

Palladium(0)-catalyzed direct cross-coupling reaction of allylic alcohols with aryl- and alkenylboronic acids

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Supplementary Material

General Procedure for the cross-coupling reaction between **4** and **3a** (Table 1): To a test tube containing cinnamyl alcohol (**4**) (1 equiv, see Table 1S), phenylboronic acid (**3a**) (1.2 equiv), and Pd(PPh₃)₄ (0.2-10 mol %) or Pd₂dba₃ (2.5 mol %)-PPh₃ (5 or 10 mol %) was added anhydrous solvent (CH₂Cl₂, Toluene, 1,4-Dioxane, DMF, THF, or tAmOH, 0.3 M) under argon. The resulting mixture was sealed with a screw cap and agitated at 80 °C for the time described in Table 1. The mixture was cooled down to room temperature, and then *N,N*-diethanolaminomethyl polystyrene (PS-DEAMTM, 1.63 mmol/g, 2.4 equiv, X g) and THF (10 x X mL) were added to remove an excess of **3a**. The mixture was agitated at room temperature for 2 h. The mixture was filtered and thoroughly washed with CHCl₃. The filtrate was concentrated *in vacuo* and the residue was purified by gel permeation chromatography (GPC) repeated four times to afford **5a** in the yield described in Table 1.

General Procedure for the cross-coupling reaction between **4** and phenylboron reagents (Table 2): To a test tube containing **4** (0.37 mmol, see Table 2S), phenylboron reagent (0.45 mmol), and Pd(PPh₃)₄ (1.8 μmol) was added anhydrous THF (1 mL) under argon. The resulting mixture was sealed with a screw cap and agitated at 80 °C for 6 h. The mixture was cooled down to room temperature, and then partitioned between EtOAc and saturated aqueous Na₂CO₃. The organic layers were washed with water, brine, dried over MgSO₄, and concentrated *in vacuo*. The residue was purified by GPC repeated four times to afford **5a** in the yield described in Table 2.

General Procedure for the cross-coupling reaction between cinnamyl derivatives and **3a** (Table 3): To a test tube containing cinnamyl derivative (0.37 mmol, see Table 3S), **3a** (0.45 mmol), and Pd(PPh₃)₄ (1.8 μmol) was added anhydrous THF (1 mL) under argon. The resulting mixture was sealed with a screw cap and agitated at 80 °C for the time described in Table 3. The mixture was cooled down to room temperature, and then PS-DEAMTM (1.63 mmol/g, 0.55 g, 0.90 mmol) and THF (5 mL) were added to remove an excess of **3a**. The mixture was agitated at room temperature for 2 h. The mixture was filtered and thoroughly washed with CHCl₃. The filtrate was concentrated *in vacuo* and the residue was purified by GPC repeated several times to afford **5a** in the yield described in Table 3.

Table 1S

	Entry	4 (mg)	3a (mg)	[Pd] (mg)	PPh ₃ (mg)	5a (mg)
	1	40.9	44.0	17.0	-	44.0
	2	40.1	44.9	6.6	-	39.2
	3	40.0	44.0	17.0	-	38.1
	4	40.6	44.5	7.6	-	43.7
	5	40.6	44.0	17.0	-	37.2
	6	40.6	44.0	7.1	-	46.9
	7	50.3	54.7	21.5	-	32.8
	8	50.9	55.7	9.1	-	51.5
	9	41.8	46.9	17.1	-	40.0
	10	40.9	44.3	7.7	-	47.9
	11	38.5	44.8	34.0	-	26.0
	12 ^a	40.7	44.5	6.9	7.8	48.8
	13 ^b	41.0	45.5	6.7	3.8	49.1
	14	41.0	45.0	3.5	-	50.2
	15	49.1	55.1	2.4	-	61.7
	16	96.1	109.4	1.8	-	88
	17	42.7	45.5	1.8	-	49.8

Table 2S

	Entry	4 (mg)	[PhB]; (mg)	[Pd] (mg)	5a (mg)
	1	49.3	(PhBO) ₃ ; 46.1	2.4	52.0
	2	49.6	PhB(pinacolato); 95.1	2.3	nd
	3	47.9	PhB(catecholato); 88.0	2.2	18.3
	4	49.9	Ph ₃ B; 108.3	2.1	45.3
	5	47.9	Ph ₄ BNa; 153.0	2.4	22.1

Table 3S

	Entry	X; (mg)	3a (mg)	[Pd] (mg)	5a (mg)
	1	OMe; 53.1	54.3	2.1	59.3
	2	OCO ₂ Me; 71.5	55.9	2.0	65.8
	3	OC ₆ H ₄ -4-OMe; 90.4	56.1	2.2	59.3
	4	OAc; 65.8	54.9	2.0	15.4

General Procedure for the cross-coupling reaction between **4** and **3a** (Table 4): To a test tube containing **4** (0.30 mmol, see Table 4S), **3a** (0.36 mmol), Pd₂dba₃ (1.5 µmol), and ligand (3 µmol) was added anhydrous THF (1 mL) under argon. The resulting mixture was sealed with a screw cap and agitated at 80 °C for 2 h. The mixture was cooled down to room temperature, and then PS-DEAM™ (1.63 mmol/g, 0.44 g, 0.72 mmol) and THF (4 mL) were added to remove an excess of **3a**. The mixture was agitated at room temperature for 2 h. The mixture was filtered and thoroughly washed with CHCl₃. The filtrate was concentrated *in vacuo* and the residue was purified by GPC repeated four times to afford **5a** in the yield described in Table 4.

Table 4S

	Entry	4 (mg)	3a (mg)	[Pd] (mg)	Ligand (mg)	5a (mg)
1	39.3	44.2	1.4	P(C ₆ H ₅) ₃ ; 0.8	49.6	
2	39.8	45.0	1.5	P(C ₆ H ₄ -4-OMe) ₃ ; 1.4	27.7	
3	39.9	45.4	1.5	P(C ₆ H ₄ -4-Cl) ₃ ; 1.1	28.4	
4	39.9	44.9	1.4	P(2-furyl) ₃ ; 0.9	41.1	
5	41.0	45.4	1.4	P(2-thienyl) ₃ ; 1.0	48.4	
6	39.2	45.1	1.4	P(OPh) ₃ ; 1.1	48.7	
7	40.3	44.1	1.6	P(OEt) ₃ ; 0.5	48.7	
8	39.6	43.9	1.5	PCy ₃ ; 0.8	12.5	
9	39.4	45.4	1.6	PBu ₃ ; 0.6	nd	
10	39.8	44.6	1.4	dppe; 0.6	nd	
11	39.1	44.1	1.6	AsPh ₃ ; 0.9	30.0	

General Procedure for the cross-coupling reaction between **4** and boronic acids **3b-z** (Table 5): To a test tube containing **4** (0.37 mmol, see Table 5S), **3b-z** (0.45 mmol), and Pd(PPh₃)₄ (1.8 µmol) was added anhydrous THF (1 mL) under argon. The resulting mixture was sealed with a screw cap and agitated at 80 °C for the time described in Table 5. The mixture was cooled down to room temperature, and then PS-DEAM™ (1.63 mmol/g, 0.55 g, 0.90 mmol) and THF (5 mL) were added to remove an excess of **3b-z**. The mixture was agitated at room temperature for 2 h. The mixture was filtered and thoroughly washed with CHCl₃. The filtrate was concentrated *in vacuo* and the residue was purified by GPC repeated four times to afford **5b-z** in the yield described in Table 5.

Table 5S

	Entry 4 (mg)	3 (mg)	[Pd] (mg)	5 (mg)
1	51.0	3b ; 68.9	2.3	5b ; 78.4
2	49.2	3c ; 75.3	1.9	5c ; 78.9
3	50.9	3d ; 75.3	2.1	5d ; 69.0
4	49.1	3e ; 80.1	4.3	5e ; 82.5
5	49.2	3f ; 62.1	2.1	5f ; 67.3
6	49.1	3g ; 61.6	2.2	5g ; 68.5
7	51.4	3h ; 61.6	2.0	5h ; 70.4
8	49.8	3i ; 68.0	2.5	5i ; 28.3
9	50.2	3j ; 67.1	2.4	5j ; 70.0
10	49.1	3k ; 64.6	2.0	5k ; 67.5
11	49.2	3l ; 70.4	2.6	5l ; 69.9
12	49.1	3m ; 85.8	1.9	5m ; 80.2
13	50.4	3n ; 67.1	2.2	5n ; 62.4
14	50.1	3o ; 87.3	2.0	5o ; 84.9
15	49.4	3p ; 73.3	2.5	5p ; 72.4
16	49.5	3q ; 66.6	2.3	5q ; 66.5
17	48.7	3r ; 75.9	2.2	5r ; 63.2
18	49.2	3s ; 77.1	2.3	5s ; 77.0
19	51.1	3t ; 76.7	2.1	5t ; 73.5
20	46.7	3u ; 96.2	2.6	5u ; nd
21	49.6	3v ; 96.5	2.0	5v ; 69.8
22	48.5	3w ; 110.1	2.1	5w ; 70.5
23	49.7	3x ; 111.2	2.4	5x ; 58.4
24	51.5	3y ; 64.2	2.1	5y ; 41.0
25	51.4	3z ; 65.7	2.1	5z ; 46.0

General Procedure for the cross-coupling reaction between **6-13** and **3a** (Table 6): To a test tube containing **6-13** (0.37 mmol, see Table 6S), **3a** (0.45 mmol), and Pd(PPh₃)₄ (1.8 μmol) was added anhydrous THF (1 mL) under argon. The resulting mixture was sealed with a screw cap and agitated at 80 °C for the time described in Table 6. The mixture was cooled down to room temperature, and then PS-DEAMTM (1.63 mmol/g, 0.55 g, 0.90 mmol) and THF (5 mL) were added to remove an excess of **3a**. The mixture was agitated at room temperature for 2 h. The mixture was filtered and thoroughly washed with CHCl₃. The filtrate was concentrated *in vacuo* and the residue was purified by GPC repeated several times to afford **5a** and **14-17** in the yield described in Table 6. The optical

rotation of **15** prepared from **10** was 0°.

Table 6S

Entry	Alcohol (mg)	3a (mg)	[Pd] (mg)	Product (mg)
1	6 ; 49.7	55.4	2.2	5a ; 65.0
2	7 ; 50.0	55.5	2.2	5a ; 63.9
3	8 ; 55.4	55.3	2.3	14 ; 53.8
4	9 ; 53.2	55.4	2.0	14 ; 59.5
5	10 ; 55.8	56.0	2.3	15 ; 62.2
6	11 ; 56.3	55.7	2.2	15 ; 58.0
7	12 ; 78.1	55.0	1.9	16 ; 80.3
8	13 ; 57.0	58.8	2.4	17 ; 52.4

General Procedure for the cross-coupling reaction between **1** or **20-25** and **3s** (Table 7): To a test tube containing **1** or **20-25** (0.45 mmol, see Table 7S), **3s** (0.52 mmol), and Pd(PPh₃)₄ (1.8 μmol) was added anhydrous THF (1 mL for Entries 1-5) or 1,4-dioxane (1 mL, for Entries 6, 7) under argon. The resulting mixture was sealed with a screw cap and agitated at 80 (for Entries 1-5) or 110 °C (Entries 6, 7) for the time described in Table 7. The mixture was cooled down to room temperature, and then PS-DEAMTM (1.63 mmol/g, 0.55 g, 0.90 mmol) and THF (5 mL) were added to remove an excess of **3s**. The mixture was agitated at room temperature for 2 h. The mixture was filtered and thoroughly washed with CHCl₃. The filtrate was concentrated *in vacuo* and the residue was purified by GPC repeated several times to afford **2s** or **26-31** in the yield described in Table 7.

Table 7S

Entry	Alcohol (mg)	3s (mg)	[Pd] (mg)	Product (mg)
1	1 ; 26.3	89.2	2.2	2s ; 61.2
2	20 ; 32.8	89.2	2.4	26+27 ; 61.1
3	21 ; 31.9	90.0	2.2	26+27 ; 68.8
4	22 ; 39.8	89.2	2.2	28 ; 53.3
				29 ; 4.5
5	23 ; 38.2	89.3	2.4	28 ; 57.1
				29 ; 7.7
6	24 ; 32.3	89.7	2.2	30 ; 62.9
7	25 ; 45.9	90.1	2.4	31 ; 22.1

Spectral data of the cross-coupling products

(*E*)-1,3-Diphenyl-1-propene (**5a**): ^1H NMR (400 MHz, CDCl_3): δ 7.34–7.15 (m, 10H), 6.43 (d, 1H, $J=16.0$ Hz), 6.34 (dt, 1H, $J=16.0$, 6.4 Hz), 3.52 (d, 2H, $J=6.4$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 140.1, 137.4, 131.0, 129.1, 128.6, 128.4, 127.0, 126.1, 126.0, 39.4; IR (neat): ν_{max} (cm^{-1}) 1654, 1600, 1495, 1451, 963; EI-MS m/z (relative intensity) 194 (M^+) (100), 179 (37), 165 (11), 115 (46), 103 (12), 91 (21), 77 (7); HRMS calcd for $\text{C}_{15}\text{H}_{14}$ (M^+) 194.1096, found 194.1086.

(*E*)-3-(4-Methoxyphenyl)-1-phenylpropene (**5b**): ^1H NMR (400 MHz, CDCl_3): δ 7.34–6.81 (m, 9H), 6.40 (d, 1H, $J=16.0$ Hz), 6.31 (dt, 1H, $J=16.0$, 6.4 Hz), 3.75 (s, 3H), 3.46 (d, 2H, $J=6.4$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 157.9, 137.4, 132.0, 130.6, 129.54, 129.48, 128.4, 126.9, 126.0, 113.8, 55.2, 38.5; IR (neat): ν_{max} (cm^{-1}) 1654, 1609, 1509, 1243, 1034, 965; EI-MS m/z (relative intensity) 224 (M^+) (100), 208 (35), 193 (50), 178 (20), 165 (15), 147 (8), 121 (21), 115 (49), 91 (21), 77 (12); HRMS calcd for $\text{C}_{16}\text{H}_{16}\text{O}$ (M^+) 224.1201, found 224.1180.

(*E*)-3-(4-Methylthiophenyl)-1-phenylpropene (**5c**): ^1H NMR (400 MHz, CDCl_3): δ 7.35–7.14 (m, 9H), 6.43 (d, 1H, $J=16.0$ Hz), 6.31 (dt, 1H, $J=16.0$, 6.4 Hz), 3.49 (d, 2H, $J=6.4$ Hz), 2.46 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 137.3, 137.1, 135.7, 131.0, 129.1, 128.9, 128.4, 127.1, 127.0, 126.0, 38.8, 16.3; IR (neat): ν_{max} (cm^{-1}) 1598, 1493, 963; EI-MS m/z (relative intensity) 240 (M^+) (100), 193 (58), 178 (20), 165 (8), 137 (20), 115 (49), 91 (18), 77 (6); HRMS calcd for $\text{C}_{16}\text{H}_{16}\text{S}$ (M^+) 240.0973, found 240.0953.

(*E*)-3-(4-*N,N*-Dimethylaminophenyl)-1-phenylpropene (**5d**): ^1H NMR (400 MHz, CDCl_3): δ 7.35 (d, 2H, $J=7.3$ Hz), 7.28 (dd, 2H, $J=7.3$, 7.3 Hz), 7.18 (t, 1H, $J=7.3$ Hz), 7.10 (d, 1H, $J=8.8$ Hz), 6.72 (d, 1H, $J=8.8$ Hz), 6.43 (d, 1H, $J=15.8$ Hz), 6.34 (dt, 1H, $J=15.8$, 6.5 Hz), 3.46 (d, 2H, $J=6.5$ Hz), 2.92 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 148.9, 137.3, 130.0, 129.8, 128.9, 128.1, 127.8, 126.5, 125.7, 112.7, 40.8, 38.3; IR (neat): ν_{max} (cm^{-1}) 3023, 2885, 1613, 1517, 1341, 964, 946, 816, 797, 747, 696; EI-MS m/z (relative intensity) 237 (M^+) (100), 193 (11), 160 (9), 134 (19), 115 (11), 91 (5); HRMS calcd for $\text{C}_{17}\text{H}_{19}\text{N}$ (M^+) 237.1517, found 237.1517.

(*E*)-3-(4-Acetamidophenyl)-1-phenylpropene (**5e**): ^1H NMR (400 MHz, CDCl_3): δ 7.42 (d, 1H, $J=8.3$ Hz), 7.34 (d, 2H, $J=7.2$ Hz), 7.28 (dd, 2H, $J=7.3$, 7.3 Hz), 7.19 (t, 1H, $J=7.3$ Hz), 7.17 (d, 1H, $J=8.3$ Hz), 6.42 (d, 1H, $J=15.9$ Hz), 6.31 (dt, 1H, $J=15.9$, 6.6 Hz), 3.50 (d, 2H, $J=6.6$ Hz), 2.15 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 168.1, 137.2, 136.0, 135.9, 130.9, 128.99, 128.97, 128.3, 126.9, 125.9, 120.0, 38.8, 24.7; IR (neat): ν_{max} (cm^{-1}) 3304, 1660, 1603, 1535, 1512, 1408, 1367, 1319, 961, 829, 740, 691; EI-MS m/z (relative intensity) 251 (M^+) (100), 209 (80), 194 (12), 132 (12), 115 (18), 106 (19), 91(10); HRMS calcd for $\text{C}_{17}\text{H}_{17}\text{NO}$ (M^+) 251.1310, found 251.1319.

(*E*)-3-(4-Methylphenyl)-1-phenylpropene (**5f**): ^1H NMR (400 MHz, CDCl_3): δ 7.34–7.11 (m, 9H), 6.42 (d, 1H, $J=16.0$ Hz), 6.32 (dt, 1H, $J=16.0$, 6.4 Hz), 3.49 (d, 2H, $J=6.4$ Hz), 2.31 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 137.4, 136.9, 135.5, 130.7, 129.4, 129.1, 128.5, 128.4, 126.9, 126.0,

38.9, 21.1; IR (neat): ν_{max} (cm^{-1}) 1654, 1598, 1513, 1495, 963; EI-MS m/z (relative intensity) 208 (M^+) (100), 193 (86), 178 (22), 165 (13), 129 (11), 115 (53), 91 (19), 77 (9); HRMS calcd for $\text{C}_{16}\text{H}_{16}$ (M^+) 208.1252, found 208.1234.

(*E*)-3-(2-Methylphenyl)-1-phenylpropene (**5g**): ^1H NMR (400 MHz, CDCl_3): δ 7.32-7.13 (m, 9H), 6.35 (d, 1H, $J=16.0$ Hz), 6.30 (dt, 1H, $J=16.0, 4.8$ Hz), 3.50 (d, 2H, $J=4.8$ Hz), 2.31 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 138.1, 137.4, 136.3, 130.8, 130.1, 129.1, 128.42, 128.37, 126.9, 126.3, 125.99, 125.96, 36.9, 19.5; IR (neat): ν_{max} (cm^{-1}) 1648, 1600, 1493, 965; EI-MS m/z (relative intensity) 208 (M^+) (100), 193 (78), 178 (26), 167 (22), 130 (15), 115 (64), 104 (44), 91 (30), 77 (17); HRMS calcd for $\text{C}_{16}\text{H}_{16}$ (M^+) 208.1252, found 208.1236.

(*E*)-3-(3-Methylphenyl)-1-phenylpropene (**5h**): ^1H NMR (400 MHz, CDCl_3): δ 7.35-7.01 (m, 9H), 6.44 (d, 1H, $J=16.0$ Hz), 6.33 (dt, 1H, $J=16.0, 6.4$ Hz), 3.50 (d, 2H, $J=6.4$ Hz), 2.32 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 140.0, 138.0, 137.4, 130.8, 129.33, 129.25, 128.4, 128.3, 127.0, 126.8, 126.0, 125.6, 39.3, 21.4; IR (neat): ν_{max} (cm^{-1}) 1654, 1605, 1493, 1447, 963; EI-MS m/z (relative intensity) 208 (M^+) (100), 193 (79), 178 (22), 165 (12), 129 (11), 115 (50), 91 (19), 77 (9); HRMS calcd for $\text{C}_{16}\text{H}_{16}$ (M^+) 208.1252, found 208.1239.

(*E*)-3-(2,6-Dimethylphenyl)-1-phenylpropene (**5i**): ^1H NMR (400 MHz, CDCl_3): δ 7.30-7.23 (m, 4H), 7.16 (t, 1H, $J=7.0$ Hz), 7.06-7.02 (m, 3H), 6.28 (dt, 1H, $J=16.1, 4.9$ Hz), 6.22 (d, 1H, $J=16.1$ Hz), 3.55 (d, 2H, $J=4.9$ Hz), 2.34 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 137.4, 136.6, 136.0, 129.8, 128.3, 127.9, 127.2, 126.8, 126.0, 125.8, 33.0, 22.1; IR (neat): ν_{max} (cm^{-1}) 3023, 1468, 1446, 963, 767, 730, 692; EI-MS m/z (relative intensity) 222 (M^+) (100), 207 (66), 129 (31), 118 (91), 115 (44), 91 (30); HRMS calcd for $\text{C}_{17}\text{H}_{18}$ (M^+) 222.1409, found 222.1390.

(*E*)-3-(4-Ethenylphenyl)-1-phenylpropene (**5j**): ^1H NMR (400 MHz, CDCl_3): δ 7.37-7.34 (m, 4H), 7.29 (dd, 2H, $J=7.8, 7.3$ Hz), 7.21-7.19 (m, 3H), 6.71 (dd, 1H, $J=17.6, 10.7$ Hz), 6.45 (d, 1H, $J=15.9$ Hz), 6.34 (dd, 1H, $J=15.9, 6.6$ Hz), 5.72 (d, 1H, $J=17.6$ Hz), 5.21 (d, 1H, $J=10.7$ Hz), 3.53 (d, 2H, $J=6.6$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 139.6, 137.3, 136.4, 135.5, 131.0, 128.9, 128.7, 128.3, 127.0, 126.2, 126.0, 113.1, 39.1; IR (neat): ν_{max} (cm^{-1}) 3024, 1510, 989, 964, 905, 832, 757, 738, 691; EI-MS m/z (relative intensity) 220 (M^+) (100), 205 (63), 129 (23), 115 (25), 91 (15); HRMS calcd for $\text{C}_{17}\text{H}_{16}$ (M^+) 220.1252, found 220.1243.

(*E*)-3-(4-Fluorophenyl)-1-phenylpropene (**5k**): ^1H NMR (400 MHz, CDCl_3): δ 7.35-6.95 (m, 9H), 6.42 (d, 1H, $J=15.6$ Hz), 6.31 (dt, 1H, $J=15.6, 6.4$ Hz), 3.50 (d, 2H, $J=6.4$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 161.4 (d, $J=243.0$ Hz), 137.2, 135.6 (d, $J=3.3$ Hz), 131.1, 129.9 (d, $J=7.5$ Hz), 128.9, 128.4, 127.1, 126.0, 115.1 (d, $J=20.7$ Hz), 38.5; IR (neat): ν_{max} (cm^{-1}) 1648, 1600, 1507, 1219, 965; EI-MS m/z (relative intensity) 212 (M^+) (100), 197 (29), 183 (8), 133 (23), 115 (24), 109 (14), 91 (11), 83 (5), 77 (5); HRMS calcd for $\text{C}_{15}\text{H}_{13}\text{F}$ (M^+) 212.1001, found 212.1013.

(*E*)-3-(4-Chlorophenyl)-1-phenylpropene (**5l**): ^1H NMR (400 MHz, CDCl_3): δ 7.34-7.13 (m, 9H), 6.42 (d, 1H, $J=15.6$ Hz), 6.28 (dt, 1H, $J=15.6, 6.8$ Hz), 3.48 (d, 2H, $J=6.8$ Hz); ^{13}C NMR (100 MHz,

CDCl_3): δ 138.5, 137.1, 131.8, 131.4, 129.9, 128.5, 128.4, 127.2, 126.0, 38.6; IR (neat): ν_{\max} (cm^{-1}) 1648, 1598, 1492, 1090, 965; EI-MS m/z (relative intensity) 228 (M^+) (87), 193 (100), 178 (35), 165 (14), 149 (10), 125 (15), 115 (75), 91 (21), 77 (10); HRMS calcd for $C_{15}\text{H}_{13}\text{Cl}$ (M^+) 228.0706, found 228.0686.

(*E*)-1-Phenyl-3-[4-(trifluoromethyl)phenyl]propene (**5m**): ^1H NMR (400 MHz, CDCl_3): δ 7.54 (d, 2H, $J=8.0$ Hz), 7.36-7.18 (m, 7H), 6.46 (d, 1H, $J=16.0$ Hz), 6.30 (dt, 1H, $J=16.0, 6.8$ Hz), 3.58 (d, 2H, $J=6.8$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 144.2, 137.0, 131.8, 128.9, 128.49 (q, $J=10.8$ Hz), 128.48, 127.8, 127.3, 126.1, 125.33, 125.32 (q, $J=4.1$ Hz), 39.1; IR (neat): ν_{\max} (cm^{-1}) 1619, 1600, 1495, 1322, 965; EI-MS m/z (relative intensity) 262 (M^+) (100), 247 (12), 193 (57), 178 (18), 165 (8), 115 (43), 91 (22), 77 (8); HRMS calcd for $C_{16}\text{H}_{13}\text{F}_3$ (M^+) 262.0969, found 262.0955.

(*E*)-3-(4-Formylphenyl)-1-phenylpropene (**5n**): ^1H NMR (400 MHz, CDCl_3): δ 9.96 (s, 1H), 7.81 (d, 2H, $J=8.0$ Hz), 7.39-7.18 (m, 7H), 6.47 (d, 1H, $J=16.0$ Hz), 6.31 (dt, 1H, $J=16.0, 7.2$ Hz), 3.60 (d, 2H, $J=7.2$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 191.7, 147.3, 136.9, 134.6, 131.9, 129.9, 129.2, 128.4, 127.4, 127.3, 126.0, 39.4; IR (neat): ν_{\max} (cm^{-1}) 1696, 1603, 1495, 965; EI-MS m/z (relative intensity) 222 (M^+) (100), 193 (70), 178 (31), 165 (11), 131 (31), 115 (61), 91 (26), 77 (17); HRMS calcd for $C_{16}\text{H}_{14}\text{O}$ (M^+) 222.1045, found 222.1030.

(*E*)-3-[4-(Ethoxycarbonyl)phenyl]-1-phenylpropene (**5o**): ^1H NMR (400 MHz, CDCl_3): δ 7.99 (d, 2H, $J=8.3$ Hz), 7.35 (d, 2H, $J=7.1$ Hz), 7.32-7.27 (m, 4H), 7.21 (t, 1H, $J=7.2$ Hz), 6.46 (d, 1H, $J=15.9$ Hz), 6.33 (dt, 1H, $J=15.9, 6.8$ Hz), 4.37 (q, 2H, $J=7.2$ Hz), 3.60 (d, 2H, $J=6.8$ Hz), 1.39 (t, 3H, $J=7.2$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 166.3, 145.3, 137.0, 131.6, 129.6, 128.49, 128.41, 128.39, 127.95, 127.2, 126.0, 60.9, 39.4, 14.5; IR (neat): ν_{\max} (cm^{-1}) 2980, 1711, 1270, 1176, 1100, 1021, 964, 754, 742, 692; EI-MS m/z (relative intensity) 266 (M^+) (55), 237 (22), 221 (29), 193 (100), 178 (26), 115 (43), 91 (11); HRMS calcd for $C_{18}\text{H}_{18}\text{O}_2$ (M^+) 266.1307, found 266.1291.

(*E*)-3-(4-Acetylphenyl)-1-phenylpropene (**5p**): ^1H NMR (400 MHz, CDCl_3): δ 7.89 (d, 2H, $J=8.4$ Hz), 7.36-7.18 (m, 7H), 6.46 (d, 1H, $J=16.0$ Hz), 6.31 (dt, 1H, $J=16.0, 6.8$ Hz), 3.58 (d, 2H, $J=6.8$ Hz), 2.57 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 197.6, 145.7, 137.0, 135.2, 131.7, 128.7, 128.5, 128.4, 127.8, 127.2, 126.0, 39.2, 26.6; IR (neat): ν_{\max} (cm^{-1}) 1677, 1605, 1495, 1449, 959; EI-MS m/z (relative intensity) 236 (M^+) (100), 221 (64), 193 (62), 178 (27), 148 (12), 133 (30), 115 (37), 105 (20), 91 (18), 77 (18), 43 (17); HRMS calcd for $C_{17}\text{H}_{16}\text{O}$ (M^+) 236.1201, found 236.1172.

(*E*)-3-(4-Cyanophenyl)-1-phenylpropene (**5q**): ^1H NMR (400 MHz, CDCl_3): δ 7.58 (d, 2H, $J=8.4$ Hz), 7.41-7.20 (m, 7H), 6.46 (d, 1H, $J=16.0$ Hz), 6.28 (dt, 1H, $J=16.0, 6.8$ Hz), 3.59 (d, 2H, $J=6.8$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 145.7, 136.8, 132.3, 132.2, 129.3, 128.5, 127.4, 127.0, 126.1, 118.9, 100.0, 39.3; IR (neat): ν_{\max} (cm^{-1}) 2227, 1605, 1503, 1449, 967; EI-MS m/z (relative intensity) 219 (M^+) (100), 204 (27), 190 (8), 141 (14), 115 (18), 103 (7), 91 (13), 77 (7); HRMS calcd for $C_{16}\text{H}_{13}\text{N}$ (M^+) 219.1048, found 219.1048.

(*E*)-3-(3-Nitrophenyl)-1-phenylpropene (**5r**): ^1H NMR (400 MHz, CDCl_3): δ 8.10-8.05 (m, 2H), 7.56

(d, 1H, $J=7.6$ Hz), 7.45 (t, 1H, $J=7.6$ Hz) 7.37-7.20 (m, 5H), 6.49 (d, 1H, $J=15.6$ Hz), 6.31 (dt, 1H, $J=15.6$, 6.8 Hz), 3.64 (d, 2H, $J=6.8$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 142.1, 136.7, 134.8, 132.3, 129.2, 128.5, 127.4, 127.1, 126.1, 123.4, 121.3, 38.9; IR (neat): ν_{max} (cm^{-1}) 1596, 1528, 1345, 971; EI-MS m/z (relative intensity) 239 (M^+) (100), 222 (68), 192 (78), 178 (22), 165 (18), 115 (37), 91 (23), 77 (10); HRMS calcd for $\text{C}_{15}\text{H}_{13}\text{NO}_2$ (M^+) 239.0946, found 239.0923.

(E)-3-(1-Naphthyl)-1-phenylpropene (**5s**): ^1H NMR (400 MHz, CDCl_3): δ 7.49-7.13 (m, 12H), 6.47-6.45 (m, 2H), 3.96 (d, 2H, $J=4.8$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 137.3, 136.1, 133.8, 131.9, 131.2, 128.7, 128.6, 128.4, 127.0, 126.3, 126.0, 125.8, 125.54, 125.47, 123.9, 36.4; IR (neat): ν_{max} (cm^{-1}) 1596, 1492, 1449, 971; EI-MS m/z (relative intensity) 244 (M^+) (100), 229 (23), 215 (10), 202 (7), 165 (36), 153 (84), 141 (14), 115 (27), 91 (20), 77 (4); HRMS calcd for $\text{C}_{19}\text{H}_{16}$ (M^+) 244.1252, found 244.1246.

(E)-3-(2-Naphthyl)-1-phenylpropene (**5t**): ^1H NMR (400 MHz, CDCl_3): δ 7.82-7.78 (m, 3H), 7.68 (s, 1H), 7.48-7.36 (m, 6H), 7.30 (dd, 2H, $J=7.8$, 7.3 Hz), 7.21 (t, 1H, $J=7.3$ Hz), 6.51 (d, 1H, $J=15.9$ Hz), 6.43 (dt, 1H, $J=15.9$, 6.1 Hz), 3.71 (d, 2H, $J=6.1$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 137.5, 137.3, 133.5, 132.0, 131.2, 128.9, 128.4, 127.9, 127.5, 127.4, 127.3, 127.0, 126.6, 126.0, 125.8, 125.2, 39.6; IR (neat): ν_{max} (cm^{-1}) 3053, 3022, 1507, 1495, 965, 818, 752, 740, 691; EI-MS m/z (relative intensity) 244 (M^+) (100), 229 (25), 165 (21), 153 (30), 115 (18), 91 (10); HRMS calcd for $\text{C}_{19}\text{H}_{16}$ (M^+) 244.1252, found 244.1237.

(E)-1-Phenyl-3-(thiophen-3-yl)propene (**5v**): ^1H NMR (400 MHz, CDCl_3): δ 7.36-6.97 (m, 8H), 6.45 (d, 1H, $J=16.0$ Hz), 6.35 (dt, 1H, $J=16.0$, 6.4 Hz), 3.55 (d, 2H, $J=6.4$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 140.4, 137.3, 131.0, 128.4, 128.3, 127.1, 126.0, 125.5, 120.8, 33.9; IR (neat): ν_{max} (cm^{-1}) 1654, 1598, 1495, 1447, 963; EI-MS m/z (relative intensity) 200 (M^+) (100), 185 (23), 167 (18), 123 (13), 167 (18), 123 (13), 115 (25), 97 (15), 91 (8), 77 (6); HRMS calcd for $\text{C}_{13}\text{H}_{12}\text{S}$ (M^+) 200.0660, found 200.0660.

(E,E)-1,5-Diphenylpenta-1,4-diene (**5w**): ^1H NMR (400 MHz, CDCl_3): δ 7.37-7.17 (m, 10H), 6.45 (d, 2H, $J=16.0$ Hz), 6.23 (dt, 2H, $J=16.0$, 6.8 Hz), 3.11 (t, 2H, $J=6.8$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 137.4, 130.9, 128.4, 128.1, 127.0, 126.0, 36.2; IR (neat): ν_{max} (cm^{-1}) 1648, 1598, 1493, 1447, 963; EI-MS m/z (relative intensity) 220 (M^+) (61), 205 (12), 178 (8), 165 (6), 142 (23), 129 (100), 115 (43), 91 (39), 77 (14); HRMS calcd for $\text{C}_{17}\text{H}_{16}$ (M^+) 220.1252, found 220.1247.

(E)-1,4-Diphenylpenta-1,4-diene (**5x**): ^1H NMR (400 MHz, CDCl_3): δ 7.47 (d, 2H, $J=8.3$ Hz), 7.35-7.25 (m, 7H), 7.19 (t, 1H, $J=7.8$ Hz), 6.47 (d, 1H, $J=15.9$ Hz), 6.30 (dt, 1H, $J=15.9$, 6.6 Hz), 5.43 (s, 1H), 5.15 (s, 1H), 3.40 (d, 2H, $J=6.6$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 146.3, 137.4, 131.5, 128.3, 128.2, 127.9, 127.4, 126.9, 125.95, 125.85, 113.2, 38.8; IR (neat): ν_{max} (cm^{-1}) 3024, 1493, 1424, 1025, 969, 893, 777, 732, 700, 688; EI-MS m/z (relative intensity) 220 (M^+) (100), 205 (56), 142 (38), 129 (76), 115 (30), 103 (47), 91 (23), 77 (20); HRMS calcd for $\text{C}_{17}\text{H}_{16}$ (M^+) 220.1252, found 220.1233.

(*1E,4E*)-1-Phenyl-1,4-hexadiene (**5y**): ^1H NMR (400 MHz, CDCl_3): δ 7.34 (d, 2H, $J=7.8$ Hz), 7.28 (dd, 2H, $J=7.8$, 7.4 Hz), 7.19 (t, 1H, $J=7.4$ Hz), 6.38 (d, 1H, $J=15.9$ Hz), 6.21 (dt, 1H, $J=15.9$, 6.6 Hz), 5.54-5.50 (m, 2H), 2.91-2.87 (m, 2H), 1.72-1.67 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 137.6, 130.0, 129.1, 128.7, 128.3x2, 126.7, 126.2, 125.8, 36.0, 18.1; IR (neat): ν_{max} (cm^{-1}) 3024, 2915, 1494, 1448, 962, 740, 691; EI-MS m/z (relative intensity) 158 (M^+) (69), 143 (60), 129 (100), 115 (30), 91 (25); HRMS calcd for $\text{C}_{12}\text{H}_{14}$ (M^+) 158.1096, found 158.1083.

(*1E,4Z*)-1-Phenyl-1,4-hexadiene (**5z**): ^1H NMR (300 MHz, CDCl_3): δ 7.36-7.16 (m, 5H), 6.41 (d, 1H, $J=15.8$ Hz), 6.20 (dt, 1H, $J=15.8$, 6.3 Hz), 5.59 (dtq, 1H, $J=10.7$, 1.4, 6.6 Hz), 5.49 (dtq, 1H, $J=10.7$, 7.0, 1.7 Hz), 2.96 (dddq, 2H, $J=6.3$, 1.4, 7.0, 0.8 Hz), 1.67 (ddt, 3H, $J=6.6$, 1.7, 0.8 Hz); ^{13}C NMR (75.4 MHz, CDCl_3): δ 137.9, 130.0, 129.0, 128.5, 127.6, 126.9, 126.1, 125.3, 30.3, 12.7; IR (neat): ν_{max} (cm^{-1}) 3024, 2917, 1683, 1648, 1600, 1493, 1447, 1436, 1401, 963, 739, 691; EI-MS m/z (relative intensity) 158 (M^+) (77), 143 (56), 129 (100), 128 (54), 115 (31), 91 (24), 77 (11); HRMS calcd for $\text{C}_{12}\text{H}_{14}$ (M^+) 158.1096, found 158.1086.

(*E*)-1,3-Diphenyl-2-butene (**14-E**)¹: ^1H NMR (400 MHz, CDCl_3): δ 7.42-7.18 (m, 10H), 5.97 (tq, 1H, $J=7.2$, 1.2 Hz), 3.57 (d, 2H, $J=7.2$ Hz), 2.14 (d, 3H, $J=1.2$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 143.5, 140.9, 128.4, 128.3, 128.1, 126.6, 125.9, 125.6, 35.0, 16.0; IR (neat): ν_{max} (cm^{-1}) 1600, 1493, 1453; EI-MS m/z (relative intensity) 208 (M^+) (100), 193 (76), 178 (22), 165 (7), 130 (18), 115 (62), 91 (26), 77 (8); HRMS calcd for $\text{C}_{16}\text{H}_{16}$ (M^+) 208.1252, found 208.1247.

(*Z*)-1,3-Diphenyl-2-butene (**14-Z**)¹: ^1H NMR (400 MHz, CDCl_3): δ 7.37-7.13 (m, 10H), 5.65 (tq, 1H, $J=7.2$, 1.6 Hz), 3.32 (d, 2H, $J=7.2$ Hz), 2.08 (d, 3H, $J=1.6$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 141.4, 137.3, 128.3, 128.2, 128.1, 127.9, 126.6, 125.7, 125.6, 35.3, 25.7; IR (neat): ν_{max} (cm^{-1}) 1600, 1493, 1453; EI-MS m/z (relative intensity) 208 (M^+) (100), 193 (75), 178 (21), 165 (8), 130 (18), 115 (62), 91 (25), 77 (8); HRMS calcd for $\text{C}_{16}\text{H}_{16}$ (M^+) 208.1252, found 208.1237.

(*E*)-1,3-Diphenyl-1-butene (**15**): ^1H NMR (400 MHz, CDCl_3): δ 7.35-7.16 (m, 10H), 6.42 (d, 1H, $J=16.0$ Hz), 6.37 (dd, 1H, $J=16.0$, 5.2 Hz), 3.63 (dq, 1H, $J=5.2$, 7.2 Hz), 1.46 (d, 3H, $J=7.2$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 145.5, 137.5, 135.1, 128.43, 128.39, 127.2, 127.0, 126.13, 126.06, 42.6, 21.3; IR (neat): ν_{max} (cm^{-1}) 1600, 1492, 1449, 963; EI-MS m/z (relative intensity) 208 (M^+) (100), 193 (84), 178 (27), 154 (42), 130 (20), 115 (71), 91 (28), 77 (11); HRMS calcd for $\text{C}_{16}\text{H}_{16}$ (M^+) 208.1252, found 208.1263.

(*E*)-1,3,3-Triphenylpropene (**16**): ^1H NMR (400 MHz, CDCl_3): δ 7.37-7.17 (m, 15H), 6.67 (dd, 1H, $J=15.6$, 7.6 Hz), 6.34 (d, 1H, $J=15.6$ Hz), 4.89 (d, 1H, $J=7.6$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 143.4, 137.2, 132.5, 131.3, 128.6, 128.42, 128.39, 127.2, 126.3, 126.2, 54.2; IR (neat): ν_{max} (cm^{-1}) 1598, 1492, 1445, 969; EI-MS m/z (relative intensity) 270 (M^+) (100), 192 (83), 179 (40), 165 (25), 152 (7), 115 (24), 91 (16), 77 (4); HRMS calcd for $\text{C}_{21}\text{H}_{18}$ (M^+) 270.1409, found 270.1413.

2-Methyl-1,3-diphenylpropene (*E/Z* mixture) (**17**)²: ^1H NMR (400 MHz, CDCl_3): δ 7.34-7.16 (m, 10H), [**17-E** is found at δ 6.37 (d, 0.7H, $J=1.2$ Hz), 3.47 (s, 1.4H), 1.80 (d, 2.1H, $J=1.2$ Hz)], [**17-Z** is

found at δ 6.51 (d, 0.3H, $J=1.6$ Hz), 3.60 (s, 0.6H), 1.81 (d, 0.9H, $J=1.6$ Hz)].

1-(2-Propenyl)naphthalene (2s): ^1H NMR (400 MHz, CDCl_3): δ 8.01-7.30 (m, 7H), 6.10 (ddt, 1H, $J=16.8$, 10.8, 6.4 Hz), 5.11-5.05 (m, 2H), 3.82 (d, 2H, $J=6.4$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 136.9, 136.0, 133.7, 131.9, 128.6, 126.9, 126.2, 125.7, 125.5, 125.4, 123.9, 116.1, 37.3; IR (neat): ν_{max} (cm^{-1}) 1596, 1509, 1395, 911; EI-MS m/z (relative intensity) 168 (M^+) (100), 153 (64), 141 (19), 115 (17), 83 (10), 63 (4); HRMS calcd for $\text{C}_{13}\text{H}_{12}$ (M^+) 168.0939, found 168.0937.

1-(2-Butenyl)naphthalene (26) and **1-(1-methyl-2-propenyl)naphthalene (27)** (**26-E/ 26-Z/ 27 mixture**)³: ^1H NMR (400 MHz, CDCl_3): δ 8.12-7.30 (m, 7H), [**26-E** is found at δ 5.76–5.68 (m, 0.55H), 5.57-5.48 (m, 0.55H), 3.75 (d, 1.10H, $J=6.0$ Hz), 1.66 (ddt, 1.65H, $J=7.0$, 1.6, 1.6 Hz)], [**26-Z** is found at δ 5.65–5.63 (m, 0.05H), 3.82 (d, 0.10H, $J=6.0$ Hz), 1.80 (d, 0.15H, $J=5.2$ Hz)], [**27** is found at δ 6.15 (ddd, 0.4H, $J=5.6$, 10.0, 17.6 Hz), 5.12 (ddd, 0.4H, $J=1.6$, 1.6, 17.6 Hz), 5.11 (ddd, 0.4H, $J=1.6$, 1.6, 10.0 Hz), 4.29 (dddq, 0.4H, $J=1.6$, 1.6, 5.6, 7.2 Hz), 1.50 (d, 1.2H, $J=7.2$ Hz)].

1-(3-Methyl-2-butenyl)naphthalene (28): ^1H NMR (400 MHz, CDCl_3): δ 8.01 (d, 1H, $J=8.0$ Hz), 7.82 (d, 1H, $J=7.6$ Hz), 7.68 (d, 1H, $J=8.0$ Hz), 7.50-7.30 (m, 4H), 5.39 (t, 1H, $J=6.8$ Hz), 3.76 (d, 2H, $J=6.8$ Hz), 1.78 (s, 3H), 1.75(s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 137.7, 133.8, 132.6, 132.0, 128.6, 126.5, 125.6, 125.55, 125.49, 125.3, 123.9, 122.8, 31.8, 25.8, 18.0; IR (neat): ν_{max} (cm^{-1}) 1598, 1509, 1449; EI-MS m/z (relative intensity) 196 (M^+) (74), 181 (100), 165 (36), 153 (31), 141 (17), 128 (25), 115 (11), 89 (4), 83 (4); HRMS calcd for $\text{C}_{15}\text{H}_{16}$ (M^+) 196.1252, found 196.1228.

1-(1,1-Dimethyl-2-propenyl)naphthalene (29): ^1H NMR (400 MHz, CDCl_3): δ 8.37-8.34 (m, 1H), 7.85-7.83 (m, 1H), 7.74 (d, 1H, $J=8.1$ Hz), 7.53 (d, 1H, $J=7.3$ Hz), 7.44-7.39 (m, 3H), 6.28 (dd, 1H, $J=10.7$, 17.6 Hz), 5.09 (d, 1H, $J=10.7$ Hz), 5.06 (d, 1H, $J=17.6$ Hz), 1.63 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 148.8, 143.6, 134.5, 131.1, 128.7, 127.4, 127.3, 124.8, 124.5, 124.0, 123.2, 111.2, 41.9, 29.9; IR (neat): ν_{max} (cm^{-1}) 2966, 1509, 1396, 1360, 1076, 996, 908, 801, 775, 662; EI-MS m/z (relative intensity) 196 (M^+) (45), 181 (100), 165 (43), 153 (39), 141 (11), 128 (8), 115 (5), 89 (6), 83 (7); HRMS calcd for $\text{C}_{15}\text{H}_{16}$ (M^+) 196.1252, found 196.1237.

1-(2-Methyl-2-propenyl)naphthalene (30): ^1H NMR (400 MHz, CDCl_3): δ 8.01-7.32 (m, 7H), 4.85 (s, 1H), 4.62 (s, 1H), 3.77 (s, 2H), 1.77 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 144.5, 135.6, 133.7, 132.3, 128.5, 127.1, 126.9, 125.6, 125.38, 125.36, 124.2, 112.2, 41.5, 22.9; IR (neat): ν_{max} (cm^{-1}) 1596, 1509, 1443, 890; EI-MS m/z (relative intensity) 182 (M^+) (61), 167 (100), 152 (14), 141 (24), 115 (16); HRMS calcd for $\text{C}_{14}\text{H}_{14}$ (M^+) 182.1096, found 182.1077.

1-(2-Cyclohexenyl)naphthalene (31): ^1H NMR (300 MHz, CDCl_3): δ 8.14 (d, 1H, $J=8.2$ Hz), 7.87 (d, 1H, $J=7.4$ Hz), 7.72 (d, 1H, $J=7.7$ Hz), 7.54-7.39 (m, 4H), 6.02 (ddd, 1H, $J=9.9$, 6.5, 3.2 Hz), 5.84 (dd, 1H, $J=9.9$, 1.9 Hz), 4.25-4.23 (m, 1H), 2.21-2.15 (m, 3H), 1.77-1.68 (m, 3H); ^{13}C NMR (75.4 MHz, CDCl_3): δ 142.0, 134.1, 131.5, 130.3, 129.0, 128.9, 126.7, 125.8, 125.5, 125.4, 125.1, 123.5, 36.9, 30.8, 25.1, 20.8; IR (neat): ν_{max} (cm^{-1}) 3018, 2927, 2858, 2833, 1596, 1509, 1445, 1432, 1393, 882, 795, 775, 760, 724; EI-MS m/z (relative intensity) 208 (M^+) (100), 179 (46), 165 (59), 152 (14),

128 (15), 89 (11); HRMS calcd for C₁₆H₁₆ (M⁺) 208.1252, found 208.1238.

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