

## Supporting Information

### **An efficient solvent and temperature tuned access to aldoxime ethers and phenolic functions by Pd-catalyzed C–O cross-coupling of aldoximes with aryl bromides and bromo-chalcones**

Reeta,<sup>a,b</sup>T. M. Rangarajan,<sup>\*c</sup>Kumar Kaushik,<sup>a</sup>Rishi Pal Singh,<sup>c</sup>ManjulaSingh,<sup>d</sup>Raj Pal Singh,<sup>\*a</sup>

<sup>a</sup>Centre for Fire, Explosive and Environment Safety, DRDO, Delhi, India.

<sup>b</sup>Department of Chemistry, University of Delhi, Delhi, India.

<sup>c</sup>Department of Chemistry, Sri Venkateswara College, University of Delhi, New Delhi, India.

<sup>d</sup>Department of Chemistry, Shivaji College, University of Delhi, New Delhi, India.

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E-mail:[rangarajan93150@gmail.com](mailto:rangarajan93150@gmail.com); [rajcfees@gmail.com](mailto:rajcfees@gmail.com)

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## General Considerations

All reactions were carried out in flame dried 10 mL two-neck R. B. flask under argon atmosphere. All phosphine ligands, Pd-catalyst such as  $[\text{Pd}_2(\text{dba})_3]$ ,  $\text{Pd}(\text{OAc})_2$ ,  $[(\pi\text{-allylPdCl})_2]$ ,  $[(\pi\text{-cinnamylPdCl})_2]$  were purchased from Sigma-Aldrich and Sterm Chemicals. Dry anhydrous toluene and  $\text{Cs}_2\text{CO}_3$  were purchased from spectrochemPvt. Ltd., India and purged with nitrogen after every use. All other substituted benzaldehydes, substituted acetophenones and other common reagents were purchased from SpectrochemPvt. Ltd., India, and other common suppliers. Chalcones were prepared by base (KOH) catalysed condensation of acetophenones with benzaldehydes in ethanol. The chalcones thus obtained were then purified either by recrystallization or column chromatography. The Pd-catalyzed cross-coupling products were purified by column chromatography on silica gel (60-120 mesh) using ethyl acetate and hexane mixture as eluent. All the reactions were monitored by thin layer chromatography (TLC) on pre-coated silica gel (Merck Silica gel 60,  $F_{254}$ ) plates and visualized under light.

## Analytical Methods

NMR data were obtained on Jeol 400 MHz spectrometers. All compounds were characterized by  $^1\text{H}$ ,  $^{13}\text{C}$  NMR (399.78 MHz, 100.5 MHz respectively), IR, and HRMS. All  $^1\text{H}$  and  $^{13}\text{C}$  chemical shifts are reported in parts per million (ppm) and were measured relative to TMS or residual  $\text{CDCl}_3$  solvent peak. FT-IR spectra were recorded on Perkin-Elmer model RXI using KBr disc. HRMS (ESI) measurements were performed on Thermo Scientific Orbitrap Elite Hybrid Ion Trap-Orbitrap Mass Spectrometer. Melting points were recorded on Buchi M-560 instruments and were uncorrected. Yields referred to isolated compounds.

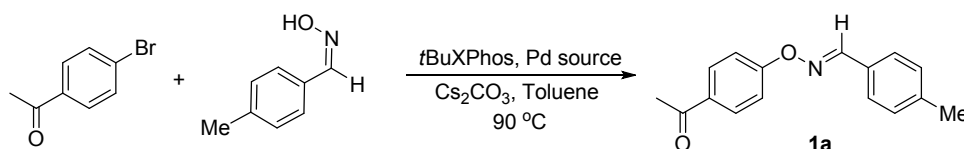
## General Procedure for the Pd-Catalyzed C O Cross-Coupling Reaction of Aryl Bromides and Bromo-chalcones with Aldoximes

An oven dried 10 mL two-neck round bottomed flask was equipped with a magnetic stir bar, a rubber septum, condenser and an argon balloon on the top of the condenser with the aid of an adaptor. The flask was charged with  $\text{Cs}_2\text{CO}_3$  and dried with hot air gun under vacuum. The R.B. flask was allowed to cool under argon atmosphere. Bromo coupling partners, aldoximes, Pd-source and ligands were added in quick succession. The flask was then evacuated and refilled with argon for three times. To this, 2.0 mL of suitable anhydrous solvent for oxime ethers or

hydroxyl compound was added via syringe and again the flask was flushed with argon for three times. The flask was placed in a pre-heated oil bath at optimized temperature. The reaction mixture was stirred vigorously until completion of the reaction as indicated by TLC analysis. The reaction mixture was allowed to cool to room temperature and the crude product was purified by column chromatography on silica gel (60-120 mesh size) using ethyl acetate in hexane as eluent. The solvent removal under reduced pressure afforded the desired compounds as a solid.

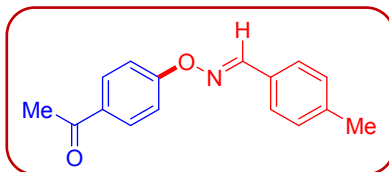
## Experimental Details and Characterization of the Compounds

**Table 1.** Palladium source screen for the Pd-catalyzed coupling of 4'-bromoacetophenone with 4-methylbenzaloxime<sup>a</sup>



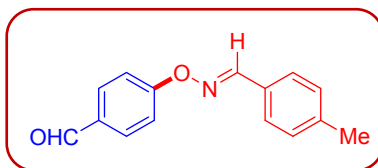
Pd Source (1.0 mol %)	Reaction Time (h)	Yield (%) <sup>b</sup>
[Pd <sub>2</sub> (dba) <sub>3</sub> ]	7 h	72
Pd(OAc) <sub>2</sub>	23 h	NR
[( $\pi$ -cinnamyl)PdCl] <sub>2</sub>	2 h	78
Pd(PPh <sub>3</sub> ) <sub>4</sub>	23 h	NR
[( $\pi$ -allyl)PdCl] <sub>2</sub>	1.5	<b>83</b>
<sup>a</sup> Reaction Conditions: 4'-Bromoacetophenone (0.5 mmol, 1.0 eq.), 4-methylbenzaloxime (0.55 mmol, 1.1 eq.), Cs <sub>2</sub> CO <sub>3</sub> (0.75 mmol, 1.5 eq.), Pd Source (1.0 mol %), <i>t</i> BuXPhos( <b>L2</b> ) (2.5 mol %), toluene (2.0 mL), Ar atm. 90 °C, <sup>b</sup> Isolated yield; NR = No Reaction. ND = Not Determined.		

**(E)-4-Methylbenzaldehyde O-(4-acetylphenyl) oxime (1c)**



The general procedure described above was followed to get the title compound from 4'-bromoacetophenone (199 mg, 1.0mmol), (E)-4-methylbenzaldehyde oxime (142 mg, 1.05mmol), Cs<sub>2</sub>CO<sub>3</sub> (488 mg, 1.5mmol), [( $\pi$ -allyl)PdCl]<sub>2</sub> (3.65 mg, 1.0 mol %), *t*BuXPhos (**L2**) (10.6 mg, 2.5 mol %), with THF as solvent (2.0 mL) were heated at 40 °C. for 24 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a creamy white solid (215 mg, 85% yield). **m.p.**: 86.9-88.9°C; **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 2.41 (s, 3H), 2.59 (s, 3H), 7.26(d, 2H, <sup>3</sup>*J* = 7.8 Hz), 7.31(d, 2H, <sup>3</sup>*J*= 8.9 Hz), 7.63(d, 2H, <sup>3</sup>*J* = 8.2 Hz), 7.98(d, 2H, <sup>3</sup>*J* = 8.7 Hz), 8.42 (s, 1H); **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 21.73, 26.57, 114.08, 127.93, 128.23, 129.82, 130.61, 131.58, 141.70, 152.99, 163.33, 197.18; **IR (KBr)**  $\nu$  = 698, 711, 822, 838, 935, 961, 1112, 1162, 1233, 1274, 1304, 1357, 1503, 1596, 1668, 2361, 2918cm<sup>-1</sup>; **HRMS (ESI)** calcd. for C<sub>16</sub>H<sub>15</sub>NO<sub>2</sub>: [M+H]<sup>+</sup> 254.1181; Found: 254.1178; [M+Na]<sup>+</sup> 276.1000; Found: 276.0992.

**(E)-4-(((4-Methylbenzylidene)amino)oxy)benzaldehyde (2c)**

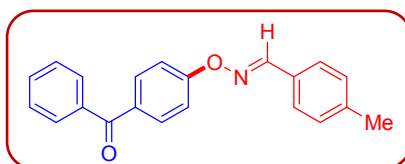


The general procedure described above was followed to get the title compound from 4-bromobenzaldehyde (185 mg, 1.0mmol), (E)-4-methylbenzaldehyde oxime (142 mg, 1.05 mmol), Cs<sub>2</sub>CO<sub>3</sub> (488 mg, 1.5 mmol), [( $\pi$ -allyl)PdCl]<sub>2</sub> (3.65 mg, 1.0 mol %), *t*BuXPhos (**L2**) (10.6 mg, 2.5 mol %), with THF as solvent (2.0 mL) were heated at 40 °C for 24 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a light yellow solid (215 mg, 90% yield). **m.p.**: 78.9-80.5°C; **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 2.41 (s, 3H), 7.26 (d, 2H, <sup>3</sup>*J* = 7.7 Hz), 7.39 (d, 2H, <sup>3</sup>*J* = 8.5 Hz), 7.63 (d, 2H, <sup>3</sup>*J* = 7.5 Hz), 7.88 (d, 2H, <sup>3</sup>*J* = 8.4 Hz), 8.43 (s, 1H), 9.92 (s, 1H); **<sup>13</sup>C NMR**



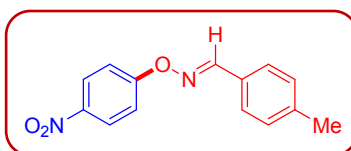
(100 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 21.72, 114.63, 127.96, 128.05, 129.83, 131.12, 132.00, 141.83, 153.26, 164.35, 191.14; IR (KBr)  $\nu$  = 2917, 2729, 1697, 1604, 1502, 1354, 1313, 1293, 1244, 1153, 1107, 1035, 963, 927, 825, 806, 758, 708, 640cm<sup>-1</sup>; HRMS (ESI)calcd. for C<sub>15</sub>H<sub>13</sub>NO<sub>2</sub>: [M+H]<sup>+</sup> 240.1025; Found: 240.1021; [M+Na]<sup>+</sup> 262.0844; Found: 262.0841.

**(*E*)-4-Methylbenzaldehyde *O*-(4-benzoylphenyl) oxime(3c)**



The general procedure described above was followed to get the title compound from 4-bromobenzophenone (261 mg, 1.0 mmol), (*E*)-4-methylbenzaldehyde oxime (142 mg, 1.05 mmol), Cs<sub>2</sub>CO<sub>3</sub> (488 mg, 1.5 mmol), [( $\pi$ -allyl)PdCl]<sub>2</sub> (3.65 mg, 1.0 mol %), *t*BuXPhos (**L2**) (10.6 mg, 2.5 mol %), with THF as solvent (2.0 mL) were heated at 40 °C for 24 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a creamy yellow solid (309 mg, 98% yield). **m.p.**: 78.5-81.2°C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 2.41 (s, 3H), 7.26 (d, 2H, <sup>3</sup>*J* = 7.6 Hz), 7.34 (d, 2H, <sup>3</sup>*J* = 8.9 Hz), 7.47-7.50 (t, 2H), 7.57 (d, 1H, <sup>3</sup>*J* = 7.3 Hz), 7.63 (d, 2H, <sup>3</sup>*J* = 8.0 Hz), 7.78 (d, 2H, <sup>3</sup>*J* = 8.3 Hz), 7.87 (d, 2H, <sup>3</sup>*J* = 8.7 Hz), 8.43 (s, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 21.71, 113.93, 127.91, 128.23, 128.33, 129.78, 129.95, 131.48, 132.11, 132.52, 138.35, 141.66, 152.96, 163.02, 195.81; IR (KBr)  $\nu$  = 2916, 2716, 1669, 1604, 1502, 1390, 1354, 1313, 1293, 1244, 1211, 1107, 1035, 963, 927, 825, 806, 758, 620cm<sup>-1</sup>; HRMS (ESI)calcd. for C<sub>21</sub>H<sub>17</sub>NO<sub>2</sub>: [M+H]<sup>+</sup> 316.1338; Found: 316.1334.

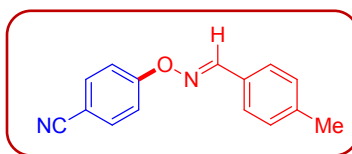
**(*E*)-4-Methylbenzaldehyde *O*-(4-nitrophenyl) oxime(4c)**



The general procedure described above was followed to get the title compound from 4-bromonitrobenzene (202 mg, 1.0 mmol), (*E*)-4-methylbenzaldehyde oxime (142 mg, 1.05 mmol), Cs<sub>2</sub>CO<sub>3</sub> (488 mg, 1.5 mmol), [( $\pi$ -allyl)PdCl]<sub>2</sub> (3.65 mg, 1.0 mol %), *t*BuXPhos (**L2**)

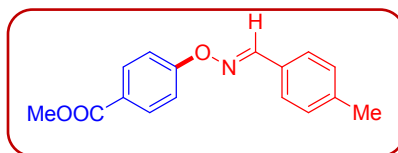
(10.6 mg, 2.5 mol %), with THF as solvent (2.0 mL) were heated at 40 °C for 24 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a yellow solid (250 mg, 97% yield). **m.p.:** 130.2-132.2 °C; **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 2.42 (s, 3H), 7.27 (d, 2H, <sup>3</sup>*J* = 7.3 Hz), 7.35 (d, 2H, <sup>3</sup>*J* = 9.4 Hz), 7.63 (d, 2H, <sup>3</sup>*J* = 7.9 Hz), 8.24 (d, 2H, <sup>3</sup>*J* = 9.1 Hz), 8.44 (s, 1H); **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 21.75, 114.36, 125.91, 127.77, 128.05, 129.89, 142.12, 142.54, 153.78, 164.27; **IR (KBr)**  $\nu$  = 2362, 1719, 1602, 1503, 1435, 1352, 1283, 1230, 1158, 1114, 1007, 971, 916, 900, 850, 811, 766, 693 cm<sup>-1</sup>; **HRMS (ESI)** calcd. for C<sub>14</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>: [M+H]<sup>+</sup> 257.0926; Found: 257.0924.

**(*E*)-4-(((4-Methylbenzylidene)amino)oxy)benzonitrile (5c)**



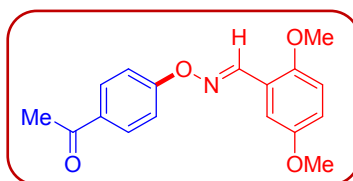
The general procedure described above was followed to get the title compound from 4-bromobenzonitrile (182 mg, 1.0 mmol), (*E*)-4-methylbenzaldehyde oxime (142 mg, 1.05 mmol), Cs<sub>2</sub>CO<sub>3</sub> (488 mg, 1.5 mmol), [( $\pi$ -allyl)PdCl]<sub>2</sub> (3.65 mg, 1.0 mol %), *t*BuXPhos (**L2**) (10.6 mg, 2.5 mol %), with THF as solvent (2.0 mL) were heated at 40 °C for 24 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a creamy white solid (189 mg, 80% yield). **m.p.:** 94.2-96.3 °C; **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 2.41 (s, 3H), 7.26 (d, 2H, <sup>3</sup>*J* = 7.9 Hz), 7.33 (d, 2H, <sup>3</sup>*J* = 8.9 Hz), 7.60-7.64 (m, 4H), 8.41 (s, 1H); **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 21.75, 105.30, 115.06, 119.36, 127.91, 127.96, 129.85, 134.02, 141.95, 153.36, 162.66; **IR (KBr)**  $\nu$  = 2366, 1719, 1602, 1503, 1435, 1391, 1352, 1230, 1193, 1179, 1158, 1114, 1036, 1007, 971, 943, 916, 900, 850, 811, 766, 693 cm<sup>-1</sup>; **HRMS (ESI)** calcd. for C<sub>15</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>: [M+H]<sup>+</sup> 237.1028; Found: 237.1021; [M+Na]<sup>+</sup> 259.0847.; Found: 259.0842.

**(E)-Methyl 4-(((4-Methylbenzylidene)amino)oxy)benzoate (6c)**



The general procedure described above was followed to get the title compound from methyl 4-bromobenzoate (215 mg, 1.0 mmol), (*E*)-4-methylbenzaldehyde oxime (142 mg, 1.05 mmol), Cs<sub>2</sub>CO<sub>3</sub> (488 mg, 1.5 mmol), [( $\pi$ -allyl)PdCl]<sub>2</sub> (3.65 mg, 1.0 mol %), *t*BuXPhos (**L2**) (10.6 mg, 2.5 mol %), with THF as solvent (2.0 mL) were heated at 40 °C for 24 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a creamy white solid (258 mg, 96% yield). **m.p.**: 86.2-87.4°C; **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 2.41 (s, 3H), 3.90 (s, 3H), 7.25 (d, 2H, <sup>3</sup>*J* = 7.8 Hz), 7.29 (d, 2H, <sup>3</sup>*J* = 9.0 Hz), 7.62 (d, 2H, <sup>3</sup>*J* = 8.0 Hz), 8.04 (d, 2H, <sup>3</sup>*J* = 8.7 Hz), 8.41 (s, 1H); **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 21.73, 52.06, 113.97, 123.93, 127.89, 128.26, 129.78, 131.60, 141.61, 152.80, 163.15, 166.99; **IR (KBr)**  $\nu$  = 2362, 1719, 1602, 1503, 1391, 1283, 1230, 1193, 1179, 1158, 1114, 1036, 971, 943, 915, 850, 766, 707, 693 cm<sup>-1</sup>; **HRMS (ESI) calcd.** for C<sub>16</sub>H<sub>15</sub>NO<sub>3</sub>: [M+H]<sup>+</sup> 270.1130; Found: 270.1129.

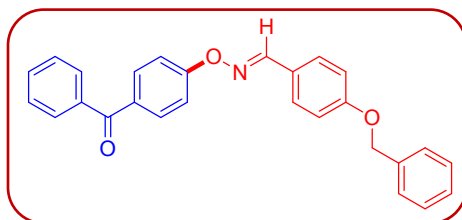
**(E)-2,5-Dimethoxybenzaldehyde O-(4-acetylphenyl) oxime (7c) *E:Z* (3.3 : 1)**



The general procedure described above was followed to get the title compound from 4'-bromoacetophenone (199 mg, 1.0 mmol), (*E*)-2,5-dimethoxybenzaldehyde oxime (190 mg, 1.05 mmol), Cs<sub>2</sub>CO<sub>3</sub> (488 mg, 1.5 mmol), [( $\pi$ -allyl)PdCl]<sub>2</sub> (3.65 mg, 1.0 mol %), *t*BuXPhos (**L2**) (10.6 mg, 2.5 mol %), with THF as solvent (2.0 mL) were heated at 40 °C for 24 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a yellow solid (250 mg, 83% yield). **m.p.**: 136.8-138.7°C; **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): **Isomer *E***: 2.85 (s, 3H), 3.84 (s, 3H), 3.85 (s, 3H), 6.98 (d, 1H, <sup>3</sup>*J* = 9.2 Hz), 6.98-7.01 (m, 1H), 7.30 (d, 2H, <sup>3</sup>*J* = 8.8 Hz), 7.47 (d, 1H, <sup>3</sup>*J* = 3.2 Hz), 7.97 (d,

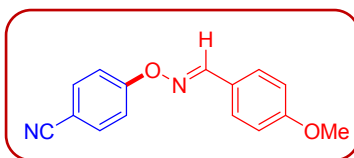
2H,  $^3J = 8.7$  Hz), 8.83 (s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 26.58, 55.38, 55.99, 110.79, 112.84, 114.07, 118.88, 130.60, 131.46, 149.06, 152.93, 153.70, 163.40, 197.30; **Isomer Z** : 26.46, 56.06, 56.52, 112.68, 115.50, 116.55, 117.66, 119.90, 120.98, 131.02, 153.24, 155.86; **IR** (KBr)  $\nu = 2918, 2847, 2225, 1665, 1596, 1499, 1462, 1417, 1353, 1228, 1162, 1144, 1042, 927, 836, 810, 722, 693, 614\text{cm}^{-1}$ ; **HRMS (ESI) calcd.** for  $\text{C}_{17}\text{H}_{17}\text{NO}_4$ :  $[\text{M}+\text{H}]^+$  300.1236; Found: 300.1232;  $[\text{M}+\text{Na}]^+$  322.1055; Found: 322.1052.

**(E)-4-(Benzyloxy)benzaldehydeO-(4-benzoylphenyl) oxime (8c)**



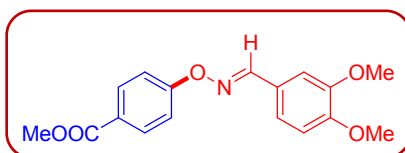
The general procedure described above was followed to get the title compound from 4-bromobenzophenone (261 mg, 1.0 mmol), (*E*)-4-(benzyloxy)benzaldehydeoxime (238 mg, 1.05 mmol),  $\text{Cs}_2\text{CO}_3$  (488 mg, 1.5 mmol),  $[(\pi\text{-allylPdCl})_2]$  (3.65 mg, 1.0 mol %), *t*BuXPhos (**L2**) (10.6 mg, 2.5 mol %), with THF as solvent (2.0 mL) were heated at 40 °C for 24 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a light brown solid (400 mg, 98% yield). **m.p.**: 89.2-91.2°C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 5.13 (s, 2H), 7.04 (d, 2H,  $^3J = 8.6$  Hz), 7.33 (d, 2H,  $^3J = 8.6$  Hz), 7.39-7.50 (m, 7H), 7.56-7.60 (t, 1H), 7.68 (d, 2H,  $^3J = 8.6$  Hz), 7.79 (d, 2H,  $^3J = 7.8$  Hz), 7.86 (d, 2H,  $^3J = 8.7$  Hz), 8.41 (s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 70.22, 113.90, 115.41, 123.75, 127.62, 128.34, 128.82, 129.58, 129.95, 131.34, 132.11, 132.55, 136.44, 138.33, 152.49, 161.16, 163.08, 195.89; **IR** (KBr)  $\nu = 2225, 1650, 1592, 1500, 1444, 1617, 1393, 1356, 1316, 1308, 1280, 1249, 1174, 1159, 1113, 994, 920, 847, 834, 737, 696, 680, 648, 630, 616\text{cm}^{-1}$ ; **HRMS (ESI) calcd.** for  $\text{C}_{27}\text{H}_{21}\text{NO}_3$ :  $[\text{M}+\text{H}]^+$  408.1600; Found: 408.1596;  $[\text{M}+\text{K}]^+$  446.1159; Found: 446.1195.

**(E)-4-(((4-Methoxybenzylidene)amino)oxy)benzonitrile(9c)**



The general procedure described above was followed to get the title compound from 4-bromobenzonitrile (182 mg, 1.0 mmol), (*E*)-4-methoxybenzaldehyde oxime (158 mg, 1.05 mmol), Cs<sub>2</sub>CO<sub>3</sub> (488 mg, 1.5 mmol), [( $\pi$ -allyl)PdCl]<sub>2</sub> (3.65 mg, 1.0 mol %), *t*BuXPhos (**L2**) (10.6 mg, 2.5 mol %), with THF as solvent (2.0 mL) were heated at 40 °C for 24 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a creamy brown solid (130 mg, 91% yield). **m.p.**: 126.5-128.9°C; **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 3.86 (s, 3H), 6.96 (d, 2H, <sup>3</sup>*J* = 8.6 Hz), 7.32 (d, 2H, <sup>3</sup>*J* = 8.8 Hz), 7.62 (d, 2H, <sup>3</sup>*J* = 8.6 Hz), 7.66 (d, 2H, <sup>3</sup>*J* = 8.7 Hz), 8.38 (s, 1H); **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 55.54, 105.20, 114.60, 115.03, 119.34, 123.22, 129.63, 133.97, 152.97, 162.22, 162.73; **IR (KBr)**  $\nu$  = 2221, 1603, 1499, 1469, 1442, 1425, 1390, 1350, 1311, 1238, 1189, 1175, 1162, 1110, 1030, 957, 921, 827, 776, 720, 649, 637 cm<sup>-1</sup>; **HRMS (ESI) calcd.** for C<sub>15</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>: [M+H]<sup>+</sup> 253.0977; Found: 253.0975; [M+Na]<sup>+</sup> 275.0796; Found: 275.0794.

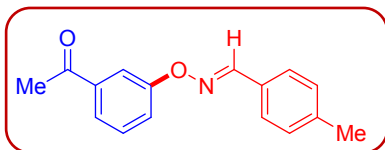
**(E)-Methyl 4-(((3,4-dimethoxybenzylidene)amino)oxy)benzoate (10c)**



The general procedure described above was followed to get the title compound from methyl 4-bromobenzoate (215 mg, 1.0 mmol), (*E*)-3,4-dimethoxybenzaldehyde oxime (190 mg, 1.05 mmol), Cs<sub>2</sub>CO<sub>3</sub> (488 mg, 1.5 mmol), [( $\pi$ -allyl)PdCl]<sub>2</sub> (3.65 mg, 1.0 mol %), *t*BuXPhos (**L2**) (10.6 mg, 2.5 mol %), with THF as solvent (2.0 mL) were heated at 40 °C for 24 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a light brown solid (285 mg, 90% yield). **m.p.**: 73.5-75.8°C; **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 3.90 (s, 3H), 3.93 (s, 3H), 3.97 (s, 3H), 6.19 (d, 1H, <sup>3</sup>*J* = 8.5 Hz), 7.16 (d, 1H, <sup>3</sup>*J* = 8.3 Hz), 7.28 (d, 2H, <sup>3</sup>*J* = 8.9 Hz), 7.37 (s, 1H), 8.04 (d, 2H, <sup>3</sup>*J* = 8.7 Hz), 8.37 (s, 1H); **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 52.05, 56.09, 56.11, 108.58, 110.93,

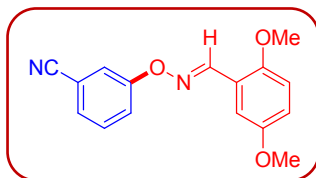
113.98, 123.03, 123.79, 123.88, 131.58, 149.55, 151.82, 152.75, 163.17, 167.03; **IR** (KBr)  $\nu$  = 2221, 1603, 1469, 1142, 1349, 1311, 1238, 1175, 1162, 1110, 1030, 957, 921, 827, 776, 720, 631, 596 $\text{cm}^{-1}$ ; **HRMS (ESI) calcd.** for  $\text{C}_{17}\text{H}_{17}\text{NO}_5$ :  $[\text{M}+\text{H}]^+$  316.1185; Found: 316.1182;  $[\text{M}+\text{Na}]^+$  338.1004; Found: 338.1002.

**(*E*)-4-Methylbenzaldehyde *O*-(3-acetylphenyl) oxime (11c)**



The general procedure described above was followed to get the title compound from 3'-bromoacetophenone (199 mg, 1.0 mmol), (*E*)-4-methylbenzaldehyde oxime (142 mg, 1.05 mmol),  $\text{Cs}_2\text{CO}_3$  (488 mg, 1.5 mmol),  $[(\pi\text{-allylPdCl})_2]$  (7.3 mg, 2.0 mol %), RockPhos (**L7**) (23.4 mg, 5.0 mol %), with toluene as solvent (2.0 mL) were heated at 90°C for 2.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a light yellow solid (244 mg, 88% yield). **m.p.**: 83.5-85.9°C;  **$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )**  $\delta$  (ppm): 2.40 (s, 3H), 2.62 (s, 3H), 7.25 (d, 2H,  $^3J = 7.8$  Hz), 7.40-7.47 (m, 2H), 7.63 (d, 3H,  $^3J = 7.8$  Hz), 7.84 (s, 1H), 8.40 (s, 1H);  **$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )**  $\delta$  (ppm): 21.68, 26.93, 114.17, 119.40, 122.35, 127.81, 128.41, 129.63, 129.74, 138.52, 141.41, 152.33, 159.77, 198.04; **IR** (KBr)  $\nu$  = 2361, 1668, 1597, 1503, 1358, 1303, 1358, 1274, 1234, 1162, 1112, 961, 935, 838, 822, 711, 698 $\text{cm}^{-1}$ ; **HRMS (ESI) calcd.** for  $\text{C}_{16}\text{H}_{15}\text{NO}_2$ :  $[\text{M}+\text{H}]^+$  254.1181; Found: 254.1184.

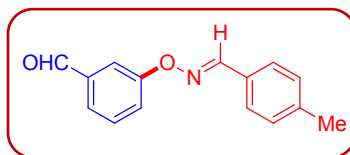
**(*E*)-3-(((2,5-Dimethoxybenzylidene)amino)oxy)benzonitrile (12c) *E:Z* (3.3:2)**



The general procedure described above was followed to get the title compound from 3-bromobenzonitrile (182 mg, 1.0 mmol), (*E*)-2,5-dimethoxybenzaldehyde oxime (190 mg, 1.05 mmol),  $\text{Cs}_2\text{CO}_3$  (488 mg, 1.5 mmol),  $[(\pi\text{-allylPdCl})_2]$  (7.3 mg, 2.0 mol %), RockPhos (**L7**)

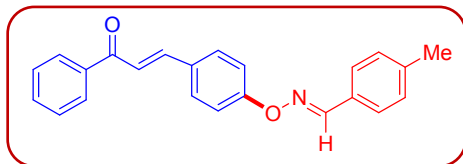
(23.4 mg, 5.0 mol %), with toluene as solvent (2.0 mL) were heated at 90 °C for 3.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a creamy white solid (240 mg, 85% yield). **m.p.**: 97.2-99.6°C; **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): **Isomer E**: 3.84 (s, H), 3.85 (s, 3H), 6.89 (d, 1H, <sup>3</sup>J = 9.1 Hz), 7.01 (d, 1H, <sup>3</sup>J = 9.0 Hz), 7.05-7.07 (m, 1H), 7.31 (d, 1H, <sup>3</sup>J = 6.6 Hz), 7.41-7.44 (m, 2H), 7.59 (s, 1H), 8.81 (s, 1H); **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 56.00, 56.35, 101.76, 110.60, 112.70, 112.87, 113.08, 119.11, 119.66, 120.97, 125.85, 130.29, 149.06, 152.91, 153.72, 159.62; **Isomer Z**: 56.03, 56.50, 117.64, 117.81, 118.87, 119.14, 120.75, 123.70, 130.38, 152.91, 153.24; **IR (KBr)**  $\nu$  = 2221, 1603, 1514, 1491, 1470, 1442, 1425, 1391, 1350, 1311, 1238, 1175, 1162, 1110, 1030, 957, 921, 827, 756, 649 cm<sup>-1</sup>; **HRMS (ESI) calcd.** for C<sub>16</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub>: [M+H]<sup>+</sup> 283.1083; Found: 283.1080; [M+Na]<sup>+</sup> 305.0902; Found: 305.0899.

**(E)-3-(((4-Methylbenzylidene)amino)oxy)benzaldehyde (13c)**



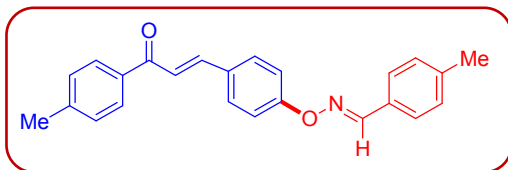
The general procedure described above was followed to get the title compound from 3-bromobenzaldehyde (185 mg, 1.0 mmol), (E)-4-methylbenzaldehyde oxime (142 mg, 1.05 mmol), Cs<sub>2</sub>CO<sub>3</sub> (488 mg, 1.5 mmol), [( $\pi$ -allyl)PdCl]<sub>2</sub> (7.3 mg, 2.0 mol %), RockPhos (**L7**) (23.4 mg, 5.0 mol %), with toluene as solvent (2.0 mL) were heated at 90 °C for 1.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a light yellow solid (234 mg, 98% yield). **m.p.**: 72.5-74.5°C; **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 2.41 (s, 3H), 7.25 (d, 2H, <sup>3</sup>J = 7.5 Hz), 7.49 (d, 2H, <sup>3</sup>J = 4.8 Hz), 7.55-7.57 (m, 1H), 7.63 (d, 2H, <sup>3</sup>J = 8.0 Hz), 7.80 (s, 1H), 8.42 (s, 1H), 10.02 (s, 1H); **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 21.72, 114.72, 120.80, 124.13, 127.85, 128.28, 129.78, 130.08, 137.78, 141.54, 152.56, 160.11, 192.31; **IR (KBr)**  $\nu$  = 1696, 1578, 1511, 1480, 1437, 1382, 1347, 1316, 1285, 1255, 1172, 1126, 1078, 1041, 1000, 966, 913, 866, 794, 676 cm<sup>-1</sup>; **HRMS (ESI) calcd.** for C<sub>15</sub>H<sub>13</sub>NO<sub>2</sub>: [M+H]<sup>+</sup> 240.1025; Found: 240.1020; [M+Na]<sup>+</sup> 262.0844; Found: 262.0839.

**(*E*)-4-Methylbenzaldehyde *O*-(4-((*E*)-3-oxo-3-phenylprop-1-en-1-yl)phenyl) oxime (16c)**



The general procedure described above was followed to get the title compound from (*E*)-3-(4-bromophenyl)-1-phenylprop-2-en-1-one (143 mg, 0.5 mmol), (*E*)-4-methylbenzaldehyde oxime (71 mg, 0.525 mmol), Cs<sub>2</sub>CO<sub>3</sub> (244 mg, 0.75 mmol), [( $\pi$ -allylPdCl)<sub>2</sub>] (5.49 mg, 3.0 mol %), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with THF as solvent (2.0 mL) were heated at 75 °C for 4.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a light yellow solid (135 mg, 79% yield). **m.p.**: 103.5-106.0°C; **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 2.41 (s, 3H), 7.25 (d, 2H, <sup>3</sup>*J* = 6.9 Hz), 7.31 (d, 2H, <sup>3</sup>*J* = 8.8 Hz), 7.45 (d, 1H, <sup>3</sup>*J* = 15.6 Hz), 7.49-7.53 (t, 2H), 7.58 (d, 1H, <sup>3</sup>*J* = 7.3 Hz), 7.63 (d, 2H, <sup>3</sup>*J* = 7.2 Hz), 7.65 (d, 2H, <sup>3</sup>*J* = 8.4 Hz), 7.82 (d, 1H, <sup>3</sup>*J* = 15.5 Hz), 8.03 (d, 2H, <sup>3</sup>*J* = 7.1 Hz), 8.41 (s, 1H); **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 21.71, 114.88, 120.22, 127.84, 128.34, 128.58, 128.71, 129.00, 129.77, 130.22, 132.75, 138.58, 141.53, 144.92, 152.60, 161.55, 190.84; **IR (KBr)**  $\nu$  = 2366, 1668, 1578, 1498, 1459, 1428, 1388, 1325, 1298, 1274, 1217, 1158, 1101, 1041, 1016, 987, 932, 842, 817, 786, 745, 676, 662 cm<sup>-1</sup>; **HRMS (ESI) calcd.** for C<sub>23</sub>H<sub>19</sub>NO<sub>2</sub>: [M+H]<sup>+</sup> 342.1494; Found: 342.1487; [M+Na]<sup>+</sup> 364.1313; Found: 364.1303.

**(*E*)-4-Methylbenzaldehyde *O*-(4-((*E*)-3-oxo-3-(*p*-tolyl)prop-1-en-1-yl)phenyl) oxime (17c)**

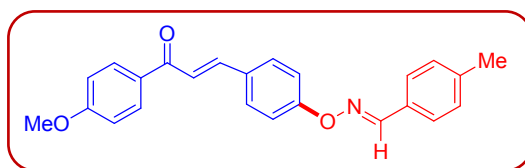


The general procedure described above was followed to get the title compound from (*E*)-3-(4-bromophenyl)-1-*p*-tolylprop-2-en-1-one (150 mg, 0.5 mmol), (*E*)-4-methylbenzaldehyde oxime (71 mg, 0.525 mmol), Cs<sub>2</sub>CO<sub>3</sub> (244 mg, 0.75 mmol), [( $\pi$ -allylPdCl)<sub>2</sub>] (5.49 mg, 3.0 mol %), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with THF as solvent (2.0 mL) were heated at 75 °C for 3.0 hour. The crude reaction mixture was purified through column chromatography (silica gel



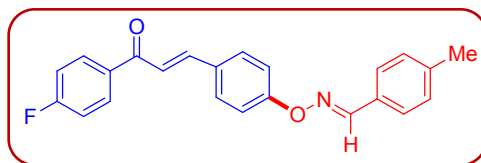
60-120 mesh) to afford the title compound as a light yellow solid (130 mg, 73% yield). **m.p.**: 105.2-107.8°C; **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 2.41 (s, 3H), 2.44 (s, 3H), 7.25(d, 2H, <sup>3</sup>J = 7.8Hz), 7.30 (d, 2H, <sup>3</sup>J = 8.3Hz), 7.46 (d, 1H, <sup>3</sup>J = 15.6Hz), 7.51-7.55 (m, 1H), 7.62(d, 2H, <sup>3</sup>J = 7.7Hz), 7.64(d, 1H, <sup>3</sup>J = 8.3Hz), 7.81 (d, 1H, <sup>3</sup>J = 15.6Hz), 7.94(d, 2H, <sup>3</sup>J = 8.0Hz), 8.40 (s, 1H); **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 21.72, 21.82, 114.85, 120.17, 127.84, 128.34, 128.75, 129.09, 129.44, 129.77, 130.18, 132.19, 135.92, 141.52, 144.56, 152.57, 161.47, 190.44; **IR** (KBr)  $\nu$  = 1668, 1596, 1558, 1508, 1450, 1425, 1390, 1338, 1295, 1254, 1218, 1168, 1109, 1035, 1016, 998, 934, 838, 777, 725, 686, 663 cm<sup>-1</sup>; C<sub>24</sub>H<sub>21</sub>NO<sub>2</sub>: [M+H]<sup>+</sup> 356.1651; Found: 356.1647; [M+K]<sup>+</sup> 394.1209; Found: 394.1221.

**(E)-4-Methylbenzaldehyde O-(4-((E)-3-(4-methoxyphenyl)-3-oxoprop-1-en-1-yl)phenyl) oxime (18c)**



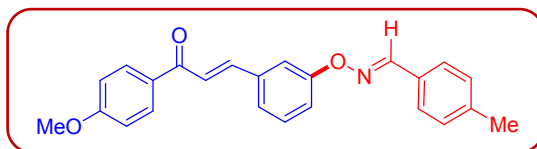
The general procedure described above was followed to get the title compound from (E)-3-(4-bromophenyl)-1-(4-methoxyphenyl)prop-2-en-1-one (158 mg, 0.5 mmol), (E)-4-methylbenzaldehyde oxime (71 mg, 0.525 mmol), Cs<sub>2</sub>CO<sub>3</sub> (244 mg, 0.75 mmol), [( $\pi$ -allyl)PdCl]<sub>2</sub> (5.49 mg, 3.0 mol %), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with THF as solvent (2.0 mL) were heated at 75 °C for 2.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a light yellow solid (144 mg, 74% yield). **m.p.**: 89.5-91.9°C; **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 2.41 (s, 3H), 3.89 (s, 3H), 6.99 (d, 2H, <sup>3</sup>J = 9.0 Hz), 7.25 (d, 2H, <sup>3</sup>J = 8.0 Hz), 7.30 (d, 2H, <sup>3</sup>J = 8.9 Hz), 7.46 (d, 1H, <sup>3</sup>J = 15.5 Hz), 7.63 (d, 2H, <sup>3</sup>J = 8.0 Hz), 7.64 (d, 2H, <sup>3</sup>J = 8.5 Hz), 7.80 (d, 1H, <sup>3</sup>J = 15.6 Hz), 8.05 (d, 2H, <sup>3</sup>J = 8.9 Hz), 8.41 (s, 1H); **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 21.74, 55.64, 113.94, 114.87, 120.00, 127.85, 128.39, 129.22, 129.79, 130.11, 130.91, 131.43, 141.53, 144.07, 152.56, 161.40, 163.45, 189.06; **IR** (KBr)  $\nu$  = 2365, 1660, 1578, 1509, 1456, 1425, 1395, 1338, 1295, 1243, 1218, 1165, 1108, 1038, 1018, 996, 930, 836, 777, 723, 686 cm<sup>-1</sup>; **HRMS (ESI) calcd.** for C<sub>24</sub>H<sub>21</sub>NO<sub>3</sub>: [M+H]<sup>+</sup> 372.1600; Found: 372.1613; [M+Na]<sup>+</sup> 394.1419; Found: 394.1430.

**(*E*)-4-Methylbenzaldehyde *O*-(4-((*E*)-3-(4-fluorophenyl)-3-oxoprop-1-en-1-yl)phenyl)oxime (19c)**



The general procedure described above was followed to get the title compound from (*E*)-3-(4-bromophenyl)-1-(4-fluorophenyl)prop-2-en-1-one (152 mg, 0.5 mmol), (*E*)-4-methylbenzaldehyde oxime (71 mg, 0.525 mmol), Cs<sub>2</sub>CO<sub>3</sub> (244 mg, 0.75 mmol), [( $\pi$ -allyl)PdCl]<sub>2</sub>] (5.49 mg, 3.0 mol %), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with THF as solvent (2.0 mL) were heated at 75 °C for 4.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a light yellow solid (134 mg, 76% yield). **m.p.**: 133.5-135.7°C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 2.41 (s, 3H), 7.16-7.20 (t, 2H), 7.25 (d, 2H, <sup>3</sup>*J* = 7.6 Hz), 7.31 (d, 2H, <sup>3</sup>*J* = 8.7 Hz), 7.42 (d, 1H, <sup>3</sup>*J* = 15.5 Hz), 7.63 (d, 2H, <sup>3</sup>*J* = 7.8 Hz), 7.64 (d, 2H, <sup>3</sup>*J* = 8.7 Hz), 7.81 (d, 1H, <sup>3</sup>*J* = 15.5 Hz), 8.04-8.08 (m, 2H), 8.41 (s, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 21.73, 114.90, 115.82 (d, <sup>3</sup>*J*<sub>C-F</sub> = 21.1 Hz), 119.64, 127.85, 128.59 (d, <sup>2</sup>*J*<sub>C-F</sub> = 54.7 Hz), 129.79, 130.27, 131.15 (d, <sup>4</sup>*J*<sub>C-F</sub> = 9.1 Hz), 134.87 (d, <sup>4</sup>*J*<sub>C-F</sub> = 2.9 Hz), 141.58, 145.14, 152.65, 161.63, 165.63, 165.63 (d, <sup>1</sup>*J*<sub>C-F</sub> = 253.1 Hz), 189.11; IR (KBr)  $\nu$  = 2369, 1656, 1591, 1571, 1504, 1446, 1419, 1390, 1337, 1292, 1243, 1216, 1162, 1109, 1034, 1016, 995, 979, 930, 834, 813, 717, 748, 723, 686 cm<sup>-1</sup>; HRMS (ESI) calcd. for C<sub>23</sub>H<sub>18</sub>FNO<sub>2</sub>: [M+H]<sup>+</sup> 360.1400; Found: 360.1415.

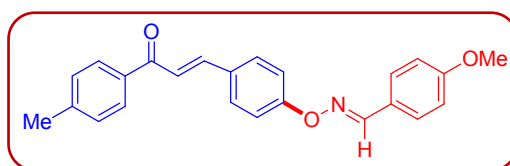
**(*E*)-4-Methylbenzaldehyde *O*-(3-((*E*)-3-(4-methoxyphenyl)-3-oxoprop-1-en-1-yl)phenyl)oxime (20c)**



The general procedure described above was followed to get the title compound from (*E*)-3-(3-bromophenyl)-1-(4-methoxyphenyl)prop-2-en-1-one (158 mg, 0.5 mmol), (*E*)-4-methylbenzaldehyde oxime (71 mg, 0.525 mmol), Cs<sub>2</sub>CO<sub>3</sub> (244 mg, 0.75 mmol), [( $\pi$ -allyl)PdCl]<sub>2</sub>] (5.49 mg, 3.0 mol %), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with THF as solvent (2.0 mL) were

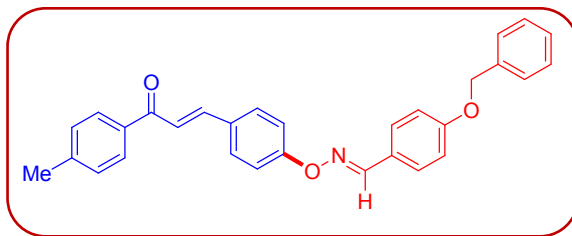
heated at 75 °C for 3.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a light yellow solid(150 mg, 81% yield). **m.p.**: 115.9-117.9°C; **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 2.41 (s, 3H), 3.89 (s, 3H), 6.99 (d, 2H,  $^3J$  = 8.9 Hz), 7.26 (d, 2H,  $^3J$  = 8.0 Hz), 7.29-7.33 (t, 2H), 7.37 (d, 1H,  $^3J$  = 7.8 Hz), 7.55 (d, 2H,  $^3J$  = 15.5 Hz), 7.63 (d, 2H,  $^3J$  = 8.3 Hz), 7.8 (d, 1H,  $^3J$  = 15.6 Hz), 8.05 (d, 2H,  $^3J$  = 8.9 Hz), 8.41 (s, 1H); **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 21.68, 55.61, 113.98, 116.73, 122.43, 122.60, 127.79, 128.51, 129.75, 129.93, 131.01, 131.16, 136.48, 141.35, 144.09, 152.20, 159.94, 163.58, 189.03; **IR (KBr)**  $\nu$  = 2917, 1668, 1576, 1509, 1456, 1419, 1392, 1338, 1286, 1203, 1116, 1045, 1019, 985, 940, 836, 825, 776, 758, 735, 696, 668 cm<sup>-1</sup>; **HRMS (ESI) calcd.** for C<sub>24</sub>H<sub>21</sub>NO<sub>3</sub>: [M+H]<sup>+</sup> 372.1600; Found: 372.1618.

**(E)-4-Methoxybenzaldehyde O-(4-((E)-3-oxo-3-(p-tolyl)prop-1-en-1-yl)phenyl) oxime (21c)**



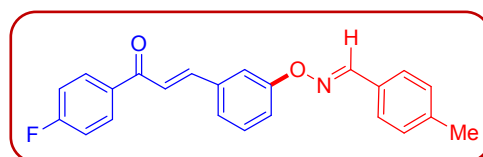
The general procedure described above was followed to get the title compound from (E)-3-(4-bromophenyl)-1-p-tolylprop-2-en-1-one (150 mg, 0.5 mmol), (E)-4-methoxybenzaldehyde oxime (79 mg, 0.525 mmol), Cs<sub>2</sub>CO<sub>3</sub> (244 mg, 0.75 mmol), [( $\pi$ -allyl)PdCl]<sub>2</sub> (5.49 mg, 3.0 mol %), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with THF as solvent (2.0 mL) were heated at 75 °C for 4.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a light yellow solid(150 mg, 81% yield). **m.p.**: 107.9-110.0°C; **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 2.44 (s, 3H), 3.86 (s, 3H), 6.96 (d, 2H,  $^3J$  = 8.5 Hz), 7.29 (d, 2H,  $^3J$  = 8.7 Hz), 7.30 (d, 2H,  $^3J$  = 8.0 Hz), 7.45 (d, 1H,  $^3J$  = 15.5 Hz), 7.64 (d, 2H,  $^3J$  = 8.4 Hz), 7.68 (d, 2H,  $^3J$  = 8.7 Hz), 7.81 (d, 1H,  $^3J$  = 15.5 Hz), 7.94 (d, 2H,  $^3J$  = 8.0 Hz), 8.37 (s, 1H); **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 21.77, 55.52, 114.48, 114.80, 120.09, 123.65, 128.74, 128.96, 129.47, 130.16, 134.10, 135.91, 143.61, 144.61, 152.17, 161.54, 161.91, 190.43; **IR (KBr)**  $\nu$  = 2921, 2342, 1652, 1600, 1505, 1334, 1293, 1247, 1216, 1165, 1100, 1030, 988, 923, 811, 737, 678 cm<sup>-1</sup>; **HRMS (ESI) calcd.** for C<sub>24</sub>H<sub>21</sub>NO<sub>3</sub>: [M+H]<sup>+</sup> 372.1600; Found: 372.1582.

**(*E*)-4-(Benzyloxy)benzaldehyde *O*-(4-((*E*)-3-oxo-3-(*p*-tolyl)prop-1-en-1-yl)phenyl) oxime (22c)**



The general procedure described above was followed to get the title compound from (*E*)-3-(4-bromophenyl)-1-*p*-tolylprop-2-en-1-one (150 mg, 0.5 mmol), (*E*)-4-(benzyloxy)benzaldehyde oxime (119 mg, 0.525 mmol), Cs<sub>2</sub>CO<sub>3</sub> (244 mg, 0.75 mmol), [( $\pi$ -allyl)PdCl]<sub>2</sub>] (5.49 mg, 3.0 mol %), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with THF as solvent (2.0 mL) were heated at 75 °C for 4.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a light brown solid (162 mg, 73% yield). **m.p.**: 102.3-105.3°C; **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 2.44 (s, 3H), 5.12 (s, 2H), 7.03 (d, 2H, <sup>3</sup>*J* = 8.7 Hz), 7.29 (d, 2H, <sup>3</sup>*J* = 8.7 Hz), 7.31 (d, 2H, <sup>3</sup>*J* = 8.0 Hz), 7.35-7.47 (m, 6H), 7.55 (d, 1H, <sup>3</sup>*J* = 8.5 Hz), 7.64 (d, 1H, <sup>3</sup>*J* = 8.9 Hz), 7.68 (d, 2H, <sup>3</sup>*J* = 8.7 Hz), 7.81 (d, 1H, <sup>3</sup>*J* = 15.4 Hz), 7.94 (d, 2H, <sup>3</sup>*J* = 8.1 Hz), 8.38 (s, 1H); **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 21.82, 70.24, 114.83, 115.41, 120.20, 123.94, 127.63, 128.35, 128.75, 128.83, 129.44, 129.52, 130.17, 130.55, 136.00, 136.49, 143.58, 144.53, 152.13, 161.10, 161.53, 190.37; **IR (KBr)**  $\nu$  = 2368, 1654, 1597, 1572, 1510, 1451, 1391, 1360, 1343, 1291, 1265, 1240, 1214, 1167, 1140, 1023, 1011, 983, 920, 863, 828, 808, 734, 670, 639 cm<sup>-1</sup>; **HRMS (ESI) calcd.** for C<sub>30</sub>H<sub>25</sub>NO<sub>3</sub>: [M+H]<sup>+</sup> 448.1913; Found: 448.1947.

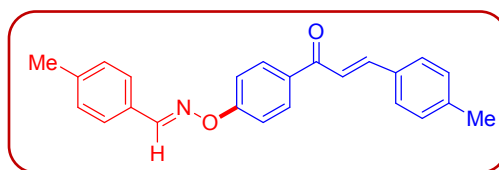
**(*E*)-4-Methylbenzaldehyde *O*-(3-((*E*)-3-(4-fluorophenyl)-3-oxoprop-1-en-1-yl)phenyl) oxime (23c)**



The general procedure described above was followed to get the title compound from (*E*)-3-(3-bromophenyl)-1-(4-fluorophenyl)prop-2-en-1-one (152 mg, 0.5 mmol), (*E*)-4-methylbenzaldehyde oxime (71 mg, 0.525 mmol), Cs<sub>2</sub>CO<sub>3</sub> (244 mg, 0.75 mmol), [( $\pi$ -

allylPdCl)<sub>2</sub>] (5.49 mg, 3.0 mol %), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with THF as solvent (2.0 mL) were heated at 75 °C for 3.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a light yellow solid (131 mg, 70% yield). **m.p.**: 110.5-112.9 °C; **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 3.86 (s, 3H), 6.97 (d, 2H, <sup>3</sup>*J* = 8.4 Hz), 7.16-7.21 (t, 2H), 7.31 (d, 2H, <sup>3</sup>*J* = 7.7 Hz), 7.38 (d, 1H, <sup>3</sup>*J* = 15.5 Hz), 7.49-7.53 (t, 2H), 7.68 (d, 2H, <sup>3</sup>*J* = 8.6 Hz), 7.81 (d, 1H, <sup>3</sup>*J* = 15.7 Hz), 8.05-8.08 (m, 2H), 8.39 (s, 1H); **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 55.51, 113.99, 114.50, 115.88 (d, <sup>3</sup>*J*<sub>C-F</sub> = 21.3 Hz), 117.04, 122.37 (d, <sup>2</sup>*J*<sub>C-F</sub> = 51.9 Hz), 123.79, 129.43, 129.98, 131.28 (d, <sup>4</sup>*J*<sub>C-F</sub> = 8.4 Hz), 134.11, 134.61, 136.13, 145.22, 151.90, 160.02, 161.87, 165.74 (d, <sup>1</sup>*J*<sub>C-F</sub> = 255.0 Hz), 189.17; **IR (KBr)**  $\nu$  = 2366, 1698, 1580, 1513, 1485, 1441, 1348, 1314, 1283, 1259, 1177, 1163, 1131, 1111, 1076, 998, 970, 916, 876, 863, 818, 797, 765, 718, 678, 642 cm<sup>-1</sup>; **HRMS (ESI)** **calcd.** for C<sub>20</sub>H<sub>20</sub>FNO<sub>3</sub>: [M+H]<sup>+</sup> 390.1505; Found: 390.1510.

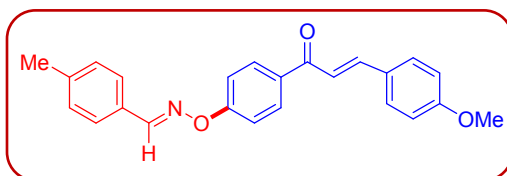
**(*E*)-4-Methylbenzaldehyde *O*-(4-((*E*)-3-(*p*-tolyl)acryloyl)phenyl) oxime (24c)**



The general procedure described above was followed to get the title compound from (*E*)-1-(4-bromophenyl)-3-*p*-tolylprop-2-en-1-one (150 mg, 0.5 mmol), (*E*)-4-methylbenzaldehyde oxime (71 mg, 0.525 mmol), Cs<sub>2</sub>CO<sub>3</sub> (244 mg, 0.75 mmol), [( $\pi$ -allylPdCl)<sub>2</sub>] (5.49 mg, 3.0 mol %), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with THF as solvent (2.0 mL) were heated at 75 °C for 3.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a light yellow solid (165 mg, 93% yield). **m.p.**: 123.2-126.1 °C; **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 2.40 (s, 3H), 2.41 (s, 3H), 7.23 (d, 2H, <sup>3</sup>*J* = 8.0 Hz), 7.25-7.27 (m, 3H), 7.36 (d, 2H, <sup>3</sup>*J* = 8.7 Hz), 7.56 (d, 2H, <sup>3</sup>*J* = 7.8 Hz), 7.64 (d, 2H, <sup>3</sup>*J* = 8.0 Hz), 7.8 (d, 1H, <sup>3</sup>*J* = 15.5 Hz), 8.07 (d, 2H, <sup>3</sup>*J* = 8.9 Hz), 8.43 (s, 1H); **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 21.68, 21.74, 114.18, 115.71, 120.99, 127.91, 128.57, 129.79, 129.81, 130.79, 132.39, 132.44, 141.05, 141.66, 144.47, 152.94, 163.17, 189.27; **IR (KBr)**  $\nu$  = 2364, 1652, 1595, 1576, 1511, 1504, 1416, 1390, 1330, 1305, 1287, 1252, 1221, 1208, 1159, 1110,

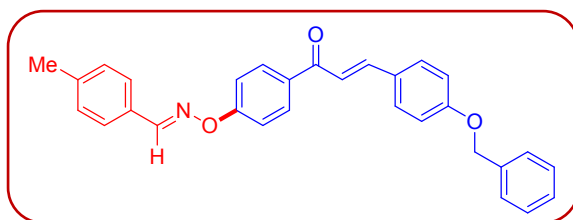
1024, 988, 928, 841, 812, 734 $\text{cm}^{-1}$ ; **HRMS (ESI) calcd.** for  $\text{C}_{24}\text{H}_{21}\text{NO}_2$ :  $[\text{M}+\text{H}]^+$  356.1651; Found: 356.1630;  $[\text{M}+\text{Na}]^+$  378.1470; Found: 378.1476.

**(E)-4-Methylbenzaldehyde O-(4-((E)-3-(4-methoxyphenyl)acryloyl)phenyl) oxime (25c)**



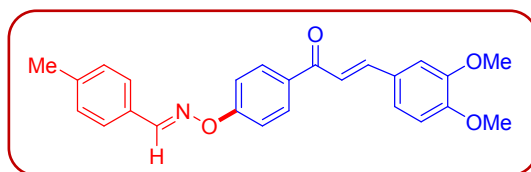
The general procedure described above was followed to get the title compound from (E)-1-(4-bromophenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (158 mg, 0.5 mmol), (E)-4-methylbenzaldehyde oxime (71 mg, 0.525 mmol),  $\text{Cs}_2\text{CO}_3$  (244 mg, 0.75 mmol),  $[(\pi\text{-allyl})\text{PdCl}]_2$  (5.49 mg, 3.0 mol%), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with THF as solvent (2.0 mL) were heated at 75  $^\circ\text{C}$  for 2.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a light yellow solid (125 mg, 67% yield). **m.p.**: 86.2-88.8 $^\circ\text{C}$ ;  **$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm)**: 2.41 (s, 3H), 3.86 (s, 3H), 6.94 (d, 2H,  $^3J = 8.7$  Hz), 7.26 (d, 2H,  $^3J = 8.0$  Hz), 7.35 (d, 2H,  $^3J = 8.7$  Hz), 7.45 (d, 1H,  $^3J = 15.5$  Hz), 7.60-7.65 (t, 4H), 7.79 (d, 1H,  $^3J = 15.5$  Hz), 8.07 (d, 2H,  $^3J = 8.9$  Hz), 8.43 (s, 1H);  **$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm)**: 21.74, 55.54, 114.16, 114.50, 119.70, 127.91, 128.24, 129.80, 130.29, 130.39, 130.69, 132.63, 141.65, 144.12, 152.90, 161.64, 163.06, 189.10; **IR (KBr)  $\nu$**  = 2366, 1653, 1606, 1550, 1503, 1420, 1383, 1337, 1289, 1244, 1221, 1162, 1031, 1014, 990, 925, 834, 810, 739, 679  $\text{cm}^{-1}$ ; **HRMS (ESI) calcd.** for  $\text{C}_{24}\text{H}_{21}\text{NO}_3$ :  $[\text{M}+\text{H}]^+$  372.1600; Found: 372.1601.

**(E)-4-Methylbenzaldehyde O-(4-((E)-3-(4-(benzyloxy)phenyl)acryloyl)phenyl) oxime (26c)**  
**E:Z (6.6 : 3.3)**



The general procedure described above was followed to get the title compound from (*E*)-3-(4-(benzyloxy)phenyl)-1-(4-bromophenyl)prop-2-en-1-one (196 mg, 0.5 mmol), (*E*)-4-methylbenzaldehyde oxime (71 mg, 0.525 mmol), Cs<sub>2</sub>CO<sub>3</sub> (244 mg, 0.75 mmol), [( $\pi$ -allyl)PdCl]<sub>2</sub>] (5.49 mg, 3.0 mol %), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with THF as solvent (2.0 mL) were heated at 75 °C for 2.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a light yellow solid (206 mg, 92% yield). **m.p.**: 132.2-134.0 °C; **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm):** Isomer *E*: 2.41 (s, 3H), 5.12 (s, 2H), 6.90 (d, 1H, <sup>3</sup>*J* = 8.4 Hz), 7.02 (d, 2H, <sup>3</sup>*J* = 8.1 Hz), 7.25-7.27 (t, 2H), 7.36 (d, 2H, <sup>3</sup>*J* = 8.4 Hz), 7.39-7.48 (m, 6H), 7.64 (d, 2H, <sup>3</sup>*J* = 8.2 Hz), 7.8 (d, 1H, <sup>3</sup>*J* = 15.6 Hz), 7.97 (d, 1H, <sup>3</sup>*J* = 8.5 Hz), 8.07 (d, 1H, <sup>3</sup>*J* = 8.8 Hz), 8.43 (s, 1H); **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm):** 21.72, 70.25, 114.20, 115.42, 119.87, 127.62, 127.92, 128.14, 128.26, 128.80, 129.80, 130.32, 130.73, 131.14, 132.60, 136.57, 141.65, 144.20, 152.94, 160.86, 163.14, 189.26; **Isomer *Z*** : 21.69, 70.23, 115.33, 115.74, 119.91, 128.14, 128.24, 128.29, 128.30, 130.24, 136.58, 143.79, 160.76, 189.11; **IR (KBr)  $\nu$**  = 2365, 1649, 1595, 1506, 1339, 1288, 1215, 1162, 1111, 1007, 981, 918, 814, 734 cm<sup>-1</sup>; **HRMS (ESI) calcd.** for C<sub>30</sub>H<sub>25</sub>NO<sub>3</sub>: [M+H]<sup>+</sup> 448.1913; Found: 448.1934.

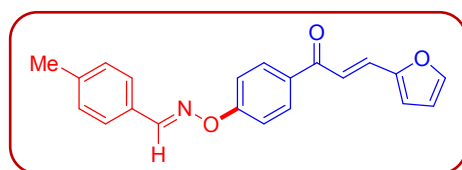
**(*E*)-4-Methylbenzaldehyde *O*-(4-((*E*)-3-(3,4-dimethoxyphenyl)acryloyl)phenyl) oxime (27c)**



The general procedure described above was followed to get the title compound from (*E*)-1-(4-bromophenyl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one (173 mg, 0.5 mmol), (*E*)-4-methylbenzaldehyde oxime (71 mg, 0.525 mmol), Cs<sub>2</sub>CO<sub>3</sub> (244 mg, 0.75 mmol), [( $\pi$ -allyl)PdCl]<sub>2</sub>] (5.49 mg, 3.0 mol %), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with THF as solvent (2.0 mL) were heated at 75 °C for 3.0 h. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a light brown solid (140 mg, 70% yield). **m.p.**: 84.2-86.9 °C; **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm):** 2.41 (s, 3H), 3.94 (s, 3H), 3.96 (s, 3H), 6.91 (d, 1H, <sup>3</sup>*J* = 8.2 Hz), 7.18 (s, 1H), 7.23-7.27 (m, 3H), 7.36

(d, 2H,  $^3J = 8.9$  Hz), 7.43 (d, 1H,  $^3J = 15.6$  Hz), 7.64 (d, 2H,  $^3J = 8.0$  Hz), 7.77 (d, 1H,  $^3J = 15.6$  Hz), 8.07 (d, 2H,  $^3J = 8.9$  Hz), 8.43 (s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 21.73, 56.09, 56.12, 110.21, 111.24, 114.18, 120.01, 123.18, 127.91, 128.17, 128.25, 129.80, 130.73, 132.58, 141.66, 144.51, 149.34, 151.41, 152.92, 163.12, 189.17; IR (KBr)  $\nu = 2367, 1656, 1574, 1504, 1492, 1391, 1335, 1304, 1250, 1217, 1147, 1112, 1086, 1032, 1017, 989, 973, 920, 837, 818, 792, 989, 973, 920, 837, 818, 792, 672\text{ cm}^{-1}$ ; HRMS (ESI) calcd. for  $\text{C}_{25}\text{H}_{23}\text{NO}_4$ :  $[\text{M}+\text{H}]^+$  402.1705; Found: 402.1708.

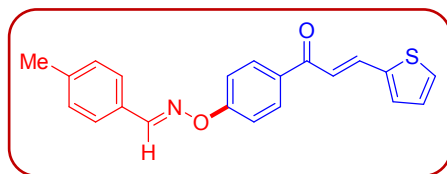
**(*E*)-4-Methylbenzaldehyde *O*-(4-((*E*)-3-(furan-2-yl)acryloyl)phenyl) oxime (28c)**



The general procedure described above was followed to get the title compound from (*E*)-1-(4-bromophenyl)-3-(furan-2-yl)prop-2-en-1-one (138 mg, 0.5 mmol), (*E*)-4-methylbenzaldehyde oxime (71 mg, 0.525 mmol),  $\text{Cs}_2\text{CO}_3$  (244 mg, 0.75 mmol),  $[(\pi\text{-allylPdCl})_2]$  (5.49 mg, 3.0 mol %), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with THF as solvent (2.0 mL) were heated at 75 °C for 2.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a yellow solid (160 mg, 98% yield). **m.p.**: 127.5-129.5°C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 2.40 (s, 3H), 6.50-6.52 (m, 1H), 6.7 (d, 1H,  $^3J = 3.4$  Hz), 7.25 (d, 2H,  $^3J = 7.7$  Hz), 7.34 (d, 2H,  $^3J = 8.6$  Hz), 7.48 (d, 1H,  $^3J = 15.6$  Hz), 7.52 (s, 1H), 7.57 (s, 1H), 7.63 (d, 2H,  $^3J = 7.7$  Hz), 8.07 (d, 2H,  $^3J = 8.4$  Hz), 8.41 (s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 21.72, 112.74, 114.17, 116.03, 119.33, 127.90, 128.21, 129.78, 130.22, 130.71, 132.33, 141.64, 144.86, 151.92, 152.91, 163.19, 188.35; IR (KBr)  $\nu = 2854, 1551, 1597, 1503, 1470, 1412, 1359, 1329, 1290, 1254, 1223, 1155, 1109, 1015, 977, 923, 817, 749, 687, 634\text{ cm}^{-1}$ ; HRMS (ESI) calcd. for  $\text{C}_{21}\text{H}_{17}\text{NO}_3$ :  $[\text{M}+\text{H}]^+$  332.1287; Found: 332.1292.

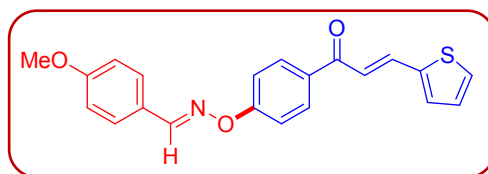


**(E)-4-Methylbenzaldehyde O-(4-((E)-3-(thiophen-2-yl)acryloyl)phenyl)oxime (29c)**



The general procedure described above was followed to get the title compound from (*E*)-1-(4-bromophenyl)-3-(thiophen-2-yl)prop-2-en-1-one (146 mg, 0.5 mmol), (*E*)-4-methylbenzaldehyde oxime (71 mg, 0.525 mmol), Cs<sub>2</sub>CO<sub>3</sub> (244 mg, 0.75 mmol), [( $\pi$ -allyl)PdCl]<sub>2</sub> (5.49 mg, 3.0 mol %), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with THF as solvent (2.0 mL) were heated at 75 °C for 1.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a yellow solid (145 mg, 84% yield). **m.p.**: 132.2-134.2°C; **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 2.41 (s, 3H), 7.08-7.11 (t, 1H), 7.26 (d, 2H, <sup>3</sup>*J* = 8.1 Hz), 7.36 (d, 2H, <sup>3</sup>*J* = 7.4 Hz), 7.38 (d, 2H, <sup>3</sup>*J* = 8.0 Hz), 7.42 (d, 1H, <sup>3</sup>*J* = 5.0 Hz), 7.64 (d, 2H, <sup>3</sup>*J* = 8.3 Hz), 7.95 (d, 1H, <sup>3</sup>*J* = 15.2 Hz), 8.06 (d, 2H, <sup>3</sup>*J* = 8.9 Hz), 8.43 (s, 1H); **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 21.74, 114.19, 120.77, 127.91, 128.20, 128.44, 128.65, 129.80, 130.70, 132.00, 132.24, 136.69, 140.68, 141.66, 152.93, 163.20, 188.38; **IR (KBr)**  $\nu$  = 2358, 1655, 1589, 1568, 1523, 1451, 1418, 1398, 1334, 1298, 1222, 1028, 1018, 973, 856, 928, 853, 840, 838, 812, 764, 752, 687, 648 cm<sup>-1</sup>; **HRMS (ESI) calcd.** for C<sub>21</sub>H<sub>17</sub>NO<sub>2</sub>S: [M+H]<sup>+</sup> 348.1058; Found: 348.1064.

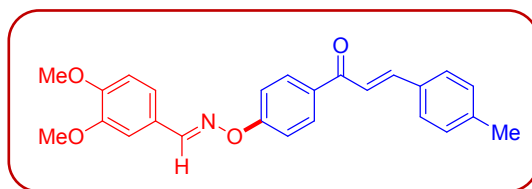
**(E)-4-methoxybenzaldehyde O-(4-((E)-3-(thiophen-2-yl)acryloyl)phenyl) oxime (30c)**



The general procedure described above was followed to get the title compound from (*E*)-1-(4-bromophenyl)-3-(thiophen-2-yl)prop-2-en-1-one (146 mg, 0.5 mmol), (*E*)-4-methoxybenzaldehyde oxime (79 mg, 0.525 mmol), Cs<sub>2</sub>CO<sub>3</sub> (244 mg, 0.75 mmol), [( $\pi$ -allyl)PdCl]<sub>2</sub> (5.49 mg, 3.0 mol %), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with THF as solvent (2.0 mL) were heated at 75 °C for 1.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a yellow solid (145

mg, 84% yield). **m.p.**: 127.2-129.0°C; **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 3.86 (s, 3H), 6.50 (q, 1H), 6.70 (d, 1H,  $^3J = 3.3$  Hz), 6.96 (d, 2H,  $^3J = 8.8$  Hz), 7.32-7.34 (m, 2H), 7.46-7.52 (m, 2H), 7.59 (d, 1H,  $^3J = 15.2$  Hz), 7.68 (d, 2H,  $^3J = 8.8$  Hz), 8.06-8.08 (m, 2H), 8.39 (s, 1H); **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 55.40, 112.58, 114.01, 114.40, 115.81, 119.27, 123.42, 129.43, 130.05, 130.57, 132.14, 144.69, 151.83, 152.39, 161.89, 163.14, 188.21; **IR (KBr)**  $\nu = 2320, 1605, 1570, 1538, 1520, 1442, 1409, 1387, 1328, 1282, 1225, 1038, 1005, 985, 856, 917, 840, 828, 812, 764, 752, 687, 665$  cm<sup>-1</sup>; **HRMS (ESI) calcd.** for C<sub>21</sub>H<sub>17</sub>NO<sub>3</sub>S: [M+H]<sup>+</sup> 363.0929; Found: 363.0936.

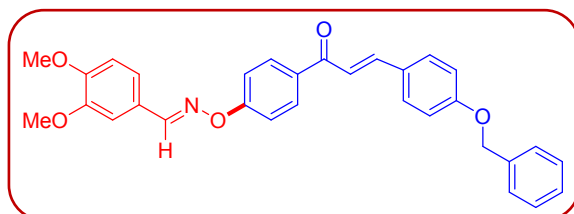
**(*E*)-3,4-Dimethoxybenzaldehyde *O*-(4-((*E*)-3-(*p*-tolyl)acryloyl)phenyl) oxime (31c) *E*:*Z* (3.3 : 1)**



The general procedure described above was followed to get the title compound from (*E*)-1-(4-bromophenyl)-3-*p*-tolylprop-2-en-1-one (150 mg, 0.5 mmol), (*E*)-3,4-dimethoxybenzaldehyde oxime (95 mg, 0.525 mmol), Cs<sub>2</sub>CO<sub>3</sub> (244 mg, 0.75 mmol), [( $\pi$ -allyl)PdCl]<sub>2</sub> (5.49 mg, 3.0 mol%), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with THF as solvent (2.0 mL) were heated at 75 °C for 2.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a light brown solid (190 mg, 95% yield). **m.p.**: 108.1-109.9°C; **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): **Isomer *E*** : 2.39 (s, 3H), 3.94 (s, 3H), 3.97 (s, 3H), 6.91 (d, 1H,  $^3J = 8.4$  Hz), 7.18 (d, 1H,  $^3J = 7.6$  Hz), 7.23 (d, 2H,  $^3J = 7.8$  Hz), 7.34-7.39 (m, 3H), 7.52-7.56 (m, 3H), 7.8 (d, 1H,  $^3J = 15.8$  Hz), 8.08 (d, 2H,  $^3J = 8.6$  Hz), 8.39 (s, 1H); **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 21.64, 56.11, 56.14, 108.69, 111.00, 114.23, 115.67, 123.09, 123.81, 128.56, 129.82, 130.78, 132.49, 132.45, 141.04, 144.49, 149.61, 151.90, 152.87, 163.23, 189.29; **Isomer *Z***: 21.62, 56.21, 56.26, 111.31, 111.40, 113.99, 114.11, 121.09, 126.61, 128.50, 129.78, 131.20, 140.87, 144.06, 189.26; **IR (KBr)**  $\nu = 2369, 1655, 1600, 1567, 1517, 1444, 1415, 1334, 1305, 1287, 1268, 1221, 1205, 1159, 1130, 1017,$

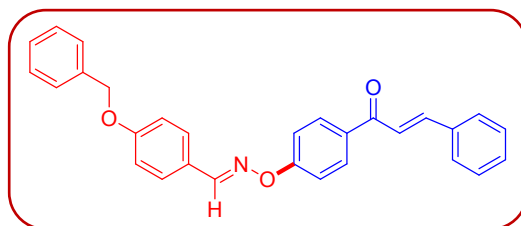
986, 920, 845, 809, 764, 733, 645, 616  $\text{cm}^{-1}$ ; **HRMS (ESI) calcd.** for  $\text{C}_{25}\text{H}_{23}\text{NO}_4$ :  $[\text{M}+\text{H}]^+$  402.1705; Found: 402.1708.

**(*E*)-3,4-Dimethoxybenzaldehyde *O*-(4-((*E*)-3-(4-(benzyloxy)phenyl)acryloyl)phenyl) oxime (32c)**



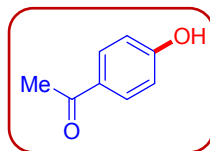
The general procedure described above was followed to get the title compound from (*E*)-3-(4-(benzyloxy)phenyl)-1-(4-bromophenyl)prop-2-en-1-one (196 mg, 0.5 mmol), (*E*)-3,4-dimethoxybenzaldehyde oxime (95 mg, 0.525 mmol),  $\text{Cs}_2\text{CO}_3$  (244 mg, 0.75 mmol),  $[(\pi\text{-allylPdCl})_2]$  (5.49 mg, 3.0 mol %), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with THF as solvent (2.0 mL) were heated at 75  $^\circ\text{C}$  for 3.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a light brown solid (180 mg, 73% yield). **m.p.:** 122.2-124.4 $^\circ\text{C}$ ;  **$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm):** 3.94 (s, 3H), 3.98 (s, 3H), 5.12 (s, 2H), 6.91 (d, 1H,  $^3J = 8.2$  Hz), 7.01 (d, 2H,  $^3J = 8.7$  Hz), 7.18 (d, 1H,  $^3J = 8.1$  Hz), 7.34-7.47 (m, 9H), 7.61 (d, 2H,  $^3J = 8.9$  Hz), 7.79 (d, 1H,  $^3J = 15.4$  Hz), 8.07 (d, 2H,  $^3J = 8.9$  Hz), 8.39 (s, 1H);  **$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm):** 56.06, 56.12, 70.19, 108.53, 110.89, 114.16, 115.37, 119.77, 123.08, 123.75, 127.60, 128.09, 128.29, 128.78, 130.29, 130.70, 132.54, 136.52, 144.14, 149.53, 151.81, 152.82, 160.82, 163.10, 189.12; **IR (KBr)  $\nu$  =** 2369, 1654, 1594, 1572, 1510, 1451, 1421, 1391, 1360, 1343, 1291, 1214, 1140, 1023, 1011, 983, 961, 920, 863, 840, 828, 808, 749, 734, 697  $\text{cm}^{-1}$ ; **HRMS (ESI) calcd.** for  $\text{C}_{31}\text{H}_{27}\text{NO}_5$ :  $[\text{M}+\text{H}]^+$  494.1967; Found: 494.1992.

**(*E*)-4-(Benzyloxy)benzaldehyde *O*-(4-cinnamoylphenyl) oxime (33c) *E:Z* (3.3 : 1)**



The general procedure described above was followed to get the title compound from (*E*)-1-(4-bromophenyl)-3-phenylprop-2-en-1-one (143 mg, 0.5 mmol), (*E*)-4-(benzyloxy)benzaldehydeoxime (119 mg, 0.525 mmol), Cs<sub>2</sub>CO<sub>3</sub> (244 mg, 0.75 mmol), [( $\pi$ -allyl)PdCl]<sub>2</sub>] (5.49 mg, 3.0 mol %), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with THF as solvent (2.0 mL) were heated at 75 °C for 3.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a light yellow solid (153 mg, 71% yield). **m.p.**: 103.3-105.5 °C; **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm):** Isomer **E**: 5.13 (s, 2H), 7.04 (d, 2H, <sup>3</sup>*J* = 8.2 Hz), 7.36 (d, 3H, <sup>3</sup>*J* = 8.9 Hz), 7.41-7.44 (m, 6H), 7.57 (d, 1H, <sup>3</sup>*J* = 15.5 Hz), 7.65-7.70 (m, 4H), 7.83 (d, 1H, <sup>3</sup>*J* = 15.4 Hz), 8.08 (d, 2H, <sup>3</sup>*J* = 8.2 Hz), 8.41 (s, 1H); **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm):** 70.26, 114.20, 115.46, 122.13, 127.61, 128.33, 128.82, 128.86, 129.03, 129.06, 129.60, 130.49, 130.82, 132.30, 135.22, 136.49, 144.28, 152.54, 161.22, 163.34, 189.11; **Isomer Z**: 70.42, 115.24, 115.71, 123.80, 128.21, 128.46, 128.90, 129.03, 130.23, 130.36, 131.20, 132.16, 134.15, 143.84, 152.32; **IR (KBr)  $\nu$  =** 2365, 1661, 1592, 1568, 1513, 1496, 1449, 1403, 1337, 1303, 1261, 1218, 1164, 1109, 1023, 978, 956, 931, 827, 761, 722, 660 cm<sup>-1</sup>; **HRMS (ESI) calcd.** for C<sub>29</sub>H<sub>23</sub>NO<sub>3</sub>: [M+H]<sup>+</sup> 434.1756; Found: 434.1759.

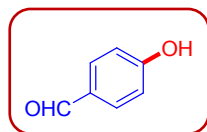
#### 4'-Hydroxyacetophenone (1p)<sup>1</sup>



The general procedure described above was followed to get the title compound from 4'-bromoacetophenone (199 mg, 1.0 mmol), (*E*)-4-methylbenzaldehyde oxime (142 mg, 1.05 mmol), Cs<sub>2</sub>CO<sub>3</sub> (488 mg, 1.5 mmol), [( $\pi$ -allyl)PdCl]<sub>2</sub>] (3.65 mg, 1.0 mol %), *t*BuXPhos (**L2**) (10.6 mg, 2.5 mol %), with THF as solvent (2.0 mL) were heated at 75 °C for 1.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a light brown solid (125 mg, 92% yield). **m.p.**: 107.2-108.5 °C (lit. 105.0-105.5 °C); **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm):** 2.58 (s, 3H), 6.92 (d, 2H, <sup>3</sup>*J* = 8.6 Hz), 7.9 (d, 2H, <sup>3</sup>*J* = 8.7 Hz); **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm):** 26.40, 115.72, 129.55,

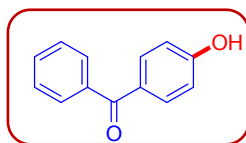
131.41, 161.92, 199.23. The  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of the compound were in good agreement with those previously reported in the literature.

#### 4-Hydroxybenzaldehyde (2p)<sup>2</sup>



The general procedure described above was followed to get the title compound from 4-bromobenzaldehyde (185 mg, 1.0 mmol), (*E*)-4-methylbenzaldehyde oxime (142 mg, 1.05 mmol),  $\text{Cs}_2\text{CO}_3$  (488 mg, 1.5 mmol),  $[(\pi\text{-allyl})\text{PdCl}]_2$  (3.65 mg, 1.0 mol %), *t*BuXPhos (**L2**) (10.6 mg, 2.5 mol %), with THF as solvent (2.0 mL) were heated at 75°C for 3.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a brown solid (120 mg, 98% yield). **m.p.**: 112.3-114.3°C (lit. 112-116 °C);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 6.98 (d, 2H,  $^3J = 8.5$  Hz), 7.81 (d, 2H,  $^3J = 8.4$  Hz), 9.85 (s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 116.28, 129.44, 132.84, 162.54, 191.92. The  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of the compound were in good agreement with those previously reported in the literature.

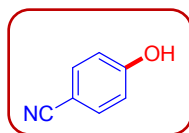
#### 4-Hydroxybenzophenone (3p)<sup>3</sup>



The general procedure described above was followed to get the title compound from 4-bromobenzophenone (261 mg, 1.0 mmol), (*E*)-4-methylbenzaldehyde oxime (142 mg, 1.05 mmol),  $\text{Cs}_2\text{CO}_3$  (488 mg, 1.5 mmol),  $[(\pi\text{-allyl})\text{PdCl}]_2$  (3.65 mg, 1.0 mol %), *t*BuXPhos (**L2**) (10.6 mg, 2.5 mol %), with THF as solvent (2.0 mL) were heated at 75°C for 3.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a creamy white solid (162 mg, 82% yield). **m.p.**: 127.9-130.5°C (lit. 132-135 °C);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 6.94 (d, 2H,  $^3J = 8.7$  Hz), 7.46 (d, 1H,  $^3J = 7.5$  Hz), 7.48 (d, 1H,  $^3J = 7.5$  Hz), 7.57 (t, 1H,  $^3J = 7.5$  Hz), 7.75 (d, 2H,  $^3J = 6.6$  Hz), 7.77 (d,

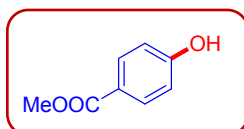
2H,  $^3J = 7.7$  Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 115.57, 128.41, 129.37, 130.00, 132.35, 133.31, 138.14, 161.29, 197.17. The  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of the compound were in good agreement with those previously reported in the literature.

#### 4-Hydroxybenzonitrile (5p)<sup>1,4</sup>



The general procedure described above was followed to get the title compound from 4-bromobenzonitrile (182 mg, 1.0 mmol), (*E*)-4-methylbenzaldehyde oxime (142 mg, 1.05 mmol),  $\text{Cs}_2\text{CO}_3$  (488 mg, 1.5 mmol),  $[(\pi\text{-allyl})\text{PdCl}]_2$  (3.65 mg, 1.0 mol %), *t*BuXPhos (**L2**) (10.6 mg, 2.5 mol %), with THF as solvent (2.0 mL) were heated at 75°C for 2.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a brown solid (117 mg, 98% yield). **m.p.**: 108.8-110.2°C (lit. 109.0-109.5 °C);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 6.93 (d, 2H,  $^3J = 8.5$  Hz), 7.55 (d, 2H,  $^3J = 8.4$  Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 102.85, 116.61, 119.46, 134.43, 160.56. The  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of the compound were in good agreement with those previously reported in the literature.

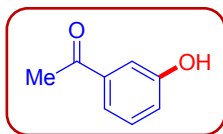
#### Methyl 4-hydroxybenzoate (6p)<sup>4</sup>



The general procedure described above was followed to get the title compound from methyl 4-bromobenzoate (215 mg, 1.0 mmol), (*E*)-4-methylbenzaldehyde oxime (142 mg, 1.05 mmol),  $\text{Cs}_2\text{CO}_3$  (488 mg, 1.5 mmol),  $[(\pi\text{-allyl})\text{PdCl}]_2$  (3.65 mg, 1.0 mol %), *t*BuXPhos (**L2**) (10.6 mg, 2.5 mol %), with THF as solvent (2.0 mL) were heated at 75 °C for 4.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a light brown solid (120 mg, 79% yield). **m.p.**: 125.6-127.8°C (lit. 127-129 °C);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 3.89 (s, 3H), 6.87 (d, 2H,  $^3J = 8.7$  Hz), 7.95 (d, 2H,  $^3J = 8.6$  Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 52.26, 115.46, 122.15, 132.08, 160.62,

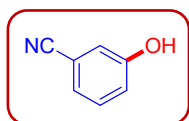
167.73. The  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of the compound were in good agreement with those previously reported in the literature.

### 3'-Hydroxyacetophenone (11p)<sup>4</sup>



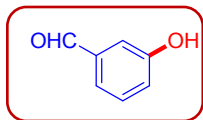
The general procedure described above was followed to get the title compound from 3'-bromoacetophenone (199 mg, 1.0 mmol), (*E*)-4-methylbenzaldehyde oxime (142 mg, 1.05 mmol),  $\text{Cs}_2\text{CO}_3$  (488 mg, 1.5 mmol),  $[(\pi\text{-allylPdCl})_2]$  (7.3 mg, 2.0 mol %), *t*BuBrettPhos (**L7**) (24.4 mg, 5.0 mol %), with DMF as solvent (2.0 mL) were heated at 90 °C for 5.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a creamy white solid (125 mg, 90% yield). **m.p.**: 93.2-95.8°C (lit. 92-94 °C);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 2.60 (s, 3H), 7.09-7.12 (m, 1H), 7.31-7.35 (t, 1H), 7.5 (d, 1H,  $^3J = 7.8\text{Hz}$ ), 7.52-7.53 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 26.90, 114.85, 121.11, 130.03, 138.31, 156.63, 156.66, 199.92.

### 3-Hydroxybenzonitrile (12p)<sup>5</sup>



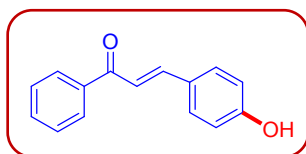
The general procedure described above was followed to get the title compound from 3-bromobenzonitrile (182 mg, 1.0 mmol), (*E*)-4-methylbenzaldehyde oxime (142 mg, 1.05 mmol),  $\text{Cs}_2\text{CO}_3$  (488 mg, 1.5 mmol),  $[(\pi\text{-allylPdCl})_2]$  (7.3 mg, 2.0 mol %), *t*BuBrettPhos (**L7**) (24.4 mg, 5.0 mol %), with DMF as solvent (2.0 mL) were heated at 90 °C for 3.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a brown solid (113 mg, 95% yield). **m.p.**: 74.8-77.2°C (lit. 78-81 °C);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.10 (d, 1H,  $^3J = 8.1\text{Hz}$ ), 7.13 (s, 1H), 7.21 (d, 1H,  $^3J = 7.6\text{Hz}$ ), 7.31-7.35 (t, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 112.63, 118.80, 118.88, 121.00, 124.40, 130.70, 156.57. The  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of the compound were in good agreement with those previously reported in the literature.

### 3-Hydroxybenzaldehyde (13p)<sup>6</sup>



The general procedure described above was followed to get the title compound from 3-bromobenzaldehyde (185 mg, 1.0 mmol), (*E*)-4-methylbenzaldehyde oxime (142 mg, 1.05 mmol), Cs<sub>2</sub>CO<sub>3</sub> (488 mg, 1.5 mmol), [( $\pi$ -allylPdCl)<sub>2</sub>] (7.3 mg, 2.0 mol %), *t*BuBrettPhos (**L7**) (24.4 mg, 5.0 mol %), with DMF as solvent (2.0 mL) were heated at 90°C for 2.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a light brown solid (112 mg, 92% yield). **m.p.**: 99.1-100.9°C (lit. 100-103 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 7.17-7.19 (m, 1H), 7.39-7.45 (m, 3H), 9.92 (s, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 114.89, 122.59, 123.75, 130.56, 137.67, 156.78, 193.34. The <sup>1</sup>H and <sup>13</sup>C NMR spectra of the compound were in good agreement with those previously reported in the literature.

### (*E*)-3-(4-Hydroxyphenyl)-1-phenylprop-2-en-1-one (16p)<sup>7</sup>

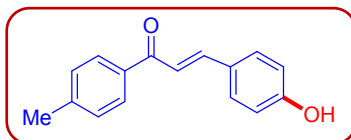


The general procedure described above was followed to get the title compound from (*E*)-3-(4-bromophenyl)-1-phenylprop-2-en-1-one (143 mg, 0.5 mmol), (*E*)-4-methylbenzaldehyde oxime (71 mg, 0.525 mmol), Cs<sub>2</sub>CO<sub>3</sub> (244 mg, 0.75 mmol), [( $\pi$ -allylPdCl)<sub>2</sub>] (5.49 mg, 3.0 mol %), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with DMF as solvent (2.0 mL) were heated at 90 °C for 1.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a brown solid (101 mg, 91% yield). **m.p.**: 179.2-181.5°C (lit. 183-187 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 6.88 (d, 2H, <sup>3</sup>J = 8.4 Hz), 7.4 (d, 1H, <sup>3</sup>J = 15.5 Hz), 7.48-7.52 (t, 2H), 7.54-7.58 (t, 3H), 7.78 (d, 1H, <sup>3</sup>J = 15.6 Hz), 8.01 (d, 2H, <sup>3</sup>J = 7.1 Hz); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 116.27, 119.58, 128.63, 128.75, 130.69, 132.85, 138.54, 145.54, 145.55, 158.87, 191.42; **HRMS (ESI) calcd.** for C<sub>15</sub>H<sub>12</sub>O<sub>2</sub>:



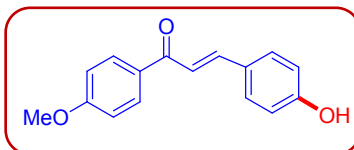
[M+H]<sup>+</sup> 225.0916; Found: 225.0907. The <sup>1</sup>H and <sup>13</sup>C NMR spectra of the compound were in good agreement with those previously reported in the literature.

**(*E*)-3-(4-Hydroxyphenyl)-1-p-tolylprop-2-en-1-one (17p)<sup>8</sup>**



The general procedure described above was followed to get the title compound from (*E*)-3-(4-bromophenyl)-1-p-tolylprop-2-en-1-one (150 mg, 0.5 mmol), (*E*)-4-methylbenzaldehyde oxime (71 mg, 0.525 mmol), Cs<sub>2</sub>CO<sub>3</sub> (244 mg, 0.75 mmol), [(π-allyl)PdCl]<sub>2</sub> (5.49 mg, 3.0 mol %), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with DMF as solvent (2.0 mL) were heated at 90 °C for 1.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a light brown solid (100 mg, 85% yield). **m.p.**: 185.2-186.8 °C (lit. 182-183 °C); **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)** δ (ppm): 2.43 (s, 3H), 6.9 (d, 2H, <sup>3</sup>J = 8.5 Hz), 7.3 (d, 2H, <sup>3</sup>J = 8.0 Hz), 7.4 (d, 1H, <sup>3</sup>J = 15.5 Hz), 7.54 (d, 2H, <sup>3</sup>J = 8.4 Hz), 7.77 (d, 1H, <sup>3</sup>J = 15.6 Hz), 7.93 (d, 2H, <sup>3</sup>J = 8.2 Hz); **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)** δ (ppm): 21.81, 116.27, 119.41, 127.29, 128.79, 129.46, 130.66, 135.84, 143.80, 145.29, 158.97, 191.04; **IR** (KBr) ν = 1656, 1572, 1503, 1467, 1386, 1378, 1286, 1256, 1232, 1126, 1029, 996, 950, 885, 756, 625 cm<sup>-1</sup>; **HRMS (ESI) calcd.** for C<sub>16</sub>H<sub>14</sub>O<sub>2</sub>: [M+H]<sup>+</sup> 239.1072; Found: 239.1069; [M+Na]<sup>+</sup> 261.0891; Found: 261.0885.

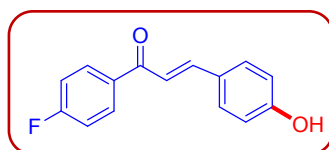
**(*E*)-3-(4-Hydroxyphenyl)-1-(4-methoxyphenyl)prop-2-en-1-one (18p)<sup>7</sup>**



The general procedure described above was followed to get the title compound from (*E*)-3-(4-bromophenyl)-1-(4-methoxyphenyl)prop-2-en-1-one (158 mg, 0.5 mmol), (*E*)-4-methylbenzaldehyde oxime (71 mg, 0.525 mmol), Cs<sub>2</sub>CO<sub>3</sub> (244 mg, 0.75 mmol), [(π-allyl)PdCl]<sub>2</sub> (5.49 mg, 3.0 mol %), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with DMF as solvent (2.0 mL) were heated at 90 °C for 1.0 hour. The crude reaction mixture was purified through

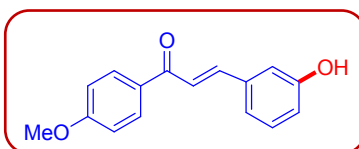
column chromatography (silica gel 60-120 mesh) to afford the title compound as a lightbrown solid (122 mg, 97% yield). **m.p.**: 182.8-183.8°C(lit. 184-186 °C); **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 3.89 (s, 3H), 6.89 (d, 2H,  $^3J = 8.5$  Hz), 6.98 (d, 2H,  $^3J = 8.9$  Hz), 7.42 (d, 1H,  $^3J = 15.6$  Hz), 7.54 (d, 2H,  $^3J = 8.6$  Hz), 7.77 (d, 1H,  $^3J = 15.6$  Hz), 8.03 (d, 2H,  $^3J = 8.9$  Hz); **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 55.65, 113.99, 116.21, 119.39, 127.64, 130.57, 130.96, 131.36, 144.56, 158.60, 163.56, 189.52; **HRMS (ESI) calcd.** for C<sub>16</sub>H<sub>14</sub>O<sub>3</sub>: [M+H]<sup>+</sup> 255.1021; Found: 255.1018. The <sup>1</sup>H and <sup>13</sup>C NMR spectra of the compound were in good agreement with those previously reported in the literature.

**(*E*)-1-(4-Fluorophenyl)-3-(4-hydroxyphenyl)prop-2-en-1-one (19p)<sup>9</sup>**



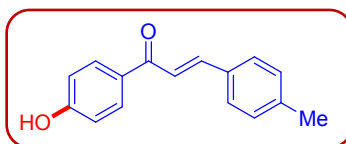
The general procedure described above was followed to get the title compound from (*E*)-3-(4-bromophenyl)-1-(4-fluorophenyl)prop-2-en-1-one (152 mg, 0.5 mmol), (*E*)-4-methylbenzaldehyde oxime (71 mg, 0.525 mmol), Cs<sub>2</sub>CO<sub>3</sub> (244 mg, 0.75 mmol), [( $\pi$ -allyl)PdCl]<sub>2</sub> (5.49 mg, 3.0 mol%), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with DMF as solvent (2.0 mL) were heated at 90 °C for 50 min. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a brown solid (96 mg, 80% yield). **m.p.**: 186.7-188.0°C; **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 6.90 (d, 2H,  $^3J = 8.6$  Hz), 7.15-7.19 (t, 2H), 7.38 (d, 1H,  $^3J = 15.6$  Hz), 7.55 (d, 2H,  $^3J = 8.5$  Hz), 7.78 (d, 1H,  $^3J = 15.6$  Hz), 8.03-8.06 (q, 2H); **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 115.87 (d,  $^2J_{C-F} = 21.6$  Hz), 116.26, 119.05, 127.28, 129.90, 130.74, 131.2 (d,  $^3J_{C-F} = 9.0$  Hz), 132.31, 145.66, 158.90, 189.62; **HRMS (ESI) calcd.** for C<sub>15</sub>H<sub>11</sub>FO<sub>2</sub>: [M+H]<sup>+</sup> 243.0821; Found: 243.0816; [M+Na]<sup>+</sup> 265.0641; Found: 265.0635. The <sup>1</sup>H and <sup>13</sup>C NMR spectra of the compound were in good agreement with those previously reported in the literature.

**(E)-3-(3-Hydroxyphenyl)-1-(4-methoxyphenyl)prop-2-en-1-one (20p)<sup>7</sup>**



The general procedure described above was followed to get the title compound from (E)-3-(3-bromophenyl)-1-(4-methoxyphenyl)prop-2-en-1-one (158 mg, 0.5 mmol), (E)-4-methylbenzaldehyde oxime (71 mg, 0.525 mmol), Cs<sub>2</sub>CO<sub>3</sub> (244 mg, 0.75 mmol), [( $\pi$ -allylPdCl)<sub>2</sub>] (5.49 mg, 3.0 mol %), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with DMF as solvent (2.0 mL) were heated at 90 °C for 1.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a brown solid (102 mg, 81% yield). **m.p.**: 189.5-192.0°C; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  (ppm): 3.91 (s, 3H), 6.90 (d, 1H, <sup>3</sup>*J* = 7.7 Hz), 7.12 (d, 2H, <sup>3</sup>*J* = 8.6 Hz), 7.25-7.29 (m, 2H), 7.32 (d, 1H, <sup>3</sup>*J* = 9.7 Hz), 7.65 (d, 1H, <sup>3</sup>*J* = 15.5 Hz), 7.88 (d, 1H, <sup>3</sup>*J* = 15.6 Hz), 8.2 (d, 2H, <sup>3</sup>*J* = 8.9 Hz), 9.66 (s, 1H); <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  (ppm): 55.71, 114.18, 115.27, 117.78, 119.95, 121.93, 130.05, 130.54, 131.07, 136.19, 143.58, 157.83, 163.37, 187.58; IR (KBr)  $\nu$  = 2365, 1646, 1603, 1561, 1509, 1466, 1383, 1339, 1285, 1254, 1221, 1166, 1035, 1020, 990, 842, 820, 738 cm<sup>-1</sup>; HRMS (ESI) **calcd.** for C<sub>16</sub>H<sub>14</sub>O<sub>3</sub>: [M+H]<sup>+</sup> 255.1021; Found: 255.1004; [M+Na]<sup>+</sup> 278.0841; Found: 278.0823.

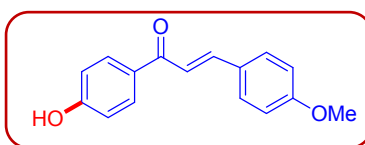
**(E)-1-(4-Hydroxyphenyl)-3-p-tolylprop-2-en-1-one (24p)**



The general procedure described above was followed to get the title compound from (E)-1-(4-bromophenyl)-3-p-tolylprop-2-en-1-one (150 mg, 0.5 mmol), (E)-4-methylbenzaldehyde oxime (71 mg, 0.525 mmol), Cs<sub>2</sub>CO<sub>3</sub> (244 mg, 0.75 mmol), [( $\pi$ -allylPdCl)<sub>2</sub>] (5.49 mg, 3.0 mol %), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with DMF as solvent (2.0 mL) were heated at 90 °C for 4.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a brown solid (116 mg, 98% yield). **m.p.**: 175.8-

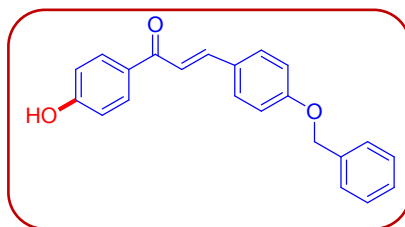
177.9°C; **<sup>1</sup>H NMR (400 MHz, DMSO-*D*<sub>6</sub>)**  $\delta$  (ppm): 2.49 (s, 3H), 5.98 (d, 2H, <sup>3</sup>*J* = 8.7 Hz), 6.34 (d, 2H, <sup>3</sup>*J* = 8.0 Hz), 6.73 (d, 1H, <sup>3</sup>*J* = 15.7 Hz), 6.83 (d, 2H, <sup>3</sup>*J* = 8.0 Hz), 6.93 (d, 1H, <sup>3</sup>*J* = 15.8 Hz), 7.14 (d, 2H, <sup>3</sup>*J* = 8.7 Hz), 9.53 (s, 1H); **<sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  (ppm): 21.16, 115.48, 121.08, 128.84, 129.29, 129.63, 131.24, 132.25, 140.45, 142.92, 162.25, 187.25; **IR (KBr)**  $\nu$  = 2334, 1668, 1510, 1466, 1338, 1285, 1265, 1222, 1184, 1003, 985, 856, 835, 725, 636 cm<sup>-1</sup>; **HRMS (ESI) calcd.** for C<sub>16</sub>H<sub>14</sub>O<sub>2</sub>: [M+H]<sup>+</sup> 239.1072; Found: 239.1068; [M+Na]<sup>+</sup> 261.0891; Found: 261.0889.

**(*E*)-1-(4-Hydroxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (25p)<sup>10</sup>**



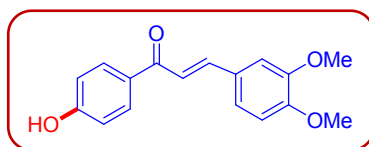
The general procedure described above was followed to get the title compound from (*E*)-1-(4-bromophenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (158 mg, 0.5 mmol), (*E*)-4-methylbenzaldehyde oxime (71 mg, 0.525 mmol), Cs<sub>2</sub>CO<sub>3</sub> (244 mg, 0.75 mmol), [( $\pi$ -allylPdCl)<sub>2</sub>] (5.49 mg, 3.0 mol %), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with DMF as solvent (2.0 mL) were heated at 90 °C for 6.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a light brown solid (122 mg, 97% yield). **m.p.**: 186.9-188.2°C (lit. 190 °C); **<sup>1</sup>H NMR (400 MHz, DMSO-*D*<sub>6</sub>)**  $\delta$  (ppm): 2.86 (s, 3H), 5.94 (d, 2H, <sup>3</sup>*J* = 8.5 Hz), 6.05 (d, 2H, <sup>3</sup>*J* = 8.5 Hz), 6.7 (d, 1H, <sup>3</sup>*J* = 15.3 Hz), 6.82 (d, 1H, <sup>3</sup>*J* = 15.6 Hz), 6.87 (d, 2H, <sup>3</sup>*J* = 8.4 Hz), 7.11 (d, 2H, <sup>3</sup>*J* = 8.4 Hz), 9.49 (s, 1H); **<sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  (ppm): 55.45, 114.49, 115.48, 119.65, 127.62, 129.47, 130.68, 131.17, 142.87, 161.25, 162.15, 187.23; **HRMS (ESI) calcd.** for C<sub>16</sub>H<sub>14</sub>O<sub>3</sub>: [M+H]<sup>+</sup> 255.1021; Found: 255.1018; [M+Na]<sup>+</sup> 277.0841; Found: 277.0838. The <sup>1</sup>H and <sup>13</sup>C NMR spectra of the compound were in good agreement with those previously reported in the literature.

**(E)-3-(4-(Benzyloxy)phenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one (26p)**



The general procedure described above was followed to get the title compound from (E)-3-(4-(benzyloxy)phenyl)-1-(4-bromophenyl)prop-2-en-1-one (196 mg, 0.5 mmol), (E)-4-methylbenzaldehyde oxime (71 mg, 0.525 mmol), Cs<sub>2</sub>CO<sub>3</sub> (244 mg, 0.75 mmol), [(π-allyl)PdCl]<sub>2</sub> (5.49 mg, 3.0 mol %), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with DMF as solvent (2.0 mL) were heated at 90°C for 50 min. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a light brown solid (161 mg, 98% yield). **m.p.**: 194.5-196.8°C; **<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)** δ (ppm): 4.22 (s, 2H), 5.95 (d, 2H, <sup>3</sup>*J* = 8.7 Hz), 6.14 (d, 2H, <sup>3</sup>*J* = 8.7 Hz), 6.39-6.53 (m, 5H), 6.7 (d, 1H, <sup>3</sup>*J* = 15.7 Hz), 6.83 (d, 1H, <sup>3</sup>*J* = 15.5 Hz), 6.87 (d, 2H, <sup>3</sup>*J* = 8.7 Hz), 7.11 (d, 2H, <sup>3</sup>*J* = 8.5 Hz), 9.49 (s, 1H); **<sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>)** δ (ppm): 69.46, 115.31, 115.45, 119.77, 127.81, 127.90, 128.08, 128.60, 129.43, 130.66, 131.17, 136.82, 142.77, 160.29, 162.13, 187.19; **IR (KBr)** ν = 2325, 1656, 1558, 1529, 1485, 1325, 1285, 1275, 1256, 1178, 1052, 1028, 980, 858, 825, 759, 662 cm<sup>-1</sup>; **HRMS (ESI) calcd.** for C<sub>22</sub>H<sub>18</sub>O<sub>3</sub>: [M+H]<sup>+</sup> 331.1334; Found 331.1315.

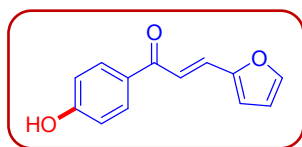
**(E)-3-(3,4-Dimethoxyphenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one (27p)**



The general procedure described above was followed to get the title compound from (E)-1-(4-bromophenyl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one (173 mg, 0.5 mmol), (E)-4-methylbenzaldehyde oxime (71 mg, 0.525 mmol), Cs<sub>2</sub>CO<sub>3</sub> (244 mg, 0.75 mmol), [(π-allyl)PdCl]<sub>2</sub> (5.49 mg, 3.0 mol %), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with DMF as solvent (2.0 mL) were heated at 90 °C for 3.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a yellow solid

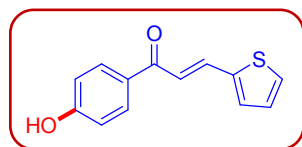
(134 mg, 95% yield). **m.p.**: 196.8-198.5°C; **<sup>1</sup>H NMR (400 MHz, DMSO-*D*<sub>6</sub>)**  $\delta$  (ppm): 2.87 (s, 3H), 2.92 (s, 3H), 5.97 (d, 2H,  $^3J = 7.4$  Hz), 6.07 (d, 1H,  $^3J = 8.2$  Hz), 6.41 (d, 1H,  $^3J = 7.7$  Hz), 6.58 (s, 1H), 6.7 (d, 1H,  $^3J = 15.5$  Hz), 6.86 (d, 1H,  $^3J = 15.7$  Hz), 7.14 (d, 2H,  $^3J = 8.0$  Hz), 9.5 (s, 1H); **<sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  (ppm): 55.65, 55.79, 110.63, 111.60, 115.43, 119.71, 123.78, 127.80, 129.47, 131.20, 143.38, 149.11, 151.12, 162.12, 187.21; **IR (KBr)**  $\nu$  = 2345, 1646, 1603, 1559, 1510, 1466, 1338, 1285, 1254, 1221, 1166, 1035, 1020, 990, 842, 820, 749, 636 cm<sup>-1</sup>; **HRMS (ESI) calcd.** for C<sub>17</sub>H<sub>16</sub>O<sub>4</sub>: [M+H]<sup>+</sup> 285.1127; Found: 285.1123.

**(*E*)-3-(Furan-2-yl)-1-(4-hydroxyphenyl)prop-2-en-1-one (28p)**



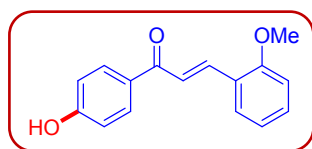
The general procedure described above was followed to get the title compound from (*E*)-1-(4-bromophenyl)-3-(furan-2-yl)prop-2-en-1-one (138 mg, 0.5 mmol), (*E*)-4-methylbenzaldehyde oxime (71 mg, 0.525 mmol), Cs<sub>2</sub>CO<sub>3</sub> (244 mg, 0.75 mmol), [( $\pi$ -allyl)PdCl]<sub>2</sub> (5.49 mg, 3.0 mol%), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with DMF as solvent (2.0 mL) were heated at 90 °C for 2.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a yellow solid (105 mg, 99% yield). **m.p.**: 165.8-168.2°C; **<sup>1</sup>H NMR (400 MHz, DMSO-*D*<sub>6</sub>)**  $\delta$  (ppm): 5.74 (s, 1H), 5.96 (d, 2H,  $^3J = 8.7$  Hz), 6.13 (d, 1H,  $^3J = 3.5$  Hz), 6.59 (s, 2H), 6.95 (s, 1H), 7.04 (d, 2H,  $^3J = 8.7$  Hz), 9.55 (s, 1H); **<sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  (ppm): 113.12, 115.58, 116.42, 118.90, 129.10, 129.54, 131.05, 145.93, 151.39, 162.29, 186.69; **IR (KBr)**  $\nu$  = 2319, 1603, 1565, 1518, 1345, 1298, 1278, 1128, 958, 853, 758, 625 cm<sup>-1</sup>; **HRMS (ESI) calcd.** for C<sub>13</sub>H<sub>10</sub>O<sub>3</sub>: [M+H]<sup>+</sup> 215.0708; Found: 215.0704; [M+Na]<sup>+</sup> 237.0528; Found: 237.0523.

**(*E*)-1-(4-Hydroxyphenyl)-3-(thiophen-2-yl)prop-2-en-1-one (29p)**



The general procedure described above was followed to get the title compound from (*E*)-1-(4-bromophenyl)-3-(thiophen-2-yl)prop-2-en-1-one (146 mg, 0.5 mmol), (*E*)-4-methylbenzaldehyde oxime (71 mg, 0.525 mmol), Cs<sub>2</sub>CO<sub>3</sub> (244 mg, 0.75 mmol), [( $\pi$ -allyl)PdCl]<sub>2</sub>] (5.49 mg, 3.0 mol %), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with DMF as solvent (2.0 mL) were heated at 90°C for 1.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a yellow solid (109 mg, 95% yield). **m.p.**: 172.6-174.8°C; **<sup>1</sup>H NMR (400 MHz, DMSO-*D*<sub>6</sub>)**  $\delta$  (ppm): 5.93 (d, 2H, <sup>3</sup>*J* = 8.6 Hz), 6.19-6.21 (q, 1H), 6.56 (d, 1H, <sup>3</sup>*J* = 15.0 Hz), 6.67 (d, 1H, <sup>3</sup>*J* = 3.9 Hz), 6.77 (d, 1H, <sup>3</sup>*J* = 5.0 Hz), 6.88 (d, 1H, <sup>3</sup>*J* = 15.3 Hz), 7.03 (d, 2H, <sup>3</sup>*J* = 9.0 Hz), 9.51 (s, 1H); **<sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  (ppm): 115.55, 120.47, 128.78, 129.06, 130.00, 131.14, 132.46, 135.68, 140.04, 162.30, 186.73; **IR (KBr)**  $\nu$  = 2317, 1610, 1573, 1509, 1486, 1376, 1316, 1253, 1228, 1169, 1095, 963, 856, 820, 729 cm<sup>-1</sup>; **HRMS (ESI) calcd.** for C<sub>13</sub>H<sub>10</sub>O<sub>2</sub>S: [M+H]<sup>+</sup> 231.0480; Found: 231.0484.

**(*E*)-1-(4-Hydroxyphenyl)-3-(2-methoxyphenyl)prop-2-en-1-one (34p)**



The general procedure described above was followed to get the title compound from (*E*)-1-(4-bromophenyl)-3-(2-methoxyphenyl)prop-2-en-1-one (158 mg, 0.5 mmol), (*E*)-4-methylbenzaldehyde oxime (71 mg, 0.525 mmol), Cs<sub>2</sub>CO<sub>3</sub> (244 mg, 0.75 mmol), [( $\pi$ -allyl)PdCl]<sub>2</sub>] (5.49 mg, 3.0 mol %), *t*BuXPhos (**L2**) (15.9 mg, 7.5 mol %), with DMF as solvent (2.0 mL) were heated at 90 °C for 4.0 hour. The crude reaction mixture was purified through column chromatography (silica gel 60-120 mesh) to afford the title compound as a brown solid (111 mg, 87% yield). **m.p.**: 194.5-196.8°C; **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 3.84 (s, 3H), 6.92 (d, 2H, <sup>3</sup>*J* = 8.7 Hz), 6.97 (d, 2H, <sup>3</sup>*J* = 8.3 Hz), 7.44 (d, 1H, <sup>3</sup>*J* = 15.9 Hz), 7.58 (d, 2H, <sup>3</sup>*J* = 8.7 Hz), 7.79 (d, 1H, <sup>3</sup>*J* = 15.5 Hz), 7.98 (d, 2H, <sup>3</sup>*J* = 8.4 Hz); **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)**  $\delta$  (ppm): 55.54, 114.52, 115.74, 115.79, 119.56, 127.78, 130.37, 130.38, 131.29, 131.33, 144.44, 144.61, 161.74, 161.75; **IR (KBr)**  $\nu$  = 2365, 1646, 1603, 1561, 1509, 1466, 1383, 1339, 1285, 1254, 1221, 1166, 1035, 1020, 990, 820, 738 cm<sup>-1</sup>; **HRMS (ESI) calcd.** for C<sub>16</sub>H<sub>14</sub>O<sub>3</sub>: [M+H]<sup>+</sup> 255.1021; Found: 255.1028.

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## **NMR Spectra of the Isolated Products**

