Supporting Information:

Chiral Olefin–Sulfoxide as Ligands for
Rhodium-Catalyzed Asymmetric Conjugate Addition of
Arylboronic Acids to Unsaturated Esters

Feng Xue\textsuperscript{a,b}, Dongping Wang\textsuperscript{a}, Xincheng Li\textsuperscript{a}, Boshun Wan\textsuperscript{*}\textsuperscript{a}

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1. Copy of NMR for the compounds (6a-6q)
Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry
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MeOOC

(+) - 6i
Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry
This journal is © The Royal Society of Chemistry 2013

\[
\text{MeOOC} \quad \text{(--)6k}
\]

\[
\begin{align*}
40.77 & \quad 46.34 & \quad 51.79 \\
76.84 & \quad 77.16 & \quad 77.48 \\
115.37 & \quad 115.58 & \quad 126.79 \\
127.64 & \quad 128.77 & \quad 139.30 \\
139.33 & \quad 143.40 & \quad 160.42 \\
162.85 & \quad 166.42 & \quad 172.18 \\
172.18 & \quad 178.77 & \quad 180.10
\end{align*}
\]
(+)-6p
MeOOC

F

(+)-6q

F

CF₃
2. Copy of HRMS for the compounds (6a-6q).

![Elemental Composition Report](image-url)
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:
C: 0-100  H: 0-150  O: 3-3  Na: 1-1

12030903 23 (0.427) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x1.09); Cr (12.23)

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Minimum: 100
Maximum: -200.0

Page 1
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100  H: 0-150  O: 3-3  Na: 1-1

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<th>Mass</th>
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<th>mDa</th>
<th>PPM</th>
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<th>i-FIT</th>
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Maximum: 5.0  5.0  200.0
Elemental Composition Report

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Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
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Elements Used:
C: 0-100  H: 0-150  O: 3-3  Na: 1-1

12030905 75 (1.395) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Cm (72.82)

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Elemental Composition Report

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Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100  H: 0-150  O: 2-2  Na: 1-1

x4-878
12000070 51 (0.948) AM (Cen,2, 80.00, H1,5000.00,0.00,1.00); Sm (Mn, 2x1.00); Cm (30:54)

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Minimum:  5.0  5.0  -200.0
Maximum:  200.0
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM  /  DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100  H: 0-150  O: 2-2  Na: 1-1

\[
\text{MeOC} \quad \text{ar} \quad \text{rBu}
\]

\((+)-6g\)

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Minimum:  5.0  -200.0
Maximum:  5.0   200.0
Elemental Composition Report

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Selected filters: None

Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100  H: 0-150  O: 2-2  Na: 1-1

Minimum:  -200.0
Maximum:   5.0  5.0  200.0

Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  Formula
313.1206 313.1204  0.2  0.6  11.5  19.3  C20 H18 O2 Na
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM  /  DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100  H: 0-150  O: 4-4  Na: 1-1

12030919 10 (0.187) AM (Cen,2, 80.00, Ht,5000.0,0.0.00,1.00); Sm (Mn, 2x1.00); Crn (10:20)

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<th>PPM</th>
<th>DBE</th>
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Minimum: -200.0
Maximum: 5.0 5.0 200.0
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM  /  DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100  H: 0-150  O: 2-2  F: 1-1  Na: 1-1

12030098 21 (0.391) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Cm (17:36)
281.0952

Minimum: 5.0  5.0  -200.0
Maximum: 200.0
Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  Formula
281.0952  281.0954  -0.2  -0.7  8.5  0.4  Cl6 H15 O2 F Na

(-)5k
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100  H: 0-150  O: 2-2  Na: 1-1  Cl: 1-1

-200.0

Minimum:
Maximum:

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Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100  H: 0-150  O: 2-2  Na: 1-1  Br: 1-1
x0.0156
12030911 15 (0.279) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Cm (14.36)

Minimum:
Maximum:
Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  Formula
341.0156  341.0153  0.3  0.9  8.5  1.8  C16 H15 O2 Na Br
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100  H: 0-150  O: 2-2  F: 3-3  Na: 1-1

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
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<th>PPM</th>
<th>DBE</th>
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Minimum: 5.0  5.0  -200.0
Maximum: 5.0  5.0  200.0
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100  H: 0-150  O: 5-5  Na: 1-1

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
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<th>PPM</th>
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<th>i-FIT</th>
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<td>C19 H22 O5 Na</td>
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Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100  H: 0-150  O: 3-3  F: 1-1  Na: 1-1

xf-4-92A
12035916 21 (0.391) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Cm (20:60)

Minimum:  5.0  -200.0
Maximum:  5.0  200.0

<table>
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<tr>
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**Elemental Composition Report**

**Single Mass Analysis (displaying only valid results)**

Tolerance = 5.0 PPM  /  DBE: min = -200.0, max = 200.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:
C: 0-100  H: 0-150  O: 2-2  F: 4-4  Na: 1-1

![Molecule Structure](image)

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3. Copy of HPLC for the Racemic and Chiral compounds (6a-6q).

**Area Percent Report**

- Sorted By: Signal
- Multiplier: 1.0000
- Dilution: 1.0000
- Use Multiplier x Dilution Factors with ETDs

Signal 1: Wavelength=230 nm

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<th>Area</th>
<th>Height</th>
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<th>mAU</th>
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End of Report

**Area Percent Report**

- Sorted By: Signal
- Multiplier: 1.0000
- Dilution: 1.0000
- Use Multiplier x Dilution Factors with ETDs

Signal 1: Wavelength=230 nm

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<tr>
<th>Peak RetTime Type</th>
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End of Report