Molecular Iodine-Mediated Reaction of 2-(2-phenylethynyl)-Morita-Baylis-Hillman Adducts: An Easy Access to Naphthyl ketones and Iodo-Substituted Isochromenes

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General Experimental information

All reactions were carried out under an atmosphere of nitrogen in oven-dried glassware. Unless otherwise noted, all reagents were commercially obtained and, where appropriate, purified prior to use. Analytical thin-layer chromatography was performed using E. Merck silica gel 60F glass plates and E. Merck silica gel 60 (230–400 mesh) was used in flash chromatography separations. $^1$H and $^{13}$C NMR spectra were recorded with Bruker Advance EX 400. Chemical shifts were reported in parts per million (δ) using TMS as internal standard and coupling constants were expressed in hertz. All substrates were prepared using literature procedures.$^{1-4}$

Preparation of the 2-(2-phenylethynyl)-Morita-Baylis-Hillman Adducts

i. The Sonogashira substrates were prepared by using 2-bromobenzaldehyde with various terminal alkynes.$^{1,2}$

ii. The MBH adducts were prepared according to the literature procedure.$^{3,4}$

Methyl 2-(hydroxy(2-(phenylethynyl)phenyl)methyl)acrylate (1a)

$^1$H NMR (400 MHz, CDCl$_3$) δH (ppm): 7.58-7.52 (m, 2H), 7.50-7.47 (m, 2H), 7.40-7.26 (m, 5H), 6.34 (s, 1H), 6.16 (d, J = 4.92 Hz, 1H), 5.68 (s, 1H), 3.74 (s, 1H), 3.31 (d, J = 5.08 Hz, 1H). $^{13}$C NMR (100 MHz, CDCl$_3$) δC (ppm): 167.3, 142.7, 141.4, 132.4, 131.6, 128.8, 128.5, 127.8, 127.0, 126.6, 123.1, 121.8, 94.8, 87.2, 70.9, 52.2.$^{3}$

Methyl 2-(hydroxy(6-(phenylethynyl)benzo[d][1,3]dioxol-5-yl)methyl)acrylate (2a)

$^1$H NMR (400 MHz, CDCl$_3$) δH (ppm): 7.46-7.45 (m, 2H), 7.34-7.32 (m, 3H), 7.03 (s, 1H), 6.96 (s, 1H), 6.33 (s, 1H), 6.10 (s, 1H), 5.99 (s, 2H), 5.71 (s, 1H), 3.75 (s, 3H) 3.20 (s, 1H). $^{13}$C NMR (100
MHz, CDCl₃) δC (ppm): 167.3, 148.5, 147.0, 141.5, 138.1, 131.5, 128.6, 128.5, 126.8, 123.3, 115.1, 111.7, 107.3, 101.7, 93.3, 87.2, 70.7, 52.2. LRMS (ESI) (m/z) (relative intensity): 359 (M⁺+Na, 100). HRMS calcd for C₂₀H₁₆O₅Na (M⁺+Na): 359.0895, found 359.0886.

3-(Hydroxy(2-(phenylethynyl)phenyl)methyl)but-3-en-2-one (3a)

![Structure of 3a](image)

¹H NMR (400 MHz, CDCl₃) δH (ppm): 7.59 (d, J = 8.0 Hz, 1H), 7.53-7.51 (m, 1H), 7.46-7.43 (m, 2H), 7.41-7.37 (m, 1H), 7.35-7.32 (m, 3H), 7.31-7.27 (m, 1H), 6.18 (d, J = 3.64 Hz, 1H), 6.16 (s, 1H), 5.75 (s, 1H), 3.45 (d, J = 3.72 Hz, 1H), 2.36 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δC (ppm): 200.9, 149.5, 143.0, 132.3, 131.7, 131.6, 128.8, 128.7, 127.7, 127.6, 126.6, 123.1, 121.6, 94.9, 87.3, 72.4, 70.5, 26.5. LRMS (EI) (m/z) (relative intensity): 276 (M⁺, 35), 215 (95), 178 (100). HRMS calcd for C₁₉H₁₆O₂ (M⁺): 276.1150, found 276.1151.

3-(Hydroxy(5-methoxy-2-(phenylethynyl)phenyl)methyl)but-3-en-2-one (4a)

![Structure of 4a](image)

¹H NMR (400 MHz, CDCl₃) δH (ppm): 7.43-7.40 (m, 4H), 7.33-7.30 (m, 2H), 7.16 (d, J = 1.95 Hz, 1H), 6.82 (dd, J = 8.48, 2.64 Hz, 1H), 6.15-6.14 (m, 2H), 5.73 (s, 1H), 3.85 (s, 3H), 3.48 (d, J = 4.2 Hz, 1H), 2.36 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δC (ppm): 200.9, 160.2, 149.3, 144.9, 133.7, 131.4, 128.6, 128.3, 127.7, 123.5, 113.7, 113.6, 112.1, 93.5, 87.4, 70.4, 55.6, 26.5. LRMS (EI) (m/z) (relative intensity): 306 (M⁺, 28), 264 (60), 207 (61), 165 (100). HRMS calcd for C₂₀H₁₈O₃ (M⁺): 306.1256, found 306.1260.

Ethyl 2-(hydroxy(2-(phenylethynyl)phenyl)methyl)acrylate (5a)

![Structure of 5a](image)

¹H NMR (400 MHz, CDCl₃) δH (ppm): 7.56 (d, J = 7.6 Hz, 1H), 7.53 (dd, J = 7.58, 0.86 Hz, 1H), 7.50-7.48 (m, 2H), 7.40-7.32 (m, 4H), 7.31-7.27 (m, 1H), 6.34 (s, 1H), 6.16 (d, J = 5.0 Hz, 1H), 5.67 (s, 1H), 4.44 (q, J = 7.14 Hz, 2H), 3.29 (d, J = 5.16 Hz, 1H), 1.24 (t, J = 7.12 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δC (ppm): 166.9, 142.8, 141.7, 132.4, 131.7, 128.8, 128.7, 128.6, 127.8, 126.7, 126.6, 123.2, 121.9, 94.7, 87.3, 71.0, 61.2, 14.2. LRMS (EI) (m/z) (relative intensity): 306 (M⁺, 22), 231 (100), 203 (91). HRMS calcd for C₂₀H₁₈O₃ (M⁺): 306.1256, found 306.1255.
2-(Hydroxy(2-(phenylethynyl)phenyl)methyl)cyclohex-2-en-1-one (6a)

\[ \text{1H NMR (400 MHz, CDCl}_3 \text{)} \delta_{\text{H}} (\text{ppm}): 7.64 (d, J = 7.40 Hz, 1H), 7.52-7.50 (m, 1H), 7.52-7.37 (m, 3H) 7.35-7.31 (m, 3H), 7.30-7.28 (m, 1H), 6.57 (t, J = 4.12 Hz, 1H), 6.14 (s, 1H), 3.67 (s, 1H), 2.53-2.40 (m, 2H), 2.33-2.29 (m, 2H), 1.99-1.91 (m, 2H). \]

\[ \text{13C NMR (100 MHz, CDCl}_3 \text{)} \delta_{\text{C}} (\text{ppm}): 200.8, 148.2, 143.1, 140.5, 132.2, 131.7, 131.6, 128.8, 128.6, 127.4, 126.6, 123.2, 121.4, 94.8, 87.5, 70.1, 38.7, 26.0, 22.7. \]

LRMS (EI) \((m/z)\) (relative intensity): 302 (M\(^+\), 2), 284 (100), 165 (74). HRMS calcd for C\(_{21}\)H\(_{18}\)O\(_2\) (M\(^+\)): 302.1307, found 302.1304.

Methyl 2-(hydroxy(1-(phenylethynyl)naphthalen-2-yl)methyl)acrylate (7a)

\[ \text{1H NMR (400 MHz, CDCl}_3 \text{)} \delta_{\text{H}} (\text{ppm}): 8.5 (d, J = 2.44 Hz, 1H), 8.15 (dd, J = 8.48, 2.4 Hz, 1H), 7.66 (d, J = 8.48 Hz, 1H), 7.51-7.49 (m, 2H), 7.40-7.37 (m, 3H), 6.38 (s, 1H), 6.17 (s, 1H), 5.66 (s, 1H), 3.77 (s, 3H), 3.41 (s, 1H). \]

\[ \text{13C NMR (100 MHz, CDCl}_3 \text{)} \delta_{\text{C}} (\text{ppm}): 167.0, 147.5, 144.7, 140.6, 133.0, 131.9, 129.7, 128.8, 128.5, 127.8, 122.8, 122.1, 122.0, 99.9, 85.7, 70.4, 52.4. \]

LRMS (ESI) \((m/z)\) (relative intensity): 360 (M\(^+\)+Na, 100), 213 (80), 105 (74). HRMS calcd for C\(_{19}\)H\(_{15}\)O\(_3\)Na (M\(^+\)+Na): 360.0848, found 360.0842.

Methyl 2-(hydroxy(5-nitro-2-(phenylethynyl)phenyl)methyl)acrylate (8a)

\[ \text{1H NMR (400 MHz, CDCl}_3 \text{)} \delta_{\text{H}} (\text{ppm}): 8.40 (s, 1H), 8.11 (d, J = 8.44 Hz, 1H), 7.82 (d, J = 8.12 Hz, 1H), 7.73-7.69 (m, 1H), 7.59-7.53 (m, 3H), 7.39-7.33 (m, 3H), 6.38 (s, 1H), 6.32 (s, 1H), 5.66 (s, 1H), 3.74 (s, 3H). \]

\[ \text{13C NMR (100 MHz, CDCl}_3 \text{)} \delta_{\text{C}} (\text{ppm}): 167.2, 147.7, 142.4, \]
141.2, 135.8, 134.1, 132.3, 130.3, 129.5, 129.1, 128.6, 128.0, 127.8, 127.6, 127.3, 122.0, 94.4, 87.3, 69.8, 52.3. LRMS (ESI) (m/z) (relative intensity): 366 (M⁺+Na, 47), 344 (M⁺+H, 100). HRMS calcd for C₂₂H₁₈NO₃ (M⁺): 344.1287, found 344.1284.

**Methyl (E)-2-(acetamidomethyl)-3-(2-(phenylethynyl)phenyl)acrylate (1c)**

\[
\begin{align*}
\text{H NMR (400 MHz, CDCl}_3\text{)} & \delta \text{H (ppm)}: 8.20 \text{ (s, 1H)}, 7.69 \text{ (d, } J = 7.56 \text{ Hz, 1H)}, 7.57 \text{ (dd, } J = 7.54, 1.06 \text{ Hz, 1H)}, 7.53-7.51 \text{ (m, 2H)}, 7.43-7.39 \text{ (m, 1H)}, 7.37-7.33 \text{ (m, 4H)}, 6.12 \text{ (bs, 1H)}, 4.30 \text{ (d, } J = 5.8 \text{ Hz, 2H)}, 3.88 \text{ (s, 3H)}, 1.94 \text{ (s, 3H)}. \\
\text{13C NMR (100 MHz, CDCl}_3\text{)} & \delta \text{C (ppm): 169.7, 168.4, 141.3, 136.3, 132.3, 131.7, 129.3, 129.2, 129.0, 128.9, 128.8, 128.6, 123.7, 123.1, 95.6, 87.7, 52.5, 37.1, 23.5. LRMS (EI) (m/z) (relative intensity): 333 (M⁺, 28), 301 (38), 290 (49), 230 (70). HRMS calcd for C₂₁H₁₉O₃N (M⁺): 333.1365, found 333.1364.
\end{align*}
\]

**Methyl (Z)-2-(iodomethyl)-3-(2-(phenylethynyl)phenyl)acrylate (1d)**

\[
\begin{align*}
\text{H NMR (400 MHz, CDCl}_3\text{)} & \delta \text{H (ppm)}: 8.18 \text{ (s, 1H)}, 7.77 \text{ (d, } J = 7.4 \text{ Hz, 1H)}, 7.61 \text{ (d, } J = 7.68 \text{ Hz, 1H)}, 7.53-7.52 \text{ (m, 2H)}, 7.49-7.45 \text{ (m, 1H)}, 7.41-7.35 \text{ (m, 4H)}, 4.30 \text{ (s, 2H)}, 3.91 \text{ (s, 3H)}. \\
\text{13C NMR (100 MHz, CDCl}_3\text{)} & \delta \text{C (ppm): 166.7, 139.5, 136.7, 132.6, 131.7, 131.1, 129.1, 128.9, 128.7, 128.6, 127.8, 124.5, 123.0, 96.2, 87.2, 70.2, 52.6. LRMS (EI) (m/z) (relative intensity): 402 (M⁺, 30), 243 (43), 215 (100). HRMS calcd for C₁₉H₁₅O₂I (M⁺): 402.0117, found 402.0113.
\end{align*}
\]

**References**


X-Ray Crystallographic Data of methyl 4-benzoylnaphthalene-2-carboxylate (1b):
[CCDC No 972525]

Identification code: a12599
Empirical formula: C19 H14 O3
Formula weight: 290.30
Temperature: 200(2) K
Wavelength: 0.71073 Å
Crystal system: Triclinic
Space group: P -1
Unit cell dimensions:

\[ \begin{align*}
a &= 8.3228(8) \text{ Å} & \alpha &= 86.924(3)^\circ \\
b &= 8.8321(9) \text{ Å} & \beta &= 69.716(2)^\circ \\
c &= 10.8845(11) \text{ Å} & \gamma &= 76.474(3)^\circ \\
\end{align*} \]

Volume: 729.33(13) Å³
Z: 2
Density (calculated): 1.322 Mg/m³
Absorption coefficient: 0.089 mm⁻¹
F(000): 304
Crystal size: 0.65 x 0.49 x 0.31 mm³
Theta range for data collection: 2.00 to 25.03°.
Index ranges: \(-9 \leq h \leq 5, -10 \leq k \leq 8, -12 \leq l \leq 10\)
Reflections collected: 5654
Independent reflections: 2524 [R(int) = 0.1362]
Completeness to theta = 25.03°: 98.4 %
Absorption correction: multi-scan
Max. and min. transmission: 0.9729 and 0.9444
Refinement method: Full-matrix least-squares on F²
Data / restraints / parameters: 2524 / 0 / 199
Goodness-of-fit on F²: 1.096
Final R indices [I>2σ(I)]: R1 = 0.0521, wR2 = 0.1588
R indices (all data): R1 = 0.0610, wR2 = 0.1764
Largest diff. peak and hole: 0.208 and -0.281 e.Å⁻³
X-Ray Crystallographic Data of Methyl 2-[(3E)-3-[iodo(phenyl)methyldene]-6-nitro-1,3-dihydro-2-benzofuran-1-yl]prop-2-enoate (4f): [CCDC No 973915]

Identification code: ch15710a
Empirical formula: C19 H14 I1 N1 O5
Formula weight: 962.46
Temperature: 200(2) K
Wavelength: 0.71073 Å
Crystal system: Monoclinic
Space group: P 21
Unit cell dimensions:
\[ \begin{align*}
a &= 5.8687(3) \text{ Å} & \alpha &= 90^\circ. \\
b &= 10.7289(6) \text{ Å} & \beta &= 95.947(3)^\circ. \\
c &= 27.8199(12) \text{ Å} & \gamma &= 90^\circ.
\end{align*} \]
Volume: 1742.24(15) Å\(^3\)
Z: 2
Density (calculated): 1.835 Mg/m\(^3\)
Absorption coefficient: 1.876 mm\(^{-1}\)
F(000): 952
Crystal size: 0.32 x 0.14 x 0.05 mm\(^3\)
Theta range for data collection: 0.74 to 25.04°.
Index ranges: -6<=h<=6, -11<=k<=12, -32<=l<=33
Reflections collected: 9825
Independent reflections: 5302 [R(int) = 0.0299]
Completeness to theta = 25.04°: 98.5 %
Absorption correction: multi-scan
Max. and min. transmission: 0.9120 and 0.5850
Refinement method: Full-matrix least-squares on F\(^2\)
Data / restraints / parameters: 5302 / 9 / 226
Goodness-of-fit on F\(^2\): 1.141
Final R indices [I>2sigma(I)]: R1 = 0.1087, wR2 = 0.3129
R indices (all data): R1 = 0.1246, wR2 = 0.3290
Absolute structure parameter: 0.40(13)
Extinction coefficient: 0.038(3)
Largest diff. peak and hole: 2.578 and -5.367 e.Å\(^{-3}\)
X-Ray Crystallographic Data of methyl ($E$)-2-(acetamidomethyl)-3-(2-(phenylethynyl)-phenyl)acrylate (1c): [CCDC No 978566]

Identification code a12825
Empirical formula C21 H19 N O3
Formula weight 333.37
Temperature 200(2) K
Wavelength 0.71073 Å
Crystal system Orthorhombic
Space group $P_{c}a_{2}1$
Unit cell dimensions $a = 9.5269(6)$ Å $\alpha = 90^\circ$.
$b = 10.7294(7)$ Å $\beta = 90^\circ$.
$c = 17.4823(13)$ Å $\gamma = 90^\circ$.
Volume 1787.0(2) Å$^3$
$Z$ 4
Density (calculated) 1.239 Mg/m$^3$
Absorption coefficient 0.083 mm$^{-1}$
$F(000)$ 704
Crystal size 0.58 x 0.48 x 0.11 mm$^3$
Theta range for data collection 1.90 to 25.08$^\circ$.
Index ranges $-11 \leq h \leq 8, -12 \leq k \leq 9, -9 \leq l \leq 20$
Reflections collected 6346
Independent reflections 2173 [R(int) = 0.0324]
Completeness to theta = 25.08$^\circ$ 97.6 %
Absorption correction multi-scan
Max. and min. transmission 0.9909 and 0.9535
Refinement method Full-matrix least-squares on $F^2$
Data / restraints / parameters 2173 / 1 / 226
Goodness-of-fit on $F^2$ 1.044
Final R indices [I>2sigma(I)] $R1 = 0.0322, wR2 = 0.0798$
R indices (all data) $R1 = 0.0361, wR2 = 0.0832$
Absolute structure parameter 0.2(13)
Largest diff. peak and hole 0.136 and -0.129 e./Å$^3$
X-Ray Crystallographic Data of Methyl (Z)-2-(iodomethyl)-3-(2-(phenylethynyl)phenyl)acrylate (1d): [CCDC No 1009697]

Identification code: ch16312a
Empirical formula: C19 H15 I O2
Formula weight: 402.21
Temperature: 200(2) K
Wavelength: 0.71073 Å
Crystal system: Monoclinic
Space group: P 21/c
Unit cell dimensions:
\[ a = 8.2342(2) \text{ Å} \quad \alpha = 90^\circ. \]
\[ b = 37.9905(8) \text{ Å} \quad \beta = 90.5910(10)^\circ. \]
\[ c = 10.4703(2) \text{ Å} \quad \delta = 90^\circ. \]

Volume: 3275.16(12) Å³
Z: 8
Density (calculated): 1.631 Mg/m³
Absorption coefficient: 1.960 mm⁻¹
F(000): 1584
Crystal size: 0.68 x 0.13 x 0.03 mm³
Theta range for data collection: 1.07 to 25.19°.
Index ranges:
\[-9\leq h\leq 8, \quad -45\leq k\leq 45, \quad -12\leq l\leq 12\]
Reflections collected: 23291
Independent reflections: 5837 [R(int) = 0.0271]
Completeness to theta = 25.19°: 99.1 %
Absorption correction: multi-scan
Max. and min. transmission: 0.9435 and 0.3492
Refinement method: Full-matrix least-squares on F²
Data / restraints / parameters: 5837 / 0 / 397
Goodness-of-fit on F²: 1.321
Final R indices [I>2sigma(I)]: R1 = 0.0292, wR2 = 0.0863
R indices (all data): R1 = 0.0342, wR2 = 0.1067
Largest diff. peak and hole: 0.452 and -0.698 e.Å⁻³
$^1$H and $^{13}$C NMR Spectral copies
Methyl (E)-2-(acetamidomethyl)-3-(2-(phenylethynyl)phenyl)acrylate (1c): $^1$H NMR (400MHz, CDCl$_3$)

![1H NMR spectrum](image)

Methyl (E)-2-(acetamidomethyl)-3-(2-(phenylethynyl)phenyl)acrylate (1c): $^{13}$C NMR (100 MHz, CDCl$_3$)

![$^{13}$C NMR spectrum](image)
Methyl (Z)-2-(iodomethyl)-3-(2-(phenylethynyl)phenyl)acrylate (1d): $^1$H NMR (400MHz, CDCl$_3$)

Methyl (Z)-2-(iodomethyl)-3-(2-(phenylethynyl)phenyl)acrylate (1d): $^{13}$C NMR (100 MHz, CDCl$_3$)
Methyl 2-(hydroxy(2-(phenylethynyl)phenyl)methyl)acrylate (1a): \(^1\)H NMR (400MHz, CDCl\(_3\))

Methyl 2-(hydroxy(2-(phenylethynyl)phenyl)methyl)acrylate (1a): \(^{13}\)C NMR (100 MHz, CDCl\(_3\))
Methyl 2-(hydroxy(6-(phenylethynyl)benzo[d][1,3]dioxol-5-yl)methyl)acrylate (2a): $^1$H NMR (400MHz, CDCl$_3$)

Methyl 2-(hydroxy(6-(phenylethynyl)benzo[d][1,3]dioxol-5-yl)methyl)acrylate (2a): $^{13}$C NMR (100 MHz, CDCl$_3$)
3-(Hydroxy(2-(phenylethynyl)phenyl)methyl)but-3-en-2-one (3a): $^1$H NMR (400MHz, CDCl$_3$)

3-(Hydroxy(2-(phenylethynyl)phenyl)methyl)but-3-en-2-one (3a): $^{13}$C NMR (100 MHz, CDCl$_3$)
3-((Hydroxy(5-methoxy-2-((phenylethynyl)phenyl)methyl)but-3-en-2-one (4a): $^1H$ NMR (400MHz, CDCl$_3$)

3-((Hydroxy(5-methoxy-2-((phenylethynyl)phenyl)methyl)but-3-en-2-one (4a): $^{13}C$ NMR (100 MHz, CDCl$_3$)
Ethyl 2-(hydroxy(2-(phenylethynyl)phenyl)methyl)acrylate (5a): $^1$H NMR (400MHz, CDCl$_3$)

Ethyl 2-(hydroxy(2-(phenylethynyl)phenyl)methyl)acrylate (5a): $^{13}$C NMR (100 MHz, CDCl$_3$)
2-(Hydroxy(2-(phenylethynyl)phenyl)methyl)cyclohex-2-en-1-one (6a): $^1$H NMR (400MHz, CDCl$_3$)

2-(Hydroxy(2-(phenylethynyl)phenyl)methyl)cyclohex-2-en-1-one (6a): $^{13}$C NMR (100 MHz, CDCl$_3$)
Methyl 2-(hydroxy(1-(phenylethynyl)naphthalen-2-yl)methyl)acrylate (7a): $^1$H NMR (400MHz, CDCl$_3$)

Methyl 2-(hydroxy(1-(phenylethynyl)naphthalen-2-yl)methyl)acrylate (7a): $^{13}$C NMR (100 MHz, CDCl$_3$)
Methyl 2-(hydroxy(5-nitro-2-(phenylethynyl)phenyl)methyl)acrylate (8a): $^1$H NMR (400MHz, CDCl$_3$)

Methyl 2-(hydroxy(5-nitro-2-(phenylethynyl)phenyl)methyl)acrylate (8a): $^{13}$C NMR (100 MHz, CDCl$_3$)
Methyl 2-(hydroxy(2-(phenylethynyl)quinolin-3-yl)methyl)acrylate (9a): $^1$H NMR (400 MHz, CDCl$_3$)

Methyl 2-(hydroxy(2-(phenylethynyl)quinolin-3-yl)methyl)acrylate (9a): $^{13}$C NMR (100 MHz, CDCl$_3$)
Methyl 2-(hydroxy(5-methoxy-2-(phenylethynyl)phenyl)methyl)acrylate (10a): $^1$H NMR (400 MHz, CDCl$_3$)

Methyl 2-(hydroxy(5-methoxy-2-(phenylethynyl)phenyl)methyl)acrylate (10a): $^{13}$C NMR (100 MHz, CDCl$_3$)
Methyl 4-benzoynaphthalene-2-carboxylate (1b): $^1$H NMR (400MHz, CDCl$_3$)

Methyl 4-benzoynaphthalene-2-carboxylate (1b): $^{13}$C NMR (100 MHz, CDCl$_3$)
Methyl 8-benzoyl-2H-naphtho[2,3-d][1,3]dioxole-6-carboxylate (2b): $^1$H NMR (400MHz, CDCl$_3$)

Methyl 8-benzoyl-2H-naphtho[2,3-d][1,3]dioxole-6-carboxylate (2b): $^{13}$C NMR (100 MHz, CDCl$_3$)
1-(4-Benzylnaphthalen-2-ylethan-1-one (3b): $^1$H NMR (400 MHz, CDCl$_3$)

1-(4-Benzylnaphthalen-2-yl)ethan-1-one (3b): $^{13}$C NMR (100 MHz, CDCl$_3$)
1-(4-Benzoyl-7-methoxynaphthalen-2-yl)ethan-1-one (4b): $^1$H NMR (400 MHz, CDCl$_3$)

1-(4-Benzoyl-7-methoxynaphthalen-2-yl)ethan-1-one (4b): $^{13}$C NMR (100 MHz, CDCl$_3$)
Ethyl 4-benzoynaphthalene-2-carboxylate (5b): $^1$H NMR (400MHz, CDCl$_3$)

Ethyl 4-benzoynaphthalene-2-carboxylate (5b): $^{13}$C NMR (100 MHz, CDCl$_3$)

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The text describes the NMR spectroscopy results for the compound Ethyl 4-benzoynaphthalene-2-carboxylate (5b). The $^1$H NMR spectrum is recorded at 400MHz in CDCl$_3$, and the $^{13}$C NMR spectrum is recorded at 100 MHz in the same solvent.
10-Benzoyl-1,2,3,4-tetrahydroanthracen-1-one (6b): $^1$H NMR (400 MHz, CDCl$_3$)

10-Benzoyl-1,2,3,4-tetrahydroanthracen-1-one (6b): $^{13}$C NMR (100 MHz, CDCl$_3$)
$^1$H NMR of methyl 4-benzoylphenanthrene-2-carboxylate (7b)

Methyl 4-benzoylphenanthrene-2-carboxylate (7b): $^{13}$C NMR (100 MHz, CDCl$_3$)
Methyl 2-(4-iodo-7-nitro-3-phenyl-1H-isochromen-1-yl)prop-2-enoate (8b): $^1$H NMR (400MHz, CDCl$_3$)

Methyl 2-(4-iodo-7-nitro-3-phenyl-1H-isochromen-1-yl)prop-2-enoate (8b): $^{13}$C NMR (100 MHz, CDCl$_3$)
Methyl 2-(4-iodo-3-phenyl-1H-pyrano[4,3-b]quinolin-1-yl)prop-2-enoate (9b): $^1$H NMR (400MHz, CDCl$_3$)

Methyl 2-(4-iodo-3-phenyl-1H-pyrano[4,3-b]quinolin-1-yl)prop-2-enoate (9b): $^{13}$C NMR (100 MHz, CDCl$_3$)
Methyl 2-(4-iodo-3-phenyl-1H-isochromen-1-yl)prop-2-enoate (1e): ¹H NMR (400 MHz, CDCl₃)

Methyl 2-(4-iodo-3-phenyl-1H-isochromen-1-yl)prop-2-enoate (1e): ¹³C NMR (100 MHz, CDCl₃)
Methyl 2-[(3E)-3-[iodo(phenyl)methylidene]-1,3-dihydro-2-benzofuran-1-yl]prop-2-enoate (1f): $^1$H NMR (400MHz, CDCl$_3$)

Methyl 2-[(3E)-3-[iodo(phenyl)methylidene]-1,3-dihydro-2-benzofuran-1-yl]prop-2-enoate (1f): $^{13}$C NMR (100 MHz, CDCl$_3$)
Methyl 2-(4-iodo-7-methoxy-3-phenyl-1H-isochromen-1-yl)prop-2-enoate (2e): $^1$H NMR (400MHz, CDCl$_3$)

Methyl 2-(4-iodo-7-methoxy-3-phenyl-1H-isochromen-1-yl)prop-2-enoate (2e): $^{13}$C NMR (100 MHz, CDCl$_3$)
Methyl 2-[3-(2H-1,3-benzodioxol-5-yl)-4-iodo-1H-isochromen-1-yl]prop-2-enoate (3e):

$^1$H NMR (400MHz, CDCl$_3$)

\[\text{Methyl 2-[3-(2H-1,3-benzodioxol-5-yl)-4-iodo-1H-isochromen-1-yl]prop-2-enoate (3e):} \]

$^{13}$C NMR (100 MHz, CDCl$_3$)
Methyl 2-[(3E)-3-[iodo(phenyl)methylidene]-6-nitro-1,3-dihydro-2-benzofuran-1-yl]prop-2-enoate (4f): $^1$H NMR (400MHz, CDCl$_3$)

Methyl 2-[(3E)-3-[iodo(phenyl)methylidene]-6-nitro-1,3-dihydro-2-benzofuran-1-yl]prop-2-enoate (4f): $^{13}$C NMR (100 MHz, CDCl$_3$)
3-(4-Iodo-3-phenyl-1H-isochromen-1-yl)but-3-en-2-one (5e): $^1$H NMR (400 MHz, CDCl$_3$)

3-(4-Iodo-3-phenyl-1H-isochromen-1-yl)but-3-en-2-one (5e): $^{13}$C NMR (100 MHz, CDCl$_3$)
3-[(3E)-3-[iodo(phenyl)methylidene]-1,3-dihydro-2-benzofuran-1-yl]but-3-en-2-one (5f):

$^1$H NMR (400MHz, CDCl$_3$)

3-[(3E)-3-[iodo(phenyl)methylidene]-1,3-dihydro-2-benzofuran-1-yl]but-3-en-2-one (5f):

$^{13}$C NMR (100 MHz, CDCl$_3$)
3-(4-Iodo-7-methoxy-3-phenyl-1H-isochromen-1-yl)but-3-en-2-one (6e): \( ^1\)H NMR (400MHz, CDCl\(_3\))

3-(4-Iodo-7-methoxy-3-phenyl-1H-isochromen-1-yl)but-3-en-2-one (6e): \( ^{13}\)C NMR (100 MHz, CDCl\(_3\))
2-(4-Iodo-3-phenyl-1H-isochromen-1-yl)cyclohex-2-en-1-one (7e): $^1$H NMR (400MHz, CDCl$_3$)

![NMR spectrum image]

2-(4-Iodo-3-phenyl-1H-isochromen-1-yl)cyclohex-2-en-1-one (7e): $^{13}$C NMR (100 MHz, CDCl$_3$)

![NMR spectrum image]
2-[(3E)-3-[iodo(phenyl)methylidene]-1,3-dihydro-2-benzofuran-1-yl]cyclohex-2-en-1-one (7f): $^1$H NMR (400MHz, CDCl$_3$)

![NMR spectrum](image1)

2-[(3E)-3-[iodo(phenyl)methylidene]-1,3-dihydro-2-benzofuran-1-yl]cyclohex-2-en-1-one (7f): $^{13}$C NMR (100 MHz, CDCl$_3$)

![NMR spectrum](image2)
Ethyl 2-(4-iodo-3-phenyl-1H-isochromen-1-yl)prop-2-enoate (8e) and ethyl 2-[(3E)-3-[iodo(phenyl)methylidene]-1,3-dihydro-2-benzofuran-1-yl]prop-2-enoate (8f): $^1$H NMR (400MHz, CDCl$_3$)

![Chemical Structure 1](image1)

Ethyl 2-(4-iodo-3-phenyl-1H-isochromen-1-yl)prop-2-enoate (8e) and ethyl 2-[(3E)-3-[iodo(phenyl)methylidene]-1,3-dihydro-2-benzofuran-1-yl]prop-2-enoate (8f): $^{13}$C NMR (100 MHz, CDCl$_3$)

![Chemical Structure 2](image2)
Methyl 2-[4-(4-methoxyphenyl)-3-phenyl-1H-pyrano[4,3-b]quinolin-1-yl]prop-2-enoate (3c): $^1$H NMR (400MHz, CDCl$_3$)

Methyl 2-[4-(4-methoxyphenyl)-3-phenyl-1H-pyrano[4,3-b]quinolin-1-yl]prop-2-enoate (3c): $^{13}$C NMR (100 MHz, CDCl$_3$)