Supporting Information

Gold-catalyzed Carboalkoxylations of 2-Ethynylbenzyl Ethers to Form 1- and 3-Substituted 2-Methoxy-1-*H*-indenes: Brønsted Acid Versus Gold Catalysis

Chun-Hao Chen,^a Chiou-Dong Wang,^a Yi-Feng Hsieh and Rai-Shung Liu^{a,*}

Department of Chemistry, National Tsing-Hua University, Hsinchu, Taiwan, ROC

E-mail: *rsliu@mx.nthu.edu.tw*

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(I) Representative Synthetic Procedures:

(a) General procedure:

Unless otherwise noted, all the reactions for the preparation of the substrates were performed in oven-dried glassware under nitrogen atmosphere with freshly distilled solvents. The catalytic reactions were performed under Nitrogen atmosphere. DCE, DCM and CH₃CN were distilled from CaH₂ under nitrogen. THF were distilled from Na metal under nitrogen. All other commercial reagents were used without further purification, unless otherwise indicated. ¹H NMR and ¹³C NMR spectra were recorded on a Varian 400 MHz, Bruker 400 and 600 MHz Spectrometers using chloroform-*d* (CDCl₃) and CD₂Cl₂ as the internal standards. All 2-ethynylbenzyl ethers were prepared from the reported procedure in the literature^[s1]

S1. C.-D. Wang, Y.-F. Hsieh, R.-S. Liu, Adv. Synth. Catal. 2014, 356, 144-152.

(II) Standard procedures for catalytic operations:

(a) Typical procedure for the synthesis of 1-phenyl-2-methoxyindene (2a)



After adding 4 Å molecular sieves (60 mg), a dichloromethane (1.0 mL) solution of AuCl(t-Bu)₂P(o-biphenyl) (6.2 mg, 5 mol %) and NaBARF (10.3 mg, 5 mol %) was stirred at rt for 10 min, and to this solution was slowly added a dichloromethane (1.3 mL) solution of 4-chloro-1-ethynyl-2-(methoxy(phenyl)methyl)benzene (**1a**) (60 mg, 0.2 mmol) at rt. The solution was stirred for 0.5 h before it was filtered over a Celite bed. The solvent was evaporated under reduced pressure, and the residue was purified on a flash silica gel column to give compound **2a** (54 mg, 90% yield) as yellow oil.

(b) Typical procedure for the synthesis of 3-phenyl-2-methoxyindene (2a')



A dichloromethane (1.0 mL) solution of AuCl(t-Bu)₂P(o-biphenyl) (6.2 mg, 5 mol%) and AgNTf₂ (4.4 mg, 5 mol %) was stirred at rt for 10 min, and to this solution slowly added a dichloromethane (1.3)mL) solution was of 4-chloro-1-ethynyl-2-(methoxy(phenyl)methyl)benzene (1a) (60 mg, 0.2 mmol) at rt. The solution was stirred for 3.5 h before it was filtered over a Celite bed. The solvent was evaporated under reduced pressure, and the residue was purified on a flash silica gel column to give compound 2a' (42.6 mg, 0.17 mmol, 71% yield) as yellow oil and **3a** (14.2 mg, 0.06 mmol, 25%) as yellow oil.

(c) Typical procedure for the ozonolysis of 1-phenyl-2-methoxyindene (5a)



A dichloromethane (2.3 ml) solution of compound **2a** (60 mg, 0.2 mmol) was cooled to -78 °C, and to this solution was introduced with a stream of O_3/O_2 (~ 1 mmol/min of O_3) for one min. The solution was stirred at rt for 1 h. The resulting mixture was allowed to reach -78 °C and carefully quenched by addition of DMS (21.8 mg, 0.4 mmol). After 1 h, the solvent was evaporated under reduced pressure, and the residue was purified on a flash silica gel column to give compound **5a** (54.7 mg, 0.19 mmol, 81% yield) as yellow oil.

(d) Typical procedure for the ozonolysis of 3-phenyl-2-methoxyindene (6a)



A dichloromethane (2.3 ml) solution of compound **2a'** (60 mg, 0.2 mmol) was cooled to -78 $^{\circ}$ C, and to this solution was introduced with a stream of O₃/O₂ (~ 1 mmol/min of O₃) for one min. The solution was stirred at rt for 1 h. The resulting mixture was allowed to reach -78 $^{\circ}$ C and carefully quenched by addition of DMS (21.8 mg, 0.4 mmol). After 1 h, the solvent was evaporated under reduced pressure,

and the residue was purified on a flash silica gel column to give compound 6a (52.6 mg, 0.18 mmol, 78% yield) as yellow oil.

(III) Spectral Data:

Spectral data for 4-(*tert*-butyl)-1-ethynyl-2-(methoxy(phenyl)methyl)benzene (1h)



¹H NMR (600 MHz, CDCl₃): δ 7.69 (d, J = 1.8 Hz, 1H), 7.51~7.55 (m, 3H), 7.38~7.40 (m, 2H), 7.30~7.33 (m, 2H), 5.92 (s, 1H), 3.49 (s, 3H), 3.36 (s, 1H), 1.38 (s, 9H); ¹³C NMR (150 MHz, CDCl₃): δ 152.5, 143.9, 141.5, 132.5, 128.1, 127.3, 126.9, 124.2, 122.9, 118.0, 82.4, 82.1, 81.4, 56.9, 34.8, 31.1. HRMS(EI) calcd. for C₂₀H₂₂O: 278.1671, found 278.1667.

Spectral data for 4-chloro-1-ethynyl-2-(methoxy(*p*-tolyl)methyl)benzene (1k)



¹H NMR (600 MHz, CDCl₃): δ 7.65 (d, J = 1.8 Hz, 1H), 7.44 (d, J = 8.4 Hz, 1H), 7.39 (d, J = 7.8 Hz, 2H), 7.22 (dd, J = 8.4, 1.8 Hz, 1H), 7.19 (d, J = 7.8 Hz, 2H), 5.80 (s, 1H), 3.44 (s, 3H), 3.43 (s, 1H), 2.37 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 146.7, 137.6, 137.3, 135.4, 133.9, 129.0, 127.4, 126.8, 126.3, 119.1, 83.1, 81.7, 80.9, 56.9, 21.0. HRMS(EI) calcd. for C₁₇H₁₅ClO: 270.0811, found 270.0818 .

for

Spectral data 4-chloro-2-((4-chlorophenyl)(methoxy)methyl)-1-ethynylbenzene (11)

> CI 1I OMe CI CI

¹H NMR (500 MHz, CDCl₃): δ 7.60 (d, J = 2.0 Hz, 1H), 7.46 (d, J = 8.0 Hz, 1H), 7.43 (d, J = 8.5 Hz, 2H), 7.35 (d, J = 8.5 Hz, 2H), 7.25 (dd, J = 8.0, 2.0 Hz, 1H), 5.81 (s,

1H), 3.46 (s, 1H), 3.44 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): δ 146.0, 139.2, 135.5, 134.0, 133.4, 128.4, 128.2, 127.7, 126.2, 119.1, 83.4, 81.0, 80.8, 56.9. HRMS(EI) calcd. for C₁₆H₁₂Cl₂O: 290.0265, found 290.0280.

Spectral data for 6-chloro-2-methoxy-1-phenyl-1*H*-indene (2a)



¹H NMR (600 MHz, CDCl₃): δ 7.27~7.30 (m, 2H), 7.23~7.26 (m, 1H), 7.05~7.14 (m, 4H), 6.98 (br, 1H), 5.69 (s, 1H), 4.45 (s, 1H), 3.75 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 170.1, 143.4, 142.3, 137.7, 128.8, 128.5, 128.1, 127.3, 127.2, 124.0, 119.8, 98.4, 57.7, 54.7. HRMS(EI) calcd. for C₁₆H₁₃ClO: 256.0655, found 256.0654.

Spectral data for 6-fluoro-2-methoxy-1-phenyl-1*H*-indene (2b)



¹H NMR (600 MHz, CDCl₃): δ 7.28~7.31 (m, 2H), 7.26 (d, J = 7.2 Hz, 1H), 7.11 (d, J = 7.2 Hz, 2H), 7.06 (dd, J = 7.8, 4.8 Hz, 1H), 6.85~6.89 (m, 1H), 6.76 (d, J = 8.4 Hz, 1H), 5.69 (s, 1H), 4.46 (s, 1H), 3.75 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 169.4, 160.2 (d, J = 240.0 Hz), 143.5 (d, J = 7.5 Hz), 139.4, 138.0, 128.8, 128.1, 127.3, 119.3 (d, J = 9.0 Hz), 113.5 (d, J = 21.0 Hz), 111.5 (d, J = 24.0 Hz), 98.2, 57.6, 54.9. HRMS(EI) calcd. for C₁₆H₁₃FO: 240.0950, found 240.0945.

Spectral data for 5-fluoro-2-methoxy-1-phenyl-1*H*-indene (2c)



¹H NMR (600 MHz, CDCl₃): δ 7.26~7.29 (m, 2H), 7.21~7.24 (m, 1H), 7.08~7.09 (m,

2H), 6.92 (dd, J = 8.4, 5.4 Hz, 1H), 6.85 (dd, J = 9.0, 2.4 Hz, 1H), 6.60~6.64 (m, 1H), 5.68 (s, 1H), 4.42 (s, 1H), 3.75 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 171.5, 162.8 (d, J = 241.5 Hz), 145.8 (d, J = 9.0 Hz), 138.3, 137.0, 128.7, 128.1, 127.2, 124.3 (d, J = 9.0 Hz), 109.1 (d, J = 22.5 Hz), 106.5 (d, J = 22.5 Hz), 98.6, 57.7, 54.1. HRMS(EI) calcd. for C₁₆H₁₃FO: 240.0950, found 240.0944.

Spectral data for 5-chloro-2-methoxy-1-phenyl-1*H*-indene (2d)



¹H NMR (600 MHz, CDCl₃): δ 7.26~7.29 (m, 2H), 7.22~7.25 (m, 1H), 7.12 (br, 1H), 7.07~7.08 (m, 2H), 6.91 (d, J = 1.2 Hz, 2H), 5.67 (s, 1H), 4.43 (s, 1H), 3.75 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 171.2, 145.7, 139.9, 138.0, 132.9, 128.8, 128.1, 127.2, 124.4, 122.8, 119.2, 98.3, 57.7, 54.3. HRMS(EI) calcd. for C₁₆H₁₃ClO: 256.0655, found 256.0656.

Spectral data for 5-bromo-2-methoxy-1-phenyl-1*H*-indene (2e)



¹H NMR (600 MHz, CDCl₃): δ 7.21~7.29 (m, 4H), 7.06~7.08 (m, 3H), 6.86 (d, *J* = 7.8 Hz, 1H), 5.66 (s, 1H), 4.40 (s, 1H), 3.75 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 171.1, 146.0, 140.5, 137.8, 128.8, 128.1, 127.3, 125.7, 124.9, 122.1, 121.1, 98.2, 57.7, 54.4. HRMS(EI) calcd. for C₁₆H₁₃BrO: 300.0150, found 300.0155.

Spectral data for 2-methoxy-1-phenyl-1*H*-indene (2f)



¹H NMR (600 MHz, CDCl₃): δ 7.25~7.27 (m, 2H), 7.19~7.22 (m, 1H), 7.15 (br, 2H), 7.09~7.11 (m, 2H), 7.01 (d, J = 7.2 Hz, 1H), 6.93~6.96 (m, 1H), 5.71 (s, 1H), 4.46 (s, 1H), 3.74 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 169.9, 143.8, 141.8, 138.6, 128.7, 128.2, 127.1, 127.0, 123.5, 123.0, 119.0, 99.0, 57.6, 54.7. HRMS(EI) calcd. for C₁₆H₁₄O: 222.1045, found 222.1044.

Spectral data for 2-methoxy-6-methyl-1-phenyl-1*H*-indene (2g)



¹H NMR (600 MHz, CDCl₃): δ 7.26~7.29 (m, 2H), 7.21~7.24 (m, 1H), 7.10~7.12 (m, 2H), 7.05 (d, *J* = 7.2 Hz, 1H), 6.98 (dt, *J* = 7.2, 0.6 Hz, 1H), 6.85 (s, 1H), 5.70 (s, 1H), 4.44 (s, 1H), 3.74 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 169.2, 142.1, 140.9, 138.9, 132.5, 128.7, 128.2, 127.6, 127.0, 124.4, 118.7, 98.8, 57.5, 54.7, 21.3. HRMS(ESI) calcd. for C₁₇H₁₇O⁺ (M+H)⁺ 237.1274, found 237.1277.

Spectral data for 6-(*tert*-butyl)-2-methoxy-1-phenyl-1*H*-indene (2h)



¹H NMR (600 MHz, CDCl₃): δ 7.27~7.29 (m,2H), 7.20~7.24 (m, 2H), 7.13 (dd, J = 7.8, 1.2 Hz, 2H), 7.09 (dd, J = 7.8, 0.6 Hz, 1H), 7.07 (d, J = 1.2 Hz, 1H), 5.68 (s, 1H), 4.46 (s, 1H), 3.73 (s, 3H), 1.23 (s, 9H); ¹³C NMR (150 MHz, CDCl₃): δ 169.5, 146.1, 141.5, 141.1, 138.9, 128.6, 128.3, 126.9, 123.8, 120.8, 118.4, 98.5, 57.5, 54.9, 34.5, 31.6. HRMS(EI) calcd. for C₂₀H₂₂O: 278.1671, found 278.1671.

Spectral data for 2-methoxy-5-methyl-1-phenyl-1*H*-indene (2i)



¹H NMR (600 MHz, CDCl₃): δ 7.27~7.30 (m, 2H), 7.22~7.25 (m, 1H), 7.12~7.13 (m,1H), 7.01 (s, 1H), 6.92 (d, J = 7.8 Hz, 1H), 6.79 (dd, J = 7.8, 1.2 Hz, 1H), 5.70 (s, 1H), 4.46 (s, 1H), 3.76 (s, 3H), 2.34 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 170.1, 143.9, 138.9 (C×2), 136.7, 128.6, 128.1, 126.9, 123.6, 123.2, 119.9, 98.9, 57.5, 54.4, 21.6. HRMS(EI) calcd. for C₁₇H₁₆O: 236.1201, found 236.1200.

Spectral data for 5-(*tert*-butyl)-2-methoxy-1-phenyl-1*H*-indene (2j)



¹H NMR (600 MHz, CDCl₃): δ 7.26~7.28 (m, 2H), 7.20~7.23 (m, 2H), 7.12~7.13 (m, 2H), 6.94~6.99 (m, 2H), 5.72 (s, 1H), 4.44 (s, 1H), 3.75 (s, 3H), 1.31 (s, 9H); ¹³C NMR (150 MHz, CDCl₃): δ 169.9, 150.2, 143.5, 138.9, 138.8, 128.6, 128.2, 126.9, 122.9, 119.9, 116.3, 99.2, 57.5, 54.4, 34.7, 31.6. HRMS(EI) calcd. for $C_{20}H_{22}O$: 278.1671, found 278.1673.

Spectral data for 6-chloro-2-methoxy-1-(*p*-tolyl)-1*H*-indene (2k)



¹H NMR (600 MHz, CDCl₃): δ 7.14 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.12 (d, *J* = 7.8 Hz, 2H), 7.07 (d, *J* = 8.4 Hz, 1H), 6.99~7.00 (m, 3H), 5.69 (s, 1H), 4.43 (s, 1H), 3.76 (s, 3H), 2.33 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 170.2, 143.6, 142.2, 136.9, 134.6, 129.5, 128.4, 128.0, 127.1, 123.9, 119.8, 98.2, 57.2, 54.4, 21.1. HRMS(EI) calcd. for C₁₇H₁₅ClO: 270.0811, found 270.0816.

Spectral data for 6-chloro-1-(4-chlorophenyl)-2-methoxy-1*H*-indene (2l)



¹H NMR (500 MHz, CDCl₃): δ 7.25 (d, J = 8.5 Hz, 2H), 7.14 (dd, J = 8.5, 1.5 Hz, 1H), 7.05 (d, J = 8.5 Hz, 1H), 7.01 (d, J = 8.5 Hz, 2H), 6.95 (br, 1H), 5.68 (s, 1H), 4.41 (s, 1H), 3.74 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): δ 169.6, 142.9, 142.2, 136.3, 133.1, 129.5, 129.0, 128.6, 127.4, 123.9, 120.0, 98.5, 57.7, 54.0. HRMS(EI) calcd. for C₁₆H₁₂Cl₂O: 290.0265, found 290.0273.

Spectral data for 5-chloro-2-methoxy-3-phenyl-1*H*-indene (2a')



¹H NMR (600 MHz, CDCl₃): δ 7.51~7.53 (m, 2H), 7.41~7.44 (m, 2H), 7.28~7.31 (m, 1H), 7.22~7.25 (m, 2H), 7.03 (dd, J = 7.8, 1.8 Hz, 1H), 3.82 (s, 3H), 3.55 (s, 2H); ¹³C NMR (150 MHz, CDCl₃): δ 161.7, 147.1, 133.6, 133.1, 132.8, 128.7, 128.4, 126.9, 124.2, 122.5, 118.5, 116.4, 57.9, 34.8. HRMS(EI) calcd. for C₁₆H₁₃ClO: 256.0655, found 256.0648.

Spectral data for 5-fluoro-2-methoxy-3-phenyl-1H-indene (2b')



¹H NMR (600 MHz, CDCl₃): δ 7.52~7.54 (m, 2H), 7.41~7.43 (m, 2H), 7.23~7.30 (m, 2H), 7.00 (dd, J = 9.6, 2.4 Hz, 1H), 6.72~6.76 (m, 1H), 3.83 (s, 3H), 3.55 (s, 2H); ¹³C NMR (150 MHz, CDCl₃): δ 162.8 (d, J = 240.0 Hz), 162.1, 147.3 (d, J = 9.0 Hz), 133.3, 130.6, 128.6, 128.4, 126.8, 124.1 (d, J = 9.0 Hz), 116.7, 109.0 (d, J = 22.5 Hz), 105.9 (d, J = 24.0 Hz), 57.8, 34.6. HRMS(EI) calcd. for C₁₆H₁₃FO: 240.0950, found

240.0955.

Spectral data for 6-fluoro-2-methoxy-3-phenyl-1*H*-indene (2c')



¹H NMR (600 MHz, CDCl₃): δ 7.54 (dt, J = 7.8, 1.8 Hz, 2H), 7.40~7.42 (m, 2H), 7.26~7.29 (m, 1H), 7.20 (dd, J = 8.4, 4.8 Hz, 1H), 7.07 (dt, J = 8.4, 1.2 Hz, 1H), 6.91 (td, J = 9.0, 2.4 Hz, 1H), 3.81 (s, 3H), 3.57 (s, 2H); ¹³C NMR (150 MHz, CDCl₃): δ 160.1 (d, J = 238.5 Hz), 159.5, 140.9, 137.2 (d, J = 7.5 Hz), 133.6, 128.7, 128.3, 126.7, 118.8 (d, J = 7.5 Hz), 116.4,.113.1 (d, J = 21.0 Hz), 111.3 (d, J = 24.0 Hz), 57.9, 35.2. HRMS(EI) calcd. for C₁₆H₁₃FO: 240.0950, found 240.0953.

Spectral data for 6-chloro-2-methoxy-3-phenyl-1*H*-indene (2d')



¹H NMR (600 MHz, CDCl₃): δ 7.52~7.54 (m, 2H), 7.42 (tt, J = 7.8, 1.2 Hz, 2H), 7.31 (br, 1H), 7.27~7.30 (m, 1H), 7.17~7.22 (m, 2H), 3.82 (s, 3H), 3.57 (s, 2H); ¹³C NMR (150 MHz, CDCl₃): δ 160.4, 143.7, 137.1, 133.3, 128.7, 128.4, 128.2, 126.8, 126.7, 123.7, 119.1, 116.4, 57.9, 35.0. HRMS(EI) calcd. for C₁₆H₁₃ClO: 256.0655, found 256.0652.

Spectral data for 6-bromo-2-methoxy-3-phenyl-1H-indene (2e')



¹H NMR (600 MHz, CDCl₃): δ 7.52~7.53 (m, 2H), 7.45 (d, *J* = 0.6 Hz, 1H), 7.41 (td, *J* = 7.8, 1.8 Hz, 2H), 7.33 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.28 (tt, *J* = 7.2, 1.2 Hz, 1H), 7.16

(d, J = 8.4 Hz, 1H), 3.82 (s, 3H), 3.56 (s, 2H); ¹³C NMR (150 MHz, CDCl₃): δ 160.4, 144.2, 137.4, 133.3, 129.6, 128.7, 128.4, 126.8, 126.5, 119.6, 116.4, 116.0, 57.9, 34.9. HRMS(EI) calcd. for C₁₆H₁₃BrO: 300.0150, found 300.0143.

Spectral data for 2-methoxy-3-phenyl-1*H*-indene (2f')



¹H NMR (600 MHz, CDCl₃): δ 7.57 (dd, J = 7.2, 1.2 Hz, 2H), 7.41 (t, J = 7.8 Hz, 2H), 7.35 (dd, J = 7.2, 0.6 Hz, 1H), 7.32 (d, J = 7.8 Hz, 1H), 7.28 (td, J = 7.2, 1.2 Hz, 1H), 7.22 (t, J = 7.8 Hz, 1H), 7.08 (td, J = 7.8, 1.2 Hz, 1H), 3.83 (s, 3H), 3.59 (s, 2H); ¹³C NMR (150 MHz, CDCl₃): δ 160.4, 145.2, 135.5, 133.8, 128.8, 128.3, 126.7, 126.6, 123.4, 122.7, 118.4, 116.9, 57.8, 35.1. HRMS(EI) calcd. for C₁₆H₁₄O: 222.1045, found 222.1047.

Spectral data for 2-methoxy-5-methyl-3-phenyl-1*H*-indene (2g')



¹H NMR (600 MHz, CDCl₃): δ 7.56 (dd, J = 7.8, 1.2 Hz, 2H), 7.41~7.43 (m, 2H), 7.28 (td, J = 7.2, 1.2 Hz, 1H), 7.23 (d, J = 7.2 Hz, 1H), 7.12 (s, 1H), 6.89 (d, J = 7.2 Hz, 1H), 3.81 (s, 3H), 3.55 (s, 2H), 2.33 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 160.7, 145.3, 136.3, 133.9, 132.5, 128.9, 128.3, 126.5, 123.4, 123.1, 119.2, 116.9, 57.8, 34.8, 21.7. HRMS(EI) calcd. for C₁₇H₁₇O: 236.1201, found 236.1205.

Spectral data for 5-(tert-butyl)-2-methoxy-3-phenyl-1H-indene (2h')



¹H NMR (600 MHz, CDCl₃): δ 7.57 (dd, J = 7.8, 1.2 Hz, 2H), 7.42~7.45 (m, 2H), 7.37 (d, J = 1.8 Hz, 1H), 7.27~7.30 (m, 2H), 7.13 (dd, J = 7.8, 1.8 Hz, 1H), 3.81 (s, 3H), 3.55 (s, 2H), 1.30 (s, 9H); ¹³C NMR (150 MHz, CDCl₃): δ 160.6., 149.9, 144.9, 133.9, 132.7, 128.8, 128.3, 126.5, 122.9, 119.7, 117.2, 115.5, 57.7, 34.8, 34.6, 31.6. HRMS(EI) calcd. for C₂₀H₂₂O: 278.1671, found 278.1669.

Spectral data for 2-methoxy-6-methyl-3-phenyl-1*H*-indene (2i')



¹H NMR (600 MHz, CDCl₃): δ 7.57 (dd, J = 8.4, 1.2 Hz, 2H), 7.39~7.42 (m, 2H), 7.25~7.28 (m, 1H), 7.21 (d, J = 7.2 Hz, 1H), 7.18 (br, 1H), 7.03 (d, J = 7.8 Hz, 1H), 3.81 (s, 3H), 3.55 (s, 2H), 2.35 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 159.5, 142.2, 135.7, 133.9, 132.2, 128.7, 128.2, 127.1, 126.4, 124.3, 118.0, 116.7, 57.7, 34.9, 21.2. HRMS(EI) calcd. for C₁₇H₁₆O: 236.1201, found 236.1199.

Spectral data for 6-(tert-butyl)-2-methoxy-3-phenyl-1H-indene (2j')



¹H NMR (600 MHz, CDCl₃): δ 7.56~7.58 (m, 2H), 7.39~7.42 (m, 3H), 7.25~7.28 (m, 3H), 3.81 (s, 3H), 3.58 (s, 2H), 1.33 (s, 9H); ¹³C NMR (150 MHz, CDCl₃): δ 159.9, 145.9, 142.5, 135.5, 134.0, 128.7, 128.2, 126.5, 123.4, 120.7, 117.9, 116.8, 57.8, 35.2, 34.5, 31.6. HRMS(EI) calcd. for C₂₀H₂₂O: 278.1671, found 278.1664.

Spectral data for 5-chloro-2-methoxy-3-(p-tolyl)-1H-indene (2k')



¹H NMR (500 MHz, CDCl₃): δ 7.41 (d, J = 8.0 Hz, 2H), 7.21~7.24 (m, 4H), 7.01 (dd, J = 7.8, 1.9 Hz, 1H), 3.81 (s, 3H), 3.52 (s, 2H), 2.37 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): δ 161.4, 147.3, 136.6, 133.6, 132.8, 130.1, 129.1, 128.6, 124.2, 122.4, 118.5, 116.3, 57.8, 34.7, 21.3. HRMS(EI) calcd. for C₁₇H₁₅ClO: 270.0811, found 270.0822.

Spectral data for 5-chloro-3-(4-chlorophenyl)-2-methoxy-1H-indene (2l')



¹H NMR (600 MHz, CDCl₃): δ 7.47 (d, J = 8.4 Hz, 2H), 7.39 (d, J = 8.4 Hz, 2H), 7.23 (d, J = 7.8 Hz, 1H), 7.22 (d, J = 1.8 Hz, 1H), 7.04 (dd. J = 7.8, 1.8 Hz, 1H), 3.84 (s, 3H), 3.55 (s, 2H); ¹³C NMR (150 MHz, CDCl₃): δ 162.1, 146.6, 133.4, 132.9, 132.4, 131.6, 130.0, 128.6, 124.4, 122.7, 118.4, 115.3, 57.9, 34.7. HRMS(EI) calcd. for C₁₆H₁₂Cl₂O: 290.0265, found 290.0260.

Spectral data for 6-(*tert*-butyl)-1-phenyl-1*H*-inden-2(3*H*)-one (3h)



¹H NMR (600 MHz, CDCl₃): δ 7.38 (dd, J = 7.8, 1.8 Hz, 1H), 7.30~7.33 (m, 3H), 7.25~7.27 (m, 1H), 7.21 (br, 1H), 7.11 (dd, J = 7.8, 1.2 Hz, 2H), 4.65 (s, 1H), 3.61 (s, 2H), 1.28 (s, 9H); ¹³C NMR (150 MHz, CDCl₃): δ 214.2, 151.2, 140.8, 138.2, 134.3, 128.7, 128.4, 127.2, 125.2, 124.4, 122.8, 60.0, 42.6, 34.8, 31.4. HRMS(EI) calcd. for C₁₉H₂₀O: 264.1514, found 264.1508.

Spectral data for 6-chloro-1-(p-tolyl)-1H-inden-2(3H)-one (3k)



¹H NMR (600 MHz, CDCl₃): δ 7.29~7.30 (m, 2H), 7.15~7.16 (m, 1H), 7.13 (d, J = 7.8 Hz, 2H), 6.96 (d, J = 7.8 Hz, 2H), 4.60 (s, 1H), 3.60 (s, 2H), 2.31 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 213.0, 143.4, 137.4, 135.5, 134.4, 133.6, 129.6, 128.3 (CH×2), 126.1 (CH×2), 59.5, 42.4, 21.1. HRMS(EI) calcd. for C₁₆H₁₃ClO: 256.0655, found 256.0648.

Spectral data for 6-chloro-1-(4-chlorophenyl)-1*H*-inden-2(3*H*)-one (3l)



¹H NMR (500 MHz, CDCl₃): δ 7.31 (br, 2H), 7.29 (d, J = 8.5 Hz, 2H), 7.14 (br, 1H), 7.01 (d, J = 8.5 Hz, 2H), 4.61 (s, 1H), 3.61 (s, 2H); ¹³C NMR (125 MHz, CDCl₃): δ 212.2, 142.4, 135.7, 135.5, 133.7, 133.6, 129.7, 129.1, 128.6, 126.2, 126.1, 59.0, 42.4. HRMS(EI) calcd. for C₁₅H₁₀Cl₂O: 276.0109, found 276.0099.

Spectral data for methyl 2-(5-chloro-2-formylphenyl)-2-phenylacetate (5a)



¹H NMR (600 MHz, CDCl₃): δ 10.05 (s, 1H), 7.75 (d, J = 8.4 Hz, 1H), 7.44 (dd, J = 7.8, 1.8 Hz, 1H), 7.35~7.38 (m, 2H), 7.30~7.33 (m, 1H), 7.23~7.24 (m, 2H), 7.15 (d, J = 1.8 Hz, 1H), 6.00 (s, 1H), 3.73 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 192.0, 172.3, 141.9, 140.5, 136.8, 136.2, 132.1, 130.8, 129.1, 129.0, 128.0, 127.8, 52.5 (CH₃×1, CH×1). HRMS(ESI) calcd. for C₁₆H₁₃ClNaO₃⁺ (M+Na)⁺ 311.0445, found 311.0446.

Spectral data for methyl 2-(5-fluoro-2-formylphenyl)-2-phenylacetate (5b)



¹H NMR (600 MHz, CDCl₃): δ 10.04 (s, 1H), 7.83 (dd, J = 8.4, 6.0 Hz, 1H), 7.30~7.38 (m, 3H), 7.24~7.25 (m, 2H), 7.11~7.15 (m, 1H), 6.87 (dd, J = 10.2, 2.4 Hz, 1H), 6.03 (s, 1H), 3.73 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 191.7, 172.3, 165.7 (d, J = 256.5 Hz), 143.6 (d, J = 9.0 Hz), 137.8 (d, J = 10.5 Hz), 136.8, 130.4, 129.0 (CH×2), 127.8, 118.2 (d, J = 24.0 Hz), 114.7 (d, J = 21.0 Hz), 52.7, 52.5. HRMS(ESI) calcd. for C₁₆H₁₃FNaO₃⁺ (M+Na)⁺ 295.0741, found 295.0742.

Spectral data for methyl 2-(4-fluoro-2-formylphenyl)-2-phenylacetate (5c)



¹H NMR (600 MHz, CDCl₃): δ 10.07 (s, 1H), 7.52 (dt, J = 9.0, 1.8 Hz, 1H), 7.34~7.36 (m, 2H), 7.28~7.31 (m, 1H), 7.21~7.23 (m, 2H), 7.19 (dd, J = 6.6, 1.8 Hz, 2H), 5.95 (s, 1H), 3.73 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 191.6, 172.7, 161.9,(d, J = 247.5 Hz), 137.4, 135.9 (d, J = 3.0 Hz), 135.3 (d, J = 6.0 Hz), 132.5 (d, J = 7.5 Hz), 128.9 (CH×2), 127.7, 120.6 (d, J = 21.0 Hz), 120.4 (d, J = 22.5 Hz), 52.5, 52.2. HRMS(ESI) calcd. for C₁₆H₁₃FNaO₃⁺ (M+Na)⁺ 295.0741, found 295.0745.

Spectral data for methyl 2-(4-chloro-2-formylphenyl)-2-phenylacetate (5d)



¹H NMR (600 MHz, CDCl₃): δ 10.05 (s, 1H), 7.78 (d, J = 1.8 Hz, 1H), 7.45 (dd, J = 8.4, 2.4 Hz, 1H), 7.34~7.36 (m, 2H), 7.29~7.31 (m, 1H), 7.21~7.22 (m, 2H), 7.13 (d, J = 8.4 Hz, 1H), 5.95 (s, 1H), 3.73 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 191.8, 172.5, 138.4, 137.1, 135.0, 134.2, 134.0, 133.6, 132.0, 129.0, 128.9, 127.7, 52.5, 52.3. HRMS(ESI) calcd. for C₁₆H₁₃ClNaO₃⁺ (M+Na)⁺ 311.0445, found 311.0445.

Spectral data for methyl 2-(4-bromo-2-formylphenyl)-2-phenylacetate (5e)



¹H NMR (600 MHz, CDCl₃): δ 10.04 (s, 1H), 7.93 (d, J = 2.4 Hz, 1H), 7.60 (dd, J = 8.4, 2.4 Hz, 1H), 7.34~7.36 (m, 2H), 7.29~7.31 (m, 1H), 7.20~7.22 (m, 2H), 7.06 (d, J = 7.8 Hz, 1H), 5.94 (s, 1H), 3.73 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 191.7, 172.4, 138.9, 137.2, 137.1, 136.6, 135.2, 132.3, 129.0 (CH×2), 127.7, 121.8, 52.5, 52.4. HRMS(ESI) calcd. for C₁₆H₁₃BrNaO₃⁺ (M+Na)⁺ 354.9940, found 354.9944.

Spectral data for methyl 2-(2-formylphenyl)-2-phenylacetate (5f)



¹H NMR (600 MHz, CDCl₃): δ 10.09 (s, 1H), 7.80 (dd, J = 7.2, 1.8 Hz, 1H), 7.44~7.50 (m, 2H), 7.31~7.34 (m, 2H), 7.27 (tt, J = 7.2, 1.2 Hz, 1H), 7.22~7.24 (m, 2H), 7.18 (d, J = 7.2 Hz, 1H), 6.04 (s, 1H), 3.71 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 193.3, 172.9, 140.0, 137.6, 135.1, 133.8, 133.7, 130.4, 129.1, 128.8, 127.7, 127.5, 52.7, 52.4. HRMS(ESI) calcd. for C₁₆H₁₄NaO₃⁺ (M+Na)⁺ 277.0835, found 277.0839.

Spectral data for methyl 2-(2-formyl-5-methylphenyl)-2-phenylacetate (5g)



¹H NMR (600 MHz, CDCl₃): δ 10.04 (s, 1H), 7.69 (d, J = 7.8 Hz, 1H), 7.34 (t, J = 7.8 Hz, 2H), 7.24~7.29 (m, 4H), 7.00 (s, 1H), 6.07 (s, 1H), 3.73 (s, 3H), 2.33 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 192.9, 173.0, 144.9, 139.9, 137.6, 135.5, 131.4, 131.1, 129.1, 128.7, 128.4, 127.4, 52.5, 52.3, 22.0. HRMS(ESI) calcd. for C₁₇H₁₆NaO₃⁺ (M+Na)⁺ 291.0992, found 291.0991.

Spectral data for methyl 2-(5-(tert-butyl)-2-formylphenyl)-2-phenylacetate (5h)



¹H NMR (600 MHz, CDCl₃): δ 10.04 (s, 1H), 7.73 (d, J = 7.8 Hz, 1H), 7.46 (dd, J = 7.8, 1.8 Hz, 1H), 7.33~7.35 (m, 2H), 7.25~7.29 (m, 3H), 7.23 (d, J = 1.8 Hz, 1H), 6.05 (s, 1H), 3.73 (s, 3H), 1.22 (s, 9H); ¹³C NMR (150 MHz, CDCl₃): δ 192.9, 173.0, 157.6, 139.6, 137.8, 135.3, 131.3, 129.1, 128.7, 127.8, 127.4, 124.5, 52.9, 52.3, 35.3, 30.9. HRMS(ESI) calcd. for C₂₀H₂₂NaO₃⁺ (M+Na)⁺ 333.1461, found 333.1465.

Spectral data for methyl 2-(2-formyl-4-methylphenyl)-2-phenylacetate (5i)



¹H NMR (600 MHz, CDCl₃): δ 10.06 (s, 1H), 7.61 (br, 1H), 7.26~7.34 (m, 4H), 7.24 (d, J = 7.2 Hz, 2H), 7.08 (d, J = 7.8 Hz, 1H), 6.01 (s, 1H), 3.72 (s, 3H), 2.40 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 193.5, 173.0, 137.8, 137.6, 137.1, 135.7, 134.5, 133.5,

130.3, 129.0, 128.8, 127.4, 52.4, 52.3, 20.7. HRMS(ESI) calcd. for $C_{17}H_{16}NaO_3^+$ (M+Na)⁺ 291.0992, found 291.0993.

Spectral data for methyl 2-(4-(tert-butyl)-2-formylphenyl)-2-phenylacetate (5j)



¹H NMR (600 MHz, CDCl₃): δ 10.10 (s, 1H), 7.81 (d, J = 2.4 Hz, 1H), 7.51 (dd, J = 7.8, 2.4 Hz, 1H), 7.33~7.35 (m, 2H), 7.27~7.30 (m, 1H), 7.24~7.26 (m, 2H), 7.09 (d, J = 8.4 Hz, 1H), 6.00 (s, 1H), 3.73 (s, 3H), 1.32(s, 9H); ¹³C NMR (150 MHz, CDCl₃): δ 193.8, 173.1, 150.8, 137.8, 137.1, 133.3, 132.3, 130.9, 130.2, 129.1, 128.8, 127.4, 52.4, 52.3, 34.5, 31.1. HRMS(ESI) calcd. for C₂₀H₂₂NaO₃⁺ (M+Na)⁺ 333.1461, found 333.1463.

Spectral data for methyl 2-(5-chloro-2-formylphenyl)-2-(p-tolyl)acetate (5k)



¹H NMR (600 MHz, CDCl₃): δ 10.05 (s, 1H), 7.74 (d, J = 8.4 Hz, 1H), 7.43 (dd, J = 8.4, 1.8 Hz, 1H), 7.16~7.18 (m, 3H), 7.12 (d, J = 7.8 Hz, 2H), 5.94 (s, 1H), 3.72 (s, 3H), 2.34 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 192.0, 172.5, 142.1, 140.5, 137.6, 136.0, 133.7, 132.1, 130.7, 129.8, 128.9, 127.9, 52.5, 52.2, 21.1. HRMS(ESI) calcd. for C₁₇H₁₆ClO₃⁺ (M+H)⁺ 303.0782, found 303.0783.

Spectral data for methyl 2-(5-chloro-2-formylphenyl)-2-(4-chlorophenyl)acetate (51)



¹H NMR (600 MHz, CDCl₃): δ 10.02 (s, 1H), 7.74 (d, J = 7.8 Hz, 1H), 7.47 (dd, J = 7.8, 1.8 Hz, 1H), 7.33 (d, J = 8.4 Hz, 2H), 7.18 (d, J = 8.4 Hz, 2H), 7.17 (d, J = 1.8 Hz, 1H), 6.02 (s, 1H), 3.73 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 192.0, 172.0, 141.3, 140.6, 136.6, 135.3, 133.9, 132.0, 130.6, 130.4, 129.2, 128.2, 52.6, 51.7. HRMS(ESI) calcd. for C₁₆H₁₃Cl₂O₃⁺ (M+H)⁺ 323.0236, found 323.0235.

Spectral data for methyl 2-(2-benzoyl-4-chlorophenyl)acetate (6a)



¹H NMR (600 MHz, CDCl₃): δ 7.79 (dd, J = 8.4, 1.8 Hz, 2H), 7.58~7.61 (m, 1H), 7.45~7.48 (m, 2H), 7.43 (dd, J = 8.4, 2.4 Hz, 1H), 7.35 (d, J = 2.4 Hz, 1H), 7.29 (d, J = 8.4 Hz, 1H), 3.82 (s, 2H), 3.53 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 196.5, 171.2, 139.9, 137.0, 133.4, 133.1, 132.7, 132.2, 130.8, 130.3, 129.6, 128.5, 52.0, 38.0. HRMS(ESI) calcd. for C₁₆H₁₄ClO₃⁺ (M+H)⁺ 289.0626, found 289.0627.

Spectral data for methyl 2-(2-benzoyl-4-fluorophenyl)acetate (6b)



¹H NMR (600 MHz, CDCl₃): δ 7.78~7.80 (m, 2H), 7.57~7.60 (m, 1H), 7.45~7.47 (m, 2H), 7.32 (dd, J = 8.4, 5.4 Hz, 1H), 7.16 (td, J = 8.4, 3.0 Hz, 1H), 7.08 (dd, J = 8.4, 3.0 Hz, 1H), 3.82 (s, 2H), 3.53 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 196.6, 171.4, 160.9 (d, J = 247.5 Hz), 140.0 (d, J = 6.0 Hz), 137.0, 133.4 (d, J = 7.5 Hz), 133.3,

130.3, 129.6, 128.5, 117.7 (d, J = 21.0 Hz), 116.8 (d, J = 24.0 Hz), 51.9, 37.8. HRMS(ESI) calcd. for $C_{16}H_{13}FNaO_3^+$ (M+Na)⁺ 295.0741, found, 295.0740.

Spectral data for methyl 2-(2-benzoyl-5-fluorophenyl)acetate (6c)



¹H NMR (600 MHz, CDCl₃): δ 7.75~7.77 (m, 2H), 7.56~7.59 (m, 1H), 7.45 (t, J = 7.8 Hz, 2H), 7.40 (dd, J = 8.4, 6.0 Hz, 1H), 7.07 (dd, J = 9.0, 3.0 Hz, 1H), 7.01 (td, J = 8.4, 3.0 Hz, 1H), 3.89 (s, 2H), 3.57 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 196.9, 171.1, 163.7 (d, J = 252.0 Hz), 137.8, 137.4 (d, J = 7.5 Hz), 134.3, 133.0, 132.6 (d, J = 9.0 Hz), 130.2, 128.4, 119.0 (d, J = 22.5 Hz), 113.4 (d, J = 21.0 Hz), 52.0, 38.7. HRMS(ESI) calcd. for C₁₆H₁₃FNaO₃⁺ (M+Na)⁺ 295.0741, found 295.0743.

Spectral data for methyl 2-(2-benzoyl-5-chlorophenyl)acetate (6d)



¹H NMR (600 MHz, CDCl₃): δ 7.76~7.77 (m, 2H), 7.56~7.59 (m, 1H), 7.44~7.46(m, 2H), 7.29~7.35 (m, 3H), 3.86 (s, 2H), 3.56 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 197.0, 171.0, 137.5, 136.9, 136.6, 136.1, 133.1, 131.9, 131.4, 130.3, 128.4, 126.7, 52.0, 38.4. HRMS(ESI) calcd. for C₁₆H₁₃ClNaO₃⁺ (M+Na)⁺ 311.0445, found 311.0448.

Spectral data for methyl 2-(2-benzoyl-5-bromophenyl)acetate (6e)



¹H NMR (600 MHz, CDCl₃): δ 7.76 (dd, J = 8.4, 1.2 Hz, 2H), 7.56~7.59 (m, 1H),

7.51 (d, J = 1.8 Hz, 1H), 7.44~7.47 (m, 3H), 7.26 (d, J = 8.4 Hz, 1H), 3.85 (s, 2H), 3.55 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 197.1, 171.0, 137.4, 137.1, 136.1, 134.8, 133.2, 131.5, 130.3, 129.7, 128.4, 125.3, 52.0, 38.3. HRMS(ESI) calcd. for C₁₆H₁₃BrNaO₃⁺ (M+Na)⁺ 354.9940, found 354.9940.

Spectral data for methyl 2-(2-benzoylphenyl)acetate (6f)



¹H NMR (600 MHz, CDCl₃): δ 7.78~7.80 (m, 2H), 7.55~7.58 (m, 1H), 7.43~7.47 (m, 3H), 7.31~7.39 (m, 3H), 3.88 (s, 2H), 3.54 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 198.0, 171.6, 138.3, 137.8, 133.9, 132.9, 131.8, 130.9, 130.3, 130.0, 128.3, 126.5, 51.9, 38.7. HRMS(ESI) calcd. for $C_{16}H_{14}NaO_3^+$ (M+Na)⁺ 277.0835, found, 277.0841.

Spectral data for methyl 2-(2-benzoyl-4-methylphenyl)acetate (6g)



¹H NMR (600 MHz, CDCl₃): δ 7.79 (dd, J = 8.4, 1.2 Hz, 2H), 7.55~7.58 (m, 1H), 7.43~7.46 (m, 2H), 7.22~7.27 (m, 2H), 7.18 (s, 1H), 3.81 (s, 2H), 3.53 (s, 3H), 2.33 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 198.2, 171.8, 138.2, 137.9, 136.4, 132.9, 131.6 (CH×2), 130.8, 130.5, 130.3, 128.3, 51.8, 38.3, 21.0. HRMS(ESI) calcd. for C₁₇H₁₇O₃⁺ (M+H)⁺ 269.1172, found 269.1175.

Spectral data for methyl 2-(2-benzoyl-4-(*tert*-butyl)phenyl)acetate (6h)



¹H NMR (600 MHz, CDCl₃): δ 7.79~7.81 (m, 2H), 7.56~7.58 (m, 1H), 7.43~7.48 (m,

3H), 7.38 (d, J = 2.4 Hz, 1H), 7.27 (d, J= 7.8 Hz, 1H); ¹³C NMR (150 MHz, CDCl₃): δ 198.4, 171.9, 149.5, 137.8 (C×2), 132.9, 131.4, 130.8, 130.4, 128.3, 127.8, 127.2, 51.8, 38.2, 34.5, 31.1. HRMS(ESI) calcd. for C₂₀H₂₂NaO₃⁺ (M+Na)⁺ 333.1461, found 333.1463.

Spectral data for methyl 2-(2-benzoyl-5-methylphenyl)acetate (6i)



¹H NMR (500 MHz, CDCl₃): δ 7.77 (d, J = 7.0 Hz, 2H), 7.55 (t, J = 7.5 Hz, 1H), 7.41~7.45 (m, 2H), 7.29 (d, J = 8.0 Hz, 1H), 7.15 (s, 1H), 7.11 (d, J = 8.0 Hz, 1H), 3.86 (s, 2H), 3.55 (s, 3H), 2.39 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): δ 198.0, 171.9, 141.5, 138.2, 135.3, 134.2, 132.7 (CH×2), 130.7, 130.3, 128.2, 127.1, 51.9, 38.8, 21.4. HRMS(ESI) calcd. for C₁₇H₁₆NaO₃⁺(M+Na)⁺ 291.0992, found 291.0990.

Spectral data for methyl 2-(2-benzoyl-5-(tert-butyl)phenyl)acetate (6j)



¹H NMR (600 MHz, CDCl₃): δ 7.79 (dd, J = 8.4, 1.2Hz, 2H), 7.54~7.57 (m, 1H), 7.42~7.45 (m, 2H), 7.30~7.34 (m, 3H), 3.92 (s, 2H), 3.55 (s, 3H), 1.34 (s, 9H); ¹³C NMR (150 MHz, CDCl₃): δ 198.0, 171.9, 154.4, 138.2, 135.3, 133.9, 132.6, 130.5, 130.3, 129.1, 128.2, 123.4, 51.8, 39.1, 34.9, 31.1. HRMS(ESI) calcd. for C₂₀H₂₃O₃⁺ (M+H)⁺ 311.1642, found 311.1644.

Spectral data for methyl 2-(4-chloro-2-(4-methylbenzoyl)phenyl)acetate (6k)



¹H NMR (500 MHz, CDCl₃): δ 7.69 (d, *J* = 8.5 Hz, 2H), 7.42 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.34 (d, *J* = 2.0 Hz, 1H), 7.25~7.29 (m, 3H), 3.79 (s, 2H), 3.53 (s, 3H), 2.42 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): δ 196.2, 171.2, 144.4, 140.1, 134.3, 132.9, 132.6, 132.0, 130.5 (CH×2), 129.4, 129.2, 51.9, 37.9, 21.7. HRMS(ESI) calcd. for C₁₇H₁₆ClO₃⁺ (M+H)⁺ 303.0782, found 303.0784 .

Spectral data for methyl 2-(4-chloro-2-(4-chlorobenzoyl)phenyl)acetate (6l)



¹H NMR (500 MHz, CDCl₃): δ 7.74 (d, J = 8.5 Hz, 2H), 7.43~7.45 (m, 3H), 7.31 (d, J = 2.0 Hz, 1H), 7.28 (d, J = 8.5 Hz, 1H), 3.83 (s, 2H), 3.54 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): δ 195.3, 171.1, 139.9, 139.4, 135.3, 133.1, 132.7, 132.2, 131.6, 130.9, 129.4, 128.8, 52.0, 37.9. HRMS(ESI) calcd. for C₁₆H₁₃Cl₂O₃⁺ (M+H)⁺ 323.0236, found 323.0237.




















































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F2 - Acquisition Parameters Date20140421 Time 21.32 INSTRUM spect PROBHD 5 mm QNP 1H/1 PULPROG 32768 SOLVENT CDC13 NS 100 DS 0 SWH 45045.047 FIDRES 1.374666 AQ 0.3637748								
Current Data Parameters NAME Hao-ph-Me-I-1 EXPNO 2 PROCNO 1								
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1D NMR plot parameters CX 20.00 cm CY 4.00 cm F1P 135.000 ppm F1 20323.34 Hz F2P 115.000 ppm F2 17312.47 Hz									
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Current Data Parameters NAME Hao-131101 EXPNO 2 PROCNO 1									
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72 - Acquisition Parameters Date20131224 Fime14.50 INSTRUMSpect PROBHD5 mm_QNP1H/1			Į								
Current Data Parameters NAME 2013-12-26 SXPNO 2 PROCNO 1											
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Current Data Parameters NAME 2014-03-26 EXPNO 2 PROCNO 1											
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214.23		134.34 128.74 128.74 127.24 124.37 122.83	77.21 77.00 76.79	- 59.99		
Current Data Parameters NAME 2013-12-12-P EXPNO 2 PROCNO 1						
F2 - Acquisition Parameters Date20131213 Time11.20 INSTRUM_spect PROBHD_5_mm_QNP1H/1 PULPROG2gpq TD32768 SOLVENTCDC13 NS505 DS0 SWH45045.047 Hz FIDRES374666 Hz AQ 0.3637748 sec RG .2048						***
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F2 - Acquisition Parameters Date20140423 Time 7.51 INSTRUM spect PROBHD 5 mm QNP 1H/1 PULPROG 2070 TD 32768 SOLVENT CDC13 NS 261 DS 0 SWH 45045.047 Hz FIDRES 1.374666 Hz AQ 0.3837748 sec RG 2048						
Current Data Parameters NAME 2014-04-25-P EXENO 2 PROCNO 1						
212.	143. 135. 137. 138. 139. 126. 126. 126.	77.2 76.7	59.4	42.4	21.0	







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F2 - Processing y SI SF 150. WDW SSB 0 LB GB 0 FC	parameters 65536 55432883 MHz EM 1.00 Hz 2.00	1						
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F2 - Acquisition Date_ 2 Time INSTRUM PROBHD 5 mm QNU PULPROG TD SOLVENT	Parameters 0131108 6.29 spect 19 1H/1 zgpg 32768 CDC13	1						
Current Data Par NAME 201 EXPNO PROCNO	ameters 3-11-08 2 1							
192	172	141 136 136 137 132 132 132 132 132 132 132 132		77. 77 76.	25			



191.70	164.84	143.67 143.67 137.86 137.79 136.80 136.80 136.80 129.03 127.84	$\bigwedge_{114.62}^{118.30}$	77.21 77.00 76.79	52.65		
Current Data Parameters NAME 2013-11-29 EXPNO 2 PROCNO 1							
F2 - Acquisition Parameters Date20131128 20131128 Time 9.22 INSTRUM spect PROBHD 5 mm QNP IL 32768 SOLVENT CDC13 NS 300 DS 45045.047 Hz FIDRES 1.374666 Hz AQ 0.3637748 sec C448 2048	3						
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190 180	170 160 150	0 140 130	120 110 100 90	80 70 60	50 40	30 20	ppm



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Current Data Pa NAME 20 EXPNO	rameters 13-12-17 2			V			$\forall$		$\vee$				
PROCNO F2 - Acquisitio Date_ Time INSTRUM 5 mm Q PULPROG TD SOLVENT NS DS SWH FIDRES AQ 0 BG	1 Parameters 20131217 6.41 spect NF 1H/1 2gpg 32768 CCC13 231 5045.047 Hz 1.374666 Hz .3637748 sec 2048							2.44504444-1446-1446-1446-1446-1446-1446-1446					
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 190	180 170		) 140 130	120	110	100 90	80	70 6	0 50	<b>40</b>	30	<b>20</b>	ppm



LB 0 PC 0	2.00 Hz 2.50		Т				
F2 - Processing para SI 65 SF 150.5432 WDW SSB 0	ameters 5536 2411 MHz EM						
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DW 11.   DE 6   TE 2.50000   dl1 0.03000   DELTA 3.40000   MCREST 0 sec   MCWRK 0.01500	6.50 usec 94.6 K 0000 sec 0000 sec 0010 sec						
INSTRUM SEP PROBHD 5 mm QNP 1 PULPRO 2 SOLVENT CD NS DS SWH 45045. FIDRES 1.374 AQ 0.3637	Dect. H/1 Zapg 2768 2013 251 0 047 Hz 4666 Hz 7748 sec 2018				ungkaning magnassis and magnassis a	<b>₩</b> ₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩	ana ny majagatani da ped
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O T Current Data Paramet				∑ ⁵² 52			

![](_page_91_Figure_0.jpeg)

![](_page_92_Figure_0.jpeg)

![](_page_93_Figure_0.jpeg)

![](_page_94_Figure_0.jpeg)

![](_page_95_Figure_0.jpeg)

192.91		144.93 139.88 137.64 131.39 131.39 131.39 131.39 132.09 123.74 128.74 127.41		77.21 77.00	52.53	21.97	
Current Data Pa NAME 20 EXPNO PROCNO	113-11-23 2 1						
F2 - Acquisitic Date Time INSTRUM PROBHD 5 mm C PULPROG TD SOLVENT NS DS SWH 4 FIDRES AQ C RG	Dn Parameters 20131123 11.26 spect NP 1H/1 22768 CDC13 200 0 15045.047 Hz 1.374666 Hz 3637748 sec 2048						
DW DE TE D1 3. d11 0. DELTA 3. MCREST 0 sec MCWRK 0.	11.100 usec 6.50 usec 297.2 K 5000000 sec 4000001 sec 01500000 sec	1					
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PL12 PL13 SF02 598 F2 - Processing	9.00 dB 14.00 dB 2.7029935 MHz				an Conner - Branzanska Schammer - Grannen Hannachen under sin Coro		
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 190	180 170 160	150 140 130 120	) 110 100 90	80 70	60 <b>50 40</b>		ppm

![](_page_97_Figure_0.jpeg)

![](_page_98_Figure_0.jpeg)

![](_page_99_Figure_0.jpeg)

and the second			**************************************				and a start of the
F2 - Processing SI SF 150 WDW SSB 0 LB GB 0 PC	parameters 65536 .5432390 MHz EM 3.00 Hz 1.00			1			
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MCWRK 0. ====== CHANNE NUC1 P1 PL1 0 dB SF01 150	L fl	1 J.					
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F2 - Acquisitio Date Time INSTRUM PROBHD 5 mm Q PULPROG TD SOLVENT NS DS DS SWH 4 FIDRES AQ 0	n Parameters 20140327 4.29 spect NP 1H/1 2276 CDC13 500 5045.047 Hz 1.374666 Hz .3637748 sec 2048						
Current Data Pa NAME 20 EXPNO PROCNO	rameters 14-04-01 2 1						
193.4		137.6 137.6 134.6 134.6 133.6 133.6 133.6 133.6 129.6 127.3		$\bigwedge_{76.7}^{77.27}$	52.38	20.77	

![](_page_101_Figure_0.jpeg)

193.79	173.08		137.77 137.77 133.31 132.28 132.28 130.92 120.09 128.76 128.76			77.21	76.78	52.42			
Current Data H NAME 2 EXPNO PROCNO	Parameters 2013-12-29 2 1										
F2 - Acquisit: Date	ion Parameters 20140102 13.32 spect QNP 1H/1 zgpc 32768 CDC13 6144 45045.047 Hz 1.374666 Hz 0.3637748 sec 2068										
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CPDPRG2 NUC1 P1 P1 PL1 0 dB SF01 1: CPDPRG2 NUC2	NEL f1 13C 4.80 usec 50.5597948 MHz NEL f2 waltz16 1H			5					I		
PCPD2 PL2 PL12 PL13 SF02 55	92.00 usec 120.00 dB 9.00 dB 14.00 dB 98.7029935 MHz						<u></u>			~~~	
F2 - Processin SI SF 15 WDW SSB 0 LB GB 0	ng parameters 65536 50.5432383 MHz EM 3.00 Hz										
PC	0.50										
				Martin Martin Lautin Martin Lautin			Contraction and procession of a second second			-	
190	180 170 160	150	140 130 12	20 110	100 90	<b>80</b>	70 60	50 4	0 30	<b>20</b>	ppm

![](_page_103_Figure_0.jpeg)

<del></del>						
lD NMR p CX CY F1P F1 F2P F2	plot parameters 20.00 cm 4.00 cm 200.000 ppm 30108.65 Hz -10.000 ppm -1505.43 Hz					
F2 - Pro SI SF WDW SSB LB GB PC	ocessing parameters 65536 150.5432404 MHz EM 0 1.00 Hz 1.00					
CPDPRG2 NUC2 PCPD2 PL2 PL12 PL13 SF02	= CHANNEL f2 ======= waltz16 192.00 usec 120.00 dB 9.00 dB 14.00 dB 598.7029935 MHz		sk O			
NUC1 P1 PL1 SF01	= CHANNEL f1 ====== 13C 4.80 usec 0.00 dB 150.5597948 MHz			I		
DW DE TE D1 d11 DELTA MCREST MCWRK	11.100 usec 6.50 usec 299.4 K 3.50000000 sec 3.4000010 sec 0.0000000 sec 0.01500000 sec	11				
F2 - Acq Date_ Time INSTRUM PROBHD PULPROG TD SOLVENT NS DS SWH FIDRES AQ RG	quisition Parameters 20140424 5.03 spect 5 mm QNP 1H/1 20pg 32768 CDC13 5120 0 45045.047 Hz 1.374666 Hz 0.3637748 sec 2048					
Current NAME EXPNO PROCNO	Data Parameters Hao-ph-Me-aldehyde 2 1					
.191.	172		77	25. 52.	21.	

![](_page_105_Figure_0.jpeg)

92.02	72.01	41.27 40.62 35.32	23.86 31.99 30.56 29.19 28.23 28.23		7.21	6.78	2.62			
1				CI	i (	$\bigvee$				
Current Data Para NAME 2014 EXPNO PROCNO	ameters 4-04-28 2 1									
F2 - Acquisition Date_ 20 Time INSTRUM PROBHD 5 mm QNE PULPROG TD	Parameters 0140425 13.10 spect 1H/1 2979 32768						Ţ			
SOLVENT NS DS SWH 450 FIDRES 1. AQ 0.3	CDC13 5120 0 045.047 Hz .374666 Hz 3637748 sec .2048.			51 0						
DW DE TE D1 3.50 d11 0.03 DELTA 3.40 MCREST 0 sec MCWRK 0.01	11.100 usec 6.50 usec 298.5 K 000000 sec 300000 sec 1000010 sec		I					The second se		
CHANNEL NUC1 P1 PL1 0 dB SF01 150.5	f1 13C 4.80 usec	ī					1			
CPDPRG2 NUC2 PCPD2 PL2 PL12	f2 ====== waltz16 1H 92.00 usec 120.00 dB 9.00 dB									
PL13 SFO2 598.7 F2 - Processing p	14.00 dB 7029935 MHz parameters									
SI SF 150.5 WDW SSB 0 LB GB 0	65536 5432363 MHz EM 3.00 Hz		II							
PC	1.00									
				***	*****	1			****	
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190		00 100 140	130 120	110 100	30 80	10	55 50	-0 50	20	phill

![](_page_107_Figure_0.jpeg)
196.54		139.85 137.02 133.36 133.66 133.66 133.67 132.24 130.76 128.49	77 21 77 .00 76.79	51.97		
Current Data Paramete NAME 2013-11- EXPNO PROCNO F2 - Acquisition Para Date_ 201311 Time 6. INSTRUM spe PROBHD 5 mm ONP 1H PULPROG 2g TD 327 SOLVENT CCO NS 3 DS SWH 45045.0 FIDRES 1.3746 AQ 0.36377 DW 11.1	ers 09 2 1 1 12 25 12 12 12 12 12 13 13 13 13 13 14 14 147 147 142 148 148 148 148 147 147 147 147 147 147 147 147				and definition of the second	A.M.2.19.19.19.19.19.19.19.19.19.19.19.19.19.
DE 6, TE 490 D1 3.500000 d11 0.030000 DELTA 3.400000 MCREST 0 sec MCWRK 0.015000 	50 usec .2 K 100 sec 100 sec 110 sec 110 sec 110 sec 110 sec 110 sec 110 sec 110 sec 111 sec 112 sec 113 sec 113 sec 113 sec 114 sec 115 se		OMe	400-0-0-0-0-0-0-0-0-0-0-0-0-0-0-0-0-0-0		
PL13 14 SFO2 598.70299 F2 - Processing param SI 655 SF 150.54323 WDW SSB 0 LB 3. GB 0 PC 2.	00 dB 355 MHz meters 336 EM 00 Hz 000 Hz					
					40 30 2	20 ppm



200 190 180	170	160	150 14	0 130	120	110	100	90	80	70	60	50	40	30	20	ppm
			<b>.</b>			***	ni ⁿ enter (en en d					مىروپ سىيا كەنتىر				in stand
F2  - Processing parameters    SI  65536    SF  150.5432370 MH    WDW  EM    SSB  0    LB  3.00 Hz    GB  0    PC  0.50	Z															
CPDPRG2  waltz16    NUC2  1H    PCPD2  92.00 us    PL2  120.00 dB    FL1  9.00 dB    PL13  14.00 dB    SF02  598.7029935 MH	== ec z				l		02	`OMe								
NUC1  13C    P1  4.80 us    FL1  0 dB    SF01  150.557948 MH	ec z					6										
DW  11,100 us    DE  6.50 us    TE  296.4 K    D1  3.5000000 se    d11  0.3300000 se    DELTA  3.4000010 se    MCREST  0 sec    MCWRK  0.0150000 se	ec ec c c c			L.		F		$\sim$								
Date  20131129    Time  13.16    INSTRUM  spect    PROHD  5 mm QNP 1H/1    PULPROG  32768    SOLVENT  CDC13    NS  6144    DS  0    SWH  45045.047 Hz    FIDRES  1.374666 Hz    AQ  0.3637748 se	c				<u>I</u>										aldrey Supposed and the otherwise	
Current Data Parameters NAME 2013-11-30 EXPNO 2 PROCNO 1 F2 - Acquisition Parameter	5															
196.		161.	L 139	137 133 133 133 133 133 133 133 129	117	×116				~ 76.						















198.01	171.62	138.31 137.80 137.80 132.91 131.76 131.76 130.87 130.87 130.87 120.93 126.53		77.21 77.00 76.78		38.68
Current Data Parameters NAME 2013-12-04 EXPNO 2 PROCNO 1						
F2  Acquisition Parameter:    Date20131204  20131204    Time  18.41    INSTRUM  spect    PROBHD  5 mm QNP 1H/1    PUDEPROG  zgpq    TD  32768    SOLVENT  CDC13    NS  5120    DS  0    SHH  45045.047    FIDRES  1.374666    AQ  0.3637748    BG  2048	S C					1914 - 1914 - 1914 - 1914 - 1914 - 1914 - 1914 - 1914 - 1914 - 1914 - 1914 - 1914 - 1914 - 1914 - 1914 - 1914 -
Dw  11.100 Usr    DE  6.50 Usr    TE  298.3 K    D1  3.5000000 sec    d11  0.33000000 sec    DELTA  3.4000010 sec    MCREST  0 sec    MCWRK  0.01500000 sec	ec ec c c c		O C C C C C C C C C C C C C C C C C C C	1		
NUC1  13C    P1  4.80 us    PL1  0 dB    SF01  150.5597948 MH:	ec z ec		6f OMe			
PL12 9.00 dB PL12 9.00 dB PL13 14.00 dB SF02 598.7029935 MH	2					
F2 - Processing parameters SI 65536 SF 150.5432363 MH: WDW EM SSB 0 LB 3.00 Hz GB 0	z	11				
PC 0.50						I
1	1				]	
200 190 180	170 160 150	140 130 120	110 100 90		50 4	40 30 20 ppm







	171.86		132.90 131.40 130.77 130.77 130.38 130.77 122.17 127.17	× 77.21	76.79		#" ⊣ - - -
Current Data Par NAME 201 EXPNO PROCNO	ameters 3-12-15 2 1	I	ו אוו ווי		¥		I
F2 - Acquisitior Date_ 2 Time 2 INSTRUM PROBHD 5 mm QN PULEROG TD SOLVENT NS DS DS SWH 45 FIDRS 1 AQ 0. HG	1 Parameters 13.27 spect 22070 22768 20768 20768 2014 6144 6144 6144 6145.047 Hz .374666 Hz 3637748 sec 2048						L
DW DE TE D1 3.5 d11 0.0 DELTA 3.4 MCREST 0 sec MCWRK 0.0	11.100 usec 6.50 usec 297.5 K 3000000 sec 33000000 sec 10000010 sec						
CHANNEI NUC1 P1 SF01 0 dB SF01 150. CHANNEI CPDPRG2 NUC2 PCPD2	, fl			6h O OMe			
PL2 PL12 PL13 SF02 598.	120.00 dB 9.00 dB 14.00 dB 7029935 MHz	ad an aid air i cuir an				***************************************	••••••••••••••••••••••••••••••••••••••
F2 - Processing SI SF 150. WDW SSB 0 LB GB 0 PC	parameters 65536 5432370 MHz EM 3.00 Hz						
	0.50					ĺ	
	Jacobara	mminim		******			L
200 190	180 170	160 150 14	0 130 120	110 100 90 80		50 40 ;	30 20 ppm















