Supporting Info

Non-Directed Allylic C–H Functionalization in the Presence of Lewis Basic Heterocycles

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General Experimental Details

Unless otherwise noted, all reactions were conducted under ambient conditions with magnetic stirring. $Pd(OAc)_2$ (Strem Chemicals, Inc.) was stored in a dry-box with desiccant. $Pd(OAc)_2/PhS(O)C_2H_4S(O)Ph$ (Strem Chemicals, Inc.) was stored in a refrigerator. AcOH (Sigma Aldrich), 1,4-dioxane (Sigma Aldrich), *p*-benzoquinone (Sigma Aldrich), 4,5-diazafluorenone (Sigma Aldrich), NaOAc (Sigma Aldrich) were used as received, stored and weighed under ambient atmosphere. All heterocycle fragments used for the high-throughput screen are commerically available.

Analytical thin layer chromatography (TLC) was performed on Kieselgel 60 F254 (250 μm silica gel) glass plates and compounds were visualized with UV light, iodine, *p*-anisaldehyde stain, ceric ammonium molybdate stain, or aqueous $KMnO_4$ solution. Flash column chromatography was performed using Kieselgel 60 (230-400 mesh) silica gel. Eluent mixtures are reported as v:v percentages of the minor constituent in the major constituent. All compounds purified by column chromatography were sufficiently pure for use in further experiments unless otherwise indicated.

^1H NMR spectra were measured at 400 MHz on a Bruker Avance instrument. The proton signal of the residual, nondeuterated solvent (δ 7.24 for $CHCl_3$) was used as an internal reference for ^1H NMR spectra. ^{13}C NMR spectra were completely hetero-decoupled and measured at 100 MHz. Residual chloroform (δ 77.0) was used as an internal reference. All tested compounds were found to be ≥95% pure (unless stated otherwise) as determined by LC/ESI-MS, recorded using an Agilent 6220 mass spectrometer with an electrospray ionization source and Agilent 1200 liquid chromatograph. The mass accuracy of the system has been found to be < 5 ppm.

General Experimental Procedures for Pd-Catalyzed Allylic C–H Acetoxylation

General Procedure A:

To a solid mixture of $Pd(OAc)_2$/$PhS(O)C_2H_4S(O)Ph$ (10 mol %), *p*-benzoquinone (2 equiv) was added the olefin substrate (1 equiv), AcOH (10 equiv), and 1,4-dioxane (0.3 M). The reaction was sealed and heated to 45 °C with stirring for 48 h. The reaction was allowed to cool to rt, quenched with saturated bicarbonate solution, and extracted with dichloromethane three times. The combined organic solvent was dried with $MgSO_4$, filtered, and the solvent was removed *in vacuo*. The crude residue was purified via flash chromatography or HPLC as indicated to afford the desired products.

General Procedure B:

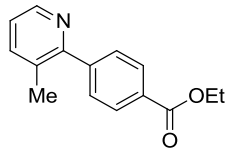
To a solid mixture of $Pd(OAc)_2$ (10 mol %), 4,5-diazafluorenone (10 mol %), NaOAc (40 mol %), *p*-benzoquinone (2 equiv) was added the olefin substrate (1 equiv), AcOH (16 equiv), and 1,4-dioxane (0.3 M). The reaction was sealed and heated to 60 °C with stirring for 48 h. The reaction was allowed to cool to rt, quenched with saturated bicarbonate solution, and extracted with dichloromethane three times. The combined organic solvent was dried with $MgSO_4$, filtered, and the solvent was removed *in vacuo*. The crude residue was purified via flash chromatography or HPLC as indicated to afford the desired products.

General Procedure C:

To a solid mixture of $Pd(OAc)_2$ (10 mol %), 4,5-diazafluorenone (10 mol %), NaOAc (40 mol %), was added the olefin substrate (1 equiv), AcOH (16 equiv), and 1,4-dioxane (0.3 M). The reaction was bubbled with O_2 for 20 minutes. The reaction was sealed under an atmosphere of O_2 (1 atm) and heated to 60 °C with stirring for 48 h. The reaction was allowed to cool to rt, quenched with saturated bicarbonate solution, and extracted with dichloromethane three times. The combined organic solvent was dried with $MgSO_4$, filtered, and the solvent was removed *in vacuo*. The crude residue was purified via flash chromatography or HPLC as indicated to afford the desired products.

Starting Materials

Ethyl 4-(3-methylpyridin-2-yl)benzoate:



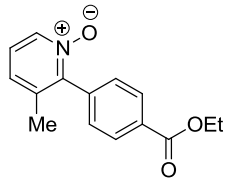
To a 20 mL microwave vial was added (4-(ethoxycarbonyl)phenyl)boronic acid (233 mg, 1.20 mmol), $Pd(PPh_3)_4$ (57.8 mg, 0.050 mmol), and K_2CO_3 (553 mg, 4.00 mmol). The reaction vessel was sealed, subjected to high vacuum and refilled with nitrogen gas three times. To the solid mixture was added 1,4-dioxane/H_2O (1:1, 0.2 M, 5 mL), and then 2-chloro-3-methylpyridine (109 µL, 1 mmol). The reaction was heated to 100 °C with stirring for 5 h in the microwave reactor. The reaction was cooled to rt, quenched with water, and extracted with EtOAc three times. The combined organic layer was washed with brine, dried with $MgSO_4$, filtered, and the solvent was removed *in vacuo*. The crude residue was purified via flash chromatography (100% heptanes to 35% EtOAc:heptanes) to afford the coupled product (240 mg, 0.995 mmol, 99% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (m, 1H), 8.22 – 8.10 (m, 2H), 7.69 – 7.59 (m, 3H), 7.25 (m, 1H), 4.43 (q, *J* = 7.1 Hz, 2H), 2.38 (s, 3H), 1.44 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.2, 157.3, 146.9, 144.7, 138.5, 130.7, 129.7, 129.19, 128.8, 122.4, 60.8, 19.7, 14.1.

HRMS (ESI) (*m*/*z*) $[M+H]^+$ calcd for $C_{15}H_{16}NO_2$, 242.1181; found 242.1168.

2-(4-(Ethoxycarbonyl)phenyl)-3-methylpyridine 1-oxide:



To a 20 mL vial was added ethyl 4-(3-methylpyridin-2-yl)benzoate (406 mg, 1.68 mmol), *m*-chloroperbenzoic acid (581 mg, 3.37 mmol), and CH_2Cl_2 (7 mL) at 0 °C with stirring and the reaction was allowed to warm to rt over 4 h. When full consumption of starting material was observed via LC-MS analysis, the reaction was quenched with saturated $NaHCO_3$ solution, and extracted with CH_2Cl_2 twice. The organic layer was dried with $MgSO_4$, filtered, and the solvent was removed *in vacuo*. The crude residue was purified via flash chromatography (100% CH_2Cl_2 to 5% MeOH:CH_2Cl_2) to afford the corresponding *N*-oxide product (221 mg, 0.859 mmol, 61% yield).

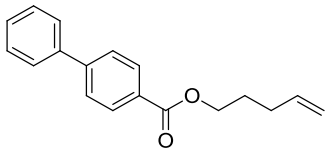
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (m, 1H), 8.21 – 8.13 (m, 2H), 7.44 (m, 2H), 7.26 – 7.16 (m, 3H), 4.40 (q, *J* = 7.1 Hz, 2H), 2.10 (s, 3H), 1.39 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.1, 148.9, 137.8, 136.6, 135.9, 131.1, 130.1, 129.3, 128.0, 124.3, 61.16, 19.72, 14.35.

HRMS (ESI) (*m*/*z*) $[M+H]^+$ calcd for $C_{15}H_{16}NO_3$, 258.1130; found 258.1132.

Substrate 1, Figure 2

Pent-4-en-1-yl [1,1'-biphenyl]-4-carboxylate:



To a 40 mL vial was added LiBr (4.09 g, 47.1 mmol), methyl [1,1'-biphenyl]-4-carboxylate (2 g, 9.42 mmol), pent-4-en-1-ol (20 mL, 194 mmol), and 1,8-diazabicyclo[5.4.0]undec-7-ene (0.710 mL, 4.71 mmol) and stirred at rt for 16 h. The residual starting material (pent-4-en-1-ol) was removed under reduced pressure. The concentrated crude residue was washed with H_2O and extracted with CH_2Cl_2 three times. The combined organic layer was washed with brine, dried with $MgSO_4$, filtered, and the organic solvent was removed *in vacuo*. The crude residue was purified via flash chromatography (100% heptanes to 30% EtOAc:heptanes) to afford the esterified product (2.2 g, 8.26 mmol, 88% yield).

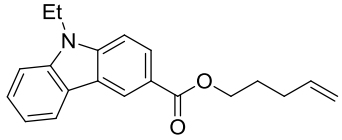
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 – 8.06 (m, 2H), 7.69 – 7.57 (m, 4H), 7.50 – 7.42 (m, 2H), 7.41 – 7.35 (m, 1H), 5.85 (ddt, *J* = 16.9, 10.2, 6.6 Hz, 1H), 5.14 – 4.95 (m, 2H), 4.34 (t, *J* = 6.6 Hz, 2H), 2.28 – 2.17 (m, 2H), 1.88 (dq, *J* = 8.2, 6.6 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.4, 145.5, 139.9, 137.4, 129.9, 129.1, 128.8, 128.0, 127.2, 126.9, 115.3, 64.3, 30.1, 27.9.

HRMS (ESI) (*m*/*z*) $[M+H]^+$ calcd for $C_{18}H_{19}O_2$, 267.1385; found 267.1285.

Entry 24 Substrate, Figure 4

Pent-4-en-1-yl 9-ethyl-9*H*-carbazole-3-carboxylate:



To a 20 mL vial containing toluene (7.7 mL) was added 1-methyl-1*H*-indole-5-carboxylic acid (553 mg, 2.31 mmol), pent-4-en-1-ol (0.24 mL, 2.31 mmol), and *p*-toluenesulfonic acid (40 mg, 0.23 mmol). The vial was sealed and the mixture was heated at 120 °C for 18 h. The organic solvent was removed *in vacuo.* The crude residue was taken up in methanol and purified via flash chromatography (100% heptanes to 100% EtOAc:heptanes) to afford the esterified product (440 mg, 1.36 mmol, 95% yield).

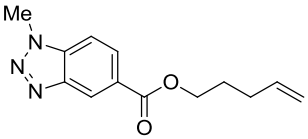
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.81 – 8.71 (m, 1H), 8.16 – 8.03 (m, 2H), 7.48 – 7.39 (m, 1H), 7.39 – 7.27 (m, 2H), 7.26 – 7.18 (m, 1H), 5.82 (ddt, *J*=17.05, 10.36, 6.63, 6.63 Hz, 1H), 5.08 – 4.99 (m, 1H), 4.99 – 4.90 (m, 1H), 4.36 – 4.30 (m, 4H), 2.28 – 2.15 (m, 2H), 1.94 – 1.79 (m, 2H), 1.38 (t, *J*=7.20 Hz, 3H),

^{13}C NMR (100 MHz, $CDCl_3$) δ 167.5, 142.6, 140.5, 137.7, 127.3, 126.4, 122.9, 120.8, 119.8, 115.3, 108.9, 107.9, 64.2, 37.8, 30.3, 28.1, 13.8

HRMS (ESI) (*m*/*z*) $[M+H]^+$ calcd for $C_{20}H_{22}NO_2$, 308.1651; found 308.1649.

Entry 24 Substrate, Figure 4

Pent-4-en-1-yl 1-methyl-1*H*-benzo[*d*][1,2,3]triazole-5-carboxylate:



To a 50 mL round bottom flask containing DMF (4.2 mL) was added 1-methyl-1*H*-benzo[*d*][1,2,3]triazole-5-carboxylic acid (0.15 g, 0.85 mmol), diisopropylethylamine (0.59 mL, 3.4 mmol), pent-4-en-1-ol (0.16 mL, 1.7 mmol), and (*O*-(7-azabenzotriazol-1-yl)-*N*,*N*,*N*′,*N*′-tetramethyluronium hexafluorophosphate) (0.64 mg, 1.7 mmol) and stirred at rt for 16 h. The DMF was removed *in vacuo*. The residue then was diluted with H_2O and extracted with EtOAc. The organic extract was dried with Na_2SO_4, filtered, and the organic solvent was removed *in vacuo*. The crude residue was purified via flash chromatography (100% Heptane to 100% EtOAc) to afford the esterified product (73 mg, 0.29 mmol, 34% yield).

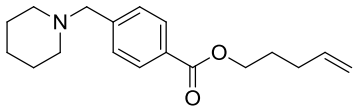
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.87 – 8.79 (m, 1H), 8.28 – 8.18 (m, 1H), 7.64 – 7.52 (m, 1H), 5.89 (ddt, *J* = 17.02, 10.26, 6.69, 6.69Hz, 1H), 5.16 – 5.08 (m, 1H), 5.08 – 5.01 (m, 1H), 4.42 (t, *J* = 6.57 Hz, 2H), 4.36 (s, 3H), 2.36 – 2.19 (m, 2H), 2.03 – 1.87 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.1, 145.7, 137.4, 135.7, 128.3, 126.6, 122.9, 115.5, 109.0, 64.8, 34.5, 30.2, 27.9

HRMS (ESI) (*m*/*z*) $[M+H]^+$ calcd for $C_{13}H_{16}N_3O_2$, 246.1243; found 246.1244.

Entry 25 Substrate, Figure 4

Pent-4-en-1-yl 4-(piperidin-1-ylmethyl)benzoate:



To a 50 mL round bottom flask containing DMF (3.9 mL) was added 4-(piperidin-1-ylmethyl)benzoic acid hydrochloride (0.2 g, 0.78 mmol), diisopropylethylamine (0.68 mL, 3.9 mmol), pent-4-en-1-ol (0.15 mL, 1.56 mmol), and (*O*-(7-azabenzotriazol-1-yl)-*N*,*N*,*N*′,*N*′-tetramethyluronium hexafluorophosphate) (0.60 mg, 1.56 mmol) and stirred at rt for 16 h. The reaction mixture was diluted with H_2O and extracted with EtOAc. The organic extract was dried with Na_2SO_4, filtered, and the organic solvent was removed *in vacuo*. The crude residue was taken up in methanol and purified via prep HPLC modified with 0.1% trifluoroacetic acid (10–30% acetonitrile in water) and concentrated *in vacuo* to afford the product as a TFA salt. The residue was taken up in methanol and loaded onto 500 mg of MP-carbonate resin which was washed with excess methanol. The filtrate was concentrated in vacuo to afford the product as a free base (43 mg, 0.15 mmol, 19% yield).

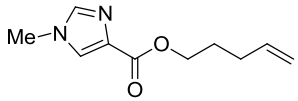
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 – 7.96 (m, 2H), 7.42 (d, *J* = 8.08 Hz, 2H), 5.87 (ddt, *J* = 17.02, 10.26, 6.57, 6.57 Hz, 1H), 5.14 – 4.99 (m, 2H), 4.35 (t, *J* = 6.57 Hz, 2H), 3.54 (s, 2H), 2.51 – 2.29 (m, 4H), 2.29 – 2.18 (m, 2H), 1.95 – 1.84 (m, 2H), 1.68 – 1.53 (m, 4H), 1.52 – 1.35 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.7, 144.1, 137.5, 129.5, 129.0, 115.4, 64.3, 63.5, 54.6, 30.2, 27.9, 25.9, 24.3.

HRMS (ESI) (*m*/*z*) $[M+H]^+$ calcd for $C_{18}H_{26}NO_2$, 288.1964; found 288.1970.

Entry 26 Substrate, Figure 4

Pent-4-en-1-yl 1-methyl-1*H*-imidazole-4-carboxylate:



To a 40 mL vial was added LiBr (0.62 g, 7.14 mmol), methyl 1-methyl-1*H*-imidazole-4-carboxylate (0.2 g, 1.43 mmol), pent-4-en-1-ol (2.9 mL, 28.5 mmol), and 1,8-diazabicyclo[5.4.0]undec-7-ene (0.108 mL, 0.71 mmol) and stirred at rt for 16 h. The reaction mixture was diluted with CH_2Cl_2 and washed with H_2O three times then with brine, dried with Na_2SO_4, filtered, and the organic solvent was removed *in vacuo*. The crude residue was purified via flash chromatography (100% dichloromethane to 10% methanol:dichloromethane) to afford the esterified product (130 mg, 0.69 mmol, 48% yield).

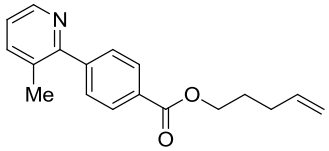
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (s, 1H), 7.49 (s, 1H), 5.84 (ddt, *J* = 17.00, 10.29, 6.56, 6.56 Hz, 1H), 5.15 – 4.92 (m, 2H), 4.32 (t, *J* = 6.78 Hz, 2H), 3.76 (s, 3H), 2.20 (m, 2H), 1.87 (tt, *J* = 7.80, 6.82 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 162.9, 138.6, 137.6, 134.2, 126.1, 115.2, 64.0, 33.1, 30.1, 27.9.

HRMS (ESI) (*m*/*z*) $[M+H]^+$ calcd for $C_{10}H_{15}N_2O_2$, 195.1134; found 195.1135.

Entry 27 Substrate, Figure 4; Entries 6 to 11 Substrate, Table 1

Pent-4-en-1-yl 4-(3-methylpyridin-2-yl)benzoate:



To a 20 mL vial was added LiBr (1490 mg, 17.16 mmol), ethyl 4-(3-methylpyridin-2-yl)benzoate (828 mg, 3.43 mmol), pent-4-en-1-ol (10 mL, 97 mmol), 1,8-diazabicyclo[5.4.0]undec-7-ene (0.259 mL, 1.716 mmol) and stirred at rt for 16 h. The residual starting material (pent-4-en-1-ol) was removed under reduced pressure. The concentrated crude residue was washed with water and extracted with CH_2Cl_2 three times. The combined organic layer was washed with brine, dried with $MgSO_4$, filtered, and the solvent was removed *in vacuo*. The crude residue was purified via flash chromatography (100% heptanes to 30% EtOAc:heptanes) to afford the esterified product (812 mg, 2.89 mmol, 84% yield).

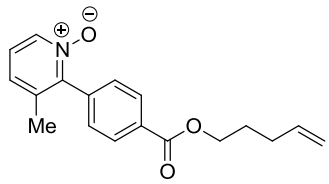
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (m, 1H), 8.24 – 8.04 (m, 2H), 7.63 (m, 2H), 7.24 (m, 1H), 5.89 (ddt, *J* = 16.9, 10.2, 6.6 Hz, 1H), 5.11 (m, 1H), 5.07 – 5.02 (m, 1H), 4.39 (t, *J* = 6.6 Hz, 2H), 2.38 (s, 3H), 2.33 – 2.22 (m, 2H), 1.93 (dq, *J* = 8.3, 6.6 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.4, 157.6, 147.1, 145.0, 138.7, 137.5, 130.9, 129.8, 129.4, 129.0, 122.6, 115.4, 64.4, 30.2, 27.9, 19.9.

HRMS (ESI) (*m*/*z*) $[M+H]^+$ calcd for $C_{18}H_{20}NO_2$, 282.1494; found 282.1483.

Entries 12 and 13 Substrate, Table 1

3-Methyl-2-(4-((pent-4-en-1-yloxy)carbonyl)phenyl)pyridine 1-oxide:



To a 50 mL round-bottom flask was added LiBr (3.60 g, 41.5 mmol), 2-(4-(ethoxycarbonyl)phenyl)-3-methylpyridine 1-oxide (2.13 g, 8.29 mmol), pent-4-en-1-ol (20 mL, 194 mmol), and 1,8-diazabicyclo[5.4.0]undec-7-ene (0.625 mL, 4.15 mmol) and stirred at rt for 48 h. The residual starting material (pent-4-en-1-ol) was removed under reduced pressure. The concentrated crude residue was washed with water and extracted with CH_2Cl_2 three times The combined organic layer was washed with brine, dried with $MgSO_4$, filtered, and the solvent was removed *in vacuo*. The crude residue was purified via flash chromatography (100% CH_2Cl_2 to 10% MeOH:CH_2Cl_2) to afford the esterified product (2.05 g, 6.89 mmol, 83% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (m, 1H), 8.20 – 8.14 (m, 2H), 7.48 – 7.39 (m, 2H), 7.22 – 7.13 (m, 2H), 5.84 (ddt, *J* = 16.9, 10.2, 6.6 Hz, 1H), 5.14 – 4.95 (m, 2H), 4.35 (t, *J* = 6.5 Hz, 2H), 2.30 – 2.17 (m, 2H), 2.09 (s, 3H), 1.87 (dq, *J* = 8.3, 6.6 Hz, 2H).

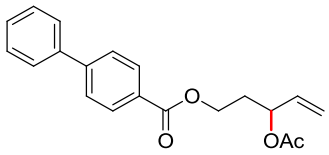
^{13}C NMR (100 MHz, $CDCl_3$) δ 166.0, 148.7, 137.7, 137.3, 136.8, 135.7, 130.8, 130.0, 129.3, 127.5, 124.2, 115.3, 64.4, 30.1, 27.8, 19.6.

HRMS (ESI) (*m*/*z*) $[M+H]^+$ calcd for $C_{18}H_{20}NO_3$, 298.1443; found 298.1443.

C–H Functionalization Products

Product 2, Figure 2; Entry 3 Product, Table 1

(±)-3-Acetoxypent-4-en-1-yl [1,1'-biphenyl]-4-carboxylate, Major Regioisomer:



Following Procedure A, pent-4-en-1-yl [1,1'-biphenyl]-4-carboxylate (50 mg, 0.188 mmol), $Pd(OAc)_2$/$PhS(O)C_2H_4S(O)Ph$ (9.44 mg, 0.019 mmol), *p*-benzoquinone (40.6 mg, 0.375 mmol), AcOH (107 µl, 1.877 mmol) afforded a crude residue which was purified via flash chromatography (100% heptanes to 20% EtOAc:heptanes) to afford a mixture of products (31 mg, 0.096 mmol, 51% yield) as a mixture of regioisomers (84:16 branched:linear).

Major Regioisomer:

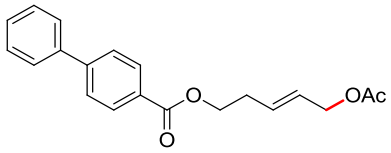
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 – 8.07 (m, 2H), 7.77 – 7.60 (m, 4H), 7.54 – 7.46 (m, 2H), 7.45 – 7.37 (m, 1H), 5.88 (ddd, *J* = 17.0, 10.5, 6.3 Hz, 1H), 5.56 – 5.46 (m, 1H), 5.40 – 5.22 (m, 2H), 4.43 (td, *J* = 6.4, 2.3 Hz, 2H), 2.20 – 2.12 (m, 2H), 2.10 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 170.2, 166.3, 145.8, 140.0, 135.7, 130.1, 128.9, 128.8, 128.2, 127.3, 127.1, 117.4, 61.0, 33.3, 21.2.

HRMS (ESI) (*m*/*z*) $[M+NH_4]^+$ calcd for $C_{20}H_{24}NO_4$, 342.1705; found 342.1694.

Product 3, Figure 2; Entry 4 Product, Table 1

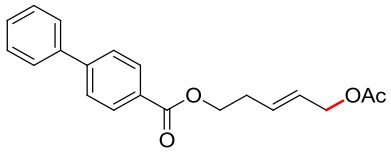
(*E*)-5-Acetoxypent-3-en-1-yl [1,1'-biphenyl]-4-carboxylate, Major Regioisomer:



Following Procedure B, pent-4-en-1-yl [1,1'-biphenyl]-4-carboxylate (50 mg, 0.188 mmol), $Pd(OAc)_2$ (4.21 mg, 0.019 mmol), 4,5-diazafluorenone (3.42 mg, 0.019 mmol), NaOAc (6.16 mg, 0.075 mmol), *p*-benzoquinone (40.6 mg, 0.375 mmol), AcOH (172 µl, 3.00 mmol) afforded a crude residue which was purified via flash chromatography (100% heptanes to 20% EtOAc:heptanes) to afford a mixture of products (40 mg, 0.123 mmol, 66% yield) as a mixture of regioisomers (19:81 branched:linear).

Entry 4 Product, Table 1

(*E*)-5-Acetoxypent-3-en-1-yl [1,1'-biphenyl]-4-carboxylate, Major Regioisomer:



Following Procedure C, pent-4-en-1-yl [1,1'-biphenyl]-4-carboxylate (50 mg, 0.188 mmol), $Pd(OAc)_2$ (4.21 mg, 0.019 mmol), 4,5-diazafluorenone (3.42 mg, 0.019 mmol), NaOAc (6.16 mg, 0.075 mmol), O_2 (1 atm), AcOH (172 µl, 3.00

mmol) afforded a crude residue which was purified via flash chromatography (100% heptanes to 20% EtOAc:heptanes) to afford a mixture of products (35 mg, 0.108 mmol, 58% yield) as a mixture of regioisomers (18:82 branched:linear).

Major Regioisomer:

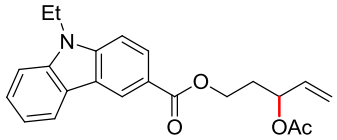
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 – 8.03 (m, 2H), 7.70 – 7.57 (m, 4H), 7.45 (m, 2H), 7.41 – 7.34 (m, 1H), 5.89 – 5.78 (m, 1H), 5.78 – 5.67 (m, 1H), 4.58 – 4.49 (m, 2H), 4.37 (t, *J* = 6.7 Hz, 2H), 2.58 – 2.50 (m, 1H), 2.03 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 170.7, 166.3, 145.7, 140.0, 131.1, 130.1, 128.93, 128.89, 128.1, 127.2, 127.0, 126.8, 64.8, 63.7, 31.7, 20.9.

HRMS (ESI) (*m*/*z*) $[M+NH_4]^+$ calcd for $C_{20}H_{24}NO_4$, 342.1705; found 342.1692.

Entry 23 Product, Reaction A, Figure 4

(±)-3-Acetoxypent-4-en-1-yl 9-ethyl-9*H*-carbazole-3-carboxylate, Major Regioisomer:



Following Procedure A, pent-4-en-1-yl 9-ethyl-9*H*-carbazole-3-carboxylate (40 mg, 0.130 mmol), $Pd(OAc)_2$/$PhS(O)C_2H_4S(O)Ph$ (6.54 mg, 0.013 mmol), *p*-benzoquinone (28.1 mg, 0.260 mmol), AcOH (74.5 µl, 1.301 mmol) afforded a crude residue which was purified via flash chromatography (100% heptanes to 20% EtOAc:heptanes) to afford a mixture of products (32 mg, 0.088 mmol, 67% yield) as a mixture of regioisomers (80:20 branched:linear).

Major Regioisomer:

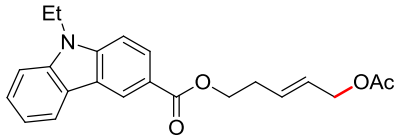
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.84 (m, 1H), 8.19 (m, 2H), 7.54 (m, 1H), 7.50 – 7.39 (m, 2H), 7.37 – 7.24 (m, 1H), 5.91 (ddd, *J* = 17.0, 10.5, 6.3 Hz, 1H), 5.61 – 5.51 (m, 1H), 5.36 (m, 1H), 5.27 (dt, *J* = 10.5, 1.1 Hz, 1H), 4.51 – 4.37 (m, 4H), 2.21 (qd, *J* = 6.4, 2.4 Hz, 2H), 2.11 (s, 2H), 1.48 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 170.2, 167.3, 142.7, 140.5, 135.8, 127.3, 126.3, 123.1, 123.0, 122.7, 120.8, 120.6, 119.9, 117.2, 108.9, 107.9, 71.9, 60.7, 37.8, 33.4, 21.2, 13.8.

HRMS (ESI) (*m*/*z*) $[M+H]^+$ calcd for $C_{22}H_{24}NO_4$, 366.1705; found 366.1697.

Entry 23 Product, Reaction B, Figure 4

(*E*)-5-Acetoxypent-3-en-1-yl 9-ethyl-9*H*-carbazole-3-carboxylate, Major Regioisomer:



Following Procedure B, pent-4-en-1-yl 9-ethyl-9H-carbazole-3-carboxylate (40 mg, 0.130 mmol), $Pd(OAc)_2$ (2.92 mg, 0.013 mmol), 4,5-diazafluorenone (2.371 mg, 0.013 mmol), NaOAc (4.27 mg, 0.052 mmol), *p*-benzoquinone (28.1 mg, 0.260 mmol), AcOH (119 µl, 2.082 mmol), afforded a crude residue which was purified via flash chromatography (100% heptanes to 20% EtOAc:heptanes) to afford a mixture of products (34 mg, 0.093 mmol, 72% yield) as a mixture of regioisomers (16:84 branched:linear).

Major Regioisomer:

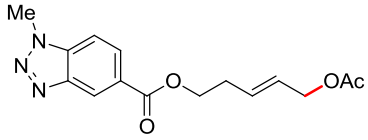
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 (m, 1H), 8.16 – 7.98 (m, 2H), 7.43 (m, 1H), 7.39 – 7.28 (m, 2H), 7.21 (m, 1H), 5.88 – 5.76 (m, 1H), 5.73 – 5.61 (m, 1H), 4.52 – 4.45 (m, 2H), 4.39 – 4.26 (m, 5H), 2.52 (dddd, *J* = 7.8, 6.7, 5.6, 1.1 Hz, 2H), 1.96 (s, 3H), 1.37 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 170.8, 167.3, 142.6, 140.5, 131.4, 127.2, 126.7, 126.3, 123.0, 122.9, 122.7, 120.7, 120.68, 119.8, 108.8, 107.9, 64.9, 63.5, 37.8, 31.9, 20.9, 13.6.

HRMS (ESI) (*m*/*z*) $[M+H]^+$ calcd for $C_{22}H_{24}NO_4$, 366.1705; found 366.1700.

Entry 24 Product, Reaction A, Figure 4

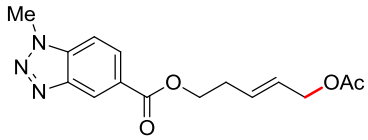
(*E*)-5-Acetoxypent-3-en-1-yl 1-methyl-1*H*-benzo[*d*][1,2,3]triazole-5-carboxylate, Major Regioisomer:



Following Procedure A, pent-4-en-1-yl 1-methyl-1*H*-benzo[*d*][1,2,3]triazole-5-carboxylate (50 mg, 0.204 mmol), $Pd(OAc)_2$/$PhS(O)C_2H_4S(O)Ph$ (10.25 mg, 0.020 mmol), *p*-benzoquinone (44.1 mg, 0.408 mmol), AcOH (117 µl, 2.039 mmol) afforded a crude residue which was purified via flash chromatography (100% heptanes to 40% EtOAc:heptanes) to afford a mixture of products (30 mg, 0.099 mmol, 49% yield) as a mixture of regioisomers (17:83 branched:linear).

Entry 24 Product, Reaction B, Figure 4

(*E*)-5-Acetoxypent-3-en-1-yl 1-methyl-1*H*-benzo[*d*][1,2,3]triazole-5-carboxylate, Major Regioisomer:



Following Procedure B, pent-4-en-1-yl 1-methyl-1*H*-benzo[*d*][1,2,3]triazole-5-carboxylate (40 mg, 0.163 mmol), $Pd(OAc)_2$ (3.66 mg, 0.016 mmol), 4,5-diazafluorenone (2.97 mg, 0.016 mmol), NaOAc (5.35 mg, 0.065 mmol), *p*-benzoquinone (35.3 mg, 0.326 mmol), and AcOH (149 µl, 2.61 mmol) afforded a crude residue which was purified via flash chromatography (100% heptanes to 40% EtOAc:heptanes) to afford a mixture of products (37 mg, 0.122 mmol, 75% yield) as a mixture of regioisomers (10:90 branched:linear).

Major Regioisomer:

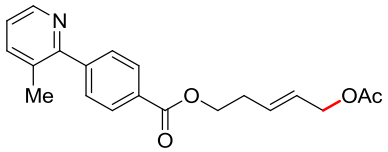
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 (m, 1H), 8.14 (m, 1H), 7.52 (m, 1H), 5.87 – 5.77 (m, 1H), 5.77 – 5.66 (m, 1H), 4.56 – 4.47 (m, 2H), 4.39 (t, *J* = 6.6 Hz, 2H), 4.30 (s, 3H), 2.58 – 2.49 (m, 2H), 2.02 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.7, 165.9, 145.6, 135.7, 130.8, 128.1, 127.0, 126.3, 122.8, 109.0, 64.7, 64.1, 34.4, 31.7, 20.9.

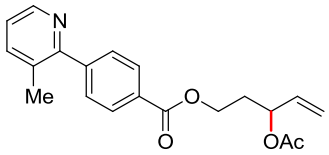
HRMS (ESI) (*m*/*z*) $[M+H]^+$ calcd for $C_{15}H_{18}N_3O_4$, 304.1297; found 304.1301.

Entry 8 Product, Table 1

(*E*)-5-Acetoxypent-3-en-1-yl 4-(3-methylpyridin-2-yl)benzoate, Major Regioisomer:



(±)-3-Acetoxypent-4-en-1-yl 4-(3-methylpyridin-2-yl)benzoate, Minor Regioisomer:



Following a modified procedure A, $BF_3 \bullet OEt_2$ (89 µl, 0.711 mmol) was added to a vial containing pent-4-en-1-yl 4-(3-methylpyridin-2-yl)benzoate (100 mg, 0.355 mmol) and 1,4-dioxane and stirred for 15 min. The resulting mixture was then transferred to a vial containing $Pd(OAc)_2$/$PhS(O)C_2H_4S(O)Ph$ (17.87 mg, 0.036 mmol), *p*-benzoquinone (77 mg, 0.711 mmol), and AcOH (203 µl, 3.55 mmol). The crude residue which was purified via flash chromatography (100% heptanes to 40% EtOAc:heptanes) to afford a mixture of products (46 mg, 0.135 mmol, 38% yield) as a mixture of regioisomers (70:30 branched:linear).

Mixture of Regioisomers:

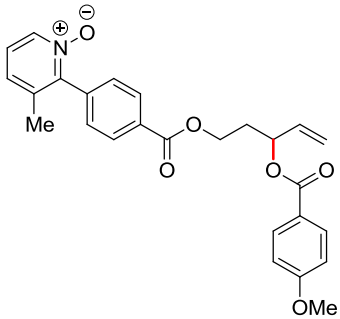
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (m, 1H), 8.04 (m, 2H), 7.68 – 7.37 (m, 2H), 7.24 – 7.03 (m, 1H), 5.89 – 5.71 (m, 1H), 5.66 (dt, *J* = 15.3, 6.1 Hz, 0.7H), 5.40 (q, *J* = 6.5 Hz, 0.3H), 5.31 – 5.20 (m, 0.3H), 5.15 (d, *J* = 10.5 Hz, 0.3H), 4.46 (d, *J* = 6.1 Hz, 1.4H), 4.32 (q, *J* = 7.0 Hz, 2H), 2.48 (q, *J* = 6.7 Hz, 1.4H), 2.27 (s, 3H), 2.06 (qd, *J* = 6.5, 3.1 Hz, 0.6H), 2.00 (s, 0.9H), 1.98 (s, 2.1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 170.76, 170.16, 166.29, 166.25, 157.40, 152.11, 151.10, 146.94, 144.90, 144.85, 138.81, 135.60, 131.04, 131.00, 129.62, 129.47, 129.44, 129.06, 129.04, 126.81, 124.66, 122.67, 117.30, 115.52, 111.80, 105.84, 71.76, 64.75, 63.81, 61.07, 33.17, 31.67, 21.10, 20.92, 19.85.

HRMS (ESI) (*m*/*z*) $[M+H]^+$ calcd for $C_{20}H_{22}NO_4$, 340.1549; found 340.1546.

Entry 12 Product, Table 1

(±)-2-(4-(((3-((4-Methoxybenzoyl)oxy)pent-4-en-1-yl)oxy)carbonyl)phenyl)-3-methylpyridine 1-oxide, Major Regioisomer:



Following a modified procedure A, 3-methyl-2-(4-((pent-4-en-1-yloxy)carbonyl)phenyl)pyridine 1-oxide (50 mg, 0.168 mmol), $Pd(OAc)_2$/$PhS(O)C_2H_4S(O)Ph$ (8.46 mg, 0.017 mmol), 4-methoxybenzoic acid (77 mg, 0.504 mmol), and *p*-benzoquinone (36.4 mg, 0.336 mmol) afforded a crude residue which was purified via HPLC modified with 0.1%

trifluoroacetic acid (10-30% acetonitrile in water) and concentrated *in vacuo* to afford a mixture of products (46 mg, 0.103 mmol, 61% yield) as a mixture of regioisomers (88:12 branched:linear).

Major Regioisomer:

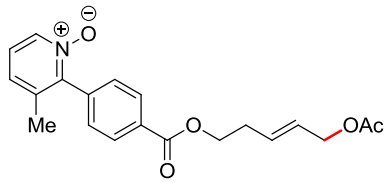
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (m, 1H), 8.27 – 8.14 (m, 2H), 8.09 – 7.95 (m, 2H), 7.77 – 7.63 (m, 1H), 7.54 – 7.36 (m, 3H), 7.08 – 6.84 (m, 2H), 5.98 (ddd, *J* = 17.0, 10.5, 6.1 Hz, 1H), 5.79 – 5.66 (m, 1H), 5.41 (dt, *J* = 17.3, 1.2 Hz, 1H), 5.29 (dt, *J* = 10.6, 1.1 Hz, 1H), 4.62 – 4.36 (m, 2H), 3.87 (s, 3H), 2.37 – 2.24 (m, 1H), 2.21 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.6, 165.4, 163.5, 149.9, 138.3, 137.3, 135.8, 135.0, 134.7, 131.6, 131.3, 130.1, 129.1, 125.0, 122.5, 117.2, 113.6, 71.9, 61.5, 55.4, 33.4, 19.7.

HRMS (ESI) (*m*/*z*) $[M+H]^+$ calcd for $C_{26}H_{26}NO_6$, 448.1760; found 448.1758.

Entry 13 Product, Table 1

(*E*)-2-(4-(((5-Acetoxypent-3-en-1-yl)oxy)carbonyl)phenyl)-3-methylpyridine 1-oxide, Major Regioisomer:



Following Procedure C, 3-methyl-2-(4-((pent-4-en-1-yloxy)carbonyl)phenyl)pyridine 1-oxide (50 mg, 0.168 mmol), $Pd(OAc)_2$ (378 mg, 1.682 mmol), 4,5-diazafluorenone (306 mg, 1.682 mmol), NaOAc (5.52 mg, 0.067 mmol), O_2 (1 atm), and AcOH (154 µl, 2.69 mmol) afforded a crude residue which was purified via flash chromatography (100% CH_2Cl_2 to 10% MeOH: CH_2Cl_2) to afford a mixture of products (46 mg, 0.129 mmol, 77% yield) as a mixture of regioisomers (9:91 branched:linear).

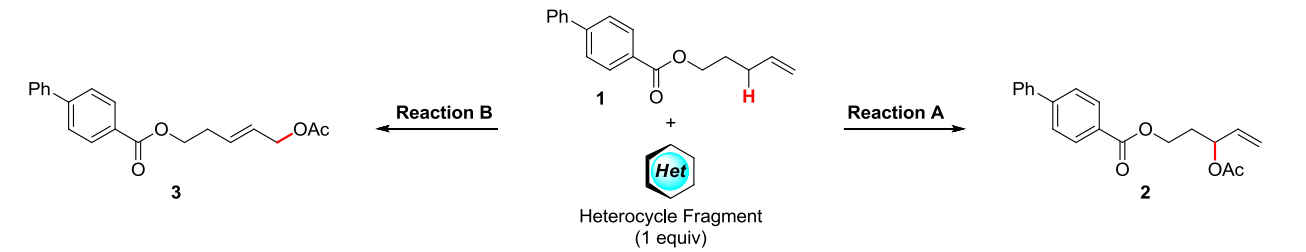
Major Regioisomer:

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (m, 1H), 8.21 – 8.12 (m, 2H), 7.46 (m, 2H), 7.27 – 7.14 (m, 2H), 5.85 (dt, *J* = 15.7, 6.5 Hz, 1H), 5.74 (dt, *J* = 15.6, 6.0 Hz, 1H), 4.55 (d, *J* = 6.0 Hz, 2H), 4.41 (t, *J* = 6.6 Hz, 2H), 2.56 (q, *J* = 6.6 Hz, 2H), 2.11 (s, 3H), 2.06 (s, 3H).

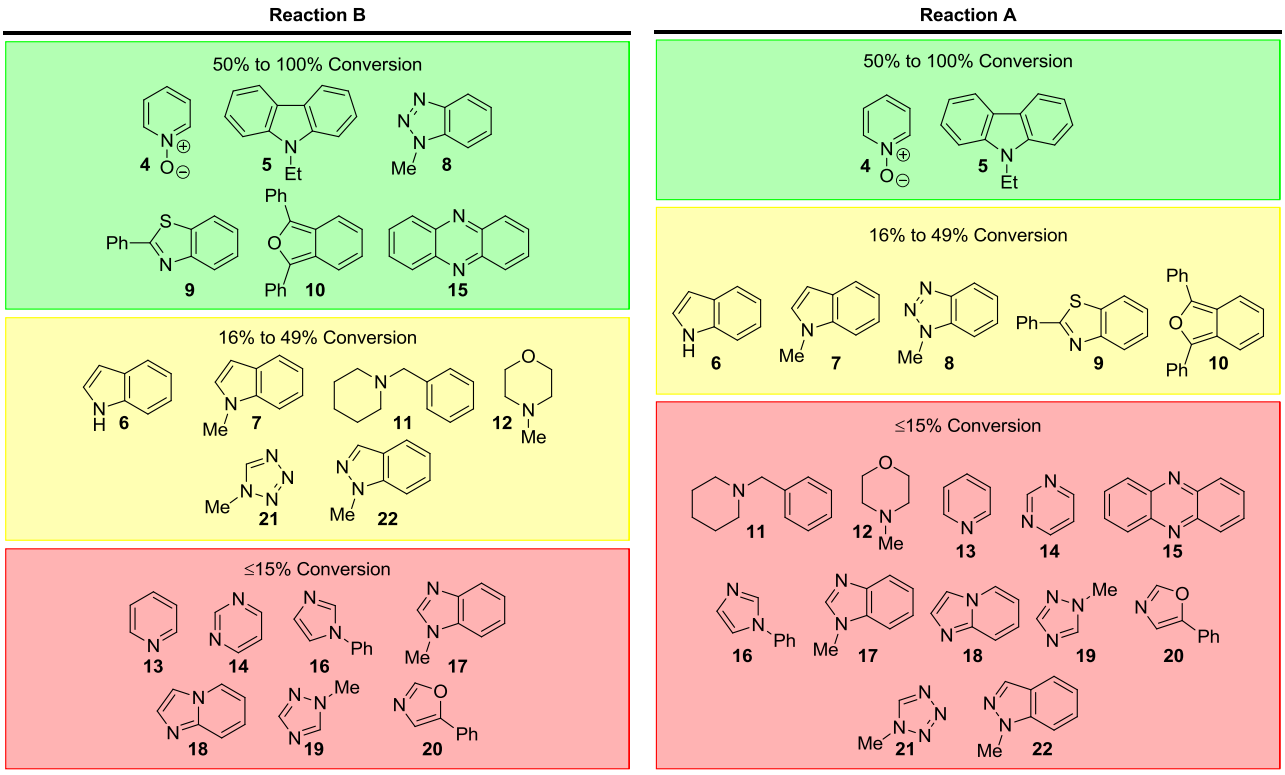
^{13}C NMR (100 MHz, $CDCl_3$) δ 170.7, 165.9, 148.7, 137.7, 136.8, 135.8, 130.9, 130.7, 130.0, 129.3, 127.8, 126.8, 124.3, 64.7, 63.9, 31.7, 20.9, 19.6.

HRMS (ESI) (*m*/*z*) $[M+H]^+$ calcd for $C_{20}H_{22}NO_5$, 356.1492; found 356.1502.

High-Throughput Heterocycle Screening Conditions and Details



Levels of Conversion for Heterocycles Screened

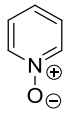
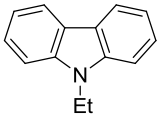
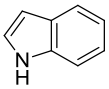
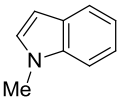
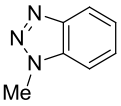
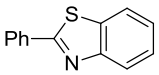
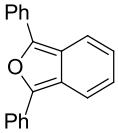
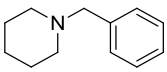
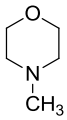
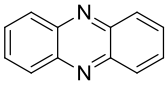


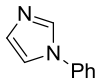
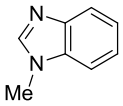
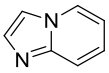
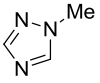
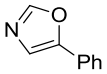
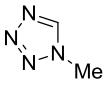
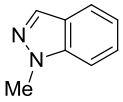
Reaction A:

To a solid mixture of $Pd(OAc)_2$/$PhS(O)C_2H_4S(O)Ph$ (10 mol %), *p*-benzoquinone (2 equiv) was added the olefin substrate (1 equiv), heterocycle fragment (1 equiv), AcOH (10 equiv), and 1,4-dioxane (0.3 M). The reaction was sealed and heated to 45 °C with stirring for 48 h. The reaction was allowed to cool to rt, and an aliquot was obtained for LC-MS analysis.

Reaction B:

To a solid mixture of $Pd(OAc)_2$ (10 mol %), 4,5-diazafluorenone (10 mol %), NaOAc (40 mol %), *p*-benzoquinone (2 equiv) was added the olefin substrate (1 equiv), heterocycle fragment (1 equiv), AcOH (16 equiv), and 1,4-dioxane (0.3 M). The reaction was sealed and heated to 60 °C with stirring for 48 h. The reaction was allowed to cool to rt, and an aliquot was obtained for LC-MS analysis.

Heterocycle Screen Results				
Entry	**Manuscript Identifier**	**Structure**	**Reaction A % Conversion**	**Reaction B % Conversion**
1	4		51	63
2	5		85	94
3	6		46	48
4	7		48	29
5	8		28	59
6	9		28	88
7	10		39	99
8	11		7	16
9	12		9	40
10	13		7	10
11	14		0	0
12	15		15	50

13	16		0	0
14	17		0	0
15	18		0	0
16	19		0	0
17	20		0	8
18	21		8	30
19	22		8	44

Lewis and Brønsted Acid Screening Conditions and Details

The screening of acidic additives was carried out in 1 mL glass vials arrayed in a 96 well aluminum block. The reactions were sealed with a Teflon-lined silicone cap mat and were mixed by orbital shaking. Stock solutions were transferred using either a TECAN 100 liquid handler or a standard micropipette with disposable plastic tips.

Brønsted Acid Screening for Reaction A:

To each reaction vial was added substrate (pent-4-en-1-yl 4-(3-methylpyridin-2-yl)benzoate (19 µL, 7 µmol, 0.356 M in 1,4-dioxane, 1 equiv), acid additive (19 µL, 7 µmol, 0.356 M in water or 1,4-dioxane, 1 equiv), and the mixtures were shaken at ambient temperature for 15 minutes. To the reaction was then added *p*-benzoquinone (20 µL, 0.014 mmol, 0.712 M in 1,4-dioxane, 2 equiv), $Pd(OAc)_2$/$PhS(O)C_2H_4S(O)Ph$ (19.97 µL, 0.711 µmol, 0.036 M in 1,4-dioxane 0.1 equiv), and AcOH (20 µL, 0.060 mmol). The reactions were heated at 45 °C for 48 h.

Lewis Acid Screening for Reaction A:

To each reaction vial was added substrate (pent-4-en-1-yl 4-(3-methylpyridin-2-yl)benzoate (19 µl, 7 µmol, 0.356 M in 1,4-dioxane, 1 equiv), acid additive (19 µL, 7 µmol, 0.356 M in water or 1,4-dioxane, 1 equiv), and the mixtures were shaken at ambient temperature for 15 min. To the reaction was added *p*-benzoquinone (20 µL, 0.014 mmol, 0.712 M in 1,4-dioxane, 2 equiv), $Pd(OAc)_2$/$PhS(O)C_2H_4S(O)Ph$ (19.97 µL, 0.711 µmol, 0.036 M in dioxane 0.1 equiv), and AcOH (20 µL, 0.060 mmol). The reactions were heated at 45 °C for 48 h.

Results:

Lewis Acids/Brønsted Acids Screened [a]

LiCl	**$AlMe_3$**	MnO	$CuBr_2$	AgCl	HCl
LiBr	**$Sc(OTf)_3$**	MnO_2	CuI	$Ag(OAc)_2$	HBr
KI	$Sc(NO_2)_3$	MnI_2	**CuO**	**AuCl**	HI
$BeSO_4•(H_2O)_4$	**Sc(O-*i*-Pr)$_3$**	$Fe(OAc)_2$	$Cu(OAc)_2$	$AuCl_3$	HNO_3
$B(C_6H_5)_3$	**ScF_3**	$FeCl_3$	$ZnCl_2$	$Lu(OTf)_3$	H_2SO_4
$B(C_6F_5)_3$	$ScCl_3$	FeO	ZnO	$La(OTf)_3$	CF_3CO_2H
(*R*)-(+)-2-Methyl-CBS-oxazaborolidine	$Y(OTf)_3$	Fe_2O_3	$Zn(OAc)_2$	**$Yb(OTf)_3$**	HBF_4
$BF_3•OEt_2$	$TiCl_2$	$CoBr_2$	YCl_3		**HCO_2H**
$B(OMe)_3$	$TiCl_4$	$NiCl_2$	$ZrCl_4$		***p*-TsOH**
BEt_3	$Ti(O-i-Pr)_4$	$CuCl_2$	$AgNO_3$		**MsOH**
		CuBr			**CSA**
					$(C_6F_5)CO_2H$

[a] Lewis or Brønsted acids highligted in bold green Indicate that product formation was observed via LC-MS analysis in reactions employing these reagents.

From the set of Lewis and Brønsted acids above, $Sc(OTf)_3$ and $BF_3•OEt_2$ provided the highest levels of desired product formation.

Theoretical Calculations

Computational Details

All calculations were performed with Gaussian 09.[1] The geometries of all heterocycles and complexes were optimized with the B3LYP[2] functional in the gas phase, using tight convergence criteria and an ultrafine integration grid. A mixed basis set of SDD (with ECP) for Pd and 6-31G(d,p) for all other atoms was used in geometry optimizations. Stationary points were confirmed by frequency analysis. Thermal corrections were calculated from unscaled vibrational frequencies at the same level of theory for a standard state of 1 atm and 298.15 K. Entropies were corrected for the breakdown of the harmonic oscillator approximation at low frequencies by raising all harmonic frequencies below 100 cm^{-1} to 100 cm^{-1}.[3] Electronic energies were obtained from single point energy calculations performed with the M06[4] functional and a mixed basis set of SDD(f) for Pd and 6-311++G(2d,p) for all other atoms. The SDD basis set (with ECP) was supplemented with an f-type polarization function (exponent 1.472).[5] The SMD[6] solvation model for 1,4-dioxane or acetic acid was used in M06 single point energy calculations.

[1] Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2010**.

[2] (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648. (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785.

[3] Ribeiro, R. F.; Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* **2011**, *115*, 14556.

[4] (a) Zhao,Y.; Truhlar, D. G. *Theor. Chem. Acc.*, **2008**, *120*, 215. (b) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.*, **2008**, *41*, 157.

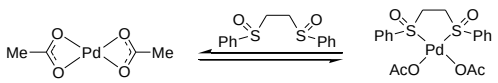
[5] Ehlers, A. W.; Böhme, M.; Dapprich, S.; Gobbi, A.; Höllwarth, A.; Jonas, V.; Köhler, K. F.; Stegmann, R.; Veldkamp, A.; Frenking, G. *Chem. Phys. Lett.* **1993**, *208*, 111.

[6] Marenich, A. V.; Cramer, C. J.; Truhlar, D. G., *J. Phys. Chem. B* **2009**, *113*, 6378.

Theoretical Binding Free Energies of $PhS(O)CH_2CH_2S(O)Ph$ and 4,5-Diazafluorenone Ligands

We considered the effect of chelating ligands $PhS(O)CH_2CH_2S(O)Ph$ and 4,5-diazafluorenone on the heterocycle binding equilibria. Here we use binding free-energies rather than enthalpies in order to compare binding of 1 equivalent ligand versus 2 equivalents heterocycle. We report free energies at a standard state of 1 atm and 298 K, but heterocycle binding will be somewhat more favorable at the experimental concentration of 0.3 M (by approximately –2.3 kcal/mol).

Binding of $PhS(O)CH_2CH_2S(O)Ph$ is endergonic by 1.9 kcal/mol. All heterocyclces except **5** and **10** are predicted to bind more strongly than the chelating ligand:

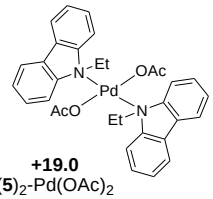


0.0
(0.0)

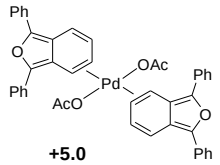
+1.9
(-12.1)

ΔG
(*ΔH*)
in kcal/mol

Heterocycles that bind <u>less favorably</u> than $PhS(O)CH_2CH_2S(O)Ph$:

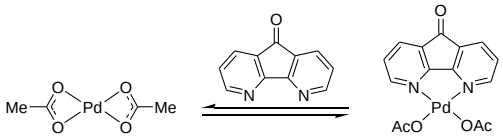


+19.0
(**5**)$_2$-Pd(OAc)$_2$



+5.0
(**10**)$_2$-Pd(OAc)$_2$

Binding of 4,5-diazafluorenone is exergonic by 4.2 kcal/mol. All heterocyclces except **4**, **5**, **6**, **7**, and **10** are predicted to bind more strongly than the chelating ligand:

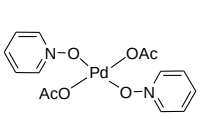


0.0
(0.0)

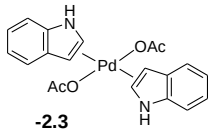
-4.2
(-17.4)

ΔG
(*ΔH*)
in kcal/mol

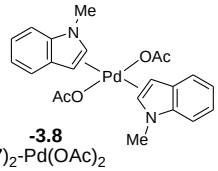
Heterocycles that bind <u>less favorably</u> than 4,5-diazafluorenone:



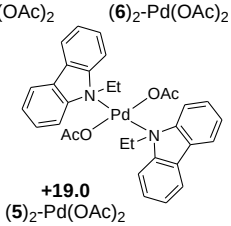
-3.3
(**4**)$_2$-Pd(OAc)$_2$



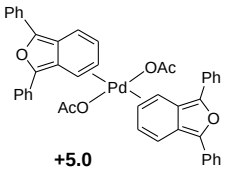
-2.3
(**6**)$_2$-Pd(OAc)$_2$



-3.8
(**7**)$_2$-Pd(OAc)$_2$



+19.0
(**5**)$_2$-Pd(OAc)$_2$



+5.0
(**10**)$_2$-Pd(OAc)$_2$

While the weakly-binding heterocycles above generally give high conversions (>50%), they are not the only heterocycles to do so. We speculate that other factors, such as binding of the olefin substrate, also contribute to successful turnover, which will be the subject of future mechanistic studies.

Theoretical Binding Affinities Using Acetic Acid in the SMD Solvation Model

We considered that acetic acid may have a significant effect on the binding affinities of heterocycles to palladium. Since parameters for solvent mixtures are not available for continuum solvent models, we computed the theoretical binding affinities in both dioxane and acetic acid individually using the SMD solvation model. Results for acetic acid appear below. The theoretical binding affinities are larger in acetic acid (by 1–4 kcal/mol for 1:1 Heterocycle:Pd complexes and 2–8 kcal/mol for 2:1 Hetrocycle:Pd complexes). The general trend is unchanged, although the correlation is somewhat poorer.

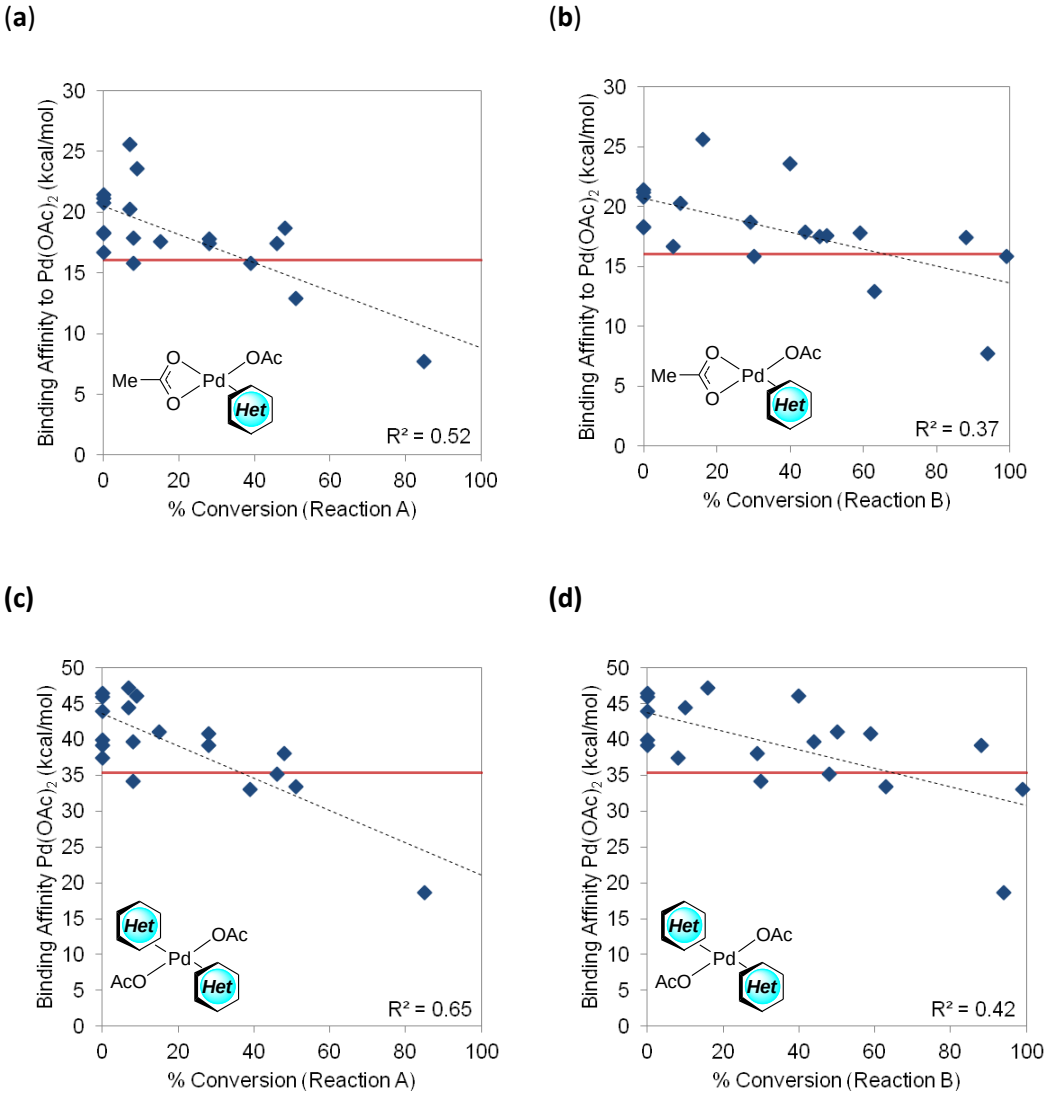


Figure S1. Theoretical binding affinities of heterocycles to $Pd(OAc)_2$ vs. product conversion (%) observed in reaction A (**a**) and reaction B (**b**); Theoretical binding affinities of heterocycles to $Pd(OAc)_2$ to form a 2:1 complex vs. product conversion (%) observed in reaction A (**c**) and reaction B (**d**). Binding affinity is defined as $-\Delta H$ for the reaction L + $Pd(OAc)_2$ → $LPd(OAc)_2$ (**a** and **b**) or 2 L + $Pd(OAc)_2$ → $L_2Pd(OAc)_2$ (**c** and **d**). The horizontal red line indicates the binding affinity of propene. The SMD solvation model for acetic acid was used.

Theoretical Binding Affinities Using the ωB97X-D Functional

In order to test the dependence of the results on choice of theoretical method, we computed binding affinities using the long-range, dispersion-corrected ωB97X-D functional.[7] In each case, the trend and correlation is similar to those computed with M06; absolute binding energies vary by 1–3 kcal/mol.

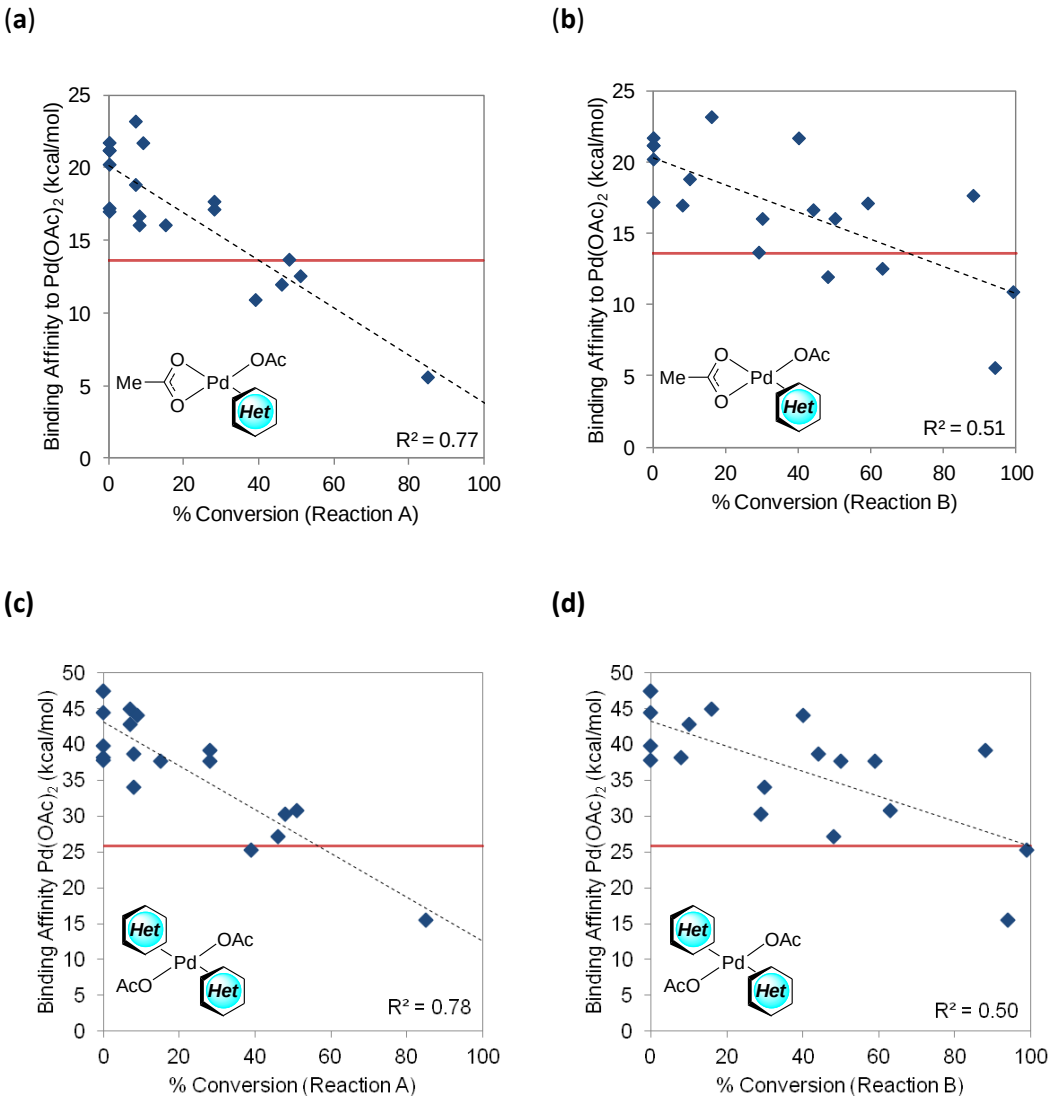


Figure S2. Theoretical binding affinities of heterocycles to $Pd(OAc)_2$ vs. product conversion (%) observed in reaction A (**a**) and reaction B (**b**); Theoretical binding affinities of heterocycles to $Pd(OAc)_2$ to form a 2:1 complex vs. product conversion (%) observed in reaction A (**c**) and reaction B (**d**). The horizontal red line indicates the binding affinity of propene. Geometries were optimized at the B3LYP/SDD–6-31G(d,p) level with single-point energies computed at the ωB97X-D/SDD(f)–6-311++G(2d,p) level with SMD solvation model (1,4-dioxane).

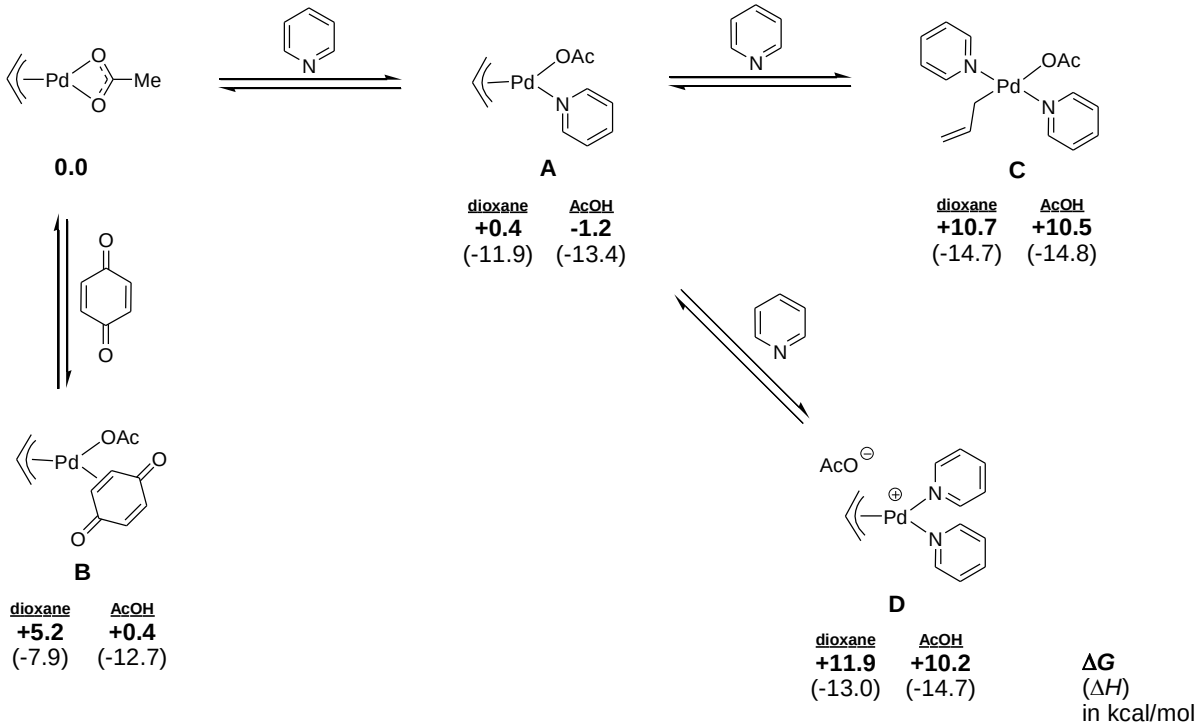
[7] Chai, J.-D.; Head-Gordon, M. *Phys. Chem. Chem. Phys.* **2008**, *10*, 6615.

Theoretical Binding Affinities to Allylpalladium Acetate

We considered an alternative pathway for catalyst arrest in which heterocycles bind to an allylpalladium intermediate following C–H activation. While the details of the subsequent C–O bond-forming process are not known, it has been proposed that benzoquinone binds to the allylpalladium intermediate to facilitate reductive elimination.[8] We therefore considered the possibility that heterocycles can compete with benzoquinone to inhibit catalyst turnover.

This mechanistic scenario is outlined below, using pyridine as an example. Coordination of one equivalent of pyridine (**A**) is more favorable than coordinate of benzoquinone (**B**), suggesting that unhindered heterocycles may bind to the catalyst and inhibit reductive elimination. A detailed examination of this and other steps in the mechanism will be the focus of future studies.

We also considered 2:1 binding of pyridine to allylpalladium acetate, to form either an η^1-allylpalladium complex (**C**) or an ion-pair (**D**), both of which are significantly endergonic. Therefore, 2:1 heterocycle:allylpalladium coordination is unlikely to contribute to catalyst arrest, and we have studied only 1:1 heterocycle:allylpalladium coordination in the following plots.



[8] Chen, M. S.; Prabagaran, N.; Labenz, N. A.; White, M. C. *J. Am. Chem. Soc.* **2005**, *127*, 6970.

We also computed binding affinities for all heterocycles to allylpalladium acetate. Similar to the results for $Pd(OAc)_2$, a reasonably good correlation is observed between heterocycle–Pd(allyl)OAc binding affinity and product conversion for reaction A, while a poor correlation is observed for reaction B. The correlation is somewhat poorer when the solvent model for acetic acid is used. It is worth noting that the binding affinities to Pd(allyl)OAc are on average 4 kcal/mol weaker than those to $Pd(OAc)_2$. More definitive determination of the process for catalyst arrest will require a more detailed examination of the reaction mechanism, which will be the subject of future studies.

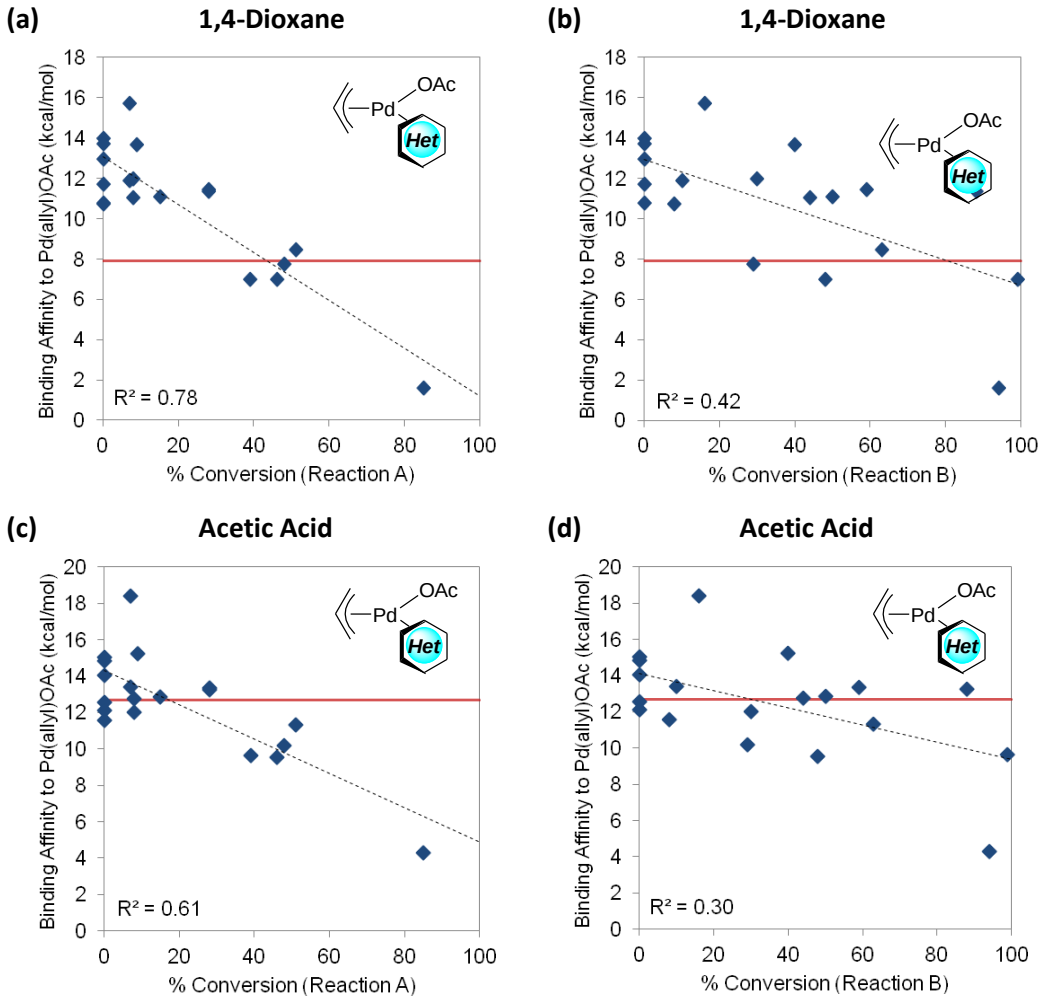
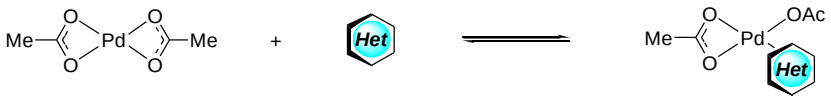


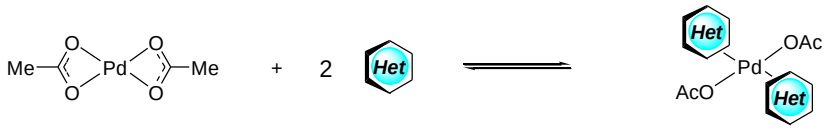
Figure S3. Theoretical binding affinities of heterocycles to Pd(allyl)OAc vs. product conversion (%) observed in reaction A and reaction B; Binding affinity is defined as $-\Delta H$ for the reaction L + Pd(allyl)OAc → LPd(allyl)OAc. The horizontal red line indicates the binding affinity of benzoquinone. The SMD solvation model for 1,4-dioxane was used for **a** and **b**, while the SMD model for acetic acid was used for **c** and **d**.

Table S1. Computed Binding Energies for a 1:1 Heterocycle:Palladium Complex (kcal/mol)



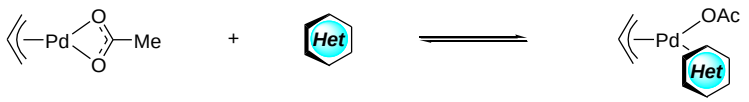
	M06/1,4-Dioxane			M06/Acetic Acid			ωB97X-D/1,4-Dioxane		
Heterocycle	**Δ*E***	**Δ*H***	**Δ*G***	**Δ*E***	**Δ*H***	**Δ*G***	**Δ*E***	**Δ*H***	**Δ*G***
propene	–16.1	–14.8	–3.3	–20.5	–16.0	–7.7	–14.9	–13.6	–2.1
4	–12.3	–10.9	+0.8	–14.3	–12.9	–1.2	–13.9	–12.6	–0.9
5	–5.4	–4.0	+9.4	–9.4	–8.0	+5.4	–7.1	–5.6	+7.7
6	–14.7	–13.4	–0.9	–18.8	–17.5	–5.0	–13.3	–12.0	+0.5
7	–16.0	–14.6	–1.9	–20.0	–18.7	–5.9	–15.0	–13.7	–0.9
8	–17.2	–15.5	–2.9	–19.5	–17.8	–5.2	–18.9	–17.1	–4.5
9	–16.5	–14.9	–1.6	–19.0	–17.4	–4.1	–19.2	–17.7	–4.3
10	–13.0	–11.6	+2.0	–17.2	–15.8	–2.2	–12.3	–10.9	+2.7
11	–23.1	–21.0	–7.4	–27.7	–25.6	–12.0	–25.3	–23.2	–9.6
12	–22.4	–20.3	–7.4	–25.6	–23.6	–10.7	–23.8	–21.7	–8.9
13	–19.6	–17.9	–5.9	–21.9	–20.2	–8.3	–20.5	–18.8	–6.9
14	–16.9	–15.3	–3.3	–19.9	–18.3	–6.3	–22.9	–21.2	–8.8
15	–16.7	–15.3	–3.1	–19.0	–17.6	–5.4	–17.5	–16.1	–3.9
16	–19.7	–18.1	–5.3	–22.4	–20.8	–7.9	–21.9	–20.2	–7.4
17	–21.2	–19.5	–6.8	–22.9	–21.2	–8.5	–23.4	–21.7	–9.0
18	–20.9	–19.2	–6.9	–23.1	–21.4	–9.1	–22.9	–21.2	–8.8
19	–16.9	–15.4	–3.5	–19.7	–18.2	–6.3	–18.7	–17.2	–5.3
20	–16.9	–15.4	–2.6	–18.2	–16.7	–3.9	–18.5	–17.0	–4.2
21	–16.4	–14.9	–2.8	–17.3	–15.8	–3.8	–17.6	–16.1	–4.0
22	–18.2	–16.5	–3.7	–19.6	–17.9	–5.0	–18.3	–16.7	–3.8

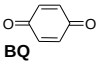
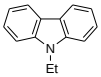
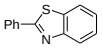
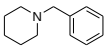
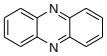
Table S2. Theoretical Binding Energies for a 2:1 Heterocycle:Palladium Complex (kcal/mol)



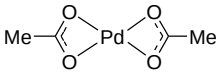
	M06/1,4-Dioxane			M06/Acetic Acid			ωB97X-D/1,4-Dioxane		
Heterocycle	**Δ*E***	**Δ*H***	**Δ*G***	**Δ*E***	**Δ*H***	**Δ*G***	**Δ*E***	**Δ*H***	**Δ*G***
propene	–30.9	–28.3	–4.7	–38.0	–35.4	–11.7	–28.4	–25.8	–2.2
4	–30.9	–28.0	–3.3	–36.2	–33.4	–8.6	–33.6	–30.8	–6.0
5	–13.3	–10.3	+18.6	–21.7	–18.7	+10.1	–18.0	–15.0	+13.8
6	–31.3	–28.6	–2.3	–37.9	–35.1	–8.9	–29.9	–27.1	–0.8
7	–33.7	–30.9	–3.8	–41.0	–38.0	–10.5	–33.1	–30.3	–3.2
8	–38.5	–35.1	–8.6	–44.2	–40.8	–14.2	–41.1	–37.7	–11.1
9	–36.0	–33.1	–4.6	–42.2	–39.2	–10.8	–42.1	–39.2	–10.7
10	–27.1	–24.4	+5.0	–35.7	–33.0	–3.6	–28.0	–25.3	+4.1
11	–44.0	–39.4	–10.2	–51.8	–47.2	–18.0	–49.6	–44.9	–15.8
12	–45.7	–41.5	–14.5	–50.3	–46.0	–19.1	–48.4	–44.1	–17.1
13	–44.1	–40.5	–15.4	–47.9	–44.4	–19.2	–46.4	–42.8	–17.6
14	–39.2	–35.9	–10.8	–43.2	–39.9	–14.8	–41.2	–37.8	–12.7
15	–39.0	–36.0	–9.9	–44.0	–41.0	–14.9	–40.7	–37.7	–11.6
16	–43.8	–40.4	–12.9	–47.2	–43.9	–16.3	–47.8	–44.4	–16.9
17	–46.6	–43.0	–16.1	–49.5	–45.9	–19.0	–51.0	–47.5	–20.5
18	–46.8	–43.3	–16.9	–49.7	–46.4	–20.2	–50.9	–47.4	–21.0
19	–39.6	–36.4	–11.3	–42.4	–39.2	–14.2	–42.9	–39.8	–14.6
20	–38.0	–34.9	–7.6	–40.6	–37.4	–10.2	–41.3	–38.1	–10.9
21	–35.5	–32.4	–7.0	–37.3	–34.2	–8.8	–37.2	–34.1	–8.7
22	–39.0	–35.7	–8.5	–43.1	–39.7	–12.5	–42.0	–38.7	–11.4

Table S3. Theoretical Binding Energies for a 1:1 Heterocycle:Allylpalladium Complex (kcal/mol)



	M06/1,4-Dioxane			M06/Acetic Acid		
Heterocycle	**Δ*E***	**Δ*H***	**Δ*G***	**Δ*E***	**Δ*H***	**Δ*G***
 **BQ**	–9.1	–7.9	+5.2	–13.9	–12.7	+0.4
4 	–9.6	–8.4	+3.4	–12.5	–11.3	+0.5
5 	–2.9	–1.6	+11.9	–5.6	–4.3	+9.2
6 	–8.1	–7.0	+5.5	–10.7	–9.5	+3.0
7 	–8.9	–7.8	+5.0	–11.3	–10.2	+2.6
8 	–13.0	–11.5	+1.4	–14.9	–13.4	–0.5
9 	–12.7	–11.4	+2.1	–14.6	–13.3	+0.2
10 	–8.2	–7.0	+6.7	–10.8	–9.6	+4.1
11 	–17.6	–15.7	–1.9	–20.3	–18.4	–4.5
12 	–15.4	–13.7	–0.6	–17.0	–15.2	–2.2
13 	–13.3	–11.9	+0.4	–14.9	–13.4	–1.2
14 	–12.2	–10.8	+1.4	–13.6	–12.1	+0.1
15 	–12.4	–11.1	+1.3	–14.1	–12.9	–0.4
16 	–14.4	–13.0	+0.3	–15.5	–14.0	–0.8
17 	–15.4	–14.0	–1.0	–16.3	–14.8	–1.9
18 	–15.2	–13.7	–1.0	–16.5	–15.0	–2.4
19 	–13.1	–11.7	+0.6	–13.9	–12.5	–0.3
20 	–12.0	–10.7	+2.3	–12.9	–11.5	+1.5
21 	–13.3	–11.9	+0.4	–13.4	–12.0	+0.3
22 	–12.5	–11.0	+2.2	–14.2	–12.7	+0.5

Cartesian coordinates (Å), energies (hartree) and thermal corrections for optimized structures



$Pd(OAc)_2$

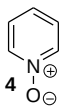
SCF Energy (M06, 1,4-dioxane): -584.7951348
SCF Energy (M06, acetic acid): -584.7882213
SCF Energy (wB97XD, 1,4-dioxane): -584.9212275
SCF Energy (B3LYP): -584.9336408
ZPE Correction: 0.103414
Enthalpy Correction: 0.115054
Free-Energy Correction: 0.067697899

Pd	0.00000	0.00000	0.00000
C	-0.00745	2.43645	0.00000
O	0.00000	1.76255	1.08808
O	0.00000	1.76255	-1.08808
C	-0.05437	3.93112	0.00000
O	0.00000	-1.76255	-1.08808
C	0.00745	-2.43645	0.00000
O	0.00000	-1.76255	1.08808
C	0.05437	-3.93112	0.00000
H	0.42669	4.32154	-0.89860
H	-1.10131	4.25345	0.00000
H	0.42669	4.32154	0.89860
H	1.10131	-4.25345	0.00000
H	-0.42669	-4.32154	0.89860
H	-0.42669	-4.32154	-0.89860

propene

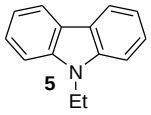
SCF Energy (M06, 1,4-dioxane): -117.8372950
SCF Energy (M06, acetic acid): -117.8374459
SCF Energy (wB97XD, 1,4-dioxane): -117.9017109
SCF Energy (B3LYP): -117.9075586
ZPE Correction: 0.080075
Enthalpy Correction: 0.085096
Free-Energy Correction: 0.055071

C	-0.13377	-0.45513	0.00000
H	-0.16480	-1.54525	0.00001
C	-1.28259	0.22051	-0.00000
H	-1.30400	1.30795	-0.00001
H	-2.24346	-0.28528	0.00000
C	1.23445	0.16280	-0.00000
H	1.81099	-0.15103	0.87938
H	1.81099	-0.15104	-0.87937
H	1.18172	1.25560	-0.00001



SCF Energy (M06, 1,4-dioxane): -323.3223811
SCF Energy (M06, acetic acid): -323.3245243
SCF Energy (wB97XD, 1,4-dioxane): -323.4356615
SCF Energy (B3LYP): -323.4550060
ZPE Correction: 0.093088
Enthalpy Correction: 0.099091
Free-Energy Correction: 0.065046

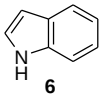
O	0.00000	0.00000	2.26140
N	0.00000	0.00000	0.98724
C	0.00000	1.18073	0.28359
C	0.00000	-1.18073	0.28359
C	0.00000	1.19439	-1.09917
H	0.00000	2.05962	0.91342
C	0.00000	-1.19439	-1.09917
H	0.00000	-2.05962	0.91342
C	0.00000	0.00000	-1.82180
H	0.00000	2.15551	-1.60275
H	0.00000	-2.15551	-1.60275
H	0.00000	0.00000	-2.90548



5

SCF Energy (M06, 1,4-dioxane): -595.7954165
SCF Energy (M06, acetic acid): -595.7956879
SCF Energy (wB97XD, 1,4-dioxane): -596.0617108
SCF Energy (B3LYP): -596.1182347
ZPE Correction: 0.233519
Enthalpy Correction: 0.246197
Free-Energy Correction: 0.196430124

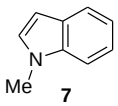
C	1.12963	0.29231	-0.17687
C	-1.12963	0.29233	-0.17686
C	0.00002	2.53822	-0.46814
C	0.72392	-1.05455	0.02403
C	2.48124	0.64862	-0.22196
C	-0.72394	-1.05454	0.02402
C	-2.48123	0.64866	-0.22194
H	0.87606	2.81127	-1.06521
H	-0.87606	2.81128	-1.06515
C	1.69423	-2.05188	0.17146
C	3.42575	-0.36469	-0.07200
H	2.79375	1.67811	-0.36506
C	-1.69426	-2.05186	0.17144
C	-3.42576	-0.36463	-0.07199
H	-2.79373	1.67816	-0.36503
C	3.04083	-1.70210	0.12249
H	1.39955	-3.08639	0.32382
H	4.48164	-0.11220	-0.10366
C	-3.04086	-1.70206	0.12249
H	-1.39961	-3.08637	0.32380
H	-4.48165	-0.11213	-0.10364
H	3.80238	-2.46725	0.23713
H	-3.80242	-2.46719	0.23711
N	0.00001	1.09305	-0.31173
C	0.00006	3.29779	0.86284
H	0.88513	3.04668	1.45437
H	0.00008	4.37823	0.68520
H	-0.88499	3.04671	1.45440



6

SCF Energy (M06, 1,4-dioxane): -363.6413666
SCF Energy (M06, acetic acid): -363.6429379
SCF Energy (wB97XD, 1,4-dioxane): -363.7974879
SCF Energy (B3LYP): -363.8300359
ZPE Correction: 0.129856
Enthalpy Correction: 0.137113
Free-Energy Correction: 0.099534

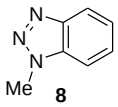
N	-1.56619	-1.08119	0.00001
C	-0.24787	-0.67180	0.00000
C	-2.38971	0.03016	-0.00001
C	-0.24999	0.75181	0.00000
C	0.93503	-1.41870	0.00000
C	-1.62589	1.16673	0.00001
H	-3.46407	-0.08547	-0.00002
C	0.98236	1.42901	-0.00000
C	2.13543	-0.71850	-0.00000
H	0.91790	-2.50505	0.00001
H	-1.99860	2.18098	0.00002
C	2.15881	0.69162	-0.00000
H	1.01119	2.51509	-0.00000
H	3.07242	-1.26748	0.00000
H	3.11545	1.20567	-0.00000
H	-1.87996	-2.03745	0.00001



7

SCF Energy (M06, 1,4-dioxane):	-402.9278297
SCF Energy (M06, acetic acid):	-402.9280645
SCF Energy (wB97XD, 1,4-dioxane):	-403.1053594
SCF Energy (B3LYP):	-403.1426986
ZPE Correction:	0.157709
Enthalpy Correction:	0.166645
Free-Energy Correction:	0.125150005

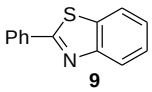
N	1.52960	-0.22381	0.00000
C	0.15159	-0.33248	0.00000
C	1.86044	1.12094	0.00000
C	-0.38898	0.98523	0.00000
C	-0.65990	-1.47311	0.00000
C	0.72640	1.88886	0.00000
H	2.90016	1.41787	0.00000
C	-1.78548	1.14341	-0.00000
C	-2.03694	-1.28116	0.00000
H	-0.23491	-2.47239	0.00000
H	0.69091	2.96881	-0.00000
C	-2.59398	0.01397	0.00000
H	-2.22491	2.13712	-0.00000
H	-2.69530	-2.14488	0.00000
H	-3.67422	0.12639	-0.00000
C	2.45962	-1.33294	0.00000
H	2.32768	-1.95948	-0.88947
H	3.47918	-0.94368	-0.00001
H	2.32769	-1.95946	0.88948



8

SCF Energy (M06, 1,4-dioxane):	-434.9880656
SCF Energy (M06, acetic acid):	-434.9917826
SCF Energy (wB97XD, 1,4-dioxane):	-435.1554483
SCF Energy (B3LYP):	-435.1937486
ZPE Correction:	0.133993
Enthalpy Correction:	0.142544
Free-Energy Correction:	0.101567

C	0.36140	-0.93591	0.00000
C	1.74834	-1.15406	0.00000
C	0.66647	1.50883	-0.00001
C	2.56927	-0.03779	-0.00000
H	2.14778	-2.16249	0.00000
C	2.03356	1.27341	-0.00000
H	0.26441	2.51657	-0.00001
H	3.64748	-0.16318	-0.00000
H	2.71541	2.11856	-0.00001
N	-0.69183	-1.82736	0.00001
C	-0.15962	0.37445	-0.00000
N	-1.79552	-1.15487	-0.00000
N	-1.51154	0.18354	-0.00000
C	-2.58429	1.15539	0.00001
H	-2.53549	1.78734	0.89222
H	-2.53552	1.78733	-0.89221
H	-3.52259	0.60081	0.00002

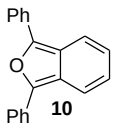


9

SCF Energy (M06, 1,4-dioxane):	-953.4826570
SCF Energy (M06, acetic acid):	-953.4833479
SCF Energy (wB97XD, 1,4-dioxane):	-953.7290326
SCF Energy (B3LYP):	-953.7777836
ZPE Correction:	0.183476
Enthalpy Correction:	0.195543
Free-Energy Correction:	0.146684483

N	0.40014	1.05980	0.00000
C	1.73931	0.72110	0.00000
C	-0.36587	0.01115	0.00000
C	2.80275	1.63665	0.00000
C	2.01488	-0.66887	0.00000
S	0.50472	-1.55505	-0.00000

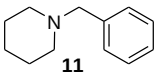
C	4.10565	1.15551	0.00000
H	2.58645	2.69968	0.00000
C	3.32483	-1.15213	-0.00000
C	4.36500	-0.22610	0.00000
H	4.93644	1.85439	0.00000
H	3.53032	-2.21759	-0.00000
H	5.39165	-0.57941	0.00000
C	-1.83386	0.06894	0.00000
C	-2.46506	1.32580	0.00000
C	-2.62621	-1.08977	-0.00000
C	-3.85316	1.41450	0.00000
H	-1.84671	2.21615	0.00000
C	-4.01600	-0.99555	-0.00000
H	-2.15947	-2.07063	-0.00000
C	-4.63442	0.25572	0.00000
H	-4.32862	2.39088	0.00000
H	-4.61570	-1.90068	-0.00000
H	-5.71795	0.32781	0.00000



10

SCF Energy (M06, 1,4-dioxane):	-845.3654653
SCF Energy (M06, acetic acid):	-845.3632192
SCF Energy (wB97XD, 1,4-dioxane):	-845.7142235
SCF Energy (B3LYP):	-845.8018889
ZPE Correction:	0.279252
Enthalpy Correction:	0.295690
Free-Energy Correction:	0.237753465

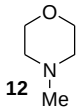
O	0.00000	0.66789	0.00000
C	1.12190	-0.10916	-0.00015
C	-1.12190	-0.10916	0.00015
C	0.72463	-1.44485	-0.00805
C	2.39740	0.58657	-0.01977
C	-0.72463	-1.44485	0.00805
C	-2.39740	0.58657	0.01977
C	1.42937	-2.68287	-0.05921
C	2.47392	1.92548	-0.45428
C	3.58239	-0.04859	0.40094
C	-1.42937	-2.68287	0.05921
C	-3.58239	-0.04859	-0.40094
C	-2.47392	1.92548	0.45428
C	0.71440	-3.85212	-0.03976
H	2.51088	-2.70172	-0.13043
C	3.69343	2.59429	-0.47890
H	1.56989	2.42809	-0.77991
C	4.80025	0.62501	0.36475
H	3.54323	-1.05931	0.79065
C	-0.71440	-3.85212	0.03975
H	-2.51088	-2.70172	0.13043
C	-4.80025	0.62501	-0.36475
H	-3.54323	-1.05931	-0.79065
C	-3.69343	2.59429	0.47890
H	-1.56989	2.42809	0.77991
H	1.23713	-4.80296	-0.08229
C	4.86489	1.94804	-0.07649
H	3.73099	3.62466	-0.82073
H	5.70132	0.11737	0.69670
H	-1.23713	-4.80296	0.08229
C	-4.86489	1.94804	0.07649
H	-5.70132	0.11737	-0.69670
H	-3.73099	3.62466	0.82073
H	5.81578	2.47154	-0.10094
H	-5.81578	2.47154	0.10094



11

SCF Energy (M06, 1,4-dioxane): -522.0023205
SCF Energy (M06, acetic acid): -522.0037329
SCF Energy (wB97XD, 1,4-dioxane): -522.2534170
SCF Energy (B3LYP): -522.2918119
ZPE Correction: 0.268426
Enthalpy Correction: 0.280676
Free-Energy Correction: 0.232123642

H	-2.56122	-1.87172	0.17753
C	-2.26501	-1.13842	-0.60181
C	-3.68886	0.70656	0.37312
C	-1.26715	0.37139	1.00507
C	-2.39102	1.39387	0.81598
N	-1.05331	-0.41109	-0.21683
C	-3.42779	-0.17427	-0.85549
H	-4.46803	1.44739	0.15959
H	-0.33148	0.87974	1.25592
H	-2.54220	1.94603	1.75097
H	-4.32418	-0.74614	-1.12293
H	-2.04738	-1.71205	-1.51027
H	-4.06559	0.08029	1.19426
H	-1.51355	-0.29314	1.85994
H	-2.08016	2.12094	0.05545
H	-3.17578	0.45879	-1.71539
C	0.10485	-1.29564	-0.10707
H	0.08869	-1.95971	-0.98183
H	0.04128	-1.95654	0.78002
C	1.42996	-0.55490	-0.08420
C	3.92011	0.75007	-0.12005
C	1.66490	0.50964	-0.96512
C	2.45606	-0.95062	0.78027
C	3.69527	-0.30691	0.76175
C	2.89872	1.15822	-0.98171
H	0.86190	0.82777	-1.62288
H	2.28327	-1.76951	1.47475
H	4.48049	-0.62724	1.44081
H	3.06528	1.98341	-1.66872
H	4.88155	1.25540	-0.13386



12

SCF Energy (M06, 1,4-dioxane): -326.9784163
SCF Energy (M06, acetic acid): -326.9817297
SCF Energy (wB97XD, 1,4-dioxane): -327.1089746
SCF Energy (B3LYP): -327.1201222
ZPE Correction: 0.163007
Enthalpy Correction: 0.170617
Free-Energy Correction: 0.132816

N	-0.54782	0.84367	0.00000
C	0.10781	0.32381	1.19950
H	1.15289	0.68305	1.28505
H	-0.43691	0.67512	2.08435
C	0.10781	0.32381	-1.19950
H	-0.43691	0.67512	-2.08435
H	1.15289	0.68305	-1.28505
C	0.10781	-1.20263	1.16971
H	0.66114	-1.60625	2.02262
H	-0.93078	-1.56845	1.21676
C	0.10781	-1.20263	-1.16971
H	0.66114	-1.60625	-2.02262
H	-0.93078	-1.56845	-1.21676
O	0.74855	-1.69582	0.00000
C	-0.61583	2.29615	0.00000
H	-1.15909	2.64068	0.88606
H	0.37938	2.78149	0.00000
H	-1.15909	2.64068	-0.88606

13

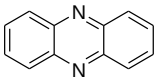
SCF Energy (M06, 1,4-dioxane): -248.1624114
SCF Energy (M06, acetic acid): -248.1640958
SCF Energy (wB97XD, 1,4-dioxane): -248.2667482
SCF Energy (B3LYP): -248.2925931
ZPE Correction: 0.088876
Enthalpy Correction: 0.094092
Free-Energy Correction: 0.061474

N	-0.00000	-1.42090	-0.00000
C	-1.14223	-0.72189	-0.00001
C	1.14223	-0.72189	0.00001
C	-1.19836	0.67292	-0.00000
H	-2.06031	-1.30707	-0.00001
C	1.19836	0.67292	0.00001
H	2.06031	-1.30707	0.00001
C	0.00000	1.38538	0.00000
H	-2.15704	1.18210	-0.00000
H	2.15705	1.18210	0.00001
H	0.00000	2.47162	0.00000

14

SCF Energy (M06, 1,4-dioxane): -264.2093447
SCF Energy (M06, acetic acid): -264.2101282
SCF Energy (wB97XD, 1,4-dioxane): -264.3081120
SCF Energy (B3LYP): -264.3294834
ZPE Correction: 0.077122
Enthalpy Correction: 0.082251
Free-Energy Correction: 0.04976

N	0.71637	-1.19904	-0.00000
C	-0.62250	-1.18442	-0.00000
C	1.30959	-0.00001	-0.00001
C	-1.35608	0.00000	0.00000
H	-1.11875	-2.15340	-0.00000
H	2.39782	-0.00001	0.00001
C	-0.62250	1.18443	0.00000
H	-2.44070	0.00001	0.00001
H	-1.11873	2.15341	0.00001
N	0.71638	1.19903	0.00000

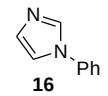


15

SCF Energy (M06, 1,4-dioxane): -571.3274815
SCF Energy (M06, acetic acid): -571.3294920
SCF Energy (wB97XD, 1,4-dioxane): -571.5553606
SCF Energy (B3LYP): -571.6190212
ZPE Correction: 0.170367
Enthalpy Correction: 0.180448
Free-Energy Correction: 0.137142703

N	0.00000	0.00000	1.42580
C	0.00000	1.14375	0.72329
C	0.00000	-1.14375	0.72329
C	0.00000	1.14375	-0.72329
C	0.00000	-1.14375	-0.72329
N	0.00000	0.00000	-1.42580
C	0.00000	-2.39347	1.41562
C	0.00000	-3.56962	0.71413
H	0.00000	-4.51802	1.24305
C	0.00000	-3.56962	-0.71413
H	0.00000	-4.51802	-1.24305
C	0.00000	-2.39347	-1.41562
C	0.00000	2.39347	1.41562
C	0.00000	2.39347	-1.41562
C	0.00000	3.56962	-0.71413
H	0.00000	4.51802	-1.24305
C	0.00000	3.56962	0.71413
H	0.00000	4.51802	1.24305
H	0.00000	-2.36707	2.50032
H	0.00000	-2.36707	-2.50032
H	0.00000	2.36707	-2.50032

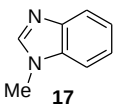
H	0.00000	2.36707	2.50032



16

SCF Energy (M06, 1,4-dioxane): -457.0568568
SCF Energy (M06, acetic acid): -457.0564632
SCF Energy (wB97XD, 1,4-dioxane): -457.2444408
SCF Energy (B3LYP): -457.2802591
ZPE Correction: 0.152116
Enthalpy Correction: 0.161141
Free-Energy Correction: 0.118790138

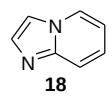
N	3.10569	-0.68611	-0.33530
C	3.12187	0.55904	0.25656
C	1.83445	-0.98752	-0.46301
C	1.84708	1.01056	0.47626
H	4.05093	1.05743	0.49561
H	1.43625	-1.88248	-0.91985
H	1.45834	1.90283	0.94056
N	1.00930	0.00551	0.01509
C	-0.41080	0.00695	0.01171
C	-1.11017	1.18445	-0.27607
C	-1.11014	-1.17231	0.29262
C	-2.50395	1.17875	-0.27482
H	-0.56238	2.08907	-0.51812
C	-2.50400	-1.17141	0.27076
H	-0.56352	-2.07420	0.54709
C	-3.20612	0.00229	-0.00740
H	-3.04118	2.09559	-0.49786
H	-3.04108	-2.08954	0.48864
H	-4.29155	0.00068	-0.01427



17

SCF Energy (M06, 1,4-dioxane): -418.9878995
SCF Energy (M06, acetic acid): -418.9887946
SCF Energy (wB97XD, 1,4-dioxane): -419.1595221
SCF Energy (B3LYP): -419.1913022
ZPE Correction: 0.146416
Enthalpy Correction: 0.155079
Free-Energy Correction: 0.113936

C	0.36922	0.95593	-0.00000
C	-1.75157	1.16328	0.00000
C	-0.15561	-0.35996	0.00000
C	1.75602	1.15000	-0.00000
H	-2.76121	1.55640	0.00000
C	0.65899	-1.49490	0.00000
C	2.57427	0.02511	-0.00000
H	2.16630	2.15453	-0.00000
C	2.03435	-1.27697	-0.00000
H	0.24813	-2.49987	0.00000
H	3.65318	0.14792	-0.00000
H	2.70636	-2.12997	-0.00000
C	-2.53014	-1.24690	0.00000
H	-2.43431	-1.87757	-0.89009
H	-2.43430	-1.87757	0.89009
H	-3.52302	-0.79321	0.00001
N	-0.66192	1.88691	0.00000
N	-1.53155	-0.19751	0.00000



18

SCF Energy (M06, 1,4-dioxane): -379.6784739
SCF Energy (M06, acetic acid): -379.6789500
SCF Energy (wB97XD, 1,4-dioxane): -379.8278851
SCF Energy (B3LYP): -379.8592681
ZPE Correction: 0.118014
Enthalpy Correction: 0.124911
Free-Energy Correction: 0.087903

C	-0.56890	-0.55492	0.00000
C	-2.19037	0.83875	0.00000

C	0.30456	-1.66736	0.00000
H	-3.21487	1.18734	0.00000
C	1.35939	0.93641	0.00000
C	1.66314	-1.46622	0.00000
H	-0.13698	-2.65705	0.00000
C	2.19447	-0.14452	0.00000
H	1.69753	1.96559	0.00000
H	2.34066	-2.31345	0.00000
H	3.26577	0.01984	0.00000
N	-1.89850	-0.49268	0.00000
C	-1.05519	1.62423	0.00000
H	-0.90520	2.69232	0.00000
N	0.00000	0.73657	0.00000

19

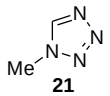
SCF Energy (M06, 1,4-dioxane): -281.4608636
SCF Energy (M06, acetic acid): -281.4602905
SCF Energy (wB97XD, 1,4-dioxane): -281.5619936
SCF Energy (B3LYP): -281.5724017
ZPE Correction: 0.087834
Enthalpy Correction: 0.093939
Free-Energy Correction: 0.059189662

N	1.50134	0.70504	0.00001
C	1.39515	-0.65298	0.00001
C	0.23439	1.08536	-0.00000
H	2.25202	-1.31231	0.00001
H	-0.13111	2.10316	-0.00000
N	-0.58514	0.00997	0.00000
C	-2.03394	-0.05121	0.00001
H	-2.38673	-0.57771	0.88991
H	-2.42865	0.96623	0.00002
H	-2.38674	-0.57770	-0.88990
N	0.15633	-1.12769	-0.00002

20

SCF Energy (M06, 1,4-dioxane): -476.9295522
SCF Energy (M06, acetic acid): -476.9290107
SCF Energy (wB97XD, 1,4 dioxane): -477.1050936
SCF Energy (B3LYP): -477.1452331
ZPE Correction: 0.139833
Enthalpy Correction: 0.148813
Free-Energy Correction: 0.106668353

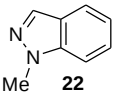
N	-3.22460	0.61463	0.00000
C	-3.03712	-0.66648	-0.00000
C	-1.94183	1.14190	-0.00000
H	-3.77505	-1.45471	-0.00000
H	-1.77371	2.20842	-0.00000
C	0.43389	0.05669	0.00000
C	1.09422	-1.18369	0.00000
C	1.20260	1.23440	0.00000
C	2.48609	-1.24067	0.00000
H	0.51034	-2.09741	-0.00000
C	2.59239	1.17006	0.00000
H	0.70950	2.20165	0.00000
C	3.24151	-0.06716	0.00000
H	2.98179	-2.20697	0.00000
H	3.17127	2.08887	0.00000
H	4.32621	-0.11467	0.00000
C	-1.02086	0.13139	0.00000
O	-1.73543	-1.04827	-0.00000



21

SCF Energy (M06, 1,4-dioxane): -297.4614012
SCF Energy (M06, acetic acid): -297.4654137
SCF Energy (wB97XD, 1,4-dioxane): -297.5591447
SCF Energy (B3LYP): -297.5730386
ZPE Correction: 0.074775
Enthalpy Correction: 0.080956
Free-Energy Correction: 0.046295256

N	1.51857	0.61843	0.00859
C	0.28245	1.07340	-0.00392
H	-0.02044	2.10950	-0.00960
N	0.16526	-1.10557	-0.00664
N	-0.57138	0.03054	-0.01725
N	1.40625	-0.73916	0.00647
C	-2.02416	-0.01450	0.01056
H	-2.34540	-0.92070	-0.50268
H	-2.39097	-0.03146	1.04029
H	-2.42381	0.85958	-0.50609

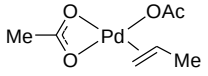


22

SCF Energy (M06, 1,4-dioxane): -418.9592494
SCF Energy (M06, acetic acid): -418.9605495
SCF Energy (wB97XD, 1,4-dioxane): -419.1316107
SCF Energy (B3LYP): -419.1702558
ZPE Correction: 0.14606
Enthalpy Correction: 0.154867
Free-Energy Correction: 0.113618317

N	1.51337	-0.20492	-0.00000
C	0.15184	-0.34489	0.00000
C	-0.38374	0.96914	0.00000
C	-0.66799	-1.48603	0.00000
C	0.76819	1.81197	0.00000
C	-1.77902	1.14994	0.00000
C	-2.03818	-1.27552	0.00000
H	-0.25138	-2.48819	0.00000
H	0.81598	2.89262	0.00000
C	-2.59085	0.02727	0.00000
H	-2.20876	2.14737	0.00000
H	-2.70643	-2.13169	0.00000
H	-3.67042	0.14216	0.00000
C	2.51827	-1.24560	0.00000
H	2.43143	-1.87656	-0.89139
H	3.49143	-0.75611	-0.00001
H	2.43144	-1.87655	0.89141
N	1.88600	1.10625	-0.00000

1:1 Heterocycle:Pd Complexes

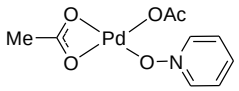


propene-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -702.6580951
SCF Energy (M06, acetic acid): -702.6582776
SCF Energy (wB97XD, 1,4-dioxane): -702.8467102
SCF Energy (B3LYP): -702.8633026
ZPE Correction: 0.185353
Enthalpy Correction: 0.202183
Free-Energy Correction: 0.143154587

Pd	0.14839	0.09458	-0.32870
C	2.35828	-0.92984	0.09756
O	2.18191	0.34380	0.01368
O	1.35068	-1.68455	-0.07617
C	3.71101	-1.48734	0.42382
O	-1.70352	-0.54272	-0.74089
C	-2.36336	-0.89606	0.34712
O	-1.96841	-0.68713	1.49073

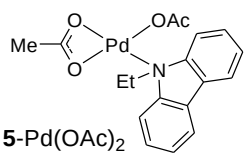
C	-3.66866	-1.61092	0.04034
H	3.85011	-2.44594	-0.07982
H	4.49379	-0.78258	0.13839
H	3.77105	-1.65901	1.50405
H	-3.44763	-2.62767	-0.30033
H	-4.27944	-1.66077	0.94255
H	-4.21232	-1.10593	-0.76197
C	-0.37202	2.01384	-1.17614
C	-0.66866	2.08733	0.17988
H	-1.67826	1.84110	0.49937
H	-1.14676	1.77465	-1.89779
H	0.55051	2.44048	-1.56353
C	0.19885	2.75840	1.20620
H	-0.20538	3.75841	1.41402
H	0.18891	2.20350	2.14864
H	1.23128	2.86528	0.86521



4-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -908.1370718
SCF Energy (M06, acetic acid): -908.1354925
SCF Energy (wB97XD, 1,4-dioxane): -908.3791096
SCF Energy (B3LYP): -908.4037983
ZPE Correction: 0.197914
Enthalpy Correction: 0.216345
Free-Energy Correction: 0.153567115

Pd	-0.90365	-0.12070	-0.37139
C	-2.09650	-2.10408	0.42570
O	-0.90200	-2.19674	-0.02455
O	-2.62912	-0.94268	0.46077
C	-2.86095	-3.31707	0.86493
O	-1.39549	1.80770	-0.58246
C	-0.90057	2.66518	0.26611
O	-0.07817	2.41652	1.15539
C	-1.46289	4.06767	0.07819
H	-3.43930	-3.69928	0.01676
H	-2.17311	-4.09761	1.19485
H	-3.55826	-3.05350	1.66241
H	-2.51229	4.08114	0.38954
H	-0.89758	4.77854	0.68206
H	-1.43078	4.35359	-0.97627
O	0.91848	0.22059	-1.28170
N	1.99286	-0.07404	-0.54655
C	2.17071	0.48217	0.67941
C	2.91687	-0.89939	-1.09754
C	3.32552	0.19528	1.39190
H	1.36204	1.14319	1.00582
C	4.08366	-1.19478	-0.41315
H	2.65363	-1.28068	-2.07487
C	4.29827	-0.64738	0.85280
H	3.44936	0.64763	2.36944
H	4.80647	-1.85728	-0.87553
H	5.20340	-0.87398	1.40583

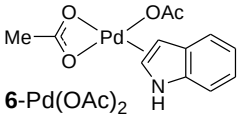


5-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -1180.599202
SCF Energy (M06, acetic acid): -1180.598952
SCF Energy (wB97XD, 1,4-dioxane): -1180.994227
SCF Energy (B3LYP): -1181.038180
ZPE Correction: 0.338453
Enthalpy Correction: 0.363540
Free-Energy Correction: 0.287729774

Pd	1.08154	0.61731	-0.17198
C	1.07970	2.89126	0.74966
O	0.00400	2.20000	0.69908
O	2.14689	2.36173	0.28653
C	1.09729	4.26061	1.35946
O	2.53455	-0.46351	-1.05055

C	3.13875	-1.37308	-0.32564
O	2.72918	-1.81499	0.75001
C	4.43970	-1.85682	-0.95069
H	1.83670	4.88640	0.85578
H	0.10532	4.71206	1.30229
H	1.38226	4.17618	2.41377
H	5.20343	-1.08191	-0.82774
H	4.77322	-2.76989	-0.45581
H	4.31689	-2.02619	-2.02358
N	-0.44792	-0.87249	-0.42717
C	-1.51717	-0.19421	-1.14554
C	-0.98578	-1.05873	0.91635
C	0.03906	-2.14157	-1.08498
C	-2.60185	0.06315	-0.29065
C	-1.51960	0.18113	-2.48348
C	-2.26506	-0.48825	1.01753
C	-0.35083	-1.67810	1.98669
H	0.50134	-1.84392	-2.02694
H	0.82988	-2.52502	-0.44224
C	-3.72347	0.73402	-0.78488
C	-2.65202	0.84241	-2.96671
H	-0.66955	-0.01659	-3.12830
C	-2.94507	-0.53775	2.23721
C	-1.05059	-1.72826	3.19568
H	0.66014	-2.06052	1.88826
C	-3.73914	1.11872	-2.12573
H	-4.56922	0.94933	-0.13884
H	-2.68439	1.15087	-4.00703
C	-2.32945	-1.16602	3.31998
H	-3.93269	-0.09837	2.34069
H	-0.58663	-2.20100	4.05590
H	-4.60456	1.63911	-2.52474
H	-2.84480	-1.21548	4.27456
C	-1.05968	-3.17925	-1.30024
H	-0.61636	-4.06747	-1.76117
H	-1.51462	-3.48513	-0.35413
H	-1.84743	-2.81274	-1.96386

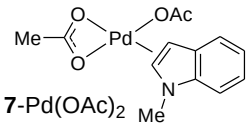


6-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -948.4598641
SCF Energy (M06, acetic acid): -948.4610576
SCF Energy (wB97XD, 1,4-dioxane): -948.7398854
SCF Energy (B3LYP): -948.7712529
ZPE Correction: 0.234540
Enthalpy Correction: 0.254248
Free-Energy Correction: 0.18915533

Pd	0.77340	0.33814	-0.19346
C	0.29983	2.76086	0.01836
O	-0.57644	1.85352	0.27033
O	1.45535	2.38920	-0.35625
C	-0.03750	4.21289	0.19325
O	2.33815	-0.75465	-0.81172
C	3.11069	-1.32793	0.08379
O	2.86363	-1.42974	1.28548
C	4.40022	-1.86483	-0.52150
H	0.44547	4.80311	-0.58842
H	-1.11861	4.35931	0.17344
H	0.34848	4.55458	1.15972
H	5.06976	-1.02540	-0.73575
H	4.88603	-2.53933	0.18464
H	4.20334	-2.37654	-1.46672
N	-1.29564	-1.00572	1.73730
C	-2.34525	-0.87080	0.82972
C	-0.15102	-1.37653	1.08729
C	-1.85304	-1.21478	-0.45131
C	-3.67287	-0.50112	1.04446
C	-0.43582	-1.51021	-0.29687
H	0.76029	-1.64000	1.61308
C	-2.72413	-1.21131	-1.54784

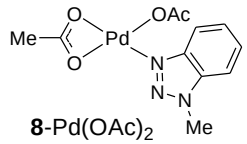
C	-4.51852	-0.50061	-0.06247
H	-4.03601	-0.23014	2.03107
H	0.16791	-2.08175	-0.98939
C	-4.05380	-0.85574	-1.34230
H	-2.36545	-1.47675	-2.53789
H	-5.56031	-0.22309	0.06702
H	-4.74437	-0.84809	-2.17980
H	-1.32195	-0.69607	2.69702



7-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -987.7483861
SCF Energy (M06, acetic acid): -987.7481857
SCF Energy (wB97XD, 1,4-dioxane): -988.0505467
SCF Energy (B3LYP): -988.0848602
ZPE Correction: 0.262394
Enthalpy Correction: 0.283829
Free-Energy Correction: 0.215305475

Pd	0.85608	0.37091	-0.29070
C	0.39613	2.78219	0.06683
O	-0.50273	1.87119	0.20039
O	1.56922	2.42484	-0.26105
C	0.05908	4.22366	0.31847
O	2.44094	-0.70628	-0.88721
C	3.15423	-1.34448	0.01252
O	2.84028	-1.51403	1.19108
C	4.46844	-1.86612	-0.55232
H	0.54426	4.85301	-0.43106
H	-1.02153	4.37339	0.30276
H	0.44658	4.51538	1.30043
H	5.15900	-1.02639	-0.68199
H	4.90691	-2.58710	0.13874
H	4.31698	-2.32037	-1.53458
N	-1.32977	-1.05836	1.47903
C	-2.32209	-0.85635	0.51419
C	-0.16574	-1.41136	0.86313
C	-1.76389	-1.12123	-0.75834
C	-3.65510	-0.47858	0.67824
C	-0.35977	-1.44270	-0.54435
H	0.71496	-1.71156	1.42075
C	-2.57130	-1.03514	-1.89776
C	-4.43885	-0.39629	-0.47159
H	-4.07152	-0.25955	1.65596
H	0.26873	-1.99686	-1.22940
C	-3.90782	-0.67581	-1.74323
H	-2.16002	-1.23975	-2.88183
H	-5.48283	-0.11133	-0.38170
H	-4.55013	-0.60480	-2.61552
C	-1.46604	-0.73784	2.88980
H	-1.57034	0.34263	3.03348
H	-2.34207	-1.24327	3.30644
H	-0.57553	-1.08207	3.41724

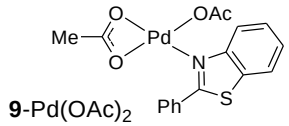


8-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -1019.81060
SCF Energy (M06, acetic acid): -1019.81107
SCF Energy (wB97XD, 1,4-dioxane): -1020.10672
SCF Energy (B3LYP): -1020.14154
ZPE Correction: 0.239245
Enthalpy Correction: 0.260314
Free-Energy Correction: 0.192073466

Pd	-1.21654	-0.19564	-0.20900
C	-3.19886	-1.34661	0.64598
O	-2.03780	-1.87760	0.73969
O	-3.28578	-0.20881	0.07054
C	-4.41045	-2.01815	1.21938
O	-0.92420	1.50717	-1.23414

C	-0.91952	2.60877	-0.52290
O	-0.87398	2.66452	0.70680
C	-0.99461	3.86255	-1.38442
H	-5.28700	-1.79435	0.60805
H	-4.25002	-3.09554	1.28566
H	-4.58913	-1.62769	2.22709
H	-2.02591	3.99639	-1.72744
H	-0.70073	4.73312	-0.79629
H	-0.36242	3.76722	-2.27058
C	1.83450	0.05331	0.34657
C	1.87621	1.19128	1.16945
C	4.26467	-0.29070	0.49634
C	3.12646	1.55868	1.63904
H	0.96868	1.74932	1.38504
C	4.29842	0.83086	1.31018
H	5.16320	-0.84372	0.24558
H	3.21700	2.43283	2.27589
H	5.25192	1.16539	1.70750
N	0.78663	-0.59457	-0.27553
C	2.99908	-0.66536	0.01999
N	1.22419	-1.62320	-0.94128
N	2.55427	-1.68679	-0.77887
C	3.31105	-2.74884	-1.41891
H	4.04147	-2.32594	-2.11405
H	3.82703	-3.35035	-0.66559
H	2.60343	-3.37210	-1.96424

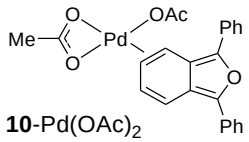


9-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -1538.304060
SCF Energy (M06, acetic acid): -1538.301807
SCF Energy (wB97XD, 1,4-dioxane): -1538.680903
SCF Energy (B3LYP): -1538.715896
ZPE Correction: 0.288385
Enthalpy Correction: 0.313049
Free-Energy Correction: 0.238135708

Pd	-0.54424	-1.16889	-0.32661
C	-2.48576	-1.63527	-1.74531
O	-1.84831	-0.52957	-1.84164
O	-2.07233	-2.48419	-0.88346
C	-3.65696	-1.93894	-2.63052
O	0.48185	-2.26306	1.00591
C	0.25371	-2.03675	2.27917
O	-0.46111	-1.14493	2.73149
C	0.97456	-3.02918	3.18202
H	-4.40875	-2.50274	-2.07410
H	-4.08192	-1.01508	-3.02593
H	-3.31986	-2.55938	-3.46787
H	2.03626	-3.07881	2.92483
H	0.85401	-2.73400	4.22486
H	0.55476	-4.02896	3.03359
N	0.81002	0.38094	-0.15491
C	2.17189	0.20755	-0.42085
C	0.47991	1.63838	0.05049
C	2.81800	-1.00968	-0.68261
C	2.90367	1.41218	-0.43553
S	1.83665	2.75058	-0.07127
C	4.18079	-0.98794	-0.95118
H	2.25630	-1.93506	-0.64755
C	4.27388	1.43136	-0.70834
C	4.90353	0.21807	-0.96548
H	4.69703	-1.92153	-1.15140
H	4.82896	2.36359	-0.71871
H	5.96795	0.20454	-1.17850
C	-0.85618	2.15145	0.37861
C	-1.67866	1.46148	1.28782
C	-1.30086	3.35673	-0.19324
C	-2.93604	1.97781	1.59977
H	-1.32194	0.55209	1.76706
C	-2.56086	3.85721	0.12334

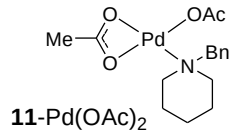
H	-0.67290	3.88269	-0.90646
C	-3.38135	3.16738	1.01962
H	-3.56457	1.44743	2.30880
H	-2.90357	4.78086	-0.33308
H	-4.36318	3.56016	1.26797



10-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -1430.181243
SCF Energy (M06, acetic acid): -1430.178785
SCF Energy (wB97XD, 1,4-dioxane): -1430.654990
SCF Energy (B3LYP): -1430.728611
ZPE Correction: 0.383736
Enthalpy Correction: 0.412873
Free-Energy Correction: 0.329255953

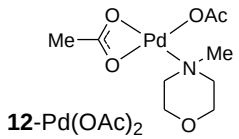
Pd	-1.99501	-1.25979	0.00420
C	-1.37412	-2.28048	2.17548
O	-0.50181	-1.97208	1.28514
O	-2.60090	-2.07062	1.90822
C	-0.94879	-2.84017	3.50057
O	-3.72239	-0.82961	-0.93037
C	-4.22795	0.36331	-0.71008
O	-3.64200	1.28662	-0.14626
C	-5.65601	0.49907	-1.21640
H	-1.69223	-3.55413	3.86082
H	0.03201	-3.31159	3.41849
H	-0.88411	-2.02180	4.22579
H	-6.32946	-0.00830	-0.51779
H	-5.92892	1.55368	-1.27155
H	-5.77306	0.02137	-2.19204
O	2.31731	1.28259	-0.03039
C	0.99329	1.52242	-0.25942
C	2.65307	0.02204	-0.44699
C	0.45147	0.39445	-0.86302
C	0.48026	2.82172	0.14610
C	1.52309	-0.57028	-0.98757
C	4.03358	-0.39069	-0.25038
C	-0.84884	0.09467	-1.39206
C	1.36960	3.89187	0.37195
C	-0.90130	3.03227	0.32447
C	1.29557	-1.81462	-1.65660
C	4.37472	-1.75356	-0.15076
C	5.05875	0.57002	-0.14782
C	-1.03649	-1.15719	-2.02237
H	-1.59007	0.87775	-1.50159
C	0.88791	5.13994	0.75266
H	2.43497	3.73680	0.24101
C	-1.37166	4.28898	0.70015
H	-1.61715	2.22683	0.20191
C	0.05456	-2.09664	-2.15071
H	2.11187	-2.51393	-1.80011
C	5.70188	-2.14012	0.01817
H	3.59471	-2.50690	-0.16627
C	6.38162	0.17597	0.02985
H	4.80838	1.62303	-0.21733
H	-1.93197	-1.31593	-2.61415
C	-0.48527	5.34627	0.91407
H	1.58539	5.95570	0.92010
H	-2.43975	4.43053	0.83431
H	-0.12858	-3.02944	-2.67373
C	6.71189	-1.17957	0.10665
H	5.94578	-3.19558	0.09727
H	7.15965	0.93034	0.10342
H	-0.85890	6.32244	1.20949
H	7.74538	-1.48381	0.24250



11-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -1106.834287
SCF Energy (M06, acetic acid): -1106.836163
SCF Energy (wB97XD, 1,4-dioxane): -1107.215037
SCF Energy (B3LYP): -1107.239644
ZPE Correction: 0.374670
Enthalpy Correction: 0.399138
Free-Energy Correction: 0.324926765

Pd	0.68075	-0.48947	0.43983
C	-0.22995	-1.65097	2.40696
O	-0.59317	-0.45715	2.11027
O	0.64514	-2.20767	1.66573
C	-0.84228	-2.37641	3.56814
O	2.12291	-0.94044	-0.89604
C	1.77537	-1.67494	-1.92728
O	0.61896	-1.92452	-2.26609
C	2.97338	-2.21988	-2.69285
H	-0.13841	-3.10825	3.96852
H	-1.14469	-1.66716	4.34096
H	-1.73458	-2.90916	3.22181
H	3.41372	-3.04462	-2.12276
H	2.65368	-2.59106	-3.66740
H	3.74524	-1.45476	-2.80977
N	0.35323	1.40438	-0.45809
C	-0.21032	2.33167	0.57642
H	-0.49375	3.26419	0.06345
H	-1.11668	1.87471	0.97412
C	1.62473	1.98353	-1.00619
H	2.01367	1.27756	-1.73900
H	1.36334	2.92081	-1.52140
C	0.78195	2.63737	1.70001
H	0.30555	3.34969	2.38367
H	0.96510	1.72224	2.27356
C	2.66226	2.25954	0.08023
H	3.54675	2.69622	-0.39784
H	2.97579	1.30778	0.52354
C	-0.61313	1.24290	-1.61468
H	-0.70542	2.22967	-2.09032
H	-0.12776	0.56204	-2.31628
C	2.10305	3.19525	1.15823
H	1.93265	4.19156	0.72614
H	2.82645	3.32362	1.97062
C	-1.98811	0.72003	-1.26057
C	-2.23637	-0.66106	-1.24905
C	-3.04421	1.60270	-0.99435
C	-3.51170	-1.14195	-0.94713
H	-1.42840	-1.34455	-1.49655
C	-4.31803	1.12047	-0.69061
H	-2.87259	2.67598	-1.03421
C	-4.55222	-0.25556	-0.66105
H	-3.69361	-2.21304	-0.94724
H	-5.12619	1.81727	-0.48701
H	-5.54432	-0.63371	-0.43049

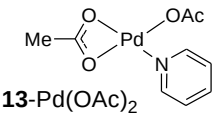


12-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -911.8091730
SCF Energy (M06, acetic acid): -911.8108212
SCF Energy (wB97XD, 1,4-dioxane): -912.0681202
SCF Energy (B3LYP): -912.0725040
ZPE Correction: 0.269296
Enthalpy Correction: 0.288974
Free-Energy Correction: 0.224299319

Pd	0.52882	0.19334	0.33371
C	2.86483	-0.35647	-0.20107
O	2.00204	-1.27641	0.04519
O	2.47594	0.85379	-0.13109
C	4.27041	-0.70304	-0.59129

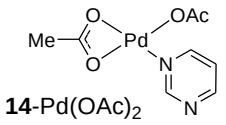
O	-0.49648	1.89474	0.66267
C	-0.79812	2.56428	-0.43262
O	-0.70382	2.11871	-1.57314
C	-1.27503	3.98091	-0.14751
H	4.95012	0.09959	-0.29990
H	4.56879	-1.64806	-0.13348
H	4.31813	-0.81653	-1.67984
H	-0.40519	4.60994	0.06933
H	-1.79115	4.38073	-1.02144
H	-1.92735	4.00954	0.72893
N	-1.19666	-0.91116	0.86272
C	-2.41809	-0.48891	0.10583
H	-3.28021	-1.01419	0.54167
H	-2.54423	0.58446	0.24621
C	-0.95405	-2.36522	0.60719
H	-0.01179	-2.64638	1.08396
H	-1.77375	-2.93359	1.06919
C	-2.29860	-0.84617	-1.37159
H	-3.23217	-0.59484	-1.88197
H	-1.48460	-0.26960	-1.83198
C	-0.90969	-2.66144	-0.89175
H	-0.82190	-3.74134	-1.04150
H	-0.03310	-2.17614	-1.34382
O	-2.10360	-2.24744	-1.53490
C	-1.40237	-0.67017	2.31410
H	-2.29028	-1.21225	2.66650
H	-0.52612	-1.01707	2.86532
H	-1.53235	0.40057	2.47568



13-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -832.9887630
SCF Energy (M06, acetic acid): -832.9872821
SCF Energy (wB97XD, 1,4-dioxane): -833.2207163
SCF Energy (B3LYP): -833.2475874
ZPE Correction: 0.194371
Enthalpy Correction: 0.211853
Free-Energy Correction: 0.150972727

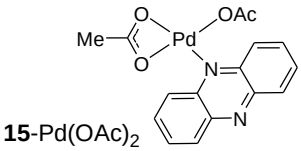
Pd	-0.61743	-0.03341	-0.16085
C	-2.78811	-1.11816	0.18518
O	-1.68839	-1.77053	0.30069
O	-2.71552	0.11199	-0.14222
C	-4.10731	-1.77494	0.46046
O	-0.08095	1.78983	-0.80777
C	0.26760	2.68743	0.08176
O	0.51083	2.45839	1.26817
C	0.34272	4.09172	-0.50127
H	-4.88953	-1.31453	-0.14587
H	-4.04524	-2.84677	0.26378
H	-4.36155	-1.63059	1.51617
H	-0.67352	4.46654	-0.66130
H	0.86294	4.75330	0.19265
H	0.84501	4.08316	-1.47191
N	1.32104	-0.68444	-0.04866
C	1.62688	-1.87124	-0.61074
C	2.27593	0.01288	0.59990
C	2.91037	-2.40075	-0.55622
H	0.81204	-2.39304	-1.09978
C	3.58015	-0.46574	0.69620
H	1.95062	0.94982	1.04318
C	3.90735	-1.68542	0.10783
H	3.11432	-3.35678	-1.02562
H	4.31952	0.12037	1.23090
H	4.91882	-2.07549	0.16798



14-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -849.0313863
SCF Energy (M06, acetic acid): -849.0300544
SCF Energy (wB97XD, 1,4-dioxane): -849.2576528
SCF Energy (B3LYP): -849.2794256
ZPE Correction: 0.182320
Enthalpy Correction: 0.199812
Free-Energy Correction: 0.139103606

Pd	0.62254	0.02430	-0.21413
C	2.86707	-0.92958	0.03416
O	1.81381	-1.65700	0.15033
O	2.70437	0.30897	-0.21730
C	4.23556	-1.52791	0.15746
O	-0.11316	1.83823	-0.65712
C	-0.45626	2.54491	0.40537
O	-0.50138	2.10865	1.55061
C	-0.78854	3.98990	0.06223
H	4.93574	-0.78526	0.54410
H	4.20742	-2.40657	0.80434
H	4.57814	-1.83924	-0.83542
H	-1.43888	4.04400	-0.81486
H	-1.26388	4.47125	0.91766
H	0.13623	4.52167	-0.18395
N	-1.26868	-0.74945	-0.12092
C	-1.45780	-1.91772	0.52063
C	-2.34127	-0.14027	-0.66548
C	-2.72763	-2.46868	0.62382
H	-0.57210	-2.38881	0.93435
H	-2.14525	0.79955	-1.16868
C	-3.77317	-1.76440	0.02908
H	-2.88834	-3.40569	1.14403
H	-4.79467	-2.13630	0.06742
N	-3.58389	-0.60780	-0.61837

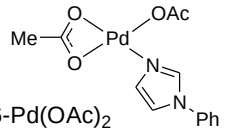


15-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -1156.149259
SCF Energy (M06, acetic acid): -1156.148003
SCF Energy (wB97XD, 1,4-dioxane): -1156.504471
SCF Energy (B3LYP): -1156.560520
ZPE Correction: 0.275011
Enthalpy Correction: 0.297777
Free-Energy Correction: 0.226527253

Pd	1.26459	-0.32768	-0.02782
C	2.90084	-0.98866	-1.72970
O	1.65280	-0.89883	-2.00828
O	3.25813	-0.75456	-0.52667
C	3.90828	-1.32328	-2.78816
O	1.34134	0.06655	1.93803
C	1.78277	1.27177	2.22405
O	2.00280	2.15758	1.39958
C	2.02425	1.46965	3.71354
H	4.75406	-1.85422	-2.34720
H	3.44502	-1.91925	-3.57652
H	4.28060	-0.39247	-3.22969
H	2.93728	0.93872	4.00240
H	2.14602	2.53194	3.92890
H	1.20150	1.05314	4.30000
N	-0.78666	-0.05097	-0.02002
C	-1.32541	1.13062	-0.40577
C	-1.60721	-1.09819	0.23265
C	-2.75447	1.22535	-0.61628
C	-0.51130	2.28287	-0.60559
C	-3.03048	-0.95648	0.02689
C	-1.09492	-2.34442	0.69523
N	-3.57419	0.18798	-0.40715
C	-3.30603	2.46428	-1.06551
C	-1.09082	3.45317	-1.02560
H	0.54583	2.22836	-0.35971
C	-3.88162	-2.07524	0.28189

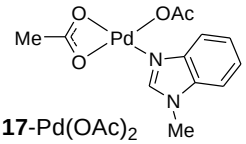
C	-1.95042	-3.38945	0.93339
H	-0.02681	-2.43389	0.86449
C	-2.49321	3.54580	-1.27094
H	-4.37819	2.50143	-1.22488
H	-0.46960	4.33301	-1.16172
C	-3.35486	-3.25910	0.72264
H	-4.94421	-1.93803	0.11311
H	-1.55314	-4.33350	1.29332
H	-2.91325	4.48815	-1.60898
H	-4.00346	-4.10724	0.91848



16-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -1041.883421
SCF Energy (M06, acetic acid): -1041.880381
SCF Energy (wB97XD, 1,4-dioxane): -1042.200497
SCF Energy (B3LYP): -1042.232627
ZPE Correction: 0.257153
Enthalpy Correction: 0.278768
Free-Energy Correction: 0.209542328

Pd	-1.71755	0.24237	-0.26886
C	-2.68914	2.48692	-0.09484
O	-1.41714	2.30991	-0.12757
O	-3.43568	1.45953	-0.18677
C	-3.27069	3.85853	0.08072
O	-2.40778	-1.63356	-0.47283
C	-2.79055	-2.18001	0.66557
O	-2.62412	-1.68824	1.77599
C	-3.49980	-3.51350	0.46169
H	-3.42991	4.04205	1.14889
H	-2.58323	4.61464	-0.30274
H	-4.23661	3.92321	-0.42374
H	-2.97386	-4.13216	-0.27041
H	-3.57889	-4.03777	1.41500
H	-4.50544	-3.32794	0.07024
N	0.17586	-0.49101	-0.34568
C	0.58298	-1.76651	-0.67508
C	1.26136	0.21485	-0.06801
C	1.94595	-1.82171	-0.59569
H	-0.14128	-2.52349	-0.92815
H	1.27737	1.26104	0.19449
H	2.64152	-2.63177	-0.74212
N	2.37087	-0.55895	-0.20481
C	3.71851	-0.13986	0.01279
C	4.71624	-0.52946	-0.88519
C	4.02560	0.65504	1.12076
C	6.03150	-0.12215	-0.66500
H	4.45938	-1.12641	-1.75425
C	5.34166	1.07120	1.31983
H	3.24713	0.92417	1.82743
C	6.34668	0.68132	0.43266
H	6.80758	-0.42366	-1.36163
H	5.58155	1.68870	2.17979
H	7.37101	1.00100	0.59647

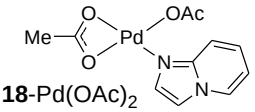


17-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -1003.816823
SCF Energy (M06, acetic acid): -1003.813445
SCF Energy (wB97XD, 1,4-dioxane): -1004.118095
SCF Energy (B3LYP): -1004.148552
ZPE Correction: 0.251695
Enthalpy Correction: 0.272839
Free-Energy Correction: 0.204566656

Pd	-1.19879	-0.18220	-0.08728
C	-2.60045	-2.12437	0.43480
O	-1.33341	-2.14437	0.63391
O	-3.10566	-1.06600	-0.06655
C	-3.45895	-3.29462	0.81211

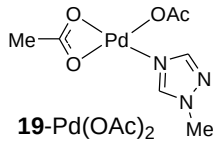
O	-1.60806	1.56945	-0.97838
C	-1.62773	2.68484	-0.29725
O	-1.20985	2.84015	0.85396
C	-2.25390	3.83276	-1.07957
H	-4.34563	-3.33049	0.17668
H	-2.88906	-4.22246	0.73443
H	-3.78365	-3.17613	1.85161
H	-3.34080	3.70099	-1.09534
H	-2.01754	4.78267	-0.59796
H	-1.90873	3.83137	-2.11636
C	1.85119	-0.61005	-0.21654
C	1.31214	1.33913	0.60284
C	3.05006	0.04975	0.12634
C	1.87535	-1.89483	-0.76816
H	0.70749	2.17477	0.93937
C	4.30254	-0.53649	-0.07030
C	3.12111	-2.48148	-0.96423
H	0.95212	-2.40595	-1.01695
C	4.31497	-1.81399	-0.62273
H	5.22275	-0.02524	0.19309
H	3.17784	-3.47880	-1.38903
H	5.26631	-2.30840	-0.79311
C	3.55308	2.32307	1.14213
H	4.14740	1.94924	1.98111
H	4.22592	2.66375	0.34955
H	2.95013	3.16572	1.48238
N	0.78853	0.23493	0.09536
N	2.66846	1.28282	0.64398



18-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -964.5069876
SCF Energy (M06, acetic acid): -964.5040237
SCF Energy (wB97XD, 1,4-dioxane): -964.7856196
SCF Energy (B3LYP): -964.8149017
ZPE Correction: 0.223287
Enthalpy Correction: 0.242675
Free-Energy Correction: 0.178024386

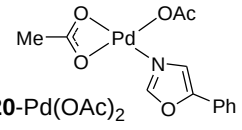
Pd	-0.97103	0.25197	0.08299
C	-1.98263	2.46279	-0.25145
O	-0.74800	2.24848	-0.52897
O	-2.65933	1.49809	0.23408
C	-2.61340	3.79604	-0.52458
O	-1.64676	-1.43678	0.92433
C	-1.99797	-2.43170	0.14707
O	-1.78616	-2.50639	-1.06408
C	-2.73222	-3.52998	0.90640
H	-3.44335	3.96735	0.16321
H	-1.87031	4.59136	-0.44038
H	-3.00620	3.79941	-1.54718
H	-3.74238	-3.18403	1.14859
H	-2.79931	-4.42560	0.28726
H	-2.22798	-3.75407	1.84989
C	2.04317	0.03868	0.05799
C	1.16562	-1.74993	-0.84998
C	2.33575	1.27510	0.67067
H	0.36168	-2.38665	-1.19266
C	4.40235	-0.44613	-0.14584
C	3.65215	1.62080	0.86381
H	1.51082	1.91732	0.95417
C	4.69646	0.74636	0.45208
H	5.14219	-1.15915	-0.48751
H	3.90098	2.56771	1.33044
H	5.73503	1.01570	0.60422
N	0.87552	-0.55026	-0.25103
C	2.52441	-1.92163	-0.91654
H	3.12766	-2.72128	-1.31463
N	3.08707	-0.79378	-0.34231



19-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -866.2829072
SCF Energy (M06, acetic acid): -866.2799317
SCF Energy (wB97XD, 1,4-dioxane): -866.5130857
SCF Energy (B3LYP): -866.5238070
ZPE Correction: 0.192832
Enthalpy Correction: 0.211402
Free-Energy Correction: 0.148250937

Pd	0.67383	-0.09933	-0.23343
C	2.53382	-1.66921	0.04307
O	1.31282	-2.06285	0.10978
O	2.74678	-0.43679	-0.20059
C	3.66637	-2.62329	0.27758
O	0.47499	1.85286	-0.65891
C	0.52795	2.63131	0.40643
O	0.54132	2.23580	1.56662
C	0.59091	4.10954	0.04438
H	3.94660	-2.58768	1.33598
H	3.36153	-3.64224	0.03261
H	4.53428	-2.32669	-0.31442
H	-0.11985	4.35144	-0.75025
H	0.39076	4.71380	0.93012
H	1.59258	4.34338	-0.33090
N	-1.35694	-0.24470	-0.20330
C	-2.29081	0.65587	-0.62997
C	-2.06694	-1.26562	0.27130
H	-2.02160	1.60351	-1.06851
H	-1.66444	-2.17251	0.69659
N	-3.36883	-0.98096	0.12954
C	-4.52796	-1.77478	0.50534
H	-5.13668	-1.97319	-0.37890
H	-4.18459	-2.71642	0.93534
H	-5.12221	-1.22892	1.24076
N	-3.52851	0.24130	-0.44543

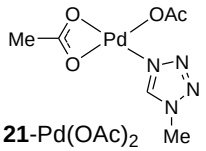


20-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -1061.751572
SCF Energy (M06, acetic acid): -1061.746226
SCF Energy (wB97XD, 1,4-dioxane): -1062.055804
SCF Energy (B3LYP): -1062.094441
ZPE Correction: 0.244794
Enthalpy Correction: 0.266257
Free-Energy Correction: 0.197187072

Pd	-1.81416	-0.27401	-0.12789
C	-2.98521	-2.39611	0.21357
O	-1.71882	-2.29495	0.39592
O	-3.61097	-1.35356	-0.17330
C	-3.70474	-3.68354	0.47924
O	-2.42191	1.49758	-0.84074
C	-2.46554	2.55313	-0.06812
O	-1.97587	2.64119	1.06059
C	-3.21986	3.71107	-0.70771
H	-4.57316	-3.77001	-0.17640
H	-3.02951	-4.52993	0.34142
H	-4.05616	-3.68583	1.51680
H	-4.29426	3.50583	-0.65800
H	-3.00807	4.63406	-0.16634
H	-2.95389	3.81450	-1.76240
N	0.13601	0.30326	0.07299
C	0.61050	1.40139	0.60070
C	1.23536	-0.47789	-0.26583
H	0.02977	2.22669	0.99204
H	1.11570	-1.45173	-0.71128
C	3.79357	-0.05365	-0.01489
C	4.72619	0.89327	0.44017
C	4.25590	-1.26301	-0.56322
C	6.09152	0.63194	0.34690

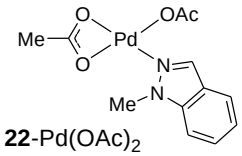
H	4.37745	1.82839	0.86445
C	5.62116	-1.51630	-0.65280
H	3.54724	-2.00501	-0.91868
C	6.54444	-0.57061	-0.19854
H	6.80306	1.37133	0.70198
H	5.96563	-2.45411	-1.07804
H	7.60919	-0.77092	-0.26972
C	2.36333	0.20604	0.07730
O	1.94840	1.40399	0.62944



21-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -882.2826091
SCF Energy (M06, acetic acid): -882.2812349
SCF Energy (wB97XD, 1,4-dioxane): -882.5083697
SCF Energy (B3LYP): -882.5263804
ZPE Correction: 0.179976
Enthalpy Correction: 0.198408
Free-Energy Correction: 0.135596324

Pd	-0.77756	-0.01563	-0.16635
C	-3.00605	-0.93163	0.23056
O	-1.96546	-1.67716	0.26019
O	-2.83124	0.31030	-0.02157
C	-4.36980	-1.48475	0.50918
O	-0.17012	1.83044	-0.68378
C	0.52933	2.58699	0.11749
O	1.10083	2.22069	1.15142
C	0.57485	4.03824	-0.34071
H	-5.11586	-0.95801	-0.08924
H	-4.39220	-2.55559	0.30061
H	-4.60835	-1.32803	1.56675
H	-0.37584	4.51851	-0.08652
H	1.38452	4.56370	0.16762
H	0.69483	4.10128	-1.42470
N	1.11446	-0.77862	-0.19157
C	2.20976	-0.29168	0.37352
H	2.23718	0.65743	0.90246
N	2.68091	-2.21328	-0.57560
N	3.18666	-1.17543	0.13972
N	1.43353	-1.96578	-0.76867
C	4.58922	-1.15025	0.53380
H	4.80393	-2.00924	1.17175
H	5.21720	-1.18842	-0.35778
H	4.77747	-0.22653	1.08068



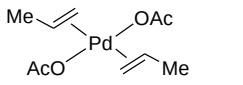
22-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -1003.783364
SCF Energy (M06, acetic acid): -1003.779928
SCF Energy (wB97XD, 1,4-dioxane): -1004.082062
SCF Energy (B3LYP): -1004.118334
ZPE Correction: 0.251371
Enthalpy Correction: 0.272563
Free-Energy Correction: 0.204441065

Pd	1.36975	-0.05076	-0.27761
C	3.25902	-1.59455	-0.04796
O	2.05179	-2.01558	0.03287
O	3.43887	-0.34491	-0.24385
C	4.41946	-2.53859	0.05019
O	1.21899	1.90494	-0.66684
C	0.84291	2.66398	0.33677
O	0.51003	2.26351	1.45148
C	0.87569	4.14557	-0.01371
H	5.27543	-2.03473	0.50324
H	4.14060	-3.42214	0.62689
H	4.70482	-2.85707	-0.95834
H	0.35527	4.32888	-0.95750
H	0.41811	4.72458	0.78916

H	1.91454	4.46393	-0.14600
N	-0.66638	-0.19364	-0.29516
N	-1.41099	-0.48820	0.80465
C	-2.81584	-0.29265	-0.93341
C	-2.73114	-0.55732	0.45988
C	-0.78834	-0.60255	2.11586
C	-4.07092	-0.29667	-1.57680
C	-3.87613	-0.82727	1.23270
H	-1.58190	-0.63037	2.86320
H	-0.19598	-1.51972	2.17945
H	-0.16001	0.27740	2.27514
C	-5.19389	-0.56129	-0.81682
H	-4.14741	-0.09600	-2.64091
C	-5.09248	-0.82282	0.57365
H	-3.81362	-1.03223	2.29580
H	-6.17322	-0.57079	-1.28463
H	-5.99823	-1.02664	1.13690
C	-1.47695	-0.07102	-1.33988
H	-1.07103	0.16994	-2.31096

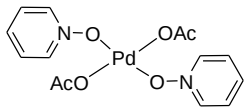
2:1 Heterocycle:Pd Complexes



(**propene**)$_2$-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -820.5190253
SCF Energy (M06, acetic acid): -820.5236311
SCF Energy (wB97XD, 1,4-dioxane): -820.7699491
SCF Energy (B3LYP): -820.7900590
ZPE Correction: 0.267192
Enthalpy Correction: 0.289409
Free-Energy Correction: 0.219687824

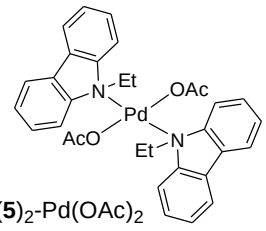
Pd	0.00968	0.00000	-0.24062
O	1.94117	0.00000	0.39608
C	2.75385	0.00000	-0.63716
O	2.36739	0.00000	-1.80666
C	4.22631	-0.00000	-0.26003
H	4.45925	-0.88071	0.34622
H	4.83930	0.00002	-1.16175
H	4.45925	0.88068	0.34625
O	-1.86399	-0.00000	-1.00790
C	-2.91270	-0.00000	-0.21705
O	-2.87583	0.00000	1.01324
C	-4.22693	-0.00000	-0.98821
H	-4.28202	-0.88016	-1.63565
H	-5.06448	-0.00001	-0.29008
H	-4.28203	0.88016	-1.63564
C	-0.38427	2.08825	0.77419
C	0.08262	2.22464	-0.51418
H	1.12516	2.46050	-0.70696
H	-0.60485	2.31798	-1.34902
C	-0.38427	-2.08825	0.77419
H	-1.45434	-1.98392	0.93746
C	0.08262	-2.22464	-0.51418
H	-0.60485	-2.31799	-1.34902
H	1.12516	-2.46050	-0.70695
C	0.45164	-2.26402	2.00700
H	0.16512	-1.54655	2.78117
H	0.26802	-3.26704	2.41601
H	1.51696	-2.15596	1.79716
H	-1.45434	1.98392	0.93746
C	0.45164	2.26402	2.00700
H	0.26802	3.26704	2.41600
H	0.16512	1.54655	2.78117
H	1.51696	2.15596	1.79716



(**4**)$_2$-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -1231.489107
SCF Energy (M06, acetic acid): -1231.494985
SCF Energy (wB97XD, 1,4-dioxane): -1231.846159
SCF Energy (B3LYP): -1231.877725
ZPE Correction: 0.292559
Enthalpy Correction: 0.317749
Free-Energy Correction: 0.241801063

Pd	0.00000	0.00000	-1.07609
O	-1.17782	1.65873	-1.13331
C	-1.27327	2.35394	-0.04009
O	-0.77891	2.05623	1.05787
C	-2.06303	3.64726	-0.20975
H	-2.91067	3.50534	-0.88434
H	-2.40254	4.01147	0.76143
H	-1.40921	4.40305	-0.65863
O	1.17782	-1.65873	-1.13332
C	1.27327	-2.35394	-0.04009
O	0.77891	-2.05622	1.05786
C	2.06304	-3.64724	-0.20975
H	2.91075	-3.50528	-0.88425
H	2.40247	-4.01151	0.76144
H	1.40928	-4.40301	-0.65875
O	1.70296	1.16583	-1.14247
N	2.55185	0.95055	-0.13702
C	3.82973	0.62880	-0.45191
C	2.14890	1.10024	1.15029
C	4.77191	0.45760	0.54843
H	4.01678	0.52309	-1.51172
C	3.06781	0.92761	2.17356
H	1.09576	1.35841	1.27287
C	4.39377	0.60494	1.88384
H	5.78792	0.20080	0.27088
H	2.72662	1.04764	3.19544
H	5.11676	0.46651	2.68053
O	-1.70296	-1.16582	-1.14248
N	-2.55185	-0.95056	-0.13702
C	-3.82974	-0.62882	-0.45191
C	-2.14889	-1.10024	1.15029
C	-4.77192	-0.45762	0.54843
H	-4.01680	-0.52311	-1.51172
C	-3.06781	-0.92762	2.17356
H	-1.09575	-1.35841	1.27287
C	-4.39377	-0.60496	1.88384
H	-5.78793	-0.20083	0.27089
H	-2.72661	-1.04764	3.19544
H	-5.11676	-0.46653	2.68053

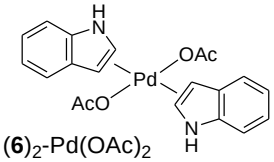


(**5**)$_2$-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -1776.407101
SCF Energy (M06, acetic acid): -1776.414188
SCF Energy (wB97XD, 1,4-dioxane): -1777.073406
SCF Energy (B3LYP): -1777.137738
ZPE Correction: 0.573949
Enthalpy Correction: 0.612232
Free-Energy Correction: 0.511265082

Pd	0.00000	0.00000	-0.00000
O	1.11288	0.76001	1.52761
C	1.29545	2.05102	1.62306
O	0.74554	2.90606	0.92292
C	2.28220	2.44005	2.71692
H	3.30016	2.31966	2.33320
H	2.13457	3.48505	2.99453
H	2.17680	1.79175	3.59016
O	-1.11288	-0.76001	-1.52761
C	-1.29545	-2.05102	-1.62307
O	-0.74554	-2.90605	-0.92292

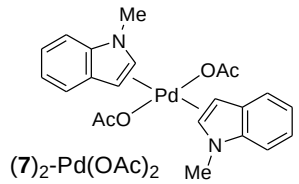
C	-2.28220	-2.44004	-2.71693
H	-2.17681	-1.79174	-3.59015
H	-2.13457	-3.48504	-2.99454
H	-3.30016	-2.31965	-2.33320
N	1.92885	-0.58237	-0.89806
C	2.60573	-1.44330	0.06677
C	2.79082	0.58870	-0.98253
C	1.73406	-1.25211	-2.24431
C	3.78398	-0.83882	0.53223
C	2.18452	-2.69451	0.49924
C	3.90650	0.44958	-0.14038
C	2.60230	1.70676	-1.78299
H	1.13197	-0.57069	-2.84620
H	1.13580	-2.13947	-2.05026
C	4.57651	-1.50400	1.47116
C	2.99281	-3.35011	1.43323
H	1.25070	-3.11852	0.14248
C	4.86674	1.46423	-0.09391
C	3.57209	2.71178	-1.73196
H	1.72252	1.81076	-2.40928
C	4.17185	-2.76337	1.91443
H	5.48944	-1.05190	1.84778
H	2.69426	-4.32896	1.79657
C	4.69103	2.59211	-0.89705
H	5.73665	1.37481	0.55035
H	3.44751	3.60223	-2.34005
H	4.77628	-3.29531	2.64335
H	5.42797	3.38928	-0.87246
N	-1.92885	0.58237	0.89806
C	-2.79082	-0.58871	0.98253
C	-2.60573	1.44329	-0.06677
C	-1.73406	1.25212	2.24431
C	-3.90650	-0.44958	0.14039
C	-2.60229	-1.70676	1.78299
C	-3.78398	0.83881	-0.53223
C	-2.18452	2.69451	-0.49924
H	-1.13197	0.57069	2.84620
H	-1.13580	2.13947	2.05026
C	-4.86674	-1.46424	0.09392
C	-3.57208	-2.71178	1.73197
H	-1.72252	-1.81076	2.40928
C	-4.57652	1.50400	-1.47116
C	-2.99281	3.35010	-1.43323
H	-1.25071	3.11852	-0.14248
C	-4.69103	-2.59212	0.89706
H	-5.73665	-1.37482	-0.55034
H	-3.44749	-3.60223	2.34005
C	-4.17185	2.76336	-1.91443
H	-5.48944	1.05189	-1.84778
H	-2.69427	4.32895	-1.79657
H	-5.42796	-3.38929	0.87247
H	-4.77629	3.29530	-2.64335
C	-3.03635	1.62044	2.95244
H	-2.78743	2.13095	3.88834
H	-3.64315	2.30318	2.35134
H	-3.63832	0.74195	3.19766
C	3.03635	-1.62044	-2.95244
H	3.64315	-2.30319	-2.35134
H	2.78743	-2.13096	-3.88834
H	3.63832	-0.74195	-3.19766



(**6**)$_2$-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane):	-1312.127776
SCF Energy (M06, acetic acid):	-1312.134502
SCF Energy (wB97XD, 1,4-dioxane):	-1312.563816
SCF Energy (B3LYP):	-1312.607883
ZPE Correction:	0.366093
Enthalpy Correction:	0.393678
Free-Energy Correction:	0.313024318

Pd	0.00000	0.00000	0.00000
O	-1.34269	-1.22900	0.90078
C	-1.88837	-2.20098	0.20997
O	-1.59245	-2.51318	-0.94530
C	-2.97851	-2.93633	0.97819
H	-3.87494	-2.30880	1.01054
H	-3.21721	-3.87412	0.47478
H	-2.66842	-3.12606	2.00912
O	1.34269	1.22899	-0.90077
C	1.88837	2.20099	-0.20998
O	1.59245	2.51320	0.94529
C	2.97850	2.93633	-0.97821
H	2.66837	3.12610	-2.00913
H	3.21724	3.87410	-0.47478
H	3.87491	2.30878	-1.01062
N	-2.46121	1.60382	1.47893
C	-3.46352	1.06678	0.68024
C	-1.35808	1.88935	0.72475
C	-2.98129	1.03967	-0.65103
C	-4.75002	0.64161	1.01824
C	-1.62064	1.54168	-0.61665
H	-0.49119	2.39601	1.13537
C	-3.82074	0.58253	-1.67598
C	-5.56404	0.19309	-0.01905
H	-5.10561	0.66581	2.04403
H	-1.05366	1.89851	-1.46567
C	-5.10713	0.16574	-1.35105
H	-3.46793	0.54741	-2.70219
H	-6.57345	-0.13960	0.20429
H	-5.77029	-0.19139	-2.13279
H	-2.47063	1.61116	2.48726
N	2.46121	-1.60381	-1.47893
C	3.46352	-1.06678	-0.68024
C	1.35808	-1.88936	-0.72475
C	2.98129	-1.03968	0.65104
C	4.75002	-0.64161	-1.01823
C	1.62064	-1.54168	0.61665
H	0.49119	-2.39600	-1.13537
C	3.82074	-0.58254	1.67599
C	5.56404	-0.19309	0.01905
H	5.10561	-0.66580	-2.04402
H	1.05367	-1.89852	1.46567
C	5.10713	-0.16575	1.35106
H	3.46794	-0.54742	2.70219
H	6.57345	0.13961	-0.20428
H	5.77029	0.19139	2.13280
H	2.47063	-1.61115	-2.48725

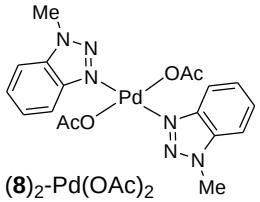


$(\mathbf{7})_2$-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -1390.704447
SCF Energy (M06, acetic acid): -1390.708418
SCF Energy (wB97XD, 1,4-dioxane): -1391.184717
SCF Energy (B3LYP): -1391.234904
ZPE Correction: 0.421922
Enthalpy Correction: 0.45283
Free-Energy Correction: 0.365655354

Pd	0.00000	0.00000	-0.00000
O	-1.35600	0.94810	-1.18100
C	-1.79950	2.13090	-0.82970
O	-1.40160	2.79030	0.13270
C	-2.90890	2.64290	-1.73940
H	-3.82720	2.08550	-1.52950
H	-3.08230	3.70320	-1.55120
H	-2.65510	2.48120	-2.79060
O	1.35600	-0.94810	1.18100
C	1.79950	-2.13090	0.82960
O	1.40160	-2.79030	-0.13280
C	2.90890	-2.64300	1.73940
H	2.65500	-2.48130	2.79060

H	3.08230	-3.70330	1.55110
H	3.82720	-2.08550	1.52950
N	-2.63390	-1.81880	-0.76760
C	-3.54110	-0.99430	-0.10620
C	-1.49920	-1.93270	-0.01760
C	-2.95740	-0.58790	1.11880
C	-4.82780	-0.60240	-0.48440
C	-1.62830	-1.16530	1.15970
H	-0.69130	-2.59990	-0.29910
C	-3.69280	0.21720	1.99790
C	-5.53870	0.19680	0.40870
H	-5.26320	-0.90860	-1.43020
H	-1.01840	-1.29210	2.04390
C	-4.98070	0.59990	1.63660
H	-3.26000	0.54240	2.93920
H	-6.54510	0.51420	0.15160
H	-5.56430	1.22390	2.30640
N	2.63380	1.81880	0.76760
C	3.54110	0.99420	0.10620
C	1.49920	1.93270	0.01760
C	2.95740	0.58790	-1.11880
C	4.82780	0.60240	0.48440
C	1.62830	1.16530	-1.15970
H	0.69130	2.59980	0.29910
C	3.69280	-0.21720	-1.99790
C	5.53880	-0.19680	-0.40870
H	5.26320	0.90860	1.43030
H	1.01850	1.29210	-2.04400
C	4.98070	-0.59990	-1.63660
H	3.26010	-0.54240	-2.93920
H	6.54510	-0.51420	-0.15160
H	5.56440	-1.22390	-2.30640
C	-2.78350	-2.29340	-2.13160
H	-3.74420	-2.80300	-2.25030
H	-2.72500	-1.45900	-2.83810
H	-1.98140	-3.00010	-2.34920
C	2.78340	2.29330	2.13160
H	2.72500	1.45890	2.83810
H	3.74420	2.80290	2.25040
H	1.98140	3.00010	2.34920

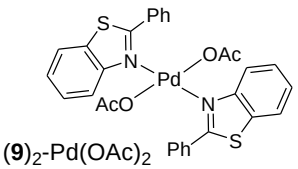


(**8**)$_2$-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane):	-1454.832695
SCF Energy (M06, acetic acid):	-1454.842153
SCF Energy (wB97XD, 1,4-dioxane):	-1455.297623
SCF Energy (B3LYP):	-1455.350552
ZPE Correction:	0.374873
Enthalpy Correction:	0.405557
Free-Energy Correction:	0.318611421

Pd	-0.00000	0.00000	0.70594
O	0.10956	2.02717	0.83436
C	-0.19856	2.71350	-0.23288
O	-0.46583	2.24138	-1.34116
C	-0.19290	4.21997	0.01271
H	0.79110	4.53700	0.37163
H	-0.43924	4.75035	-0.90810
H	-0.91721	4.47357	0.79284
O	-0.10958	-2.02717	0.83434
C	0.19857	-2.71349	-0.23291
O	0.46589	-2.24135	-1.34117
C	0.19291	-4.21996	0.01267
H	-0.79106	-4.53699	0.37169
H	0.43916	-4.75033	-0.90817
H	0.91730	-4.47357	0.79272
N	2.04565	-0.09439	0.62955
C	2.84550	0.32869	-0.41042
N	2.76882	-0.62151	1.57029
C	2.53645	0.94624	-1.63310

C	4.16918	0.02089	-0.05056
N	4.05503	-0.56386	1.18439
C	3.60991	1.23275	-2.46003
H	1.50912	1.19262	-1.88563
C	5.25573	0.31061	-0.88993
C	5.09368	-1.08791	2.05207
C	4.94425	0.91930	-2.09596
H	3.42910	1.71140	-3.41719
H	6.27775	0.07297	-0.61553
H	5.63757	-1.89174	1.54800
H	5.79168	-0.29357	2.33145
H	4.60726	-1.47896	2.94499
H	5.74680	1.16507	-2.78498
N	-2.04566	0.09439	0.62954
C	-2.84550	-0.32869	-0.41043
N	-2.76883	0.62148	1.57030
C	-2.53645	-0.94620	-1.63312
C	-4.16919	-0.02091	-0.05056
N	-4.05504	0.56382	1.18440
C	-3.60990	-1.23271	-2.46006
H	-1.50911	-1.19257	-1.88566
C	-5.25573	-0.31061	-0.88994
C	-5.09369	1.08786	2.05208
C	-4.94425	-0.91928	-2.09599
H	-3.42908	-1.71134	-3.41723
H	-6.27776	-0.07299	-0.61554
H	-5.63757	1.89172	1.54803
H	-5.79171	0.29352	2.33142
H	-4.60729	1.47886	2.94502
H	-5.74679	-1.16504	-2.78501

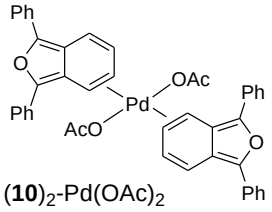


($\mathbf{9}$)$_2$-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -2491.817860
SCF Energy (M06, acetic acid): -2491.821784
SCF Energy (wB97XD, 1,4-dioxane): -2492.446423
SCF Energy (B3LYP): -2492.494001
ZPE Correction: 0.473204
Enthalpy Correction: 0.510876
Free-Energy Correction: 0.411154226

Pd	-0.02800	-0.27800	-0.01120
O	-0.38080	-0.97360	1.86740
C	-0.32120	-0.12610	2.86240
O	-0.05980	1.07410	2.77120
C	-0.60960	-0.77860	4.21030
H	0.16280	-1.52160	4.43320
H	-0.62490	-0.02170	4.99530
H	-1.56740	-1.30610	4.17910
O	0.26470	0.36940	-1.91610
C	0.60340	-0.55310	-2.78280
O	0.74940	-1.74980	-2.52840
C	0.80530	-0.00100	-4.18920
H	1.53190	0.81660	-4.17420
H	1.14840	-0.79340	-4.85530
H	-0.13770	0.40970	-4.56400
N	2.03640	-0.40510	0.27630
C	2.61560	-1.65550	0.52320
C	2.92750	0.53460	0.05620
C	1.93240	-2.84820	0.80180
C	4.02360	-1.65430	0.46220
S	4.59220	-0.03680	0.12250
C	2.68490	1.96700	-0.16030
C	2.67400	-4.00390	1.00830
H	0.85250	-2.84600	0.86880
C	4.76880	-2.81880	0.66440
C	1.71330	2.64250	0.59680
C	3.48790	2.68190	-1.06720
C	4.07810	-3.99390	0.93860
H	2.15760	-4.93320	1.22780
H	5.85250	-2.80500	0.61090

C	1.56500	4.02120	0.44400
H	1.10060	2.10000	1.31380
C	3.31830	4.05500	-1.22130
H	4.22830	2.15760	-1.66440
H	4.63210	-4.91320	1.10220
C	2.35960	4.72890	-0.46010
H	0.82290	4.54000	1.04240
H	3.93450	4.59770	-1.93200
H	2.23720	5.80300	-0.57000
N	-2.09190	-0.44410	-0.32330
C	-2.61760	-1.72100	-0.54280
C	-3.01440	0.44770	-0.04590
C	-1.88850	-2.85530	-0.92940
C	-4.01320	-1.80270	-0.36350
S	-4.64620	-0.21660	0.01760
C	-2.82110	1.89270	0.12170
C	-2.57610	-4.05180	-1.09310
H	-0.82740	-2.76640	-1.14310
C	-4.70010	-3.00890	-0.52220
C	-1.89200	2.57380	-0.68430
C	-3.62050	2.61470	1.02460
C	-3.96380	-4.13340	-0.88190
H	-2.03050	-4.93790	-1.40220
H	-5.77400	-3.06510	-0.37780
C	-1.78270	3.95980	-0.58710
H	-1.27560	2.02060	-1.38590
C	-3.49320	3.99740	1.12240
H	-4.32390	2.08960	1.66410
H	-4.47330	-5.08280	-1.01550
C	-2.57860	4.67360	0.31150
H	-1.06900	4.48050	-1.21730
H	-4.10590	4.54570	1.83140
H	-2.48750	5.75390	0.38080

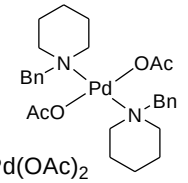


(**10**)$_2$-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -2275.569214
SCF Energy (M06, acetic acid): -2275.571507
SCF Energy (wB97XD, 1,4-dioxane): -2276.394252
SCF Energy (B3LYP): -2276.518222
ZPE Correction: 0.664009
Enthalpy Correction: 0.710687
Free-Energy Correction: 0.594252515

Pd	0.00000	1.34660	-0.00000
O	-1.45620	1.46900	1.41850
C	-1.77540	0.35710	2.03330
O	-1.21660	-0.72850	1.85980
C	-2.93590	0.51920	3.00440
H	-3.85730	0.70540	2.44370
H	-3.05080	-0.38770	3.59920
H	-2.77240	1.38120	3.65710
O	1.45620	1.46900	-1.41850
C	1.77540	0.35710	-2.03330
O	1.21660	-0.72850	-1.85970
C	2.93590	0.51910	-3.00440
H	3.85730	0.70530	-2.44370
H	3.05080	-0.38780	-3.59920
H	2.77240	1.38110	-3.65720
O	4.67440	-0.82360	0.63420
C	3.39290	-0.94610	1.08390
C	5.00040	0.49430	0.45900
C	2.86020	0.33180	1.21090
C	2.91450	-2.29620	1.33580
C	3.89220	1.25930	0.79680
C	6.33760	0.77420	-0.04010
C	1.60610	0.82630	1.69390
C	3.83640	-3.35260	1.48280
C	1.53710	-2.57390	1.43000

C	3.62710	2.66340	0.79030
C	6.94830	2.02640	0.16830
C	7.05610	-0.21550	-0.74110
C	1.40640	2.21660	1.71240
H	0.91030	0.16350	2.19620
C	3.39120	-4.64780	1.72620
H	4.89890	-3.14600	1.41250
C	1.10350	-3.87440	1.67970
H	0.79510	-1.79700	1.28910
C	2.41880	3.12120	1.23630
H	4.37590	3.36120	0.43210
C	8.22240	2.28550	-0.33040
H	6.43970	2.78480	0.75300
C	8.33280	0.04850	-1.22820
H	6.59870	-1.18500	-0.90570
H	0.54720	2.61920	2.23790
C	2.02300	-4.91460	1.82930
H	4.11400	-5.45070	1.84070
H	0.03740	-4.06900	1.74310
H	2.20780	4.18570	1.24480
C	8.92100	1.30070	-1.03240
H	8.67740	3.25640	-0.15640
H	8.86930	-0.72580	-1.76920
H	1.67760	-5.92650	2.02150
H	9.91580	1.50460	-1.41690
O	-4.67440	-0.82360	-0.63420
C	-3.39290	-0.94610	-1.08390
C	-5.00040	0.49420	-0.45900
C	-2.86020	0.33180	-1.21090
C	-2.91450	-2.29630	-1.33570
C	-3.89220	1.25930	-0.79680
C	-6.33760	0.77420	0.04010
C	-1.60610	0.82630	-1.69390
C	-3.83640	-3.35260	-1.48270
C	-1.53710	-2.57390	-1.42990
C	-3.62710	2.66340	-0.79040
C	-6.94830	2.02640	-0.16840
C	-7.05610	-0.21540	0.74110
C	-1.40640	2.21650	-1.71240
H	-0.91030	0.16340	-2.19620
C	-3.39120	-4.64780	-1.72600
H	-4.89890	-3.14600	-1.41240
C	-1.10350	-3.87440	-1.67950
H	-0.79510	-1.79700	-1.28910
C	-2.41880	3.12110	-1.23650
H	-4.37590	3.36120	-0.43230
C	-8.22240	2.28550	0.33030
H	-6.43970	2.78480	-0.75310
C	-8.33280	0.04850	1.22820
H	-6.59870	-1.18500	0.90570
H	-0.54720	2.61910	-2.23800
C	-2.02300	-4.91460	-1.82910
H	-4.11400	-5.45080	-1.84050
H	-0.03740	-4.06910	-1.74290
H	-2.20780	4.18560	-1.24490
C	-8.92100	1.30080	1.03240
H	-8.67740	3.25640	0.15630
H	-8.86930	-0.72570	1.76920
H	-1.67760	-5.92650	-2.02120
H	-9.91580	1.50470	1.41680

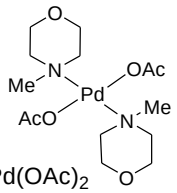


(**11**)$_2$-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane):	-1628.869918
SCF Energy (M06, acetic acid):	-1628.878308
SCF Energy (wB97XD, 1,4-dioxane):	-1629.507039
SCF Energy (B3LYP):	-1629.531150
ZPE Correction:	0.646706
Enthalpy Correction:	0.68378
Free-Energy Correction:	0.585822498

Pd	-0.00030	0.00070	0.00660
O	-1.27390	-0.18270	-1.57770
C	-0.87930	-0.55950	-2.76250
O	0.28150	-0.83170	-3.08780
C	-2.01620	-0.61370	-3.77810
H	-2.30980	0.40660	-4.04880
H	-1.69110	-1.13980	-4.67670
H	-2.89740	-1.09700	-3.34820
O	1.26940	0.18910	1.59460
C	0.86270	0.56490	2.77570
O	-0.30500	0.81560	3.09420
C	1.99970	0.69210	3.78430
H	2.62260	1.55500	3.52510
H	1.59640	0.83120	4.78810
H	2.64450	-0.19020	3.75140
N	0.92390	1.81800	-0.86860
C	-0.02370	2.54780	-1.77890
C	1.37680	2.78350	0.18520
C	2.10150	1.42150	-1.73680
H	0.54760	3.36320	-2.25120
H	-0.32810	1.86150	-2.56540
C	-1.23080	3.13040	-1.05200
H	2.06050	2.25390	0.84540
H	1.93910	3.57980	-0.32980
C	0.22100	3.40570	0.97210
H	1.67770	0.84590	-2.55970
H	2.51960	2.35640	-2.13870
C	3.20970	0.61770	-1.09480
H	-1.85930	3.63990	-1.79250
H	-1.82830	2.31490	-0.63400
C	-0.78820	4.09910	0.05020
H	0.64910	4.11950	1.68660
H	-0.27860	2.63250	1.56220
C	4.26390	1.23260	-0.40540
C	3.24740	-0.77130	-1.28170
H	-0.32780	4.98740	-0.40580
H	-1.65120	4.45250	0.62560
C	5.31170	0.47590	0.12030
H	4.27680	2.31360	-0.29220
C	4.29990	-1.52890	-0.76500
H	2.45100	-1.24150	-1.85100
C	5.32980	-0.90910	-0.05490
H	6.12060	0.96900	0.65230
H	4.32100	-2.60320	-0.92680
H	6.15080	-1.49840	0.34400
N	-0.92260	-1.82010	0.87760
C	-1.35320	-2.79260	-0.17950
C	0.01840	-2.54060	1.80230
C	-2.11460	-1.43120	1.72910
H	-1.91380	-3.59300	0.33080
H	-2.03420	-2.27200	-0.84930
C	-0.18150	-3.40450	-0.95040
H	0.30400	-1.85130	2.59320
H	-0.55250	-3.36100	2.26620
C	1.24120	-3.11240	1.09320
H	-2.53220	-2.36890	2.12530
H	-1.70570	-0.85310	2.55770
C	-3.21880	-0.63460	1.07170
H	-0.59350	-4.12390	-1.66880
H	0.31530	-2.62670	-1.53680
C	0.82330	-4.08580	-0.01470
H	1.86320	-3.61610	1.84300
H	1.83730	-2.29170	0.68350
C	-3.26800	0.75410	1.25790
C	-4.25880	-1.25600	0.36660
H	0.36680	-4.97900	0.43570
H	1.69760	-4.43010	-0.57850
C	-4.31760	1.50510	0.72610
H	-2.48250	1.22960	1.83800
C	-5.30340	-0.50580	-0.17460

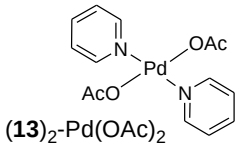
H	-4.26310	-2.33710	0.25320
C	-5.33300	0.87910	0.00070
H	-4.34790	2.57920	0.88760
H	-6.10150	-1.00390	-0.71830
H	-6.15170	1.46330	-0.41020



(**12**)$_2$-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -1238.824847
SCF Energy (M06, acetic acid): -1238.831865
SCF Energy (wB97XD, 1,4-dioxane): -1239.216233
SCF Energy (B3LYP): -1239.209917
ZPE Correction: 0.435359
Enthalpy Correction: 0.463093
Free-Energy Correction: 0.383140687

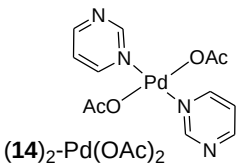
Pd	0.00000	0.00000	0.17650
O	-0.19240	-2.04020	0.07220
C	-0.31330	-2.70720	1.19630
O	-0.35220	-2.20440	2.31910
C	-0.39020	-4.21640	0.99060
H	0.57650	-4.59150	0.63690
H	-0.64180	-4.70840	1.93070
H	-1.12990	-4.46540	0.22430
O	0.19240	2.04020	0.07220
C	0.31330	2.70720	1.19630
O	0.35230	2.20440	2.31910
C	0.39020	4.21640	0.99060
H	-0.57660	4.59150	0.63700
H	0.64190	4.70840	1.93070
H	1.12980	4.46550	0.22420
N	-2.15950	0.23380	0.24850
C	-2.62630	1.46090	-0.46610
C	-2.89430	-0.92180	-0.34990
C	-2.47910	0.33630	1.70120
H	-3.69810	1.58850	-0.25640
H	-2.07770	2.31860	-0.08240
C	-2.41330	1.33010	-1.97040
H	-2.55700	-1.83940	0.12730
H	-3.96570	-0.78390	-0.14420
C	-2.67200	-0.98980	-1.85700
H	-3.56200	0.46560	1.83690
H	-2.13860	-0.57050	2.20240
H	-1.94320	1.18520	2.12710
H	-2.81590	2.21190	-2.47670
H	-1.33590	1.26610	-2.18570
O	-3.09920	0.20390	-2.49910
H	-3.26540	-1.80540	-2.27970
H	-1.61000	-1.18620	-2.06490
N	2.15950	-0.23380	0.24850
C	2.62630	-1.46090	-0.46610
C	2.89430	0.92180	-0.34990
C	2.47910	-0.33630	1.70120
H	3.69810	-1.58850	-0.25640
H	2.07770	-2.31860	-0.08240
C	2.41330	-1.33010	-1.97040
H	2.55700	1.83940	0.12730
H	3.96570	0.78380	-0.14420
C	2.67200	0.98980	-1.85700
H	3.56200	-0.46560	1.83690
H	2.13860	0.57050	2.20240
H	1.94320	-1.18520	2.12710
H	2.81590	-2.21190	-2.47670
H	1.33590	-1.26610	-2.18570
O	3.09920	-0.20390	-2.49910
H	3.26540	1.80540	-2.27970
H	1.61000	1.18620	-2.06490



(**13**)$_2$-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -1081.190259
SCF Energy (M06, acetic acid): -1081.192824
SCF Energy (wB97XD, 1,4-dioxane): -1081.528589
SCF Energy (B3LYP): -1081.567083
ZPE Correction: 0.285618
Enthalpy Correction: 0.308939
Free-Energy Correction: 0.236453847

Pd	0.00000	0.00000	0.00000
O	-0.00000	1.83861	-0.88959
C	-0.00000	2.87611	-0.10114
O	-0.00001	2.83133	1.13617
C	-0.00001	4.20370	-0.85011
H	-0.87973	4.26703	-1.49785
H	0.00003	5.03422	-0.14312
H	0.87965	4.26701	-1.49793
O	0.00000	-1.83861	0.88959
C	0.00000	-2.87611	0.10114
O	0.00001	-2.83133	-1.13617
C	0.00001	-4.20370	0.85011
H	-0.87968	-4.26702	1.49790
H	0.00000	-5.03422	0.14312
H	0.87971	-4.26702	1.49788
N	-2.05736	0.00000	0.00000
C	-2.73197	0.96144	0.65983
C	-2.73197	-0.96144	-0.65983
C	-4.12315	0.98763	0.68316
C	-4.12315	-0.98764	-0.68316
C	-4.83175	-0.00001	0.00000
H	-5.91767	-0.00001	0.00000
N	2.05736	0.00000	0.00000
C	2.73197	0.96144	0.65983
C	2.73197	-0.96144	-0.65983
C	4.12315	0.98764	0.68316
C	4.12315	-0.98763	-0.68316
C	4.83176	0.00001	0.00000
H	5.91767	0.00001	0.00000
H	-2.12297	-1.70588	-1.16303
H	-4.63221	-1.77389	-1.22986
H	2.12298	-1.70588	-1.16303
H	4.63222	-1.77388	-1.22987
H	-4.63222	1.77388	1.22987
H	-2.12298	1.70588	1.16303
H	2.12297	1.70588	1.16303
H	4.63221	1.77389	1.22987

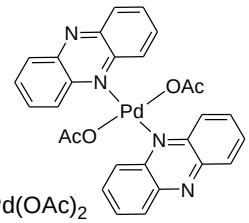


(**14**)$_2$-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -1113.276345
SCF Energy (M06, acetic acid): -1113.277397
SCF Energy (wB97XD, 1,4-dioxane): -1113.603050
SCF Energy (B3LYP): -1113.633622
ZPE Correction: 0.261749
Enthalpy Correction: 0.284925
Free-Energy Correction: 0.212606023

Pd	0.00000	0.00000	0.00000
O	-0.06621	1.83782	-0.88326
C	0.00043	2.87045	-0.08787
O	0.12904	2.80934	1.14155
C	-0.11398	4.20390	-0.81426
H	-1.13398	4.32567	-1.19350
H	0.11533	5.02291	-0.13152
H	0.55642	4.22873	-1.67754
O	0.06621	-1.83782	0.88326
C	-0.00043	-2.87045	0.08787
O	-0.12904	-2.80934	-1.14155
C	0.11398	-4.20390	0.81426
H	-0.55640	-4.22873	1.67755
H	-0.11534	-5.02291	0.13152
H	1.13399	-4.32568	1.19349

N	-2.05718	-0.03085	0.01892
C	-2.74220	-0.98671	-0.63709
C	-2.74964	0.92567	0.66985
C	-4.13208	-0.97175	-0.63964
H	-2.14451	-1.74236	-1.13984
H	-2.16106	1.67897	1.18513
N	-4.07542	1.00087	0.72047
C	-4.75906	0.05412	0.06363
H	-4.69509	-1.73192	-1.16872
H	-5.84397	0.12434	0.10690
N	2.05718	0.03085	-0.01892
C	2.74220	0.98671	0.63709
C	2.74964	-0.92567	-0.66985
C	4.13208	0.97175	0.63965
H	2.14451	1.74236	1.13984
H	2.16107	-1.67897	-1.18514
N	4.07543	-1.00087	-0.72047
C	4.75906	-0.05413	-0.06363
H	4.69508	1.73191	1.16873
H	5.84397	-0.12434	-0.10690

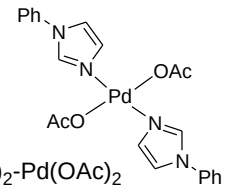


(**15**)$_2$-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane):	-1727.512233
SCF Energy (M06, acetic acid):	-1727.517312
SCF Energy (wB97XD, 1,4-dioxane):	-1728.096821
SCF Energy (B3LYP):	-1728.190204
ZPE Correction:	0.446955
Enthalpy Correction:	0.480747
Free-Energy Correction:	0.388377886

Pd	0.07670	0.00000	0.00000
O	0.10300	-0.30970	2.01130
C	-0.31160	-1.47740	2.43410
O	-0.64480	-2.41960	1.71180
C	-0.35630	-1.57730	3.95400
H	-1.12600	-0.90340	4.34400
H	-0.58430	-2.60060	4.25440
H	0.59880	-1.26230	4.38360
O	0.10300	0.30970	-2.01130
C	-0.31160	1.47740	-2.43410
O	-0.64480	2.41960	-1.71180
C	-0.35630	1.57730	-3.95400
H	-1.12600	0.90340	-4.34400
H	-0.58430	2.60060	-4.25440
H	0.59890	1.26230	-4.38360
N	-2.01260	0.00000	0.00000
C	-2.70080	-0.96100	-0.66030
C	-2.70080	0.96100	0.66030
C	-4.14650	-0.94210	-0.65030
C	-2.03200	-2.00230	-1.36620
C	-4.14650	0.94210	0.65030
C	-2.03200	2.00230	1.36620
N	-4.84030	0.00000	-0.00000
C	-4.86150	-1.96150	-1.35160
C	-2.75830	-2.95930	-2.02520
H	-0.95030	-2.01490	-1.36660
C	-4.86150	1.96150	1.35160
C	-2.75830	2.95930	2.02520
H	-0.95030	2.01490	1.36660
C	-4.18450	-2.94290	-2.02180
H	-5.94480	-1.91560	-1.32200
H	-2.23870	-3.74960	-2.55830
C	-4.18450	2.94290	2.02180
H	-5.94480	1.91560	1.32200
H	-2.23870	3.74960	2.55830
H	-4.72790	-3.71800	-2.55360

H	-4.72790	3.71800	2.55360
N	2.17510	0.00000	0.00000
C	2.86390	-1.16370	0.07920
C	2.86390	1.16370	-0.07920
C	4.31060	-1.14300	0.06170
C	2.19350	-2.41760	0.18350
C	4.31060	1.14310	-0.06170
C	2.19350	2.41760	-0.18350
N	5.00450	0.00000	0.00000
C	5.02560	-2.37880	0.11750
C	2.92340	-3.57770	0.24090
H	1.11090	-2.43640	0.26500
C	5.02560	2.37880	-0.11750
C	2.92340	3.57770	-0.24090
H	1.11090	2.43640	-0.26500
C	4.34870	-3.56510	0.19890
H	6.10870	-2.32520	0.09530
H	2.40270	-4.52610	0.33110
C	4.34870	3.56510	-0.19890
H	6.10870	2.32520	-0.09530
H	2.40270	4.52610	-0.33110
H	4.89260	-4.50380	0.24240
H	4.89250	4.50380	-0.24240

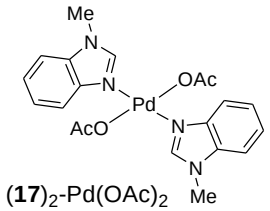


(**16**)$_2$-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -1498.978582
SCF Energy (M06, acetic acid): -1498.976433
SCF Energy (wB97XD, 1,4-dioxane): -1499.486225
SCF Energy (B3LYP): -1499.539024
ZPE Correction: 0.411201
Enthalpy Correction: 0.442705
Free-Energy Correction: 0.354533029

Pd	-0.01260	0.08440	-0.06120
O	0.31230	1.90580	0.79490
C	1.12400	2.76620	0.25060
O	1.78180	2.60140	-0.78330
C	1.21640	4.06990	1.04120
H	1.66050	3.87460	2.02280
H	1.82780	4.79430	0.50110
H	0.21770	4.47930	1.21760
O	-0.35930	-1.72180	-0.94140
C	-0.99820	-2.63990	-0.27650
O	-1.47570	-2.51200	0.85840
C	-1.13270	-3.94990	-1.04820
H	-0.14620	-4.31000	-1.35450
H	-1.62900	-4.70040	-0.43130
H	-1.71120	-3.78340	-1.96240
N	-1.94860	0.68540	-0.37390
C	-2.38600	1.87240	-0.92340
C	-3.01890	0.00280	0.00200
C	-3.75120	1.89740	-0.88500
H	-1.69270	2.61080	-1.29260
H	-2.98650	-0.97830	0.45600
N	-4.14740	0.70620	-0.28990
H	-4.46440	2.64730	-1.18530
C	-5.48490	0.28610	-0.02920
C	-6.49020	0.55440	-0.96310
C	-5.77990	-0.39230	1.15740
C	-7.79760	0.14720	-0.70030
H	-6.24510	1.05670	-1.89320
C	-7.08760	-0.81110	1.39980
H	-4.99720	-0.57510	1.88630
C	-8.09980	-0.53910	0.47740
H	-8.57760	0.35580	-1.42630
H	-7.31510	-1.33980	2.32030
H	-9.11770	-0.86030	0.67490
N	1.89330	-0.56300	0.32180

C	2.22940	-1.71220	1.00910
C	3.01830	0.00420	-0.08200
C	3.58990	-1.83250	1.02060
H	1.47210	-2.34560	1.44420
H	3.06020	0.92460	-0.64720
N	4.08580	-0.73560	0.32580
H	4.24150	-2.55700	1.48060
C	5.45520	-0.42470	0.08070
C	6.36960	-1.45430	-0.16060
C	5.87270	0.91030	0.08120
C	7.70910	-1.14320	-0.39170
H	6.03080	-2.48470	-0.18930
C	7.21110	1.20910	-0.17010
H	5.15930	1.70180	0.28570
C	8.13350	0.18660	-0.40080
H	8.41790	-1.94400	-0.57900
H	7.53310	2.24580	-0.17240
H	9.17600	0.42480	-0.58790

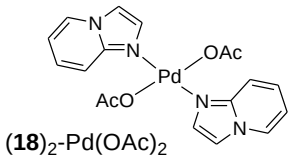


(**17**)$_2$-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -1422.845145
SCF Energy (M06, acetic acid): -1422.844703
SCF Energy (wB97XD, 1,4-dioxane): -1423.321568
SCF Energy (B3LYP): -1423.365833
ZPE Correction: 0.400403
Enthalpy Correction: 0.430880
Free-Energy Correction: 0.34413627

Pd	0.00000	0.00000	0.00000
O	-0.34920	1.58910	1.22880
C	-0.35300	2.79060	0.73460
O	-0.13520	3.09090	-0.44890
C	-0.70420	3.86310	1.76030
H	-0.28010	3.62600	2.73860
H	-0.35640	4.83880	1.41650
H	-1.79370	3.90160	1.87080
O	0.34920	-1.58910	-1.22870
C	0.35300	-2.79060	-0.73450
O	0.13520	-3.09090	0.44890
C	0.70420	-3.86310	-1.76020
H	1.79370	-3.90150	-1.87080
H	0.35640	-4.83880	-1.41640
H	0.28010	-3.62600	-2.73850
N	1.99950	0.46690	-0.11070
C	3.09950	-0.30640	0.25010
C	2.47320	1.58840	-0.62260
C	4.26880	0.41450	-0.07410
C	3.17970	-1.57050	0.84490
H	1.84020	2.39890	-0.96350
N	3.83330	1.61330	-0.62770
C	5.54720	-0.09130	0.17380
C	4.45260	-2.07510	1.09240
H	2.27990	-2.12700	1.08890
C	4.66970	2.69640	-1.11380
C	5.61640	-1.35050	0.76300
H	6.44370	0.46650	-0.07700
H	4.55390	-3.05340	1.55210
H	5.30170	3.08330	-0.30860
H	5.30700	2.35050	-1.93330
H	4.02970	3.50080	-1.47870
H	6.58930	-1.78350	0.97500
N	-1.99950	-0.46690	0.11080
C	-3.09950	0.30640	-0.25010
C	-2.47320	-1.58840	0.62270
C	-4.26880	-0.41450	0.07410
C	-3.17960	1.57050	-0.84490
H	-1.84020	-2.39890	0.96350
N	-3.83330	-1.61330	0.62770
C	-5.54720	0.09130	-0.17380

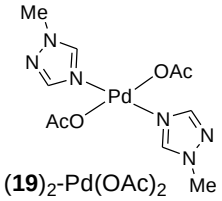
C	-4.45250	2.07500	-1.09240
H	-2.27990	2.12700	-1.08890
C	-4.66970	-2.69640	1.11380
C	-5.61630	1.35050	-0.76310
H	-6.44370	-0.46650	0.07690
H	-4.55380	3.05340	-1.55210
H	-5.30710	-2.35050	1.93330
H	-5.30170	-3.08330	0.30860
H	-4.02970	-3.50080	1.47880
H	-6.58930	1.78350	-0.97510



(**18**)$_2$-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -1344.226667
SCF Energy (M06, acetic acid): -1344.225479
SCF Energy (wB97XD, 1,4-dioxane): -1344.658149
SCF Energy (B3LYP): -1344.702136
ZPE Correction: 0.343486
Enthalpy Correction: 0.370466
Free-Energy Correction: 0.291168758

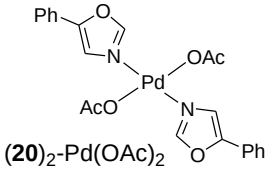
Pd	-0.00000	-0.00000	-0.00000
O	0.43565	-1.66224	1.09989
C	0.68603	-2.77679	0.47981
O	0.76059	-2.92120	-0.74911
C	0.88048	-3.95856	1.42466
H	-0.07898	-4.21819	1.88451
H	1.26071	-4.82073	0.87492
H	1.56557	-3.69285	2.23425
O	-0.43565	1.66224	-1.09989
C	-0.68603	2.77679	-0.47981
O	-0.76059	2.92119	0.74911
C	-0.88044	3.95857	-1.42465
H	-1.56529	3.69281	-2.23442
H	-1.26092	4.82067	-0.87496
H	0.07910	4.21837	-1.88425
N	-1.89220	-0.72723	-0.35093
C	-3.05700	-0.19002	0.04650
C	-2.18563	-1.86669	-1.05298
C	-3.34517	0.96818	0.80049
N	-4.10278	-0.99471	-0.40786
H	-1.38900	-2.48038	-1.44840
C	-3.54391	-2.05300	-1.10372
C	-4.66116	1.26602	1.06504
H	-2.51957	1.59444	1.12690
C	-5.41669	-0.69107	-0.14009
H	-4.14805	-2.82179	-1.55745
C	-5.70732	0.42602	0.58991
H	-4.90758	2.15225	1.64001
H	-6.15667	-1.37634	-0.53449
H	-6.74450	0.66129	0.79905
N	1.89220	0.72723	0.35093
C	3.05699	0.19002	-0.04650
C	2.18562	1.86670	1.05297
C	3.34516	-0.96818	-0.80048
N	4.10278	0.99471	0.40786
H	1.38899	2.48039	1.44839
C	3.54391	2.05300	1.10371
C	4.66116	-1.26602	-1.06503
H	2.51957	-1.59444	-1.12689
C	5.41669	0.69107	0.14009
H	4.14805	2.82180	1.55744
C	5.70731	-0.42602	-0.58991
H	4.90758	-2.15226	-1.64000
H	6.15666	1.37634	0.53449
H	6.74450	-0.66130	-0.79904



(**19**)$_2$-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -1147.779945
SCF Energy (M06, acetic acid): -1147.776349
SCF Energy (wB97XD, 1,4-dioxane): -1148.113628
SCF Energy (B3LYP): -1148.125669
ZPE Correction: 0.282677
Enthalpy Correction: 0.307953
Free-Energy Correction: 0.231220736

Pd	0.00000	0.00000	0.00001
O	0.20999	-1.89614	0.71239
C	0.85340	-2.80115	0.03002
O	1.42394	-2.62571	-1.05310
C	0.85647	-4.16524	0.71353
H	-0.16816	-4.48494	0.92418
H	1.35376	-4.90079	0.08008
H	1.37448	-4.09580	1.67534
O	-0.20999	1.89614	-0.71237
C	-0.85341	2.80115	-0.02999
O	-1.42397	2.62570	1.05311
C	-0.85646	4.16525	-0.71349
H	-1.37447	4.09582	-1.67530
H	-1.35374	4.90079	-0.08004
H	0.16817	4.48494	-0.92414
N	2.00017	0.42613	0.18445
C	2.57264	1.53150	0.74594
C	3.02430	-0.27140	-0.30642
H	2.00486	2.30855	1.23332
N	3.88562	1.54973	0.63545
H	2.92279	-1.21913	-0.82138
N	4.15445	0.39687	-0.03815
C	5.52315	0.04178	-0.37316
H	6.11321	-0.05106	0.54100
H	5.51594	-0.91000	-0.90547
H	5.95903	0.81576	-1.00830
N	-2.00016	-0.42613	-0.18444
C	-2.57262	-1.53150	-0.74594
C	-3.02431	0.27140	0.30640
H	-2.00482	-2.30855	-1.23331
N	-3.88561	-1.54974	-0.63548
H	-2.92281	1.21912	0.82137
N	-4.15445	-0.39687	0.03811
C	-5.52316	-0.04178	0.37308
H	-5.95907	-0.81576	1.00820
H	-5.51597	0.91000	0.90538
H	-6.11319	0.05105	-0.54110

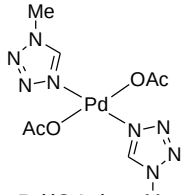


(**20**)$_2$-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -1538.714828
SCF Energy (M06, acetic acid): -1538.710933
SCF Energy (wB97XD, 1,4-dioxane): -1539.197199
SCF Energy (B3LYP): -1539.257829
ZPE Correction: 0.386291
Enthalpy Correction: 0.417694
Free-Energy Correction: 0.329526603

Pd	0.02020	0.09900	0.12890
O	-0.43470	-1.61910	1.12210
C	-0.54400	-2.72660	0.44390
O	-0.36340	-2.84210	-0.77480
C	-0.91660	-3.92430	1.31080
H	-1.82900	-3.71280	1.87570
H	-1.05810	-4.80840	0.68790
H	-0.12370	-4.11220	2.04160
O	0.51910	1.82350	-0.82680
C	0.40300	2.95920	-0.19440
O	-0.00360	3.10330	0.96340
C	0.80710	4.15740	-1.04710
H	0.04910	4.32420	-1.81980

H	0.88560	5.04940	-0.42410
H	1.75350	3.96630	-1.55950
N	-1.97300	0.57730	0.23420
C	-2.53520	1.63150	0.76020
C	-3.00450	-0.23980	-0.21110
H	-2.02890	2.48480	1.18930
O	-3.87160	1.57450	0.69270
H	-2.79800	-1.18280	-0.69100
C	-4.18590	0.37930	0.07010
C	-5.59100	0.05750	-0.13820
C	-6.60200	0.92990	0.29810
C	-5.95010	-1.13950	-0.78280
C	-7.94200	0.60800	0.09280
H	-6.33310	1.85510	0.79600
C	-7.29070	-1.45370	-0.98390
H	-5.17980	-1.82290	-1.12740
C	-8.29220	-0.58210	-0.54730
H	-8.71450	1.29030	0.43480
H	-7.55450	-2.38110	-1.48330
H	-9.33740	-0.82990	-0.70580
N	1.98530	-0.45840	-0.07270
C	2.40150	-1.57620	-0.60430
C	3.12050	0.28130	0.22620
H	1.78660	-2.38980	-0.96480
O	3.73740	-1.63470	-0.67290
H	3.04950	1.26010	0.66990
C	4.21190	-0.44900	-0.14090
C	5.65290	-0.24400	-0.08850
C	6.53670	-1.21540	-0.58760
C	6.17600	0.93780	0.46570
C	7.91290	-1.00500	-0.53250
H	6.14130	-2.12960	-1.01650
C	7.55170	1.14040	0.51660
H	5.50600	1.69700	0.85780
C	8.42600	0.17070	0.01810
H	8.58580	-1.76320	-0.92180
H	7.94270	2.05730	0.94730
H	9.49900	0.33140	0.05950

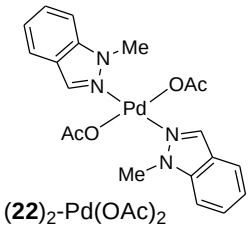


(**21**)$_2$-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -1179.774467
SCF Energy (M06, acetic acid): -1179.778431
SCF Energy (wB97XD, 1,4-dioxane): -1180.098719
SCF Energy (B3LYP): -1180.120172
ZPE Correction: 0.256797
Enthalpy Correction: 0.281874
Free-Energy Correction: 0.205635299

Pd	0.00000	0.00000	0.00000
O	0.15936	1.89110	-0.72144
C	0.74863	2.83561	-0.04390
O	1.45874	2.68154	0.95837
C	0.46982	4.22529	-0.60094
H	-0.52604	4.53938	-0.27076
H	1.20708	4.93564	-0.22370
H	0.46815	4.21582	-1.69345
O	-0.15935	-1.89110	0.72144
C	-0.74863	-2.83561	0.04390
O	-1.45874	-2.68154	-0.95837
C	-0.46982	-4.22529	0.60094
H	-0.46814	-4.21582	1.69345
H	-1.20708	-4.93564	0.22370
H	0.52604	-4.53938	0.27076
N	-2.01083	0.37206	0.17376
C	-3.00499	-0.37918	-0.27464
N	-2.54606	1.49979	0.70598
H	-2.85507	-1.35013	-0.74100
N	-4.13694	0.28514	-0.01358

N	-3.82745	1.45681	0.60072
C	-5.52004	-0.06846	-0.30104
H	-6.09830	-0.04538	0.62393
H	-5.94070	0.64232	-1.01481
H	-5.53892	-1.07247	-0.72476
N	2.01083	-0.37206	-0.17376
C	3.00499	0.37918	0.27464
N	2.54606	-1.49978	-0.70600
H	2.85507	1.35013	0.74101
N	4.13694	-0.28513	0.01356
N	3.82745	-1.45680	-0.60074
C	5.52004	0.06844	0.30109
H	5.94047	-0.64197	1.01538
H	6.09845	0.04469	-0.62376
H	5.53899	1.07271	0.72420



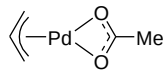
(**22**)$_2$-Pd(OAc)$_2$

SCF Energy (M06, 1,4-dioxane): -1422.775856
SCF Energy (M06, acetic acid): -1422.777960
SCF Energy (wB97XD, 1,4-dioxane): -1423.251404
SCF Energy (B3LYP): -1423.306867
ZPE Correction: 0.399507
Enthalpy Correction: 0.430145
Free-Energy Correction: 0.343672759

Pd	-0.01970	0.04130	-0.10670
O	0.08910	1.80390	0.90210
C	-0.09260	2.87140	0.16470
O	-0.35160	2.86810	-1.04040
C	0.05830	4.16960	0.94900
H	1.09810	4.28580	1.27170
H	-0.22270	5.01760	0.32350
H	-0.56130	4.14480	1.85000
O	-0.07900	-1.72050	-1.12750
C	0.22560	-2.80060	-0.46640
O	0.44210	-2.86140	0.75170
C	0.30700	-4.04210	-1.34590
H	1.20320	-3.98310	-1.97240
H	0.36160	-4.93810	-0.72620
H	-0.55510	-4.09460	-2.01590
N	2.02890	0.03090	-0.21670
N	2.83790	-0.16620	0.85770
C	2.78230	0.28380	-1.27890
C	4.14450	-0.03820	0.48030
C	2.27200	-0.48650	2.16020
C	4.15090	0.25560	-0.91010
H	2.31690	0.47520	-2.23430
C	5.33790	-0.15170	1.21790
H	3.09130	-0.76130	2.82540
H	1.74230	0.38180	2.56060
H	1.58750	-1.33120	2.04510
C	5.37490	0.44170	-1.58490
C	6.52240	0.03580	0.52770
H	5.33530	-0.37300	2.27970
C	6.54580	0.33010	-0.85960
H	5.39150	0.66760	-2.64670
H	7.46350	-0.04310	1.06380
H	7.50260	0.46910	-1.35280
N	-2.07560	0.12560	-0.08370
N	-2.90400	-0.68250	0.64110
C	-2.81310	0.90850	-0.86000
C	-4.20500	-0.38700	0.34070
C	-2.40880	-1.51950	1.72160
C	-4.18880	0.63370	-0.64490
H	-2.31830	1.62830	-1.49670
C	-5.40800	-0.91660	0.84170
H	-2.39490	-0.96580	2.66740
H	-3.06960	-2.38360	1.81880

H	-1.40300	-1.87250	1.48320
C	-5.40170	1.13100	-1.16220
C	-6.58320	-0.40680	0.31610
H	-5.41940	-1.68770	1.60450
C	-6.58480	0.60490	-0.67680
H	-5.40140	1.90830	-1.92000
H	-7.53300	-0.79160	0.67570
H	-7.53420	0.96960	-1.05610

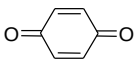
1:1 Heterocycle:Allylpalladium Complexes



Pd(allyl)OAc

SCF Energy (M06, 1,4-dioxane): -473.6206479
SCF Energy (M06, acetic acid): -473.6203659
SCF Energy (B3LYP): -473.7656868
ZPE Correction: 0.122450
Enthalpy Correction: 0.133028
Free-Energy Correction: 0.087363871

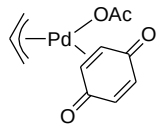
Pd	-0.38878	-0.00000	-0.00357
C	2.11607	0.00001	-0.01086
O	1.47127	1.10083	-0.02411
O	1.47129	-1.10083	-0.02410
C	3.62044	0.00002	0.05543
H	4.02108	-0.89758	-0.41905
H	4.02104	0.89840	-0.41758
H	3.92905	-0.00089	1.10657
C	-2.47359	0.00000	0.45178
H	-2.69366	-0.00000	1.51726
C	-2.14084	1.21192	-0.19801
H	-2.17414	2.14390	0.35838
H	-2.23657	1.30601	-1.27810
C	-2.14086	-1.21191	-0.19802
H	-2.23659	-1.30599	-1.27811
H	-2.17416	-2.14389	0.35836



BQ

SCF Energy (M06, 1,4-dioxane): -381.3265538
SCF Energy (M06, acetic acid): -381.3209206
SCF Energy (B3LYP): -381.4577386
ZPE Correction: 0.085181
Enthalpy Correction: 0.092364
Free-Energy Correction: 0.054674052

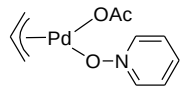
C	0.00000	1.44486	0.00000
C	0.00000	0.67138	1.26937
C	0.00000	0.67138	-1.26937
C	0.00000	-0.67138	1.26937
H	0.00000	1.25917	2.18250
C	0.00000	-0.67138	-1.26937
H	0.00000	1.25917	-2.18250
C	0.00000	-1.44486	0.00000
H	0.00000	-1.25917	2.18250
H	0.00000	-1.25917	-2.18250
O	0.00000	-2.66979	0.00000
O	0.00000	2.66979	0.00000



BQ-Pd(allyl)OAc

SCF Energy (M06, 1,4-dioxane): -854.9617727
SCF Energy (M06, acetic acid): -854.9634865
SCF Energy (B3LYP): -855.214761
ZPE Correction: 0.208980
Enthalpy Correction: 0.227377
Free-Energy Correction: 0.164918068

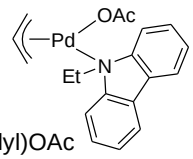
C	-2.50590	0.22175	0.32158
O	-1.86361	0.35994	1.37459
O	-2.02026	-0.33696	-0.74886
C	-3.92326	0.75093	0.18272
H	-4.40374	0.79604	1.16146
H	-3.86570	1.76657	-0.22329
H	-4.51023	0.14123	-0.50711
C	0.58641	-2.91240	0.14513
H	0.71501	-3.53273	-0.73878
C	1.62287	-2.04864	0.55873
H	2.58352	-2.05714	0.05538
H	1.62746	-1.65122	1.57172
C	-0.70235	-2.68252	0.66368
H	-0.84329	-2.29500	1.66935
Pd	-0.01753	-0.84658	-0.28333
H	0.49818	3.22076	1.63362
C	0.86408	2.49044	0.91853
C	0.40382	1.16981	-1.20764
C	2.54906	0.89662	0.05803
C	1.62748	0.53666	-1.06458
C	2.05209	1.87644	1.05601
C	-0.00591	2.25603	-0.26411
H	-0.17266	1.10974	-2.12542
H	2.07826	-0.02953	-1.87485
H	2.71758	2.07579	1.89104
O	-0.97134	2.96721	-0.49904
O	3.67227	0.41227	0.13684
H	-1.56505	-3.15204	0.20308



4-Pd(allyl)OAc

SCF Energy (M06, 1,4-dioxane): -796.9584040
SCF Energy (M06, acetic acid): -796.9648633
SCF Energy (B3LYP): -797.2270193
ZPE Correction: 0.216371
Enthalpy Correction: 0.234030
Free-Energy Correction: 0.173160043

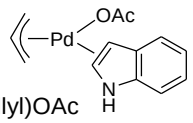
Pd	-1.37720	-0.17635	-0.11096
C	0.54143	1.87531	0.29031
O	0.48844	1.42544	1.44397
O	-0.06888	1.35997	-0.73450
C	1.35807	3.12574	-0.02729
H	0.67830	3.95076	-0.26528
H	1.97534	3.40678	0.82744
H	1.98530	2.96262	-0.90850
C	-3.48214	-0.43829	-0.31672
H	-3.81094	-0.70244	-1.31963
C	-2.99487	-1.43622	0.55587
H	-3.00864	-2.47636	0.24354
H	-2.97159	-1.26615	1.63054
C	-3.19034	0.91505	0.00443
H	-3.21131	1.25102	1.03962
H	-3.35434	1.68727	-0.74133
O	0.20728	-1.65828	-0.00621
N	1.45055	-1.21822	-0.05297
C	2.18684	-1.20491	1.08655
C	1.98790	-0.81262	-1.23141
C	3.51649	-0.82156	1.05948
H	1.64431	-1.50518	1.97149
C	3.31378	-0.41626	-1.29655
H	1.30391	-0.82750	-2.06764
C	4.09950	-0.42206	-0.14371
H	4.07806	-0.82668	1.98662
H	3.71526	-0.10212	-2.25337
H	5.13887	-0.11461	-0.18048



5-Pd(allyl)OAc

SCF Energy (M06, 1,4-dioxane): -1069.420684
SCF Energy (M06, acetic acid): -1069.424988
SCF Energy (B3LYP): -1069.864675
ZPE Correction: 0.357105
Enthalpy Correction: 0.381310
Free-Energy Correction: 0.307323847

Pd	1.14971	-0.66674	-0.63875
C	3.25291	0.53797	0.85081
O	2.78666	1.55886	0.31673
O	2.72268	-0.64208	0.76745
C	4.53084	0.60139	1.67953
H	5.32761	0.05674	1.16233
H	4.83960	1.63716	1.82710
H	4.38220	0.11125	2.64621
C	0.91866	-1.88751	-2.38149
H	0.62911	-2.91576	-2.17557
C	-0.05971	-0.87330	-2.43136
H	-1.10877	-1.13400	-2.33175
H	0.14966	0.07205	-2.92782
C	2.27420	-1.48623	-2.23848
H	2.64249	-0.60174	-2.75510
H	3.02642	-2.22193	-1.97092
N	-0.43660	0.23754	0.80477
C	-1.50224	-0.72827	0.86118
C	-0.98833	1.34880	0.06740
C	0.21081	0.57925	2.11547
C	-2.62600	-0.26998	0.14388
C	-1.49425	-1.96393	1.50326
C	-2.29862	1.05671	-0.35905
C	-0.35527	2.55025	-0.24187
H	0.69663	-0.32936	2.47407
H	1.00399	1.28873	1.88358
C	-0.75973	1.14544	3.15056
C	-3.75996	-1.08316	0.03989
C	-2.63905	-2.75764	1.40097
H	-0.62483	-2.30682	2.05479
C	-3.00083	1.99239	-1.12699
C	-1.07769	3.47659	-0.99733
H	0.67281	2.72987	0.05527
H	-0.20826	1.38315	4.06584
H	-1.23131	2.06607	2.79467
H	-1.54644	0.43023	3.40713
C	-3.75810	-2.32551	0.67269
H	-4.63105	-0.74876	-0.51627
H	-2.65943	-3.72619	1.89150
C	-2.38329	3.20319	-1.43580
H	-4.00987	1.78284	-1.47044
H	-0.61289	4.42262	-1.25859
H	-4.63300	-2.96514	0.60581
H	-2.91597	3.94316	-2.02576

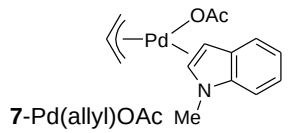


6-Pd(allyl)OAc

SCF Energy (M06, 1,4-dioxane): -837.2749931
SCF Energy (M06, acetic acid): -837.2803129
SCF Energy (B3LYP): -837.5923618
ZPE Correction: 0.253074
Enthalpy Correction: 0.271964
Free-Energy Correction: 0.208678997

C	-3.05399	-1.22575	0.04849
O	-2.76845	-1.29452	-1.15789
O	-2.39872	-0.53010	0.92770
C	-4.25076	-1.98219	0.61517
H	-5.02218	-1.26706	0.91945
H	-4.66238	-2.65855	-0.13512
H	-3.95974	-2.54188	1.50858
C	-0.57125	2.77391	0.03814

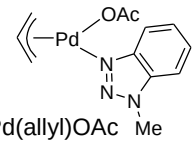
H	-0.25689	3.19802	0.98960
C	0.38299	2.15697	-0.80423
H	1.43470	2.19177	-0.53731
H	0.16776	2.02614	-1.86349
C	-1.93895	2.50131	-0.18873
H	-2.31825	2.36837	-1.19975
H	-2.67491	2.76471	0.56395
Pd	-0.86758	0.63903	0.08113
N	1.39160	-1.25295	-1.46783
C	2.47833	-0.84505	-0.71073
C	0.28782	-1.41423	-0.66078
C	2.04994	-0.76478	0.64008
C	3.78831	-0.54659	-1.09771
C	0.64320	-1.11508	0.65891
H	-0.64711	-1.79744	-1.05445
C	2.97484	-0.39833	1.62966
C	4.68206	-0.17995	-0.09612
H	4.10066	-0.60620	-2.13634
H	0.04960	-1.35906	1.52924
C	4.28215	-0.11008	1.25330
H	2.67129	-0.34026	2.67106
H	5.70955	0.05237	-0.35989
H	5.00920	0.17326	2.00834
H	1.37536	-1.33305	-2.47234



7-Pd(allyl)OAc

SCF Energy (M06, 1,4-dioxane): -876.5626770
SCF Energy (M06, acetic acid): -876.5664821
SCF Energy (B3LYP): -876.9051482
ZPE Correction: 0.280921
Enthalpy Correction: 0.301515
Free-Energy Correction: 0.234682724

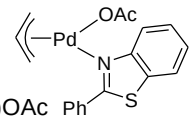
C	3.09744	-1.15847	-0.40780
O	2.75476	-1.56937	0.71268
O	2.49850	-0.21520	-1.06901
C	4.30377	-1.75502	-1.12573
H	5.09781	-1.00378	-1.18987
H	4.67465	-2.62699	-0.58537
H	4.03856	-2.03147	-2.15020
C	0.71835	2.74888	0.69066
H	0.48393	3.45718	-0.10143
C	-0.31112	1.95224	1.24569
H	-1.33984	2.11999	0.94227
H	-0.17568	1.49792	2.22600
C	2.05814	2.35554	0.90165
H	2.36210	1.89889	1.84115
H	2.85193	2.80062	0.31063
Pd	0.95102	0.71593	0.01119
N	-1.39533	-1.50659	0.84630
C	-2.44104	-0.84155	0.21973
C	-0.27628	-1.43630	0.04968
C	-1.96759	-0.34875	-1.02464
C	-3.75546	-0.63508	0.65142
C	-0.56917	-0.71767	-1.11599
H	0.63578	-1.95202	0.32955
C	-2.85025	0.34048	-1.86850
C	-4.60792	0.05815	-0.20379
H	-4.10454	-1.00488	1.61051
H	0.04541	-0.70747	-2.00590
C	-4.16311	0.53661	-1.45157
H	-2.51137	0.71583	-2.82999
H	-5.63742	0.22976	0.09635
H	-4.85815	1.06728	-2.09531
C	-1.44065	-2.07863	2.17933
H	-1.59764	-1.30358	2.93832
H	-2.24993	-2.81206	2.25306
H	-0.49203	-2.57768	2.38103



8-Pd(allyl)OAc

SCF Energy (M06, 1,4-dioxane): -908.6293800
SCF Energy (M06, acetic acid): -908.6358407
SCF Energy (B3LYP): -908.9662844
ZPE Correction: 0.257824
Enthalpy Correction: 0.277985
Free-Energy Correction: 0.211800511

Pd	1.42405	-0.58601	-0.00437
C	1.59685	2.21569	0.56432
O	1.57759	2.30240	-0.67553
O	1.47367	1.11579	1.23600
C	1.75000	3.46358	1.43048
H	2.57805	3.33499	2.13364
H	1.92362	4.34150	0.80658
H	0.84292	3.61237	2.02569
C	2.94770	-2.01710	-0.49647
H	3.16991	-2.72673	0.29815
C	1.83247	-2.23637	-1.33692
H	1.26276	-3.15564	-1.23666
H	1.77269	-1.74790	-2.30782
C	3.51077	-0.71911	-0.45482
H	3.56620	-0.10646	-1.35189
H	4.21423	-0.46661	0.33248
N	-0.71482	-0.68709	0.13277
C	-1.64356	0.24790	-0.27881
N	-1.32302	-1.69978	0.67632
C	-1.49129	1.49104	-0.91678
C	-2.91411	-0.25909	0.05161
N	-2.65017	-1.46599	0.64230
C	-2.65890	2.18069	-1.20103
H	-0.50044	1.88088	-1.14003
C	-4.09568	0.44148	-0.23562
C	-3.57252	-2.43696	1.20068
C	-3.93715	1.66521	-0.86783
H	-2.59779	3.14804	-1.68962
H	-5.07532	0.05193	0.01940
H	-4.13959	-1.99323	2.02399
H	-4.26441	-2.79059	0.43085
H	-2.98183	-3.27293	1.57388
H	-4.81874	2.24959	-1.11394

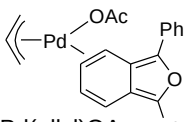


9-Pd(allyl)OAc

SCF Energy (M06, 1,4-dioxane): -1427.123593
SCF Energy (M06, acetic acid): -1427.127022
SCF Energy (B3LYP): -1427.540564
ZPE Correction: 0.307072
Enthalpy Correction: 0.330746
Free-Energy Correction: 0.257738331

Pd	0.35298	-1.34059	-0.68766
C	0.07955	-2.39525	1.95456
O	1.20074	-1.88129	2.08826
O	-0.63518	-2.35223	0.87271
C	-0.57870	-3.14606	3.10799
H	-0.83950	-4.16158	2.79510
H	0.09029	-3.18337	3.96868
H	-1.51085	-2.64575	3.38953
C	1.18502	-2.08584	-2.51939
H	0.44456	-2.36889	-3.26495
C	1.56028	-0.73048	-2.38082
H	1.16997	0.00455	-3.07869
H	2.49606	-0.46613	-1.89359
C	1.49171	-2.97499	-1.46098
H	2.42045	-2.87312	-0.90370
H	1.03432	-3.95917	-1.43788
N	-0.63212	0.52083	-0.13817
C	-2.02456	0.61099	-0.16780

C	-0.06063	1.66811	0.13893
C	-2.90994	-0.44771	-0.41995
C	-2.52775	1.90699	0.07368
S	-1.19623	2.99945	0.38221
C	1.38241	1.90657	0.28092
C	-4.27337	-0.18182	-0.43283
H	-2.51807	-1.44704	-0.56877
C	-3.89944	2.17299	0.05785
C	2.20203	0.94290	0.89718
C	1.94593	3.11196	-0.17454
C	-4.76530	1.11473	-0.19957
H	-4.97172	-0.99159	-0.61992
H	-4.27816	3.17281	0.24318
C	3.56808	1.19113	1.03462
H	1.77864	0.01811	1.28693
C	3.31182	3.34540	-0.03420
H	1.31819	3.85359	-0.66035
H	-5.83599	1.29429	-0.21497
C	4.12636	2.38405	0.56980
H	4.19301	0.44753	1.52021
H	3.73974	4.27419	-0.39944
H	5.19101	2.56813	0.68229

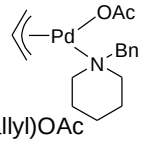


10-Pd(allyl)OAc

SCF Energy (M06, 1,4-dioxane): -1318.999146
SCF Energy (M06, acetic acid): -1319.000851
SCF Energy (B3LYP): -1319.551955
ZPE Correction: 0.402417
Enthalpy Correction: 0.430656
Free-Energy Correction: 0.348895316

O	3.87042	-0.98659	-0.79676
C	4.24891	0.24973	-0.68732
O	3.62743	1.11976	-0.05479
C	5.55646	0.57876	-1.39666
H	5.55566	0.16895	-2.41036
H	5.71211	1.65797	-1.42600
H	6.38760	0.11051	-0.85878
O	-2.37154	1.16553	-0.04160
C	-1.04212	1.36739	-0.28119
C	-2.72447	-0.12129	-0.33803
C	-0.50895	0.17833	-0.76521
C	-0.51584	2.69453	0.00200
C	-1.59423	-0.78119	-0.80701
C	-4.11448	-0.48783	-0.12028
C	0.79111	-0.18886	-1.25153
C	-1.39438	3.78912	0.13466
C	0.86841	2.91182	0.15292
C	-1.36892	-2.08902	-1.34011
C	-4.49714	-1.83354	0.04639
C	-5.11382	0.50447	-0.06234
C	0.97464	-1.48500	-1.73621
H	1.55832	0.56381	-1.39266
C	-0.90147	5.06279	0.39958
H	-2.46172	3.63248	0.02261
C	1.35018	4.19376	0.41118
H	1.58093	2.09591	0.09791
C	-0.11668	-2.42781	-1.77255
H	-2.18806	-2.79368	-1.43243
C	-5.83383	-2.17323	0.23896
H	-3.74249	-2.61214	0.05929
C	-6.44636	0.15783	0.13896
H	-4.83480	1.54522	-0.18483
H	1.90183	-1.73372	-2.24196
C	0.47372	5.27345	0.53470
H	-1.59277	5.89532	0.49592
H	2.42063	4.33695	0.52367
H	0.06562	-3.41115	-2.19496
C	-6.81629	-1.18180	0.28426

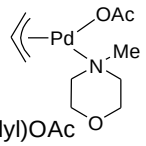
H	-6.10692	-3.21665	0.36815
H	-7.20162	0.93765	0.17706
H	0.85616	6.26947	0.73849
H	-7.85743	-1.44919	0.43775
Pd	2.14391	-1.33456	0.36631
C	0.67307	-1.73458	1.89999
C	1.83082	-2.50277	2.15822
H	0.56223	-0.74599	2.34149
H	-0.25037	-2.23168	1.62041
H	1.81553	-3.57833	1.99508
C	3.06700	-1.82529	2.26030
H	3.99657	-2.38425	2.22726
H	3.12063	-0.83603	2.70994



11-Pd(allyl)OAc

SCF Energy (M06, 1,4-dioxane): -995.6510122
SCF Energy (M06, acetic acid): -995.6564095
SCF Energy (B3LYP): -996.0596717
ZPE Correction: 0.393273
Enthalpy Correction: 0.416732
Free-Energy Correction: 0.344566947

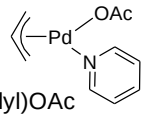
Pd	0.72051	-0.32320	0.73606
C	1.52300	-2.45007	-1.08353
O	0.47847	-3.00337	-0.71743
O	1.90980	-1.25841	-0.72940
C	2.49446	-3.15740	-2.02547
H	3.43733	-3.35023	-1.50330
H	2.07072	-4.10144	-2.37036
H	2.72726	-2.51750	-2.88210
C	0.69972	-0.49720	2.88400
H	1.50643	0.03271	3.38739
C	-0.45668	0.20862	2.48163
H	-0.57308	1.24713	2.77789
H	-1.38140	-0.32467	2.27284
C	0.94692	-1.76540	2.31157
H	0.13252	-2.44422	2.07431
H	1.92261	-2.22625	2.43103
N	0.18447	1.24240	-0.79699
C	-0.31724	2.51046	-0.19500
C	1.39281	1.54088	-1.62856
C	-0.85201	0.65152	-1.71287
H	-0.63544	3.18140	-1.01216
H	-1.20064	2.27667	0.40093
C	0.74248	3.21793	0.65175
H	1.74224	0.59342	-2.03926
H	1.08551	2.20130	-2.45726
C	2.50446	2.20929	-0.82138
H	-1.07808	1.39662	-2.49187
H	-0.37220	-0.20168	-2.19772
C	-2.13809	0.20305	-1.05224
H	0.30977	4.14665	1.04253
H	0.99095	2.58831	1.51383
C	2.01357	3.50106	-0.15763
H	3.34651	2.41002	-1.49383
H	2.86293	1.50323	-0.06273
C	-2.25930	-1.10700	-0.56199
C	-3.23888	1.06611	-0.95933
H	1.79538	4.25103	-0.93092
H	2.79112	3.92862	0.48519
C	-3.45125	-1.52648	0.03331
H	-1.42191	-1.79818	-0.64970
C	-4.42883	0.64646	-0.36142
H	-3.16943	2.07174	-1.36767
C	-4.53517	-0.65168	0.14116
H	-3.53466	-2.54509	0.40212
H	-5.27255	1.32800	-0.29852
H	-5.46233	-0.98393	0.59992



12-Pd(allyl)OAc

SCF Energy (M06, 1,4-dioxane): -800.6236164
SCF Energy (M06, acetic acid): -800.6291397
SCF Energy (B3LYP): -800.8923666
ZPE Correction: 0.287640
Enthalpy Correction: 0.306434
Free-Energy Correction: 0.24373888

Pd	0.37958	0.71790	-0.06497
C	2.37636	-1.30594	-0.01285
O	2.51861	-0.85334	1.13245
O	1.44522	-0.93548	-0.84219
C	3.31718	-2.37428	-0.56028
H	3.90353	-1.95684	-1.38537
H	3.99159	-2.72465	0.22211
H	2.74570	-3.21428	-0.96657
C	0.49579	2.79306	-0.61290
H	-0.00461	3.04743	-1.54515
C	-0.25420	2.68420	0.58213
H	-1.30374	2.96512	0.57361
H	0.24432	2.77027	1.54629
C	1.78998	2.22542	-0.64214
H	2.42997	2.25326	0.23697
H	2.29718	2.09629	-1.59311
N	-1.16109	-0.64484	0.84151
C	-2.51336	-0.03445	0.94528
C	-1.28396	-1.89597	0.04052
C	-0.64600	-0.96205	2.19621
H	-3.17254	-0.71400	1.50847
H	-2.43241	0.90424	1.49959
C	-3.11066	0.20363	-0.43885
H	-0.28659	-2.31340	-0.09851
H	-1.91234	-2.61097	0.59396
C	-1.91527	-1.60488	-1.31603
H	-1.28996	-1.70386	2.69183
H	0.37598	-1.33584	2.11654
H	-0.63282	-0.04878	2.79588
H	-4.12844	0.59354	-0.34318
H	-2.50010	0.94306	-0.98267
O	-3.19900	-1.00310	-1.17672
H	-2.06529	-2.53891	-1.86406
H	-1.24622	-0.95822	-1.90328

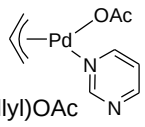


13-Pd(allyl)OAc

SCF Energy (M06, 1,4-dioxane): -721.8043104
SCF Energy (M06, acetic acid): -721.8081757
SCF Energy (B3LYP): -722.0690242
ZPE Correction: 0.212873
Enthalpy Correction: 0.229471
Free-Energy Correction: 0.170678483

Pd	-0.76834	-0.57066	-0.08378
C	-1.10634	2.25391	-0.02429
O	-0.89041	2.06403	1.18577
O	-1.06851	1.33438	-0.93523
C	-1.44841	3.64536	-0.54777
H	-2.47698	3.65248	-0.92300
H	-1.34811	4.38674	0.24619
H	-0.79779	3.90404	-1.38834
C	-2.04689	-2.29476	-0.05371
H	-2.09925	-2.83759	-0.99556
C	-0.96266	-2.52003	0.82661
H	-0.24613	-3.30420	0.59753
H	-1.04760	-2.25943	1.87997
C	-2.82516	-1.12688	0.12686
H	-3.04440	-0.75692	1.12644
H	-3.51410	-0.81650	-0.65239
N	1.37054	-0.28404	-0.03964

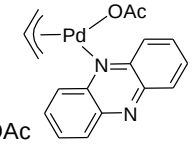
C	1.88118	0.73137	0.68587
C	2.21374	-1.07807	-0.72551
C	3.25202	0.97346	0.75147
H	1.14883	1.35089	1.19712
C	3.59264	-0.89389	-0.71429
H	1.75757	-1.87796	-1.29881
C	4.12427	0.15082	0.04181
H	3.61764	1.80086	1.35018
H	4.22889	-1.55906	-1.28830
H	5.19645	0.32027	0.07354



14-Pd(allyl)OAc

SCF Energy (M06, 1,4-dioxane): -737.8494647
SCF Energy (M06, acetic acid): -737.8520914
SCF Energy (B3LYP): -738.1042945
ZPE Correction: 0.201078
Enthalpy Correction: 0.217570
Free-Energy Correction: 0.15889814

Pd	-0.76433	-0.57063	-0.07986
C	-1.09277	2.26404	-0.00808
O	-0.81130	2.08540	1.19099
O	-1.09086	1.33801	-0.91271
C	-1.48278	3.64628	-0.52036
H	-2.54560	3.64891	-0.78414
H	-1.30188	4.40173	0.24556
H	-0.92463	3.88740	-1.42942
C	-2.02963	-2.30603	-0.07085
H	-2.07808	-2.83708	-1.01947
C	-0.94450	-2.53430	0.80689
H	-0.22204	-3.31025	0.56884
H	-1.03131	-2.28566	1.86302
C	-2.81466	-1.14488	0.12487
H	-3.03745	-0.79094	1.12958
H	-3.50452	-0.82725	-0.65061
N	1.37544	-0.26818	-0.03560
C	1.89894	0.76913	0.64888
C	2.23283	-1.07722	-0.68491
C	3.27489	0.97458	0.67868
H	1.17716	1.41488	1.14551
H	1.79382	-1.90449	-1.23401
N	3.55541	-0.95139	-0.71471
C	4.07118	0.07770	-0.02756
H	3.70003	1.80577	1.22975
H	5.15423	0.18005	-0.05027

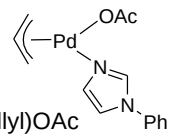


15-Pd(allyl)OAc

SCF Energy (M06, 1,4-dioxane): -1044.967861
SCF Energy (M06, acetic acid): -1044.972388
SCF Energy (B3LYP): -1045.384501
ZPE Correction: 0.293752
Enthalpy Correction: 0.315526
Free-Energy Correction: 0.246336206

Pd	1.33978	-0.67337	-0.38474
C	2.59743	0.90153	1.62363
O	2.86821	1.61225	0.64241
O	1.89460	-0.18890	1.58121
C	3.09106	1.27037	3.01896
H	3.75764	0.48769	3.39499
H	3.62230	2.22272	2.99532
H	2.24543	1.33227	3.71055
C	2.24593	-1.95983	-1.85490
H	2.09614	-3.02362	-1.67994
C	1.22795	-1.20603	-2.48265
H	0.34868	-1.71445	-2.86764
H	1.46424	-0.25468	-2.95545
C	3.25601	-1.26992	-1.14550

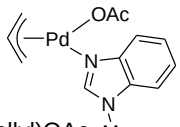
H	3.63154	-0.31222	-1.49690
H	3.91511	-1.81999	-0.48122
N	-0.70831	-0.01752	-0.04093
C	-1.06590	1.26919	-0.25561
C	-1.67597	-0.90689	0.27561
C	-2.46256	1.64875	-0.21991
C	-0.07844	2.26559	-0.51627
C	-3.05989	-0.49498	0.31656
C	-1.34998	-2.26277	0.57277
N	-3.43186	0.76519	0.05237
C	-2.81828	3.00587	-0.49051
C	-0.46955	3.55804	-0.75743
H	0.97477	1.99562	-0.45771
C	-4.06180	-1.46244	0.63608
C	-2.34233	-3.15675	0.88274
H	-0.30234	-2.54800	0.56417
C	-1.84681	3.93215	-0.75777
H	-3.87311	3.25781	-0.46693
H	0.28608	4.31653	-0.93805
C	-3.71158	-2.75714	0.91058
H	-5.09211	-1.12339	0.65326
H	-2.08494	-4.18504	1.11812
H	-2.11776	4.96430	-0.95879
H	-4.47453	-3.48914	1.15718



16-Pd(allyl)OAc

SCF Energy (M06, 1,4-dioxane): -930.7004517
SCF Energy (M06, acetic acid): -930.7015151
SCF Energy (B3LYP): -931.0576835
ZPE Correction: 0.275911
Enthalpy Correction: 0.296470
Free-Energy Correction: 0.229502514

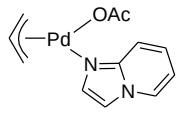
Pd	-2.20038	-0.29410	-0.01385
C	-1.19752	2.42313	-0.25698
O	-0.66331	2.20268	0.84468
O	-1.87055	1.56363	-0.94986
C	-1.08958	3.79974	-0.90948
H	-2.08453	4.25070	-0.98181
H	-0.43826	4.44984	-0.32343
H	-0.70511	3.70498	-1.92945
C	-4.05543	-1.31307	0.33574
H	-4.49127	-1.77109	-0.55016
C	-3.02757	-1.98583	1.03864
H	-2.75596	-2.99577	0.74417
H	-2.81180	-1.72952	2.07426
C	-4.23112	0.07110	0.56643
H	-4.10012	0.48658	1.56378
H	-4.85156	0.65277	-0.10800
N	-0.17976	-0.94463	-0.29498
C	0.30490	-2.13557	-0.79809
C	0.87200	-0.21684	0.04751
C	1.67101	-2.11920	-0.76109
H	-0.35499	-2.91399	-1.14805
H	0.80327	0.78434	0.45497
N	2.02610	-0.89308	-0.21592
H	2.40772	-2.85769	-1.03194
C	3.34838	-0.41497	0.02108
C	4.36684	-0.70780	-0.89110
C	3.61601	0.34597	1.16345
C	5.65936	-0.24325	-0.65033
H	4.14313	-1.27318	-1.78984
C	4.90841	0.82068	1.38315
H	2.82377	0.55228	1.87542
C	5.93379	0.52407	0.48318
H	6.44898	-0.47103	-1.35991
H	5.11372	1.41409	2.26876
H	6.93991	0.88984	0.66319



17-Pd(allyl)OAc

SCF Energy (M06, 1,4-dioxane): -892.6331637
SCF Energy (M06, acetic acid): -892.6351440
SCF Energy (B3LYP): -892.9701446
ZPE Correction: 0.270258
Enthalpy Correction: 0.290458
Free-Energy Correction: 0.224332422

Pd	1.32820	-0.69931	-0.04315
C	2.26738	2.00966	0.43230
O	1.94426	2.20887	-0.75303
O	2.08309	0.91056	1.08688
C	2.95087	3.10938	1.24221
H	3.99280	2.82857	1.42873
H	2.92758	4.05484	0.69800
H	2.46806	3.22164	2.21714
C	2.13903	-2.66903	-0.31317
H	2.00800	-3.33252	0.53961
C	1.07620	-2.48699	-1.22898
H	0.17599	-3.08612	-1.12814
H	1.27377	-2.10950	-2.23061
C	3.19111	-1.72392	-0.30834
H	3.54604	-1.28692	-1.23977
H	3.89686	-1.71115	0.51627
N	-0.64414	0.13476	-0.12217
C	-1.88112	-0.41304	0.19967
C	-0.88705	1.34909	-0.58225
C	-2.88689	0.53463	-0.09390
C	-2.22134	-1.65898	0.73642
H	-0.09909	2.02571	-0.89908
N	-2.21710	1.64527	-0.59087
C	-4.24190	0.27542	0.12418
C	-3.56974	-1.92278	0.95555
H	-1.44985	-2.38242	0.97822
C	-2.81492	2.89513	-1.02688
C	-4.56486	-0.97160	0.65281
H	-5.00991	1.00771	-0.10361
H	-3.86507	-2.88067	1.37269
H	-3.50569	2.72139	-1.85769
H	-3.35854	3.36864	-0.20356
H	-2.02279	3.56682	-1.36018
H	-5.60626	-1.21531	0.83930

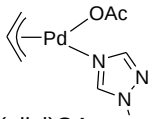


18-Pd(allyl)OAc

SCF Energy (M06, 1,4-dioxane): -853.3232796
SCF Energy (M06, acetic acid): -853.3256240
SCF Energy (B3LYP): -853.6367468
ZPE Correction: 0.241811
Enthalpy Correction: 0.260266
Free-Energy Correction: 0.197825479

Pd	-1.32685	-0.49996	-0.05160
C	-1.10715	2.34278	-0.35772
O	-0.98872	2.30854	0.87982
O	-1.19575	1.30646	-1.12742
C	-1.14500	3.67717	-1.09897
H	-2.07992	3.76455	-1.66107
H	-1.05899	4.50697	-0.39601
H	-0.32818	3.72227	-1.82631
C	-3.02910	-1.70135	0.47336
H	-3.44097	-2.28644	-0.34690
C	-1.89816	-2.18170	1.17485
H	-1.51597	-3.17386	0.95145
H	-1.67145	-1.80802	2.17168
C	-3.36564	-0.33329	0.59287
H	-3.23380	0.19412	1.53483
H	-4.08329	0.10264	-0.09513
N	0.74519	-0.93351	-0.39529

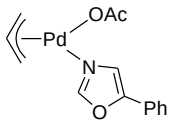
C	1.79333	-0.23788	0.07555
C	1.26088	-1.96621	-1.12889
C	1.85263	0.92032	0.88233
N	2.97918	-0.83688	-0.35714
H	0.61659	-2.67575	-1.62601
C	2.63369	-1.93380	-1.12492
C	3.08844	1.41672	1.22314
H	0.91786	1.39483	1.17546
C	4.21268	-0.33501	-0.01186
H	3.37345	-2.56825	-1.58575
C	4.27991	0.77980	0.77364
H	3.15966	2.30880	1.83628
H	5.07313	-0.86934	-0.39505
H	5.25328	1.17303	1.04367



19-Pd(allyl)OAc

SCF Energy (M06, 1,4-dioxane): -755.1023563
SCF Energy (M06, acetic acid): -755.1028308
SCF Energy (B3LYP): -755.3518716
ZPE Correction: 0.211697
Enthalpy Correction: 0.229162
Free-Energy Correction: 0.168318929

Pd	-1.03154	-0.41710	-0.07181
C	-0.43997	2.44354	0.03008
O	0.08175	2.20055	1.13343
O	-0.93406	1.56363	-0.77817
C	-0.54828	3.88072	-0.47399
H	-1.59613	4.19744	-0.44122
H	0.04549	4.54970	0.15085
H	-0.22368	3.94682	-1.51614
C	-2.71862	-1.74283	-0.02933
H	-2.99062	-2.15679	-0.99837
C	-1.66445	-2.32731	0.71145
H	-1.20574	-3.24361	0.35034
H	-1.58834	-2.16019	1.78433
C	-3.13665	-0.43662	0.31683
H	-3.16857	-0.12466	1.35909
H	-3.77747	0.11890	-0.36055
N	1.09053	-0.70654	-0.19184
C	1.84357	-1.71221	-0.72541
C	1.99005	0.13508	0.31858
H	1.42120	-2.56913	-1.22822
N	3.14330	-1.54155	-0.57747
H	1.73209	1.06133	0.82213
N	3.21680	-0.35858	0.09184
C	4.50592	0.20348	0.45725
H	5.09635	0.38853	-0.44267
H	4.33833	1.14204	0.98670
H	5.04239	-0.49375	1.10433

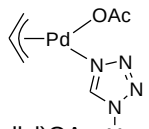


20-Pd(allyl)OAc

SCF Energy (M06, 1,4-dioxane): -950.5694005
SCF Energy (M06, acetic acid): -950.5699115
SCF Energy (B3LYP): -950.9176187
ZPE Correction: 0.263451
Enthalpy Correction: 0.283979
Free-Energy Correction: 0.216928487

Pd	-2.04230	-0.65156	-0.05138
C	-2.68893	2.15653	-0.19673
O	-2.33664	2.15509	0.99663
O	-2.63736	1.13558	-0.98967
C	-3.24219	3.42346	-0.84238
H	-4.31031	3.29109	-1.04431
H	-3.10645	4.27911	-0.17935
H	-2.75264	3.60749	-1.80284

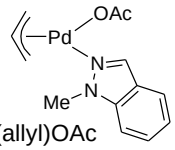
C	-3.01035	-2.56615	-0.04771
H	-2.91178	-3.12454	-0.97659
C	-1.96185	-2.59111	0.90082
H	-1.11079	-3.24599	0.73585
H	-2.15379	-2.32920	1.93969
C	-3.98127	-1.54125	0.05568
H	-4.32526	-1.20303	1.03136
H	-4.66098	-1.36094	-0.77114
N	0.00717	-0.01478	0.13107
C	0.37666	1.10653	0.68850
C	1.18127	-0.65193	-0.24933
H	-0.27980	1.86621	1.09458
O	1.71072	1.25872	0.70446
H	1.16855	-1.60939	-0.74394
C	2.23938	0.13440	0.10182
C	3.68732	0.03135	-0.02014
C	4.52452	1.04201	0.48169
C	4.26623	-1.08775	-0.64463
C	5.90813	0.93152	0.36027
H	4.08631	1.90881	0.96406
C	5.64896	-1.19115	-0.76181
H	3.63327	-1.87633	-1.04062
C	6.47614	-0.18262	-0.26009
H	6.54394	1.71981	0.75222
H	6.08247	-2.06058	-1.24699
H	7.55477	-0.26543	-0.35326



21-Pd(allyl)OAc

SCF Energy (M06, 1,4-dioxane):	-771.1032689
SCF Energy (M06, acetic acid):	-771.1070852
SCF Energy (B3LYP):	-771.3533077
ZPE Correction:	0.198663
Enthalpy Correction:	0.216165
Free-Energy Correction:	0.155458434

Pd	-1.02345	-0.42869	-0.04957
C	-0.46457	2.49995	0.04988
O	0.24212	2.30708	1.05770
O	-1.02622	1.58644	-0.66908
C	-0.74473	3.92346	-0.42605
H	-1.77235	4.19427	-0.16048
H	-0.06069	4.62695	0.05135
H	-0.66262	3.98950	-1.51407
C	-2.63482	-1.84446	-0.11829
H	-2.85195	-2.22055	-1.11607
C	-1.56951	-2.40339	0.62381
H	-1.02697	-3.25529	0.22543
H	-1.53261	-2.28427	1.70531
C	-3.13206	-0.58009	0.27954
H	-3.21256	-0.32695	1.33521
H	-3.78221	-0.02360	-0.38816
N	1.10187	-0.65933	-0.14862
C	2.01041	0.21823	0.24893
N	1.76635	-1.75849	-0.59596
H	1.75504	1.19121	0.66693
N	3.21163	-0.33920	0.04339
N	3.03684	-1.57556	-0.48841
C	4.54560	0.19215	0.28426
H	5.12274	-0.53385	0.85860
H	5.04558	0.38738	-0.66673
H	4.45145	1.11983	0.84878

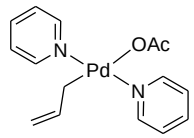


22-Pd(allyl)OAc

SCF Energy (M06, 1,4-dioxane):	-892.5997716
SCF Energy (M06, acetic acid):	-892.6034936
SCF Energy (B3LYP):	-892.9416142
ZPE Correction:	0.269996
Enthalpy Correction:	0.290176

Free-Energy Correction: 0.224282871

Pd	-1.53868	-0.55666	-0.15368
C	-1.79148	2.26595	-0.16467
O	-1.71241	2.08204	1.06271
O	-1.73138	1.33224	-1.05942
C	-1.97602	3.66950	-0.73249
H	-2.91626	3.72290	-1.29021
H	-1.98370	4.40785	0.07035
H	-1.17040	3.89519	-1.43781
C	-2.88559	-2.22499	-0.10002
H	-2.94736	-2.78274	-1.03241
C	-1.82638	-2.47950	0.80100
H	-1.13496	-3.29164	0.59603
H	-1.91992	-2.19450	1.84740
C	-3.61388	-1.01963	0.04719
H	-3.82978	-0.62123	1.03645
H	-4.27942	-0.69545	-0.74662
N	0.60607	-0.38567	-0.18796
N	1.37952	0.04328	0.84725
C	1.40397	-0.65485	-1.21363
C	2.69758	0.03711	0.48411
C	0.79001	0.41453	2.12391
C	2.75671	-0.40886	-0.86237
H	0.98129	-0.99507	-2.14764
C	3.85694	0.38302	1.20248
H	0.63463	-0.46795	2.75438
H	1.47365	1.09897	2.62960
H	-0.15771	0.93002	1.93713
C	4.00165	-0.50741	-1.51608
C	5.06466	0.27485	0.53458
H	3.81167	0.71676	2.23354
C	5.14075	-0.16500	-0.81103
H	4.06070	-0.84359	-2.54680
H	5.98175	0.53294	1.05587
H	6.11282	-0.23177	-1.28955

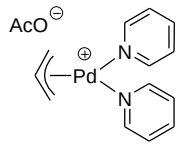


(**13**)$_2$-Pd(σ-allyl)OAc

SCF Energy (M06, 1,4-dioxane): -969.9738959
SCF Energy (M06, acetic acid): -969.9771645
SCF Energy (B3LYP): -970.3654087
ZPE Correction: 0.303850
Enthalpy Correction: 0.326226
Free-Energy Correction: 0.255725749

Pd	-0.03437	-0.26973	0.00400
C	0.29030	-3.21001	0.06007
H	-0.53960	-3.41396	0.74089
C	0.08007	-2.12844	-0.92573
H	-0.87520	-2.23806	-1.45040
H	0.88954	-2.08573	-1.66189
C	1.39699	-3.95951	0.20710
H	2.25107	-3.84606	-0.45697
O	-0.14952	1.62345	1.02737
C	-0.23561	2.67972	0.29285
O	-0.26635	2.69036	-0.95494
C	-0.29539	3.99290	1.07203
H	-1.12286	3.96663	1.78783
H	0.62411	4.11983	1.65288
H	-0.41828	4.83812	0.39290
H	1.47028	-4.72781	0.97135
N	2.02874	-0.05216	-0.07296
C	2.50295	1.04009	-0.71035
C	2.89193	-0.87776	0.54440
C	3.86379	1.32749	-0.75526
H	1.75505	1.68427	-1.16453
C	4.26450	-0.64387	0.54993

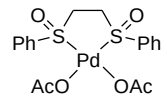
H	2.46038	-1.75150	1.02077
C	4.76239	0.47589	-0.11341
H	4.20192	2.21215	-1.28398
H	4.92148	-1.33515	1.06697
H	5.82854	0.68196	-0.12870
N	-2.11565	-0.33949	-0.03760
C	-2.74597	0.67342	-0.66999
C	-2.85379	-1.29372	0.55867
C	-4.13500	0.74948	-0.72923
H	-2.09941	1.42802	-1.11062
C	-4.24491	-1.27587	0.54938
H	-2.30390	-2.08475	1.05452
C	-4.90050	-0.23730	-0.11038
H	-4.59826	1.57868	-1.25297
H	-4.79409	-2.06517	1.05135
H	-5.98527	-0.19769	-0.13914



(**13**)$_2$-Pd(π-allyl)OAc

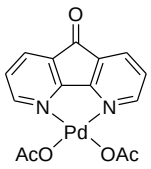
SCF Energy (M06, 1,4-dioxane): -969.9706492
SCF Energy (M06, acetic acid): -969.976477
SCF Energy (B3LYP): -970.3540368
ZPE Correction: 0.303059
Enthalpy Correction: 0.325730
Free-Energy Correction: 0.254462113

Pd	-0.00000	0.32597	-1.03807
C	-0.00003	1.41480	-2.91877
C	-1.20638	1.66006	-2.22178
H	-0.00003	0.81421	-3.82626
C	1.20633	1.66009	-2.22181
H	-2.14417	1.30193	-2.63867
H	-1.26904	2.47935	-1.50969
H	1.26896	2.47937	-1.50970
O	0.00002	1.40427	2.61855
C	0.00004	2.39200	1.83321
O	0.00010	2.33601	0.56441
C	-0.00002	3.79883	2.44882
H	-0.87979	4.35309	2.10462
H	0.00008	3.75403	3.53973
H	0.87958	4.35326	2.10445
H	2.14412	1.30200	-2.63872
N	-1.57584	-0.83178	-0.08695
C	-2.29969	-1.73327	-0.77867
C	-1.85192	-0.63927	1.21974
C	-3.32348	-2.47691	-0.20174
H	-2.03974	-1.85100	-1.82553
C	-2.86582	-1.34986	1.86425
H	-1.23436	0.09470	1.74731
C	-3.61463	-2.28065	1.14910
H	-3.87627	-3.19059	-0.80366
H	-3.05300	-1.16143	2.91614
H	-4.40910	-2.84361	1.63049
N	1.57584	-0.83178	-0.08696
C	1.85192	-0.63929	1.21973
C	2.29969	-1.73326	-0.77869
C	2.86580	-1.34988	1.86424
H	1.23436	0.09469	1.74731
C	3.32348	-2.47692	-0.20176
H	2.03975	-1.85098	-1.82556
C	3.61462	-2.28067	1.14908
H	3.05299	-1.16147	2.91613
H	3.87626	-3.19059	-0.80368
H	4.40908	-2.84364	1.63047



SCF Energy (M06, 1,4-dioxane): -2073.191997
SCF Energy (M06, acetic acid): -2073.194973
SCF Energy (B3LYP): -2073.591071
ZPE Correction: 0.352971
Enthalpy Correction: 0.383247
Free-Energy Correction: 0.297656711

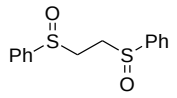
Pd	0.00000	0.48048	0.00000
O	-1.08856	1.90761	0.96938
O	1.08855	1.90762	-0.96937
S	-1.39058	-1.16016	0.84837
C	-0.43652	2.26432	2.05235
C	0.43650	2.26433	-2.05235
O	-1.51491	-1.51573	2.29750
C	-0.75935	-2.66189	-0.04550
C	-3.02846	-0.94971	0.12503
O	0.61808	1.75156	2.43351
C	-1.10594	3.40178	2.80593
O	-0.61809	1.75156	-2.43351
C	1.10592	3.40179	-2.80592
H	-1.20562	-3.51985	0.46450
H	-1.10826	-2.61546	-1.08101
C	0.75936	-2.66189	0.04547
C	-4.10649	-1.54920	0.77854
C	-3.17912	-0.18846	-1.03782
H	-2.16247	3.17695	2.97480
H	-0.59874	3.56425	3.75756
H	-1.05698	4.31447	2.20381
H	2.16245	3.17699	-2.97477
H	0.59873	3.56426	-3.75755
H	1.05694	4.31449	-2.20379
H	1.20563	-3.51984	-0.46454
H	1.10827	-2.61547	1.08098
S	1.39058	-1.16014	-0.84838
C	-5.37948	-1.40504	0.22786
H	-3.94436	-2.09281	1.70377
C	-4.46279	-0.06031	-1.57247
H	-2.33377	0.31773	-1.50250
O	1.51492	-1.51570	-2.29751
C	3.02847	-0.94970	-0.12503
C	-5.55415	-0.66757	-0.94668
H	-6.23335	-1.86160	0.71901
H	-4.60558	0.53076	-2.47147
C	3.17912	-0.18846	1.03783
C	4.10650	-1.54919	-0.77854
H	-6.54857	-0.55466	-1.36843
C	4.46279	-0.06030	1.57248
H	2.33377	0.31773	1.50250
C	5.37949	-1.40503	-0.22785
H	3.94437	-2.09280	-1.70377
C	5.55415	-0.66757	0.94669
H	4.60558	0.53075	2.47148
H	6.23336	-1.86159	-0.71900
H	6.54857	-0.55466	1.36844



SCF Energy (M06, 1,4-dioxane): -1192.075779
SCF Energy (M06, acetic acid): -1192.076938
SCF Energy (B3LYP): -1192.453994
ZPE Correction: 0.251324
Enthalpy Correction: 0.274117
Free-Energy Correction: 0.202502531

Pd	-0.99543	0.00000	-0.00000
C	-2.59054	2.38233	0.35623
O	-1.76029	2.79887	1.16575

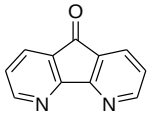
O	-2.48136	1.29729	-0.36815
C	-3.90198	3.11559	0.09896
O	-2.48136	-1.29729	0.36815
C	-2.59054	-2.38233	-0.35623
O	-1.76029	-2.79887	-1.16575
C	-3.90198	-3.11559	-0.09896
H	-4.71657	2.56165	0.57659
H	-3.85522	4.11980	0.52274
H	-4.12092	3.16050	-0.97085
H	-4.71657	-2.56164	-0.57659
H	-3.85523	-4.11980	-0.52275
H	-4.12092	-3.16051	0.97085
N	0.62544	1.39854	-0.20845
C	1.76006	0.71315	-0.10606
C	0.77560	2.73223	-0.37533
C	3.06239	1.19695	-0.17022
C	2.04258	3.32502	-0.45877
H	-0.13591	3.31363	-0.39871
C	3.22084	2.56442	-0.36042
H	2.09738	4.39956	-0.59405
H	4.20037	3.02785	-0.42365
N	0.62544	-1.39854	0.20845
C	1.76006	-0.71315	0.10606
C	0.77560	-2.73223	0.37533
C	3.06239	-1.19695	0.17022
C	2.04258	-3.32502	0.45877
H	-0.13592	-3.31363	0.39871
C	3.22084	-2.56442	0.36042
H	2.09738	-4.39956	0.59405
H	4.20037	-3.02785	0.42366
C	3.98947	-0.00000	-0.00000
O	5.19969	-0.00000	-0.00001



SCF Energy (M06, 1,4-dioxane): -1488.375385
SCF Energy (M06, acetic acid): -1488.378499
SCF Energy (B3LYP): -1488.668828
ZPE Correction: 0.248096
Enthalpy Correction: 0.265979
Free-Energy Correction: 0.205398604

S	-1.90394	0.36072	1.14772
O	-2.06820	-1.11073	1.47588
C	-0.57418	0.47084	-0.14639
H	-0.24026	1.50952	-0.21334
H	-1.07821	0.20351	-1.07948
C	-0.97170	1.11060	2.52732
C	0.33327	2.21510	4.71289
C	-0.70032	2.48055	2.54119
C	-0.62011	0.29081	3.59717
C	0.03988	0.85057	4.69330
C	-0.03715	3.02912	3.63868
H	-1.00030	3.11508	1.71107
H	-0.87542	-0.76370	3.55175
H	0.32203	0.22137	5.53237
H	0.18616	4.09157	3.65759
H	0.84435	2.64816	5.56749
S	1.90394	-0.36072	-1.14772
O	2.06820	1.11073	-1.47588
C	0.57418	-0.47084	0.14639
H	1.07821	-0.20351	1.07948
H	0.24026	-1.50952	0.21334
C	0.97170	-1.11060	-2.52732
C	-0.33327	-2.21510	-4.71289
C	0.62011	-0.29081	-3.59717
C	0.70032	-2.48055	-2.54119
C	0.03715	-3.02912	-3.63868
C	-0.03988	-0.85057	-4.69330
H	0.87542	0.76370	-3.55175

H	1.00030	-3.11508	-1.71107
H	-0.18616	-4.09157	-3.65759
H	-0.32203	-0.22137	-5.53237
H	-0.84435	-2.64816	-5.56749



SCF Energy (M06, 1,4-dioxane):	-607.2501032
SCF Energy (M06, acetic acid):	-607.2505198
SCF Energy (B3LYP):	-607.5135686
ZPE Correction:	0.146001
Enthalpy Correction:	0.156267
Free-Energy Correction:	0.111007381

N	0.00000	-1.71733	1.54712
C	-0.00000	-0.65724	0.74624
C	0.00000	-1.43894	2.86487
C	-0.00000	0.68097	1.18718
C	0.00000	-0.14944	3.40661
H	0.00000	-2.30185	3.52745
C	0.00000	0.95381	2.54552
H	0.00000	-0.01871	4.48366
H	0.00000	1.97557	2.91307
N	0.00000	-1.71733	-1.54712
C	-0.00000	-0.65724	-0.74624
C	0.00000	-1.43894	-2.86487
C	-0.00000	0.68097	-1.18718
C	0.00000	-0.14944	-3.40661
H	0.00000	-2.30185	-3.52745
C	0.00000	0.95381	-2.54552
H	0.00000	-0.01871	-4.48366
H	0.00000	1.97557	-2.91307
C	-0.00001	1.59470	0.00000
O	-0.00000	2.81180	0.00000

NMR Binding Conditions and Details

NMR binding experiments were carried out as follows:

A 0.35 M solution of pentafluoroanisole standard in CD_2Cl_2 was prepared and used to prepare 0.35 M solutions of $Pd(OAc)_2$ and each heterocycle. To the stock solutions of each heterocycle was added an equal volume of 0.35 M $Pd(OAc)_2$ solution to yield an NMR sample with 1:1:2 heterocycle:$Pd(OAc)_2$:pentafluoroanisole. ^{1}H NMR spectra were acquired and analyzed for the loss of the free heterocycle resonances. In cases where incomplete binding was observed, ratios of bound to free heterocycle were determined relative to the pentafluoroanisole internal standard.

Heterocycle ^{1}H NMR Binding to $Pd(OAc)_2$ Results					
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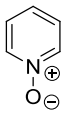
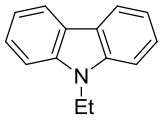
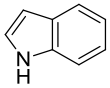
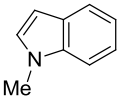
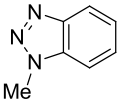
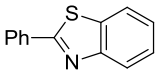
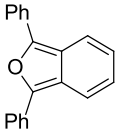
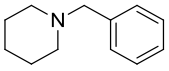
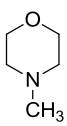
1	4		51	63	0
2	5		85	94	0
3	6		46	48	0
4	7		48	29	0
5	8		28	59	95
6	9		28	88	22
7	10		39	99	0
8	11		7	16	100
9	12		9	40	100

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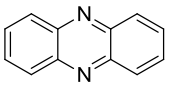
12	15		15	50	68
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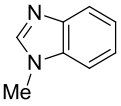
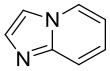
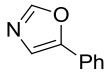
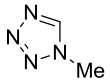
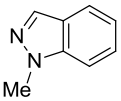
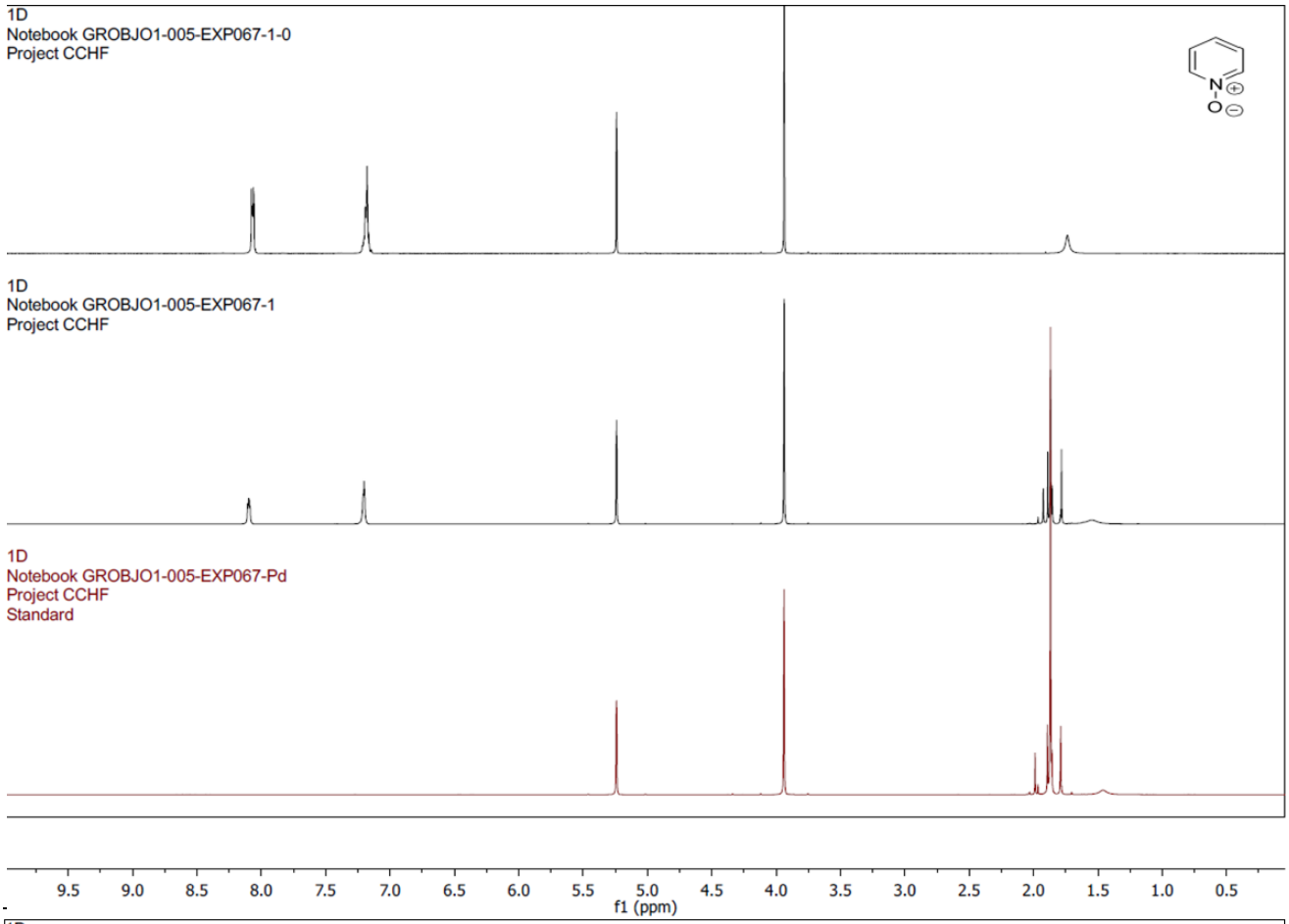
14	17		0	0	100
15	18		0	0	100
17	20		0	8	100
18	21		8	30	80
19	22		8	44	100

^{1}H NMR Pd-Binding Spectra

The following ^{1}H NMR spectra were used in the heterocycle binding experiments with $Pd(OAc)_2$. All plots show (1) heterocycle ligand with pentafluoroanisole (standard) in CD_2Cl_2, (2) 1:1 ligand /$Pd(OAc)_2$ with pentafluoroanisole in CD_2Cl_2, and (3) $Pd(OAc)_2$ with pentafluoroanisole in CD_2Cl_2.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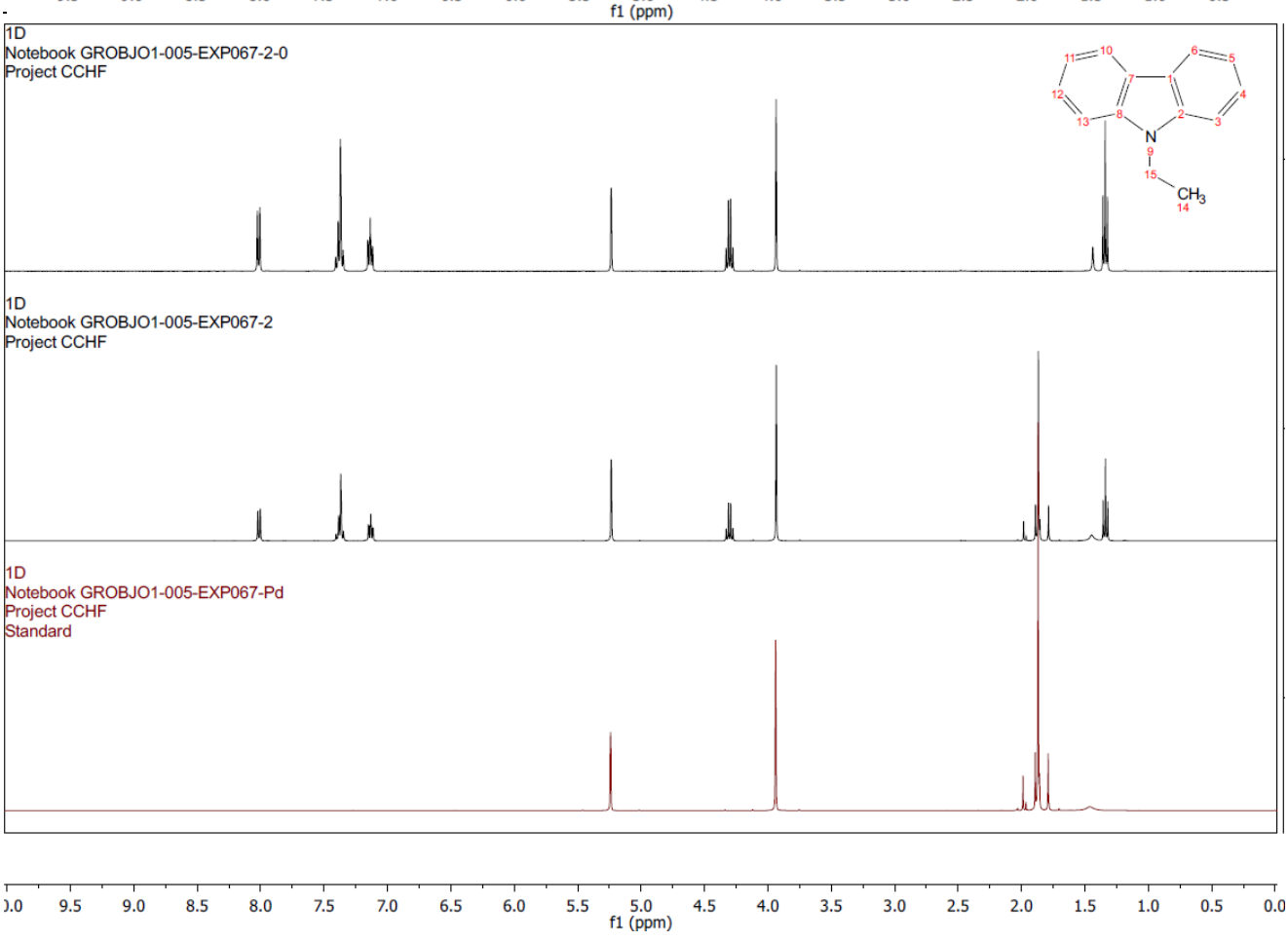
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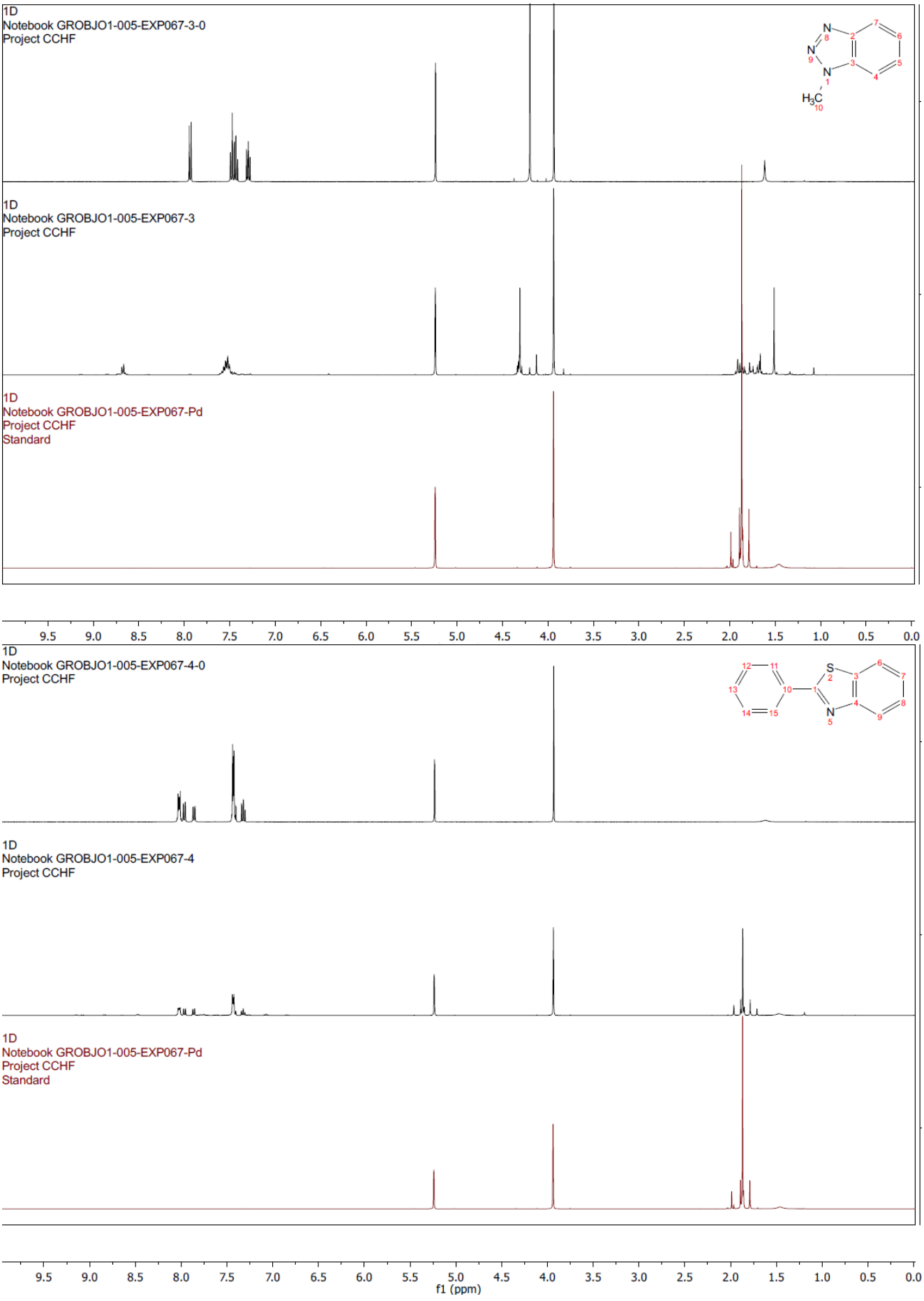
f1 (ppm)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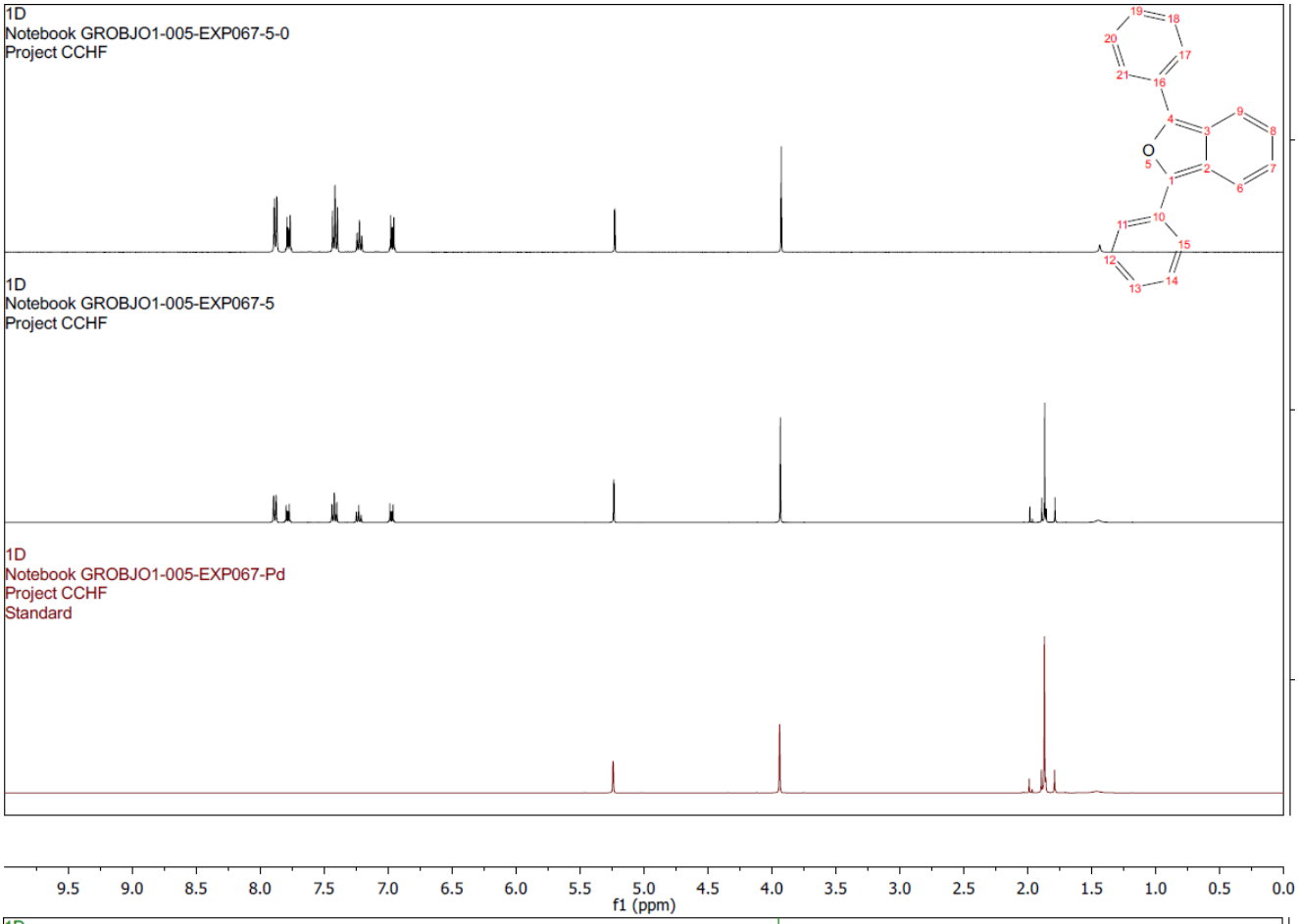
f1 (ppm)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Standard

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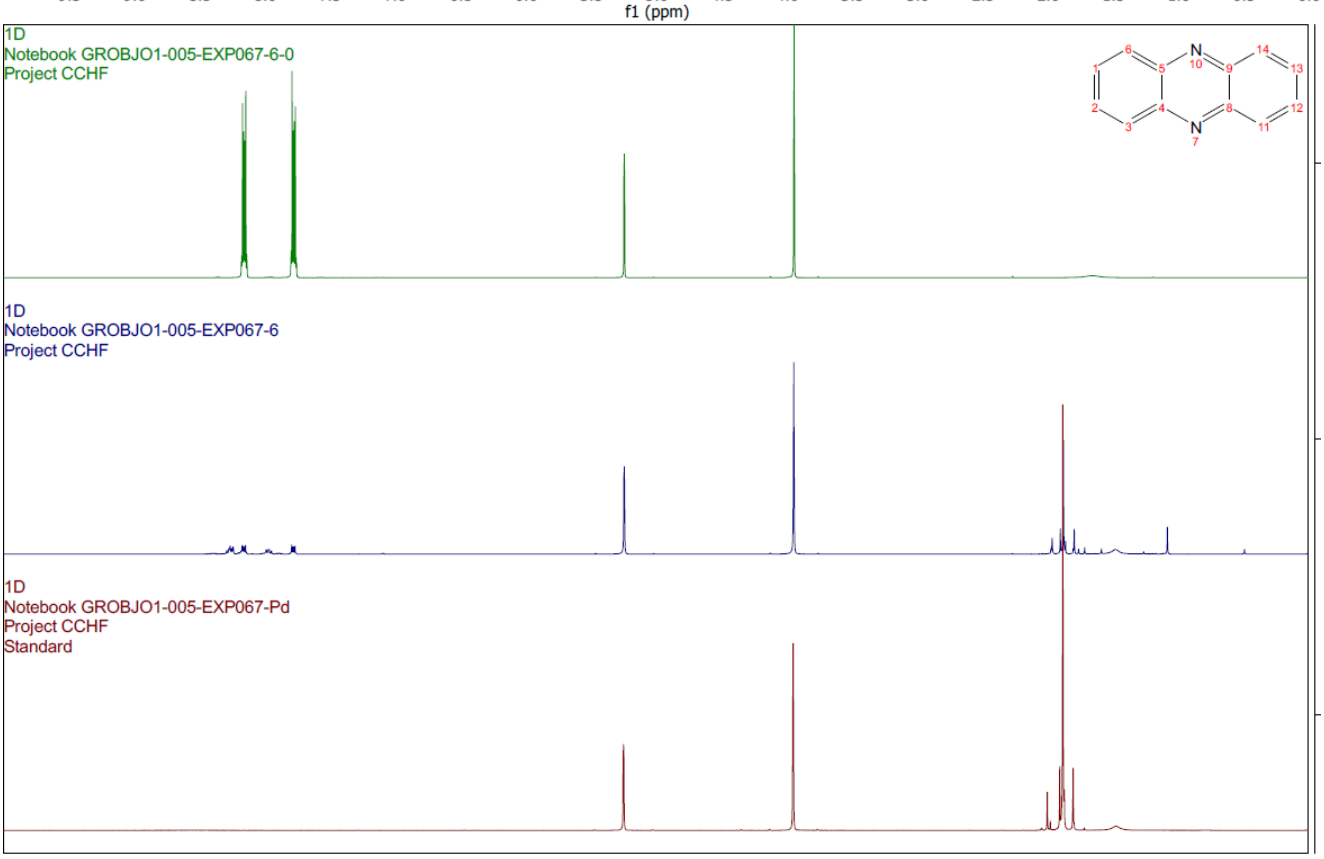
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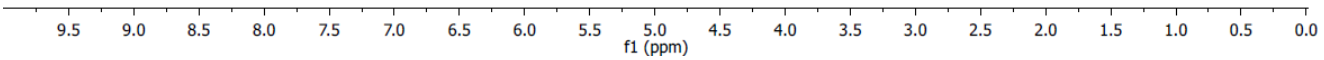
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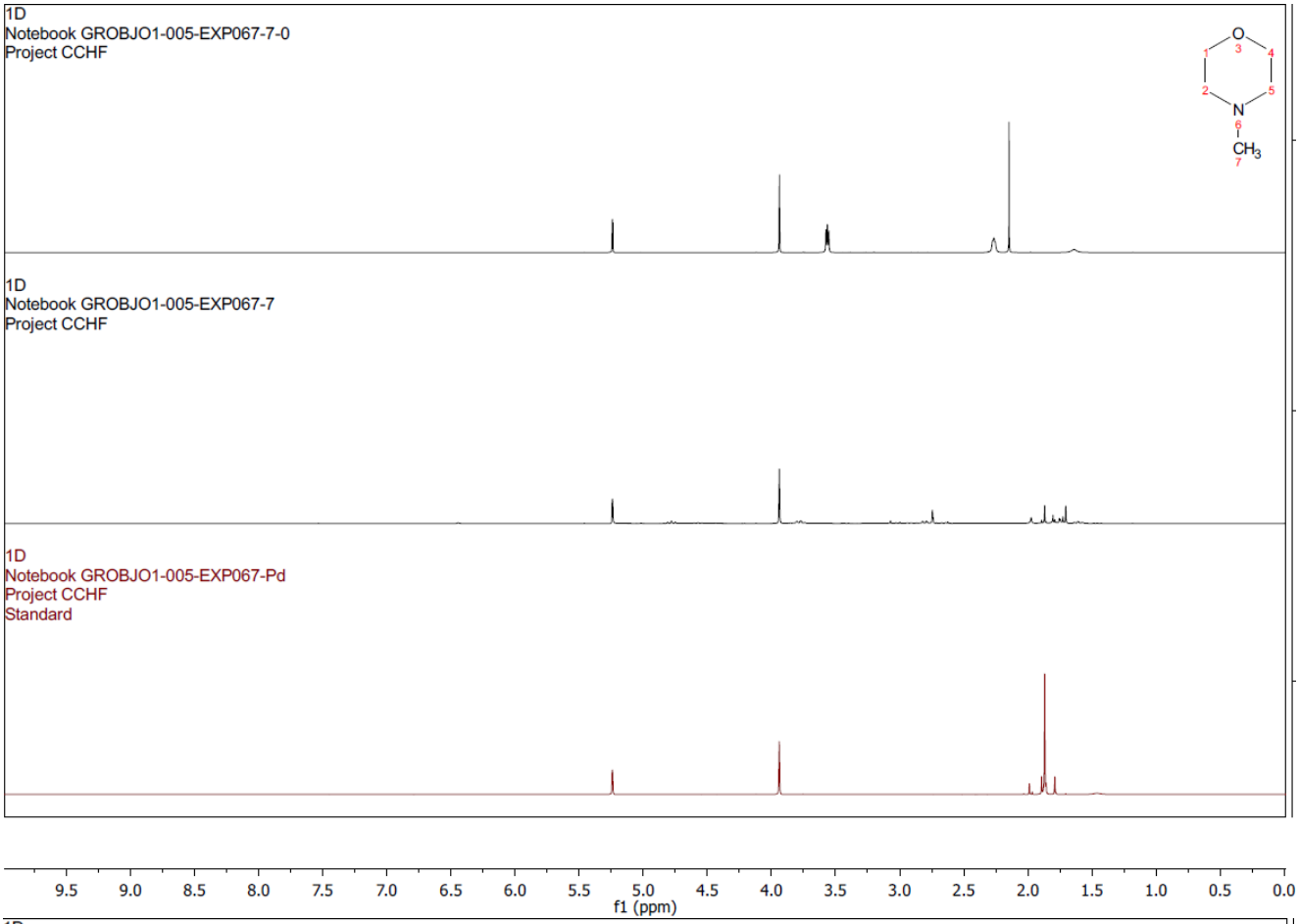
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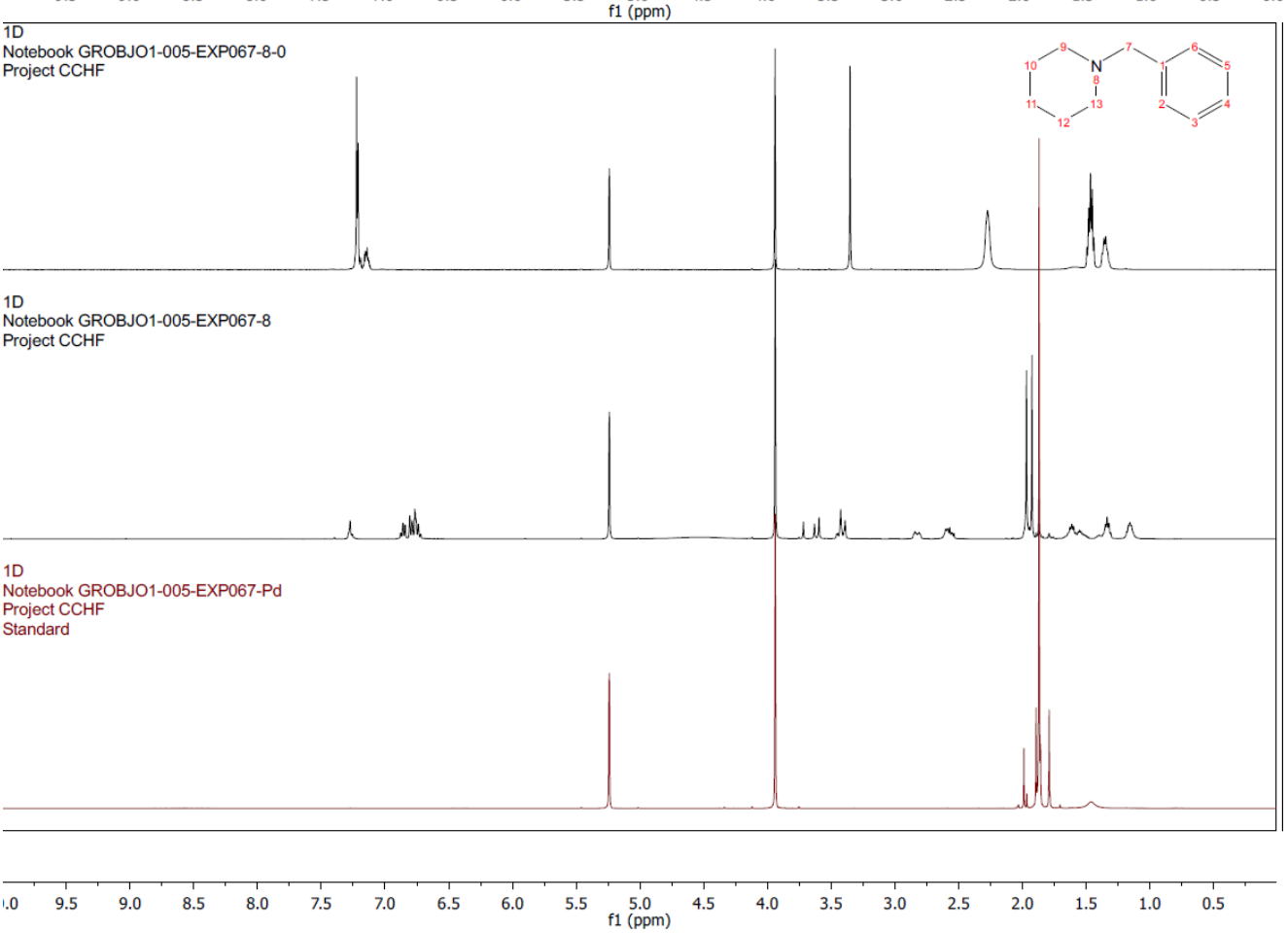
f1 (ppm)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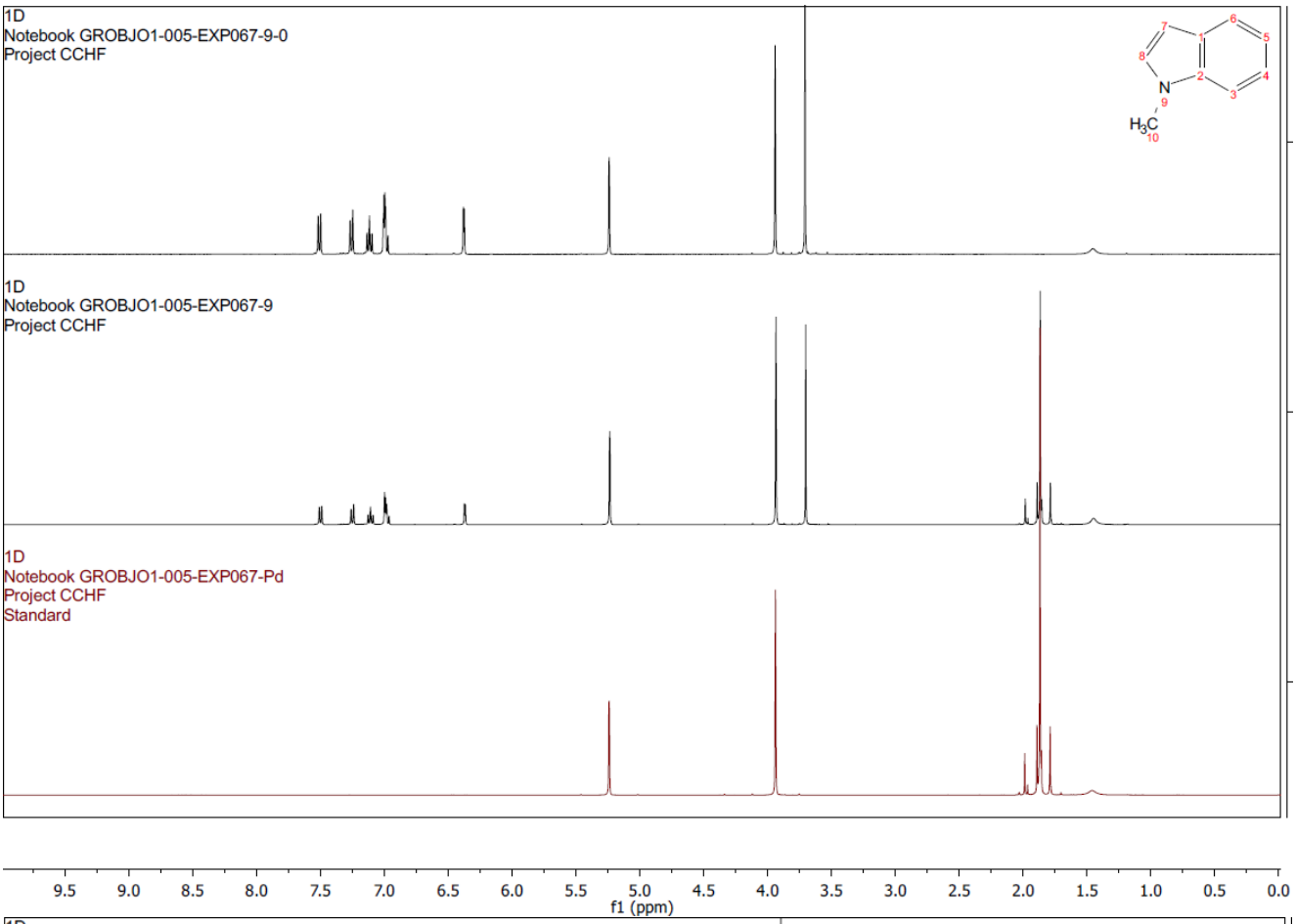
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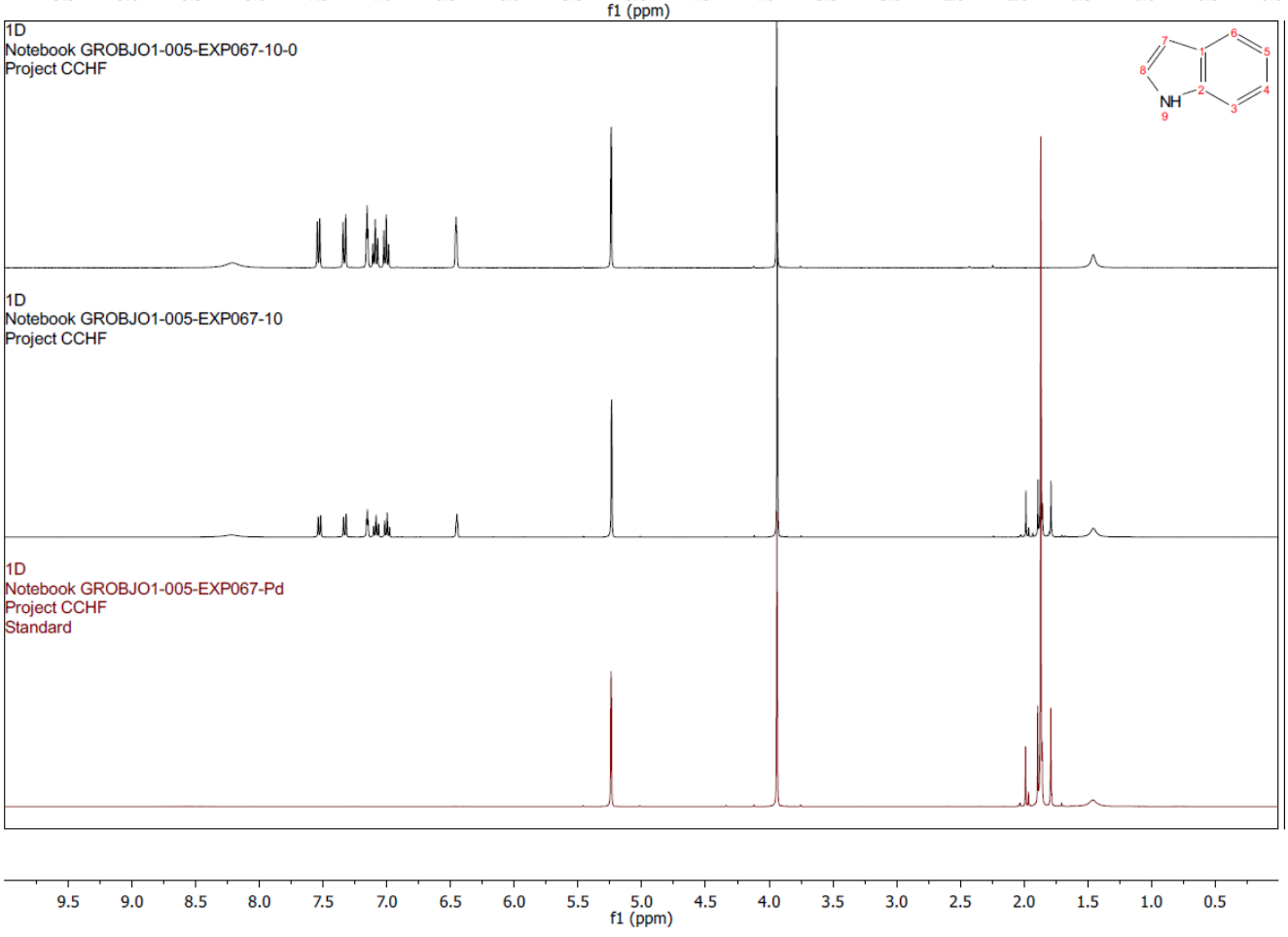
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Project CCHF
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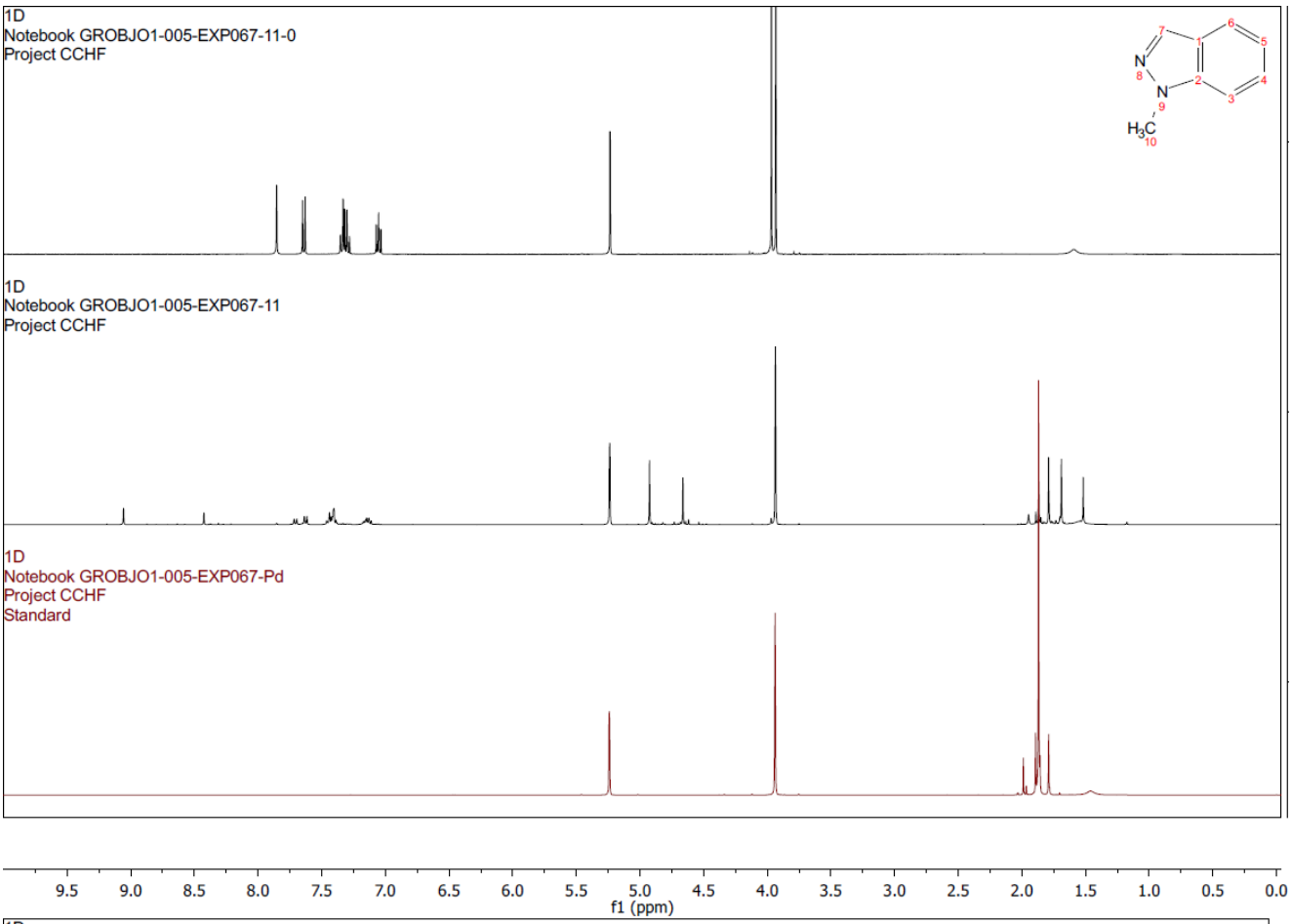
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Project CCHF
Standard

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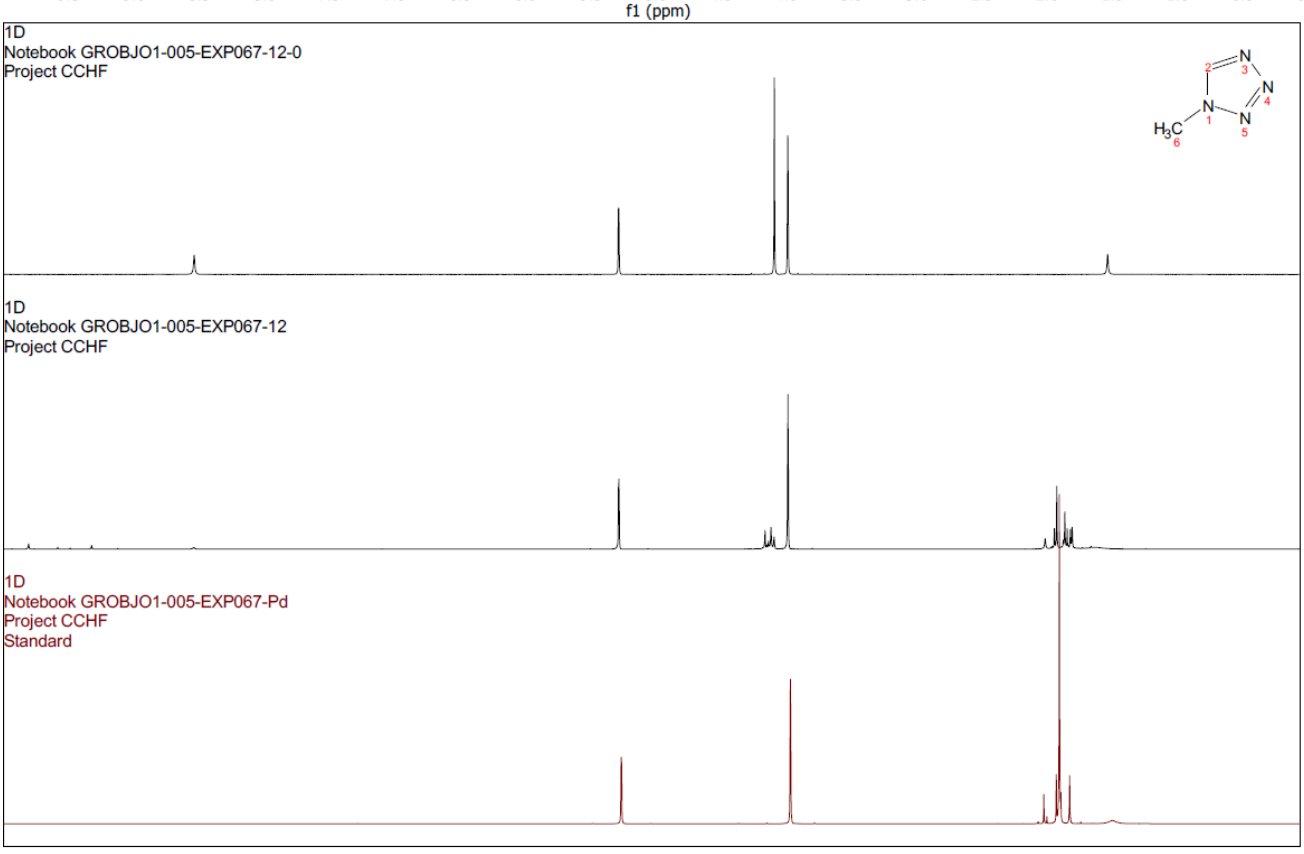
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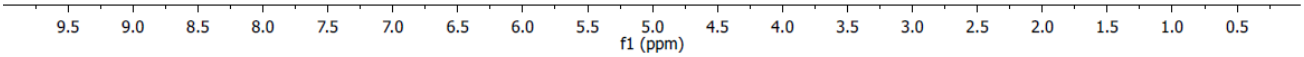
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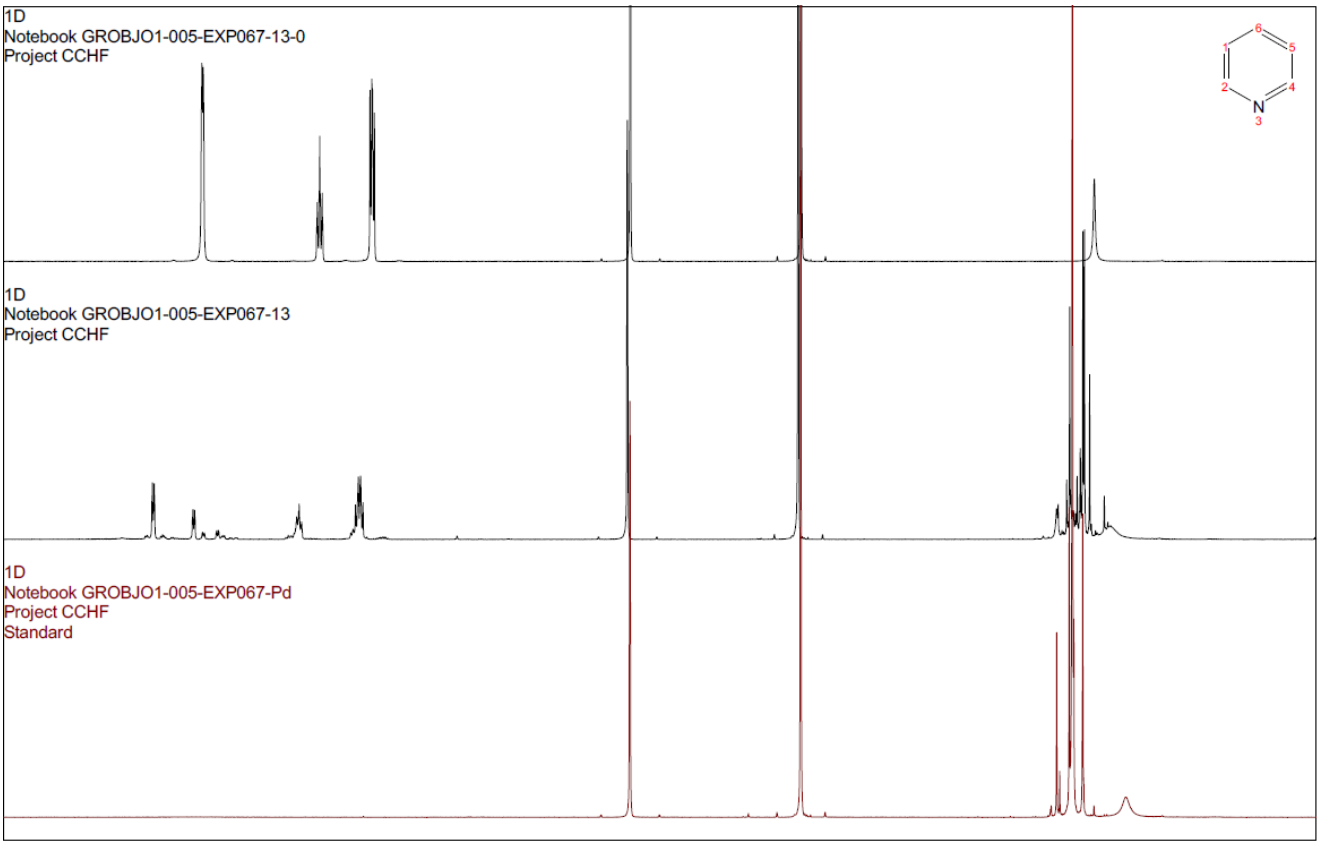
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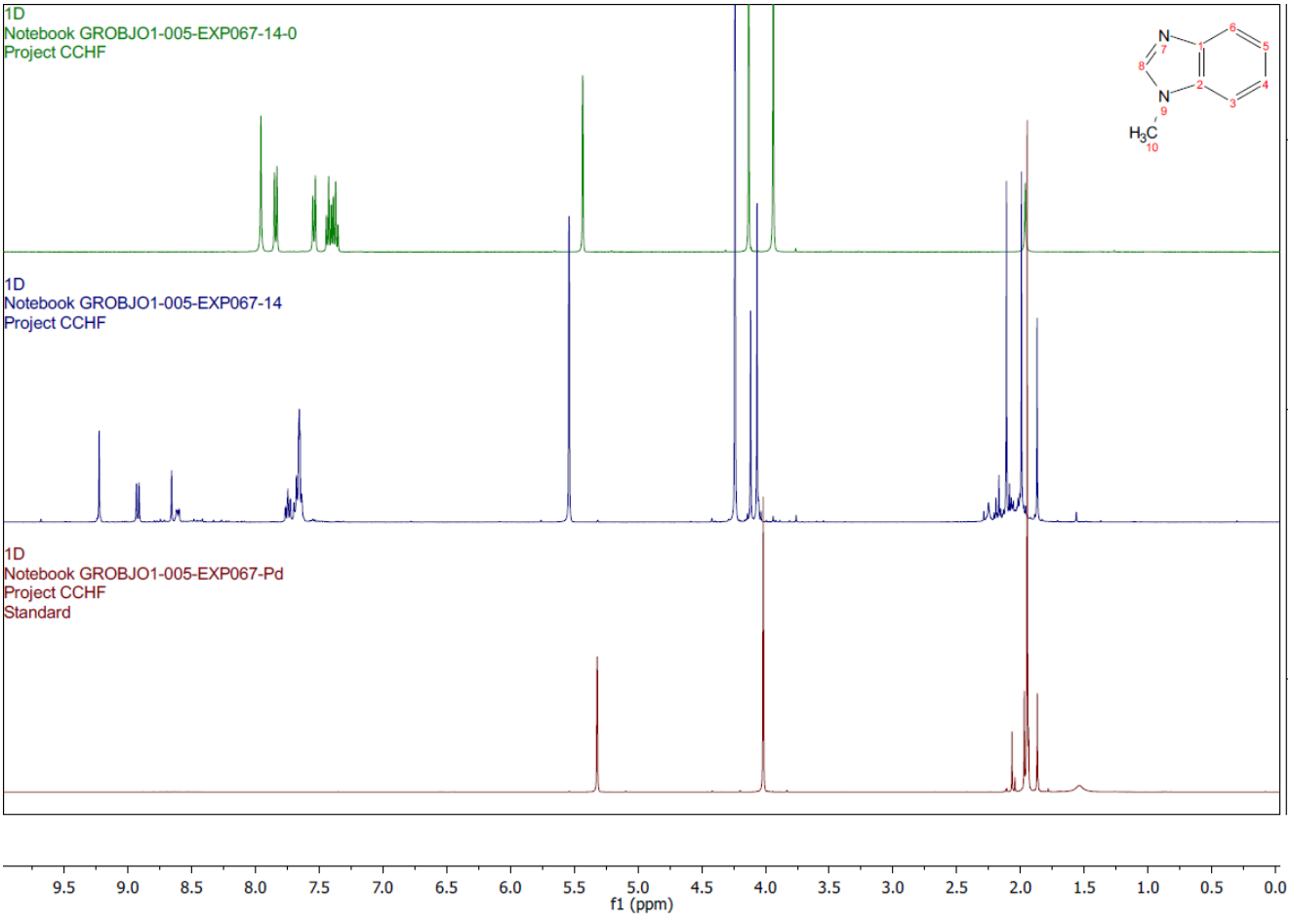
f1 (ppm)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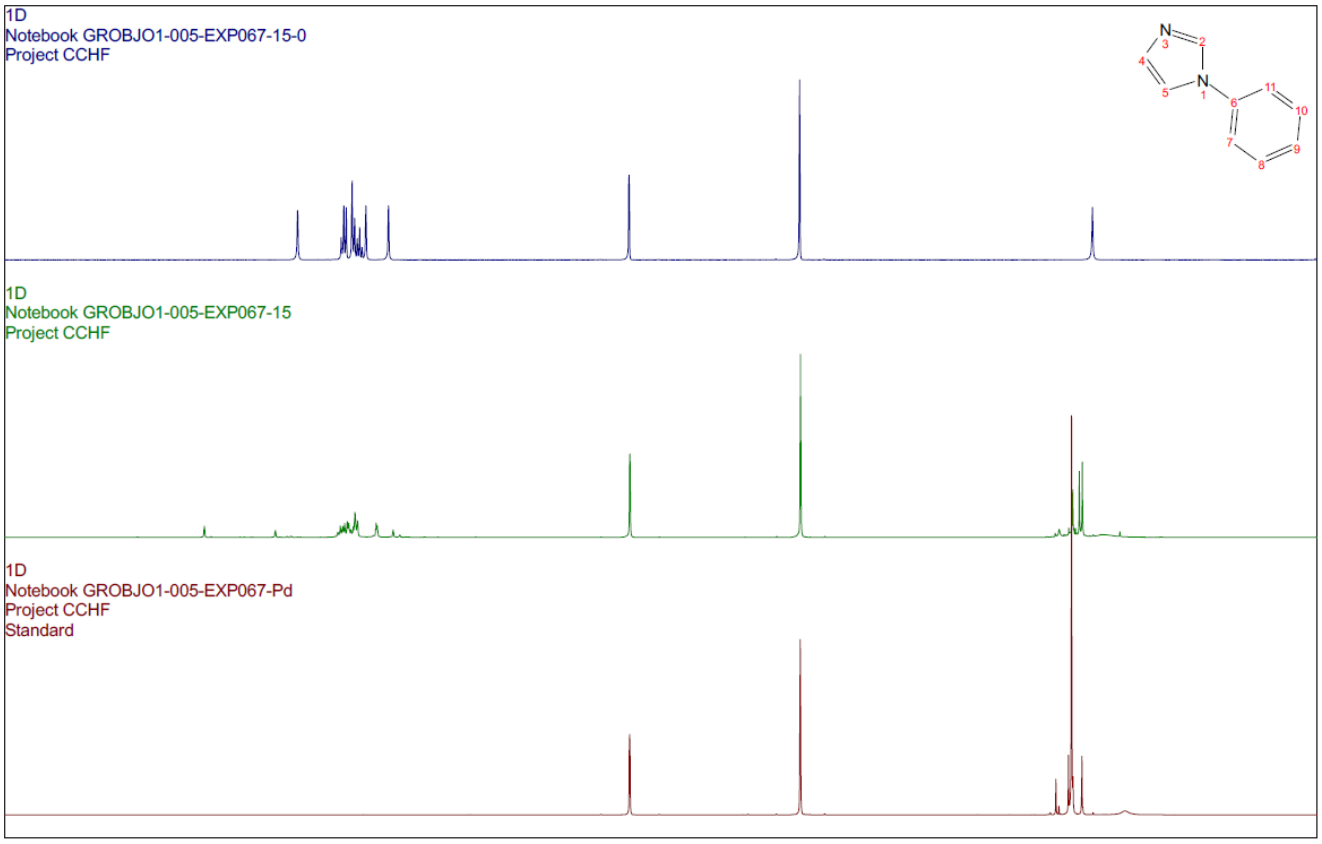
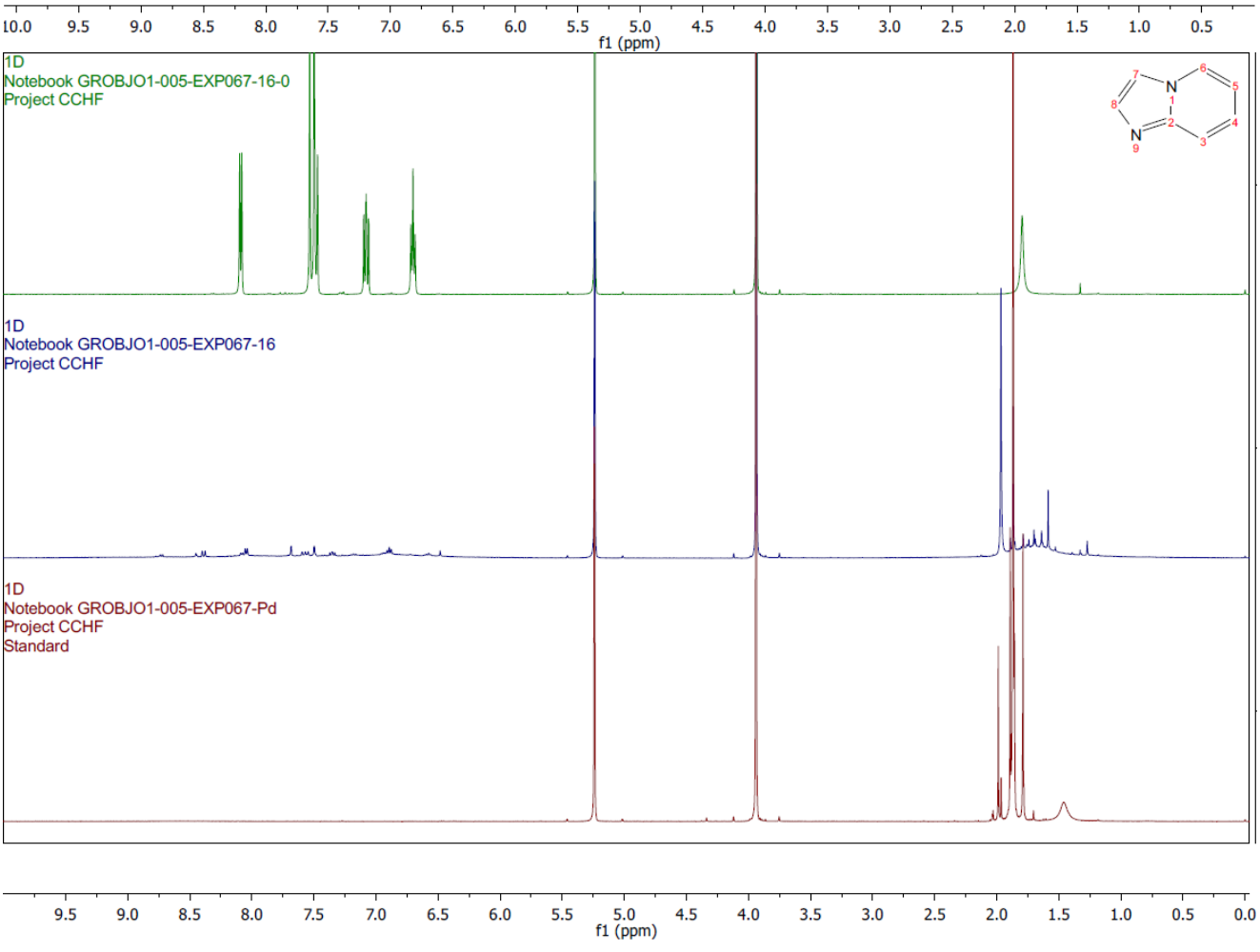
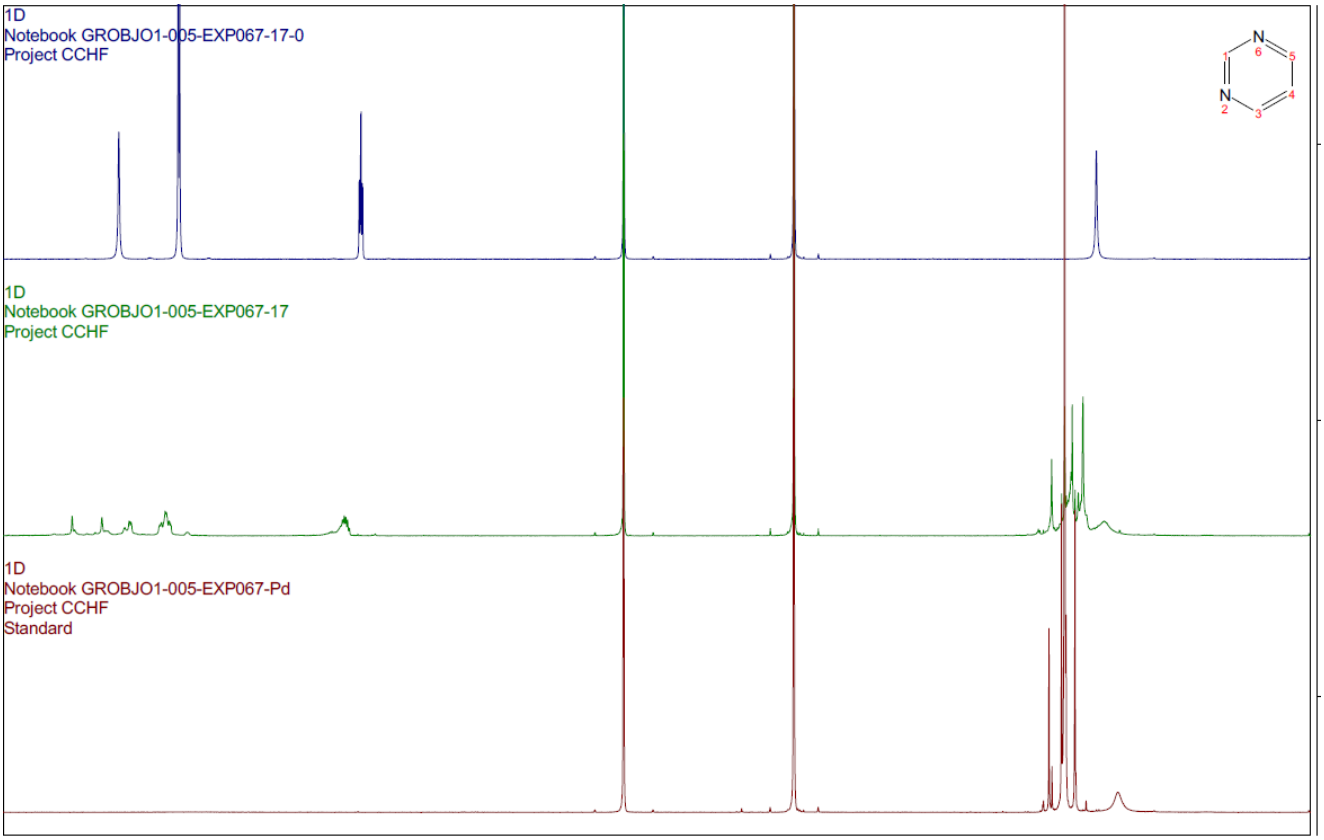
Project CCHF
1D
Notebook GROBJO1-005-EXP067-Pd
Project CCHF
Standard
f1 (ppm)


1D
Notebook GROBJO1-005-EXP067-15-0
Project CCHF
1D
Notebook GROBJO1-005-EXP067-15
Project CCHF
1D
Notebook GROBJO1-005-EXP067-Pd
Project CCHF
Standard


10.0 9.5 9.0 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
f1 (ppm)
1D
Notebook GROBJO1-005-EXP067-16-0
Project CCHF
1D
Notebook GROBJO1-005-EXP067-16
Project CCHF
1D
Notebook GROBJO1-005-EXP067-Pd
Project CCHF
Standard
9.5 9.0 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 0.0
f1 (ppm)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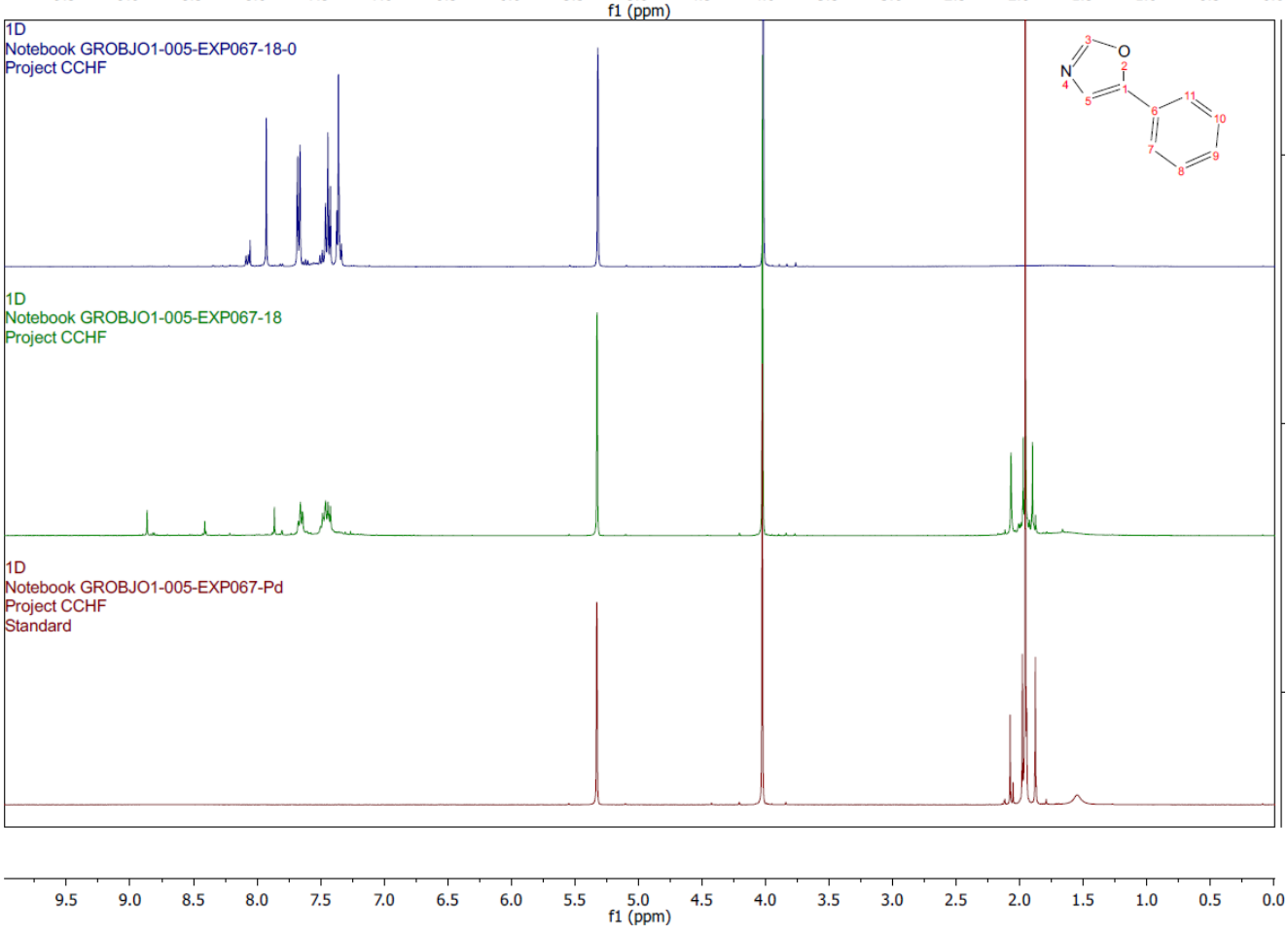
Project CCHF
1D
Notebook GROBJO1-005-EXP067-17
Project CCHF
1D
Notebook GROBJO1-005-EXP067-Pd
Project CCHF
Standard
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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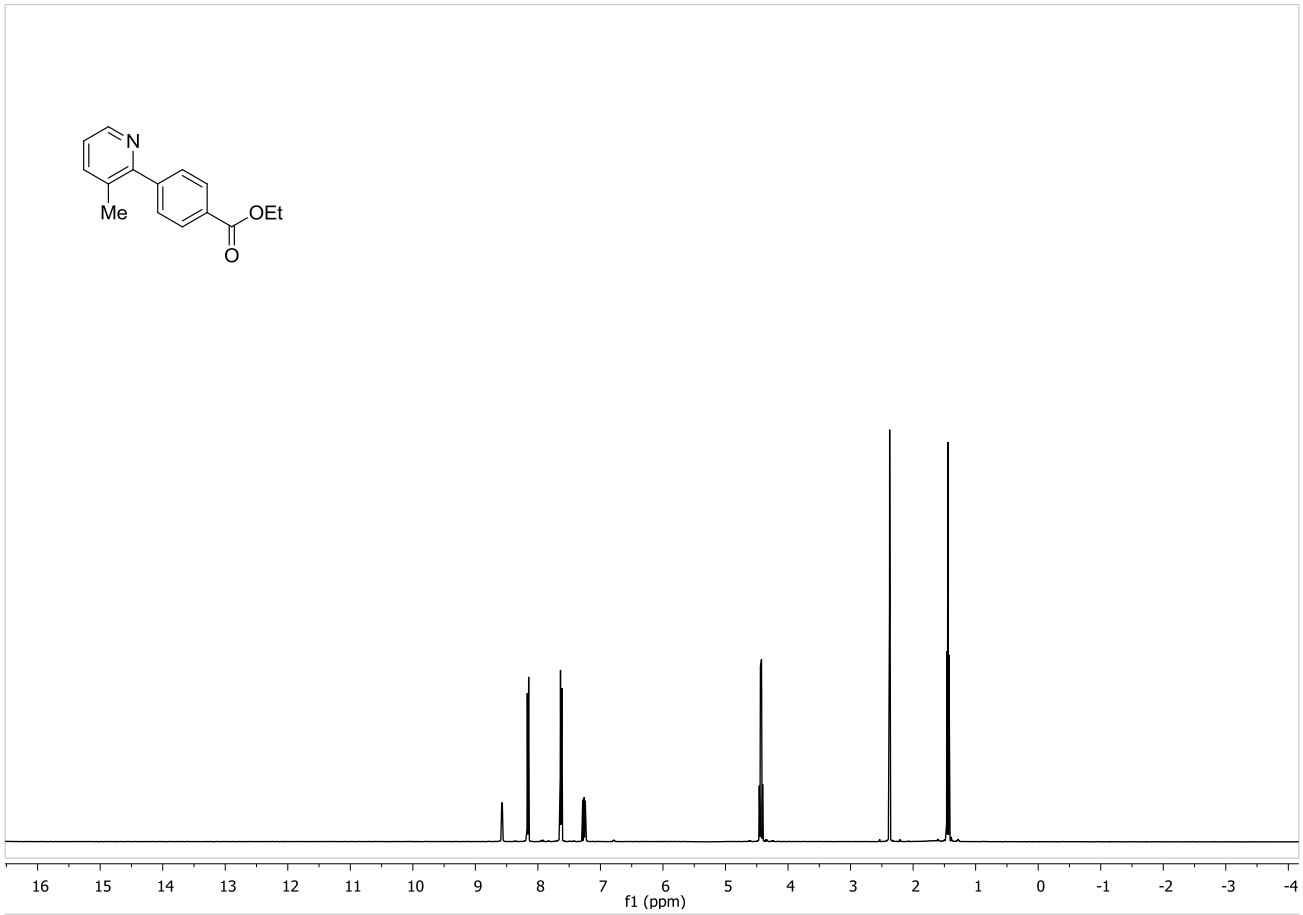
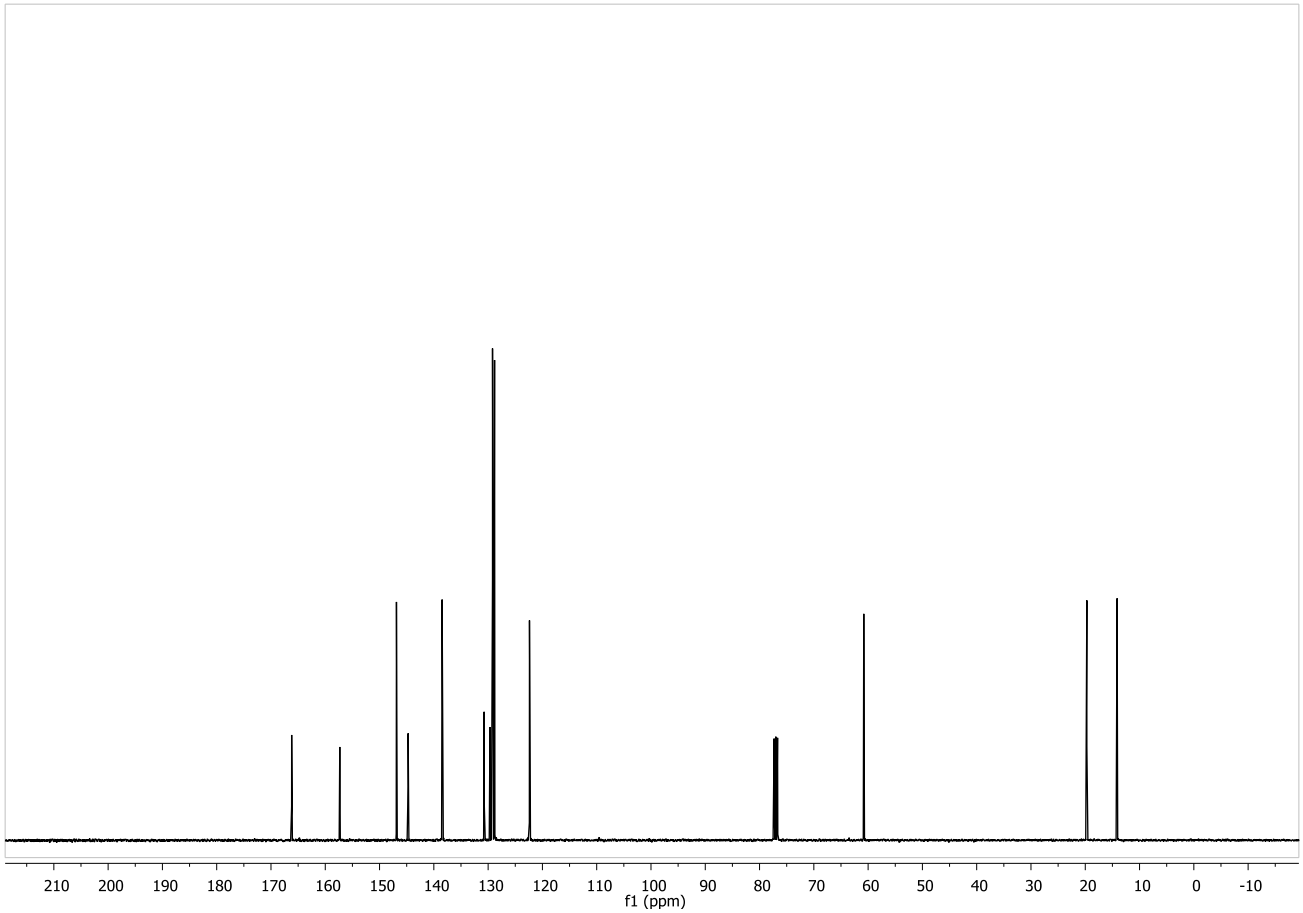
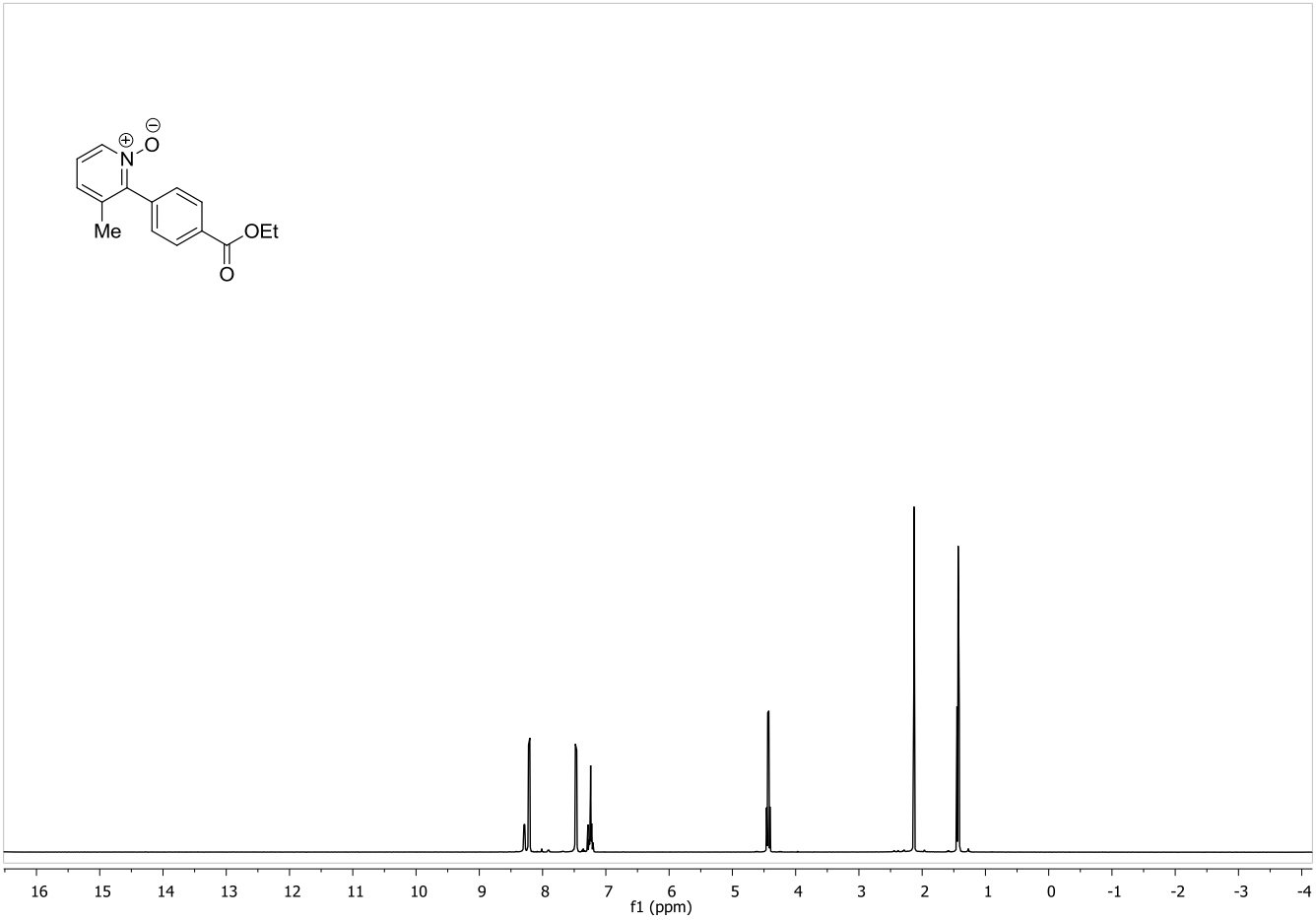
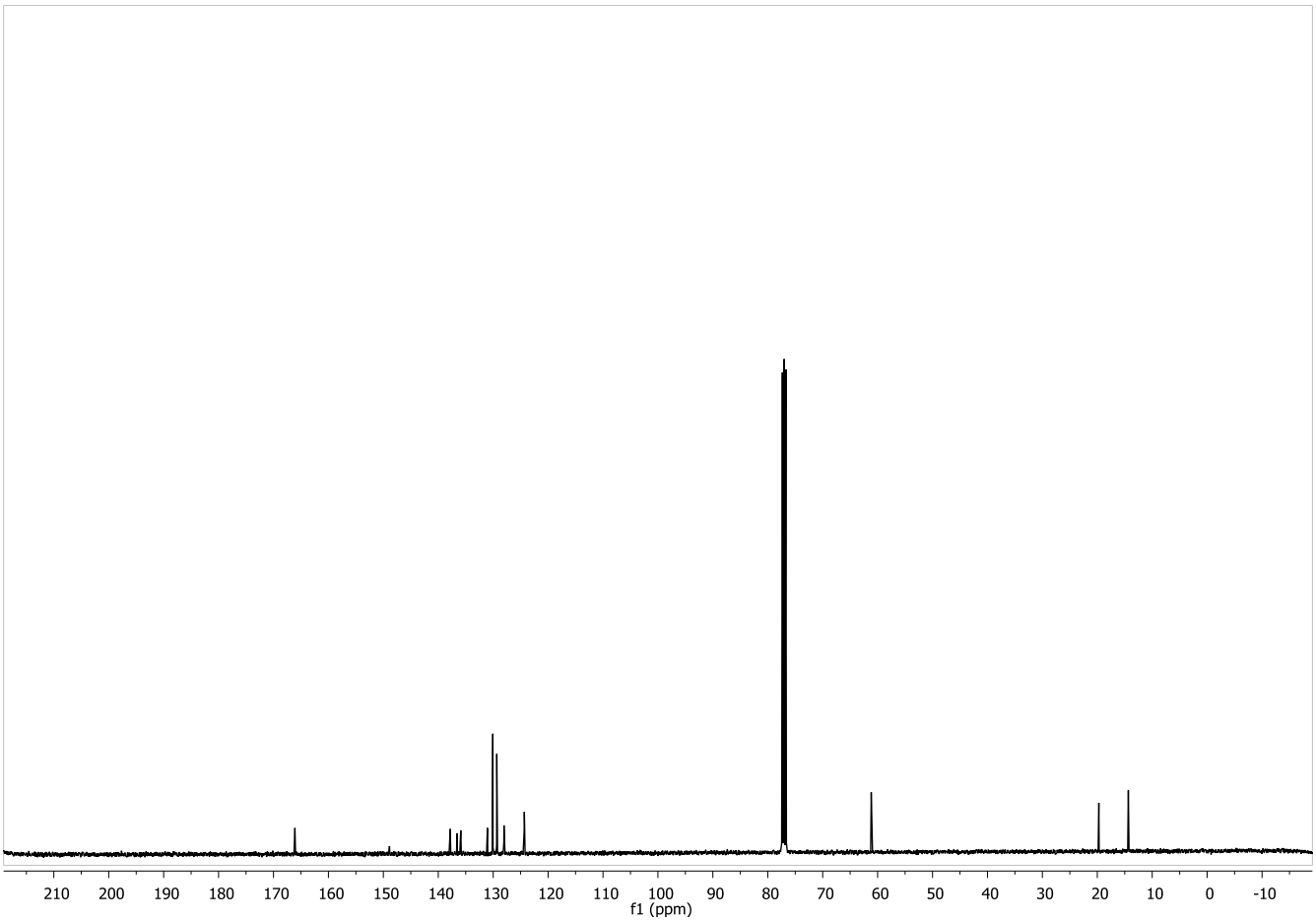
Project CCHF
1D
Notebook GROBJO1-005-EXP067-18
Project CCHF
1D
Notebook GROBJO1-005-EXP067-Pd
Project CCHF
Standard
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

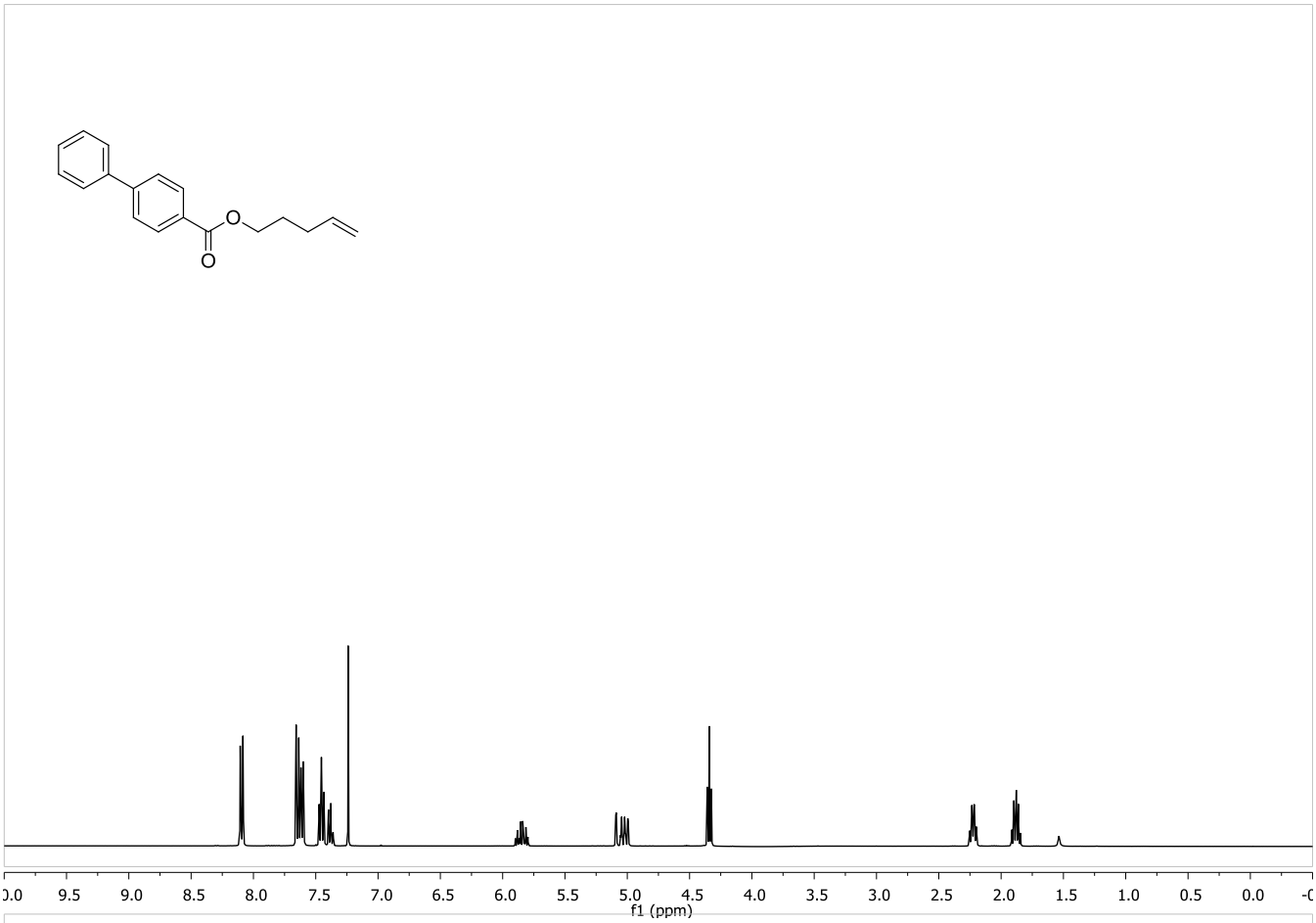
^{1}H & ^{13}C NMR Spectra

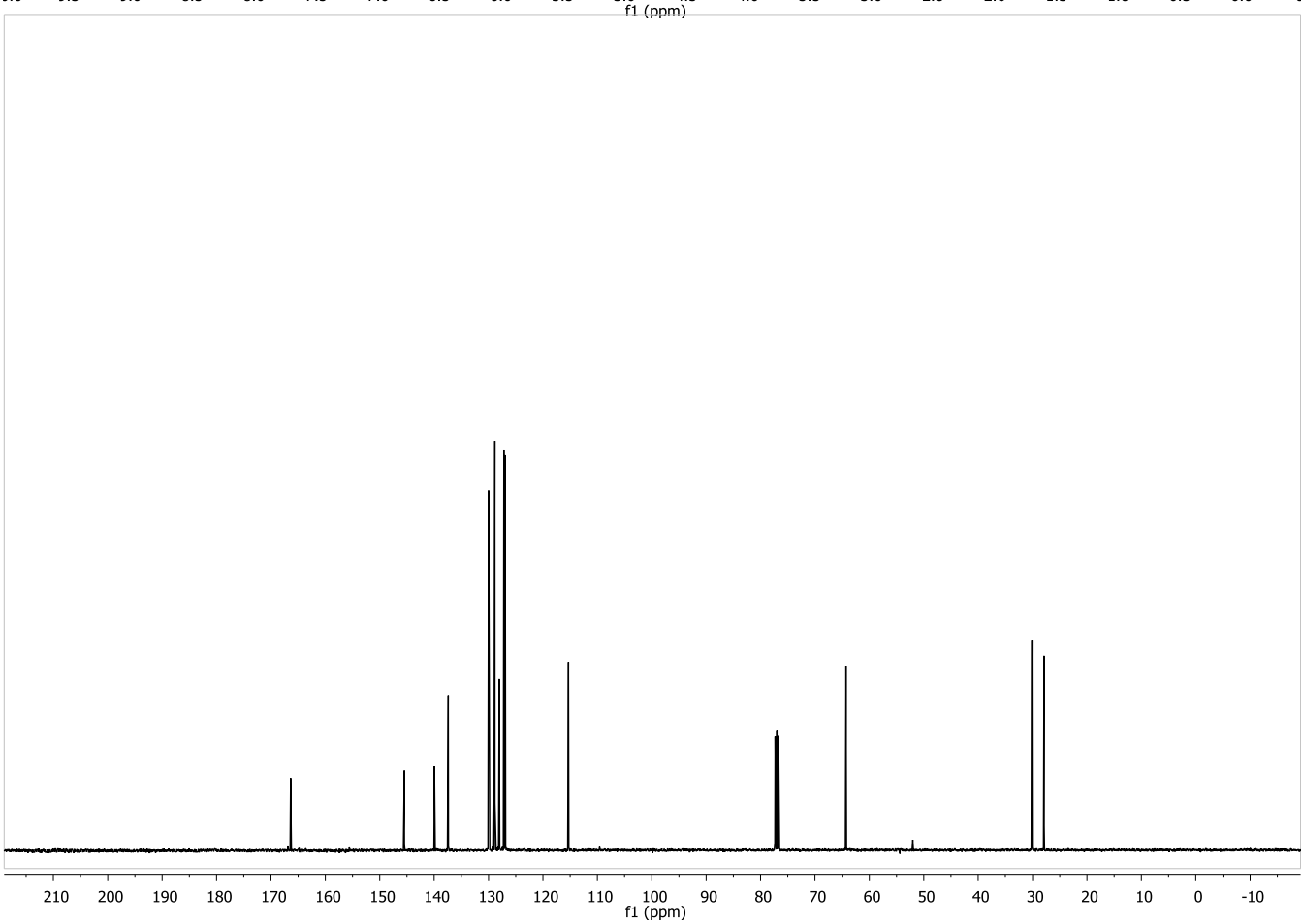


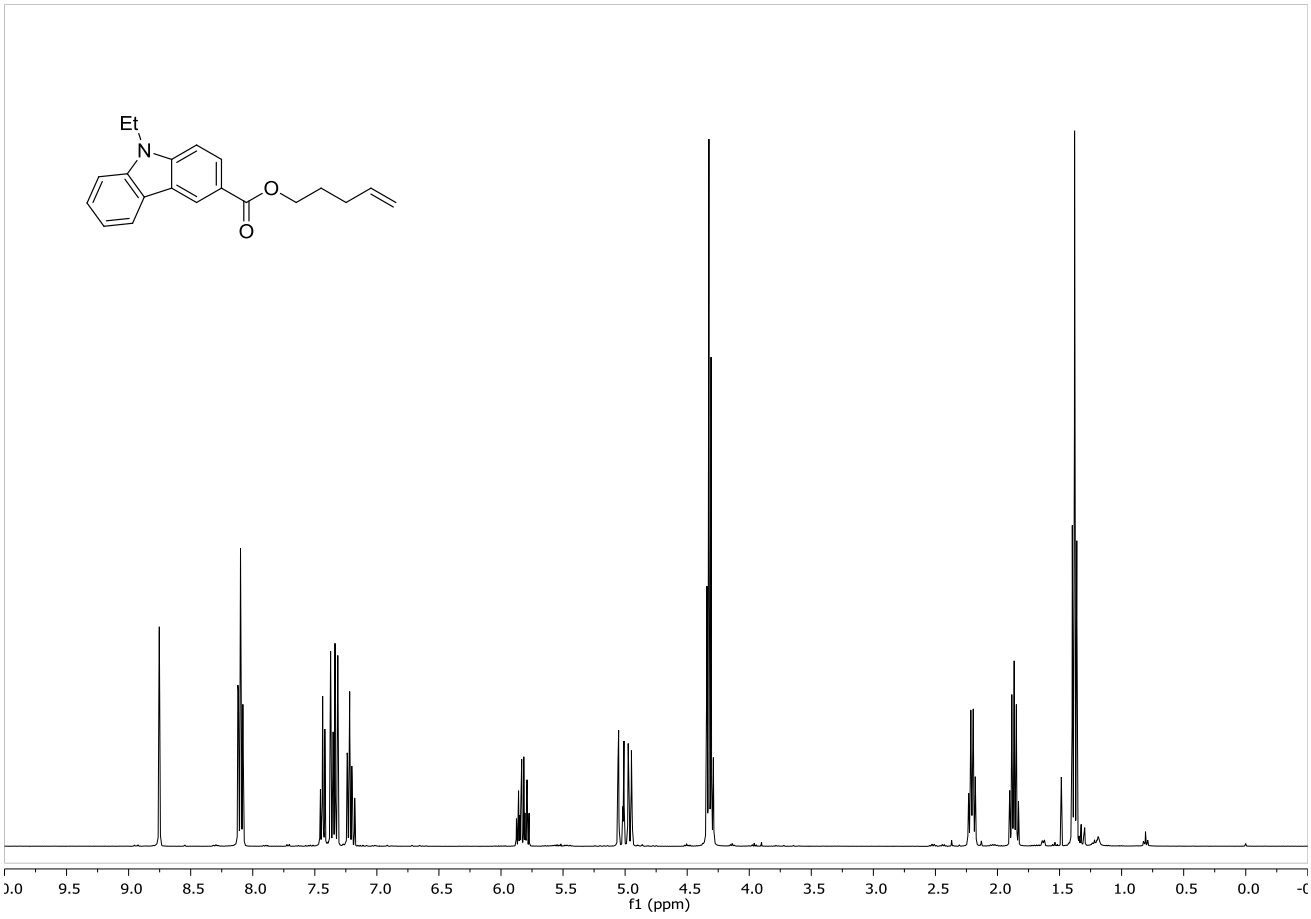


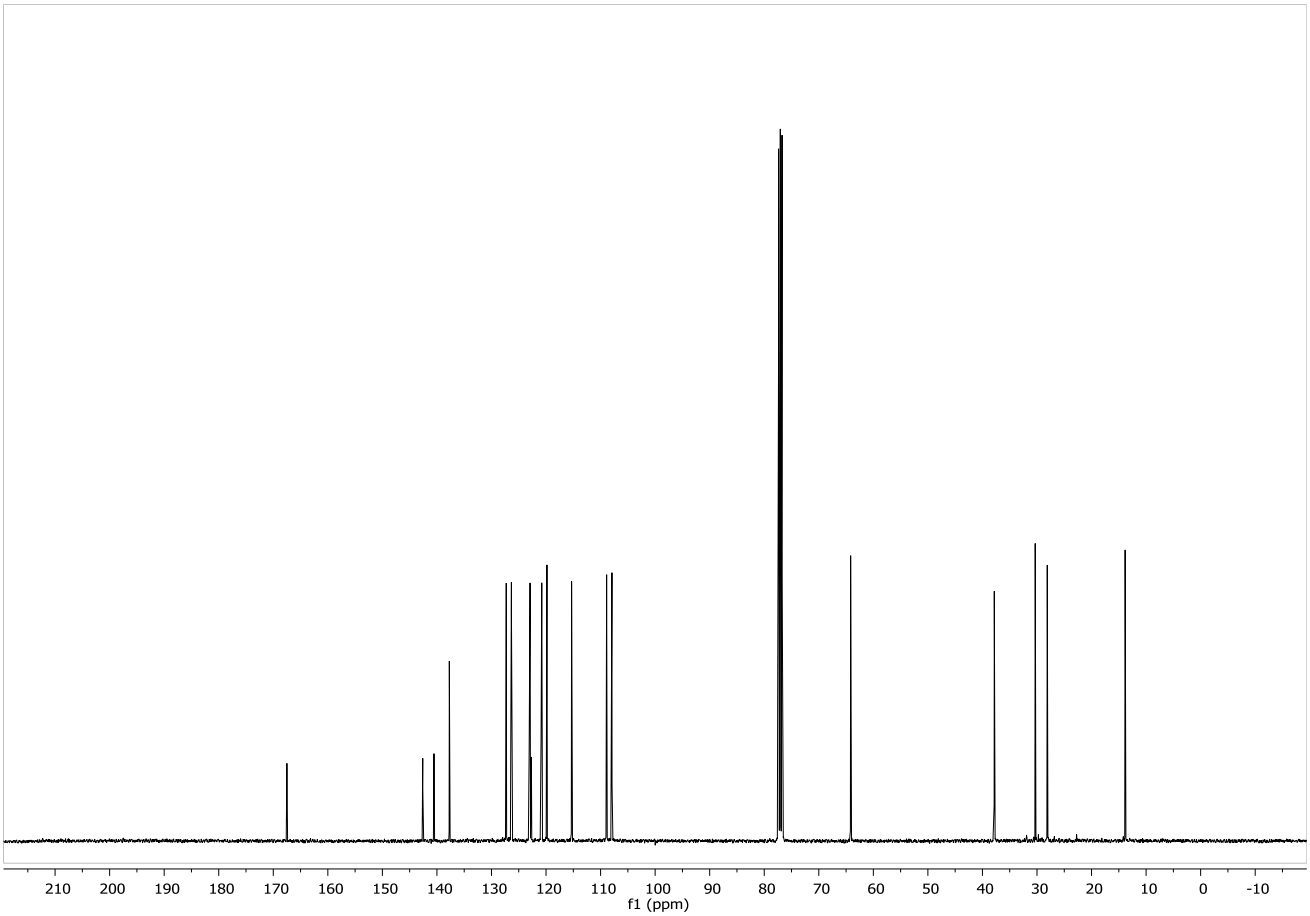

Me
OEt
O
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

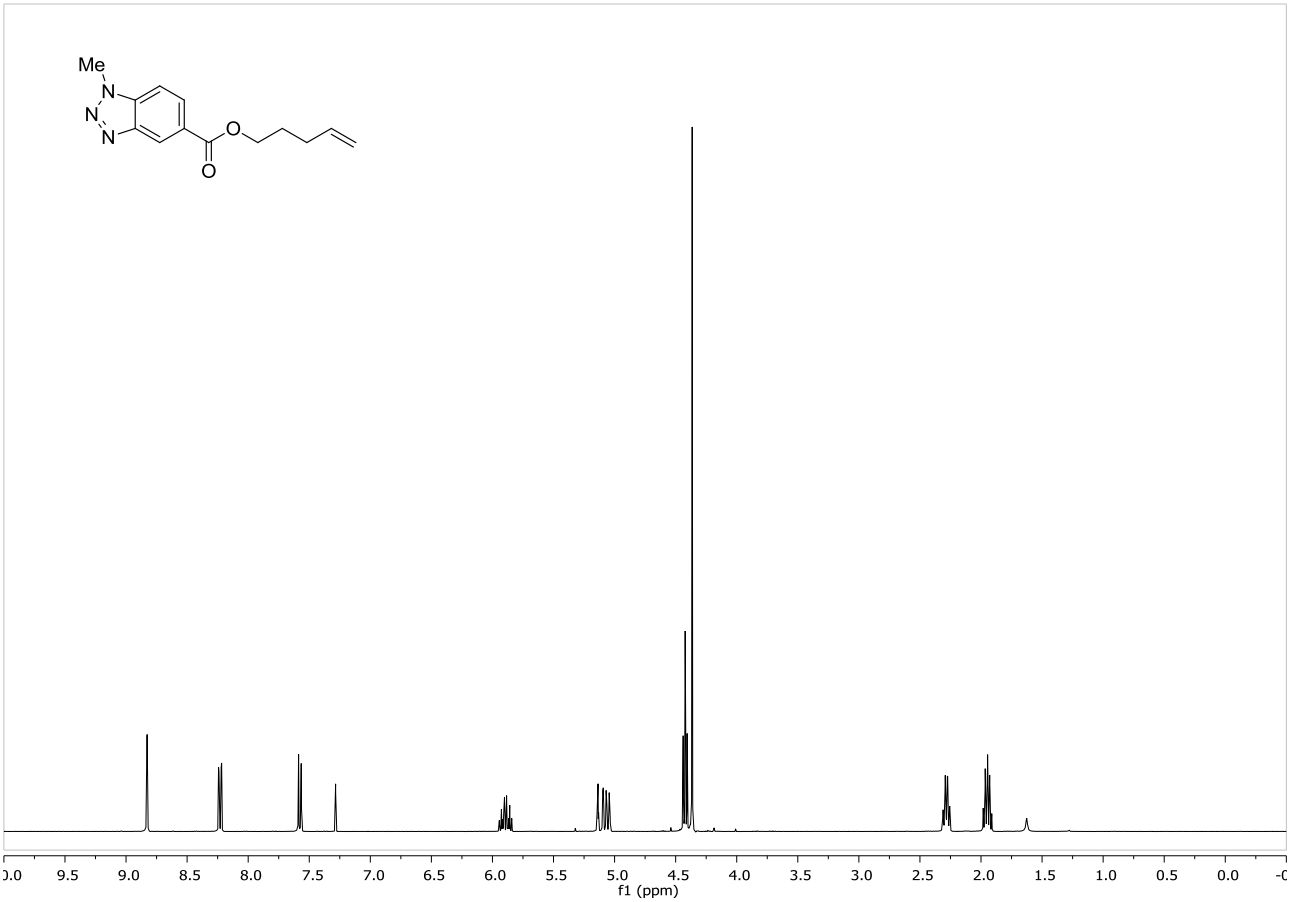

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

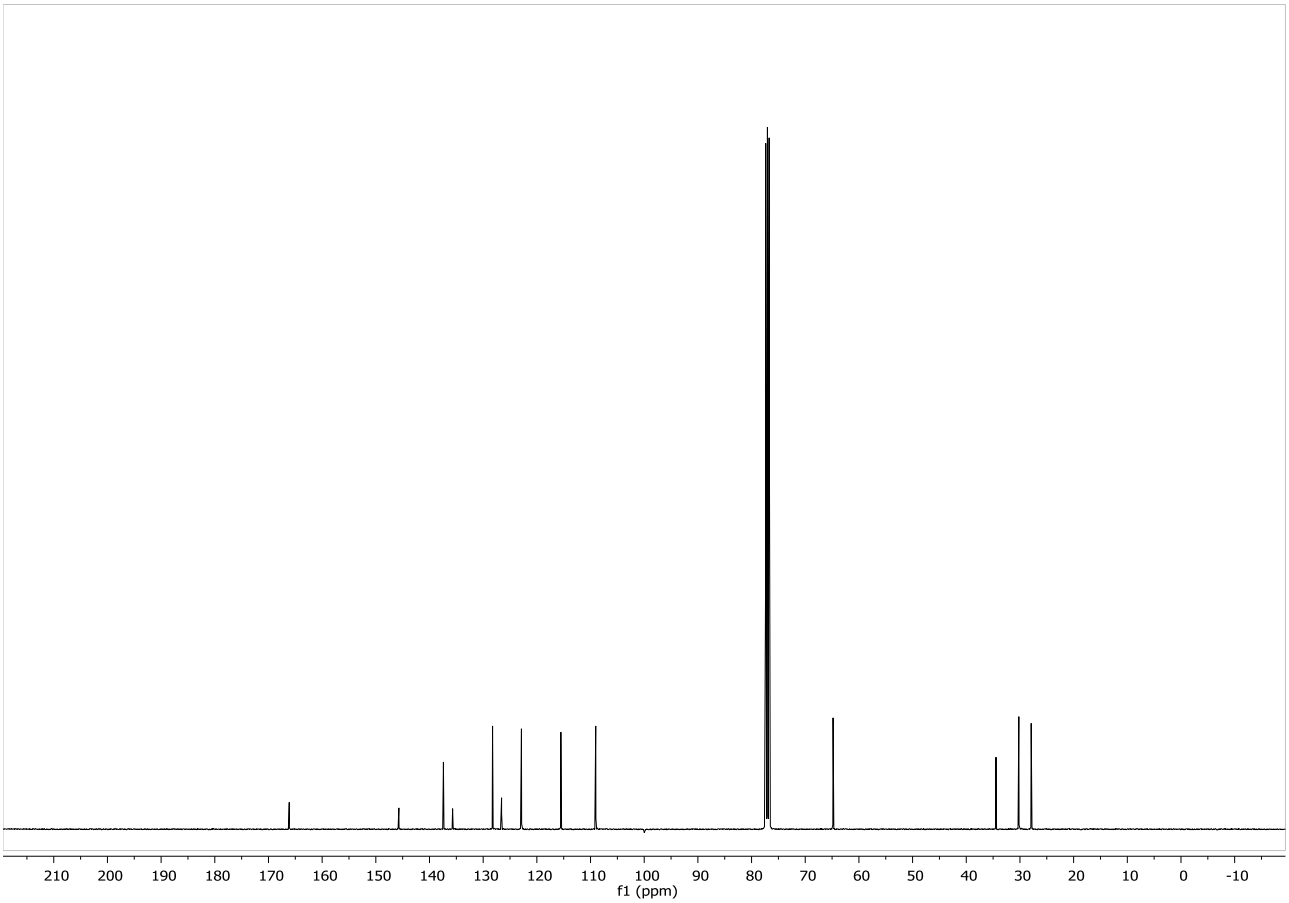

O
O
f1 (ppm)

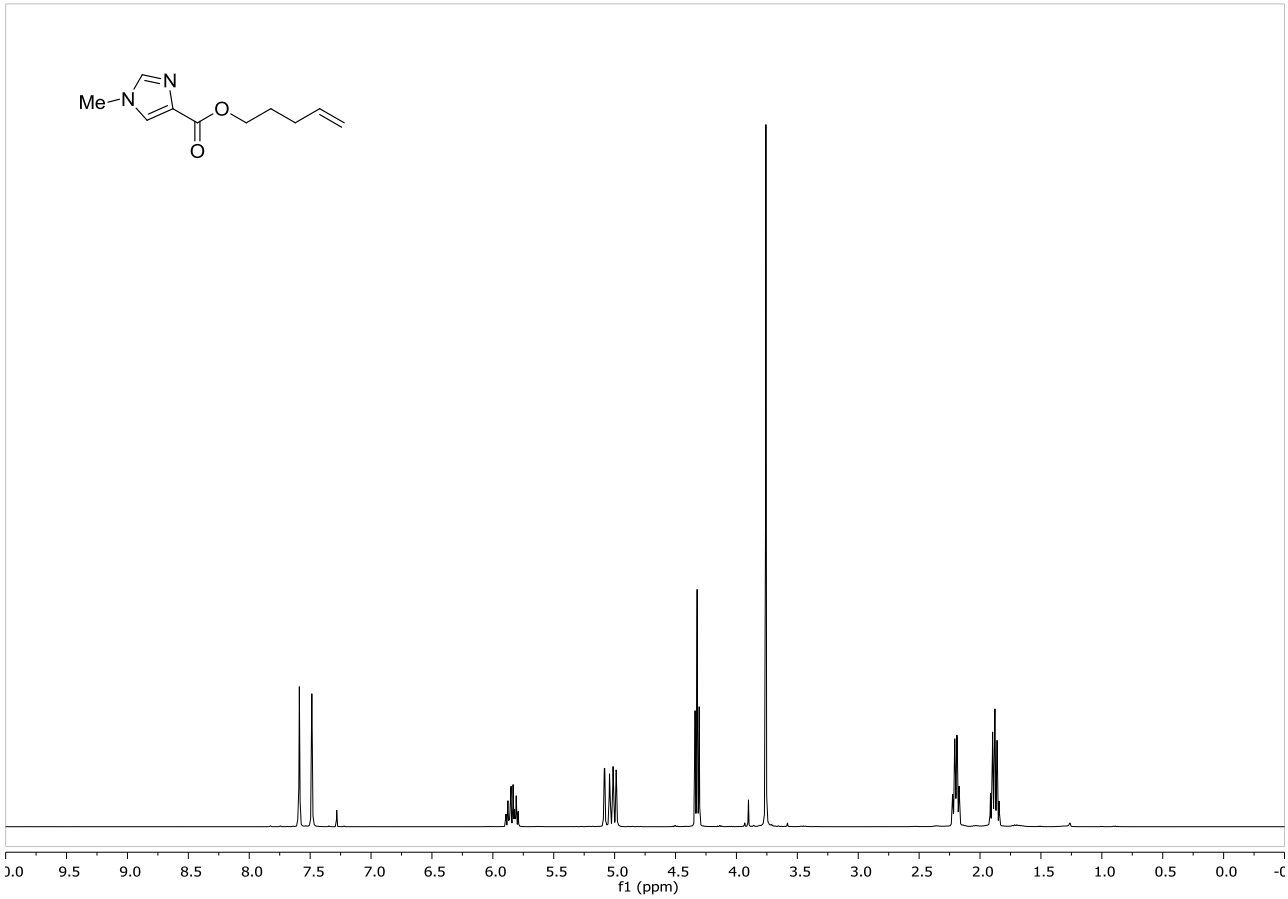

f1 (ppm)

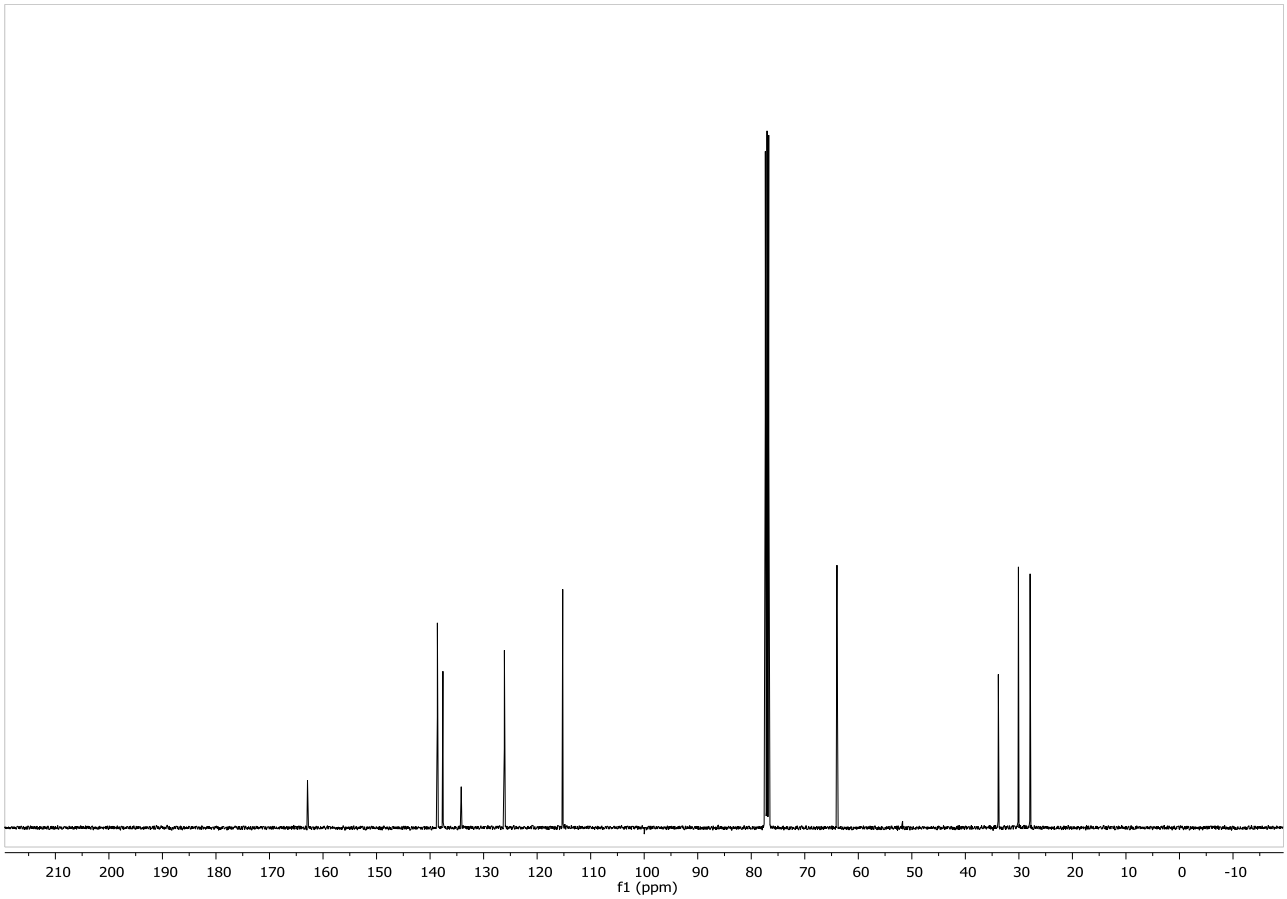

Et
N
O
O
f1 (ppm)

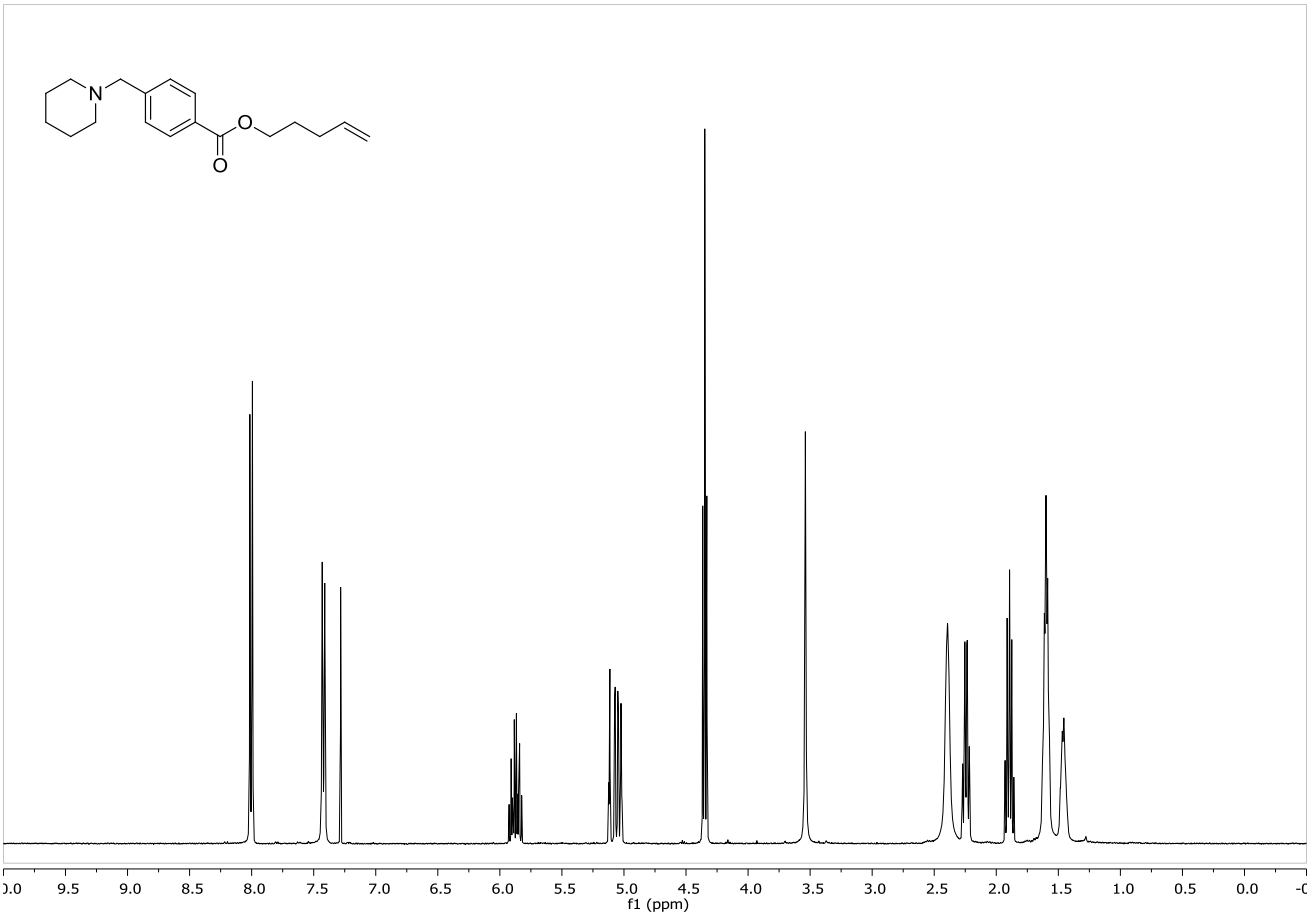

f1 (ppm)

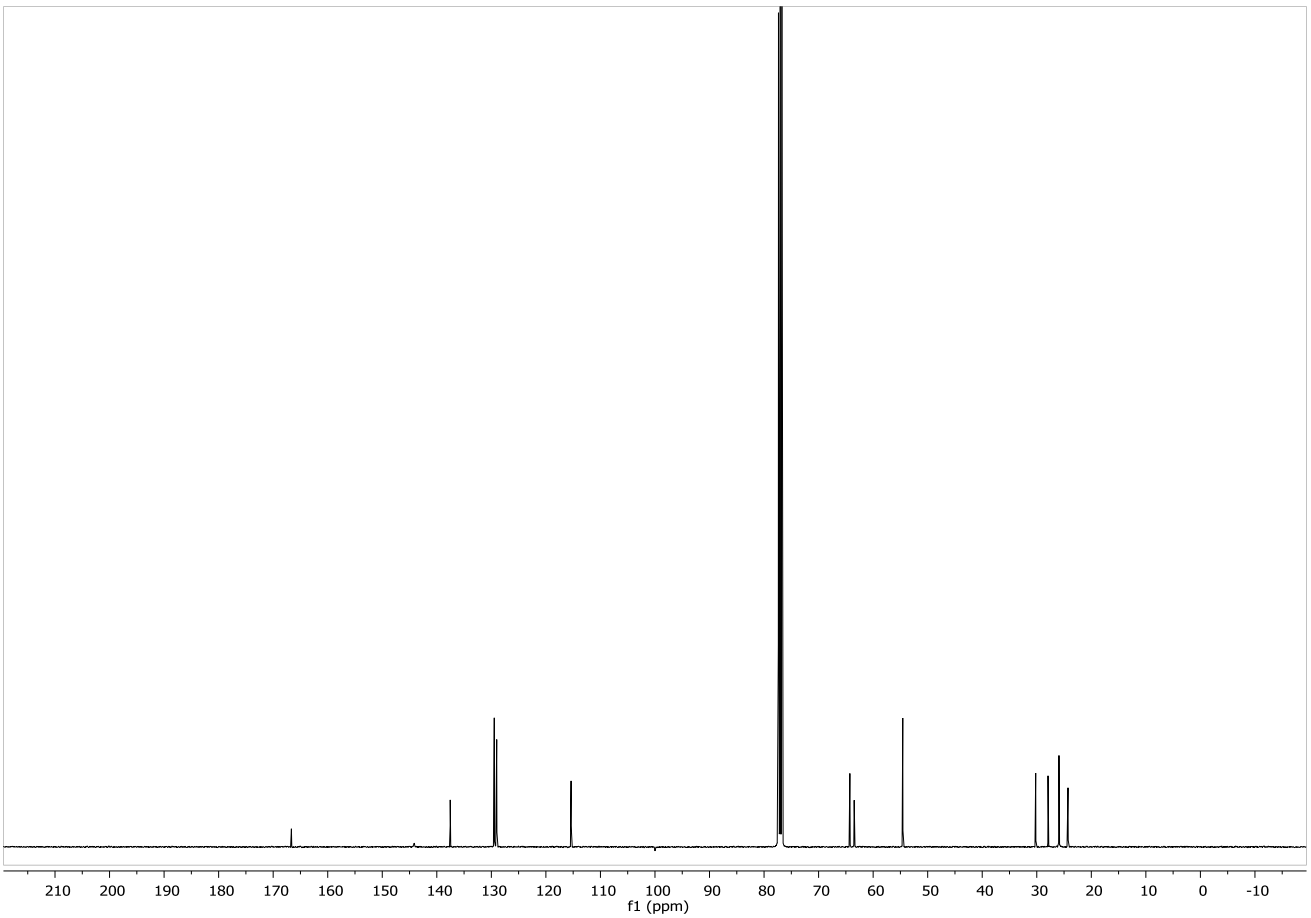

Me
N
N
N
O
O
f1 (ppm)


f1 (ppm)


Me
N
N
O
O
f1 (ppm)


f1 (ppm)


N
O
O
9.5
9.0
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
0.0
f1 (ppm)


210
200
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180
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120
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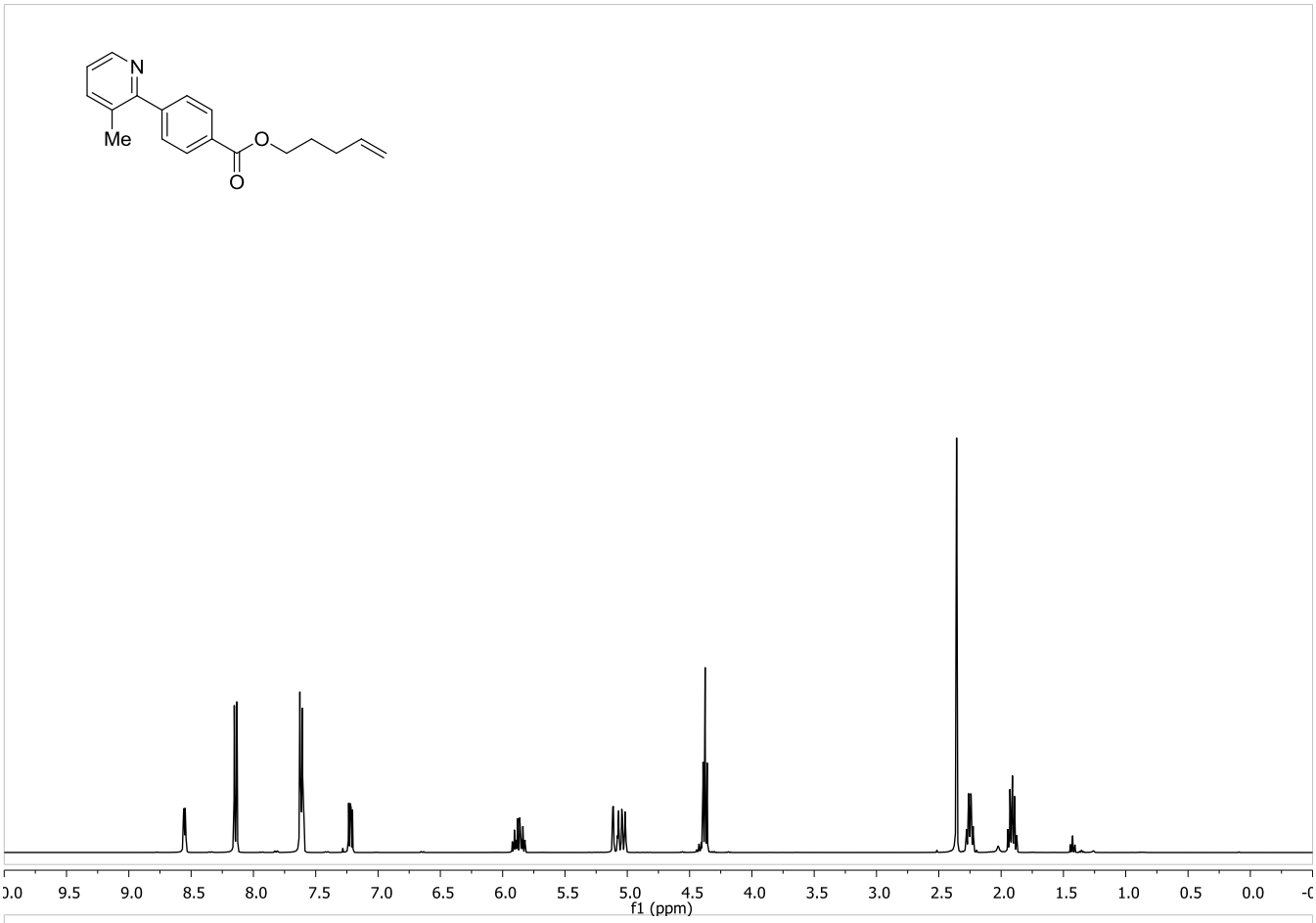
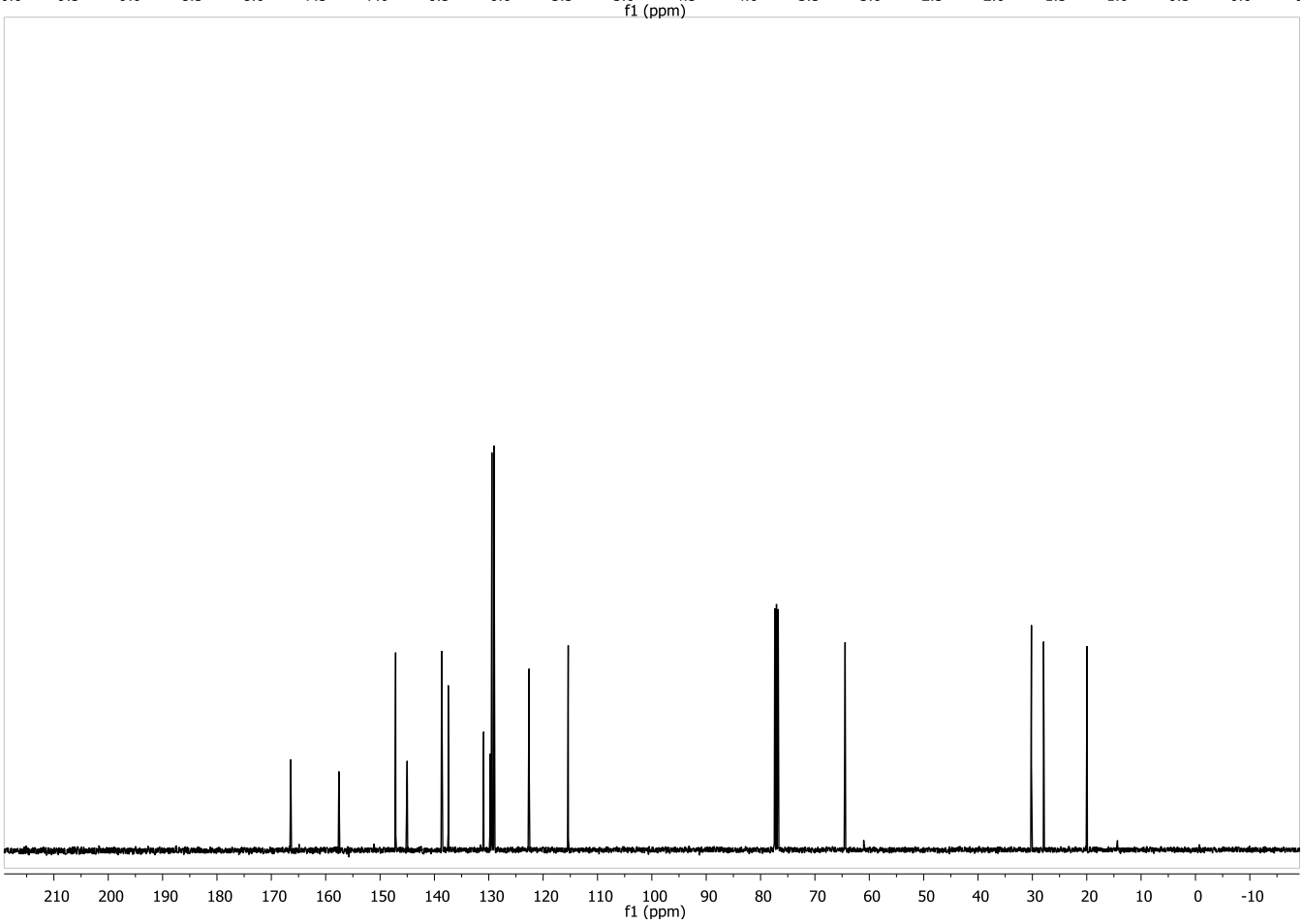
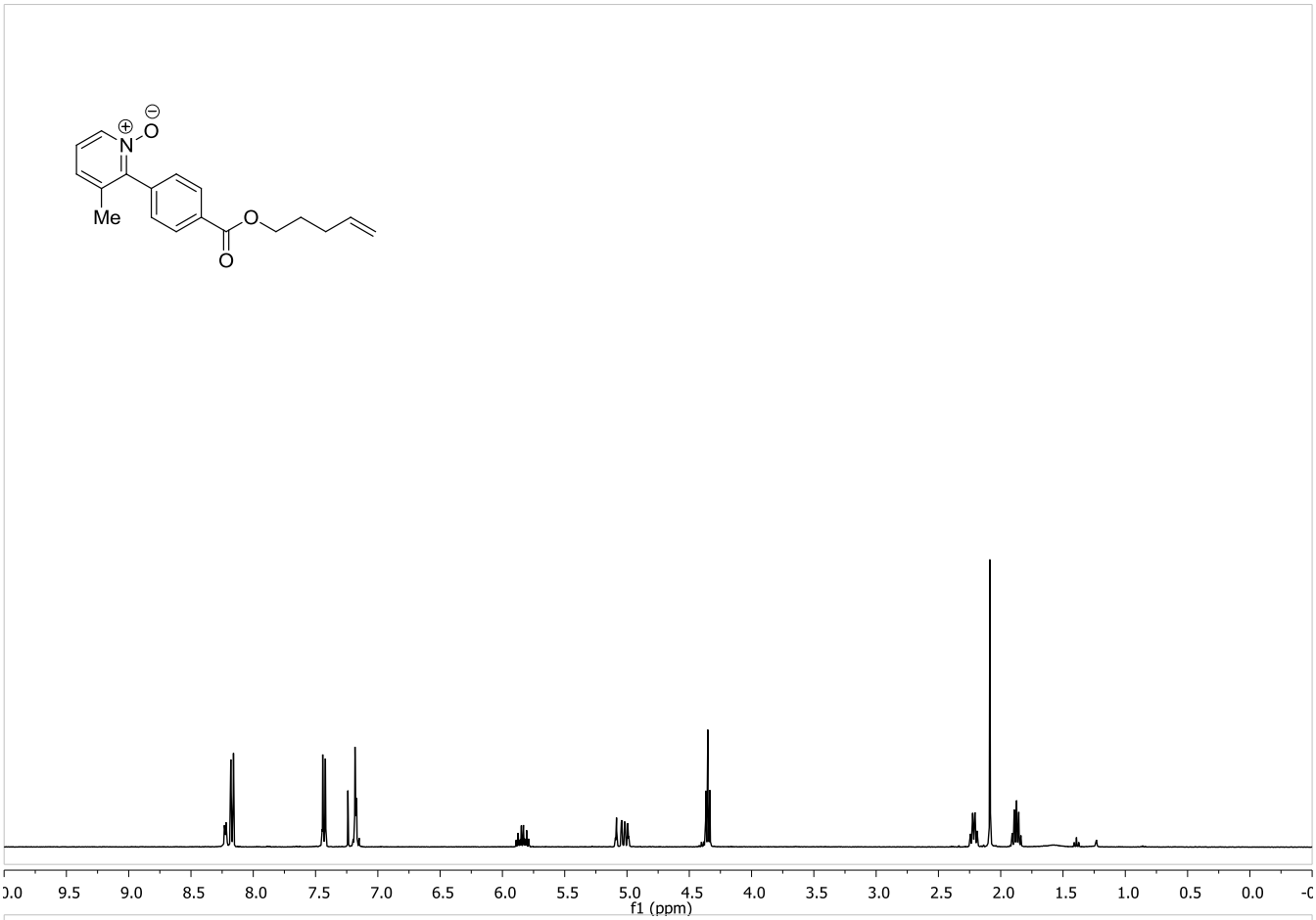
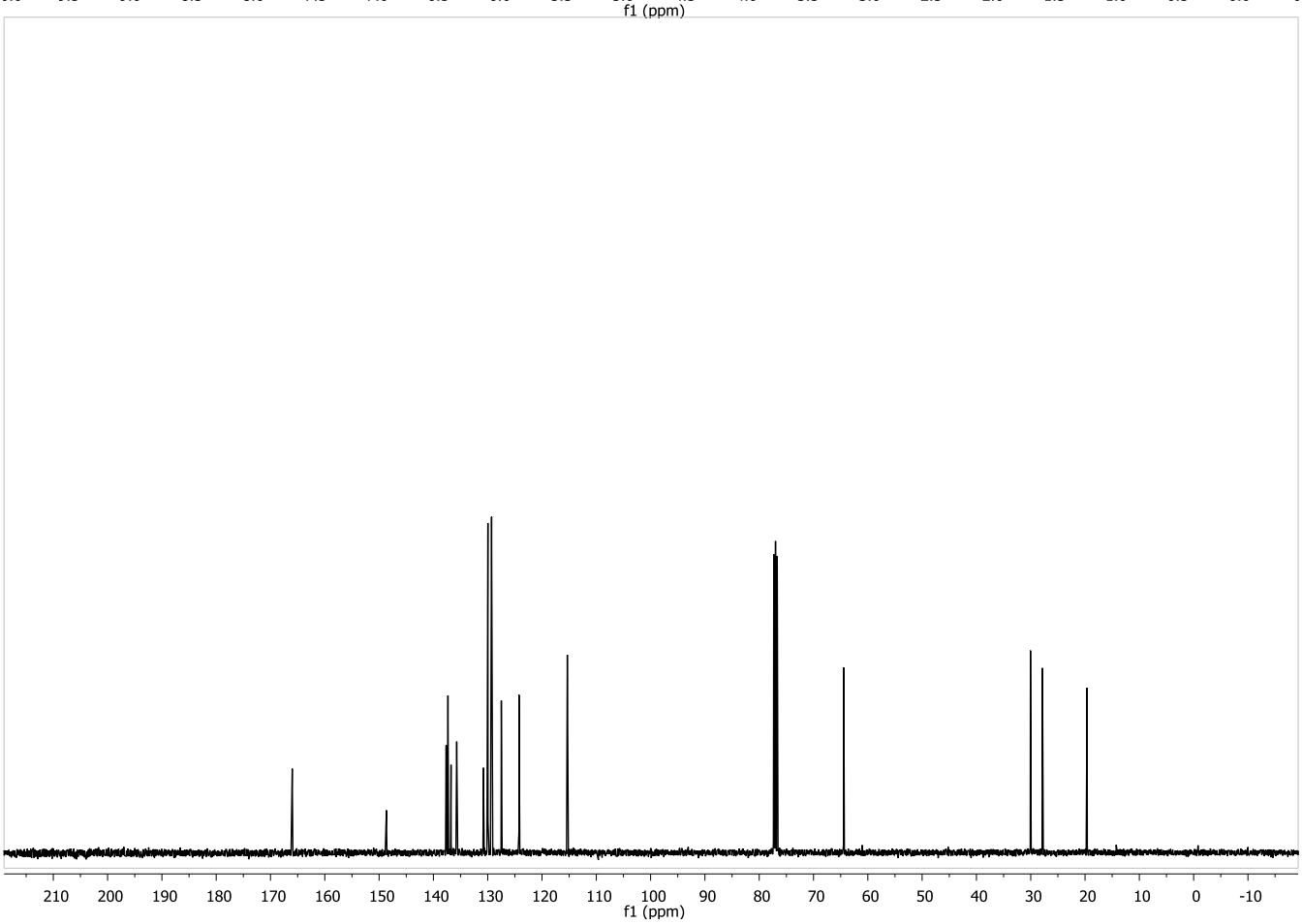
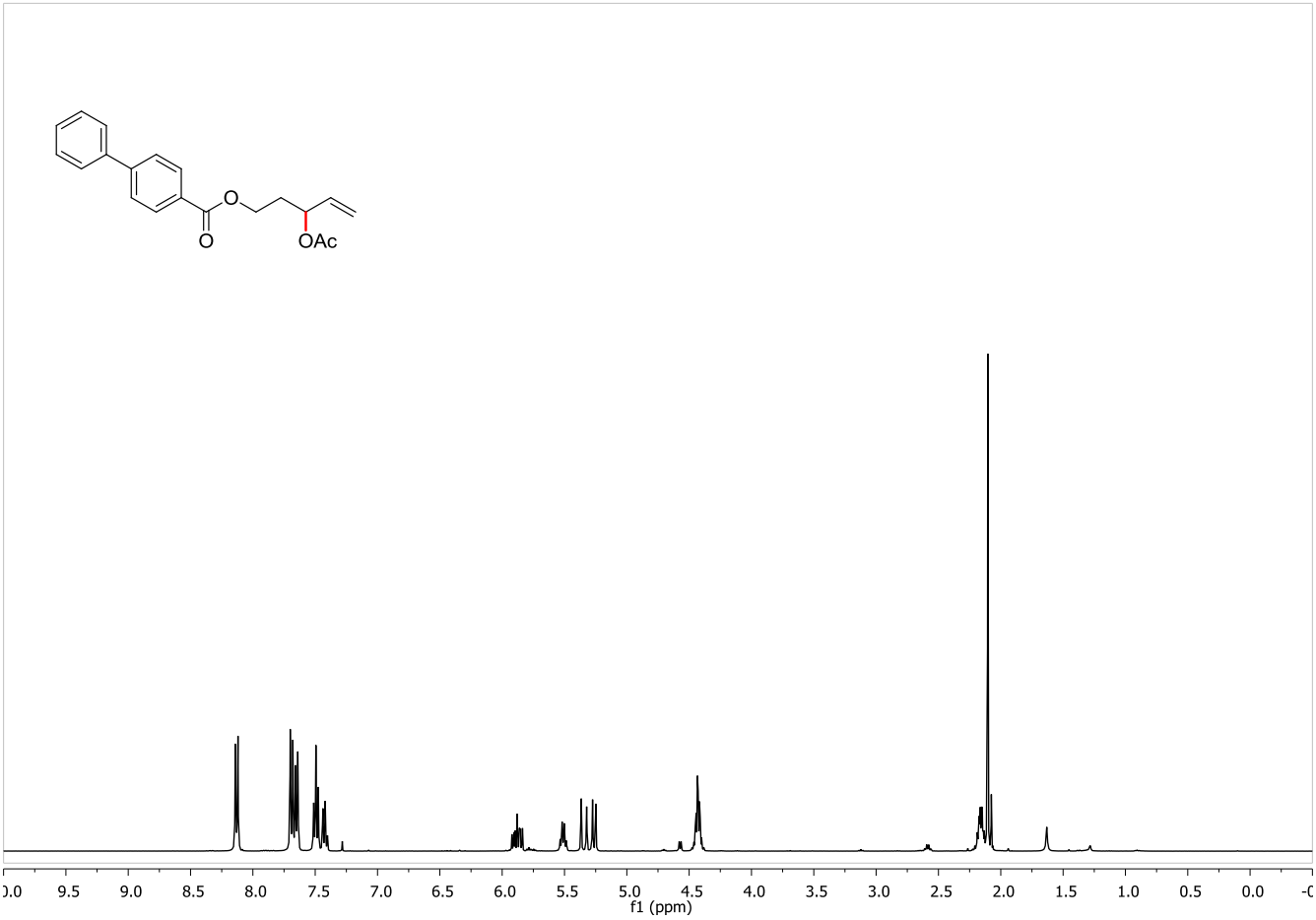
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

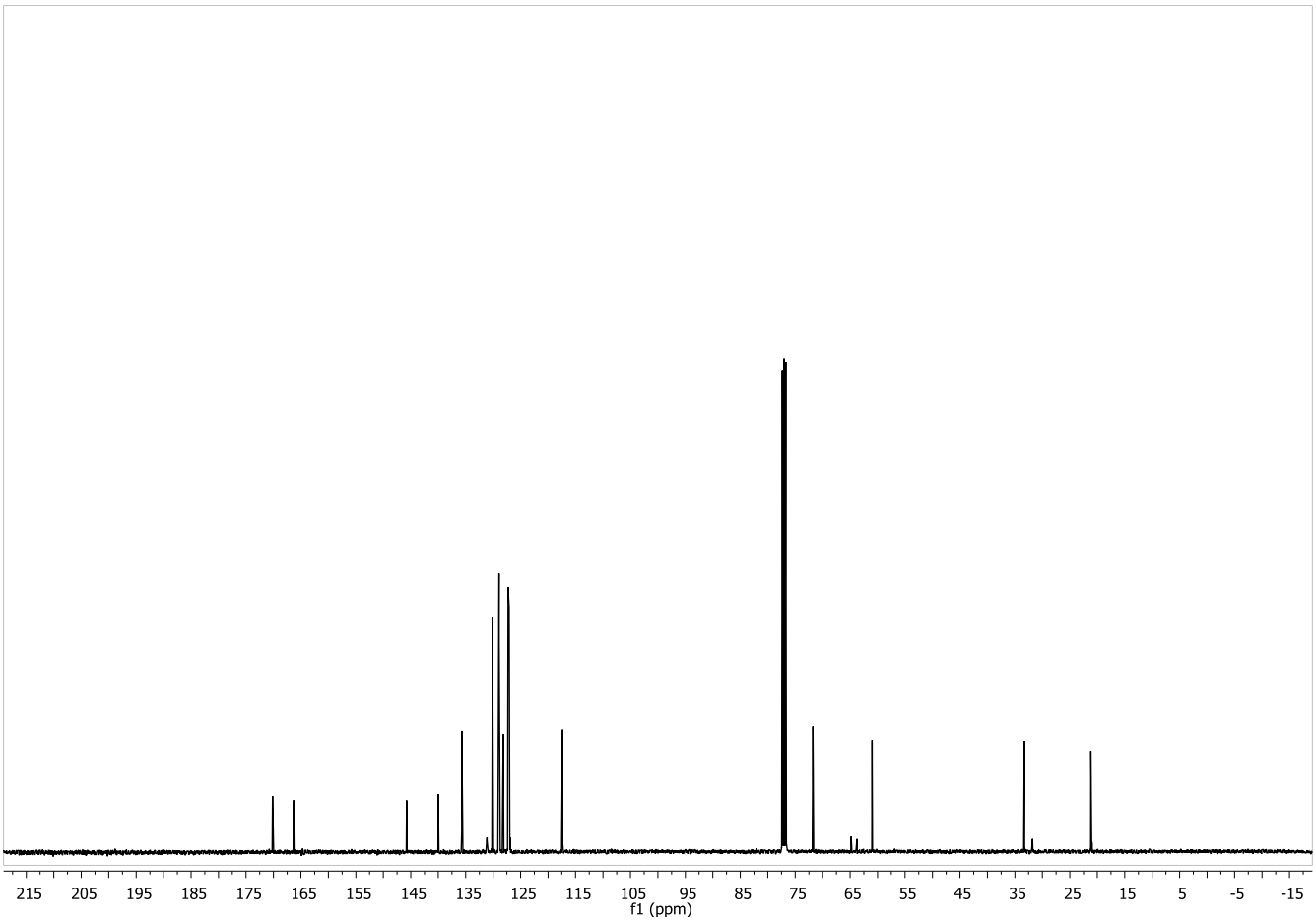

N
Me
O
O
f1 (ppm)


f1 (ppm)


Me
O
O
O
f1 (ppm)


f1 (ppm)


O
O
OAc
9.5
9.0
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
0.0
f1 (ppm)


215
205
195
185
175
165
155
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135
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105
95
85
75
65
55
45
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25
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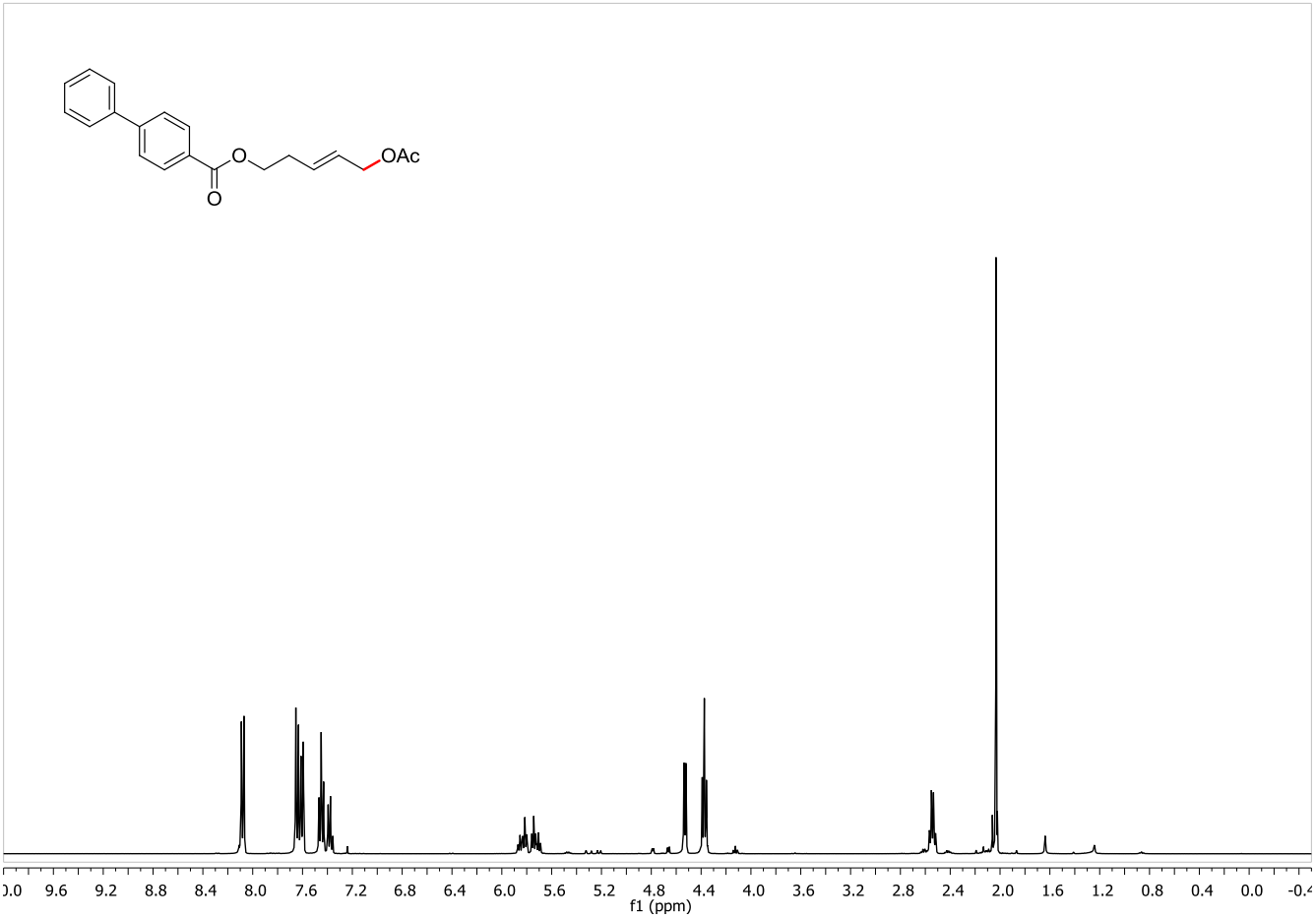
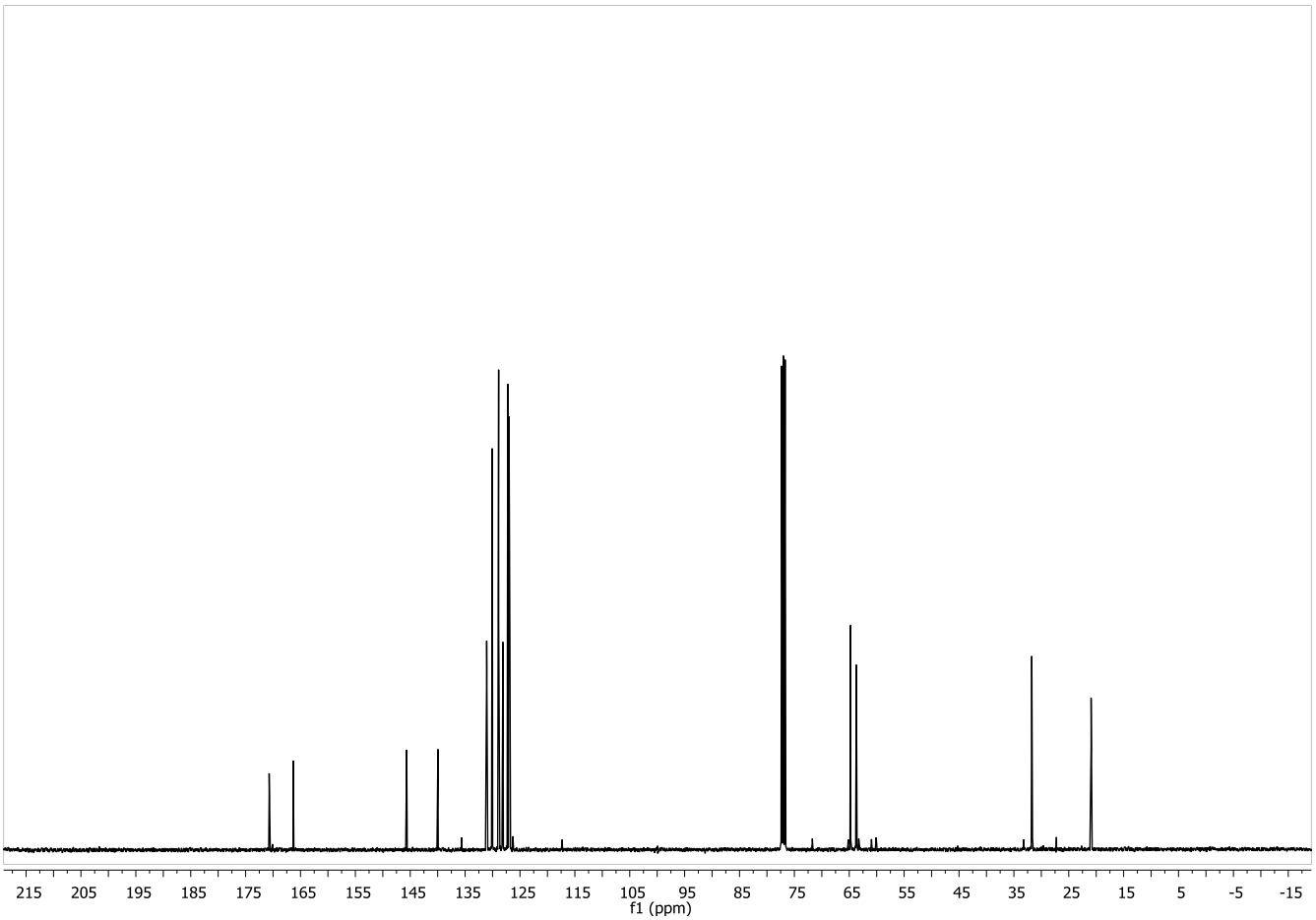
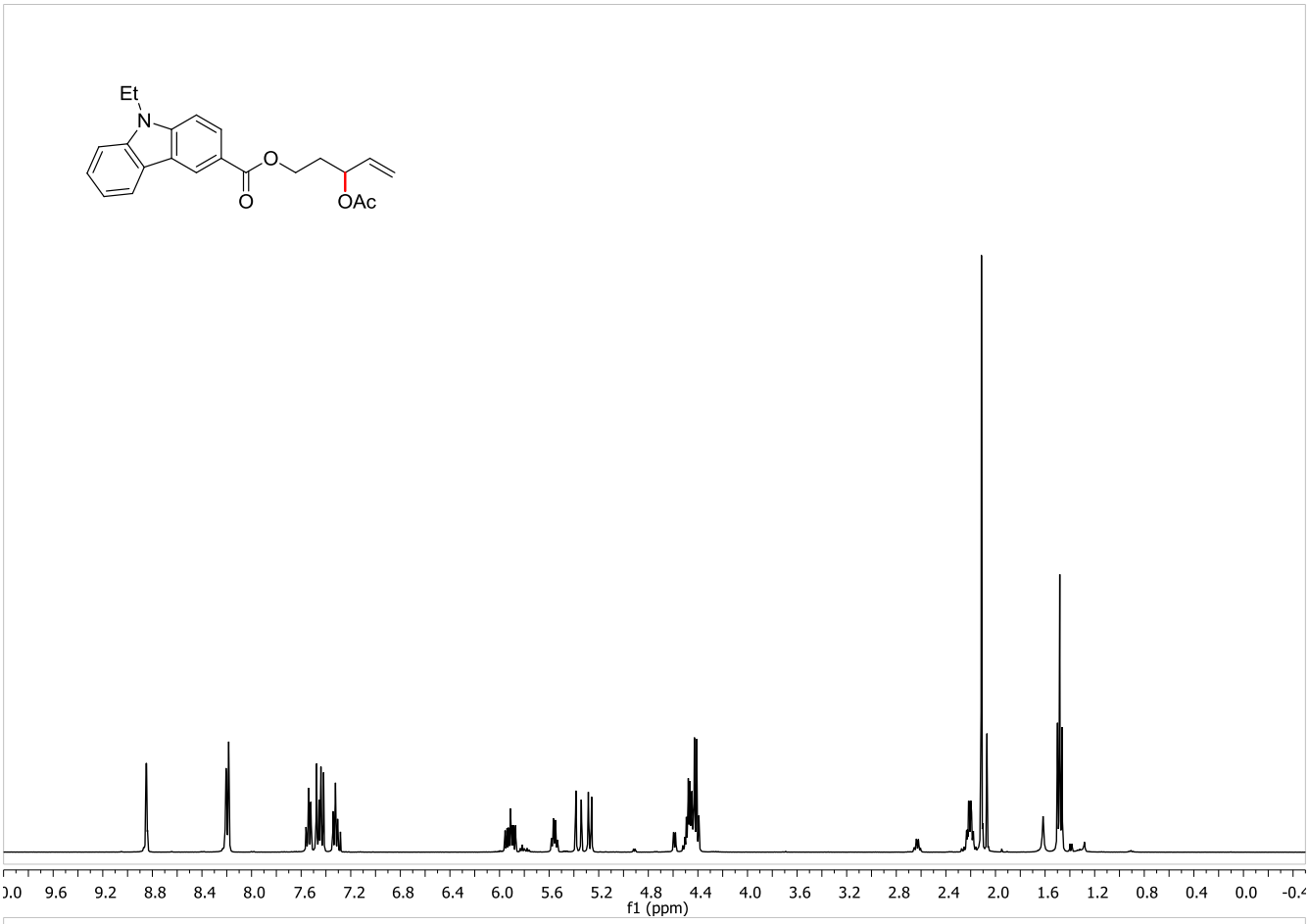
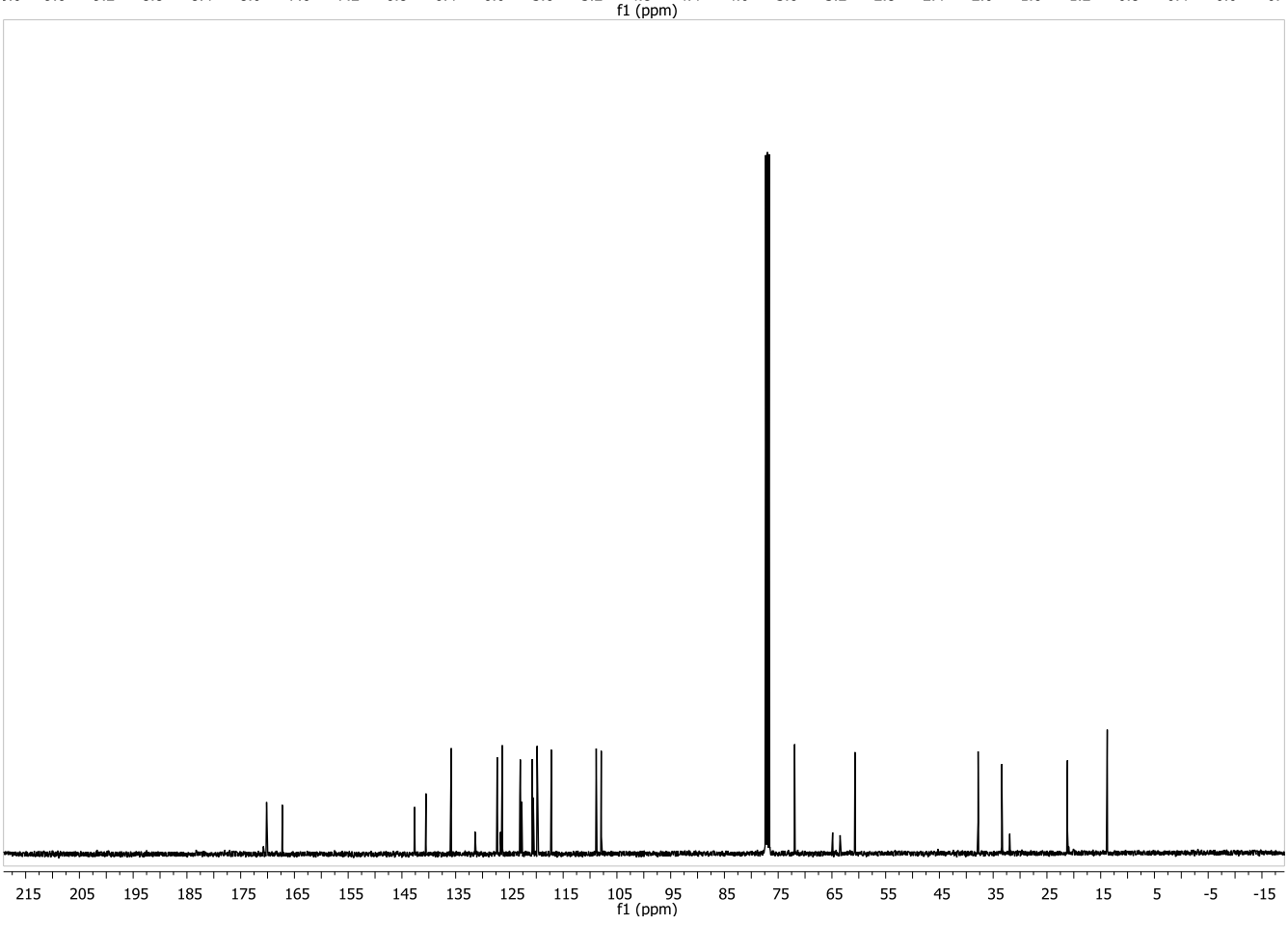
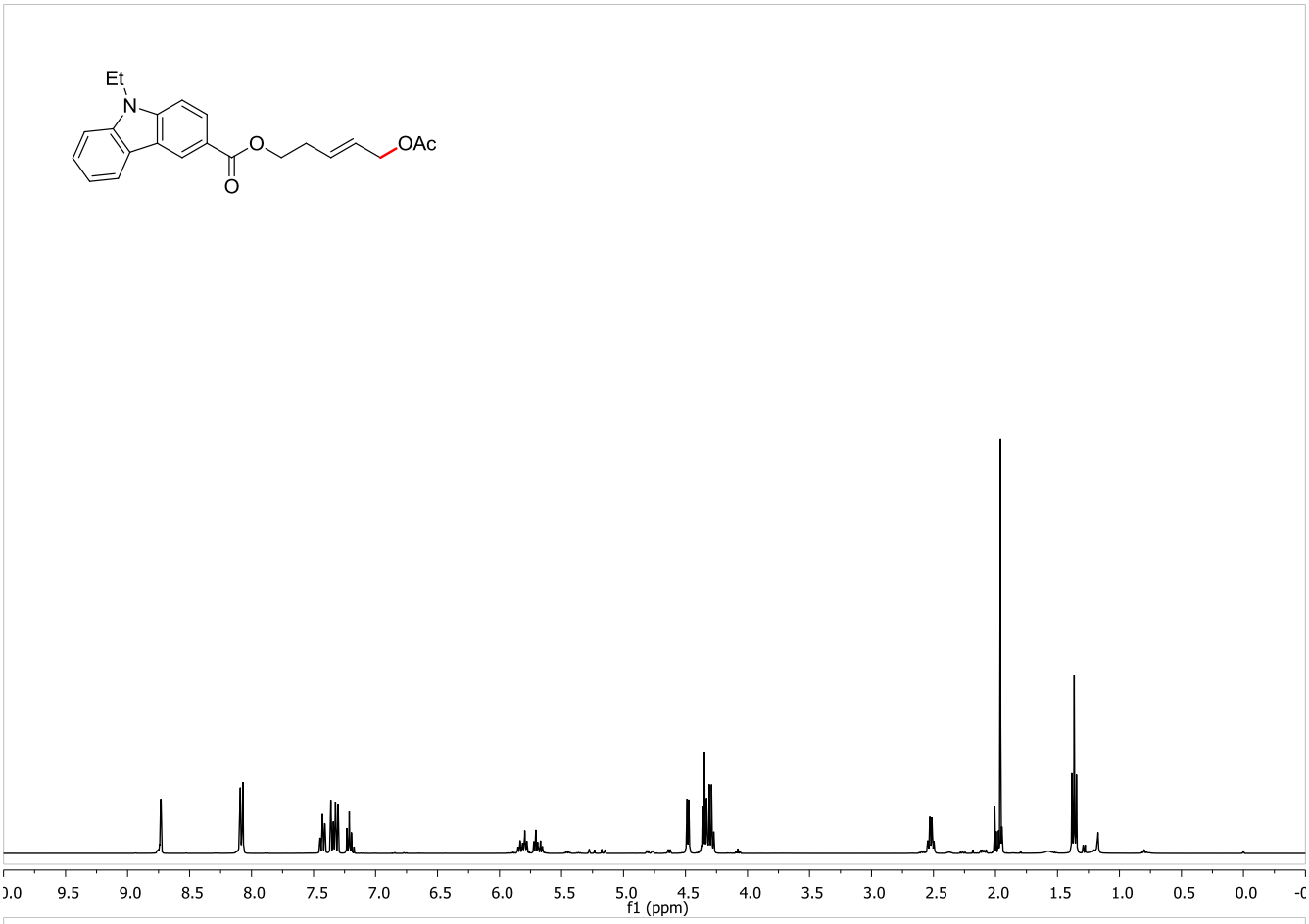
5
-5
-15
f1 (ppm)


O
O
OAc
9.6 9.2 8.8 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4 0.0
f1 (ppm)


215 205 195 185 175 165 155 145 135 125 115 105 95 85 75 65 55 45 35 25 15 5 -5 -15
f1 (ppm)


Et
N
O
O
OAc
9.6 9.2 8.8 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4 0.0
f1 (ppm)


215 205 195 185 175 165 155 145 135 125 115 105 95 85 75 65 55 45 35 25 15 5 -5 -15
f1 (ppm)


Et
N
O
O
OAc
9.5
9.0
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
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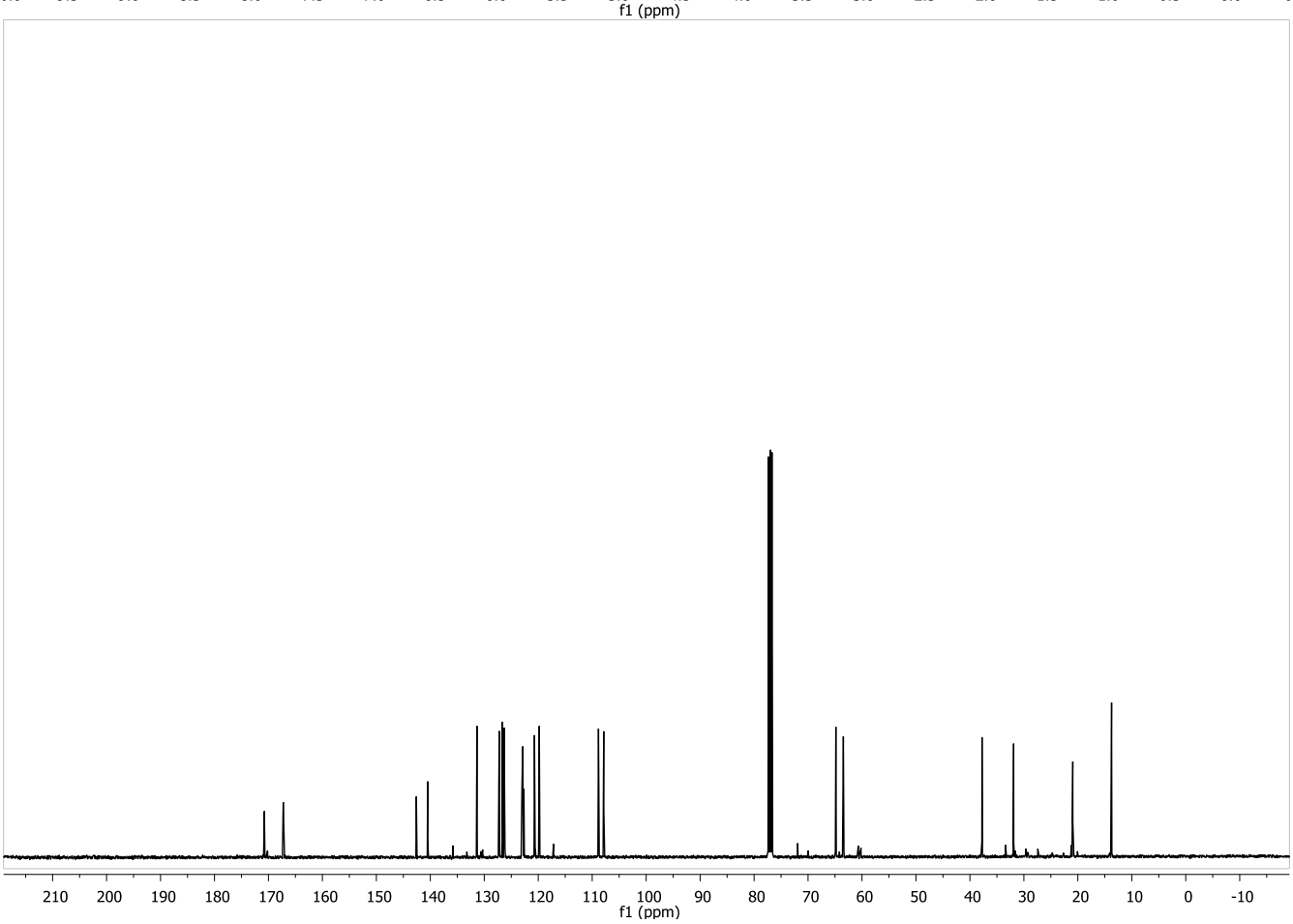
0.0
f1 (ppm)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170
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140
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60
50
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30
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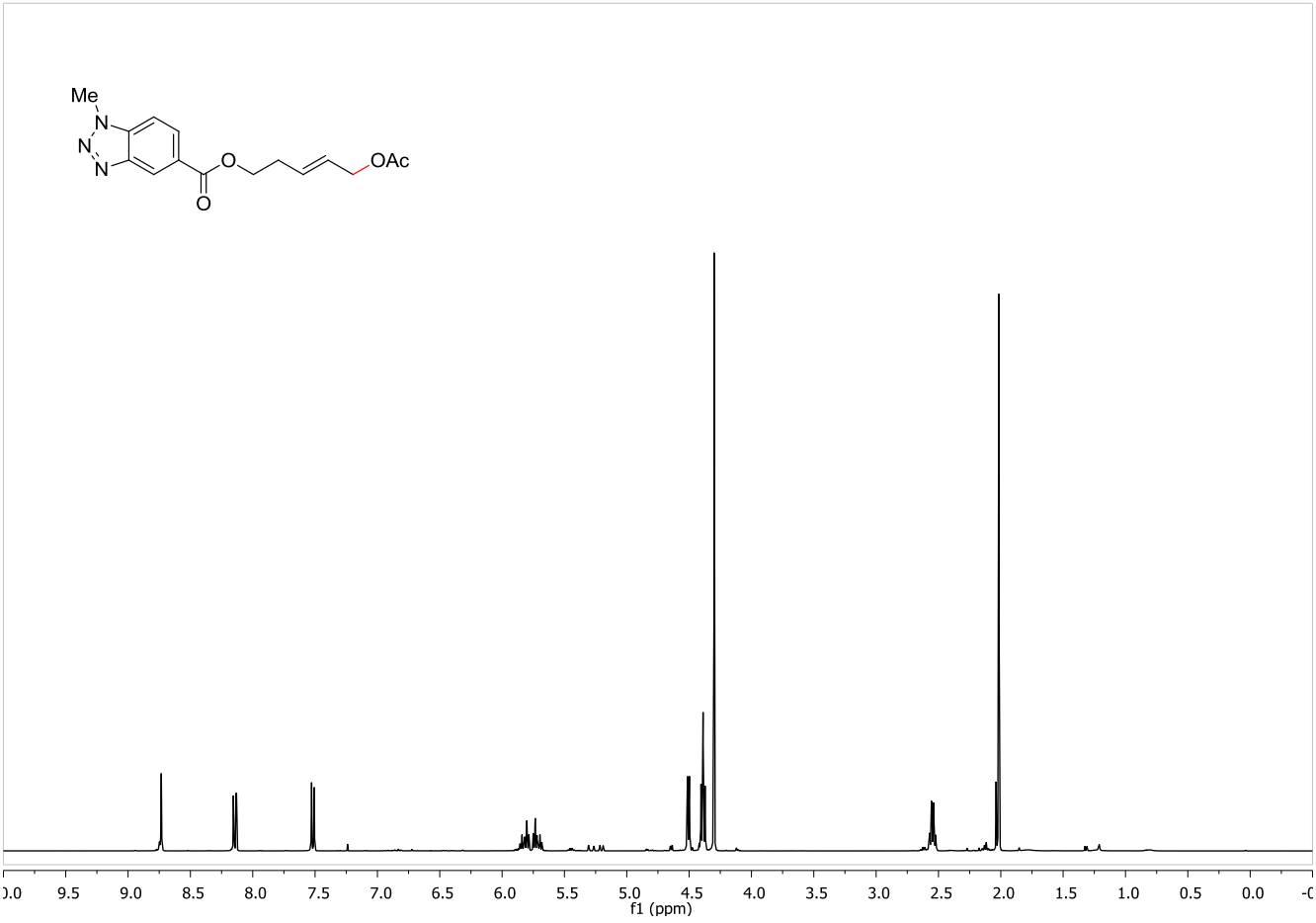
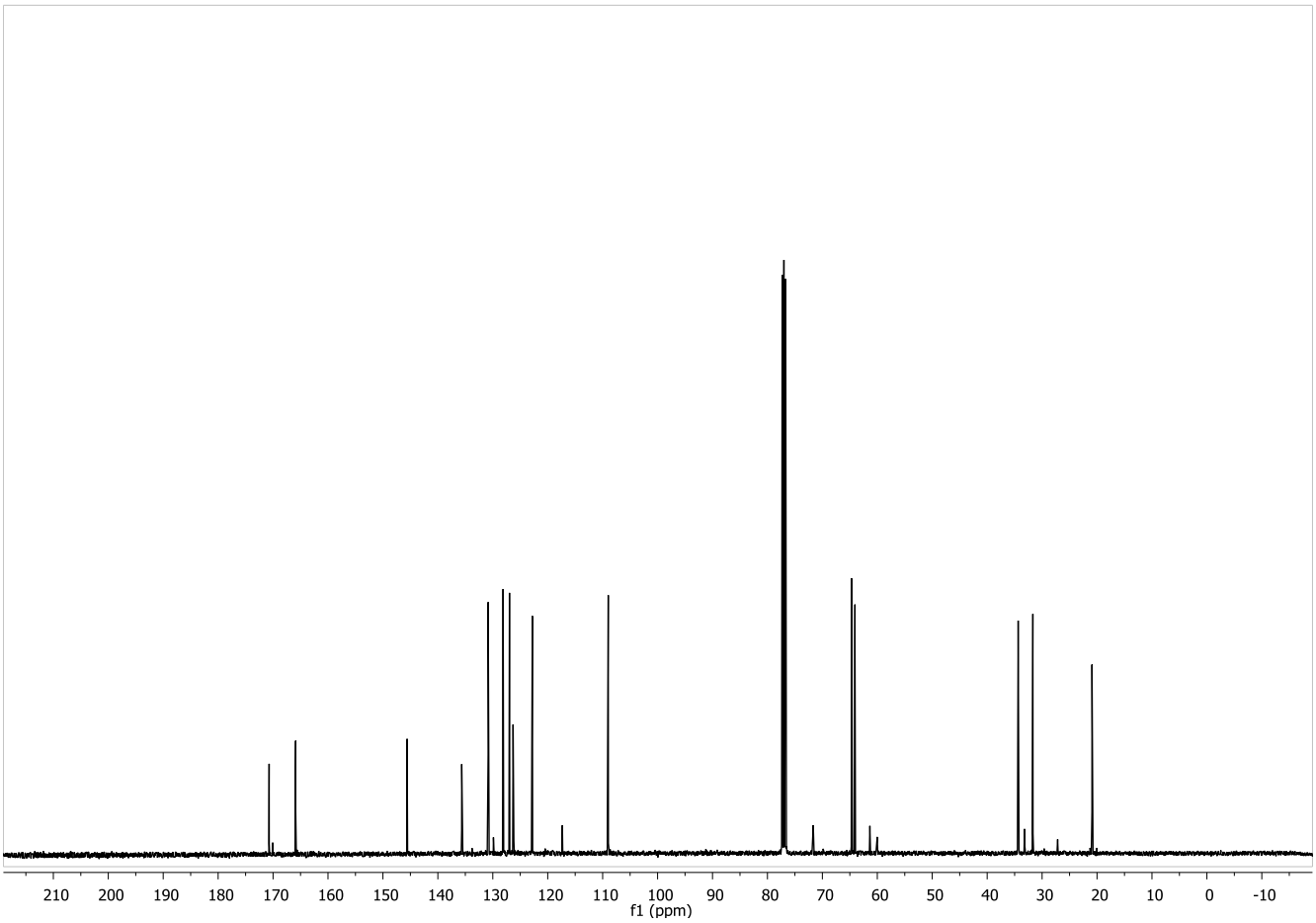
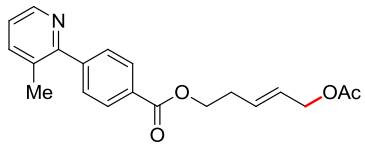
10
0
-10
f1 (ppm)

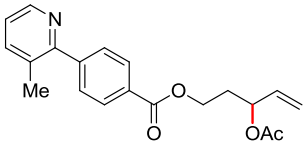

Me
N
N
N
O
O
OAc
f1 (ppm)

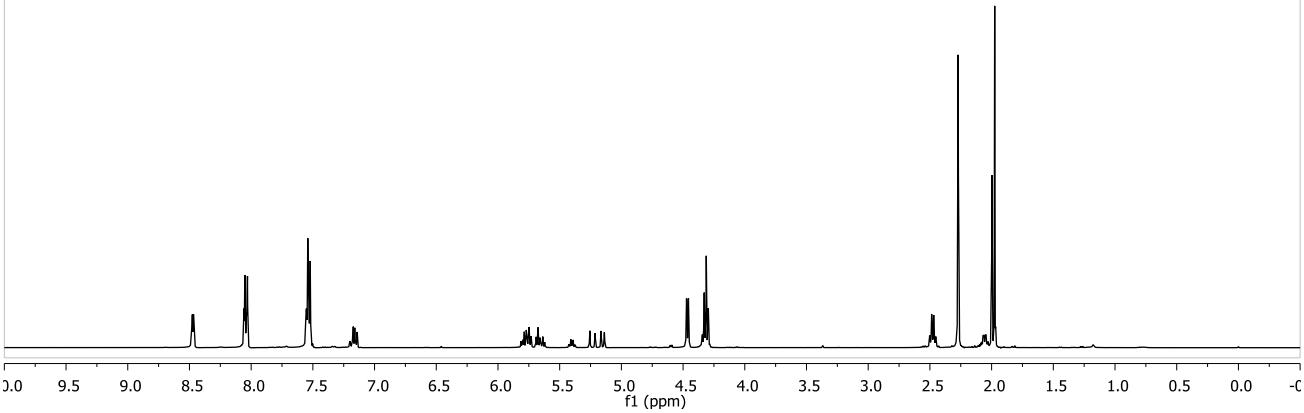

f1 (ppm)

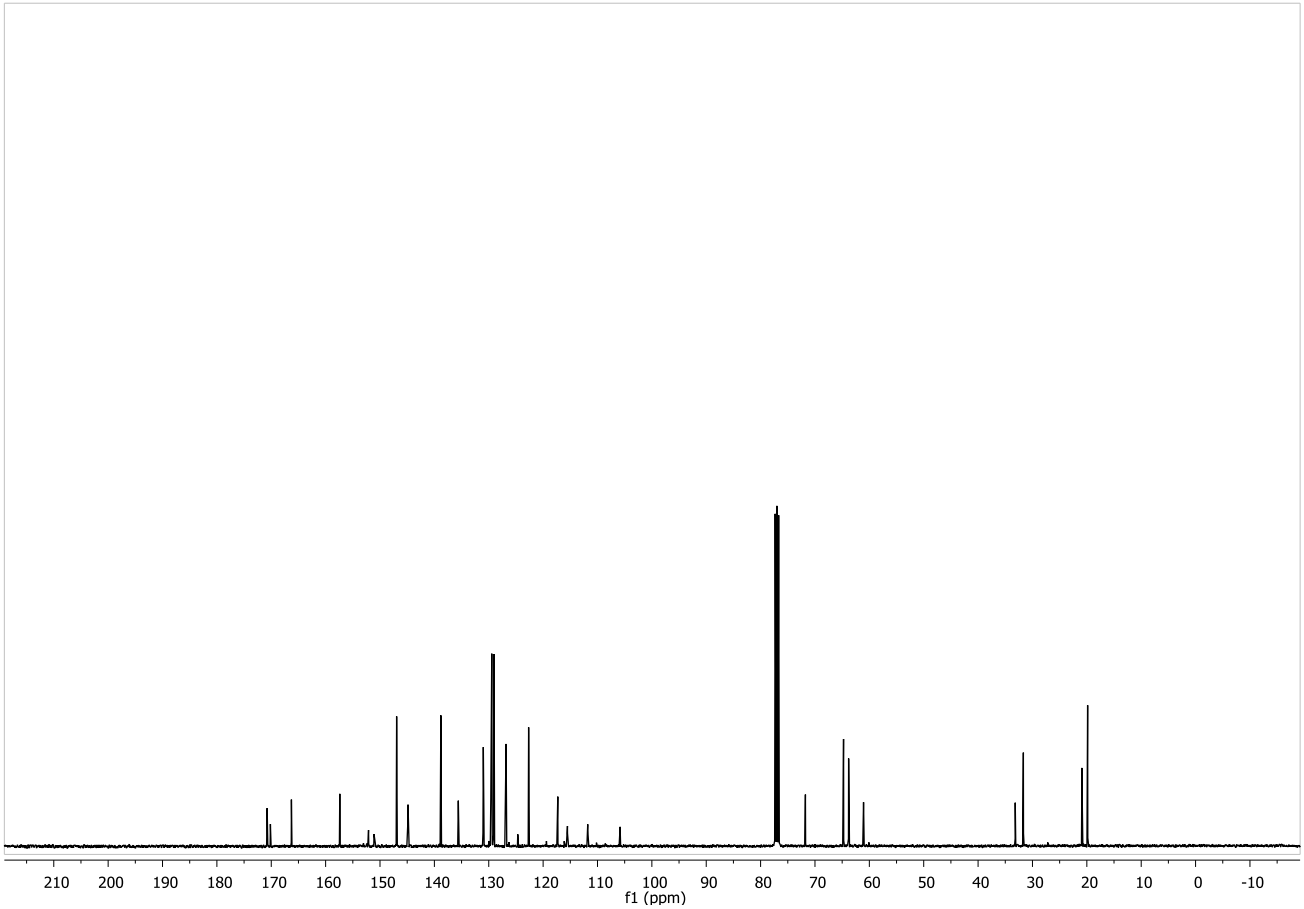
Major Regioisomer:

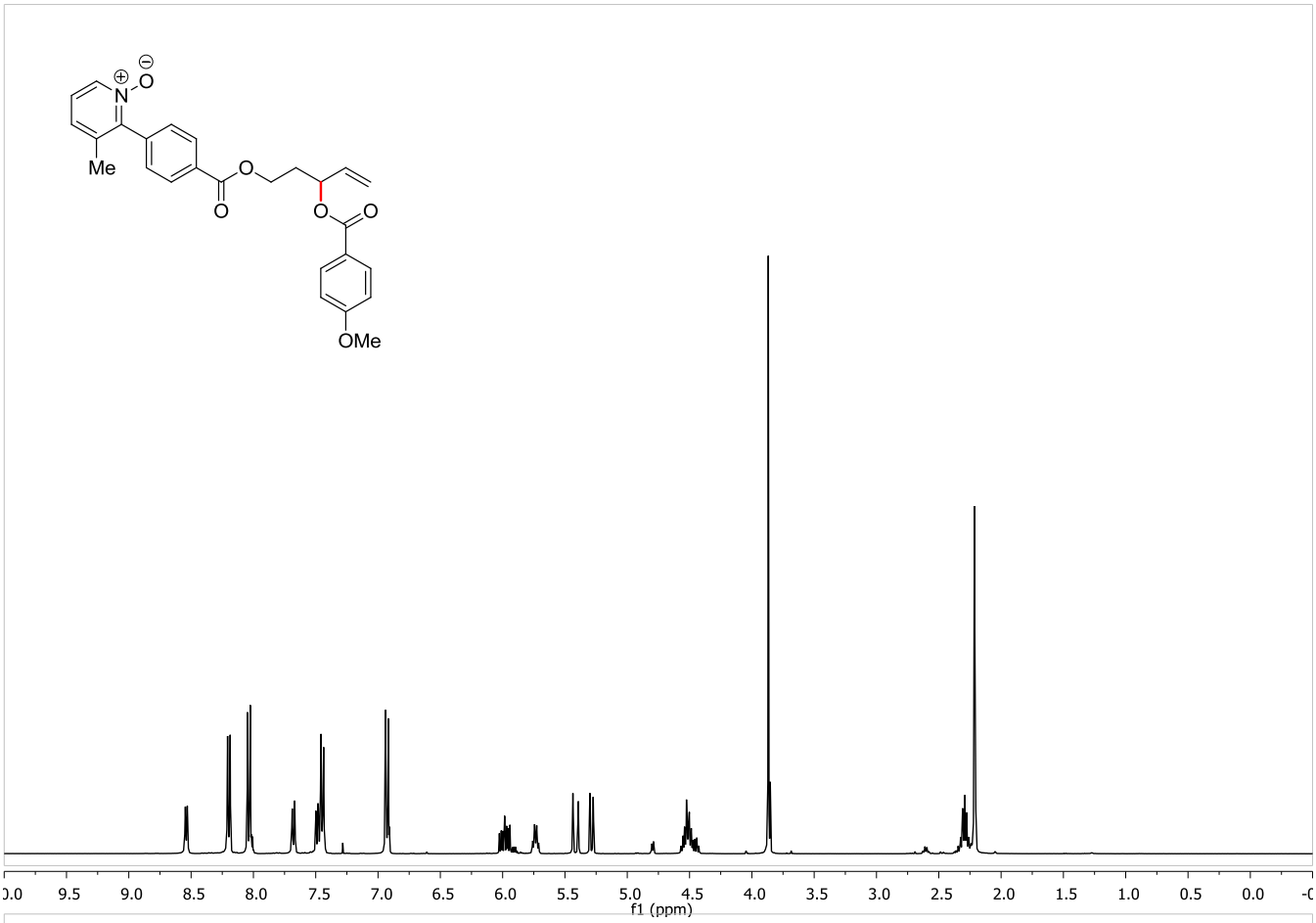


Minor Regioisomer:








Me
O
O
O
O
O
OMe
9.5
9.0
8.5
8.0
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7.0
6.5
6.0
5.5
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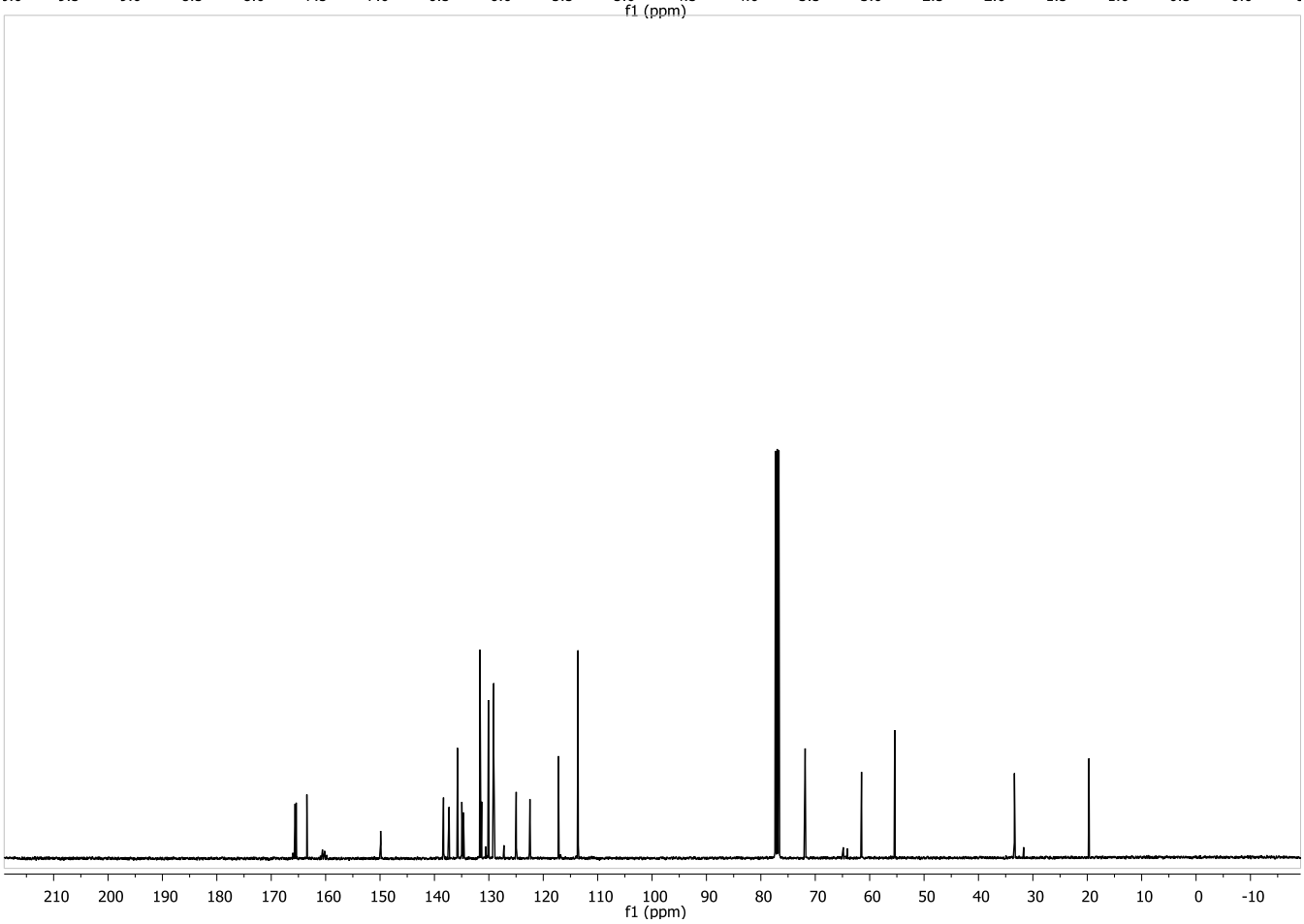
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


210
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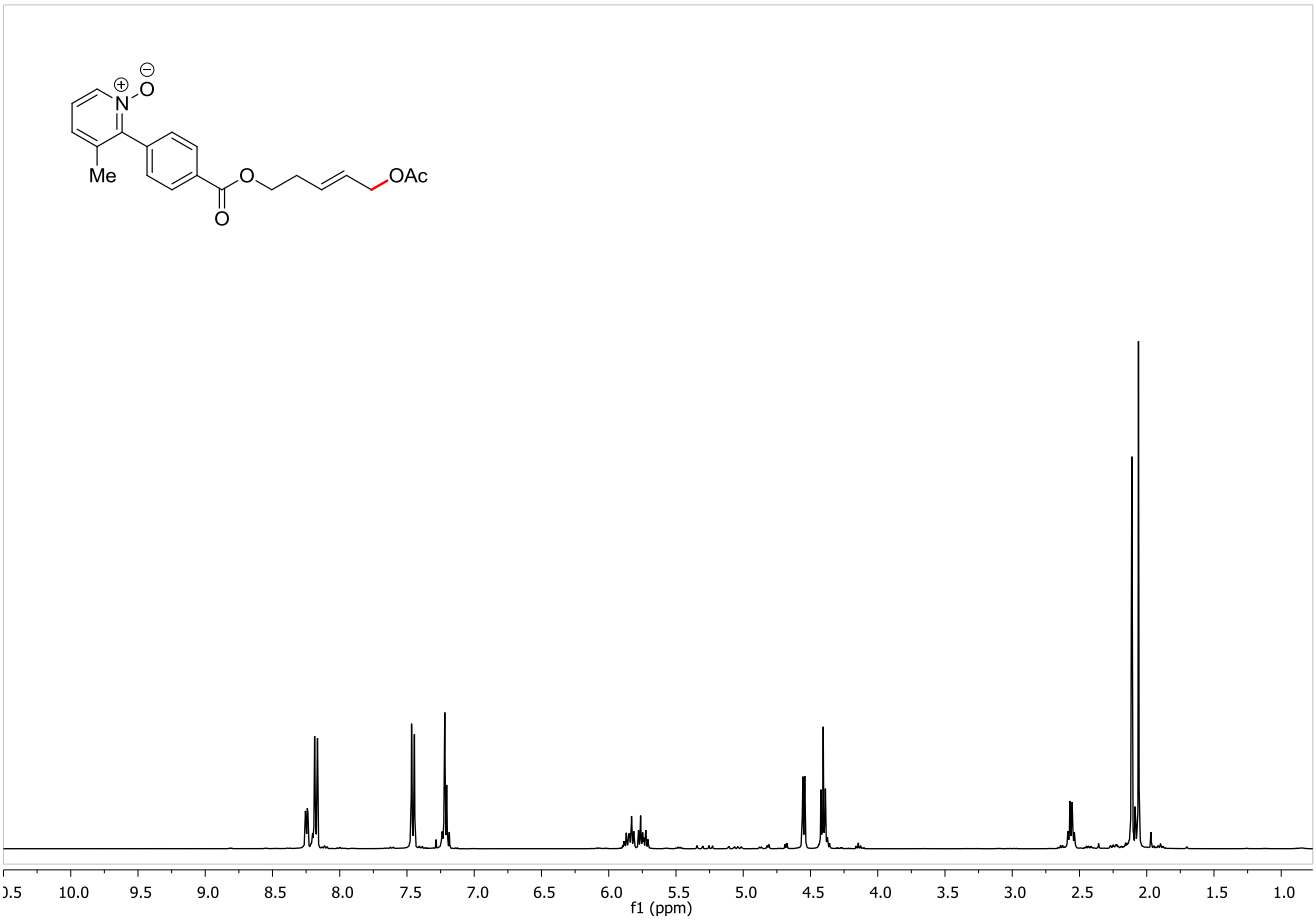
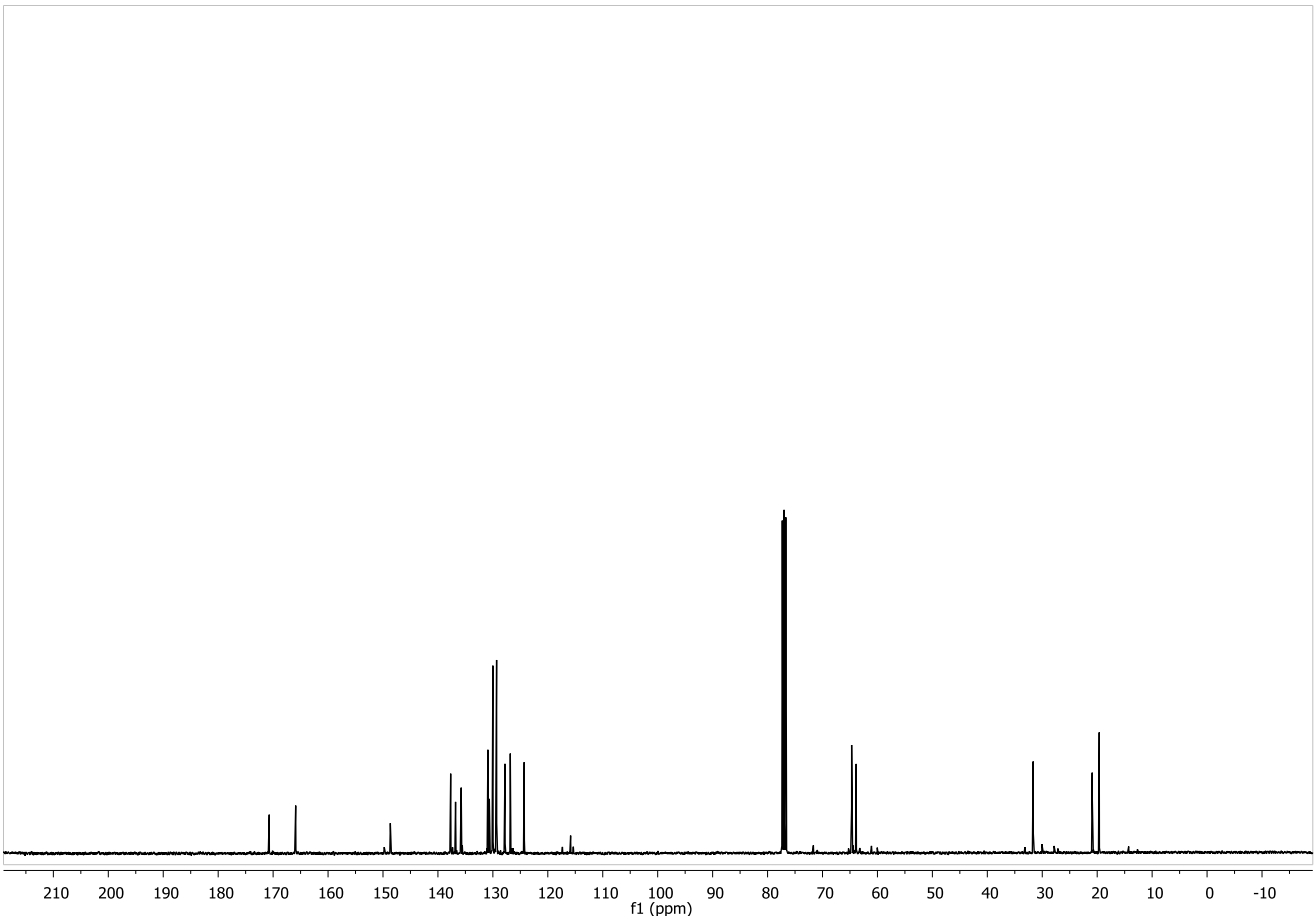
0
-10
f1 (ppm)


Me
O
OAc
O
O
10.0
9.5
9.0
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
f1 (ppm)


210
200
190
180
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130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)