Supporting Information
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Dehydrogenative Cross-Coupling Reactions of
N-Aryl α-Amino Acid Esters and Nitroalkanes for the
Synthesis of β-Nitro α-Amino Acid Esters

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Supporting Information

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1. General Information

Unless otherwise indicated, all reagents were purchased from commercial distributors and used without further purification. $^1$H NMR and $^{13}$C NMR were recorded at 400 MHz and 100 MHz respectively, using tetramethylsilane as an internal reference. Mass spectroscopy data were obtained on an HRMS-EI instrument. Melting points were uncorrected. Flash column chromatography was performed over silica gel 200-300 mesh. N-aryl glycine esters 1 were prepared according to the previous reported procedures.$^1$

2. General Procedure

**General procedure for the DCC reaction of N-aryl glycine esters 1 with nitroalkanes 2 for the synthesis of β-nitro α-amino acid esters 3:** To a mixture of CuI (3.8 mg, 0.02 mmol), N-aryl glycine esters 1 (0.2 mmol) and nitroalkanes 2 (2 mmol) in dichloromethane (1 mL) was added Et$_3$N (2.0 mg, 0.02 mmol). The reaction mixture was stirred at 30 °C under oxygen atmosphere for 24 h. After the reaction was completed, the resulting mixture was concentrated under vacuum, and the residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate as an eluent) to afford the corresponding products 3.

3. Characterization Data

**Ethyl 2-(p-tolylamino)-3-nitropropanoate (3aa)**

![Structure of ethyl 2-(p-tolylamino)-3-nitropropanoate (3aa)](image)

Brown oil; $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 7.03 (d, $J = 8.4$ Hz, 2H), 6.60 (dd, $J = 6.8$ Hz, $J = 2.0$ Hz, 2H), 4.87-4.75 (m, 2H), 4.63-4.58 (m, 1H), 4.39 (d, $J = 8.0$ Hz, 1H), 4.32-4.24 (m, 2H), 2.25 (s, 3H), 1.29 (t, $J = 7.2$, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 169.7, 142.9, 130.1, 129.1, 114.2, 75.7, 62.6, 55.4, 20.4, 14.1; HRMS (EI-TOF) $m/z$ calcd for C$_{12}$H$_{16}$N$_2$O$_4$ 252.1110, found 252.1107.

**Ethyl 2-(4-methoxyphenylamino)-3-nitropropanoate (3ba)**

![Structure of ethyl 2-(4-methoxyphenylamino)-3-nitropropanoate (3ba)](image)

Brown oil; $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 6.80 (dd, $J = 6.4$, $J = 2.0$, 2H), 6.66 (dd, $J = 6.8$, $J = 2.4$, 2H), 4.84-4.74
(m, 2H), 4.57-4.53 (m, 1H), 4.31-4.22 (m 3H), 3.74 (s, 3H), 1.28 (t, J = 7.2, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$): δ 169.8, 153.7, 139.3, 116.0, 115.0, 75.9, 62.6, 56.4, 55.7, 14.1; MS (EI) m/z (%) 268 (M$^+$), 208, 149(100%), 134, 77.

**Ethyl 2-(3,4-dimethoxyphenylamino)-3-nitropropanoate (3ca)**

![Ethyl 2-(3,4-dimethoxyphenylamino)-3-nitropropanoate (3ca)](image)

Brown oil; $^1$H NMR (400 MHz, CDCl$_3$): δ 6.75 (d, J = 8.4 Hz, 1H), 6.34 (d, J = 2.4 Hz, 1H), 6.20 (dd, J = 8.8 Hz, J = 2.8 Hz, 1H), 4.86-4.76 (m, 2H), 4.60-4.55 (m, 1H), 4.31-4.24 (m, 3H), 3.84 (s, 3H), 3.81 (s, 3H), 1.29 (t, J = 7.0, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$): δ 169.7, 150.2, 143.2, 139.8, 112.8, 104.8, 100.8, 75.8, 62.6, 56.5, 56.1, 55.8, 14.1; HRMS (EI-TOF) m/z calcd for C$_{13}$H$_{18}$N$_2$O$_6$ 298.1165, found 298.1165.

**Ethyl 2-(m-tolylamino)-3-nitropropanoate (3da)**

![Ethyl 2-(m-tolylamino)-3-nitropropanoate (3da)](image)

Brown oil; $^1$H NMR (400 MHz, CDCl$_3$): δ 7.10 (t, J = 7.6 Hz, 1H), 6.66 (d, J = 7.6 Hz, 1H), 6.48 (dd, J = 12.0 Hz, J = 4.0 Hz, 2H), 4.90-4.77 (m, 2H), 4.65-4.61 (m, 1H), 4.47(d, J = 8.0 Hz, 1H), 4.32-4.26 (m, 2H), 2.29 (s, 3H), 1.29 (t, J = 7.2 Hz, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$): δ 169.6, 145.2, 139.5, 129.5, 120.6, 114.7, 110.8, 75.6, 62.7, 54.9, 21.6, 14.1; HRMS (EI-TOF) m/z calcd for C$_{12}$H$_{16}$N$_2$O$_4$ 252.1110, found 252.1104.

**Ethyl 3-nitro-2-(phenylamino)propanoate (3ea)**

![Ethyl 3-nitro-2-(phenylamino)-3-nitropropanoate (3ea)](image)

Brown oil; $^1$H NMR (400 MHz, CDCl$_3$): δ 7.22 (t, J = 7.8 Hz, 2H), 6.83 (t, J = 7.4 Hz, 1H), 6.67 (d, J = 7.6 Hz, 2H), 4.89-4.76 (m, 2H), 4.67-4.62 (m, 1H), 4.52 (d, J = 8.0 Hz, 1H), 4.33-4.25 (m, 2H), 1.29 (t, J = 7.0 Hz, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$): δ 169.5, 145.2, 129.6, 119.7, 113.8, 75.6, 62.6, 54.9, 14.1; HRMS (EI-TOF) m/z calcd for C$_{11}$H$_{14}$N$_2$O$_4$ 238.0954, found 238.0956.

**Ethyl 2-[(1,1'-biphenyl)-4-ylamino)-3-nitropropanoate (3fa)**

![Ethyl 2-[(1,1'-biphenyl)-4-ylamino)-3-nitropropanoate (3fa)](image)

Light yellow soild; $^1$H NMR (400 MHz, CDCl$_3$): δ 7.53 (d, J = 8.4 Hz, 2H), 7.48 (dd, J = 6.4 Hz, J = 2.0 Hz, 2H), 7.41 (t, J = 7.8 Hz, 2H), 7.29 (t, J = 7.8 Hz, 1H), 6.76 (dd, J = 6.8 Hz, J = 2.0 Hz, 2H), 4.93-4.08 (m, 2H), 4.69 (t, J = 4.6 Hz, 1H), 4.35-4.28 (m, 2H), 1.31 (t, J = 7.2, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$): δ 169.5, 144.6, 140.7, 132.7,
128.8, 128.3, 126.6, 126.5, 114.1, 75.6, 62.8, 54.9, 14.1; HRMS (EI-TOF) m/z calcd for C_{17}H_{18}N_{2}O_{4} 314.1267, found 314.1264.

**Ethyl 2-(4-chlorophenylamino)-3-nitropropanoate (3ga)**

![Chemical Structure]

Brown oil; ^1^H NMR (400 MHz, CDCl₃): δ 7.17 (dd, J = 7.2 Hz, J = 2.0 Hz, 2H), 6.61 (d, J = 6.4 Hz, J = 2.0 Hz, 2H), 4.88-4.75 (m, 2H), 4.61-4.57 (m, 1H), 4.53 (d, J = 8.4 Hz, 1H), 4.33-4.25 (m, 2H), 1.30 (t, J = 7.2, 3H); ^1^C NMR (100 MHz, CDCl₃): δ 169.2, 143.9, 129.5, 124.5, 115.1, 75.5, 62.8, 55.0, 14.0; HRMS (EI-TOF) m/z calcd for C_{11}H_{13}ClN_{2}O_{4} 272.0564, found 272.0561.

**Ethyl 2-(4-bromophenylamino)-3-nitropropanoate (3ha)**

![Chemical Structure]

Brown oil; ^1^H NMR (400 MHz, CDCl₃): δ 7.30 (dd, J = 6.8 Hz, J = 2.4 Hz, 2H), 6.56 (d, J = 8.8 Hz, J = 2.0 Hz, 2H), 4.88-4.75 (m, 2H), 4.61-4.54 (m, 2H), 4.33-4.25 (m, 2H), 1.30 (t, J = 7.2, 3H); ^1^C NMR (100 MHz, CDCl₃): δ 169.2, 144.3, 132.4, 115.5, 111.6, 75.4, 62.9, 54.9, 14.1; HRMS (EI-TOF) m/z calcd for C_{11}H_{13}BrN_{2}O_{4} 316.0059, found 316.0056.

**Methyl 2-(p-tolylamino)-3-nitropropanoate (3ia)**

![Chemical Structure]

Brown oil; ^1^H NMR (400 MHz, CDCl₃): δ 7.03 (d, J = 8.0 Hz, 2H), 6.59 (dd, J = 6.8 Hz, J = 2.0 Hz, 2H), 4.87-4.76 (m, 2H), 4.65-4.61 (m, 1H), 4.38 (d, J = 8.4 Hz, 1H), 3.81 (s, 3H), 2.25 (s, 3H); ^1^C NMR (100 MHz, CDCl₃): δ 170.2, 142.9, 130.1, 129.2, 114.2, 75.6, 55.3, 53.3, 20.4; HRMS (EI-TOF) m/z calcd for C_{11}H_{16}N_{2}O_{4} 238.0954, found 238.0960.

**Isopropyl 2-(p-tolylamino)-3-nitropropanoate (3ja)**

![Chemical Structure]

Brown oil; ^1^H NMR (400 MHz, CDCl₃): δ 7.02 (d, J = 8.0 Hz, 2H), 6.59 (dd, J = 10.8 Hz, J = 2.4 Hz, 2H), 5.15-5.09 (m, 1H), 4.86-4.73 (m, 2H), 4.58-4.54 (m, 1H), 4.39 (d, J = 8.0 Hz, 1H), 2.25 (s, 3H), 1.27 (d, J = 3.6 Hz, 3H), 1.26 (d, J = 3.6 Hz, 3H); ^1^C NMR (100 MHz, CDCl₃): δ 169.1, 143.0, 130.1, 129.0, 114.1, 75.7, 70.7, 55.5, 21.6, 21.7, 20.4; HRMS (EI-TOF) m/z calcd for C_{13}H_{18}N_{2}O_{4} 266.1267, found 266.1264.
**tert-Butyl 2-(p-tolylamino)-3-nitropropanoate (3ka)**

Brown oil; $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 7.01 (d, $J = 8.0$ Hz, 2H), 6.58 (dd, $J = 9.2$ Hz, $J = 2.8$ Hz, 2H), 4.82-4.68 (m, 2H), 4.52-4.47 (m, 1H), 4.39 (d, $J = 7.6$ Hz, 1H), 2.24 (s, 3H), 1.47 (s, 9H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 168.6, 143.1, 130.1, 128.8, 114.0, 83.9, 75.8, 55.8, 27.9, 20.4; HRMS (EI-TOF) $m/z$ calcd for C$_{14}$H$_{20}$N$_2$O$_4$ 280.1423, found 266.1431.

**Benzyl 2-(p-tolylamino)-3-nitropropanoate (3la)**

Brown oil; $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 7.36-7.32 (m, 3H), 7.30-7.27 (m, 2H), 7.00 (d, $J = 8.4$ Hz, 2H), 6.57 (d, $J = 8.4$ Hz, 2H), 5.21 (s, 2H), 4.84-4.73 (m, 2H), 4.66-4.61 (m, 1H), 4.37 (d, $J = 8.4$ Hz, 1H), 4.32-4.24 (m, 2H), 2.24 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 169.7, 142.9, 134.7, 130.1, 129.2, 128.8, 128.7, 128.5, 114.3, 75.7, 55.5, 20.5; HRMS (EI-TOF) $m/z$ calcd for C$_{17}$H$_{18}$N$_2$O$_4$ 314.1267, found 314.1273.

**Ethyl 2-(p-tolylamino)-3-nitrobutanoate (3ab)**

Brown oil; $^1$H NMR (400 MHz, CDCl$_3$): dr = 2:1. Major diastereomer: $\delta$ 7.00 (d, $J = 8.0$ Hz, 2H), 6.61 (dd, $J = 6.4$ Hz, $J = 2.0$ Hz, 2H), 4.95-4.88 (m, 1H), 4.72-4.69 (m, 1H), 4.27-4.19 (m, 3H), 2.24 (s, 3H), 1.63 (d, $J = 6.8$ Hz, 3H), 1.27 (t, $J = 7.2$, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 169.9, 143.6, 130.0, 129.4, 114.9, 83.0, 62.4, 60.9, 20.4, 14.3, 14.1; Minor diastereomer: $\delta$ 7.02 (d, $J = 8.0$ Hz, 2H), 6.65 (dd, $J = 6.4$ Hz, $J = 2.0$ Hz, 2H), 4.99-4.93 (m, 1H), 4.56-4.54 (m, 1H), 4.34 (d, $J = 9.2$ Hz, 1H), 4.28-4.18 (m, 2H), 2.25 (s, 3H), 1.60 (d, $J = 6.8$ Hz, 3H), 1.26 (t, $J = 7.0$, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 169.8, 143.4, 130.6, 129.0, 114.2, 82.5, 62.3, 60.5, 20.4, 14.6, 14.1; HRMS (EI-TOF) $m/z$ calcd for C$_{13}$H$_{18}$N$_2$O$_4$ 266.1267, found 266.1262.

**Ethyl 2-(4-methoxyphenylamino)-3-nitrobutanoate (3bb)**

Brown oil; $^1$H NMR (400 MHz, CDCl$_3$): dr = 2:1. Major diastereomer: $\delta$ 6.80 (dd, $J = 6.8$ Hz, $J = 2.4$ Hz, 2H), 6.70 (dd, $J = 6.8$ Hz, $J = 2.4$ Hz, 2H), 4.98-4.91 (m, 1H), 4.48-4.46 (m, 1H), 4.28-4.18 (m, 3H), 3.74 (s, 3H), 1.62 (d, $J = 6.8$ Hz, 3H), 1.27 (t, $J$
= 7.2, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 170.0, 153.6, 139.7, 116.0, 115.0, 82.8, 62.3, 61.6, 55.7, 14.9, 14.1; Minor diastereomer: $\delta$ 6.78 (dd, $J = 6.4$ Hz, $J = 2.4$ Hz, 2H), 6.70 (dd, $J = 6.8$ Hz, $J = 2.4$ Hz, 2H), 4.94-4.88 (m, 1H), 4.67-4.64 (m, 1H), 4.27-4.19 (m, 2H), 4.15 (d, $J = 6.0$ Hz, 1H), 3.74 (s, 3H), 1.62 (d, $J = 7.2$ Hz, 3H), 1.27 (t, $J = 7.2$, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 170.1, 153.9, 139.9, 116.9, 114.9, 82.9, 62.4, 62.1, 55.7, 14.1(2C); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 169.8, 143.4, 130.6, 129.0, 114.2, 82.5, 62.3, 60.5, 20.4, 14.6, 14.1; HRMS (EI-TOF) m/z calcd for C$_{13}$H$_{18}$N$_2$O$_5$ 266.1216, found 266.1212.

4. References
5. $^1$H NMR, $^{13}$C NMR and HR-MS Spectra of Products

$^1$H NMR Spectra of ethyl 2-(p-tolylamino)-3-nitropropanoate (3aa)
\(^{13}\)C NMR Spectra of ethyl 2-(p-tolylamino)-3-nitropropanoate (3aa)
Elemental Composition Report

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
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$^1$H NMR Spectra of ethyl 2-(4-methoxyphenylamino)-3-nitropropanoate (3ba)
$^{13}$C NMR Spectra of ethyl 2-(4-methoxyphenylamino)-3-nitropropanoate (3ba)
$^1$H NMR Spectra of ethyl 2-(3,4-dimethoxyphenylamino)-3-nitropropanoate (3ca)
$^{13}$C NMR Spectra of ethyl 2-(3,4-dimethoxyphenylamino)-3-nitropropanoate (3ca)
Elemental Composition Report

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
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$^{13}$C NMR Spectra of ethyl 2-($m$-tolylamino)-3-nitropropanoate (3da)
### Elemental Composition Report

**Monoisotopic Mass, Odd and Even Electron Ions**
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TOF MS El^+ 3.55e+03
$^1$H NMR Spectra of ethyl 3-nitro-2-(phenylamino)propanoate (3ea)
$^{13}$C NMR Spectra of ethyl 3-nitro-2-(phenylamino)propanoate (3ea)
Elemental Composition Report

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
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$^1$H NMR Spectra of ethyl 2-([1,1'-biphenyl]-4-ylamino)-3-nitropropanoate (3fa)
$^{13}$C NMR Spectra of ethyl 2-(4-chlorophenylamino)-3-nitropropanoate (3fa)
**Spectra of ethyl 2-(4-chlorophenylamino)-3-nitropropanoate (3fa)**

Tolerance = 1.0 mDa  /  DBE: min = -1.5, max = 50.0  
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions  
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GCT Premier ZJU  
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22-Apr-2016  

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$^1$H NMR Spectra of ethyl 2-(4-bromophenylamino)-3-nitropropanoate (3ga)
$^{13}$C NMR Spectra of ethyl 2-(4-bromophenylamino)-3-nitropropanoate (3ga)
Elemental Composition Report

Tolerance = 0.4 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
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$^1$H NMR Spectra of ethyl 2-(4-chlorophenylamino)-3-nitropropanoate (3ha)
$^{13}$C NMR Spectra of ethyl 2-(4-chlorophenylamino)-3-nitropropanoate (3ha)
Elemental Composition Report

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
78 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
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<td>5548162.0 C11 H13 N2 O4 Cl</td>
<td></td>
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</table>
$^1$H NMR Spectra of methyl 2-(p-tolylamino)-3-nitropropanoate (3ia)
$^{13}$C NMR Spectra of methyl 2-(p-tolylamino)-3-nitropropanoate (3ia)
Elemental Composition Report

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron ions
95 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-100  H: 0-200  N: 0-4  O: 0-5
Default file
zzq010613192 (2.162)

Minimum: 1.0  10.0  50.0
Maximum: -1.5

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<th>Formula</th>
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<td>238.0960</td>
<td>238.0954</td>
<td>0.6</td>
<td>2.5</td>
<td>6.0</td>
<td>5549967.0</td>
<td>C11 H14 N2 O4</td>
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$^1$H NMR Spectra of isopropyl 2-(p-tolylamino)-3-nitropropanoate (3ja)
\(^{13}\)C NMR Spectra of isopropyl 2-(p-tolylamino)-3-nitropropanoate (3ja)
Elemental Composition Report

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
96 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:
C: 0-100   H: 0-200   N: 0-3   O: 0-6

Default file
zzq01062 189 (2.136)

TOF MS El+
3.84e+002

Minimum:
Maximum:

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<td>266.1267</td>
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<td>5546192.5</td>
<td>C13 H18 N2 O4</td>
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$^1$H NMR Spectra of tert-butyl 2-((p-tolylamino)-3-nitropropanoate (3ka)
$^{13}$C NMR Spectra of tert-butyl 2-(p-tolylamino)-3-nitropropanoate (3ka)
**Elemental Composition Report**

**Tolerance** = 1.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
101 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-100  H: 0-200  N: 0-3  O: 0-6
Default file
zzq01063 186 (2.110)

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$^1$H NMR Spectra of benzyl 2-($p$-tolylamino)-3-nitropropanoate (3la)
\( ^{13} \text{C NMR Spectra of benzyl 2-(p-tolylamino)-3-nitropropanoate (3la)} \)
**Elemental Composition Report**

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
112 formula(s) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:
C: 0-100  H: 0-200  N: 0-3  O: 0-6

Default file
zzq01064 255 (2.708)

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<th>DBE</th>
<th>i-FIT</th>
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<tbody>
<tr>
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<td>1.9</td>
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<td>5546835.0</td>
<td>C17 H18 N2 O4</td>
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TOF MS El+ 1.68e+003
$^1$H NMR Spectra of major diastereomer: Ethyl 2-(p-tolylamino)-3-nitrobutanoate (3ab)
$^{13}$C NMR Spectra of major diastereomer: Ethyl 2-(p-tolylamino)-3-nitrobutanoate (3ab)
$^1$H NMR Spectra of minor diastereomer: Ethyl 2-(p-tolylamino)-3-nitrobutanoate (3ab)
$^{13}$C NMR Spectra of minor diastereomer: Ethyl 2-($p$-tolylamino)-3-nitrobutanoate (3ab)
Elemental Composition Report

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
86 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-100  H: 0-200  N: 0-3  O: 0-5
Default file
zzq010612 189 (2.136)  

TOF MS EI-
6.72e+003

Minimum: 1.0 10.0 -1.5
Maximum: 0 10.0 50.0

Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  Formula
266.1262 266.1267  -0.5  -1.9  6.0  5549380.0  C13  H18  N2  O4

IR-MS Spectra of ethyl 2-(p-tolylamino)-3-nitrobutanoate (3ab)
$^1$H NMR Spectra of major diastereomer: Ethyl 2-(4-methoxyphenylamino)-3-nitrobutanoate (3bb)
$^{13}$C NMR Spectra of major diastereomer: Ethyl 2-(4-methoxyphenylamino)-3-nitrobutanoate (3bb)
$^1$H NMR Spectra of minor diastereomer: Ethyl 2-(4-methoxyphenylamino)-3-nitrobutanoate (3bb)
$^{13}$C NMR Spectra of minor diastereomer: Ethyl 2-(4-methoxyphenylamino)-3-nitrobutanoate (3bb)
Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
102 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-100   H: 0-200   N: 0-3   O: 0-6
Default file
zze01065 203 (2.258)

TOF MS El+
9.22e+002

Minimum: 1.0 10.0 -1.5
Maximum: 50.0

Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  Formula
282.1212  282.1216  -0.4  -1.4  6.0  5546460.5  C13 H18 N2 O5