Supplementary Materials: Suzuki-Miyaura C-C Coupling Reactions Catalyzed by Supported Pd Nanoparticles for the Preparation of Fluorinated Biphenyl Derivatives

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Table S1. Experimental quantities of reagents for the Pd loading study.

Final Material	Theoretical Pd (wt %)	G-COOH (g)	Pd (mg)	[$PdCl_2$(cod)] (mg)	Experimental Pd wt %)
G-COOH-Pd-5	5	1.0	52.6	141.2	3.06
G-COOH-Pd-10	10	1.0	111.1	298.1	7.93
G-COOH-Pd-15	15	1.0	176.4	473.4	11.20

Table S2. Adsorptive parameters of the materials G-COOH and G-COOH-Pd-10.

Material	BET surface area (m^2/g)	BJH Adsorption cumulative surface area of pores (m^2/g)	BJH Desorption cumulative surface area of pores (m^2/g)	BJH Adsorption cumulative volume of pores (cm^3/g)	BJH Desorption cumulative volume of pores (cm^3/g)
G-COOH	7.7	4.874	7.286	0.0350	0.0357
G-COOH-Pd-10	4.1	3.838	6.167	0.0383	0.0385

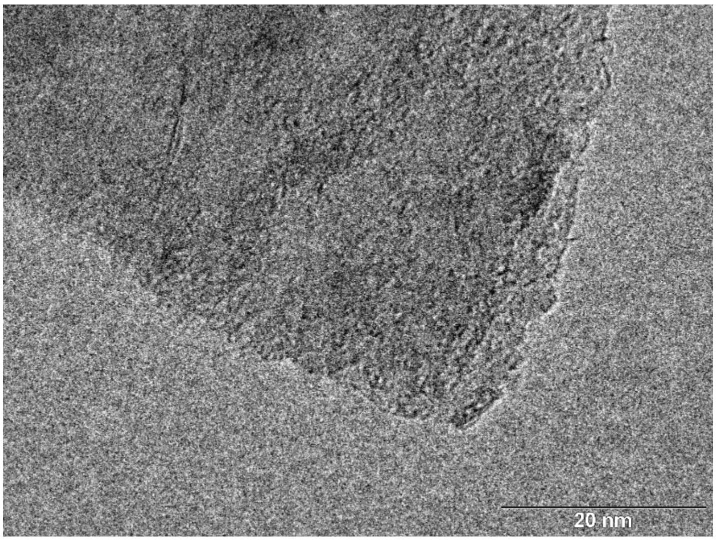


Figure S1. TEM image of G-COOH showing the single layer of graphene.

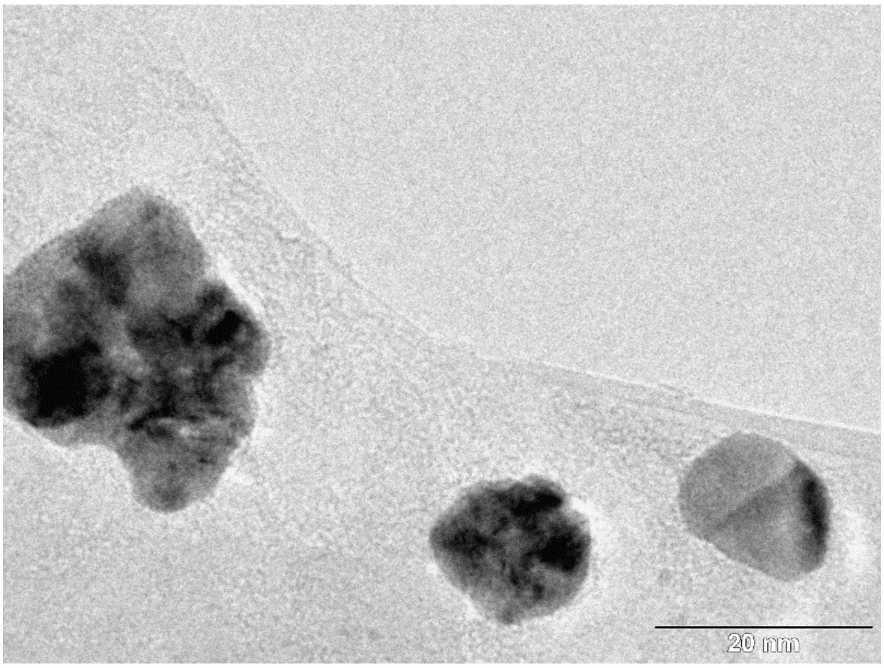


Figure S2. TEM image of a cluster of agglomerated Pd nanoparticles.

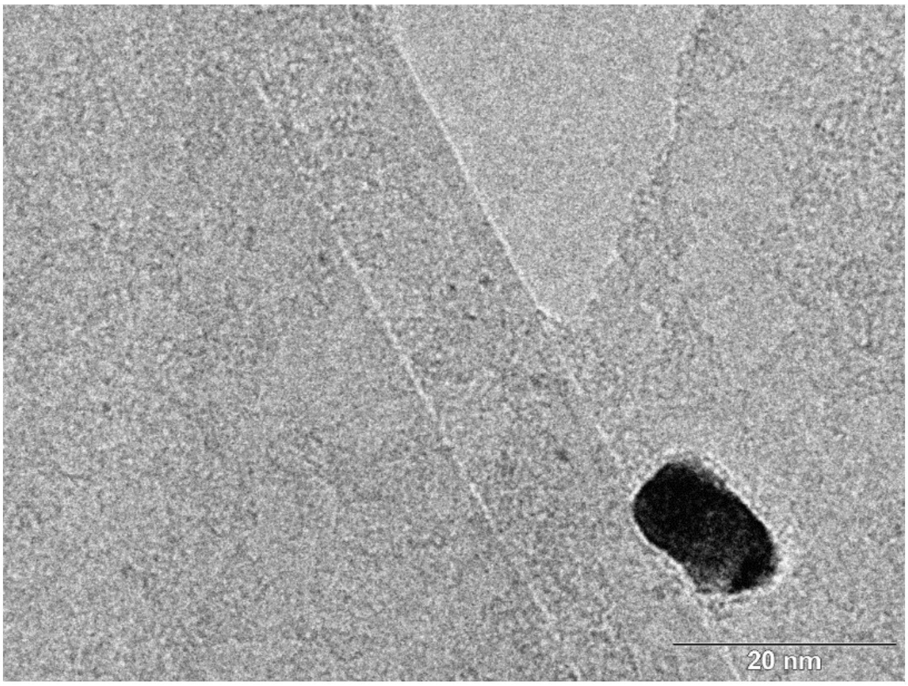


Figure S3. TEM image showing the impregnation of a cluster of Pd nanoparticles at the edge of the graphene layer.

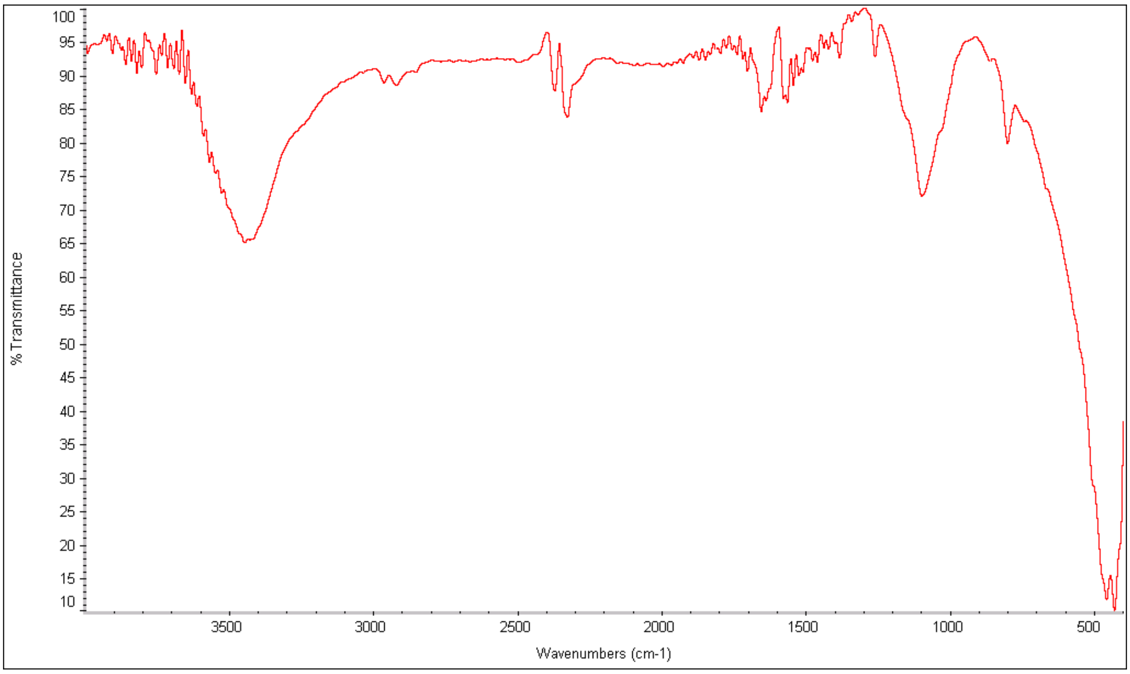


Figure S4. FT-IR spectrum of G-COOH-Pd-10.

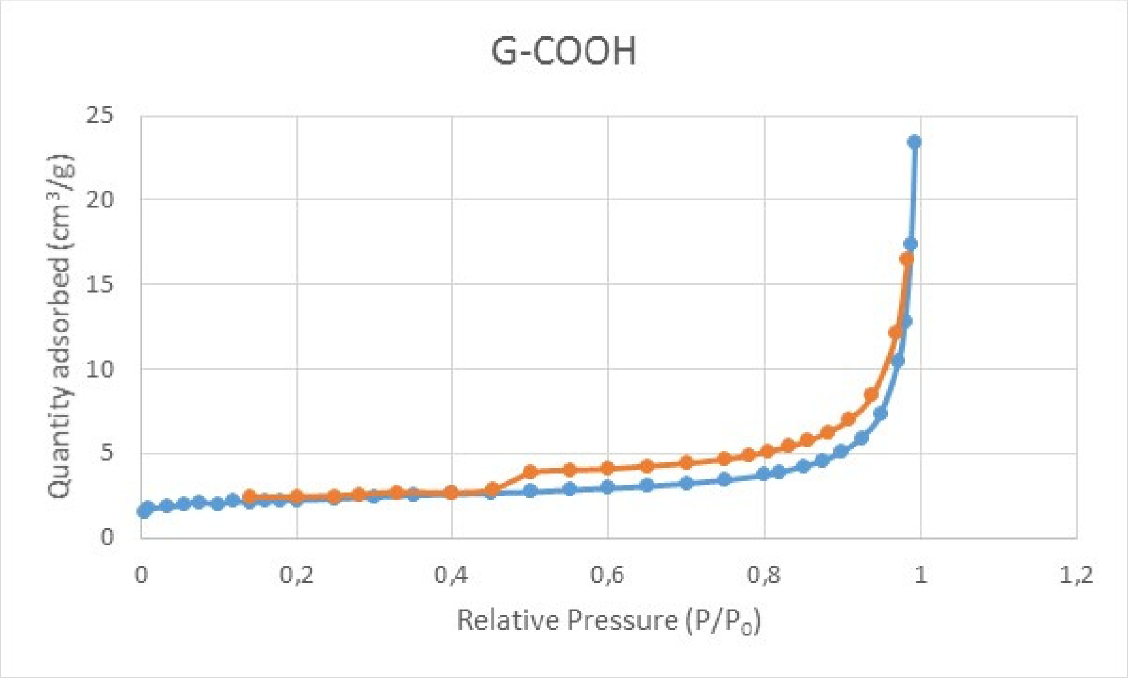


Figure S5. Nitrogen adsorption desorption isotherm of G-COOH.

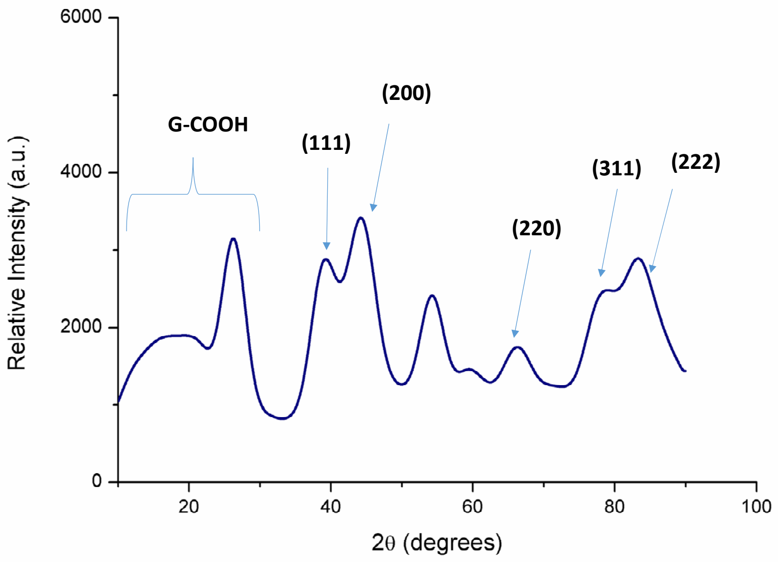


Figure S6. XRD of the material G-COOH-Pd-10

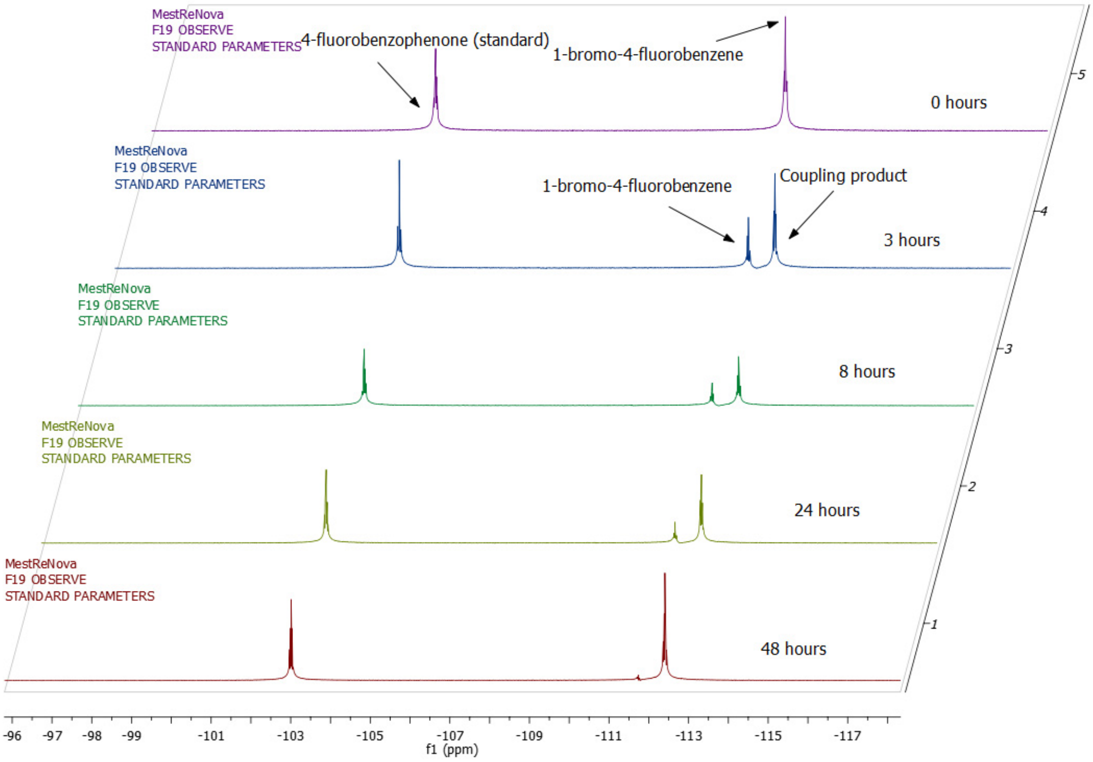


Figure S7. Comparison of the ^{19}F NMR spectra of the reaction between 1-bromo-4-fluorobenzene and phenylboronic acid catalyzed by G-COOH-Pd-10 in the presence of a constant quantity of standard (4-fluorobenzophenone) at different reaction time periods.

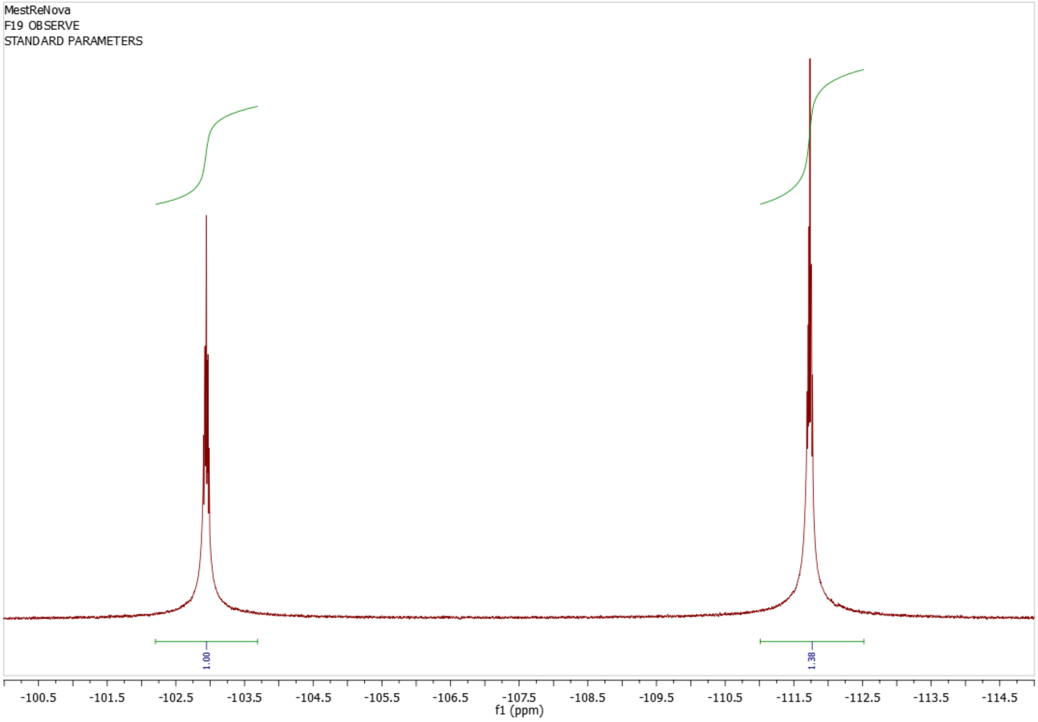


Figure S8. ^{19}F NMR spectrum of the starting solution of 1-bromo-4-fluorobenzene in the presence of a constant quantity of standard (4-fluorobenzophenone) (0 hours).

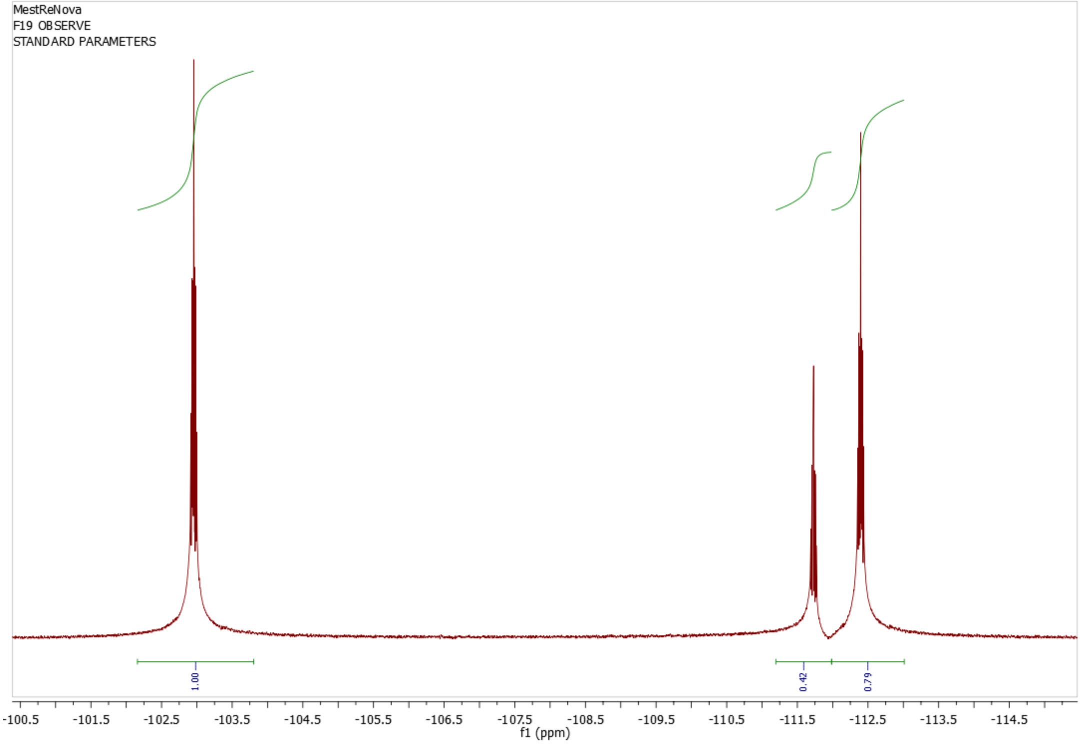


Figure S9. ^{19}F NMR spectrum of the reaction between 1-bromo-4-fluorobenzene and phenylboronic acid catalyzed by G-COOH-Pd-10 after three hours of reaction in the presence of a constant quantity of standard (4-fluorobenzophenone).

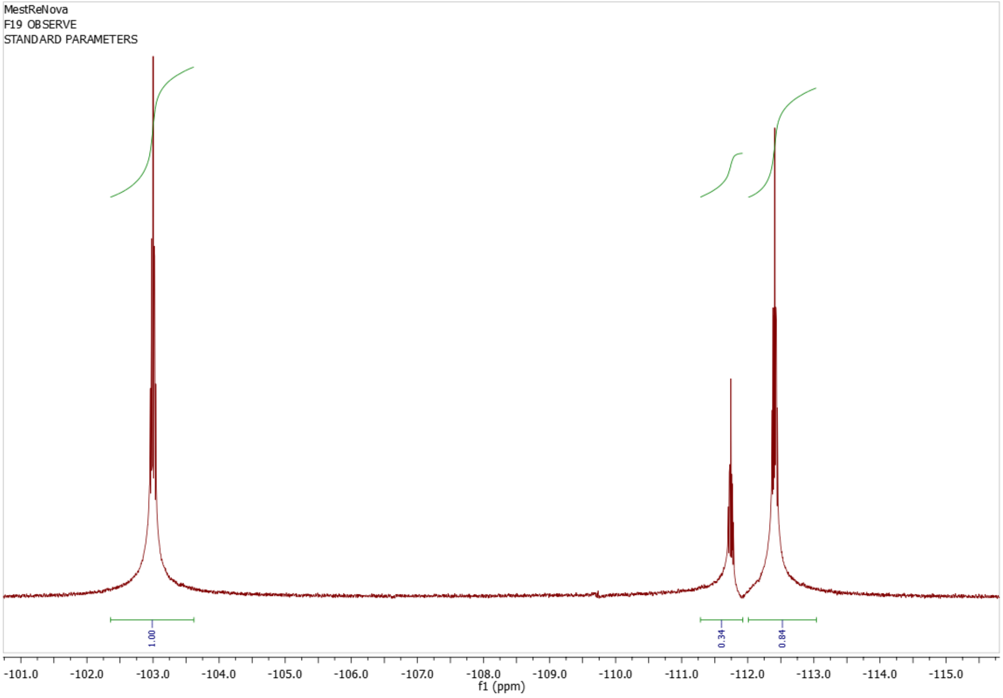


Figure S10. ^{19}F NMR spectrum of the reaction between 1-bromo-4-fluorobenzene and phenylboronic acid catalyzed by G-COOH-Pd-10 after eight hours of reaction in the presence of a constant quantity of standard (4-fluorobenzophenone).

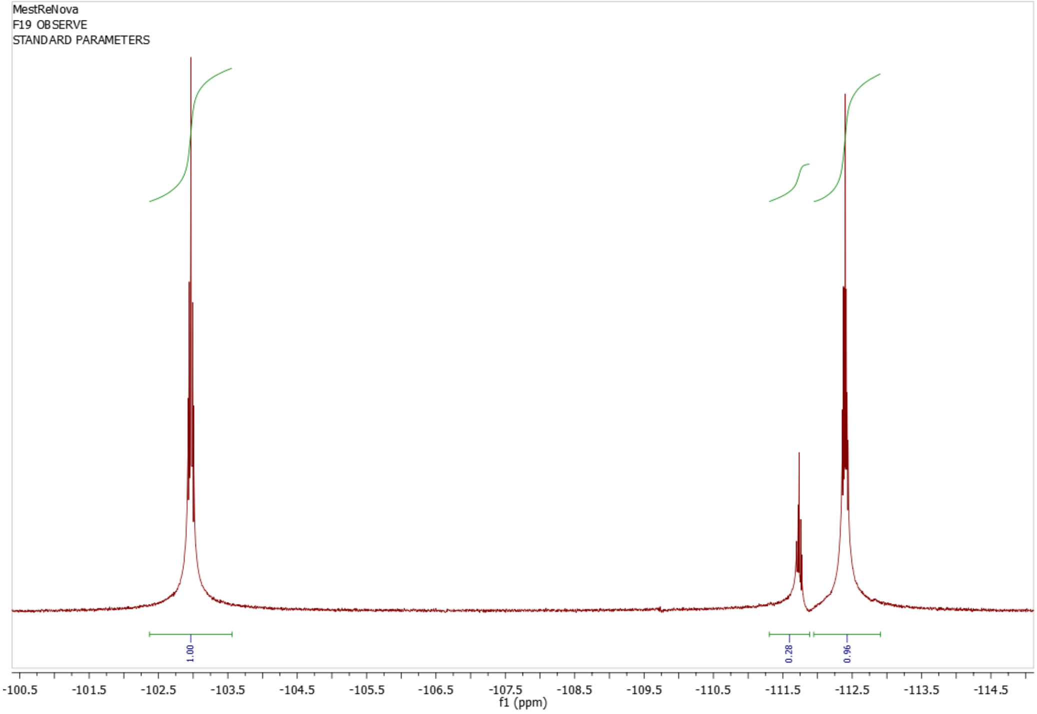


Figure S11. ^{19}F NMR spectrum of the reaction between 1-bromo-4-fluorobenzene and phenylboronic acid catalyzed by G-COOH-Pd-10 after 24 hours of reaction in the presence of a constant quantity of standard (4-fluorobenzophenone).

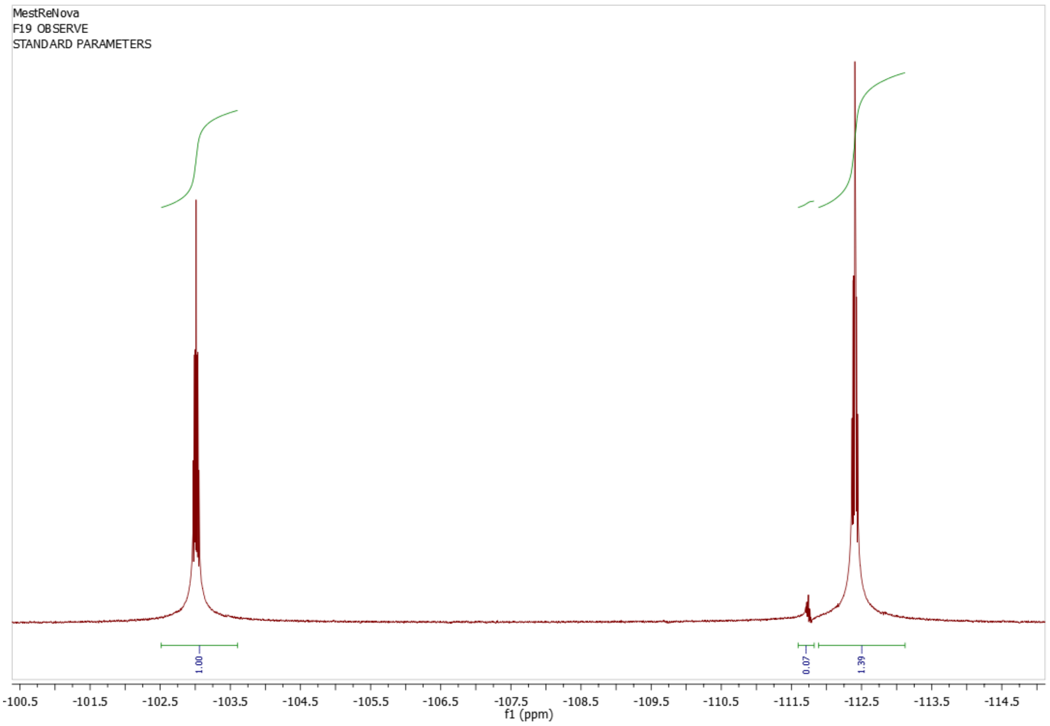


Figure S12. ^{19}F NMR spectrum of the reaction between 1-bromo-4-fluorobenzene and phenylboronic acid catalyzed by G-COOH-Pd-10 after 48 hours of reaction in the presence of a constant quantity of standard (4-fluorobenzophenone).

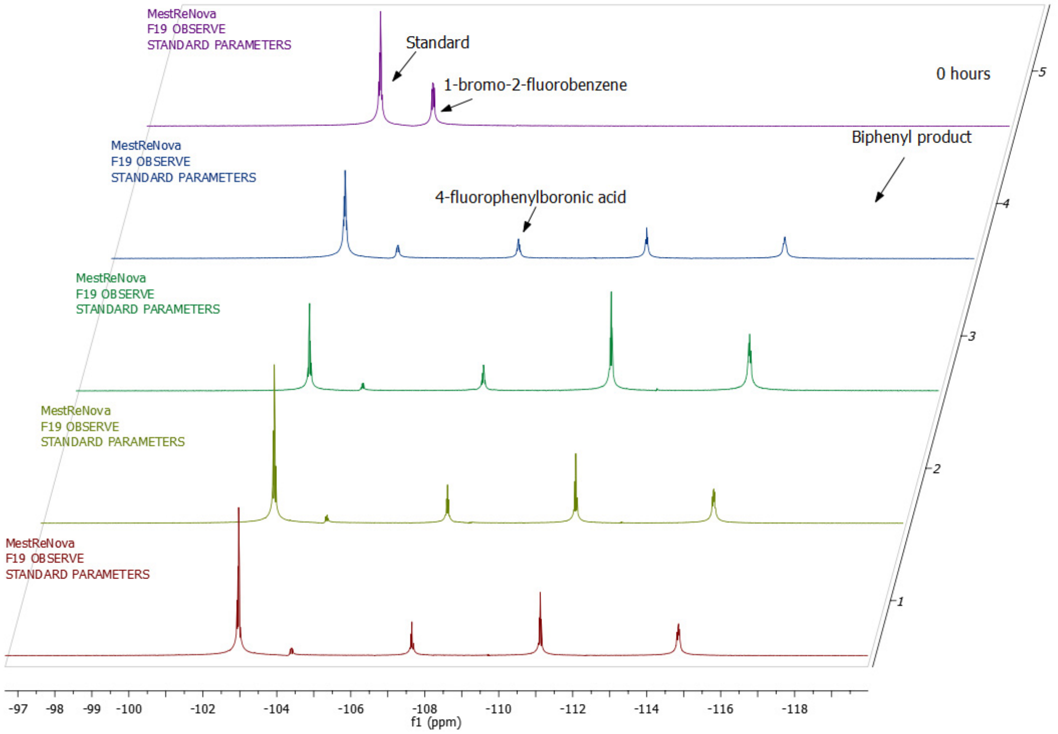
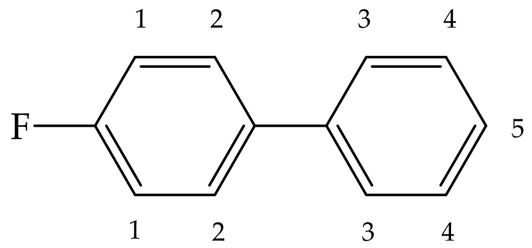
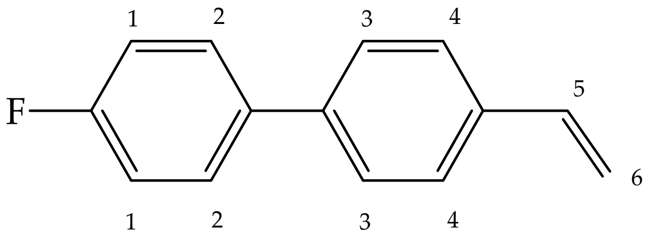


Figure S13. Comparison of the ^{19}F NMR spectra of the reaction between 1-bromo-2-fluorobenzene and 4-fluorophenylboronic acid catalyzed by G-COOH-Pd-10 in the presence of a constant quantity of standard (4-fluorobenzophenone) at different reaction time periods.

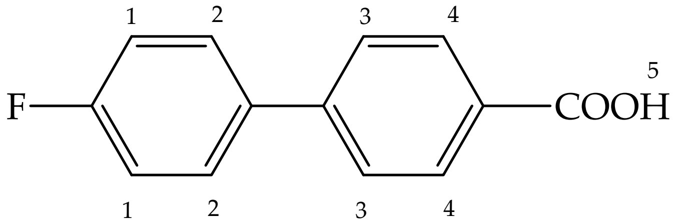
Spectroscopic Data (^{1}H and ^{19}F NMR) of all the Synthesized Fluorinated Biaryl Derivatives



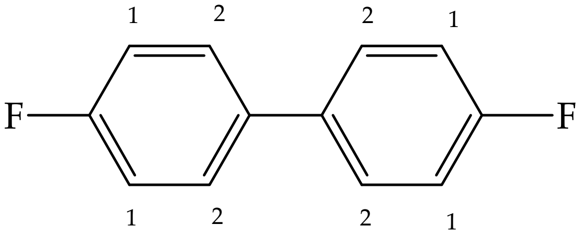
The spectroscopic data found for this compound are the same tan those found in the literature [1]. In addition, it is a commercial compound with CAS Number: 324-74-3. ^{1}H NMR (400 MHz, CDCl$_3$) δ: 7.60–7.54 (m, 4H, H2 and H3), 7.50–7.34 (m, 3H, H4, and H5), 7.20–7.12 (m, 2H, H1). ^{19}F NMR (376 MHz, CDCl$_3$) δ: −116.2 (m).



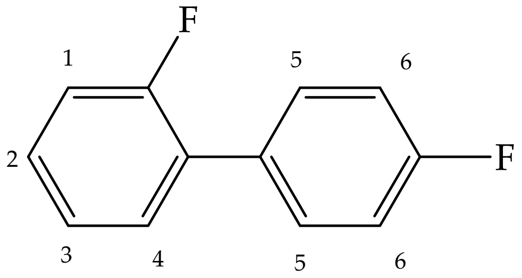
The spectroscopic data found for this compound are the same than those found in the literature [2]. ^{1}H NMR (400 MHz, CDCl$_3$) δ: 7.53–7.47 (m, 6 H, H2, H3, and H4), 7.15–7.10 (m, 2 H, H1), 6.75 (dd, *J* = 10.8, 17.6 Hz, 1 H, H5), 5.80 (d, J = 17.6 Hz, 1 H, H6), 5.28 (d, J = 11.6 Hz, 1 H, H6). ^{19}F NMR (376 MHz, CD$_3$COCD$_3$): –112.2 (m).



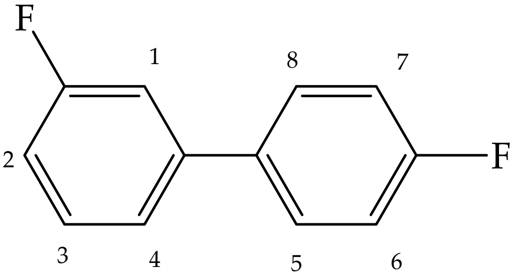
The spectroscopic data found for this compound are the same than those found in the literature [3]. In addition, it is a commercial compound with CAS Number: 5731-10-2. ^{1}H NMR (400 MHz, CDCl$_3$): 7.30 (t, 2H, *J* = 9.0 Hz, H1), 7.76 (m, 4H, H2, and H3), 7.99 (d, 2H, *J* =8.8 Hz, H4), 12.94 (1H, br s). ^{19}F NMR (376 MHz, CD$_3$COCD$_3$): –112.4 (m).



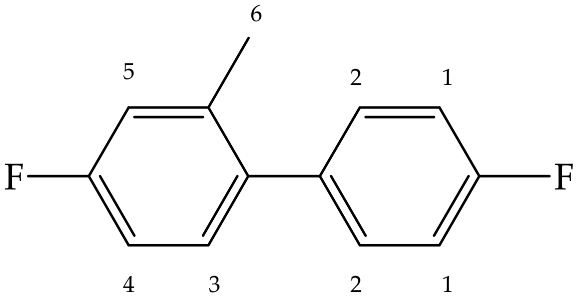
The spectroscopic data found for this compound are the same tan those found in the literature [4]. In addition, it is a commercial compound with CAS Number: 398-23-2. ^{1}H NMR (400 MHz, CDCl$_3$): 7.13 (t, 4H, *J* = 9 Hz, H1), 7.48 (dd, 4H, *J* = 9 and 5 Hz, H2). ^{19}F NMR (376 MHz, CD$_3$COCD$_3$): –112.3 (m).



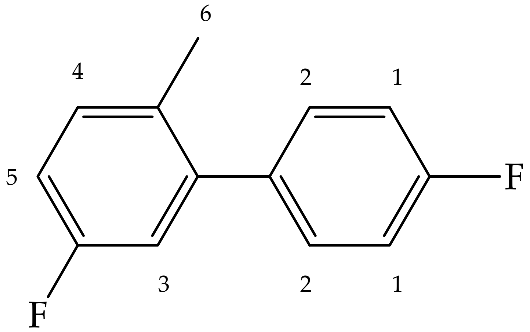
The spectroscopic data found for this compound are the same tan those found in the literature [5]. ^{1}H NMR (400 MHz, CDCl$_3$): δ = 7.20 (m, 1H, H1), 7.37 (m, 1H, H2), 7.25 (m, 1H, H3), 7.45 (d, 1H, H4), 7.57 (m, 2H, H5), 7.18 (m, 2H, H6). ^{19}F NMR (376 MHz, CD$_3$COCD$_3$): –111.1 (m), –114.8 (m).



The spectroscopic data found for this compound are the same tan those found in the literature [6]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (dd, 2H, *J* = 8.5, 5.0 Hz, H5, and H8), 7.38 (td, 1H, *J* = 8.0, 6.0 Hz, H3), 7.31 (d,1H, *J* = 7.5 Hz, H4), 7.23 (dt, 1H, *J* = 10.0, 3.5 Hz, H2), 7.13 (t,2H, *J* = 8.5 Hz, H6 and H7), 7.03 (td, 1H, *J* = 10.0, 2.5 Hz, H1). ^{19}F NMR (376 MHz, CD_3COCD_3): –109.3 (m), –111.4 (m).



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26–7.21 (m, 2H, H2), 7.16–7.13 (m, 1H, H3), 7.11–7.06 (m, 2H, H1), 6.98–6.89 (m, 2H, H4, and H5), 2.22 (s, 3H, methyl group (6)). ^{19}F NMR (376 MHz, CD_3COCD_3): –112.3 (m), –112.5 (m).



^{1}H NMR (400 MHz, CD_3COCD_3) δ 7.41–7.34 (m, 2H, H2), 7.26–7.18 (m, 2H, H3 and H4), 7.12–7.01 (m, 2H, H1), 6.94–6.99 (dd, 1H, H5), 2.20 (s, 3H, Methyl group (6)). ^{19}F NMR (376 MHz, CD_3COCD_3): –111.8 (m), –114.5 (m).

References

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