

Supporting Information

Regioselective Palladium-Catalyzed Direct Cross-Coupling of Coumarins with Simple Arenes

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I.	General Methods and Materials	S2
II.	Experimental Procedures	S2
III.	Compound characterizations	S3

Appendix I

Spectral Copies of ^1H- and ^{13}C-NMR Data Obtained in this Study	S10
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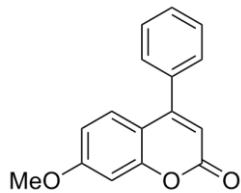
I. General Methods and Materials. Unless stated otherwise, reactions were performed in flame-dried glassware under a positive pressure of nitrogen. Analytical thin layer chromatography (TLC) was performed on precoated silica gel 60 F₂₅₄ plates and visualization on TLC was achieved by UV light (254 and 354nm). Flash column chromatography was undertaken on silica gel (400-630 mesh). ¹H NMR was recorded on 400 MHz or 300 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 75 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*. Mass spectral data were obtained from the KAIST Basic Science Institute by using EI method. Commercial grade reagents and solvents were used without further purification except as indicated below. Dichloromethane was distilled from calcium hydride. Unless otherwise stated, all commercial reagents and solvents were used without additional purification.

II. Experimental Procedures

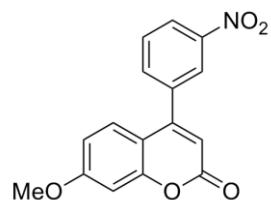
General Procedure for Coumarin Arylation:

Coumarin derivative (0.1 mmol), Arene (0.5 mL), Pd(OPIV)₂ (0.2 eq), AgOPiv (3.0 eq), and CsOPiv (3.0 eq) were combined in PivOH (0.7 mL) in a cap test tube. The reaction mixture was heated to 100 °C. The reaction was stirred for 6–12 h until the starting material, coumarin derivative disappeared (monitored by TLC using methylene chloride and ethyl acetate : *n*-hexane = 1 : 1 : 6 as the mobile phase). The reaction mixture was diluted with CH₂Cl₂ and the excess NaHCO₃ was added to neutralize PivOH. After stirring the mixture for 10 min, the residue was washed with sequentially aqueous NaHCO₃ and NH₄Cl. The organic layer was dried over MgSO₄. After removal of solvent, the residue was purified by flash chromatography on silica gel to give desired product.

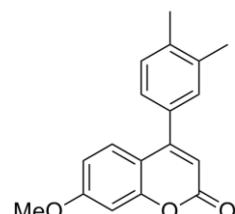
Compound Characterizations:



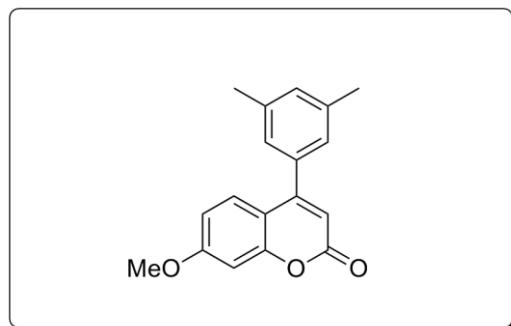
7-methoxy-4-phenyl-2H-chromen-2-one (2a). Yield 83% (20.7 mg). mp 106–107 °C. IR: ν = 1727, 1607, 1377, 1282 cm⁻¹. ¹H NMR (400 MHz, CDCl₃) δ 7.53 – 7.46 (m, 3H), 7.44 – 7.39 (m, 2H), 7.36 (d, *J* = 8.9 Hz, 1H), 6.87 (d, *J* = 2.5 Hz, 1H), 6.77 (dd, *J* = 8.9, 2.6 Hz, 1H), 6.19 (s, 1H), 3.86 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 162.8, 161.2, 156.0, 155.8, 135.6, 129.6, 128.8, 128.3, 127.9, 112.5, 112.3, 111.9, 101.1, 55.8. [Ref]. *J. Org. Chem.* **2012**, 77, 2053.



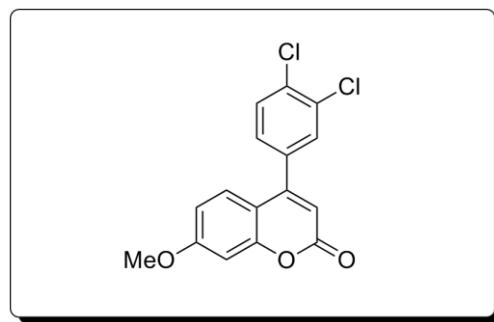
7-methoxy-4-(3-nitrophenyl)-2H-chromen-2-one (2b). Yield 52% (15.4 mg). mp 191–194 °C. IR: ν = 1714, 1598, 1526, 1345 cm⁻¹. ¹H NMR (400 MHz, CDCl₃) δ 8.39 – 8.35 (m, 1H), 8.32 – 8.29 (m, 1H), 7.78 – 7.69 (m, 2H), 7.21 (d, *J* = 8.9 Hz, 1H), 6.90 (d, *J* = 2.5 Hz, 1H), 6.81 (dd, *J* = 8.9, 2.5 Hz, 1H), 6.23 (s, 1H), 3.88 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 163.3, 160.4, 156.1, 153.1, 148.4, 137.1, 134.2, 130.2, 127.2, 124.4, 123.4, 112.8, 112.7, 111.7, 101.4, 55.9. HRMS (ESI+) m/z calcd. for C₁₆H₁₁NNaO₅⁺ [M+Na]⁺: 320.0529, found: 320.0528.



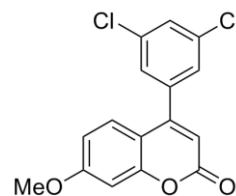
4-(3,4-dimethylphenyl)-7-methoxy-2H-chromen-2-one (2c). Yield 82% (22.9 mg). mp 115–117 °C. IR: ν = 1714, 1603, 1363, 814 cm⁻¹. ¹H NMR (400 MHz, CDCl₃) δ 7.41 (d, J = 8.9 Hz, 1H), 7.24 (d, J = 7.7 Hz, 1H), 7.20 – 7.13 (m, 2H), 6.86 (d, J = 2.5 Hz, 1H), 6.77 (dd, J = 8.9, 2.5 Hz, 1H), 6.17 (s, 1H), 3.86 (s, 3H), 2.33 (s, 3H), 2.32 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 162.7, 161.3, 156.0, 155.9, 138.4, 137.2, 133.1, 129.9, 129.4, 128.1, 125.8, 112.7, 112.2, 111.5, 101.0, 55.7, 19.8, 19.6. HRMS (ESI+) m/z calcd. for C₁₈H₁₆NaO₃⁺ [M+Na]⁺: 303.0992, found: 303.0986.



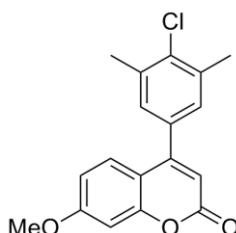
4-(3,5-dimethylphenyl)-7-methoxy-2H-chromen-2-one (2d). Yield 85% (23.8 mg). mp 97–100 °C. IR: ν = 1714, 1610, 1594, 1255 cm⁻¹. ¹H NMR (400 MHz, CDCl₃) δ 7.38 (d, J = 8.9 Hz, 1H), 7.11 (s, 1H), 7.01 (s, 2H), 6.86 (d, J = 2.5 Hz, 1H), 6.77 (dd, J = 8.9, 2.5 Hz, 1H), 6.16 (s, 1H), 3.86 (s, 3H), 2.37 (s, 6H). ¹³C NMR (100 MHz, CDCl₃) δ 162.7, 161.3, 156.2, 155.9, 138.4, 135.5, 131.1, 128.1, 126.1, 112.7, 112.2, 111.6, 101.0, 55.7, 21.3. HRMS (ESI+) m/z calcd. for C₁₈H₁₆NaO₃⁺ [M+Na]⁺: 303.0992, found: 303.0987.



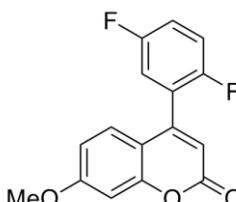
4-(3,4-dichlorophenyl)-7-methoxy-2H-chromen-2-one (2e). Yield 83% (26.5 mg). mp 155–157 °C. IR: ν = 1723, 1716, 1611, 1542, 1295 cm⁻¹. ¹H NMR (400 MHz, CDCl₃) δ 7.58 (d, J = 8.3 Hz, 1H), 7.52 (d, J = 1.8 Hz, 1H), 7.29 – 7.24 (m, 2H), 6.87 (d, J = 2.5 Hz, 1H), 6.80 (ddd, J = 8.9, 2.5, 0.6 Hz, 1H), 6.16 (s, 1H), 3.87 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 163.1, 160.6, 156.0, 153.2, 135.4, 134.1, 133.3, 130.9, 130.2, 127.6, 127.4, 112.6, 112.3, 111.8, 101.3, 55.9. HRMS (ESI+) m/z calcd. for C₁₆H₁₀Cl₂NaO₃⁺ [M+Na]⁺: 342.9899, found: 342.9894.



4-(3,5-dichlorophenyl)-7-methoxy-2H-chromen-2-one (2f). Yield 73% (23.2 mg). mp 178–179 °C. IR: ν = 1717, 1619, 1603, 1365 cm⁻¹. ¹H NMR (400 MHz, CDCl₃) δ 7.49 (t, J = 1.9 Hz, 1H), 7.30 (d, J = 1.9 Hz, 2H), 7.25 (d, J = 9.0 Hz, 1H), 6.88 (d, J = 2.5 Hz, 1H), 6.81 (dd, J = 8.9, 2.5 Hz, 1H), 6.17 (s, 1H), 3.87 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 163.2, 160.4, 156.0, 152.8, 138.3, 135.7, 129.6, 127.3, 126.7, 112.7, 112.4, 111.7, 101.3, 55.8. HRMS (ESI+) m/z calcd. for C₁₆H₁₀Cl₂NaO₃⁺ [M+Na]⁺: 342.9899, found: 342.9901.

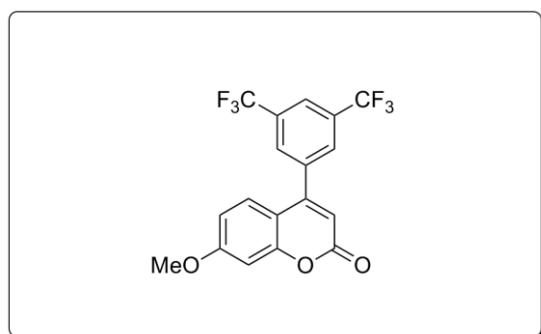


4-(4-chloro-3,5-dimethylphenyl)-7-methoxy-2H-chromen-2-one (2g). Yield 66% (20.6 mg). mp 210–212 °C. IR: ν = 1724, 1617, 1605, 1363 cm⁻¹. ¹H NMR (400 MHz, CDCl₃) δ 7.35 (d, J = 8.9 Hz, 1H), 7.13 (s, 2H), 6.86 (d, J = 2.5 Hz, 1H), 6.78 (dd, J = 8.9, 2.6 Hz, 1H), 6.15 (s, 1H), 3.86 (s, 3H), 2.43 (s, 6H). ¹³C NMR (100 MHz, CDCl₃) δ 162.8, 161.1, 156.0, 155.0, 137.0, 136.2, 133.3, 128.2, 127.9, 112.4, 112.3, 111.7, 101.1, 55.8, 20.8. HRMS (ESI+) m/z calcd. for C₁₈H₁₅ClNaO₃⁺ [M+Na]⁺: 337.0602, found: 337.0594.

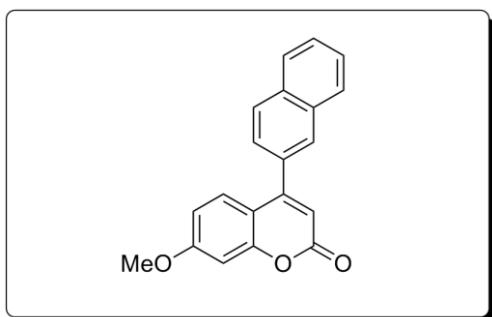


4-(2,5-difluorophenyl)-7-methoxy-2H-chromen-2-one (2h). Yield 71% (20.4 mg). mp 154–157 °C. IR: ν = 1716, 1601, 1484, 1428 cm⁻¹. ¹H NMR (400 MHz, CDCl₃) δ 7.20 – 7.15 (m, 2H), 7.12 (dd, J = 8.9, 2.4 Hz, 1H), 7.08 – 7.02 (m, 1H), 6.87 (d, J = 2.5 Hz, 1H), 6.78 (dd, J = 8.9, 2.5 Hz, 1H), 6.22 (s, 1H), 3.86 (s, 3H). ¹³C NMR (100

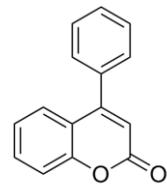
MHz, CDCl₃) δ 163.1, 160.5, 158.6 (dd, *J* = 245.0, 2.4 Hz), 155.7, 155.1 (dd, *J* = 245.8, 2.6 Hz), 149.1, 127.4, 127.4, 124.3 (dd, *J* = 18.5, 8.2 Hz), 118.1, 118.0, 117.8, 117.8, 117.7, 117.6, 117.5, 117.4, 117.1, 117.1, 116.8, 116.8, 113.7, 112.6, 111.8, 101.0, 55.8. HRMS (ESI+) m/z calcd. for C₁₆H₁₀F₂NaO₃⁺ [M+Na]⁺: 311.0490, found: 311.0490.



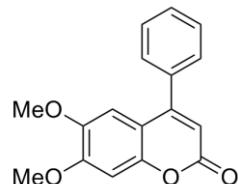
4-(3,5-bis(trifluoromethyl)phenyl)-7-methoxy-2H-chromen-2-one (2i). Yield 55% (21.2 mg). mp 151–154 °C. IR: ν = 1706, 1601, 1279 cm⁻¹. ¹H NMR (400 MHz, CDCl₃) δ 8.02 (s, 1H), 7.88 (s, 2H), 7.13 (d, *J* = 8.9 Hz, 1H), 6.91 (d, *J* = 2.5 Hz, 1H), 6.83 (dd, *J* = 8.9, 2.5 Hz, 1H), 6.23 (s, 1H), 3.89 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 163.4, 160.1, 156.1, 152.4, 137.6, 132.6 (q, *J* = 33.9 Hz), 128.5, 128.5, 126.9, 123.4 (hept, *J* = 4.0 Hz), 122.8 (q, *J* = 271.0 Hz), 113.0, 112.9, 111.5, 101.5, 55.9. HRMS (ESI+) m/z calcd. for C₁₈H₁₀F₆NaO₃⁺ [M+Na]⁺: 411.0426, found: 411.0428.



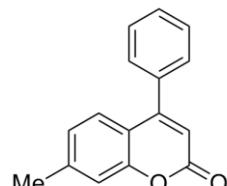
7-methoxy-4-(naphthalen-2-yl)-2H-chromen-2-one (2j). Yield 60% (18.1 mg). mp 147–150 °C. IR: ν = 1721, 1603, 1504, 1142 cm⁻¹. ¹H NMR (400 MHz, CDCl₃) δ 7.96 (d, *J* = 8.4 Hz, 1H), 7.93 – 7.88 (m, 3H), 7.59 – 7.54 (m, 2H), 7.50 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.41 (d, *J* = 8.9 Hz, 1H), 6.90 (d, *J* = 2.5 Hz, 1H), 6.78 (dd, *J* = 8.9, 2.5 Hz, 1H), 6.30 (s, 1H), 3.87 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 162.8, 161.2, 156.1, 155.8, 133.5, 133.0, 133.0, 128.6, 128.3, 128.1, 128.0, 127.8, 127.2, 127.0, 125.7, 112.7, 112.4, 112.2, 101.2, 55.8. HRMS (ESI+) m/z calcd. for C₂₀H₁₄NaO₃⁺ [M+Na]⁺: 325.0835, found: 325.0836.



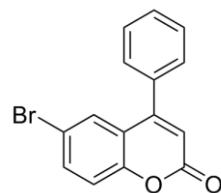
4-phenyl-2H-chromen-2-one (2k). Yield 66% (14.6 mg). IR: ν = 1718, 1603, 1369 cm^{-1} . ^1H NMR (400 MHz, CDCl_3) δ 7.56 – 7.37 (m, 8H), 7.21 (ddd, J = 8.2, 7.2, 1.2 Hz, 1H), 6.36 (s, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 160.7, 155.6, 154.2, 135.2, 131.9, 129.7, 128.8, 128.4, 127.0, 124.1, 119.0, 117.3, 115.2. [Ref]. *J. Org. Chem.* **2012**, 77, 2053.



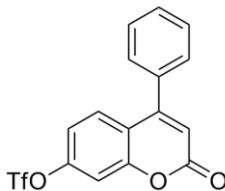
6,7-dimethoxy-4-phenyl-2H-chromen-2-one (2l). Yield 84% (23.7 mg). mp 140–142 °C. IR: ν = 1713, 1510, 1259 cm^{-1} . ^1H NMR (400 MHz, CDCl_3) δ 7.53 – 7.41 (m, 5H), 6.89 (s, 1H), 6.84 (s, 1H), 6.21 (s, 1H), 3.94 (s, 3H), 3.73 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 161.3, 155.6, 152.9, 150.1, 146.1, 135.7, 129.6, 128.9, 128.2, 112.3, 111.3, 107.4, 100.3, 56.4, 56.3. HRMS (ESI+) m/z calcd. for $\text{C}_{17}\text{H}_{14}\text{NaO}_4^+ [\text{M}+\text{Na}]^+$: 305.0784, found: 305.0775. [Ref]. *Eur. J. Org. Chem.* **2010**, 21, 4130.



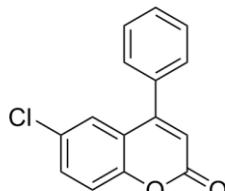
7-methyl-4-phenyl-2H-chromen-2-one (2m). Yield 74% (17.4 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.51 – 7.48 (m, 3H), 7.44 – 7.40 (m, 2H), 7.34 (d, J = 8.1 Hz, 1H), 7.19 (s, 1H), 7.02 (d, J = 8.1 Hz, 1H), 6.29 (s, 1H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 161.0, 155.6, 154.3, 143.2, 135.4, 129.6, 128.8, 128.4, 126.6, 125.3, 117.4, 116.5, 114.0, 21.6. [Ref]. *Eur. J. Org. Chem.* **2010**, 20, 3945–3955.



6-bromo-4-phenyl-2H-chromen-2-one (2n). Yield 44% (13.2 mg). mp 152–155 °C. IR: ν = 1763, 1718, 1595, 1550 cm⁻¹. ¹H NMR (400 MHz, CDCl₃) δ 7.62 (dd, *J* = 8.7, 2.4 Hz, 1H), 7.57 (d, *J* = 2.3 Hz, 1H), 7.55 – 7.52 (m, 3H), 7.44 – 7.40 (m, 2H), 7.28 (d, *J* = 8.8 Hz, 1H), 6.38 (s, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 159.9, 154.5, 153.1, 134.7, 134.5, 130.0, 129.3, 129.1, 128.3, 120.6, 119.0, 117.0, 116.1. HRMS (ESI+) m/z calcd. for C₁₅H₉BrNaO₂⁺ [M+Na]⁺: 322.9678, found: 322.9669.

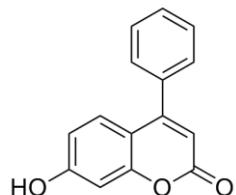


2-oxo-4-phenyl-2H-chromen-7-yl trifluoromethanesulfonate (2o). Yield 51% (18.8 mg). Colorless oil. IR: ν = 1731, 1608, 1418, 1205 cm⁻¹. ¹H NMR (400 MHz, CDCl₃) δ 7.58 (d, *J* = 8.9 Hz, 1H), 7.55 – 7.52 (m, 3H), 7.43 – 7.40 (m, 2H), 7.33 (d, *J* = 2.5 Hz, 1H), 7.14 (dd, *J* = 8.9, 2.5 Hz, 1H), 6.41 (s, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 159.4, 154.7, 154.6, 150.8, 134.4, 130.1, 129.1, 128.8, 128.3, 120.3, 119.1, 117.3, 117.1, 115.9, 110.7. HRMS (ESI+) m/z calcd. for C₁₆H₉F₃NaO₅S⁺ [M+Na]⁺: 393.0015, found: 393.0012.

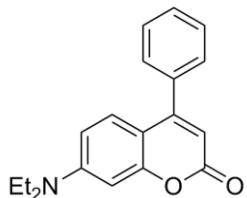


6-chloro-4-phenyl-2H-chromen-2-one (2p). Yield 72% (18.3 mg). IR: ν = 1727, 1554, 1354 cm⁻¹. ¹H NMR (400 MHz, CDCl₃) δ 7.55 – 7.52 (m, 3H), 7.48 (dd, *J* = 8.8, 2.5 Hz, 1H), 7.44 – 7.40 (m, 3H), 7.34 (dd, *J* = 8.8, 0.4 Hz,

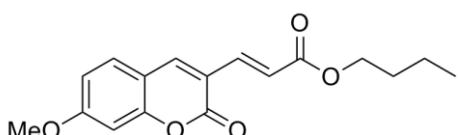
1H), 6.39 (s, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 160.0, 154.6, 152.6, 134.5, 131.9, 130.0, 129.7, 129.1, 128.3, 126.3, 120.2, 118.7, 116.1. [Ref]. *J. Org. Chem.* **2012**, *77*, 2053.



7-hydroxy-4-phenyl-2H-chromen-2-one (2q). Yield 41% (9.7 mg). ^1H NMR (400 MHz, DMSO-d_6) δ 10.65 (s, 1H), 7.59 – 7.48 (m, 5H), 7.27 (d, $J = 8.6$ Hz, 1H), 6.80 (dd, $J = 6.3, 2.2$ Hz, 1H), 6.77 (d, $J = 2.4$ Hz, 1H), 6.15 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.4, 160.1, 155.5, 155.4, 135.2, 129.5, 128.8, 128.4, 128.1, 113.2, 110.7, 110.3, 102.7. [Ref]. *J. Org. Chem.* **2012**, *77*, 2053.



7-(diethylamino)-4-phenyl-2H-chromen-2-one (2r). Yield 53% (15.5 mg). Orange oil. IR: $\nu = 1729, 1703, 1585, 1520, 1405$ cm^{-1} . ^1H NMR (400 MHz, CDCl_3) δ 7.49 – 7.39 (m, 5H), 7.23 (d, $J = 9.0$ Hz, 1H), 6.55 (d, $J = 2.6$ Hz, 1H), 6.49 (dd, $J = 9.1, 2.6$ Hz, 1H), 5.99 (s, 1H), 3.39 (q, $J = 7.1$ Hz, 4H), 1.19 (t, $J = 7.1$ Hz, 6H). ^{13}C NMR (100 MHz, CDCl_3) δ 162.1, 156.8, 156.1, 150.6, 136.2, 129.2, 128.6, 128.3, 127.9, 108.5, 108.3, 107.9, 97.9, 44.8, 12.4. [Ref]. *J. Org. Chem.* **2012**, *77*, 2053.



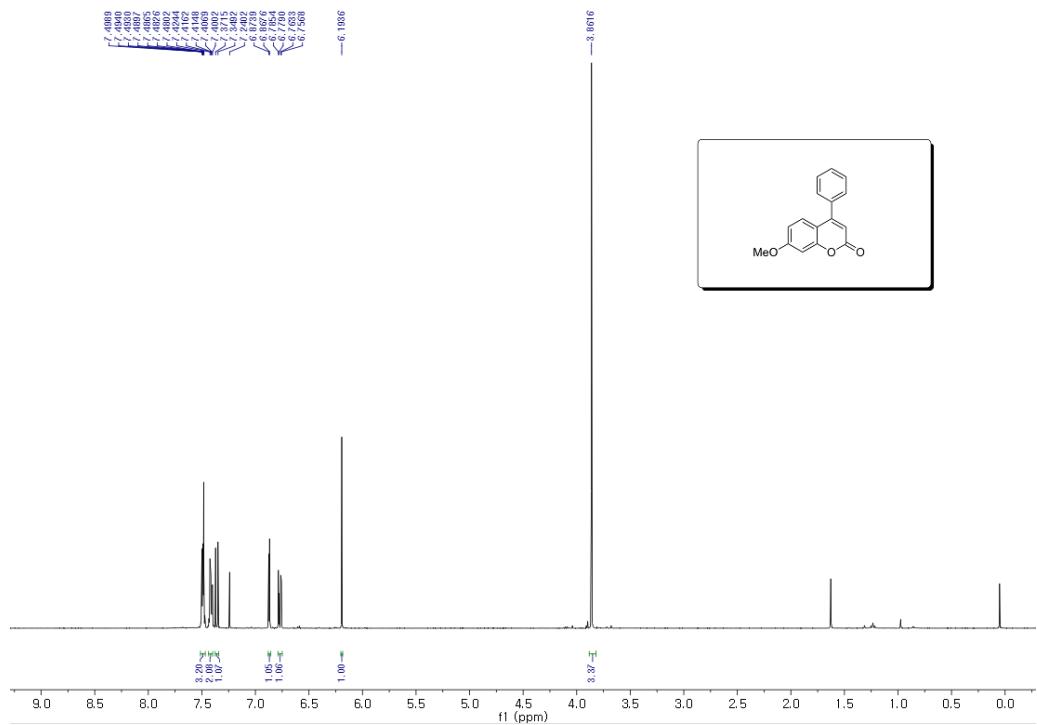
(E)-butyl 3-(7-methoxy-2-oxo-2H-chromen-3-yl)acrylate (4). Yield 63% (18.9 mg). mp 120–122 °C. IR: ν = 1723, 1706, 1601, 1156 cm⁻¹. δ 7.79 (s, 1H), 7.51 (dd, J = 15.9, 0.6 Hz, 1H), 7.42 (d, J = 8.6 Hz, 1H), 7.02 (d, J = 15.8 Hz, 1H), 6.86 (dd, J = 8.6, 2.4 Hz, 1H), 6.81 (d, J = 2.5 Hz, 1H), 4.18 (t, 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, CDCl₃) 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. HRMS (ESI+) m/z calcd. for C₁₇H₁₈NaO₅⁺ [M+Na]⁺: 325.1046, found: 325.1048.

Appendix I

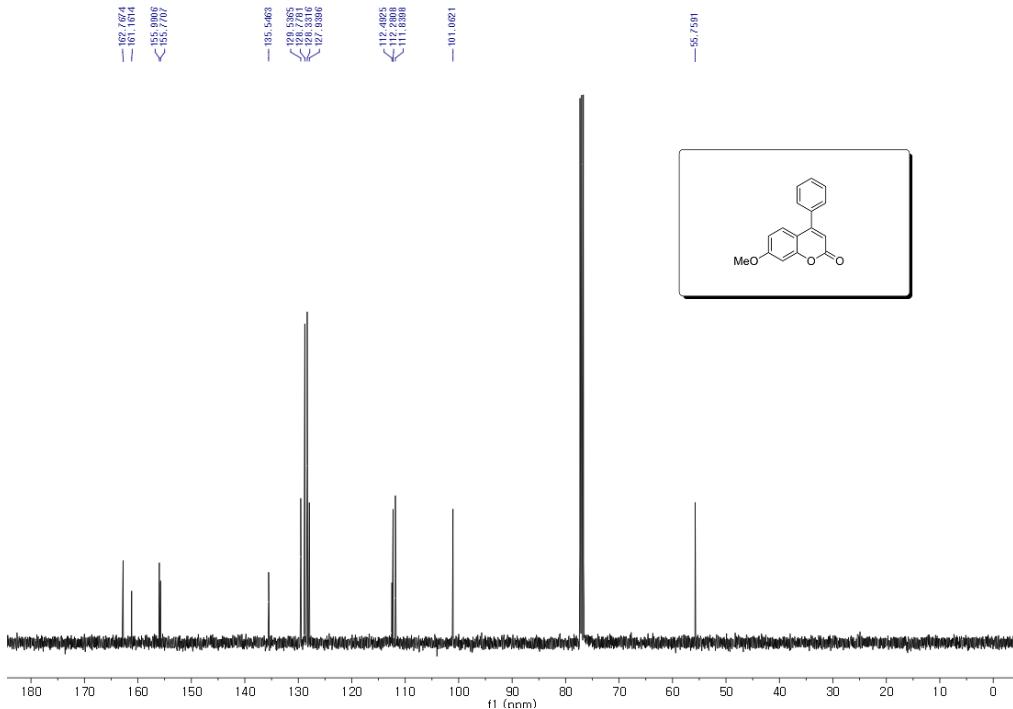
Spectral Copies of ^1H and ^{13}C NMR Data

Obtained in this Study

7-methoxy-4-phenyl-2H-chromen-2-one (2a).

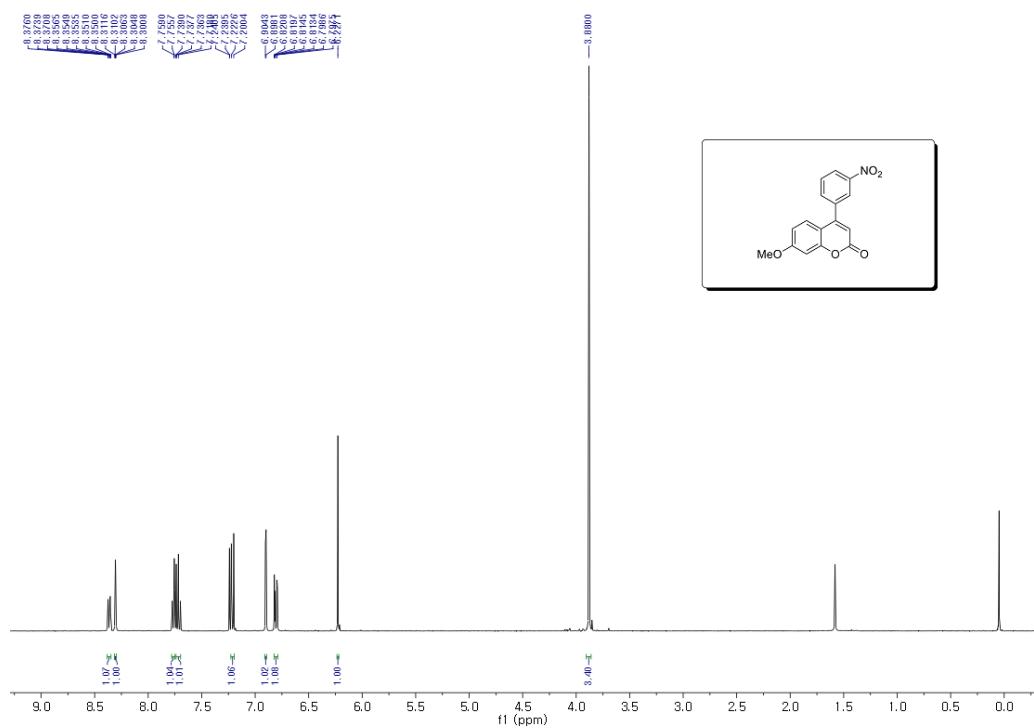


400 MHz, ^1H NMR in CDCl_3

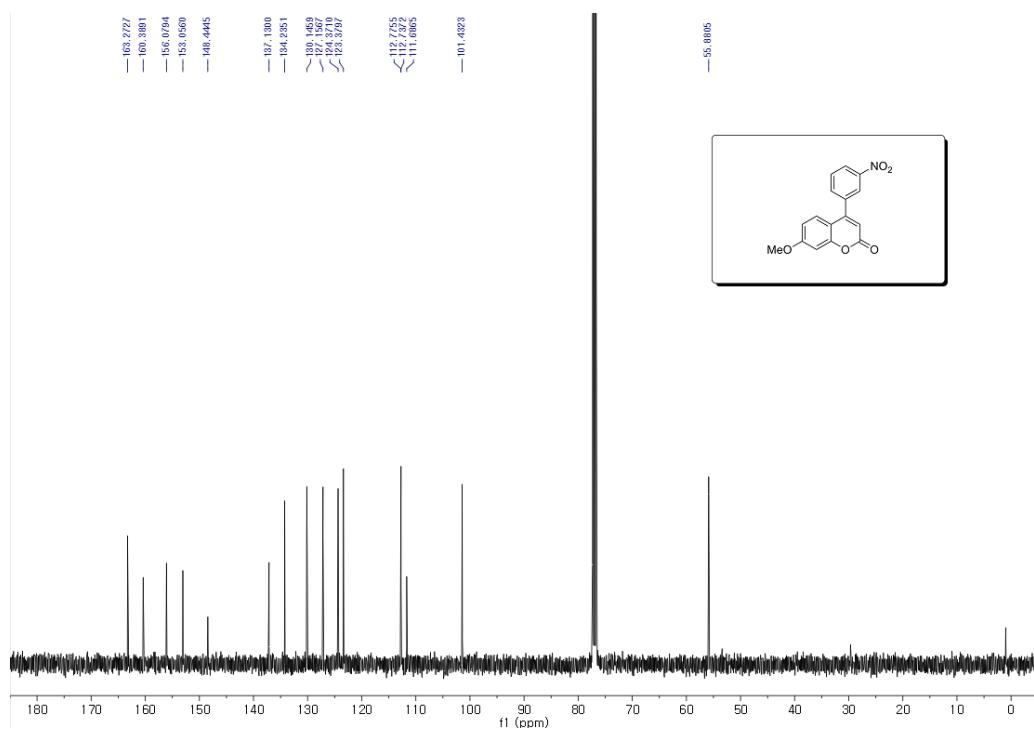


100 MHz, ^{13}C NMR in CDCl_3

7-methoxy-4-(3-nitrophenyl)-2H-chromen-2-one (2b).

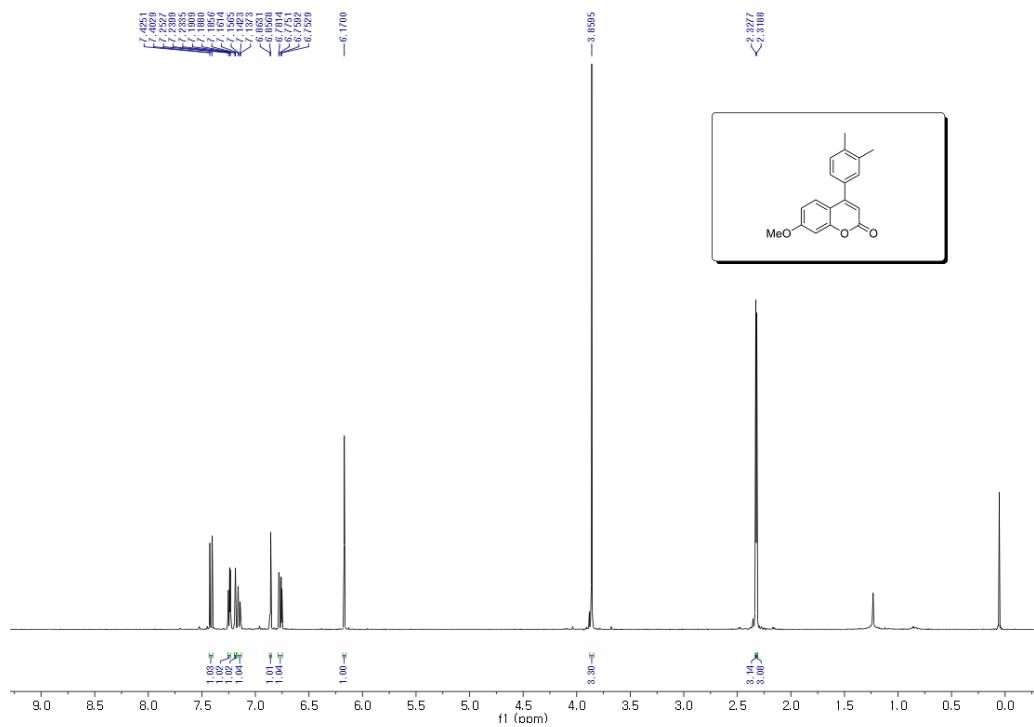


400 MHz, ¹H NMR in CDCl₃,

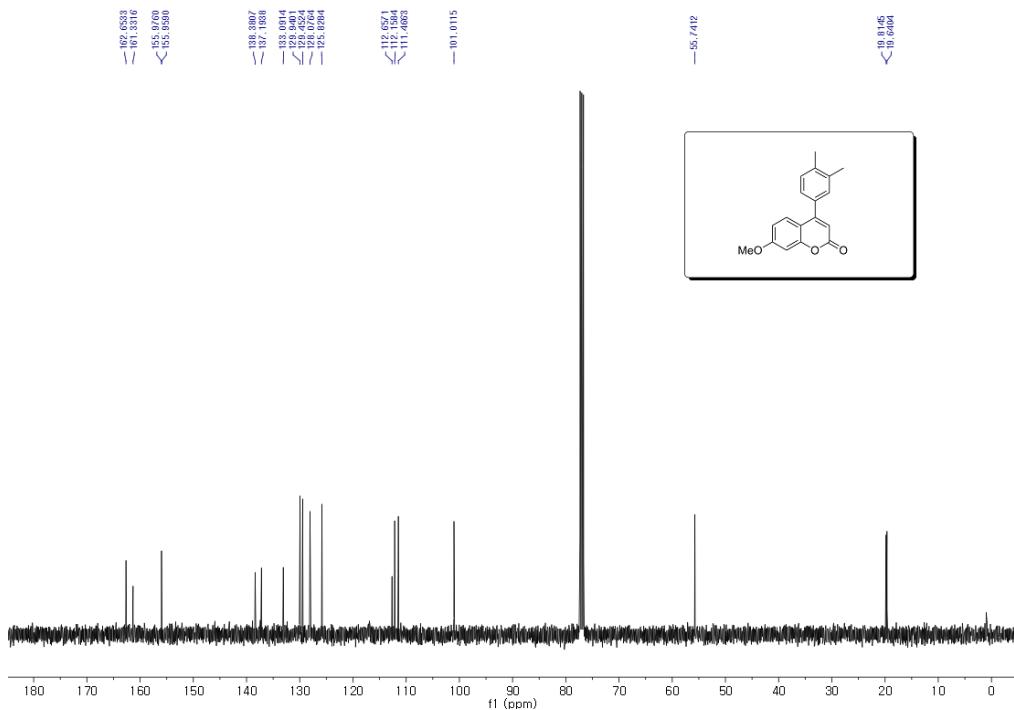


100 MHz, ¹³C NMR in CDCl₃

4-(3,4-dimethylphenyl)-7-methoxy-2H-chromen-2-one (2c).

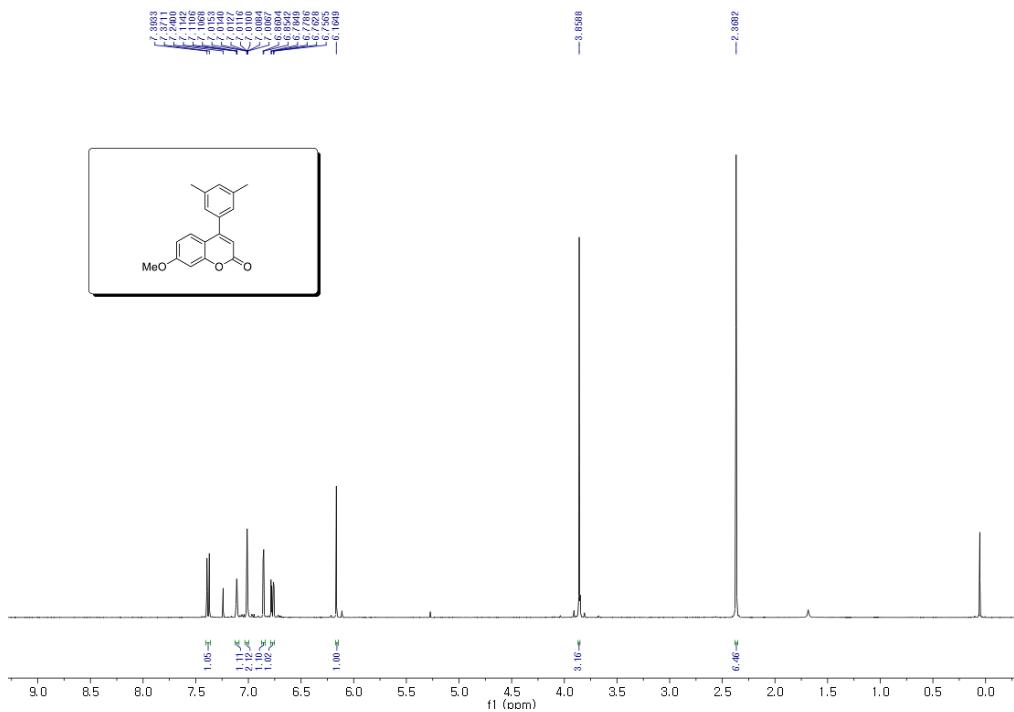


400 MHz, ^1H NMR in CDCl_3

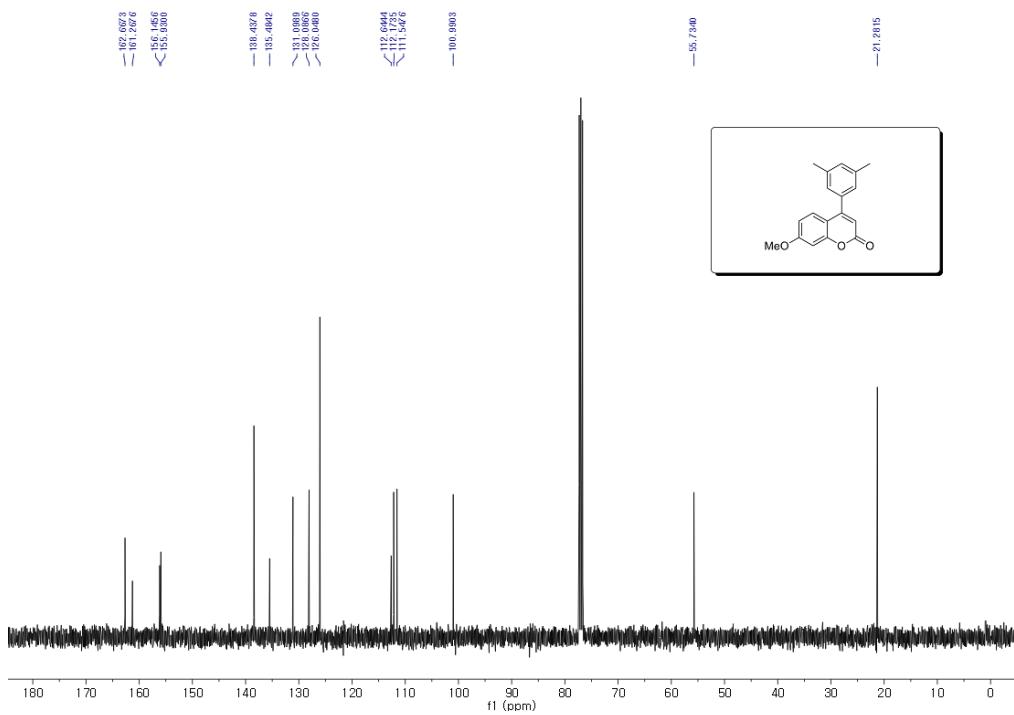


100 MHz, ^{13}C NMR in CDCl_3

4-(3,5-dimethylphenyl)-7-methoxy-2H-chromen-2-one (2d).

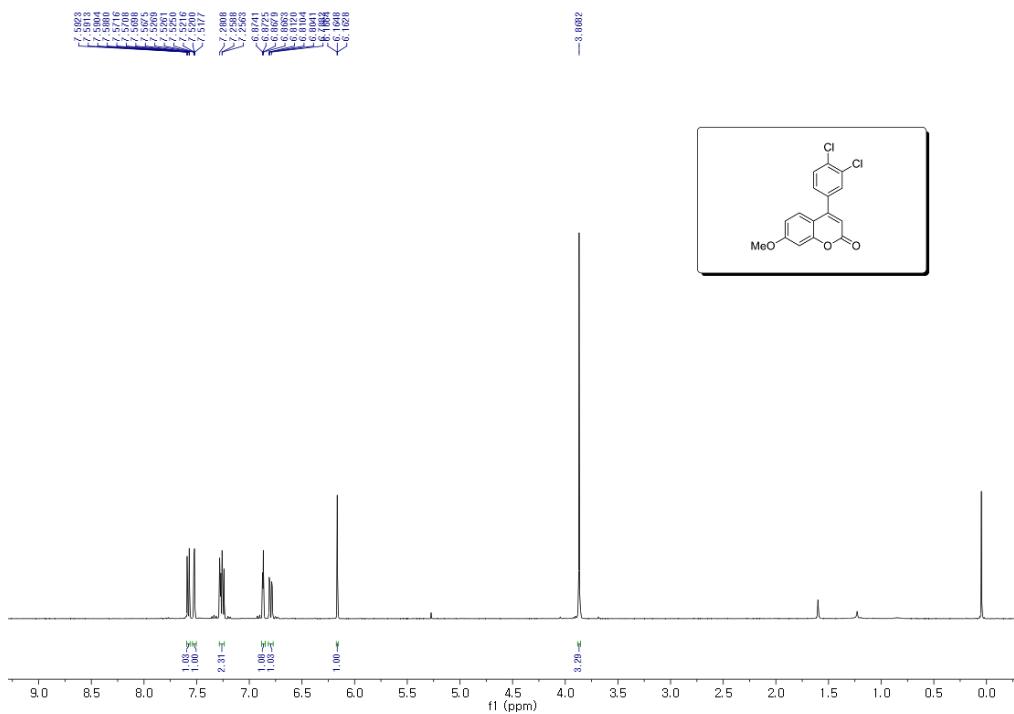


400 MHz, ¹H NMR in CDCl₃

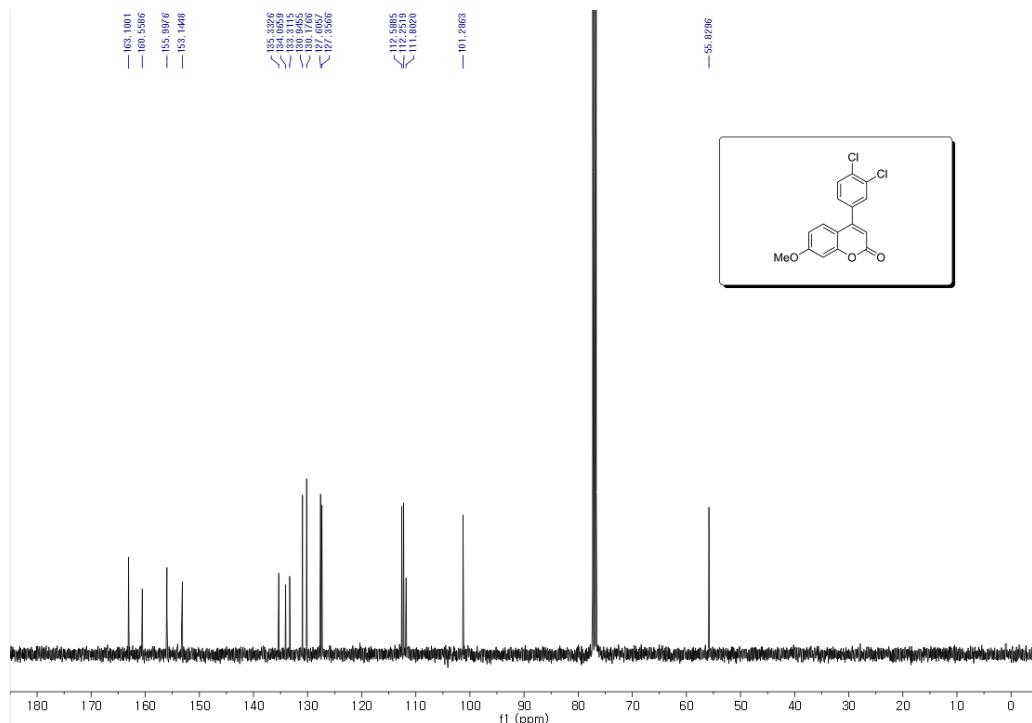


100 MHz, ¹³C NMR in CDCl₃

4-(3,4-dichlorophenyl)-7-methoxy-2H-chromen-2-one (2e).

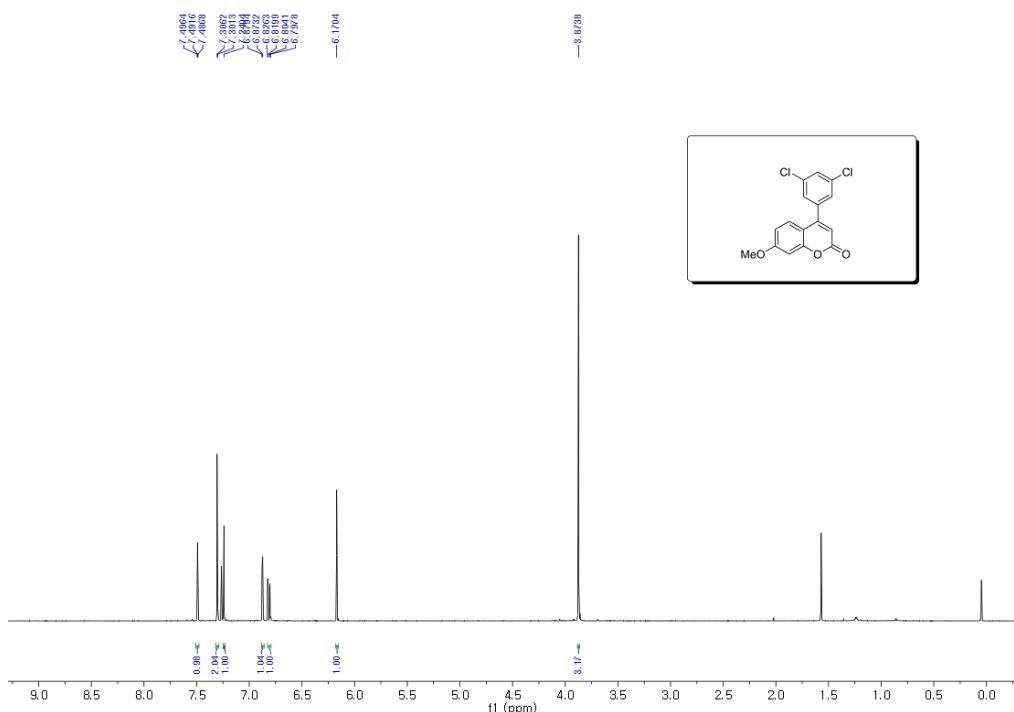


400 MHz, ^1H NMR in CDCl_3

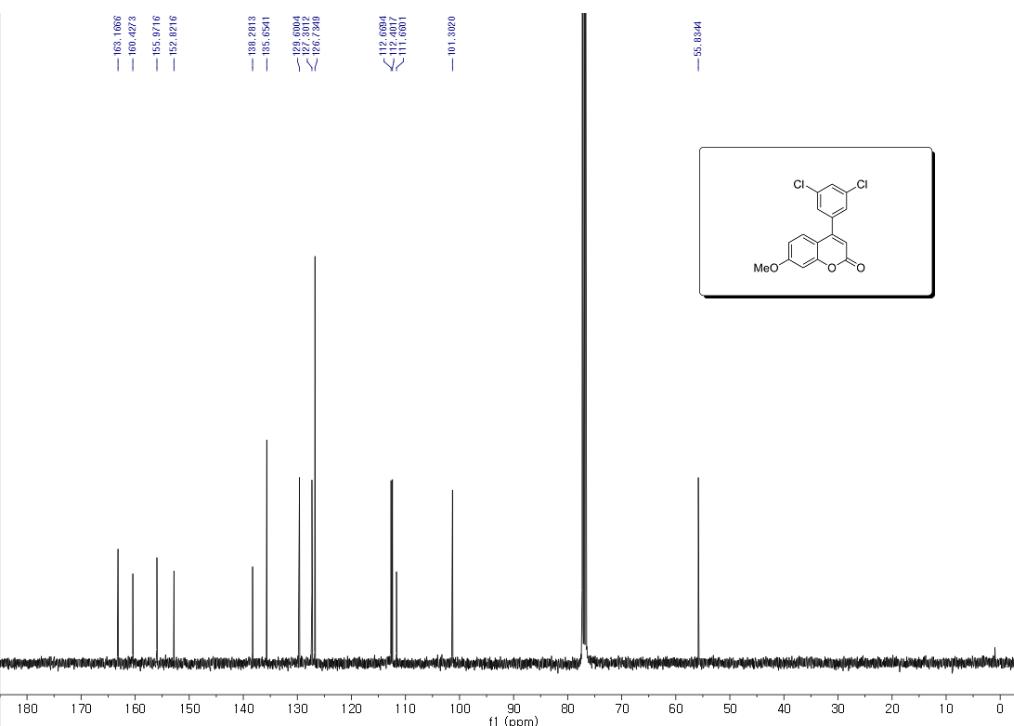


100 MHz, ^{13}C NMR in CDCl_3

4-(3,5-dichlorophenyl)-7-methoxy-2H-chromen-2-one (2f).

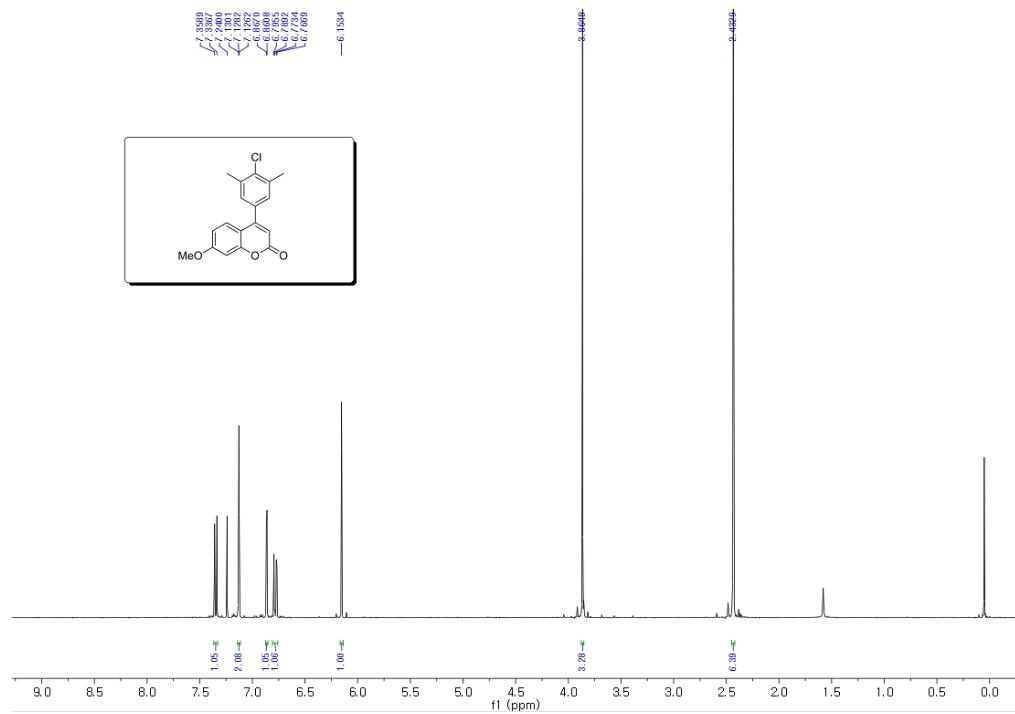


400 MHz, ¹H NMR in CDCl₃

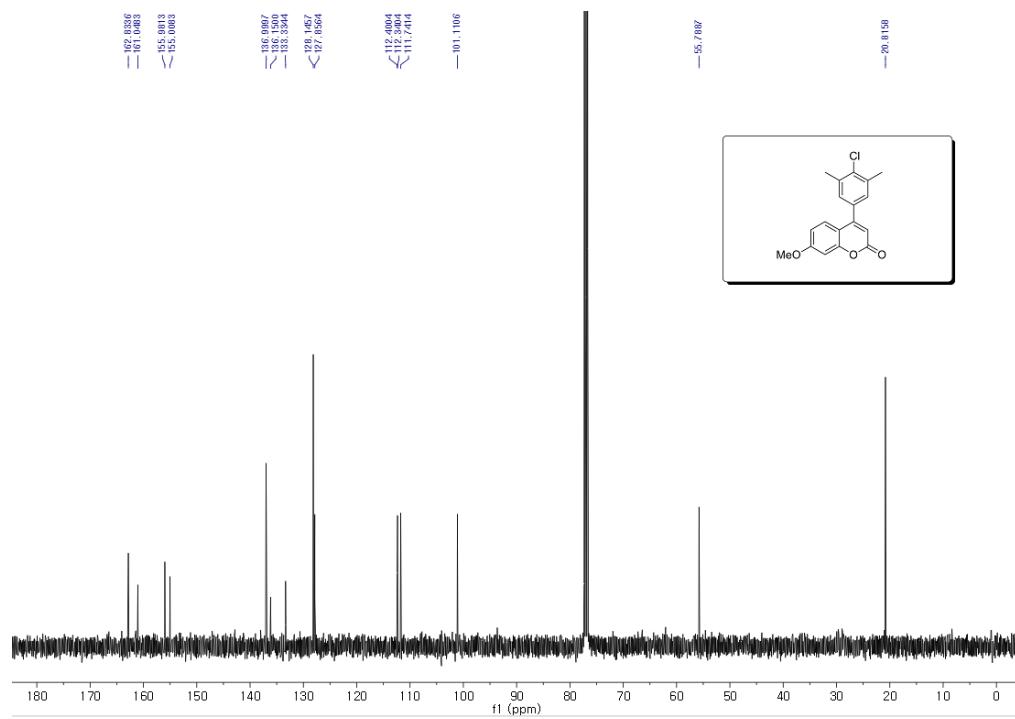


100 MHz, ¹³C NMR in CDCl₃

4-(4-chloro-3,5-dimethylphenyl)-7-methoxy-2H-chromen-2-one (2g).

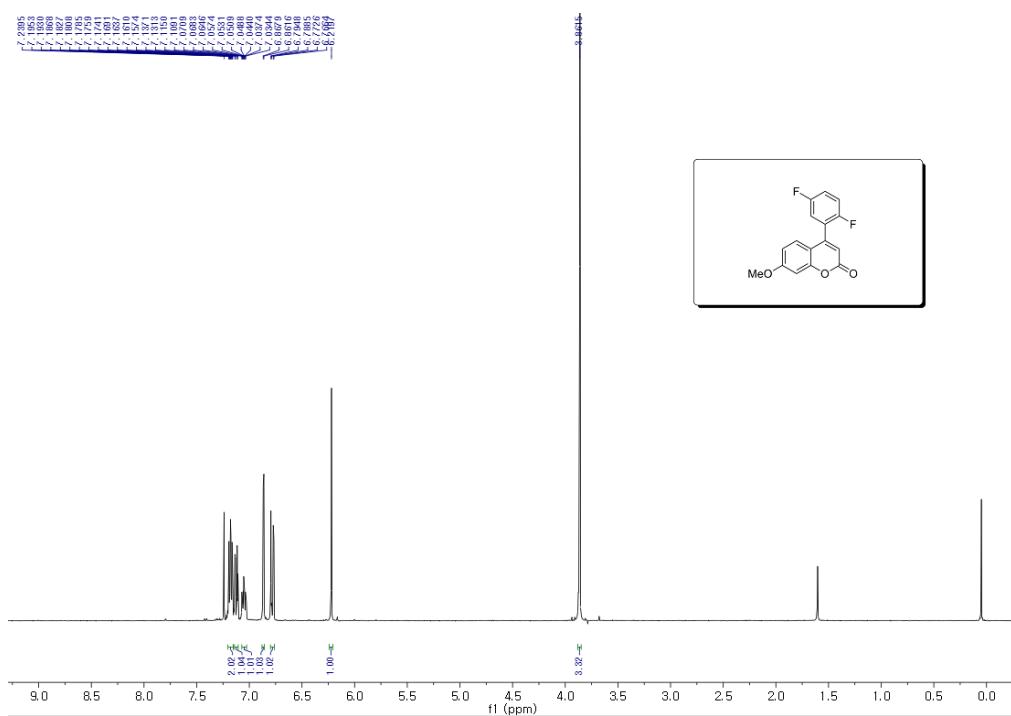


400 MHz, ^1H NMR in CDCl_3



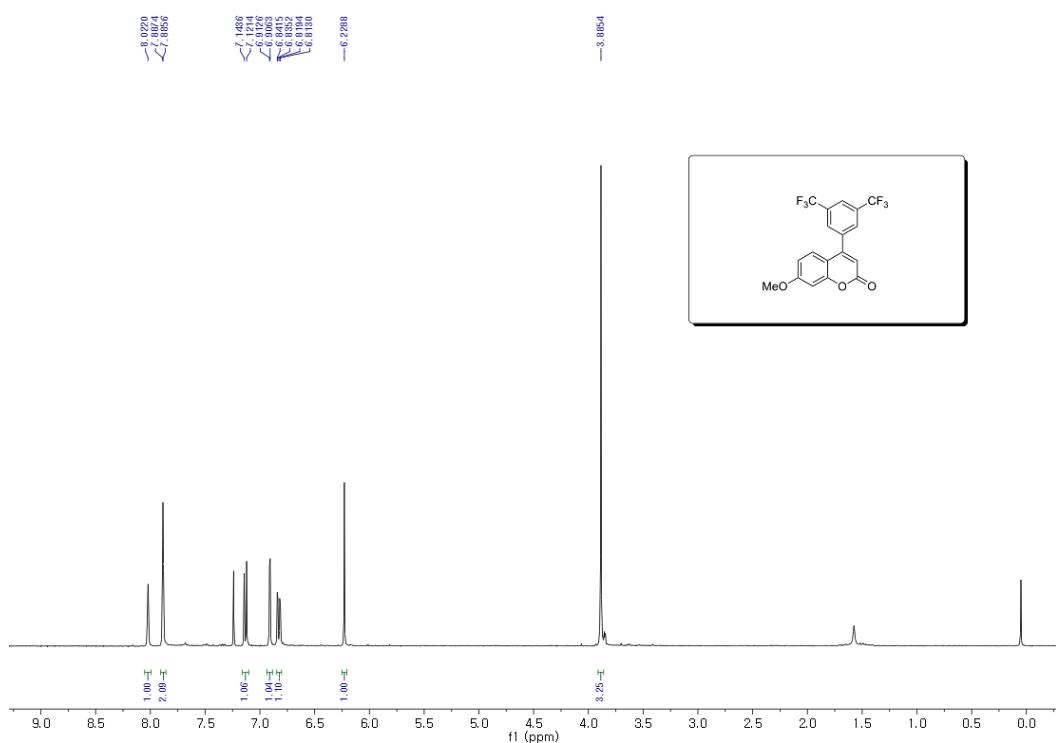
100 MHz, ^{13}C NMR in CDCl_3

4-(2,5-difluorophenyl)-7-methoxy-2H-chromen-2-one (2h).

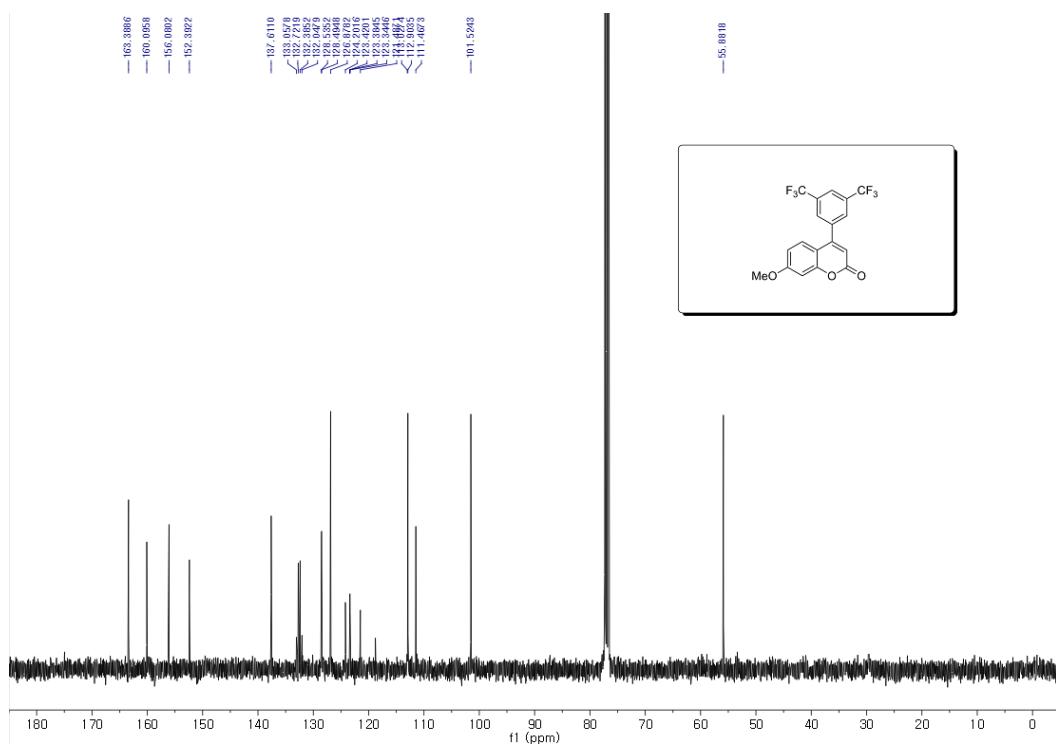


100 MHz, ^{13}C NMR in CDCl_3

4-(3,5-bis(trifluoromethyl)phenyl)-7-methoxy-2H-chromen-2-one (2i).

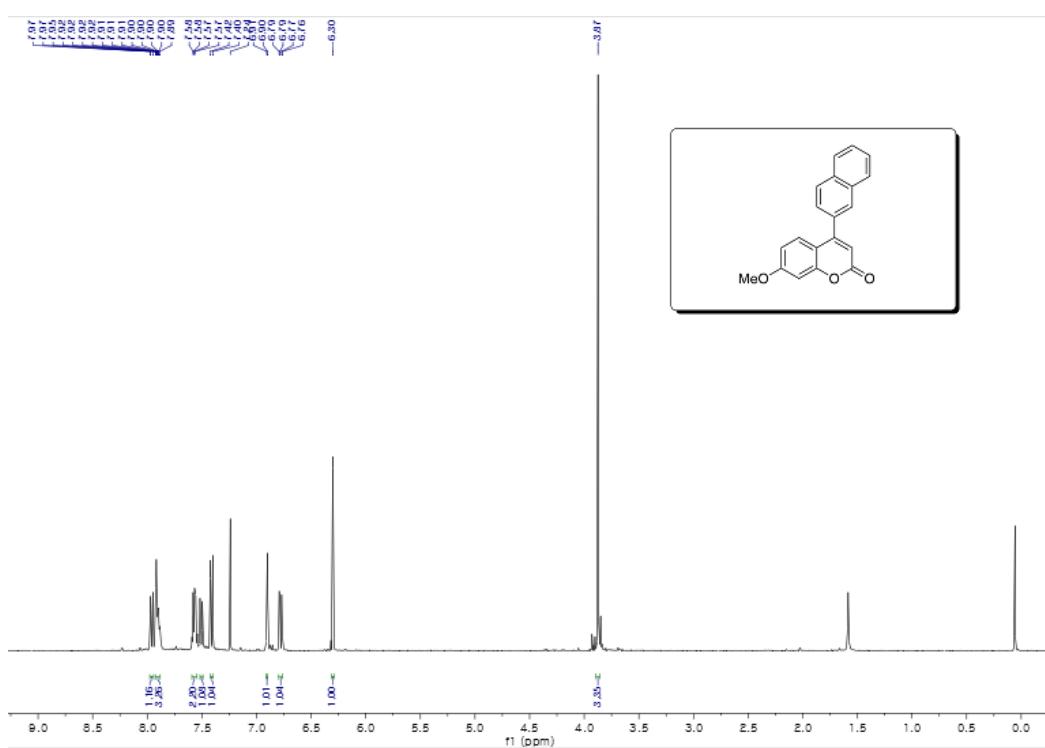


400 MHz, ^1H NMR in CDCl_3

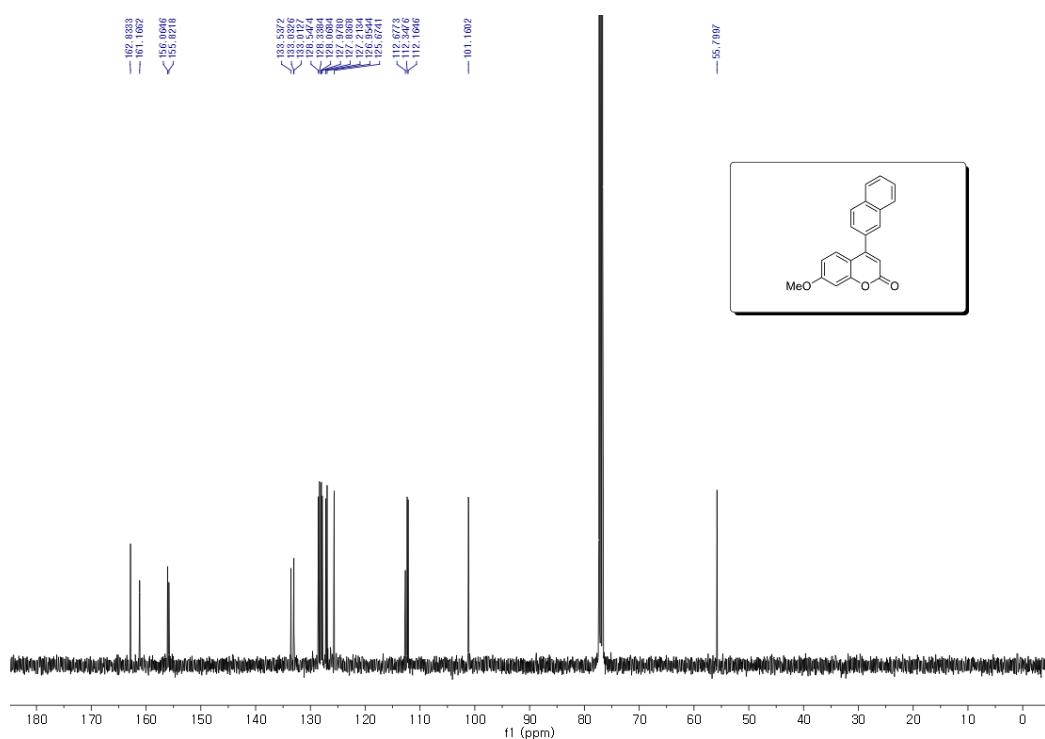


100 MHz, ^{13}C NMR in CDCl_3

7-methoxy-4-(naphthalen-2-yl)-2H-chromen-2-one (2j).

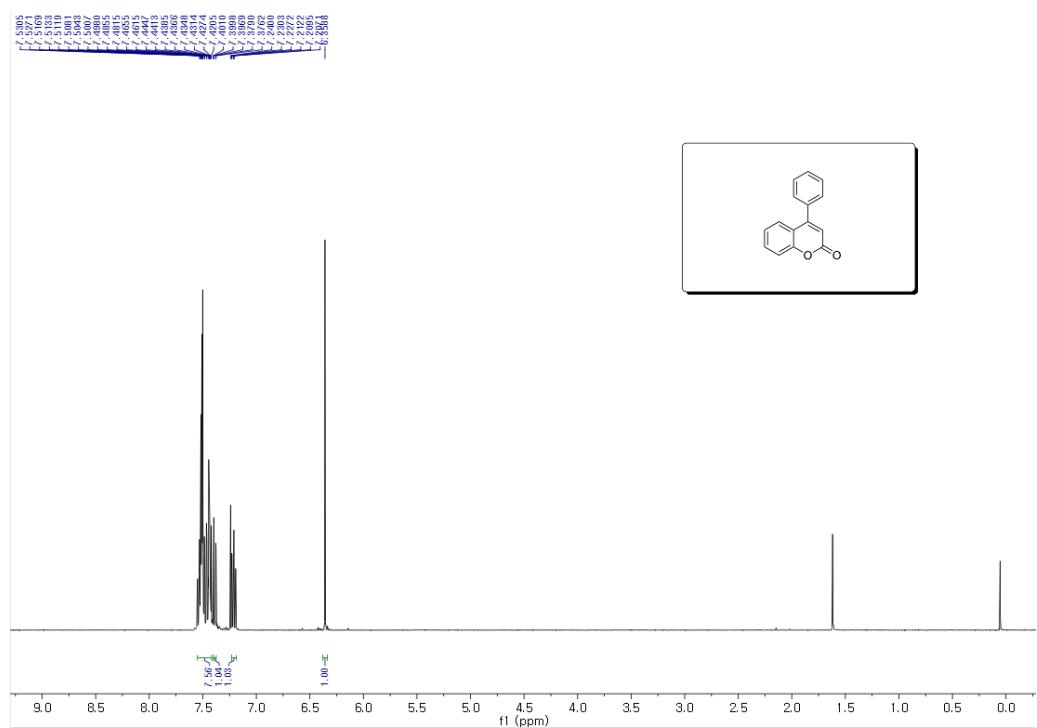


400 MHz, ^1H NMR in CDCl_3

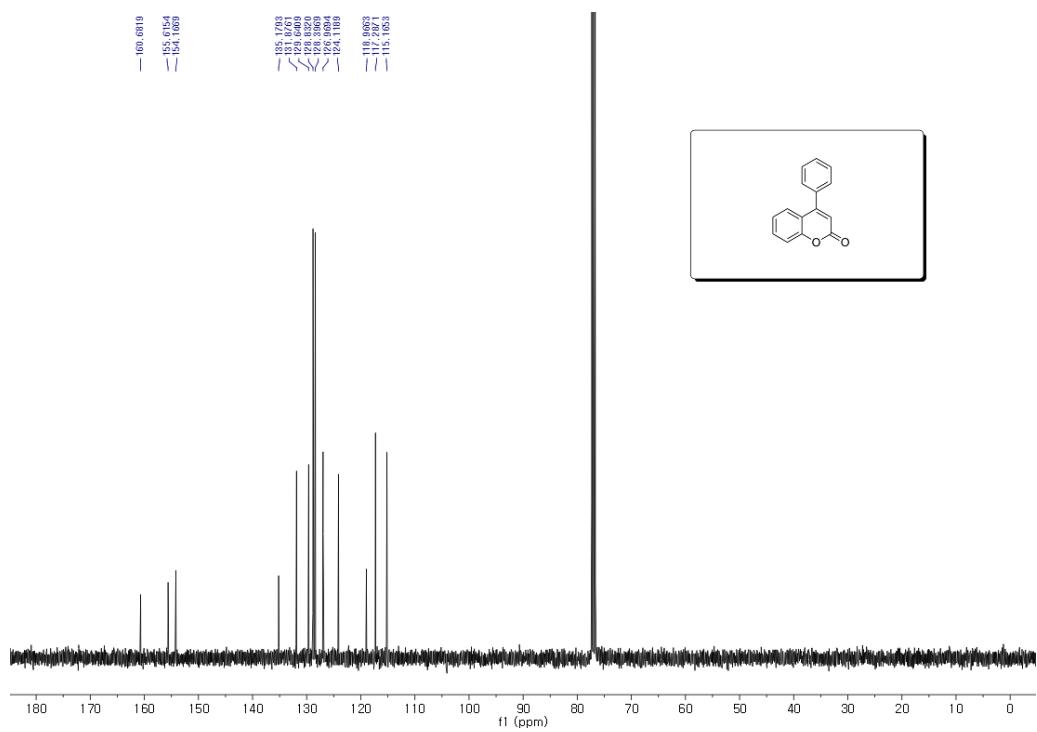


100 MHz, ^{13}C NMR in CDCl_3

4-phenyl-2H-chromen-2-one (2k).

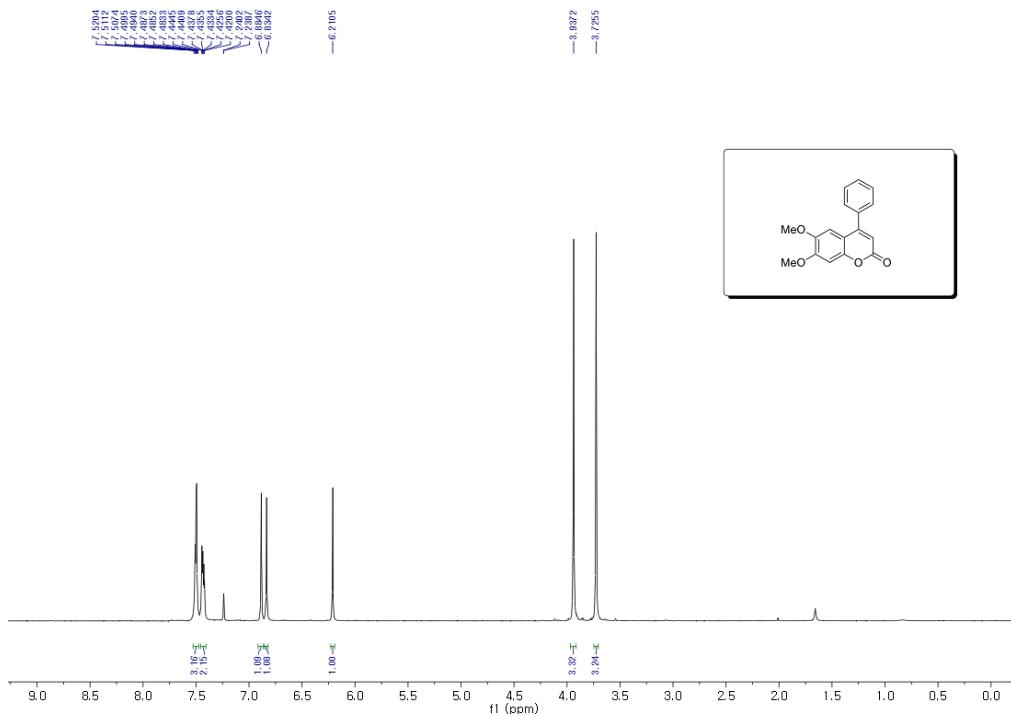


400 MHz, ^1H NMR in CDCl_3

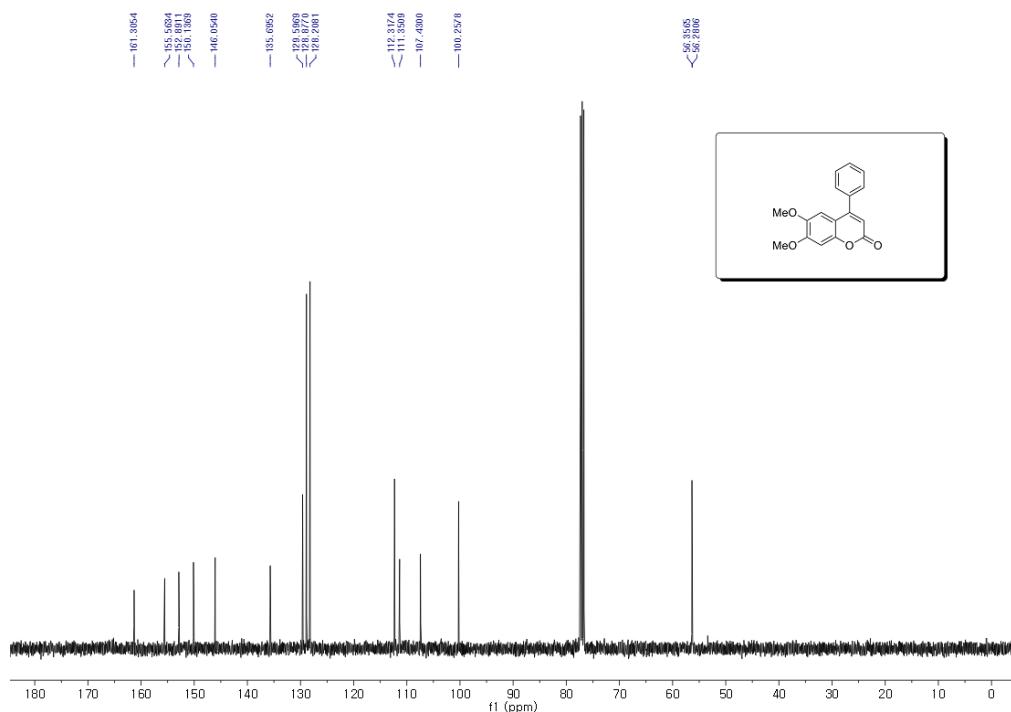


100 MHz, ^{13}C NMR in CDCl_3

6,7-dimethoxy-4-phenyl-2H-chromen-2-one (2l).

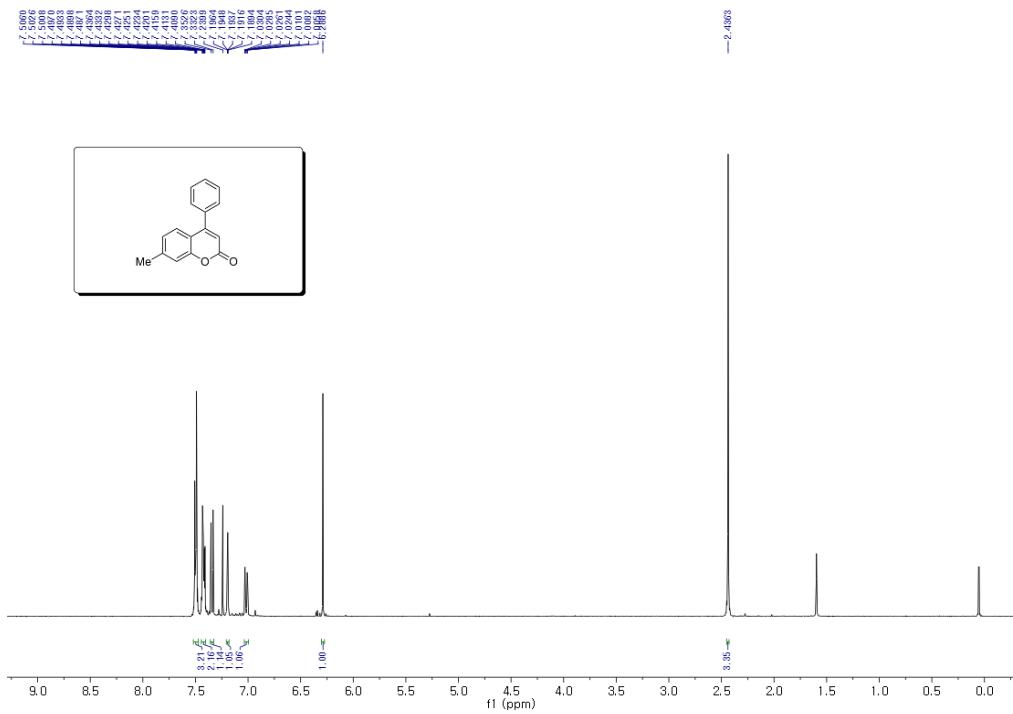


400 MHz, ^1H NMR in CDCl_3

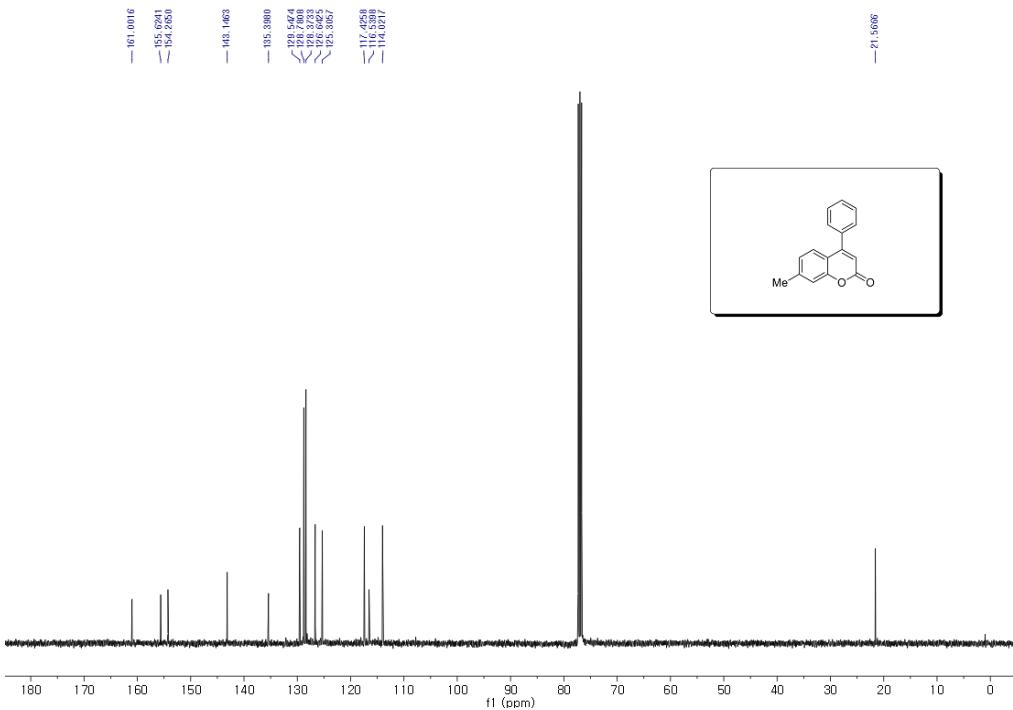


100 MHz, ^{13}C NMR in CDCl_3

7-methyl-4-phenyl-2H-chromen-2-one (2m).

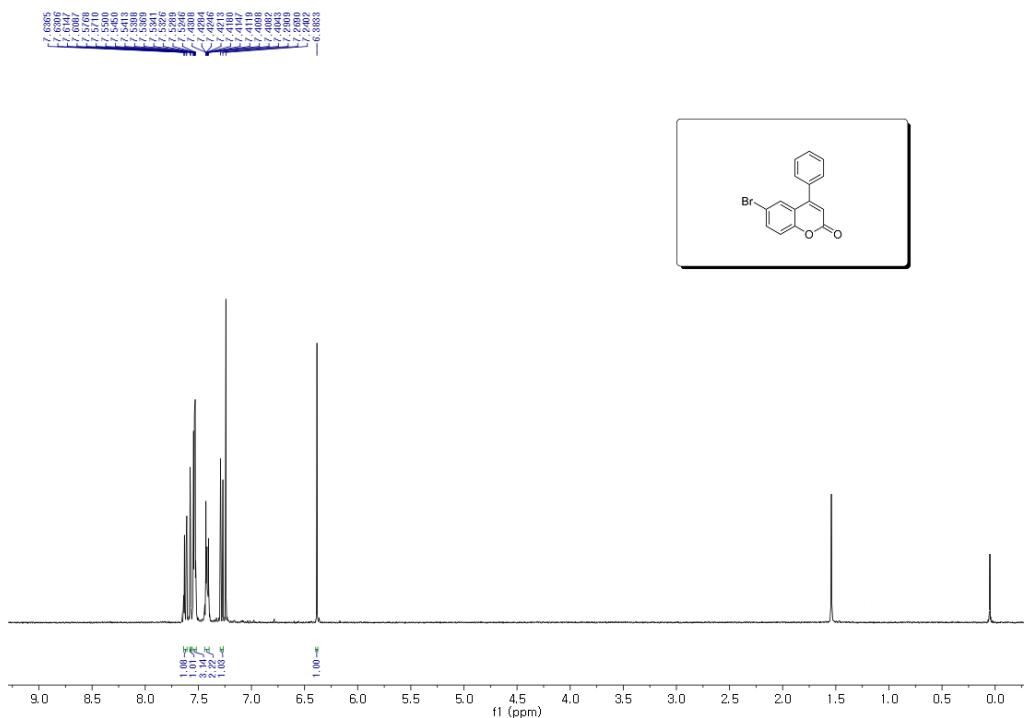


400 MHz, ^1H NMR in CDCl_3

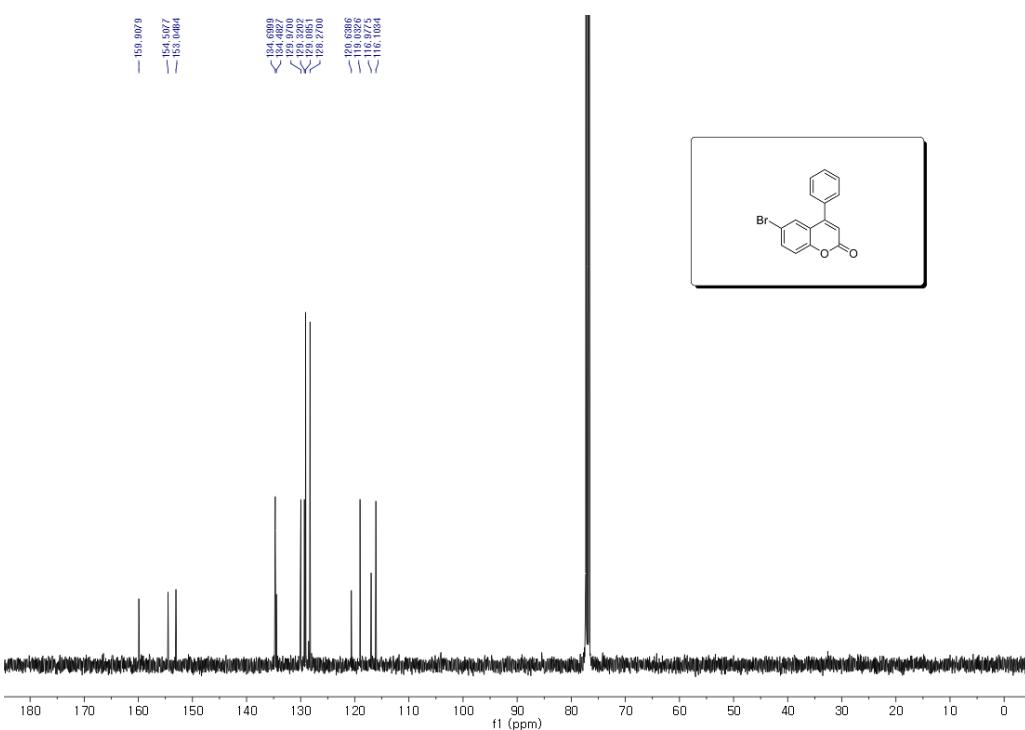


100 MHz, ^{13}C NMR in CDCl_3

6-bromo-4-phenyl-2H-chromen-2-one (2n).

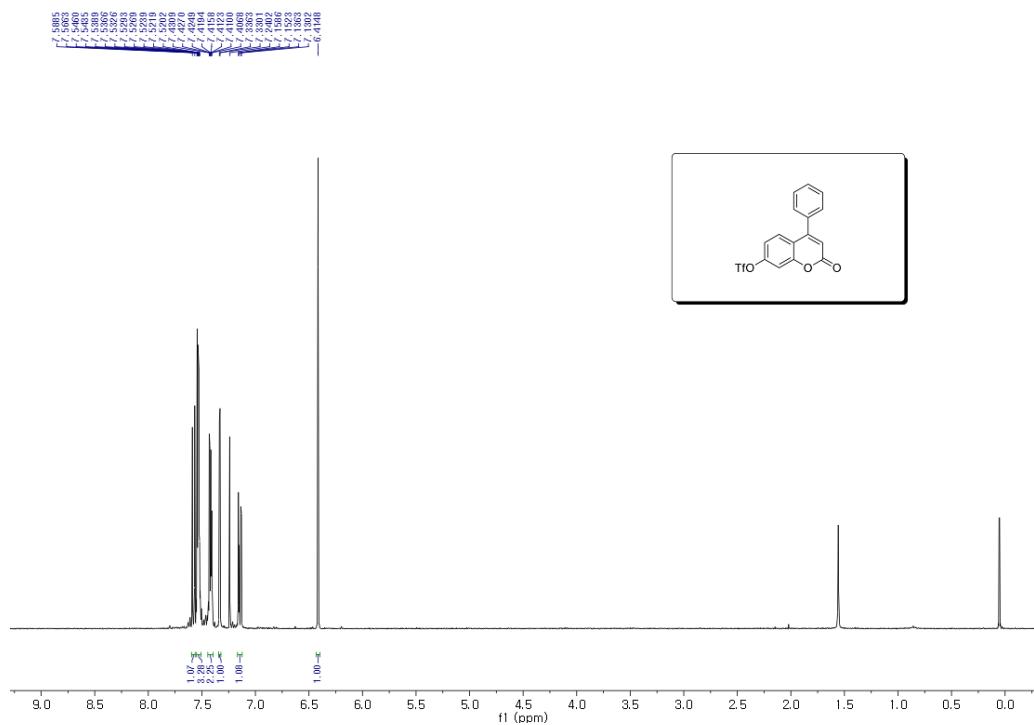


400 MHz, ¹H NMR in CDCl₃

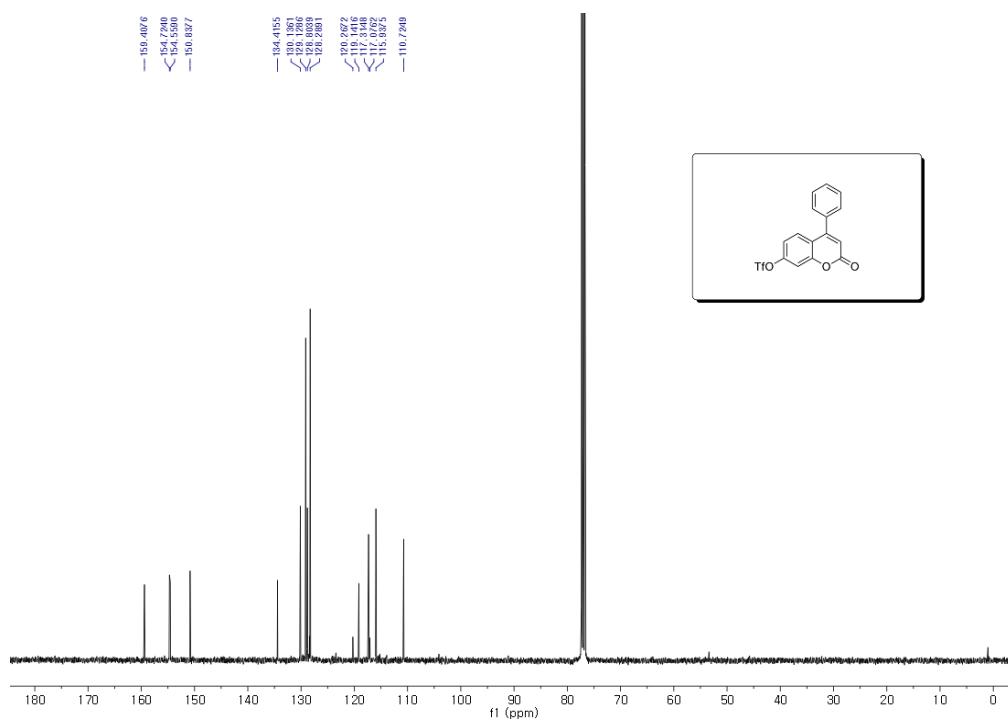


100 MHz, ¹³C NMR in CDCl₃

2-oxo-4-phenyl-2H-chromen-7-yl trifluoromethanesulfonate (2o).

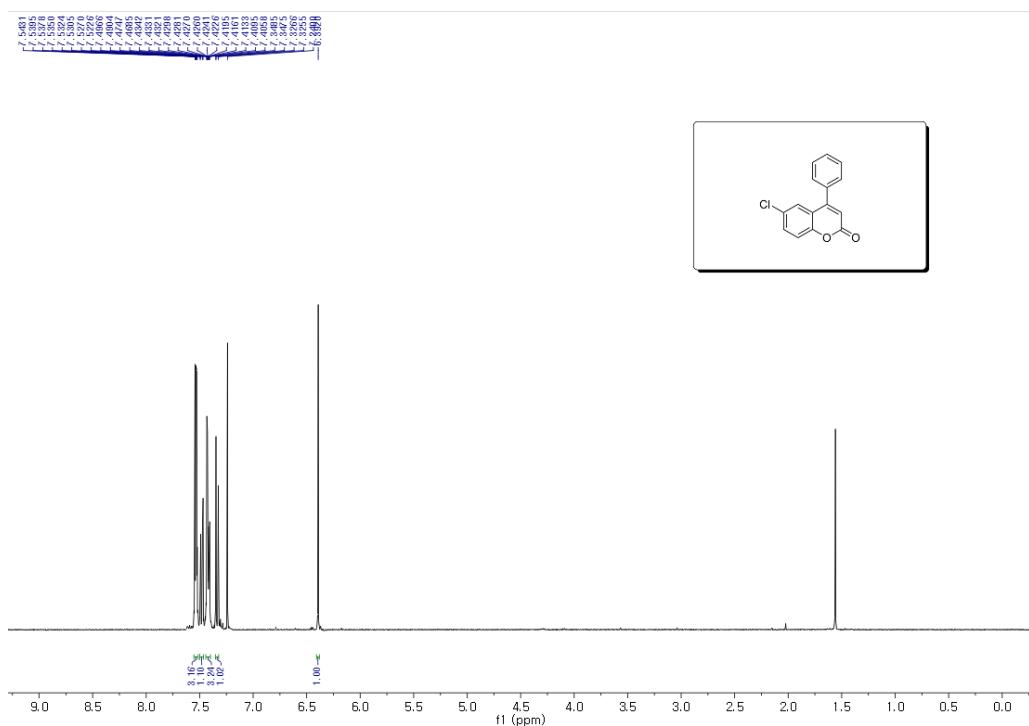


400 MHz, ¹H NMR in CDCl₃

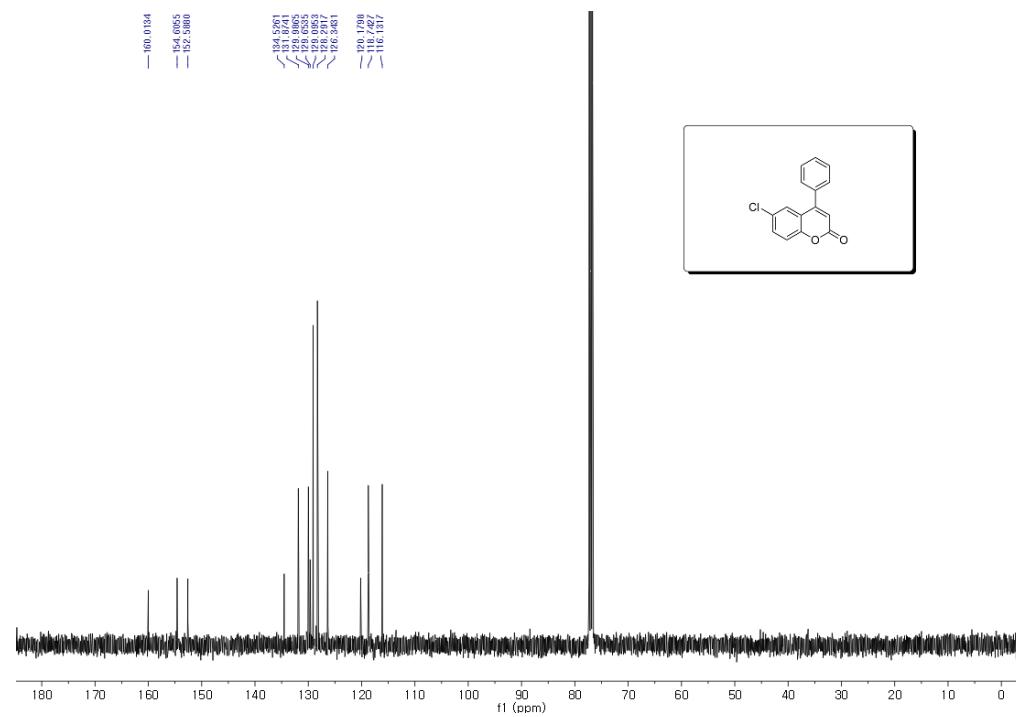


100 MHz, ^{13}C NMR in CDCl_3

6-chloro-4-phenyl-2H-chromen-2-one (2p).

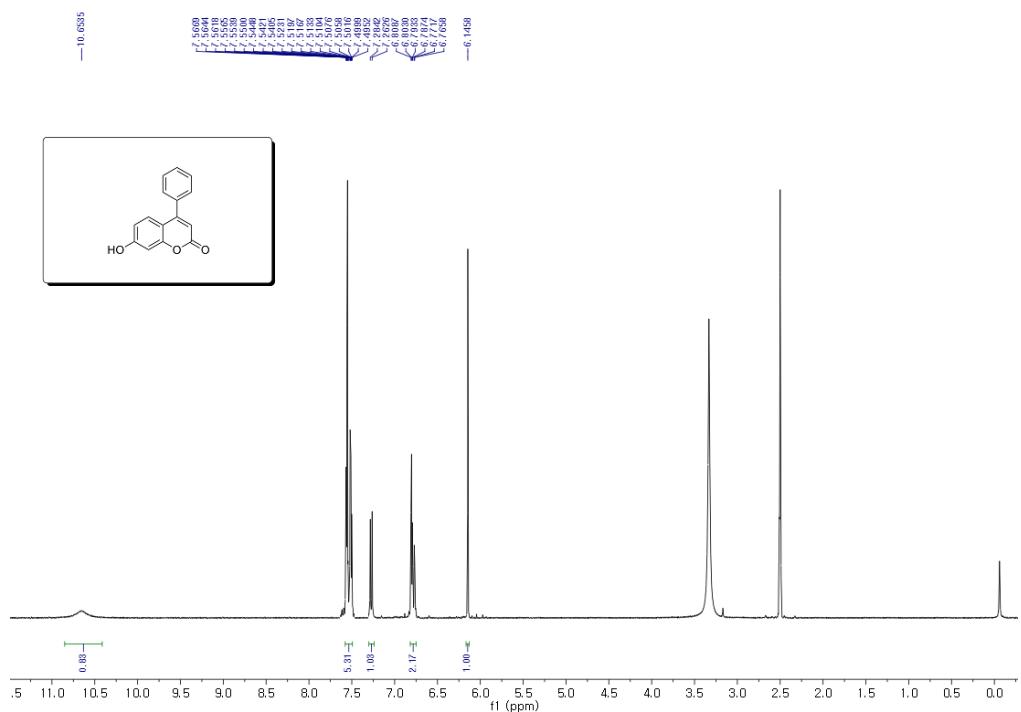


400 MHz, ^1H NMR in CDCl_3

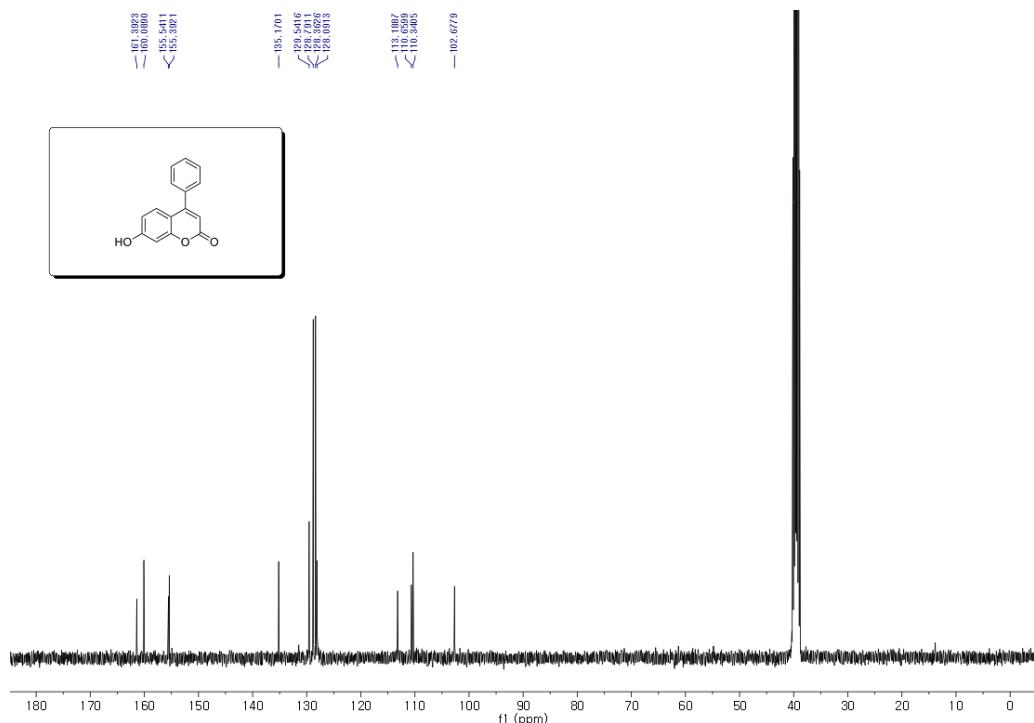


100 MHz, ^{13}C NMR in CDCl_3

7-hydroxy-4-phenyl-2H-chromen-2-one (2q).

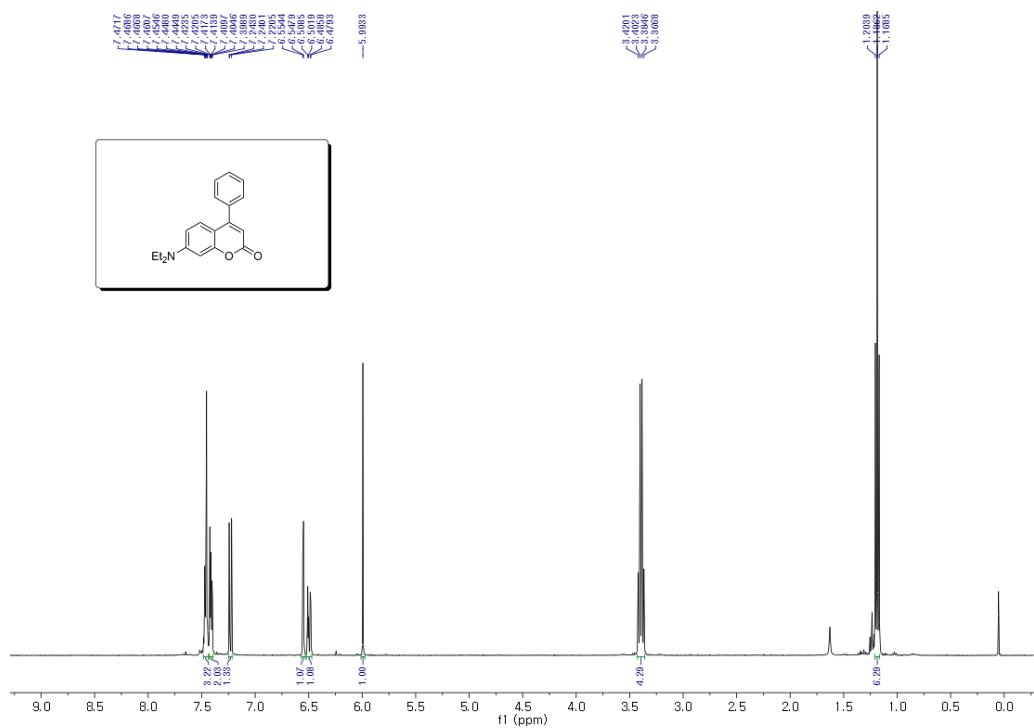


400 MHz, ¹H NMR in DMSO-d₆

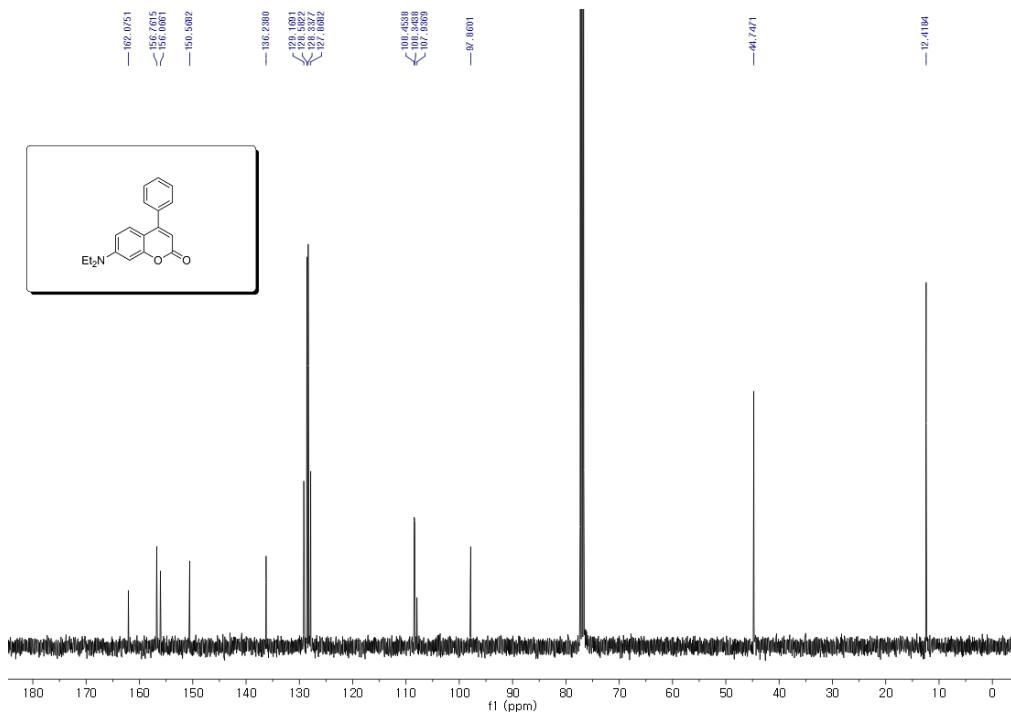


100 MHz, ¹³C NMR in DMSO-d₆

7-(diethylamino)-4-phenyl-2H-chromen-2-one (2r).

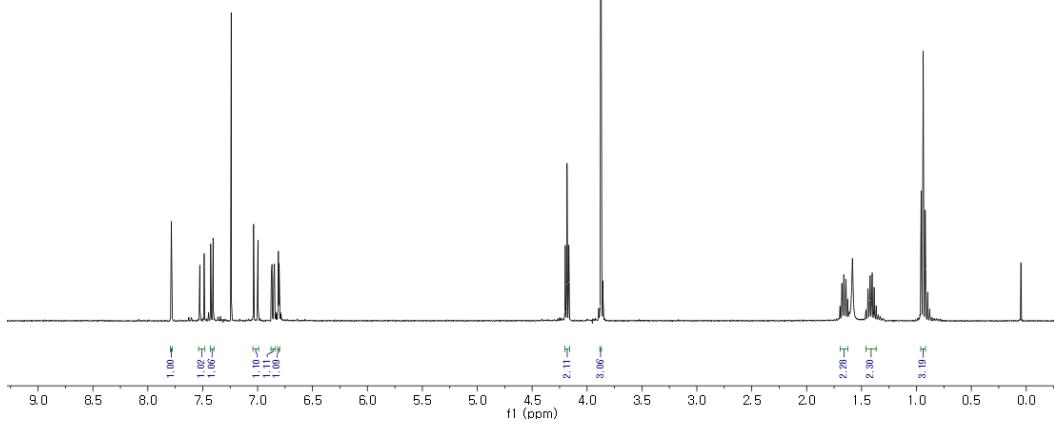
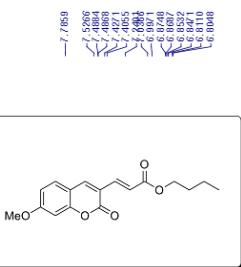


400 MHz, ¹H NMR in CDCl₃

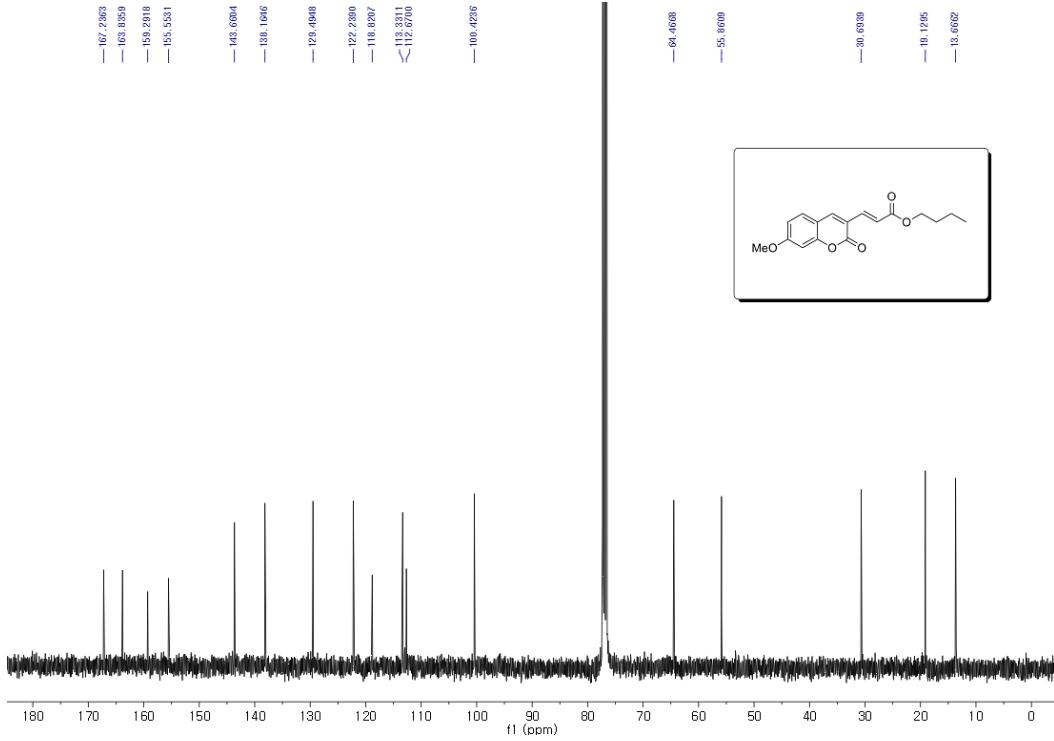
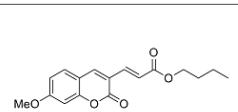


100 MHz, ¹³C NMR in CDCl₃

(E)-butyl 3-(7-methoxy-2-oxo-2H-chromen-3-yl)acrylate (4).



400 MHz, ^1H NMR in CDCl_3



100 MHz, ^{13}C NMR in CDCl_3