One-Pot Catalysis of Dehydrogenation of Cyclohexanones to Phenols and Oxidative Heck Coupling: Expedient Synthesis of Coumarins

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I. General Methods and Materials. Unless stated otherwise, reactions were performed in flame-dried glassware under a positive pressure of nitrogen. Analytical thin layer chromatography (TLC) was performed on precoated silica gel 60 F_{254} plates and visualization on TLC was achieved by UV light (254 and 354nm). Flash column chromatography was undertaken on silica gel (400-630 mesh). ¹H NMR was recorded on 400 MHz and chemical shifts were quoted in parts per million (ppm) referenced to the appropriate solvent peak or 0.0 ppm for tetramethylsilane. The following abbreviations were used to describe peak splitting patterns when appropriate: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublet. Coupling constants, *J*, were reported in hertz unit (Hz). ¹³C NMR was recorded on 100 MHz and was fully decoupled by broad band proton decoupling. Chemical shifts were reported in ppm referenced to the center line of a triplet at 77.0 ppm of chloroform-*d*. High resolution mass spectra were obtained from the Korea Basic Science Institute (Daegu) by using EI method. Dichloromethane was distilled from calcium hydride. Unless otherwise stated, all commercial reagents and solvents were used without additional purification.

II. Optimization Study

Table S1. Screen of Pd^a

$Pd^{2+}, Cu(OAc)_2$ Ph $+ On-Bu$ $PivOH, 110 °C, O_2$ Ph						
ontry	Palladium	Oxidant	Yield			
entry	(0.2 eq)	(1 eq)	$(\%)^{\mathrm{b}}$			
1	$Pd(acac)_2$	Cu(OAc) ₂	52			
2	PdCl ₂	Cu(OAc) ₂	Trace			
3	Pd(dppf)Cl ₂	Cu(OAc) ₂	N.R			
4	$(IPr)Pd(OAc)_2$	$Cu(OAc)_2$	30			
5	$Pd(OAc)_2$	$Cu(OAc)_2$	63			
6	Pd(TFA) ₂	Cu(OAc) ₂	81			

[a] Reactions were conducted with 4-phenylcyclohexaneone (1.0 equiv), *n*-butylacrylate (1.2 equiv), PdL₂ (0.2 equiv), and oxidant (1.0 equiv) in PivOH at 110 °C for 20 h under 1 atm O₂. [b] Yield of isolated product.

Table S2. Screen of oxidants.^a



entry	Oxidant (1 eq)	additive (eq)	Yield $(\%)^{b}$
1	$O_2(1 \text{ atm})$	-	N.R.
2	Oxone	-	Trace
3	$K_2S_2O_8$	-	Trace
4	HPMV	-	N.R
5	CAN	-	S.M. decomposed
6	DDQ	-	Trace
7	$Fe(acac)_3$	-	N.R.
8	Cu(OTf) ₂	-	S.M. decomposed
9	CuCl ₂	-	S.M. decomposed
10	CuBr ₂	-	S.M. decomposed
11	CuI	-	Trace
12	$Cu(SO_4)_2 \cdot 5H_2O$	-	Trace
13	$Cu(BF_4)_2$	-	20
14	CuO	-	68
15	Cu(OMe) ₂	-	63
16	-	<i>p</i> -TsOH (0.4)	phenol (68%)
	-	CSA (0.4)	phenol (~20%)
17	-	DMSO (0.5 eq)	only cyclohexnone
1/			(~50%)
18	Cu(OAc) ₂	<i>p</i> -TsOH (0.4)	27
19	Cu(OAc) ₂	2-Me ₂ N-pyridine (0.4)	<10
20	Cu(OAc) ₂	NaOAc (1)	45
21	$CuCO_3 \cdot Cu(OH)_2$	-	80
22	Cu(OAc) ₂	-	81

[a] Reactions were conducted with 4-phenylcyclohexaneone (1.0 equiv), *n*-butylacrylate (1.2 equiv), PdL₂ (0.2 equiv), and oxidant (1.0 equiv) in PivOH at 110 °C for 20 h under 1 atm O₂. [b] Yield of isolated product.

III. Reaction Profiles



Figure S1. Reaction profile of the Pd(II)-catalyzed dehydrogentation of 4-phenylcyclohexanone. (a) Reactions were conducted with 4-phenylcyclohexanone (1.0 equiv), Pd(TFA)₂ (0.2 equiv), and TsOH (0.4 eq) in PivOH at 110 °C under 1 atm O₂. (b) Reactions were conducted with 4-phenylcyclohexanone (1.0 equiv), Pd(TFA)₂ (0.2 equiv), and Cu(OAc)₂ (1 eq) in PivOH at 110 °C under 1 atm O₂.

IV. Experimental Procedure

General Procedure (GP) for Oxidation and Oxidative Heck coupling of Cyclohexanone to Coumarin.

Cyclohexanone (1.0 eq), Pd(TFA)₂ (0.2 eq) and Cu(OAc)₂ (1.0 eq) were combined in PivOH (0.1 M) under O₂ (1 atm, balloon). The reaction mixture was heated to 110 $^{\circ}$ C. The mixture was monitored by TLC using EtOAc and *n*-hexane as the mobile. Acrylate (1.2 eq) was added to the reaction mixture and the reaction mixture was stirred until corresponding phenol disappeared. The reaction mixture was diluted with CH₂Cl₂ and the excess aqueous NaHCO₃ was added to neutralize the PivOH. After stirring the mixture for 10 min, the residue was extracted with aqueous NaHCO₃, NH₄Cl three times. The organic layer was dried over MgSO₄. After removal of solvent, the residue was purified by flash chromatography on silica gel to give the desired product.

V. Compound characterizations



6-Phenyl-2H-chromen-2-one (**3a**). **4**-Phenylcyclohexanone (31.0 mg, 0.178 mmol) was oxidized to phenol according to GP for 6 h. *n*-Butylacrylate (1.2 eq) was added, and the reaction mixture was stirred for 15 h. The

residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product. (32.3 mg, 81%); This compound is known.; ¹H NMR (400 MHz, Chloroform-d) δ 7.76–7.70 (m, 2H), 7.64 (d, *J* = 2.2 Hz, 1H), 7.58–7.52 (m, 2H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.40–7.34 (m, 2H), 6.44 (d, *J* = 9.5 Hz, 1H).; ¹³C NMR (100 MHz, Chloroform-d) δ 160.6, 153.4, 143.4, 139.3, 137.8, 130.7, 129.0, 127.7, 127.0, 126.0, 119.0, 117.2, 117.0.; [Ref]. *J. Org. Chem.* **1988**, *53*, 3936-3943.



2H-Chromen-2-one (3b). Cyclohexenone (20.0 mg, 0.208 mmol) was oxidized to phenol according to GP for 5 h. *n*-Butylacrylate (1.2 eq) was added, and the reaction mixture was stirred for 12 h. The residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product. (17.6 mg, 72%); ¹H NMR (400 MHz, Chloroform-d) δ 7.67 (d, *J* = 9.5 Hz, 1H), 7.48 (td, *J* = 8.0, 1.6 Hz, 1H), 7.45 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.27 (d, *J* = 8.4 Hz, 1H), 7.23 (td, *J* = 7.5, 1.2 Hz, 1H), 6.37 (d, *J* = 9.5 Hz, 1H).; ¹³C NMR (100 MHz, Chloroform-d) δ 160.6, 153.9, 143.4, 131.7, 127.8, 124.3, 118.7, 116.7, 116.5.; [Ref]. *J. Org. Chem.* **1988**, *53*, 3936-3943.



7-Methyl-2H-chromen-2-one (3c). 3-Methylcyclohexanone (24.3 mg, 0.199 mmol) was oxidized to phenol according to GP for 11 h. *n*-Butylacrylate (1.2 eq) was added, and the reaction mixture was stirred for 12 h. The residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product. (18.7 mg, 59%); This compound is known.; ¹H NMR (400 MHz, Chloroform-d) δ 7.64 (d, *J* = 9.5 Hz, 1H), 7.33 (d, *J* = 7.8 Hz, 1H), 7.11 (s, 1H), 7.06 (d, *J* = 7.9 Hz, 1H), 6.32 (d, *J* = 9.5 Hz, 1H), 2.42 (s, 3H).; ¹³C NMR (100 MHz, Chloroform-d) δ 161.0, 154.1, 143.3, 143.1, 127.5, 125.6, 117.0, 116.4, 115.4, 21.7.; [Ref]. *J. Org. Chem.* **1988**, *53*, 3936-3943.



7-Phenyl-2H-chromen-2-one (**3d**) 3-Phenylcyclohexanone (31.0 mg, 0.178 mmol) was oxidized to phenol according to GP for 5 h. *n*-Butylacrylate (1.2 eq) was added, and the reaction mixture was stirred for 14 h. The residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product. (22.2 mg, 56%); ¹H NMR (400 MHz, Chloroform-d) δ 7.70 (d, *J* = 12.0 Hz, 1H), 7.61–7.57 (m, 2H), 7.53–7.43 (m, 5H), 7.42–7.36 (m, 1H), 6.39 (d, *J* = 9.5 Hz, 1H).; ¹³C NMR (100 MHz, Chloroform-d) δ 160.8, 154.4, 145.0, 143.0, 139.1, 129.0, 128.5, 128.1, 127.1, 123.3, 117.7, 116.2, 115.0.; [Ref]. *J. Org. Chem.* **1988**, *53*, 3936-3943.



7-(4-Methoxyphenyl)-2H-chromen-2-one (3e). 3-Phenylcyclohexanone (36.0 mg, 0.176 mmol) was oxidized to phenol according to GP for 5 h. *n*-Butylacrylate (1.2 eq) was added, and the reaction mixture was stirred for 14 h. The residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product. (23.1 mg, 52%); This compound is known.; ¹H NMR (400 MHz, Chloroform-d) δ 7.70 (d, *J* = 9.5 Hz, 1H), 7.55 (d, *J* = 8.9 Hz, 2H), 7.51–7.43 (m, 3H), 6.99 (d, *J* = 8.9 Hz, 2H), 6.37 (d, *J* = 9.5 Hz, 1H), 3.85 (s, 3H).; ¹³C NMR (100 MHz, Chloroform-d) δ 161.0, 160.1, 154.6, 144.7, 143.1, 131.5, 128.3, 128.1, 122.8, 117.3, 115.9, 114.5, 114.4, 55.4.; [Ref]. *J. Med. Chem.* **2011**, *54*, 248-261.



7-(4-Acetylphenyl)-2H-chromen-2-one (3f). 3-(4-Acetylphenyl)cyclohexanone (71.0 mg, 0.328 mmol) was oxidized to phenol according to GP for 11 h. *n*-Butylacrylate (1.2 eq) was added, and the reaction mixture was stirred for 24 h. The residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product. (60.7 mg, 64%); mp 158-160 °C.; ¹H NMR (400 MHz, Chloroform-d) δ 8.02 (d, *J* = 9.5 Hz, 2H), 7.72 (d, *J* = 9.6, 1H), 7.67 (d, *J* = 8.0 Hz, 2H), 7.57–7.48 (m, 3H), 6.41 (d, *J* = 9.5 Hz, 1H), 2.61 (s, 3H).; ¹³C NMR (100 MHz, Chloroform-d) δ 197.4, 160.5, 154.4, 143.4, 142.8, 136.7, 129.0, 128.3, 127.3, 123.3, 118.4, 116.8, 115.2, 26.6.; HRMS (EI⁺) m/z calcd. for C₁₇H₁₂O₃⁺ [M]⁺: 264.0786, found: 264.0786.



7-(3-Fluorophenyl)-2H-chromen-2-one (3g). 3-(3-Fluorophenyl)cyclohexanone (49.0 mg, 0.245 mmol) was oxidized to phenol according to GP for 9 h. *n*-Butylacrylate (1.2 eq) was added, and the reaction mixture was stirred for 23 h. The residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product. (27.1 mg, 46%); mp 129–132 °C.; ¹H NMR (400 MHz, Chloroform-d) δ 7.72 (d, *J* = 9.5 Hz 1H), 7.55–7.45 (m, 3H), 7.45–7.36 (m, 2H), 7.33–7.27 (m, 1H), 7.09 (tdd, *J* = 8.1, 2.5, 1.2 Hz, 1H), 6.42 (d, *J* = 9.5 Hz, 1H).; ¹³C NMR (100 MHz, Chloroform-d) δ 163.2 (d, *J* = 246.8 Hz), 160.6, 154.4, 143.6, 142.9, 141.4 (d, *J* = 7.7 Hz), 130.6 (d, *J* = 8.4 Hz), 128.3, 123.2, 122.9 (d, *J* = 2.8 Hz), 118.2, 116.7, 115.4 (d, *J* = 21.2 Hz), 115.1, 114.2 (d, *J* = 22.4 Hz).; HRMS (EI⁺) m/z calcd. for C₁₅H₉FO₂⁺ [M]⁺ : 240.0587, found: 240.0585.



7-Methoxy-2H-chromen-2-one (3h). 3-Methoxycyclohexanone (30.0 mg, 0.234 mmol), Pd(TFA)₂ (0.2 eq) and Cu(OAc)₂ (1.0 eq) were combined in 1,4-dioxane : PivOH (5 : 1) under O₂. The reaction mixture was heated to 110 ^oC for 8 h. The mixture was monitored by TLC using EtOAc and *n*-hexane as the mobile phase. *n*-Butylacrylate (1.2 eq) was added to the reaction mixture under O₂, and the reaction mixture was stirred for 10 h. The residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product (24.7 mg, 56%); This compound is known; ¹H NMR (400 MHz, Chloroform-d) δ 7.61 (d, *J* = 9.4 Hz, 1H), 7.34 (d, *J* = 8.5 Hz, 1H), 6.83–6.77 (m, 2H), 6.22 (d, *J* = 9.4 Hz, 1H), 3.84 (s, 3H).; ¹³C NMR (100 MHz, Chloroform-d) δ 162.8, 161.1, 155.9, 143.4, 128.7, 113.1, 112.5, 112.5, 100.8, 55.7.; [Ref]. *J. Am. Chem. Soc.* **2003**, *125*, 4518-4526.



6-Methyl-2H-chromen-2-one (**3i**). 4-Methylcyclohexanone (27.5 mg, 0.245 mmol) was oxidized to phenol according to GP for 4 h. *n*-Butylacrylate (1.2 eq) was added, and the reaction mixture was stirred for 14 h. The

residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product. (30.2 mg, 77%); This compound is known; ¹H NMR (400 MHz, Chloroform-d) δ 7.62 (d, *J* = 9.5 Hz, 1H), 7.29 (dd, *J* = 8.4, 2.2 Hz, 1H), 7.23 (s, 1H), 7.18 (d, *J* = 8.4 Hz, 1H), 6.35 (d, *J* = 9.6 Hz, 1H), 2.36 (s, 3H).; ¹³C NMR (100 MHz, Chloroform-d) δ 161.0, 152.1, 143.3, 134.1, 132.7, 127.6, 118.5, 116.5, 116.5, 20.6.; [Ref]. *J. Org. Chem.* **1988**, *53*, 3936-3943.



6-(*tert*-**Butyl**)-**2H**-chromen-2-one (**3**j). 4-*tert*-Butylcyclohexanone (27.5 mg, 0.178 mmol) was oxidized to phenol according to GP for 4 h. *n*-Butylacrylate (1.2 eq) was added, and the reaction mixture was stirred for 14 h. The residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product. (28.1 mg, 78%); This compound is known.; ¹H NMR (400 MHz, Chloroform-d) δ 7.68 (d, J = 9.5 Hz, 1H), 7.55 (dd, J = 8.7, 2.4 Hz, 1H), 7.42 (d, J = 2.4 Hz, 1H), 7.24 (d, J = 8.8 Hz, 1H), 6.38 (d, J = 9.5 Hz, 1H), 1.33 (s, 9H).; ¹³C NMR (100 MHz, Chloroform-d) δ 161.1, 152.0, 147.5, 143.8, 129.5, 124.1, 118.2, 116.4, 116.4, 34.5, 31.3.; [Ref]. *J. Org. Chem.* **2004**, *69*, 3669-3671.



Ethyl 2-oxo-2H-chromene-6-carboxylate (3k). Ethyl 4-oxocyclohexanecarboxylate (32.5 mg, 0.190 mmol) was oxidized to phenol according to GP for 6 h. *n*-Butylacrylate (1.2 eq) was added, and the reaction mixture was stirred for 18 h. The residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product. (33.5 mg, 81%); mp 125-127 °C.; ¹H NMR (400 MHz, Chloroform-d) δ 8.22–8.11 (m, 2H), 7.73 (d, J = 8.0 Hz, 1H), 7.33 (d, J = 8.2 Hz, 1H), 6.45 (d, J = 9.6 Hz, 1H), 4.38 (q, J = 7.1 Hz, 2H), 1.39 (t, J = 7.2 Hz, 3H).; ¹³C NMR (100 MHz, Chloroform-d) δ 165.1, 159.8, 156.8, 143.1, 132.7, 129.8, 126.9, 118.5, 117.4, 117.0, 61.4, 14.3.; HRMS (EI⁺) m/z calcd. for C₁₂H₁₀O₄⁺ [M]⁺ : 218.0579, found: 218.0577.



Ethyl 7-methyl-2-oxo-2H-chromene-6-carboxylate (3l). Ethyl 2-methyl-4-oxocyclohex-2-enecarboxylate (32.5 mg, 0.160 mmol) was oxidized to phenol according to GP for 4 h. *n*-Butylacrylate (1.2 eq) was added, and the reaction mixture was stirred for 14 h. The residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product (31.5 mg, 85%); mp 121-123 °C.; ¹H NMR (400 MHz, Chloroform-d) δ 8.07 (s, 1H), 7.68 (d, J = 9.6 Hz, 1H), 7.15 (s, 1H), 6.37 (d, J = 9.5 Hz, 1H), 4.35 (q, J = 7.1 Hz, 2H), 2.66 (s, 3H), 1.39 (t, J = 7.1 Hz, 3H).; ¹³C NMR (100 MHz, Chloroform-d) δ 166.0, 160.2, 155.7, 145.1, 142.9, 130.9, 126.4, 119.5, 116.5, 116.4, 61.1, 22.3, 14.3.; HRMS (EI⁺) m/z calcd. for C₁₃H₁₂O₄⁺ [M]⁺ : 232.0736, found: 232.0734.



Benzyl (2-oxo-2H-chromen-6-yl)carbamate (3m). Benzyl (4-oxocyclohexyl)carbamate (44.0 mg, 0.177 mmol) was oxidized to phenol according to GP for 5 h. *n*-Butylacrylate (1.2 eq) was added, and the reaction mixture was stirred for 12 h. The residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product. (19.9 mg, 38%); mp 138-141 °C.; ¹H NMR (400 MHz, Chloroform-d) δ 7.76 (bs, 1H), 7.63 (d, *J* = 9.5 Hz, 1H), 7.40–7.30 (m, 6H), 7.24 (d, *J* = 12.0 Hz, 1H), 6.86 (bs, 1H), 6.41 (d, *J* = 9.5 Hz, 1H), 5.20 (s, 2H).; ¹³C NMR (100 MHz, Chloroform-d) δ 160.7, 153.3, 150.0, 143.2, 135.7, 134.3, 128.6, 128.5, 128.3, 122.5, 119.1, 117.3, 116.9, 67.3.; HRMS (EI⁺) m/z calcd. for C₁₇H₁₃NO₄⁺ [M]⁺ : 295.0845, found: 295.0842.



6,7,8,9-Tetrahydro-2H-benzo[g]chromen-2-one (3n). Octahydronaphthalen-2(1H)-one (29.5 mg, 0.184 mmol) was oxidized to phenol according to GP for 4 h. *n*-Butylacrylate (1.2 eq) was added, and the reaction mixture was stirred for 14 h. The residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product. (17.6 mg, 48%); mp 123-125 °C.; ¹H NMR (400 MHz, Chloroform-d) δ 7.59 (d, *J* = 9.5 Hz, 1H), 7.12 (s, 1H), 6.99 (s, 1H), 6.29 (d, *J* = 9.5 Hz, 1H), 2.80 (d, *J* = 20.9 Hz, 4H), 1.83–1.75 (m, 4H).; ¹³C NMR (100 MHz, Chloroform-d) δ 161.3, 152.0, 143.3, 142.4, 133.7, 127.5, 116.7, 116.4, 115.4, 29.8, 28.7, 22.9, 22.6.; HRMS (EI⁺) m/z calcd. for C₁₃H₁₂O₂⁺ [M]⁺ : 200.0837, found: 200.0839.



2H-Benzo[h]chromen-2-one (**3o**). 3,4-Dihydronaphthalen-1(2H)-one (33.0 mg, 0.225 mmol), *n*-butylacrylate (1.2 eq), Pd(TFA)₂ (0.2 eq) and Cu(OAc)₂ (2.0 eq) were combined in PivOH (0.1 M) under O₂ (1 atm, balloon pressure). The reaction mixture was heated to 110 °C. The mixture was monitored by TLC using EtOAc and *n*-hexane as the mobile phase and stirred until starting material disappeared. The residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product (24.7 mg, 56%); ¹H NMR (400 MHz, Chloroform-d) δ 8.55–8.46 (m, 1H), 7.88–7.82 (m, 1H), 7.80 (d, *J* = 9.5 Hz, 1H), 7.65 (d, *J* = 8.4 Hz, 1H), 7.64–7.59 (m, 2H), 7.43 (d, *J* = 8.5 Hz, 1H), 6.49 (d, *J* = 9.5 Hz, 1H).; ¹³C NMR (100 MHz, Chloroform-d) δ 160.9, 151.3, 144.1, 134.8, 128.7, 127.8, 127.2, 124.4, 123.5, 123.1, 122.3, 115.9, 114.2.; [Ref]. *J. Org. Chem.* **1988**, *53*, 3936-3943.



4,6-Diphenyl-2H-chromen-2-one (**4a**). 4-Phenylcyclohexanone (31.0 mg, 0.178 mmol) was oxidized to phenol according to GP for 7 h. Methyl cinnamate (1.2 eq) was added, and the reaction mixture was stirred for 13 h. The residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product. (31.3 mg, 59%); This compound is known.; ¹H NMR (400 MHz, Chloroform-d) δ 7.75 (dd, *J* = 8.6, 2.2 Hz, 1H), 7.66 (d, *J* = 2.2 Hz, 1H), 7.55–7.51 (m, 3H), 7.51–7.43 (m, 5H), 7.43–7.37 (m, 2H), 7.36–7.30 (m, 1H), 6.40 (s, 1H).; ¹³C NMR (100 MHz, Chloroform-d) δ 160.6, 155.6, 153.6, 139.6, 137.5, 135.1, 130.8, 129.7, 128.9, 128.9, 128.4, 127.6, 127.0, 125.2, 119.1, 117.7, 115.5.; [Ref]. *J. Org. Chem.* **2004**, *69*, 3669-3671.



4-(3-Fluorophenyl)-6-phenyl-2H-chromen-2-one (4b). 4-Phenylcyclohexanone (31.0 mg, 0.178 mmol) was oxidized to phenol according to GP for 7 h. (*E*)-Methyl 3-(3-fluorophenyl)acrylate (1.2 eq) was added, and the reaction mixture was stirred for 26 h. The residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product. (32.1 mg, 57%); mp 138-140 °C.; ¹H NMR (400 MHz, Chloroform-d) δ 7.76 (dd, *J* = 8.6, 2.2 Hz, 1H), 7.59 (d, *J* = 2.2 Hz, 1H), 7.54–7.37 (m, 6H), 7.37–7.31 (m, 1H), 7.26 (dt, *J* = 7.6, 1.3 Hz, 1H), 7.24–7.17 (m, 2H), 6.40 (s, 1H).; ¹³C NMR (100 MHz, Chloroform-d) δ 162.8 (d, *J* = 248.6 Hz), 160.3, 154.3, 153.6, 139.5, 137.8, 137.1 (d, *J* = 7.9 Hz), 131.1, 130.8 (d, *J* = 8.3 Hz), 129.0, 127.8, 127.1, 124.9, 124.2, 118.8, 117.8, 116.8 (d, *J* = 20.9 Hz), 115.9, 115.6 (d, *J* = 22.8 Hz).; HRMS (EI⁺) m/z calcd. for C₂₁H₁₃FO₂⁺ [M]⁺ : 316.0900, found: 316.0896.



4-(3-Methoxyphenyl)-6-phenyl-2H-chromen-2-one (4c). 4-Phenylcyclohexanone (31.0 mg, 0.178 mmol) was oxidized to phenol according to GP for 7 h. (*E*)-Methyl 3-(3-methoxyphenyl)acrylate (1.2 eq) was added, and the reaction mixture was stirred for 26 h. The residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product. (36.2 mg, 62%); yellowish oil.; ¹H NMR (400 MHz, Chloroform-d) δ 7.75 (dd, *J* = 8.6, 2.2 Hz, 1H), 7.68 (d, *J* = 2.2 Hz, 1H), 7.48–7.37 (m, 6H), 7.36–7.32 (m, 1H), 7.07–7.03 (m, 2H), 7.01–6.98 (m, 1H), 6.41 (s, 1H), 3.85 (s, 3H).; ¹³C NMR (100 MHz, Chloroform-d) δ 160.7, 159.9, 155.6, 153.5, 139.6, 137.6, 136.4, 130.9, 130.0, 128.9, 127.7, 127.1, 125.2, 120.7, 119.1, 117.7, 115.5, 115.2, 114.0, 55.4.; HRMS (EI⁺) m/z calcd. for C₂₂H₁₆O₃⁺ [M]⁺ : 328.1099, found: 328.1100.



3,6-Diphenyl-2H-chromen-2-one (4d). 4-Phenylcyclohexanone (31.0 mg, 0.178 mmol) was oxidized to phenol according to GP for 7 h. 2-Phenylacrylic acid (1.2 eq) was added, and the reaction mixture was stirred for 14 h. The

residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product. (35.5 mg, 67%); yellowish oil.; ¹H NMR (400 MHz, Chloroform-d) δ 7.83 (s, 1H), 7.74–7.69 (m, 4H), 7.61–7.56 (m, 2H), 7.49–7.36 (m, 7H).; ¹³C NMR (100 MHz, Chloroform-d) δ 160.5, 152.8, 139.9, 139.5, 137.8, 134.6, 130.3, 129.0, 128.9, 128.6, 128.5, 128.5, 127.8, 127.0, 126.0, 119.8, 116.8.; HRMS (EI⁺) m/z calcd. for C₂₁H₁₄O₂⁺ [M]⁺ : 298.0994, found: 298.0991.



3-(4-Methoxyphenyl)-6-phenyl-2H-chromen-2-one (4e). 4-Phenylcyclohexanone (31 mg, 0.178 mmol) was oxidized to phenol according to GP for 7 h. Methyl 2-(4-methoxyphenyl)acrylate (1.2 eq) was added, and the reaction mixture was stirred for 22 h. The residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product. (42.1 mg, 73%); mp 146-149 °C.; ¹H NMR (400 MHz, Chloroform-d) δ 7.80 (s, 1H), 7.73–7.64 (m, 4H), 7.61–7.55 (m, 2H), 7.46 (t, *J* = 7.5 Hz, 2H), 7.43–7.34 (m, 2H), 6.97 (d, *J* = 8.8 Hz, 2H), 3.84 (s, 3H).; ¹³C NMR (100 MHz, Chloroform-d) δ 160.2, 152.6, 139.6, 138.5, 137.8, 129.9, 129.8, 129.0, 128.1, 127.7, 127.0, 127.0, 125.8, 120.0, 116.7, 113.9, 55.4.; HRMS (EI⁺) m/z calcd. for C₂₂H₁₆O₃⁺ [M]⁺ : 328.1099, found: 328.1098.



3-(3-Fluorophenyl)-6-phenyl-2H-chromen-2-one (4f). 4-Phenylcyclohexanone (31.0 mg, 0.178 mmol) was oxidized to phenol according to GP for 7 h. Methyl 2-(3-fluorophenyl)acrylate (1.2 eq) was added, and the reaction mixture was stirred for 16 h. The residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product. (41.7 mg, 75%); mp 131-133 °C.; ¹H NMR (400 MHz, Chloroform-d) δ 7.88 (s, 1H), 7.75 (dd, *J* = 8.5, 2.2 Hz, 1H), 7.72 (d, *J* = 2.1 Hz, 1H), 7.61–7.56 (m, 2H), 7.52–7.44 (m, 4H), 7.44–7.35 (m, 3H), 7.10 (td, *J* = 8.2, 2.6 Hz, 1H).; ¹³C NMR (100 MHz, Chloroform-d) δ 162.6 (d, *J* = 246.2 Hz), 160.1, 152.9, 140.4, 139.3, 138.0, 136.6 (d, *J* = 8.2 Hz), 130.7, 130.0 (d, *J* = 8.4 Hz), 129.0, 127.8, 127.3 (d, *J* = 2.4 Hz), 127.0, 126.2,

124.1 (d, J = 3.0 Hz), 119.6, 116.8, 115.8 (d, J = 13.5 Hz), 115.6 (d, J = 15.5 Hz).; HRMS (EI⁺) m/z calcd. for $C_{21}H_{13}FO_2^+$ [M]⁺ : 316.0900, found: 316.0897.



3-(4-Nitrophenyl)-6-phenyl-2H-chromen-2-one (4g). 4-Phenylcyclohexanone (31.0 mg, 0.178 mmol) was oxidized to phenol according to GP for 7 h. Methyl 2-(4-nitrophenyl)acrylate (1.2 eq) was added, and the reaction mixture was stirred for 16 h. The residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product (37.5 mg, 62%); mp 216-219 °C.; ¹H NMR (400 MHz, Chloroform-d) δ 8.30 (d, *J* = 8.7 Hz, 2H), 7.99 (s, 1H), 7.92 (d, *J* = 8.6 Hz, 2H), 7.80 (dd, *J* = 8.6, 2.2 Hz, 1H), 7.77 (s, 1H), 7.58 (d, *J* = 7.2 Hz, 2H), 7.53–7.43 (m, 3H), 7.40 (t, *J* = 7.3 Hz, 1H).; ¹³C NMR (100 MHz, Chloroform-d) δ 159.8, 153.2, 147.8, 141.7, 141.0, 139.2, 138.3, 131.5, 129.5, 129.1, 128.0, 127.0, 126.4, 126.4, 123.7, 119.3, 117.0.; HRMS (EI⁺) m/z calcd. for C₂₁H₁₃NO₄⁺ [M]⁺ : 343.0845, found: 343.0847.



3-(4-Acetylphenyl)-6-phenyl-2H-chromen-2-one (4h). 4-Phenylcyclohexanone (31.0 mg, 0.178 mmol) was oxidized to phenol according to GP for 7 h. Methyl 2-(4-acetylphenyl)acrylate (1.2 eq) was added, and the reaction mixture was stirred for 12 h. The residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product. (34.1 mg, 63%); mp 176-178 °C.; ¹H NMR (400 MHz, Chloroform-d) δ 8.02 (d, *J* = 8.4 Hz, 2H), 7.93 (s, 1H), 7.82 (d, *J* = 8.4 Hz, 2H), 7.78–7.71 (m, 2H), 7.58 (d, *J* = 6.9 Hz, 2H), 7.46 (t, *J* = 7.5 Hz, 2H), 7.42 (d, *J* = 8.5 Hz, 1H), 7.41–7.35 (m, 1H), 2.62 (s, 3H).; ¹³C NMR (100 MHz, Chloroform-d) δ 197.5, 160.1, 153.0, 140.8, 139.3, 139.1, 138.1, 137.0, 130.9, 129.0, 128.7, 128.4, 127.9, 127.4, 127.0, 126.3, 119.5, 116.9, 26.7.; HRMS (EI⁺) m/z calcd. for C₂₃H₁₆O₃⁺ [M]⁺ : 340.1099, found: 340.1097.



4-(2-Oxo-6-phenyl-2H-chromen-3-yl)benzaldehyde (**4i**). 4-Phenylcyclohexanone (31.0 mg, 0.178 mmol) was oxidized to phenol according to GP for 7 h. Methyl 2-(4-formylphenyl)acrylate (1.2 eq) was added, and the reaction mixture was stirred for 10 h. The residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product. (40.4 mg, 70%); mp 171-173 °C.; ¹H NMR (400 MHz, Chloroform-d) δ 10.06 (s, 1H), 7.96 (d, J = 2.2 Hz, 3H), 7.90 (d, J = 8.3 Hz, 2H), 7.78 (dd, J = 8.5, 2.2 Hz, 1H), 7.75 (d, J = 2.1 Hz, 1H), 7.61–7.55 (m, 2H), 7.51–7.43 (m, 3H), 7.42–7.36 (m, 1H).; ¹³C NMR (100 MHz, Chloroform-d) δ 191.6, 159.9, 153.1, 141.2, 140.5, 139.3, 138.2, 136.2, 131.1, 129.7, 129.2, 129.4, 127.9, 127.3, 127.0, 126.3, 119.5, 116.9.; HRMS (EI⁺) m/z calcd. for C₂₂H₁₄O₃⁺ [M]⁺: 326.0943, found: 326.0943.



3-(3,5-Bis(trifluoromethyl)phenyl)-6-phenyl-2H-chromen-2-one (4j). 4-Phenylcyclohexanone (34.8 mg, 0.200 mmol) was oxidized to phenol according to GP for 7 h. Methyl 2-(3,5-bis(trifluoromethyl)phenyl)acrylate (1.2 eq) was added, and the reaction mixture was stirred for 19 h. The residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product (48.4 mg, 56%); mp 116-118 °C.; ¹H NMR (400 MHz, Chloroform-d) δ 8.20 (s, 2H), 8.00 (s, 1H), 7.92 (s, 1H), 7.82 (dd, *J* = 8.5, 2.2 Hz, 1H), 7.79 (d, *J* = 2.2 Hz, 1H), 7.59 (d, *J* = 6.9 Hz, 2H), 7.48 (t, *J* = 7.5 Hz, 3H), 7.40 (t, *J* = 7.3 Hz, 1H).; ¹³C NMR (100 MHz, Chloroform-d) δ 159.7, 153.1, 141.6, 139.1, 138.4, 136.6, 131.9 (q, *J* = 33.0 Hz), 131.5, 129.1, 128.7, 128.0, 127.0, 126.4, 125.7, 123.1 (q, *J* = 272.0 Hz), 122.5, 119.2, 117.1.; HRMS (EI⁺) m/z calcd. for C₂₃H₁₂F₆O₂⁺ [M]⁺ : 434.0741, found: 434.0742.



3-(3,4-Dichlorophenyl)-6-phenyl-2H-chromen-2-one (4k). 4-Phenylcyclohexanone (34.8 mg, 0.200 mmol) was oxidized to phenol according to GP for 7 h. Methyl 2-(3,4-dichlorophenyl)acrylate (1.2 eq) was added, and the reaction mixture was stirred for 10 h. The residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product (47.3 mg, 65%); mp 164-166 °C.; ¹H NMR (400 MHz, Chloroform-d) δ 7.86 (s, 1H), 7.82 (d, *J* = 2.1 Hz, 1H), 7.75 (dd, *J* = 8.6, 2.2 Hz, 1H), 7.71 (d, *J* = 2.2 Hz, 1H), 7.60–7.54 (m, 3H), 7.49 (d, *J* = 6.9 Hz, 1H), 7.47 (d, *J* = 8.0 Hz, 1H), 7.45 (d, *J* = 6.3 Hz, 1H), 7.42–7.36 (m, 2H).; ¹³C NMR (100 MHz, Chloroform-d) δ 159.9, 152.9, 140.4, 139.2, 138.1, 134.4, 133.1, 132.7, 130.9, 130.4, 130.3, 129.0, 127.9, 127.8, 127.0, 126.2, 126.1, 119.4, 116.9.; HRMS (EI⁺) m/z calcd. for C₂₁H₁₂Cl₂O₂⁺ [M]⁺ : 366.0214, found: 366.0218.



6-Phenyl-3-(4-(trimethylsilyl)phenyl)-2H-chromen-2-one (4l). 4-Phenylcyclohexanone (34.8 mg, 0.200 mmol) was oxidized to phenol according to GP for 7 h. Methyl 2-(4-(trimethylsilyl)phenyl)acrylate (1.2 eq) was added, and the reaction mixture was stirred for 15 h. The residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product (42.6 mg, 58%); mp 152-155 °C.; ¹H NMR (400 MHz, Chloroform-d) δ 7.86 (s, 1H), 7.76–7.67 (m, 4H), 7.64–7.57 (m, 4H), 7.47 (t, *J* = 7.5 Hz, 2H), 7.44–7.35 (m, 2H), 0.30 (s, 9H).; ¹³C NMR (100 MHz, Chloroform-d) δ 160.5, 152.9, 141.6, 139.7, 139.5, 137.8, 135.0, 133.5, 130.3, 129.0, 128.7, 127.7, 127.0, 126.1, 119.9, 116.8, -1.2.; HRMS (EI⁺) m/z calcd. for C₂₄H₂₂O₂Si⁺ [M]⁺ : 370.1389, found: 370.1385.



3-(2-Oxo-6-phenyl-2H-chromen-3-yl)benzonitrile (4m). 4-Phenylcyclohexanone (34.8 mg, 0.200 mmol) was oxidized to phenol according to GP for 7 h. Methyl 2-(3-cyanophenyl)acrylate (1.2 eq) was added and the reaction mixture was stirred for 12 h. The residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product (26.5 mg, 41%); mp 140-143 °C.; ¹H NMR (400 MHz, Chloroform-d) δ 8.02 (t, *J* = 1.6 Hz, 1H), 7.98 (dt, *J* = 7.7, 1.4 Hz, 1H), 7.92 (s, 1H), 7.79 (dd, *J* = 8.6, 2.2 Hz, 1H), 7.75 (d, *J* = 2.1 Hz, 1H), 7.69 (dt, *J* = 7.7, 1.4 Hz, 1H), 7.61–7.54 (m, 3H), 7.52–7.42 (m, 3H), 7.43–7.36 (m, 1H).; ¹³C NMR (100 MHz, Chloroform-d) δ 159.9, 153.0, 141.0, 139.2, 138.3, 135.9, 132.9, 132.2, 132.1, 131.2, 129.3, 129.1, 127.9, 127.0, 126.4, 126.3, 119.4, 117.0, 112.9.; HRMS (EI⁺) m/z calcd. for C₂₂H₁₃NO₂⁺ [M]⁺ : 323.0946, found: 323.0947.



3-(Naphthalen-2-yl)-6-phenyl-2H-chromen-2-one (4n). 4-Phenylcyclohexanone (31.0 mg, 0.178 mmol) was oxidized to phenol according to GP for 7 h. Methyl 2-(naphthalen-2-yl)acrylate (1.2 eq) was added, and the reaction mixture was stirred for 28 h. The residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product. (37.8 mg, 61%); mp 155-158 °C.; ¹H NMR (400 MHz, Chloroform-d) δ 8.24 (d, *J* = 1.7 Hz, 1H), 7.96 (s, 1H), 7.93–7.88 (m, 2H), 7.86–7.83 (m, 1H), 7.79 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.74 (dd, *J* = 8.0, 1.8 Hz, 1H), 7.73 (s, 1H), 7.63–7.57 (m, 2H), 7.54–7.37 (m, 6H).; ¹³C NMR (100 MHz, Chloroform-d) δ 160.6, 152.8, 140.1, 139.5, 137.8, 133.3, 133.1, 132.0, 130.3, 129.0, 128.5, 128.1, 128.0, 127.,3 127.6, 127.0, 126.7, 126.4, 126.1, 125.8, 119.9, 116.8.; HRMS (EI⁺) m/z calcd. for C₂₅H₁₆O₂⁺ [M]⁺ : 348.1150, found: 348.1148.



3-*n***-Butylacrylated 7-methoxycoumarin (5a).** 3-Methoxycyclohexanone (30.0 mg, 0.234 mmol), $Pd(TFA)_2$ (0.3 eq) and $Cu(OAc)_2$ (1.0 eq) were combined in 1,4-dioxane : PivOH (5 : 1) under O₂. The reaction mixture was heated to 110 °C. The mixture was monitored by TLC using EtOAc and *n*-hexane as the mobile phase. *n*-Butylacrylate (1.2 eq) was then added to the reaction mixture. After 10 h, *n*-butylacrylate (2 eq) and K₂CO₃ (3 eq) were added and stirred for another 8 h. The residue was purified by flash column chromatography (EtOAc and *n*-

hexane) to produce the desired product (23.8 mg, 33%); ¹H NMR(400 MHz, Chloroform-d) δ 7.79 (s, 1H), 7.51 (dd, *J* = 15.9, 0.6 Hz, 1H), 7.42 (d, *J* = 8.6 Hz, 1H), 7.02 (d, *J* = 15.8 Hz, 1H), 6.86 (dd, *J* = 8.6, 2.4 Hz, 1H), 6.81 (d, *J* = 2.5 Hz, 1H), 4.18 (t, *J* = 6.6 Hz, 2H), 3.88 (s, 3H), 1.70–1.62 (m, 2H), 1.46–1.36 (m, 2H), 0.94 (t, *J* = 7.4 Hz, 3H).; ¹³C NMR (100 MHz, Chloroform-d) δ 167.3, 163.9, 159.3, 155.6, 143.7, 138.2, 129.6, 122.3, 118.9, 113.4, 112.7, 100.5, 64.5, 55.9, 30.8, 19.2, 13.7.; [Ref]. *Chem. Comm.* **2013**, *49*, 196-198.



(*E*)-Butyl 3-(2-oxo-6-phenyl-2H-chromen-3-yl)acrylate (5b). 4-Phenylclohexanone (32.8 mg, 0.200 mmol), Pd(TFA)₂ (0.3 eq) and Cu(OAc)₂ (1.0 eq) were combined in PivOH (0.1 M) under O₂. The reaction mixture was heated to 110 °C. The mixture was monitored by TLC using EtOAc and *n*-hexane. *n*-Butylacrylate (1.2 eq) was added to the reaction mixture. After 12 h, *n*-butylacrylate (2 eq) and K₂CO₃ (3 eq) were added and stirred for another 9 h. The residue was purified by flash column chromatography (EtOAc and *n*-hexane) to produce the desired product (26.1 mg, 38%); mp 135-138 °C.; ¹H NMR (400 MHz, Methylene Chloride-d₂) δ 7.96 (s, 1H), 7.82 (dd, *J* = 8.6, 2.2 Hz, 1H), 7.76 (d, *J* = 2.2 Hz, 1H), 7.64–7.59 (m, 2H), 7.56 (dd, *J* = 15.9, 0.7 Hz, 1H), 7.52–7.46 (m, 2H), 7.44–7.37 (m, 2H), 7.05 (d, *J* = 15.9 Hz, 1H), 4.20 (t, *J* = 6.7 Hz, 2H), 1.74–1.64 (m, 2H), 1.51–1.38 (m, 2H), 0.97 (t, *J* = 7.4 Hz, 3H).; ¹³C NMR (100 MHz, Methylene Chloride-d₂) δ 167.0, 159.3, 153.3, 143.9, 139.5, 138.3, 138.0, 132.0, 129.4, 128.2, 127.3, 126.9, 123.9, 123.0, 119.6, 117.2, 64.9, 31.1, 19.6, 13.9.; HRMS (EI⁺) m/z calcd. for C₂₂H₂₀O₄⁺ [M]⁺ : 348.1362, found: 348.1360.

Appendix I

Spectral Copies of ¹H and ¹³C NMR Data Obtained in this Study

6-phenyl-2H-chromen-2-one (3a)





400 MHz, ¹H NMR in CDCl₃



100 MHz, ¹³C NMR in CDCl₃









100 MHz, ¹³C NMR in CDCl₃

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7-methyl-2H-chromen-2-one (3c)



100 MHz, ¹³C NMR in CDCl₃

7-phenyl-2H-chromen-2-one (3d)





400 MHz, ¹H NMR in CDCl₃



7-(4-methoxyphenyl)-2H-chromen-2-one (3e)







100 MHz, ¹³C NMR in CDCl₃

7-(4-acetylphenyl)-2H-chromen-2-one (3f)







100 MHz, ¹³C NMR in CDCl₃

7-(3-fluorophenyl)-2H-chromen-2-one (3g)









100 MHz, ¹³C NMR in CDCl₃

7-methoxy-2H-chromen-2-one (3h)



100 MHz, ¹³C NMR in CDCl₃

6-methyl-2H-chromen-2-one (3i)







100 MHz, ¹³C NMR in CDCl₃

6-(tert-butyl)-2H-chromen-2-one (3j)







100 MHz, ¹³C NMR in CDCl₃

ethyl 2-oxo-2H-chromene-6-carboxylate (3k)







100 MHz, ¹³C NMR in CDCl₃

ethyl 7-methyl-2-oxo-2H-chromene-6-carboxylate (3l)







100 MHz, ¹³C NMR in CDCl₃

benzyl (2-oxo-2H-chromen-6-yl)carbamate (3m)



400 MHz, ¹H NMR in CDCl₃



100 MHz, ¹³C NMR in CDCl₃

6,7,8,9-tetrahydro-2H-benzo[g]chromen-2-one (3n)







S32

2H-benzo[h]chromen-2-one (3o)







100 MHz, ¹³C NMR in CDCl₃

4,6-diphenyl-2H-chromen-2-one (4a)









100 MHz, ¹³C NMR in CDCl₃

4-(3-fluorophenyl)-6-phenyl-2H-chromen-2-one (4b)







100 MHz, ¹³C NMR in CDCl₃

4-(3-methoxyphenyl)-6-phenyl-2H-chromen-2-one (4c)



400 MHz, ¹H NMR in CDCl₃





3,6-diphenyl-2H-chromen-2-one (4d)









100 MHz, ¹³C NMR in CDCl₃

3-(4-methoxyphenyl)-6-phenyl-2H-chromen-2-one (4e)







100 MHz, ¹³C NMR in CDCl₃

3-(3-fluorophenyl)-6-phenyl-2H-chromen-2-one (4f)





400 MHz, ¹H NMR in CDCl₃



100 MHz, ¹³C NMR in CDCl₃

3-(4-nitrophenyl)-6-phenyl-2H-chromen-2-one (4g)







100 MHz, ¹³C NMR in CDCl₃

3-(4-acetylphenyl)-6-phenyl-2H-chromen-2-one (4h)







100 MHz, ¹³C NMR in CDCl₃

4-(2-oxo-6-phenyl-2H-chromen-3-yl)benzaldehyde (4i)







100 MHz, ¹³C NMR in CDCl₃

3-(3,5-bis(trifluoromethyl)phenyl)-6-phenyl-2H-chromen-2-one (4j)







100 MHz, ¹³C NMR in CDCl₃

3-(3,4-dichlorophenyl)-6-phenyl-2H-chromen-2-one (4k)







100 MHz, ¹³C NMR in CDCl₃

6-phenyl-3-(4-(trimethylsilyl)phenyl)-2H-chromen-2-one (4l)







100 MHz, ¹³C NMR in CDCl₃

3-(2-oxo-6-phenyl-2H-chromen-3-yl)benzonitrile (4m)











100 MHz, ¹³C NMR in CDCl₃

3-(naphthalen-2-yl)-6-phenyl-2H-chromen-2-one (4n)







100 MHz, ¹³C NMR in CDCl₃

(E)-butyl 3-(7-methoxy-2-oxo-2H-chromen-3-yl)acrylate (5a)



(E)-butyl 3-(2-oxo-6-phenyl-2H-chromen-3-yl)acrylate (5b)



400 MHz, ¹H NMR in CD₂Cl₂



100 MHz, ¹³C NMR in CD₂Cl₂