

Support Information (SI)

For

Direct Cross Coupling of Benzyl Alcohols to Construct Diarylmethanes *via* Palladium Catalysis

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Table of Contents

I. Experimental Section	
Part 1. General Information	S2
Part 2. Typical procedures for the benzylic Arylation.....	S2
Part 3. Evidences of the weak interaction (naphthmethanol and phenylboroxine).....	S3
Part 4. Synthesis and analytical data for the products.....	S6
II. Spectral data for new compounds.....	S14

I. Experimental Section

Part 1. General Information

All the reactions were carried out under nitrogen atmosphere using standard Schlenk technique in the oil bath. 1-naphthylmethanol was purchased from Aldrich, (4'-(dimethylamino)biphenyl-4-yl)methanol was prepared directly from (4-bromophenyl)methanol.¹ Naphthalene-2,6-diyl dimethanol, 2-naphthylmethanol, phenanthren-9-ylmethanol, (6-methoxynaphthalen-2-yl)methanol, and 6-(hydroxymethyl)naphthalen-2-ol were prepared from corresponding aryl aldehydes or ketones.² 6-(hydroxymethyl)naphthalen-2-yl acetate was prepared from 6-(hydroxymethyl)naphthalen-2-ol via the reported procedure³. The catalyst Pd(PPh₃)₄ was purchased from Acros and stored in the glovebox without further purification. THF was freshly distilled over sodium under N₂ with the use of diphenyl ketone as an indicator, aryl boronic acids were prepared from corresponding boric acid via the reported paths⁴. ¹H NMR (400 MHz)/¹³C NMR (100 MHz) were registered on Bruker 400 M spectrometers with CDCl₃ as solvent and tetramethylsilane (TMS) as internal standard. Chemical shifts were reported in units (ppm) by assigning TMS resonance in the ¹H spectrum as 0.00 ppm. All coupling constants (J values) were reported in Hertz (Hz). Column chromatography was performed on silica gel 200-300 mesh. MS and HRMS were performed by the State-authorized Analytical Center in Peking University.

Part 2: Typical Procedure for Pd-catalyzed Cross-Coupling

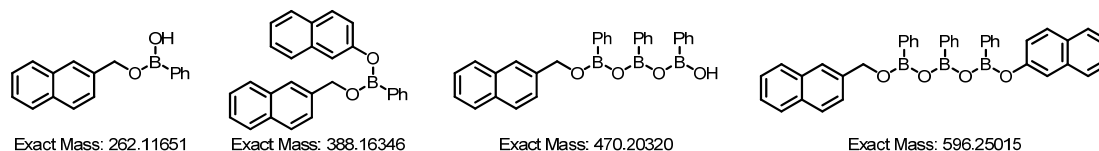
An oven-dried Schlenk tube containing a stirbar was charged with 2-naphthylmethanol (**1a**) (31.7mg, 0.2 mmol) and (PhBO)₃ (62.4mg, 0.2 mmol) and removed into the glove box after the tube was degassed and refilled with N₂ for 3 times. The catalyst Pd(PPh₃)₄ (23.1mg, 0.02 mmol) and THF (1.0 mL) were added in the glove box (Caution: the amount of oxygen is crucial to the yield) and then removed out and reacted in an oil bath. Then the mixture was cooled to room temperature and quenched by EtOAc (1 mL). The solvent was removed and the product was purified by flash column chromatography.

Part 3. Evidences of the weak interaction

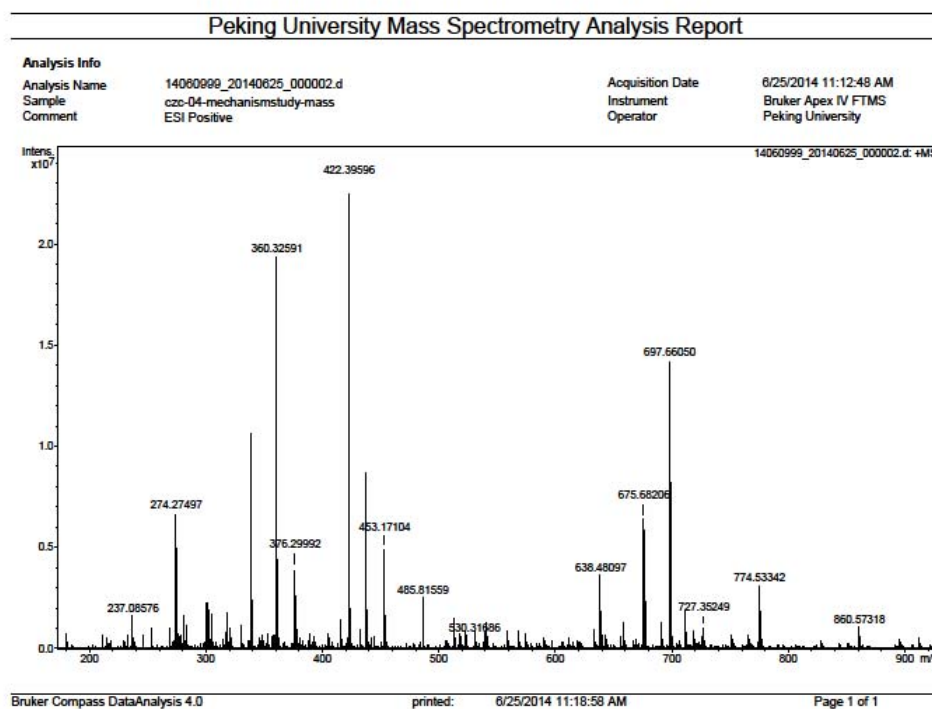
(naphthmethanol and phenylboroxine)

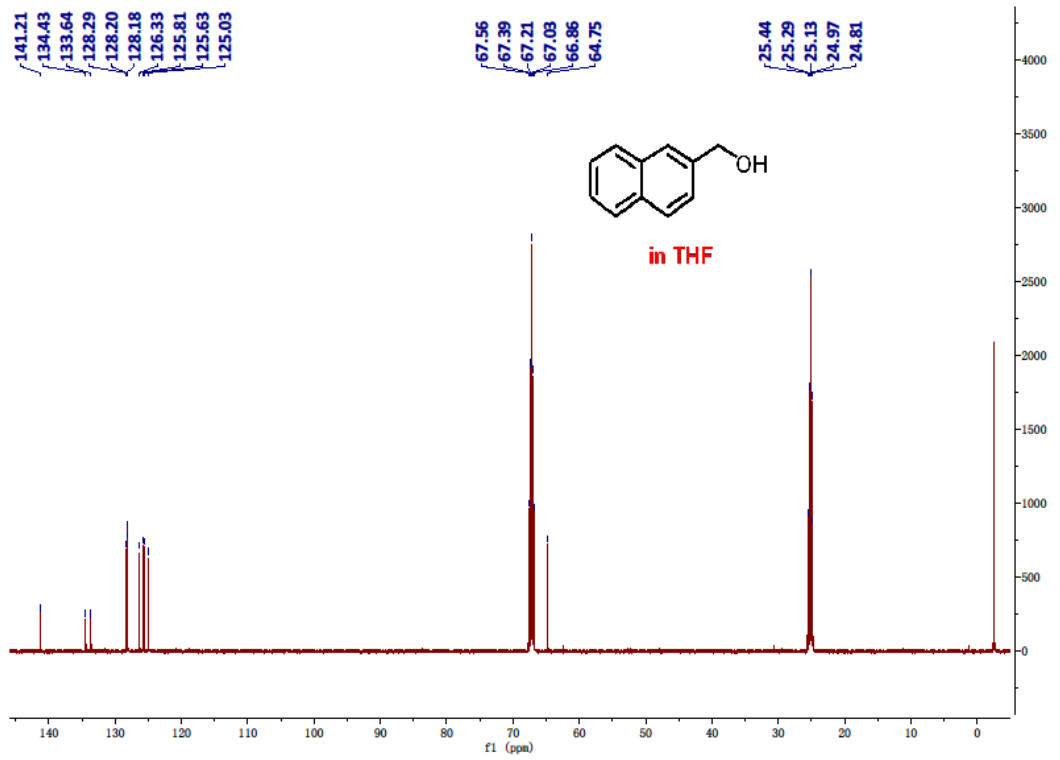
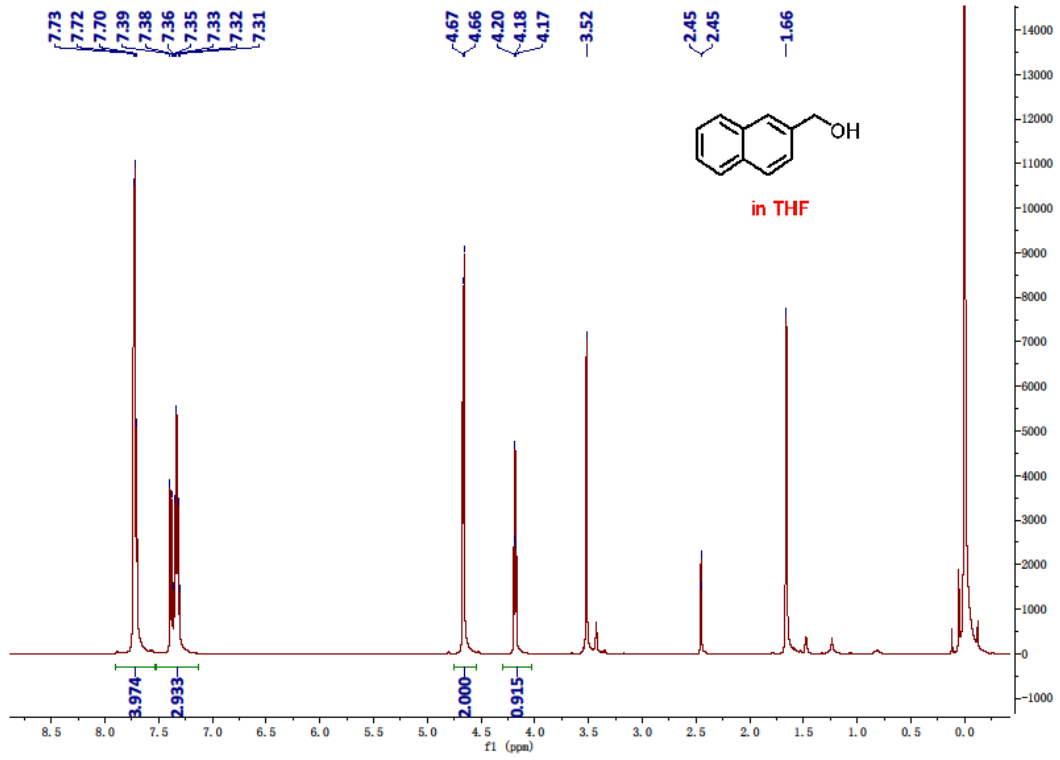
The mixture of naphthmethanol and phenylboroxine was detected by NMR and HRMS after heated at 80 °C with *d*⁸-THF as solvent for 12 h. From both ¹H NMR and ¹³C NMR, we found that ¹H NMR and ¹³C NMR signal of benzylic-CH₂ moved downfield in the presence of the phenylboroxine. And from the HRMS, we failed to get the value of the following possible benzyloboronic esters.

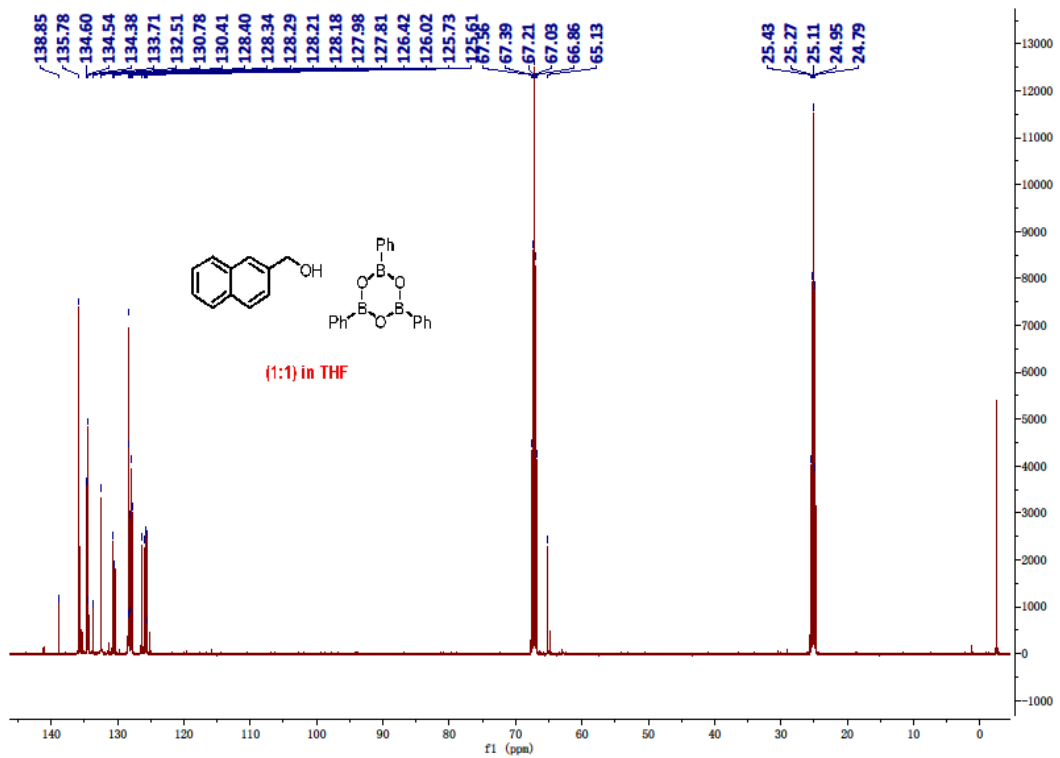
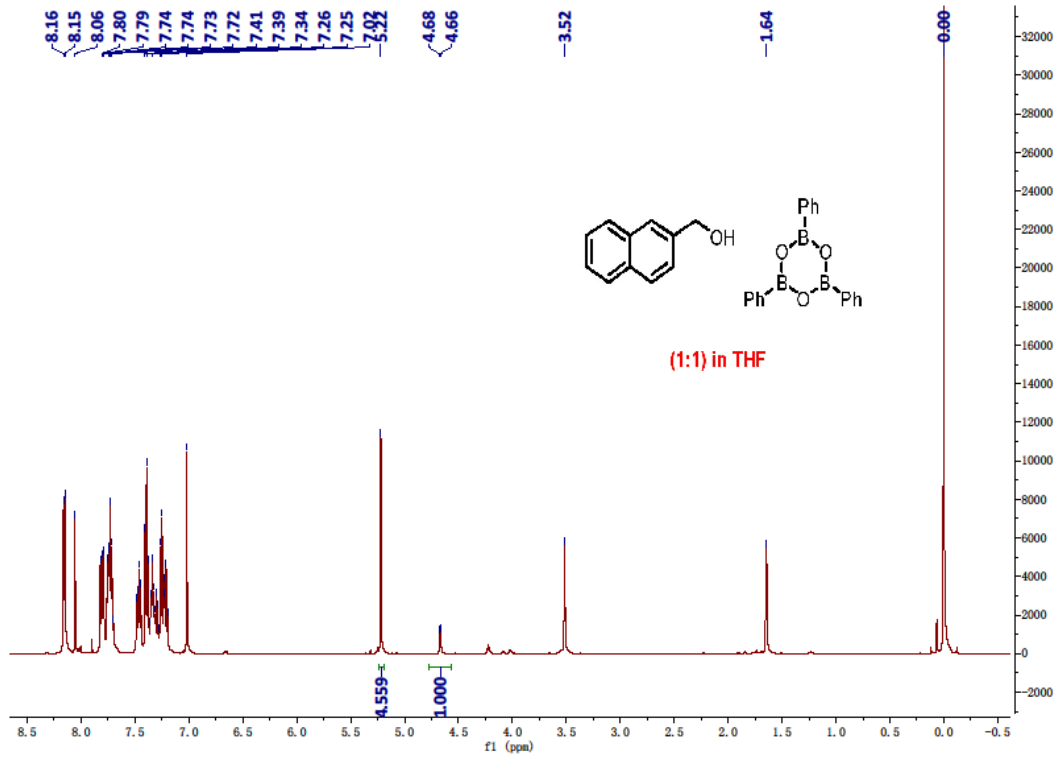
Scheme 1. Possible benzyloboronic ester



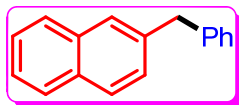
All possible intermediates are excluded!







Part 4. Synthesis and Analytical Data for Products

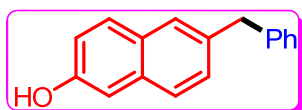


2-benzyl-naphthalene⁵ (colorless oil)

¹H NMR (CDCl₃, 400 MHz): δ 7.78-7.71 (m, 3 H), 7.61 (s, 1 H), 7.43-7.39 (m, 2 H), 7.31-7.25 (m, 3 H), 7.22-7.18 (m, 3 H), 4.13 (s, 2 H);

¹³C NMR (CDCl₃, 100 MHz): δ 140.97, 138.59, 133.60, 132.08, 129.02, 128.48, 128.06, 127.62, 127.61, 127.54, 127.08, 126.14, 125.96, 125.33, 42.10;

MS (EI) m/z: 218 (M⁺)

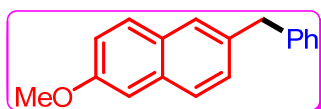


6-benzyl-2-naphthalenol (white oil)

¹H NMR (400 MHz, CDCl₃): δ 7.67 (d, *J* = 8.8 Hz, 1H), 7.59 (d, *J* = 8.5 Hz, 1H), 7.55 (s, 1H), 7.33 – 7.16 (m, 6H), 7.10 (d, *J* = 2.4 Hz, 1H), 7.06 (dd, *J* = 8.8, 2.5 Hz, 1H), 5.02 (s, 1H), 4.10 (s, 2H)

¹³C NMR (100 MHz, CDCl₃): δ 153.06, 141.16, 136.32, 133.83, 133.16, 129.46, 129.08, 129.00, 128.48, 128.35, 127.01, 126.58, 126.11, 118.15, 117.80, 109.38, 41.92.

HRMS (ESI) Anal. Calcd. (M+H⁺) 235.11174, Found: 235.11173

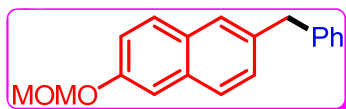


2-benzyl-6-methoxynaphthalene (white solid)

¹H NMR (400 MHz, CDCl₃): δ 7.66 (d, *J* = 2.7 Hz, 1H), 7.64 (d, *J* = 2.4 Hz, 1H), 7.55 (s, 1H), 7.32 – 7.16 (m, 7H), 7.11 (dd, *J* = 8.8, 2.6 Hz, 2H), 4.10 (s, 2H), 3.89 (s, 4H).

¹³C NMR (100 MHz, CDCl₃): δ 157.36, 141.24, 136.30, 133.14, 129.11, 129.05, 129.01, 128.48, 128.15, 126.98, 126.97, 126.09, 118.74, 105.74, 55.31, 41.93

HRMS (ESI) Anal. Calcd. (M+H⁺) 249.12739, Found: 249.12709

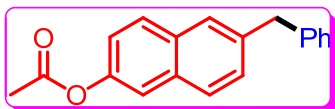


2-benzyl-6-(methoxymethoxy)naphthalene (colorless oil)

¹H NMR (400 MHz, CDCl₃): δ 7.67 (dd, *J* = 10.8, 8.8 Hz, 1H), 7.56 (s, 1H), 7.36 (d, *J* = 2.3 Hz, 1H), 7.32 – 7.15 (m, 4H), 5.27 (s, 1H), 4.10 (s, 2H), 3.51 (s, 2H).

¹³C NMR (100 MHz, CDCl₃): δ 154.78, 141.18, 136.78, 133.03, 129.68, 129.06, 129.01, 128.48, 128.19, 127.27, 126.92, 126.11, 119.05, 110.01, 94.64, 56.04, 41.96.

HRMS (ESI) Anal. Calcd. (M+H⁺) 279.13796, Found: 279.13840

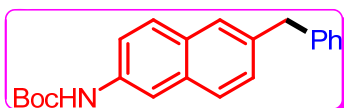


6-benzyl-2-naphthyl acetate (white solid)

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.73 (dd, $J = 23.4, 8.7$ Hz, 2H), 7.62 (s, 1H), 7.50 (d, $J = 2.0$ Hz, 1H), 7.34 – 7.24 (m, 3H), 7.20 (dt, $J = 11.1, 4.5$ Hz, 4H), 4.12 (s, 2H), 2.33 (s, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 157.36, 141.24, 136.30, 133.14, 129.11, 129.05, 129.01, 128.48, 128.15, 126.98, 126.97, 126.09, 118.74, 105.74, 55.31, 41.93.

HRMS (ESI) Anal. Calcd. ($\text{M}+\text{H}^+$) 277.12231, Found: 277.12283

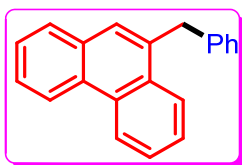


tert-butyl 6-benzyl-2-naphthylcarbamate (flavescent solid)

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.93 (s, 1H), 7.67 (d, $J = 8.5$ Hz, 2H), 7.53 (s, 1H), 7.37 – 7.14 (m, 7H), 6.60 (s, 1H), 4.10 (s, 2H), 1.54 (s, 9H)

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 152.85, 141.06, 137.24, 135.42, 132.64, 130.20, 129.04, 128.49, 128.38, 128.25, 127.58, 126.76, 126.13, 119.30, 114.48, 80.65, 41.99, 28.40.

HRMS (ESI) Anal. Calcd. ($\text{M}+\text{Na}^+$) 356.16210, Found: 356.16183

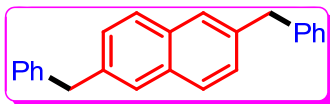


9-benzylphenanthrene (white solid)

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 8.68 (dd, $J = 23.8, 8.2$ Hz, 2H), 8.02 (d, $J = 8.0$ Hz, 1H), 7.83 – 7.77 (m, 1H), 7.66 – 7.48 (m, 5H), 7.32 – 7.15 (m, 5H), 4.47 (s, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 140.31, 134.81, 131.86, 131.43, 130.87, 129.99, 128.84, 128.53, 128.30, 127.96, 126.68, 126.66, 126.28, 126.20, 125.07, 123.15, 122.51, 99.99, 39.64.

HRMS (ESI) Anal. Calcd. ($\text{M}+\text{H}^+$) 269.13248, Found: 269.13191

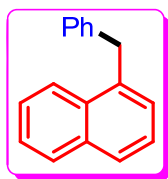


2,6-dibenzyl-1-naphthalene (white solid)

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.67 (d, $J = 8.3$ Hz, 2H), 7.58 (s, 2H), 7.33 – 7.14 (m, 12H), 4.11 (s, 4H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 141.09, 138.14, 132.28, 129.03, 128.49, 127.82, 127.77, 126.91, 126.13, 42.09.

HRMS (ESI) Anal. Calcd. ($\text{M}+\text{H}^+$) 309.16378, Found: 309.16420

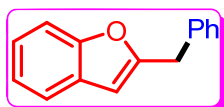


1-benzyl-naphthalene (colorless oil)

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 8.05 – 7.94 (m, 1H), 7.92 – 7.80 (m, 1H), 7.76 (d, $J = 8.2$ Hz, 1H), 7.52 – 7.35 (m, 3H), 7.34 – 7.11 (m, 6H), 4.45 (s, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 140.65, 136.64, 133.97, 132.17, 128.75, 128.67, 128.45, 127.34, 127.15, 126.06, 125.96, 125.55, 124.28, 39.05.

HRMS (ESI) Anal. Calcd. ($\text{M}+\text{Na}^+$) 241.09877, Found: 241.09946

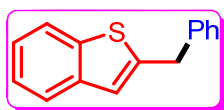


2-benzylbenzofuran⁶ (colorless oil)

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.49 – 7.43 (m, 1H), 7.43 – 7.37 (m, 1H), 7.35 – 7.13 (m, 7H), 6.36 (d, $J = 0.9$ Hz, 1H), 4.09 (s, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 157.83, 155.02, 137.28, 128.94, 128.85, 128.64, 126.79, 123.44, 122.55, 120.44, 110.94, 103.39, 35.04.

MS (EI) m/z : 208 (M^+)

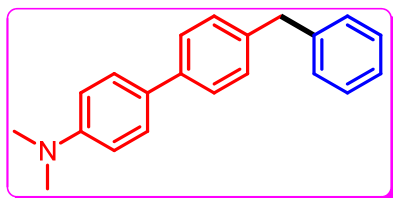


2-benzylbenzo[b]thiophene⁷ (colorless oil)

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.72 (d, $J = 7.9$ Hz, 1H), 7.64 (d, $J = 7.7$ Hz, 1H), 7.41 – 7.15 (m, 7H), 6.99 (s, 1H), 4.21 (s, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 145.17, 140.10, 139.88, 139.58, 128.81, 128.66, 126.76, 124.17, 123.67, 122.98, 122.19, 121.69, 37.02.

MS (EI) m/z : 224 (M^+)

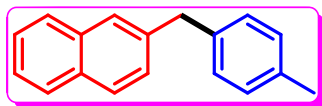


4'-benzyl-*N,N*-dimethylbiphenyl-4-amine⁸ (Yellowish solid)

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.52 – 7.43 (m, 4H), 7.33 – 7.16 (m, 7H), 6.79 (d, $J = 8.8$ Hz, 2H), 4.00 (s, 2H), 2.97 (s, 6H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 149.89, 141.28, 139.09, 138.88, 129.24, 129.14, 128.99, 128.50, 127.59, 126.37, 126.08, 112.82, 41.59, 40.62.

HRMS (ESI) Anal. Calcd. ($\text{M}+\text{H}^+$) 288.17468, Found: 288.17407.

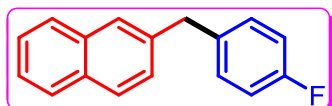


2-(4-methylbenzyl)naphthalene (colorless oil)

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.83 – 7.71 (m, 3H), 7.62 (s, 1H), 7.49 – 7.37 (m, 2H), 7.30 (dd, $J = 8.4$, 1.6 Hz, 1H), 7.15 – 7.06 (m, 4H), 4.10 (s, 2H), 2.31 (s, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 138.91, 137.95, 135.65, 133.65, 132.09, 129.20, 128.92, 128.05, 127.65, 127.63, 127.56, 127.01, 125.94, 125.30, 41.71, 21.03.

HRMS (ESI) Anal. Calcd. ($\text{M}+\text{H}^+$) 232.12465, Found: 232.12406

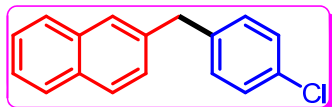


2-(4-fluorobenzyl)naphthalene (white solid)

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.85 – 7.70 (m, 3H), 7.60 (s, 1H), 7.52 – 7.38 (m, 2H), 7.27 (dd, $J = 8.4$, 1.6 Hz, 1H), 7.21 – 7.12 (m, 2H), 4.10 (s, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 161.48, (d, $J = 242.0$ Hz), 138.39, 136.61, (d, $J = 3.0$ Hz), 133.59, 132.12, 130.37 (d, $J = 8.0$ Hz), 128.17, 127.63, 127.53, 127.43, 127.02, 126.06, 125.44, 115.24 (d, $J = 21.0$ Hz), 41.23.

HRMS (ESI) Anal. Calcd. ($\text{M}+\text{Na}^+$) 255.11497, Found: 255.11432

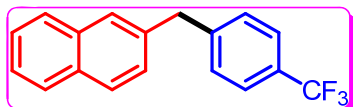


2-(4-chlorobenzyl)naphthalene (colorless oil)

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.84 – 7.72 (m, 1H), 7.60 (s, 1H), 7.50 – 7.39 (m, 1H), 7.31 – 7.22 (m, 1H), 7.15 (d, $J = 8.4$ Hz, 1H), 4.10 (s, 1H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 139.45, 138.02, 133.61, 132.16, 132.01, 130.36, 128.62, 128.25, 127.66, 127.55, 127.42, 127.13, 126.12, 125.52, 41.42.

HRMS (EI) m/z : Anal. Calcd. 252.0706, Found: 252.0710 (M^+).

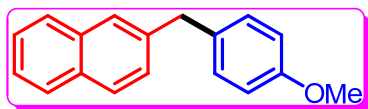


2-(4-(trifluoromethyl)benzyl)naphthalene (colorless oil)

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.84 – 7.75 (m, 1H), 7.63 (s, 1H), 7.54 (d, $J = 8.1$ Hz, 1H), 7.50 – 7.41 (m, 1H), 7.34 (d, $J = 8.0$ Hz, 1H), 7.28 (dd, $J = 8.4$, 1.6 Hz, 1H), 4.19 (s, 1H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 145.07, 137.41, 133.59, 132.20, 129.28, 128.58 (q, $J = 32.0$ Hz), 128.36, 127.66, 127.55, 127.36, 127.28, 126.19, 125.84 (q, $J = 271.0$ Hz), 125.62, 125.43 (q, $J = 4.0$ Hz), 41.87.

HRMS (EI) m/z : Anal. Calcd. 286.0969, Found: 286.0973 (M^+).

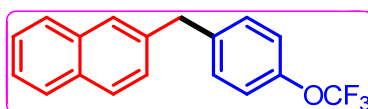


2-(4-methoxybenzyl)naphthalene (white solid)

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.84 – 7.71 (m, 3H), 7.61 (s, 1H), 7.43 (p, $J = 6.7$ Hz, 2H), 7.30 (d, $J = 8.4$ Hz, 1H), 7.14 (d, $J = 8.3$ Hz, 2H), 6.84 (d, $J = 8.4$ Hz, 2H), 4.08 (s, 2H), 3.78 (s, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 158.05, 139.08, 133.63, 133.11, 132.08, 129.98, 128.05, 127.62, 127.60, 127.55, 126.92, 125.95, 125.30, 113.94, 55.28, 41.22.

HRMS (ESI) Anal. Calcd. ($\text{M}+\text{Na}^+$) 271.10934, Found: 271.10888

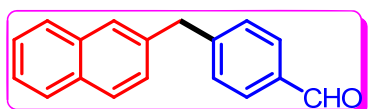


2-(4-(trifluoromethoxy)benzyl)naphthalene (white solid)

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.85 – 7.73 (m, 3H), 7.62 (s, 1H), 7.49 – 7.39 (m, 2H), 7.28 (dd, $J = 8.4$, 1.6 Hz, 1H), 7.26 – 7.19 (m, 2H), 7.13 (d, $J = 8.1$ Hz, 2H), 4.13 (s, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 147.66, 139.73, 137.87, 133.59, 132.17, 130.20, 128.28, 127.65, 127.54, 127.41, 127.17, 126.13, 125.54, 120.51 (q, $J = 255.0$ Hz), 121.02, 41.36.

HRMS (EI) m/z : Anal. Calcd. 302.0918, Found: 302.0923 (M^+).

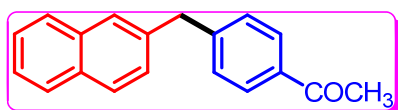


4-(naphthalen-2-ylmethyl)benzaldehyde (colorless oil)

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 9.97 (s, 1H), 7.84 – 7.74 (m, 5H), 7.63 (s, 1H), 7.50 – 7.41 (m, 2H), 7.39 (d, $J = 8.0$ Hz, 2H), 7.28 (dd, $J = 8.4$, 1.6 Hz, 1H), 4.21 (s, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 191.91, 148.27, 137.22, 134.80, 133.62, 132.24, 130.07, 129.67, 128.41, 127.68, 127.56, 127.37, 126.23, 125.67, 42.26.

HRMS (ESI) Anal. Calcd. ($\text{M}+\text{H}^+$) 247.11174, Found: 247.11226

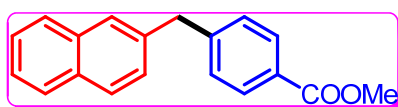


1-(4-(naphthalen-2-ylmethyl)phenyl)ethanone (colorless oil)

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.84 – 7.73 (m, 3H), 7.61 (s, 1H), 7.49 – 7.39 (m, 2H), 7.29 (dd, $J = 8.4$, 1.6 Hz, 1H), 7.06 – 6.96 (m, 2H), 6.95 – 6.87 (m, 1H), 4.06 (s, 2H), 2.22 (d, $J = 1.7$ Hz, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 197.79, 146.65, 137.51, 135.38, 133.61, 132.20, 129.22, 128.68, 128.33, 127.67, 127.56, 127.41, 127.28, 126.17, 125.60, 42.07, 26.56.

HRMS (ESI) Anal. Calcd. ($\text{M}+\text{H}^+$) 261.12739, Found: 261.12731

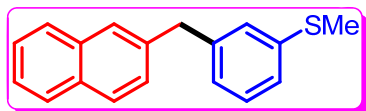


methyl 4-(naphthalen-2-ylmethyl)benzoate (white solid)

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 8.00 – 7.93 (m, 2H), 7.83 – 7.73 (m, 3H), 7.61 (s, 1H), 7.49 – 7.39 (m, 2H), 7.32 – 7.23 (m, 3H), 4.18 (s, 2H), 3.89 (s, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 167.06, 146.37, 137.61, 133.62, 132.20, 129.87, 129.06, 128.30, 128.24, 127.67, 127.57, 127.45, 127.28, 126.15, 125.57, 52.00, 42.09.

HRMS (ESI) Anal. Calcd. ($\text{M}+\text{H}^+$) 277.12231, Found: 277.12254

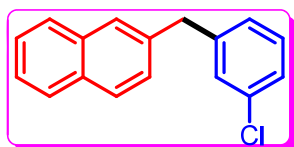


methyl(3-(naphthalen-2-ylmethyl)phenyl)sulfane (colorless oil)

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.82 – 7.72 (m, 3H), 7.62 (s, 1H), 7.48 – 7.38 (m, 2H), 7.30 (dd, $J = 8.4$, 1.6 Hz, 1H), 7.21 (dd, $J = 14.1$, 6.4 Hz, 1H), 7.16 – 7.07 (m, 2H), 6.99 (d, $J = 7.5$ Hz, 1H), 4.10 (s, 2H), 2.44 (s, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 141.67, 138.59, 138.20, 133.63, 132.15, 128.97, 128.15, 127.65, 127.59, 127.57, 127.29, 127.16, 126.04, 125.93, 125.43, 124.36, 42.02, 15.84.

HRMS (ESI) Anal. Calcd. ($\text{M}+\text{H}^+$) 265.10455, Found: 265.10458

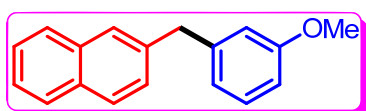


2-(3-chlorobenzyl)naphthalene (colorless oil)

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.82 – 7.73 (m, 3H), 7.61 (s, 1H), 7.49 – 7.39 (m, 2H), 7.27 (dd, $J = 8.4$, 1.7 Hz, 1H), 7.24 – 7.15 (m, 3H), 7.13 – 7.06 (m, 1H), 4.09 (s, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 143.06, 137.69, 134.35, 133.63, 132.22, 129.75, 129.13, 128.32, 127.69, 127.61, 127.46, 127.26, 127.22, 126.43, 126.15, 125.58, 41.76.

HRMS (ESI) Anal. Calcd. ($\text{M}+\text{H}^+$) 253.07785, Found: 253.07751

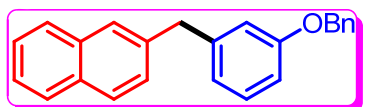


2-(3-methoxybenzyl)naphthalene (colorless oil)

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.76 (dd, $J = 14.9$, 8.6 Hz, 3H), 7.63 (s, 1H), 7.48 – 7.37 (m, 2H), 7.31 (d, $J = 8.4$ Hz, 1H), 7.21 (dd, $J = 12.8$, 4.9 Hz, 1H), 6.82 (d, $J = 7.5$ Hz, 1H), 6.75 (d, $J = 10.9$ Hz, 2H), 4.10 (s, 2H), 3.75 (s, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 159.81, 142.59, 138.44, 133.65, 132.15, 129.46, 128.09, 127.64, 127.62, 127.59, 127.12, 125.98, 125.37, 121.51, 114.92, 111.46, 55.17, 42.16.

HRMS (ESI) Anal. Calcd. ($\text{M}+\text{Na}^+$) 249.12739, Found: 249.12736

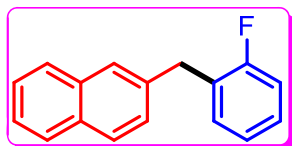


2-(3-(benzyloxy)benzyl)naphthalene (colorless oil)

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.83 – 7.69 (m, 3H), 7.61 (s, 1H), 7.47 – 7.14 (m, 9H), 6.89 – 6.78 (m,

3H), 4.99 (s, 2H), 4.09 (s, 2H).

^{13}C NMR (100 MHz, CDCl_3): δ 159.06, 142.68, 138.40, 137.08, 133.68, 132.18, 129.51, 128.57, 128.13, 127.93, 127.66, 127.63, 127.56, 127.18, 126.01, 125.40, 121.77, 115.86, 112.44, 69.97, 42.17.
HRMS (ESI) Anal. Calcd. ($\text{M}+\text{H}^+$) 325.15869, Found: 325.15794

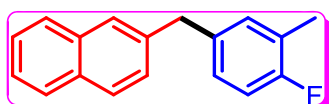


2-(2-fluorobenzyl)naphthalene (colorless oil)

^1H NMR (400 MHz, CDCl_3): δ 7.77 (dd, $J = 12.4, 7.8$ Hz, 3H), 7.64 (s, 1H), 7.48 – 7.37 (m, 2H), 7.34 (dd, $J = 8.4, 1.3$ Hz, 1H), 7.25 – 7.12 (m, 2H), 7.09 – 6.99 (m, 2H), 4.15 (s, 2H).

^{13}C NMR (100 MHz, CDCl_3): δ 161.00 (d, $J = 244.0$ Hz), 159.78, 137.33, 133.60, 132.14, 131.10 (d, $J = 5.0$ Hz), 128.12, 128.00 (d, $J = 8.0$ Hz), 127.85, 127.58 (d, $J = 5.0$ Hz), 127.39, 127.04, 125.99, 125.40, 124.08 (d, $J = 4.0$ Hz), 115.33 (d, $J = 21.0$ Hz), 34.91 (d, $J = 3.0$ Hz).

HRMS (ESI) Anal. Calcd. ($\text{M}+\text{H}^+$) 237.10741, Found: 237.10769

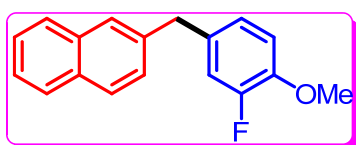


2-(4-fluoro-3-methylbenzyl)naphthalene (colorless oil)

^1H NMR (400 MHz, CDCl_3): δ 7.84 – 7.71 (m, 3H), 7.60 (s, 1H), 7.49 – 7.38 (m, 2H), 7.28 (dt, $J = 9.3, 4.7$ Hz, 1H), 7.06 – 6.95 (m, 2H), 6.95 – 6.87 (m, 1H), 4.06 (s, 2H), 2.22 (d, $J = 1.7$ Hz, 3H).

^{13}C NMR (100 MHz, CDCl_3): δ 160.01 (d, $J = 242.0$ Hz), 138.60, 136.30 (d, $J = 4.0$ Hz), 133.60, 132.10, 131.92 (d, $J = 5.0$ Hz), 128.13, 127.62 (d, $J = 8.0$ Hz), 127.63, 127.53, 127.48, 126.98, 126.02, 125.39, 124.69 (d, $J = 18.0$ Hz), 114.83 (d, $J = 22.0$ Hz), 41.28, 14.51 (d, $J = 3.0$ Hz).

HRMS (ESI) Anal. Calcd. ($\text{M}+\text{H}^+$) 273.10500, Found: 273.10542



2-(3-fluoro-4-methoxybenzyl)naphthalene (colorless oil)

^1H NMR (400 MHz, CDCl_3): δ 7.84 – 7.72 (m, 3H), 7.60 (s, 1H), 7.49 – 7.38 (m, 2H), 7.28 (dd, $J = 8.4, 1.6$ Hz, 1H), 6.98 – 6.83 (m, 3H), 4.05 (s, 2H), 3.85 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3): δ 152.40 (d, $J = 244.0$ Hz), 146.98 (d, $J = 10.0$ Hz), 138.21, 134.14 (d, $J = 6.0$ Hz), 133.59, 132.13, 128.18, 127.62, 127.53, 127.39, 127.01, 126.05, 125.44, 124.42 (d, $J = 4.0$ Hz), 116.70 (d, $J = 18.0$ Hz), 113.53 (d, $J = 2.0$ Hz), 56.36, 41.10 (d, $J = 1.0$ Hz).

HRMS (ESI) Anal. Calcd. ($\text{M}+\text{Na}^+$) 289.09991, Found: 289.09945.

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II. Spectral Data for Compounds

