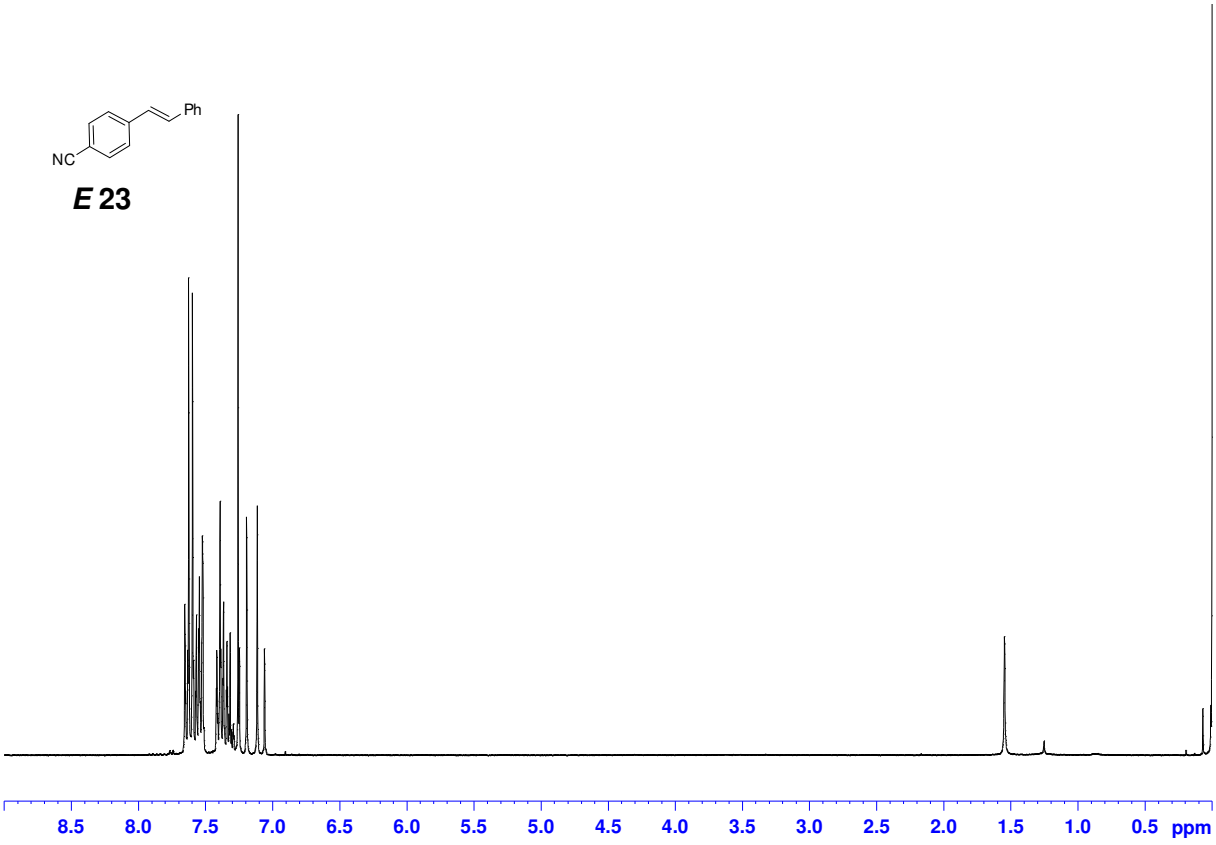
***E* 20**



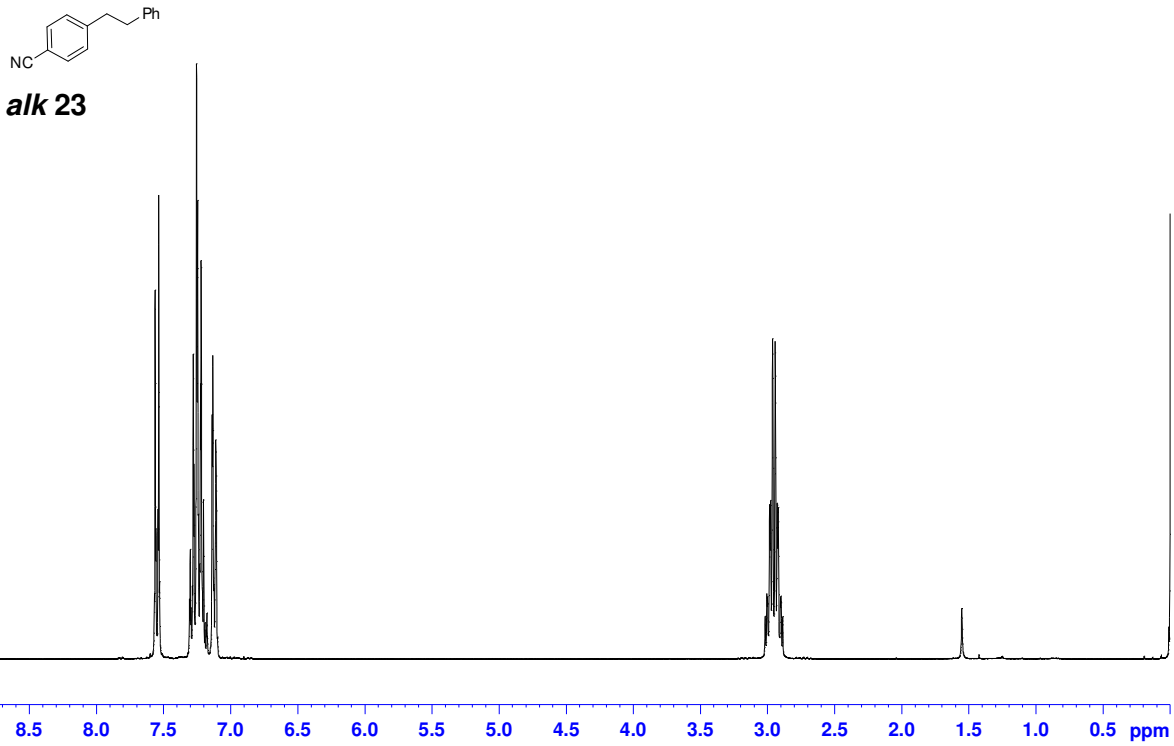
***E* 21**


Ph
HO
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

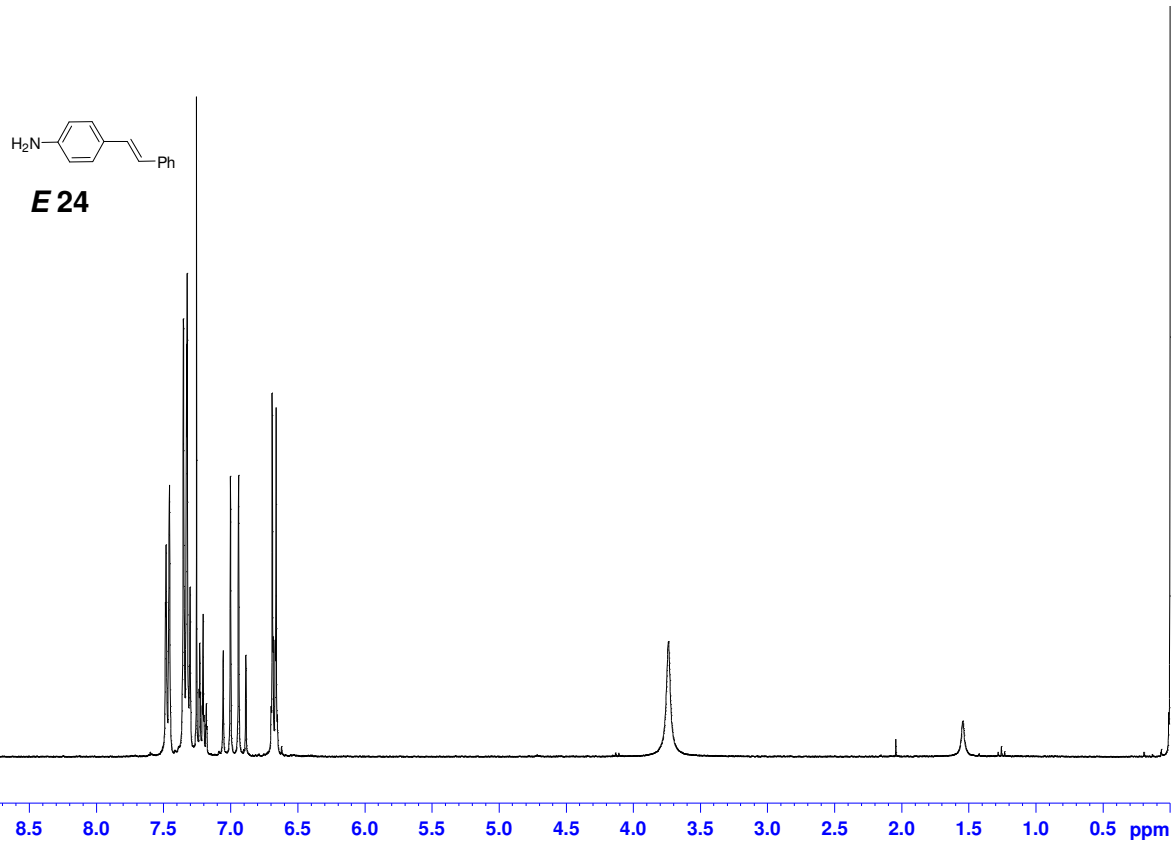
***E* 22**


Ph
NC
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

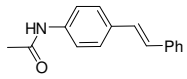
***E* 23**



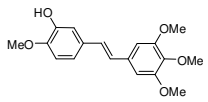
***alk* 23**



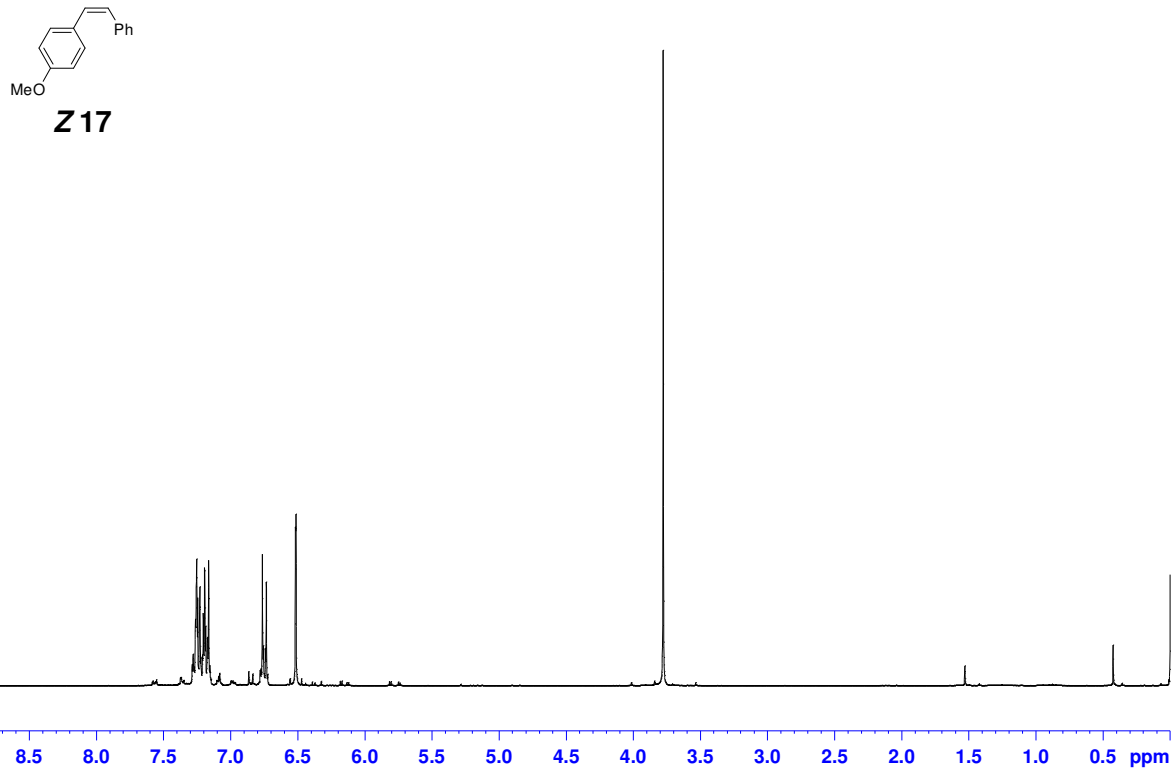
***E* 24**



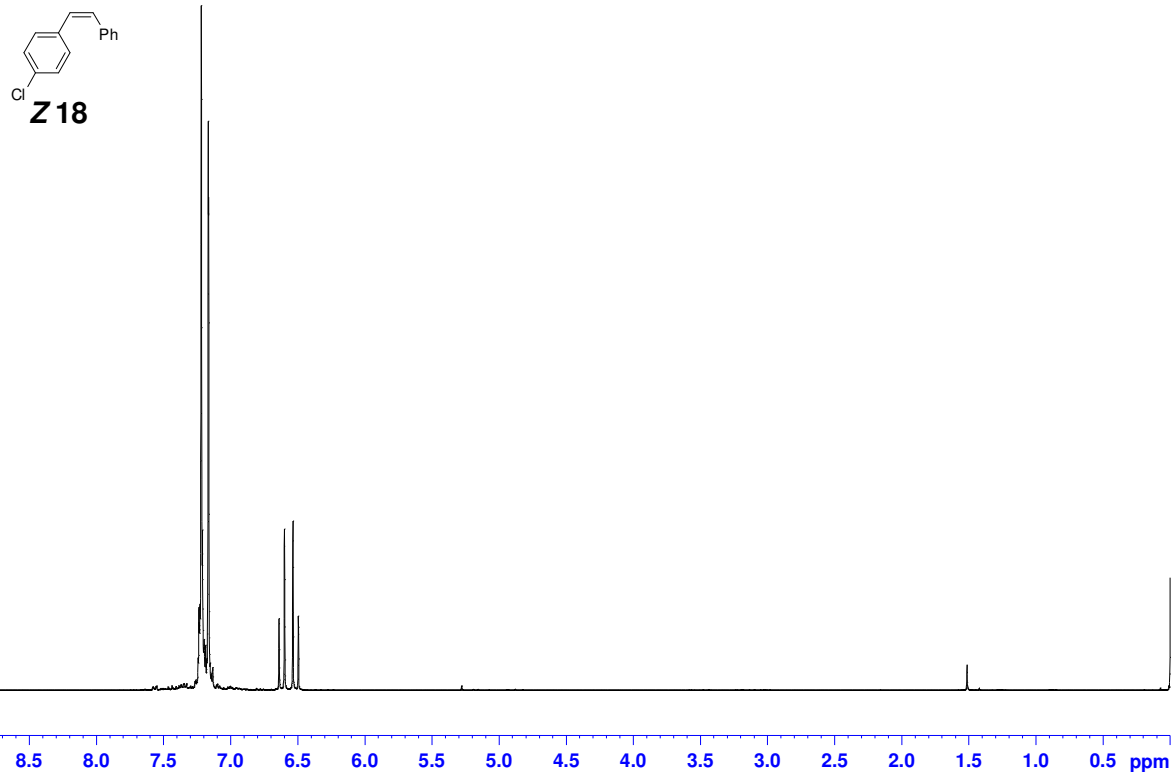
***E* 25**



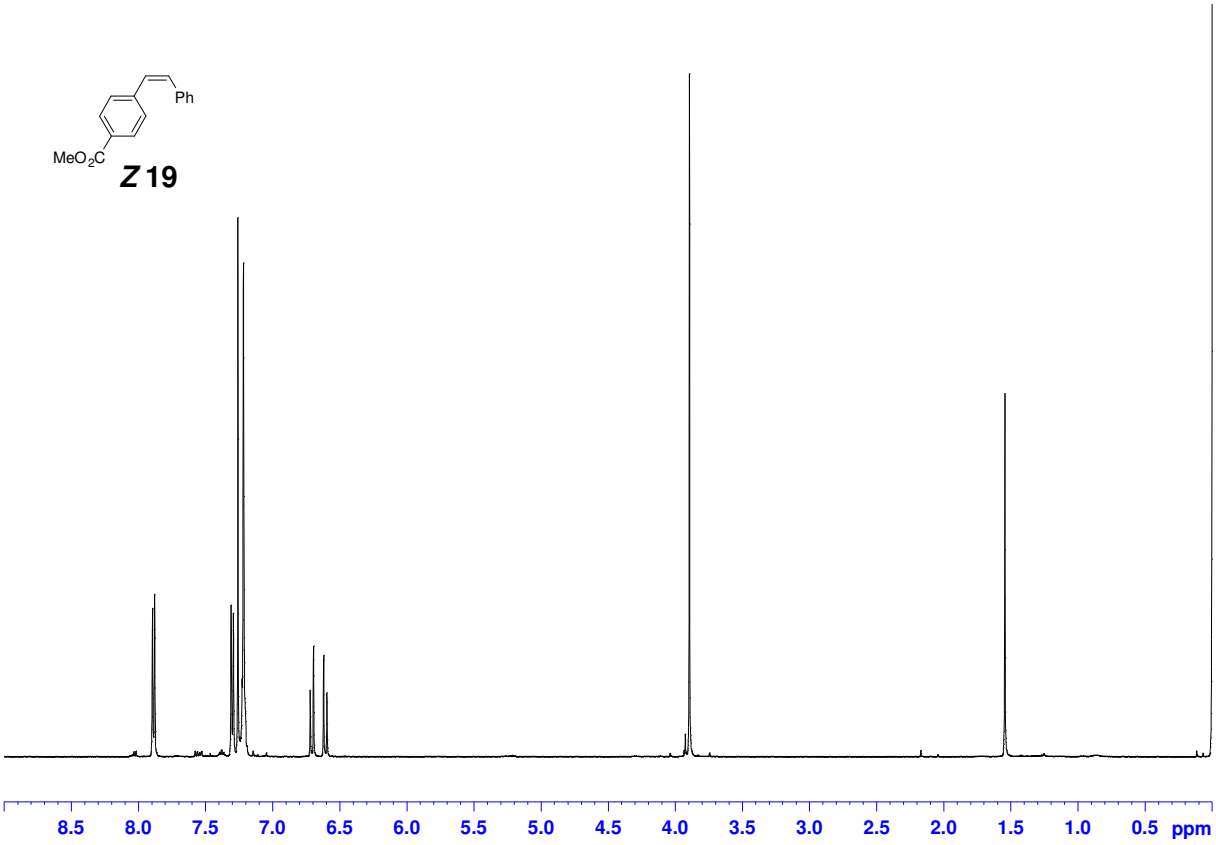
***E* 27**

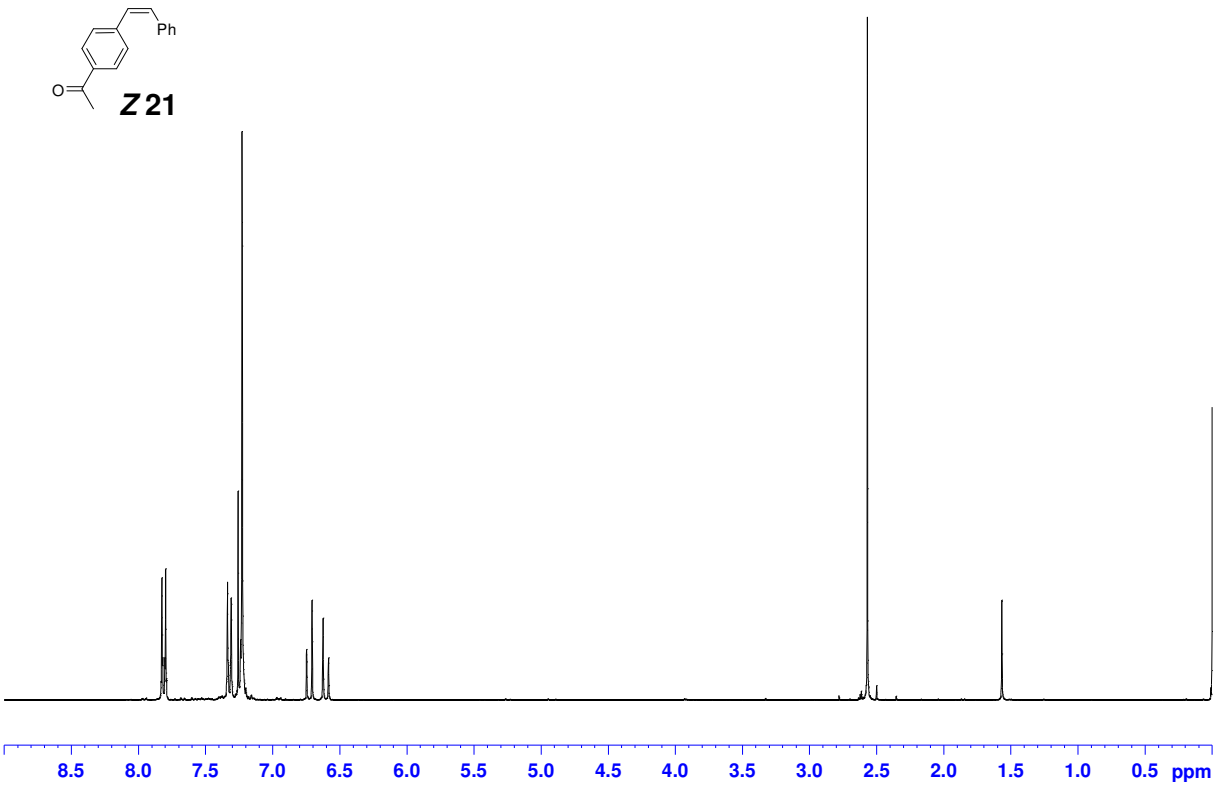


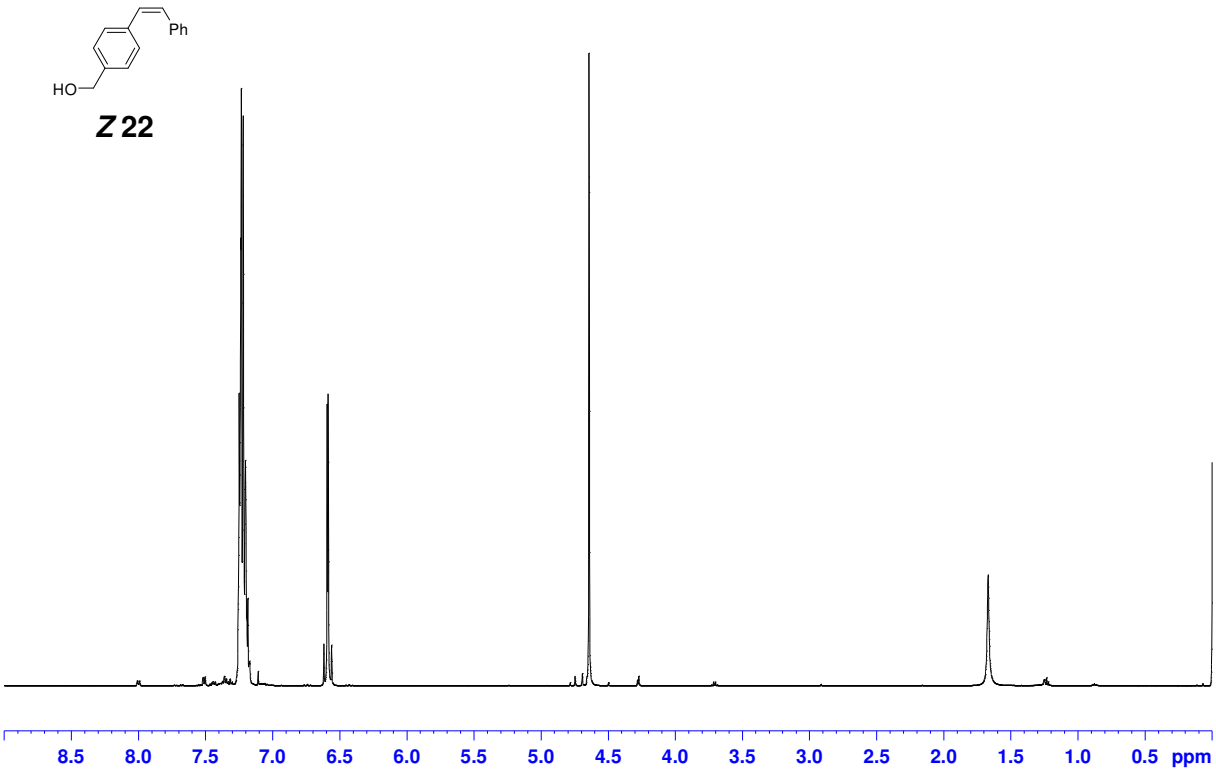
***Z* 17**



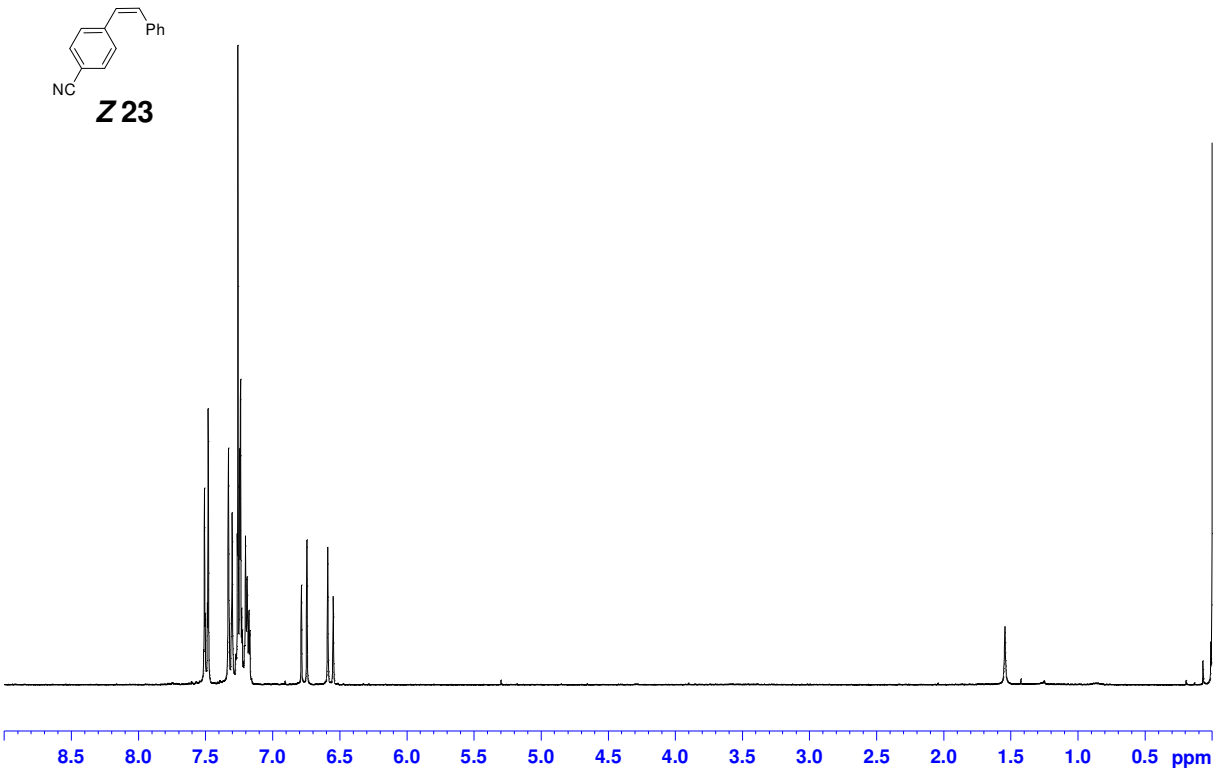
***Z* 18**


Ph
MeO2C
Z 19
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

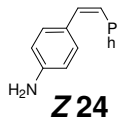

Ph
O
Z 21
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm



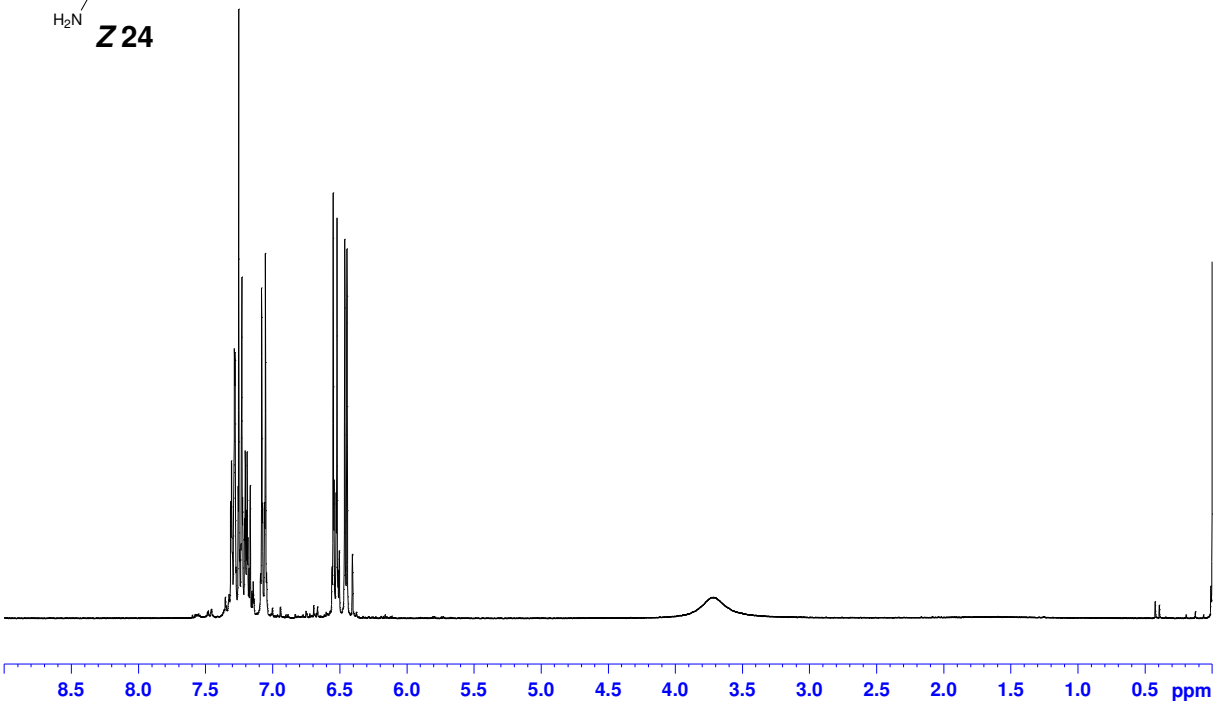
***Z* 22**

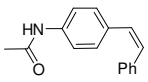


***Z* 23**


Ph
H2N

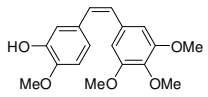
***Z* 24**


8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm


HN
O
Ph

***Z* 25**

10
9
8
7
6
5
4
3
2
1
ppm



***Z* 27**