

Supporting Information for

Aminoindanol-based chiral derivatizing agents for the determination of the absolute configuration of carboxylic acids

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Characterization Data for 2a and 2b Esters:

(1R,2S)-2a ester of (S)-2-methylbutyric acid ((1R,2S)-2a-A)

¹H NMR (400 MHz, CDCl₃): δ = 7.81-7.83 (m, 2 H), 7.71-7.74 (m, 2 H), 7.31-7.33 (m, 2 H), 7.21-7.23 (m, 2 H), 5.98 [d, ³J(H,H) = 8.1 Hz, 1 H], 5.65-5.71 (m, 1 H), 3.49 [d, ³J(H,H) = 7.4 Hz, 2 H], 2.15-2.23 (m, 1 H), 1.33-1.44 (m, 1 H), 1.11-1.21 (m, 1 H), 0.92 [d, ³J(H,H) = 7.0 Hz, 3 H], 0.59 [t, ³J(H,H) = 7.4 Hz, 3 H]. MS(ESI): *m/z* 386.1 [M+Na]⁺.

(1S,2R)-2a ester of (S)-2-methylbutyric acid ((1S,2R)-2a-A)

¹H NMR (400 MHz, CDCl₃): δ = 7.80-7.83 (m, 2 H), 7.70-7.74 (m, 2 H), 7.30-7.33 (m, 2 H), 7.20-7.23 (m, 2 H), 5.98 [d, ³J(H,H) = 8.1 Hz, 1H], 5.64-5.70 (m, 1 H), 3.49 [d, ³J(H,H) = 7.5 Hz, 2 H], 2.14-2.23 (m, 1 H), 1.38-1.49 (m, 1 H), 1.20-1.30 (m, 1 H), 0.81 [d, ³J(H,H) = 7.0 Hz, 3 H], 0.72 [t, ³J(H,H) = 7.4 Hz, 3 H]. MS(ESI): *m/z* 386.1 [M+Na]⁺.

(1R,2S)-2a ester of Boc-L-valine ((1R,2S)-2a-B)

¹H NMR (400 MHz, CDCl₃): δ = 7.80-7.83 (m, 2 H), 7.70-7.75 (m, 2 H), 7.30-7.35 (m, 2 H), 7.19-7.24 (m, 2 H), 5.99 [d, ³J(H,H) = 8.2 Hz, 1 H], 5.67-5.77 (m, 1 H), 4.89 [d, ³J(H,H) = 9.3 Hz, 1H], 4.13-4.17 (m, 1 H), 3.58 [dd, ²J(H,H) = 16.2 Hz, ³J(H,H) = 6.9 Hz, 1 H], 3.48 [dd, ²J(H,H) = 16.2 Hz, ³J(H,H) = 7.9 Hz, 1 H], 1.71-1.78 (m, 1 H), 1.39 (s, 9 H), 0.71 [d, ³J(H,H) = 6.8 Hz, 3 H], 0.44 [d, ³J(H,H) = 6.8 Hz, 3 H]. MS(ESI): *m/z* 501.2 [M+Na]⁺.

(1S,2R)-2a ester of Boc-L-valine ((1S,2R)-2a-B)

¹H NMR (400 MHz, CDCl₃): δ = 7.80-7.84 (m, 2 H), 7.69-7.73 (m, 2 H), 7.29-7.34 (m, 2 H), 7.19-7.24 (m, 2 H), 5.98 [d, ³J(H,H) = 8.0 Hz, 1 H], 5.65-5.74 (m, 1 H), 4.83 [d, ³J(H,H) = 8.9 Hz, 1H], 3.95-3.98 (m, 1 H), 3.49-3.52 (m, 2 H), 1.90-1.98 (m, 1 H), 1.35 (s, 9 H), 0.79 [d, ³J(H,H) = 6.8 Hz, 3H], 0.73 [d, ³J(H,H) = 6.9 Hz, 3H]. MS(ESI): *m/z* 501.2 [M+Na]⁺.

(1R,2S)-2a ester of (S)-2-phenylbutyric acid ((1R,2S)-2a-C)

¹H NMR (400 MHz, CDCl₃): δ = 7.60-7.67 (m, 4 H), 7.27-7.29 (m, 2 H), 7.10-7.19 (m, 2 H), 6.95 [d, ³J(H,H) = 7.0 Hz, 2 H], 6.83 [t, ³J(H,H) = 7.2 Hz, 2 H], 6.75-6.79 (m, 1 H), 5.89 [d, ³J(H,H) = 8.2 Hz, 1 H], 5.64-5.72 (m, 1 H), 3.57 [dd, ²J(H,H) = 16.0 Hz, ³J(H,H) = 7.0 Hz, 1 H], 3.44 [dd, ²J(H,H) = 16.0 Hz, ³J(H,H) = 8.0 Hz, 1 H], 3.30 [t, ³J(H,H) = 7.7 Hz, 1 H], 1.89-2.00 (m, 1 H), 1.56-1.68 (m, 1 H), 0.74 [t, ³J(H,H) = 7.3 Hz, 3 H]. MS(ESI): *m/z* 448.1 [M+Na]⁺.

(1S,2R)-2a ester of (S)-2-phenylbutric acid ((1S,2R)-2a-C)

¹H NMR (400 MHz, CDCl₃): δ = 7.71-7.79 (m, 4 H), 7.28-7.31 (m, 2 H), 7.17-7.21 (m, 2 H), 7.05 (s, 5 H), 5.94 [d, ³J(H,H) = 8.0 Hz, 1H], 5.56-5.66 (m, 1 H), 3.42 [d, ³J(H,H) = 7.6 Hz, 2H], 3.27 [t, ³J(H,H) = 7.7 Hz, 1 H], 1.79-1.91 (m, 1 H), 1.53-1.64 (m, 1 H), 0.62 [t, ³J(H,H) = 7.4 Hz, 3H]. MS(ESI): *m/z* 448.1 [M+Na]⁺.

(1R,2S)-2a ester of N,N-dimethyl-L-phenylalanine ((1R,2S)-2a-D)

¹H NMR (400 MHz, CDCl₃): δ = 7.78-7.81 (m, 2 H), 7.70-7.73 (m, 2 H), 7.28-7.34 (m, 2 H), 7.18-7.23 (m, 2 H), 7.06-7.13 (m, 3 H), 6.96 [d, ³J(H,H) = 7.5 Hz, 2 H], 5.92 [d, ³J(H,H) = 8.0 Hz, 1 H], 5.58-5.64 (m, 1 H), 3.48 [dd, ²J(H,H) = 16.2 Hz, ³J(H,H) = 7.6 Hz, 1 H], 3.40 [dd, ²J(H,H) = 16.2 Hz, ³J(H,H) = 6.4 Hz, 1 H], 3.27-3.31 (m, 1 H), 2.76 [dd, ²J(H,H) = 13.6 Hz, ³J(H,H) = 8.6 Hz, 1H], 2.67 [dd, ²J(H,H) = 13.6 Hz, ³J(H,H) = 6.8 Hz, 1 H], 2.18 (s, 6 H). MS(ESI): *m/z* 477.1 [M+Na]⁺.

(1S,2R)-2a ester of N,N-dimethyl-L-phenylalanine ((1S,2R)-2a-D)

¹H NMR (400 MHz, CDCl₃): δ = 7.78-7.81 (m, 2 H), 7.68-7.73 (m, 2 H), 7.27-7.31 (m, 2 H), 7.18-7.25 (m, 5 H), 7.5 [d, ³J(H,H) = 7.2 Hz, 2 H], 5.94 [d, ³J(H,H) = 8.0 Hz, 1 H], 5.54-5.62 (m, 1 H), 3.23-3.30 (m, 2 H), 3.16 [dd, ²J(H,H) = 16.2 Hz, ³J(H,H) = 6.7 Hz, 1 H], 2.85 [dd, ²J(H,H) = 13.4 Hz, ³J(H,H) = 9.2 Hz, 1 H], 2.76 [dd, ²J(H,H) = 13.4 Hz, ³J(H,H) = 6.3 Hz, 1 H], 2.03 (s, 6 H). MS(ESI): *m/z* 477.2 [M+Na]⁺.

(1R,2S)-2b of (S)-2-methylbutyric acid ((1R,2S)-2b-A)

¹H NMR (400 MHz, [D₆]DMSO): δ = 8.31-8.63 (m, 4 H), 7.80-7.96 (m, 2 H), 7.14-7.33 (m, 4 H), 6.75 [d, ³J(H,H) = 9.0 Hz, 1 H], 5.72-5.78 (m, 1 H), 3.51 [dd, ²J(H,H) = 16.1 Hz, ³J(H,H) = 8.4 Hz, 1 H], 3.40 [dd, ²J(H,H) = 16.1 Hz, ³J(H,H) = 6.4 Hz, 1 H], 1.98-2.06 (m, 1 H), 1.02-1.13 (m, 1 H), 0.83-0.93 (m, 1 H), 0.69 [d, ³J(H,H) = 6.7 Hz, 3 H], 0.19 [t, ³J(H,H) = 7.4 Hz, 3 H]. MS(ESI): *m/z* 436.3 [M+Na]⁺.

(1S,2R)-2b ester of (S)-2-methylbutyric acid ((1S,2R)-2b-A)

¹H NMR (400 MHz, [D₆]DMSO): δ = 8.33-8.62 (m, 4 H), 7.82-7.94 (m, 2 H), 7.13-7.33 (m, 4 H), 6.75 [d, ³J(H,H) = 9.4 Hz, 1 H], 5.71-5.77 (m, 1 H), 3.51 [dd, ²J(H,H) = 16.1 Hz, ³J(H,H) = 8.3 Hz, 1 H], 3.38 [dd, ²J(H,H) = 16.1 Hz, ³J(H,H) = 6.5 Hz, 1 H], 1.99-2.07 (m, 1 H), 0.98-1.19 (m, 2 H), 0.49 [d, ³J(H,H) = 7.1 Hz, 3 H], 0.46 [t, ³J(H,H) = 7.4 Hz, 3 H]. MS(ESI): *m/z* 436.3 [M+Na]⁺.

(1R,2S)-2b ester of Boc-L-valine ((1R,2S)-2b-B)

¹H NMR (400 MHz, [D₆]DMSO): δ = 8.33-8.61 (m, 4 H), 7.82-7.94 (m, 2 H), 7.13-7.33 (m, 4 H), 6.87 [d, ³J(H,H) = 8.4 Hz, 1H], 6.77 [d, ³J(H,H) = 9.3 Hz, 1 H], 5.78-5.84 (m, 1 H), 3.67-3.70 (m, 1 H), 3.52 [dd, ²J(H,H) = 16.2 Hz, ³J(H,H) = 7.9 Hz, 1 H], 3.42 [dd, ²J(H,H) = 16.2 Hz, ³J(H,H) = 6.5 Hz, 1 H], 1.42-1.50 (m, 1 H), 1.30 (s, 9 H), 0.30 [d, ³J(H,H) = 6.6 Hz, 3 H], 0.04 [d, ³J(H,H) = 6.6 Hz, 3 H]. MS(ESI): *m/z* 551.3 [M+Na]⁺.

(1S,2R)-2b ester of Boc-L-valine ((1S,2R)-2b-B)

¹H NMR (400 MHz, [D₆]DMSO): δ = 8.29-8.58 (m, 4 H), 7.79-7.90 (m, 2 H), 7.12-7.32 (m, 4 H), 6.89 [d, ³J(H,H) = 7.3, 1 H], 6.76 [d, ³J(H,H) = 9.1 Hz, 1 H], 5.74-5.80 (m, 1 H), 3.50 [dd, ²J(H,H) = 16.3 Hz, ³J(H,H) = 8.2 Hz, 1 H], 3.36-3.43 (m, 2 H), 1.62-1.72 (m, 1 H), 1.07 (s, 9 H), 0.66 [d, ³J(H,H) = 6.8 Hz, 3 H], 0.55 [d, ³J(H,H) = 6.8 Hz, 3 H]. MS(ESI): *m/z* 551.4 [M+Na]⁺.

(1R,2S)-2b ester of (S)-2-phenylbutric acid ((1R,2S)-2b-C)

¹H NMR (400 MHz, [D₆]DMSO): δ = 8.14-8.47 (m, 4 H), 7.74-7.91 (m, 2 H), 7.06-7.31 (m, 4 H), 6.66-6.70 (m, 3 H), 6.26-6.34 (m, 3 H), 5.73-5.83 (m, 1 H), 3.48 [dd, ²J(H,H) = 14.6 Hz, ³J(H,H) = 7.3 Hz, 1 H], 3.43 [dd, ²J(H,H) = 14.6 Hz, ³J(H,H) = 6.0 Hz, 1 H], 3.21-3.28 (m, 1 H), 1.62-1.75 (m, 1 H), 1.32-1.43 (m, 1 H), 0.55 [t, ³J(H,H) = 7.2 Hz, 3 H]. MS(ESI): *m/z* 498.3 [M+Na]⁺.

(1S,2R)-2b ester of (S)-2-phenylbutric acid ((1S,2R)-2b-C)

¹H NMR (400 MHz, [D₆]DMSO): δ = 8.30-8.59 (m, 4 H), 7.84-7.96 (m, 2 H), 7.10-7.30 (m, 4 H), 6.86 [d, ³J(H,H) = 7.7 Hz, 2 H], 6.70-6.77 (m, 4 H), 5.65-5.74 (m, 1 H), 3.48 [dd, ²J(H,H) = 16.2 Hz, ³J(H,H) = 8.5 Hz, 1 H], 3.26 [dd, ²J(H,H) = 16.2 Hz, ³J(H,H) = 7.8 Hz, 1 H], 3.16-3.22 (m, 1 H), 1.47-1.59 (m, 1 H), 1.20-1.30 (m, 1 H), 0.33 [t, ³J(H,H) = 7.3 Hz, 3 H]. MS(ESI): *m/z* 498.3 [M+Na]⁺.

(1R,2S)-2b ester of N,N-dimethyl-L-phenylalanine ((1R,2S)-2b-D)

¹H NMR (400 MHz, [D₆]DMSO): δ = 8.34-8.62 (m, 4 H), 7.82-7.95 (m, 2 H), 7.10-7.35 (m, 5 H), 6.97 [d, ³J(H,H) = 5.1 Hz, 2 H], 6.76 [d, ³J(H,H) = 9.0 Hz, 1 H], 6.73 [d, ³J(H,H) = 5.8 Hz, 2 H], 5.69-5.75 (m, 1 H), 3.50 [dd, ²J(H,H) = 16.2 Hz, ³J(H,H) = 8.3 Hz, 1 H], 3.31 [dd, ²J(H,H) = 16.2 Hz, ³J(H,H) = 6.2 Hz, 1 H], 3.16 [t, ³J(H,H) = 7.4 Hz, 1 H], 2.30-2.42 (m, 2 H), 1.89 (s, 6 H). MS(ESI): *m/z* 505.3 [M+H]⁺.

(1S,2R)-2b ester of N,N-dimethyl-L-phenylalanine ((1S,2R)-2b-D)

¹H NMR (400 MHz, [D₆]DMSO): δ = 8.30-8.62 (m, 4 H), 7.80-7.93 (m, 2 H), 7.16-7.29 (m, 5 H), 7.13 [d, ³J(H,H) = 6.7 Hz, 2 H], 6.88 [d, ³J(H,H) = 7.2 Hz, 2 H], 6.75 [d, ³J(H,H) = 9.1 Hz, 1 H], 5.66-5.73 (m, 1 H), 3.38 [dd, ²J(H,H) = 16.0 Hz, ³J(H,H) = 8.6 Hz, 1 H], 3.20 [dd, ²J(H,H) = 16.0 Hz, ³J(H,H) = 6.5 Hz, 1 H], 3.10 [t, ³J(H,H) = 7.6 Hz, 1 H], 2.49-2.60 (m, 2 H), 1.65 (s, 6 H). MS(ESI): *m/z* 505.3 [M+H]⁺.

(1R,2S)-2b ester of (R)-2-phenoxypropionic acid ((1R,2S)-2b-E)

¹H NMR (400 MHz, [D₆]DMSO): δ = 8.30-8.61 (m, 4 H), 7.82-7.86 (m, 2 H), 7.12-7.31 (m, 4 H), 6.76 [d, ³J(H,H) = 9.1 Hz, 1 H], 6.70 [t, ³J(H,H) = 7.2 Hz, 2 H], 6.63-6.68 (m, 1 H), 6.31 [d, ³J(H,H) = 7.8 Hz, 2 H], 5.76-5.82 (m, 1 H), 4.60-4.65 (m, 1 H), 3.32-3.51 (m, 2 H), 1.16 [d, ³J(H,H) = 6.8 Hz, 3 H]. MS(ESI): *m/z* 500.2 [M+Na]⁺.

(1S,2R)-2b ester of (R)-2-phenoxypropionic acid ((1S,2R)-2b-E)

¹H NMR (400 MHz, [D₆]DMSO): δ = 8.30-8.55 (m, 4 H), 7.82-7.94 (m, 2 H), 7.12-7.34 (m, 4 H), 6.94 [t, ³J(H,H) = 7.5 Hz, 2 H], 6.73 [d, ³J(H,H) = 8.9 Hz, 1 H], 6.66 [t, ³J(H,H) = 7.3 Hz, 1 H], 6.45 [d, ³J(H,H) = 8.3 Hz, 2 H], 5.76-5.85 (m, 1 H), 4.70-4.79 (m, 1 H), 3.55 [dd, ²J(H,H) = 16.1 Hz, ³J(H,H) = 8.3 Hz, 1 H], 3.47 [dd, ²J(H,H) = 16.1 Hz, ³J(H,H) = 6.6 Hz, 1 H], 0.94 [d, ³J(H,H) = 6.8 Hz, 3 H]. MS(ESI): *m/z* 500.2 [M+Na]⁺.

(1R,2S)-2b ester of Boc-L-leucine ((1R,2S)-2b-F)

¹H NMR (400 MHz, [D₆]DMSO): δ = 8.34-8.61 (m, 4 H), 7.81-7.95 (m, 2 H), 7.13-7.34 (m, 4 H), 7.05 [d, ³J(H,H) = 8.1 Hz, 1 H], 6.75 [d, ³J(H,H) = 9.2 Hz, 1 H], 5.78-5.86 (m, 1 H), 3.66-3.72 (m, 1 H), 3.49 [d, ³J(H,H) = 7.8 Hz, 2 H], 1.31 (s, 9 H), 1.02-1.10 (m, 1 H), 0.69-0.76 (m, 1 H), 0.44-0.52 (m, 1 H), 0.12 [d, ³J(H,H) = 6.5 Hz, 3 H], -0.30 [d, ³J(H,H) = 6.6 Hz, 3 H]. MS(ESI): *m/z* 565.4 [M+Na]⁺.

(1S,2R)-2b ester of Boc-L-leucine ((1S,2R)-2b-F)

^1H NMR (400 MHz, $[\text{D}_6]\text{DMSO}$): δ = 8.31-8.62 (m, 4 H), 7.80-7.93 (m, 2 H), 7.13-7.33 (m, 4 H), 7.07 [d, $^3J(\text{H,H})$ = 7.3 Hz, 1 H], 6.78 [d, $^3J(\text{H,H})$ = 9.3 Hz, 1 H], 5.64-5.72 (m, 1 H), 3.45-3.56 (m, 2 H), 3.37 [dd, $^2J(\text{H,H})$ = 16.0 Hz, $^3J(\text{H,H})$ = 6.3 Hz, 1 H], 1.22 (s, 9 H), 1.18-1.21 (m, 1 H), 1.03-1.10 (m, 1 H), 0.72-0.79 (m, 1 H), 0.27 [d, $^3J(\text{H,H})$ = 6.4 Hz, 3 H], 0.19 [d, $^3J(\text{H,H})$ = 6.5 Hz, 3 H]. MS(ESI): m/z 565.3 $[\text{M}+\text{Na}]^+$.

(1R,2S)-2b ester of (S)-2-acetoxypionic acid ((1R,2S)-2b-G)

^1H NMR (400 MHz, $[\text{D}_6]\text{DMSO}$): δ = 8.31-8.64 (m, 4 H), 7.83-7.94 (m, 2 H), 7.13-7.33 (m, 4 H), 6.76 [d, $^3J(\text{H,H})$ = 8.9 Hz, 1 H], 5.76-5.84 (m, 1 H), 4.70-4.79 (m, 1 H), 3.52 [dd, $^2J(\text{H,H})$ = 16.2 Hz, $^3J(\text{H,H})$ = 8.3 Hz, 1 H], 3.45 [dd, $^2J(\text{H,H})$ = 16.2 Hz, $^3J(\text{H,H})$ = 7.4 Hz, 1 H], 1.63 (s, 3 H), 0.81 [d, $^3J(\text{H,H})$ = 7.1 Hz, 3 H]. MS(ESI): m/z 466.2 $[\text{M}+\text{Na}]^+$.

(1S,2R)-2b ester of (S)-2-acetoxypionic acid ((1S,2R)-2b-G)

^1H NMR (400 MHz, $[\text{D}_6]\text{DMSO}$): δ = 8.32-8.62 (m, 4 H), 7.81-7.95 (m, 2 H), 7.13-7.33 (m, 4 H), 6.77 [d, $^3J(\text{H,H})$ = 9.2 Hz, 1 H], 5.72-5.80 (m, 1 H), 4.63-4.71 (m, 1 H), 3.52 [dd, $^2J(\text{H,H})$ = 16.1 Hz, $^3J(\text{H,H})$ = 8.5 Hz, 1 H], 3.35 [dd, $^2J(\text{H,H})$ = 16.1 Hz, $^3J(\text{H,H})$ = 6.6 Hz, 1 H], 1.61 (s, 3 H), 0.99 [d, $^3J(\text{H,H})$ = 7.0 Hz, 3 H]. MS(ESI): m/z 466.2 $[\text{M}+\text{Na}]^+$.

(1R,2S)-2b ester of Cbz-L-alanine ((1R,2S)-2b-H)

^1H NMR (400 MHz, $[\text{D}_6]\text{DMSO}$): δ = 8.31-8.61 (m, 4 H), 7.79-7.94 (m, 2 H), 7.52 [d, $^3J(\text{H,H})$ = 7.0 Hz, 1 H], 7.25-7.35 (m, 5 H), 7.24 [d, $^3J(\text{H,H})$ = 6.8 Hz, 2 H], 7.13-7.20 (m, 2 H), 6.77 [d, $^3J(\text{H,H})$ = 9.0 Hz, 1 H], 5.73-5.83 (m, 1 H), 4.82 [d, $^2J(\text{H,H})$ = 12.6 Hz, 1 H], 4.76 [d, $^2J(\text{H,H})$ = 12.6 Hz, 1 H], 3.80-3.91 (m, 1 H), 3.50 [d, $^3J(\text{H,H})$ = 7.4 Hz, 2 H], 0.57 [d, $^3J(\text{H,H})$ = 7.2 Hz, 3 H]. MS(ESI): m/z 557.3 $[\text{M}+\text{Na}]^+$.

(1S,2R)-2b ester of Cbz-L-alanine ((1S,2R)-2b-H)

^1H NMR (400 MHz, $[\text{D}_6]\text{DMSO}$): δ = 8.29-8.57 (m, 4 H), 7.77-7.88 (m, 2 H), 7.50 [d, $^3J(\text{H,H})$ = 6.7 Hz, 1 H], 7.14-7.34 (m, 7 H), 7.10 [d, $^3J(\text{H,H})$ = 6.6 Hz, 2 H], 6.79 [d, $^3J(\text{H,H})$ = 9.0 Hz, 1 H], 5.67-5.73 (m, 1 H), 4.46 (s, 2 H), 3.65-3.72 (m, 1 H), 3.39-3.53 (m, 2 H), 0.93 [d, $^3J(\text{H,H})$ = 7.2 Hz, 3 H]. MS(ESI): m/z 557.3 $[\text{M}+\text{Na}]^+$.

(1R,2S)-2b ester of (R)- α -methoxyphenylacetic acid ((1R,2S)-2b-I)

^1H NMR (400 MHz, $[\text{D}_6]\text{DMSO}$): δ = 8.29-8.56 (m, 4 H), 7.84-7.94 (m, 2 H), 7.12-7.30 (m, 4 H), 6.91 [d, $^3J(\text{H,H})$ = 8.2 Hz, 2 H], 6.86-6.91 (m, 1 H), 6.78 [t, $^3J(\text{H,H})$ = 7.4 Hz, 2 H], 6.74 [d, $^3J(\text{H,H})$ = 9.7 Hz, 1 H], 5.71-5.77 (m, 1 H), 4.57 (s, 1 H), 3.49 [dd, $^2J(\text{H,H})$ = 16.1 Hz, $^3J(\text{H,H})$ = 8.3 Hz, 1 H], 3.34 [dd, $^2J(\text{H,H})$ = 16.1 Hz, $^3J(\text{H,H})$ = 6.0 Hz, 1 H], 2.84 (s, 3 H). MS(ESI): m/z 500.2 $[\text{M}+\text{Na}]^+$.

(1S,2R)-2b ester of (R)- α -methoxyphenylacetic acid ((1S,2R)-2b-I)

^1H NMR (400 MHz, $[\text{D}_6]\text{DMSO}$): δ = 8.14-8.50 (m, 4 H), 7.77-7.92 (m, 2 H), 7.09-7.30 (m, 4 H), 6.78 [d, $^3J(\text{H,H})$ = 6.2 Hz, 2 H], 6.66 [d, $^3J(\text{H,H})$ = 9.1 Hz, 1 H], 6.29 [t, $^3J(\text{H,H})$ = 7.3 Hz, 2 H], 6.25-6.30 (m, 1 H), 5.81-5.87 (m, 1 H), 4.64 (s, 1 H), 3.42-3.53 (m, 2 H), 3.03 (s, 3 H). MS(ESI): m/z 500.2 $[\text{M}+\text{Na}]^+$.

(1R,2S)-2b ester of (S)-3-acetylthio-2-methylpropionic acid ((1R,2S)-2b-J)

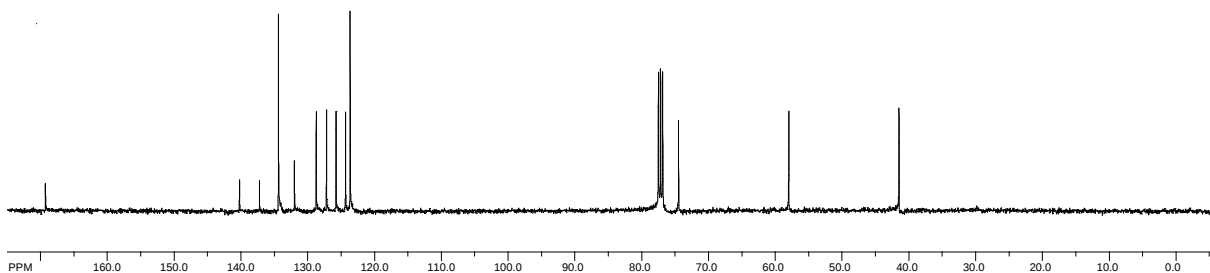
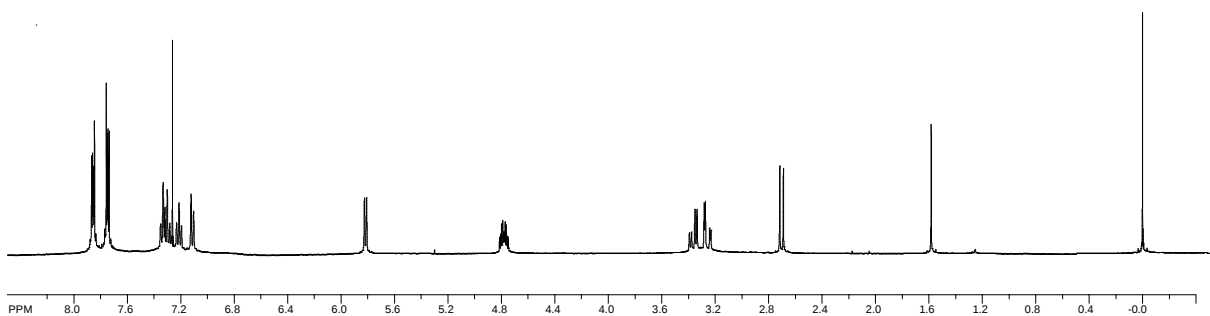
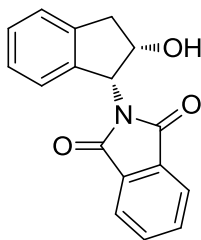
^1H NMR (400 MHz, $[\text{D}_6]\text{DMSO}$): δ = 8.31-8.64 (m, 4 H), 7.81-7.95 (m, 2 H), 7.13-7.33 (m, 4 H), 6.76 [d, $^3J(\text{H,H})$ = 8.9 Hz, 1 H], 5.71-5.77 (m, 1 H), 3.51 [dd, $^2J(\text{H,H})$ = 16.0 Hz, $^3J(\text{H,H})$ = 8.1 Hz, 1 H], 3.41 [dd, $^2J(\text{H,H})$ = 16.0 Hz, $^3J(\text{H,H})$ = 6.4 Hz, 1 H], 2.68 [d, $^3J(\text{H,H})$

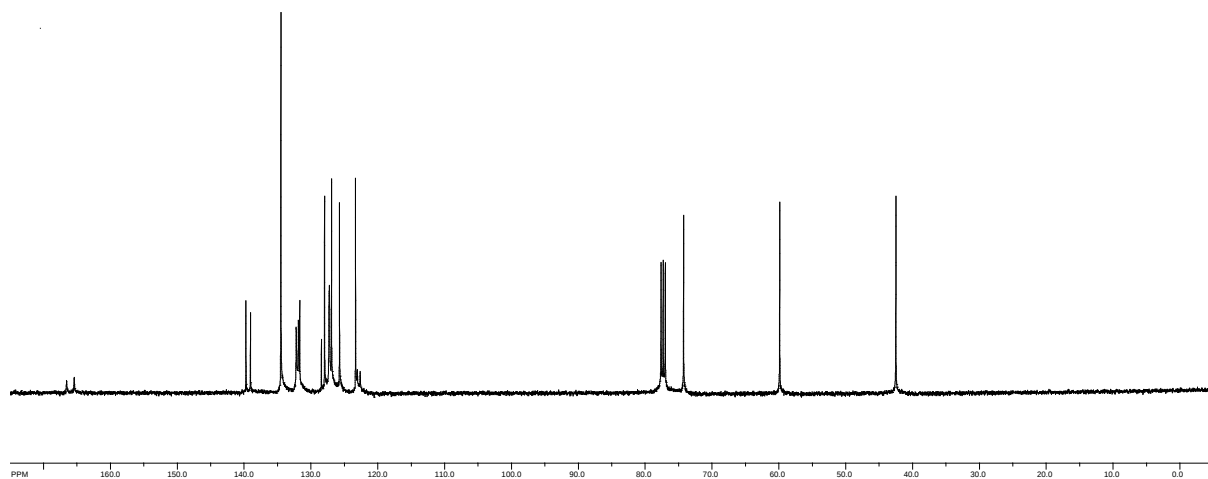
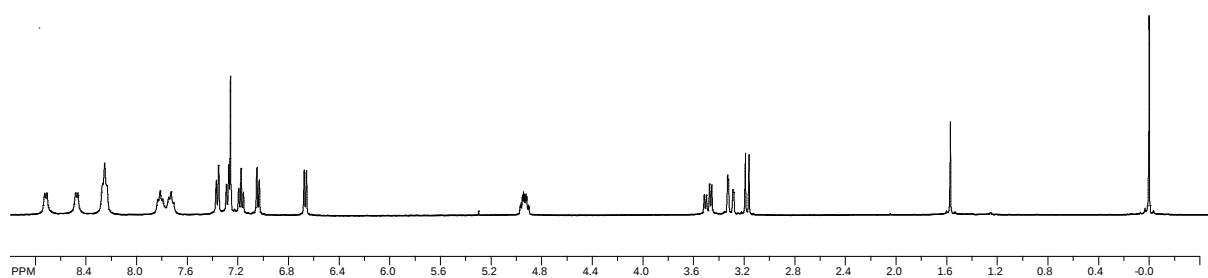
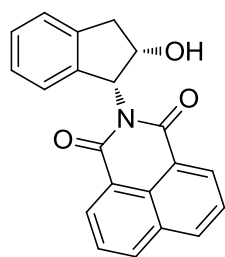
= 6.2 Hz, 2 H], 2.44-2.50 (m, 1 H), 1.98 (s, 3 H), 0.55 [d, $^3J(\text{H,H}) = 7.1$ Hz, 3 H]. MS(ESI): m/z 496.2 $[\text{M}+\text{Na}]^+$.

(1*S*,2*R*)-2b ester of (S)-3-acetylthio-2-methylpropionic acid ((1*S*,2*R*)-2b-J)

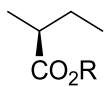
^1H NMR (400 MHz, $[\text{D}_6]\text{DMSO}$): δ = 8.32-8.64 (m, 4 H), 7.80-7.96 (m, 2 H), 7.12-7.33 (m, 4 H), 6.76 [d, $^3J(\text{H,H}) = 9.0$ Hz, 1 H], 5.70-5.76 (m, 1 H), 3.51 [dd, $^2J(\text{H,H}) = 16.0$ Hz, $^3J(\text{H,H}) = 8.3$ Hz, 1 H], 3.41 [dd, $^2J(\text{H,H}) = 16.0$ Hz, $^3J(\text{H,H}) = 6.7$ Hz, 1 H], 2.63 [dd, $^2J(\text{H,H}) = 13.5$ Hz, $^3J(\text{H,H}) = 8.0$ Hz, 1 H], 2.57 [dd, $^2J(\text{H,H}) = 13.5$ Hz, $^3J(\text{H,H}) = 5.6$ Hz, 1 H], 2.29-2.38 (m, 1 H), 1.74 (s, 3 H), 0.82 [d, $^3J(\text{H,H}) = 7.0$ Hz, 3 H]. MS(ESI): m/z 496.2 $[\text{M}+\text{Na}]^+$.

NMR Spectra:

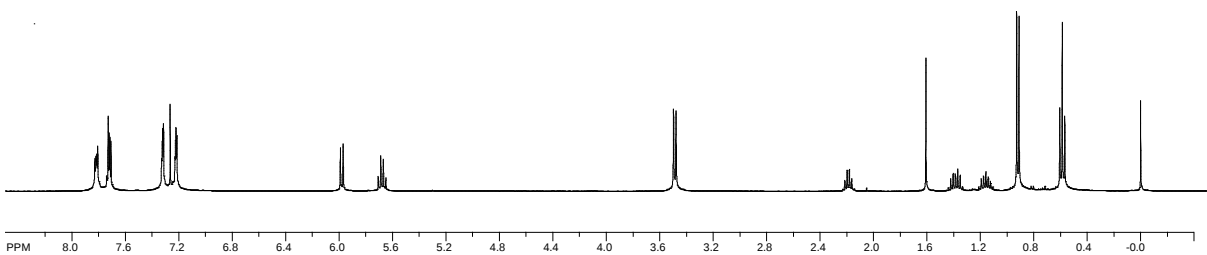




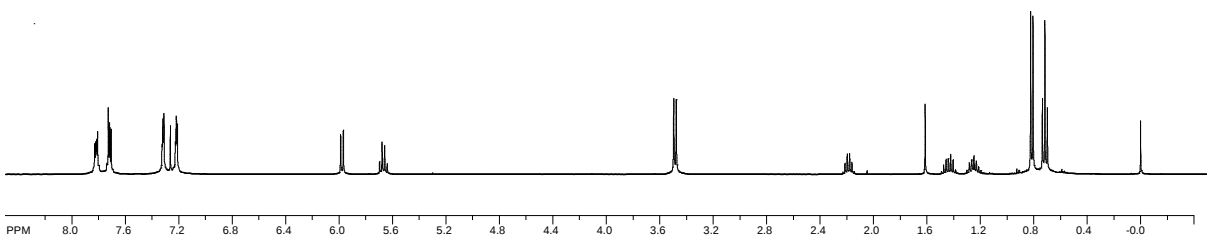
2a ester of (*S*)-2-methylbutyric acid



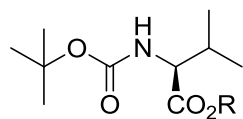
(1*R*,2*S*)-2a-A



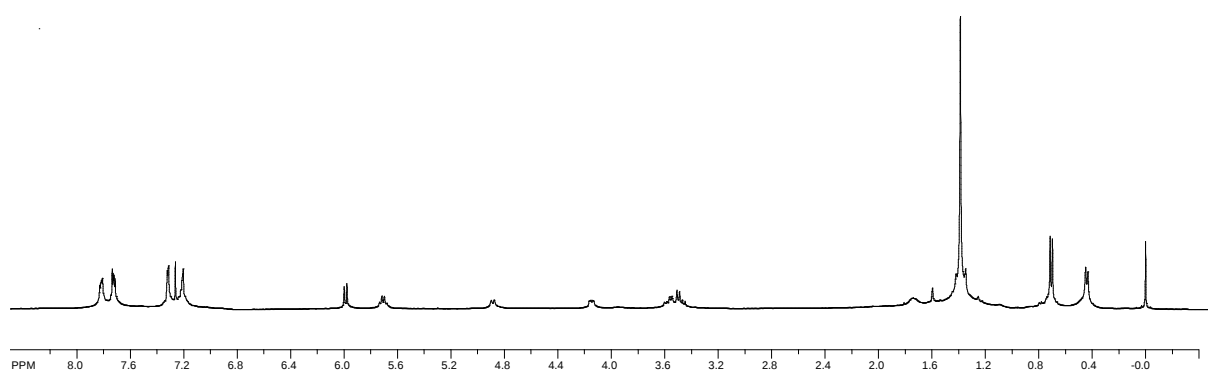
(1*S*,2*R*)-2a-A



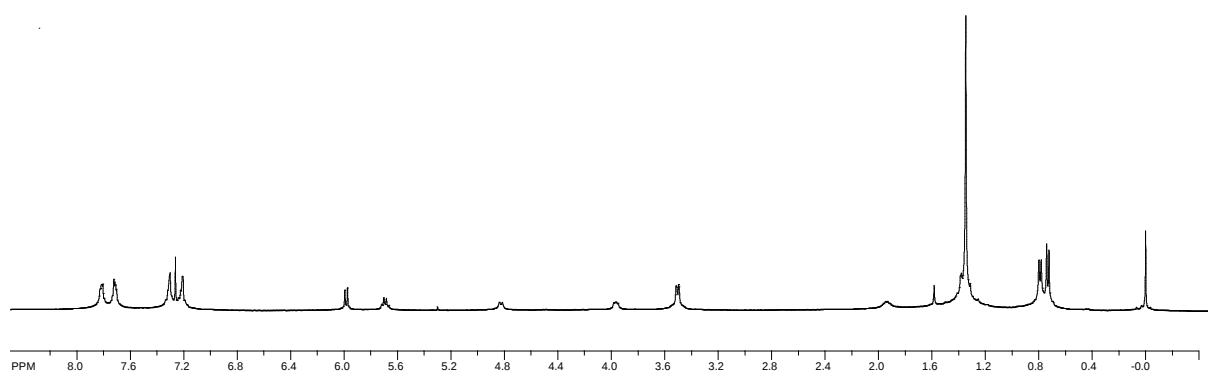
2a ester of Boc-L-valine



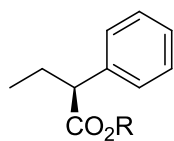
(1*R*,2*S*)-2a-B



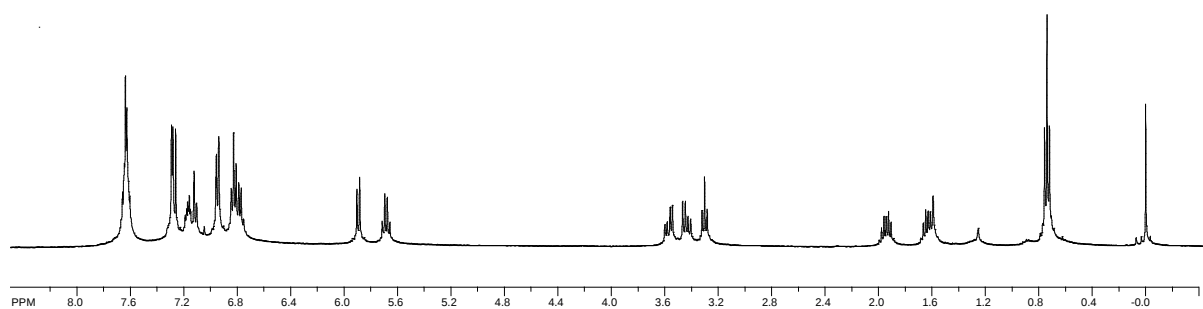
(1*S*,2*R*)-2a-B



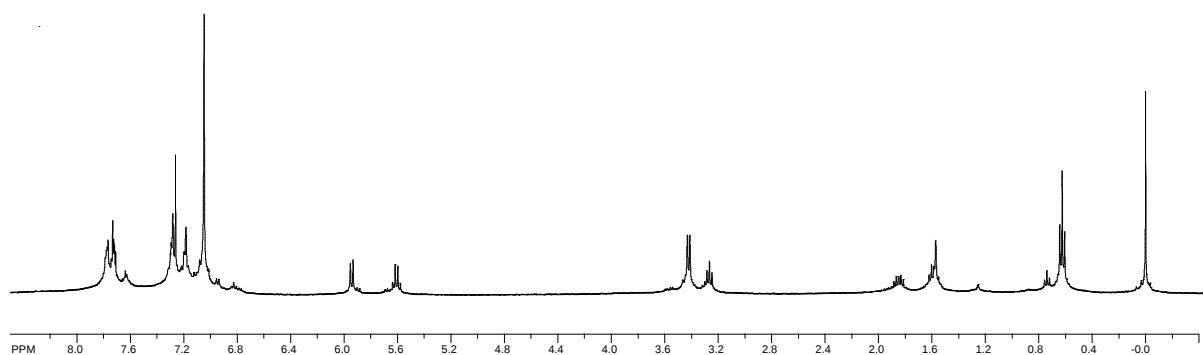
2a ester of (*S*)-2-phenylbutric acid



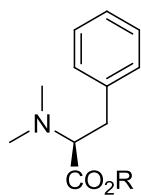
(1*R*,2*S*)-2a-C



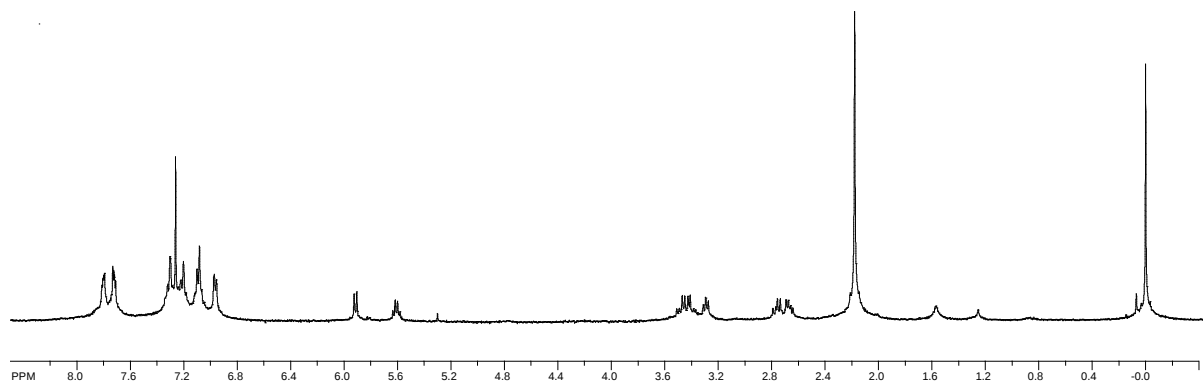
(1*S*,2*R*)-2a-C



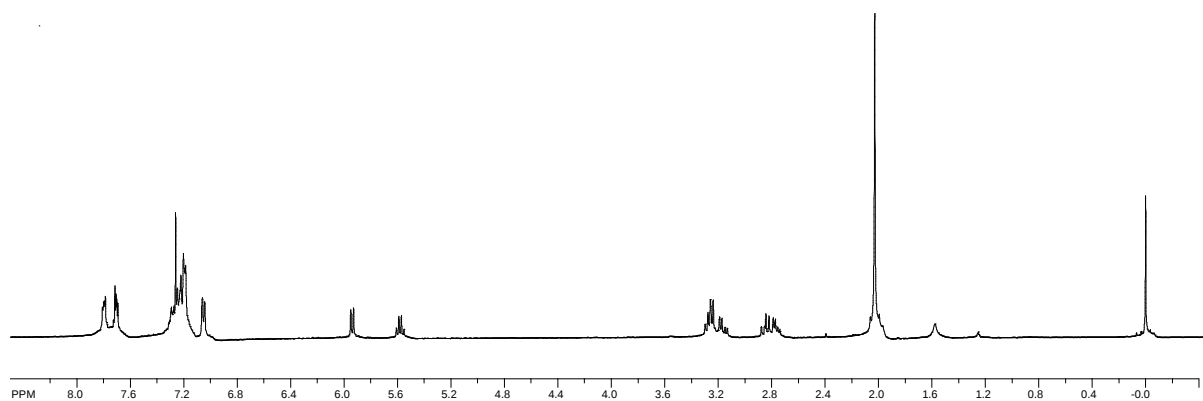
2a ester of *N,N*-dimethyl-L-phenylalanine



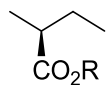
(1*R*,2*S*)-2a-D



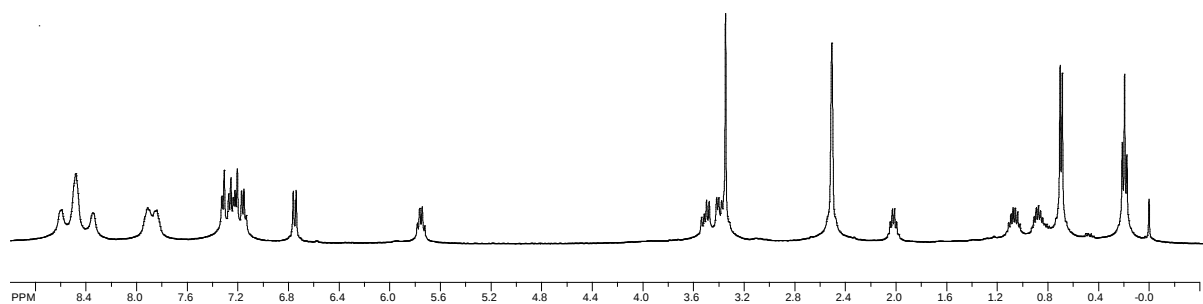
(1*S*,2*R*)-2a-D



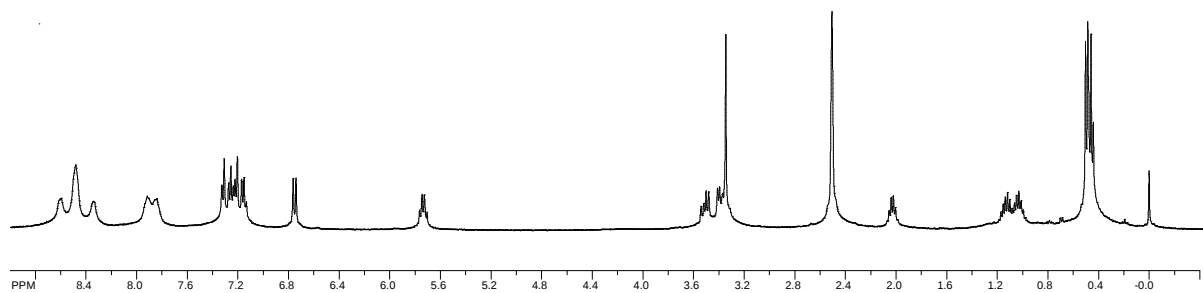
2b ester of (*S*)-2-methylbutyric acid



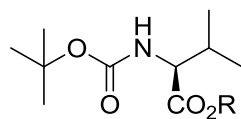
(1*R*,2*S*)-2b-A



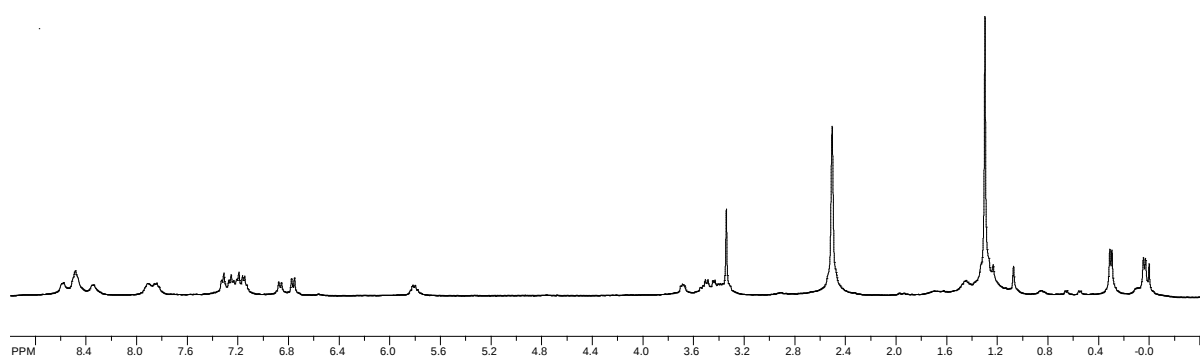
(1*S*,2*R*)-2b-A



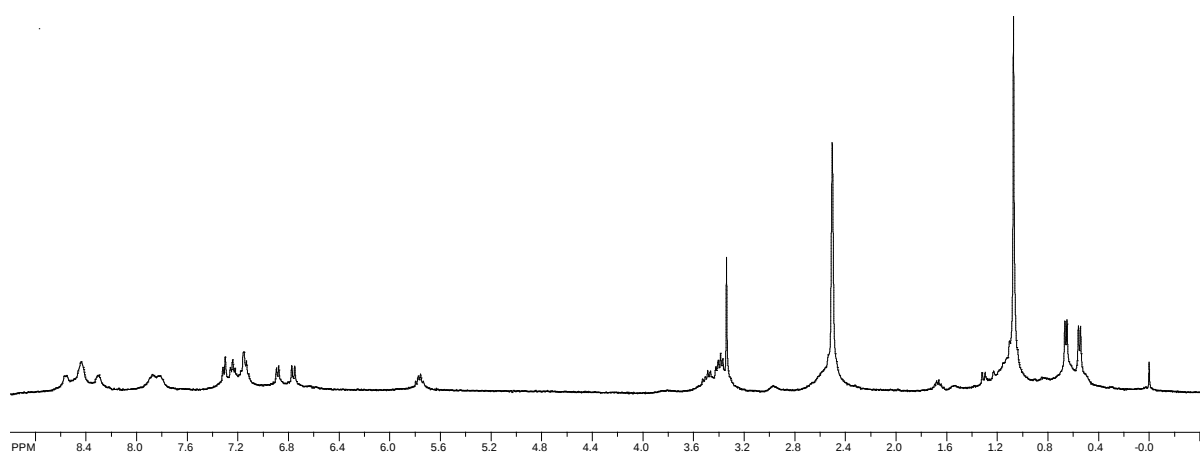
2b ester of Boc-L-valine



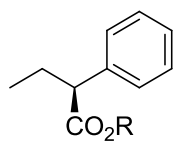
(1R,2S)-2b-B



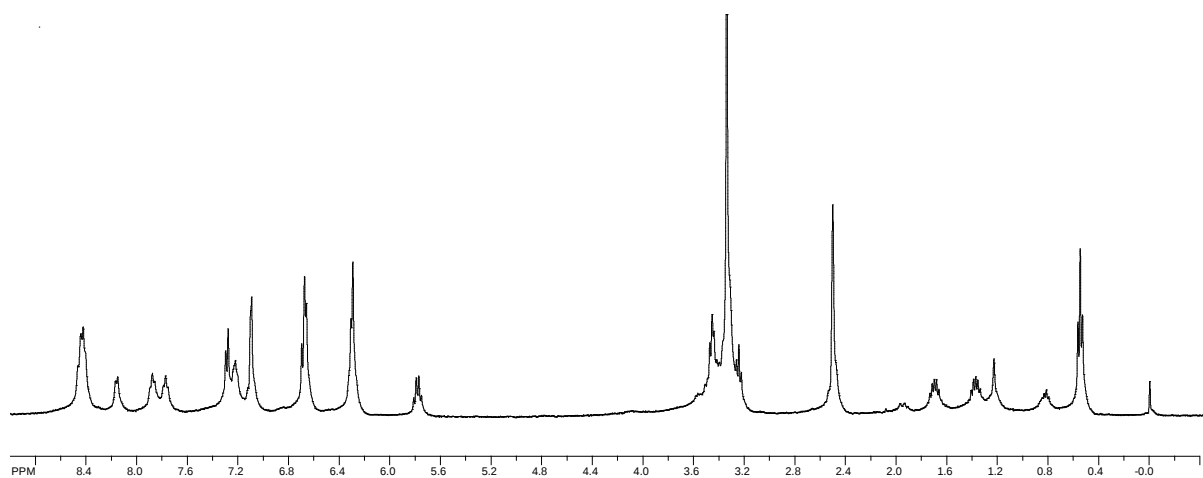
(1S,2R)-2b-B



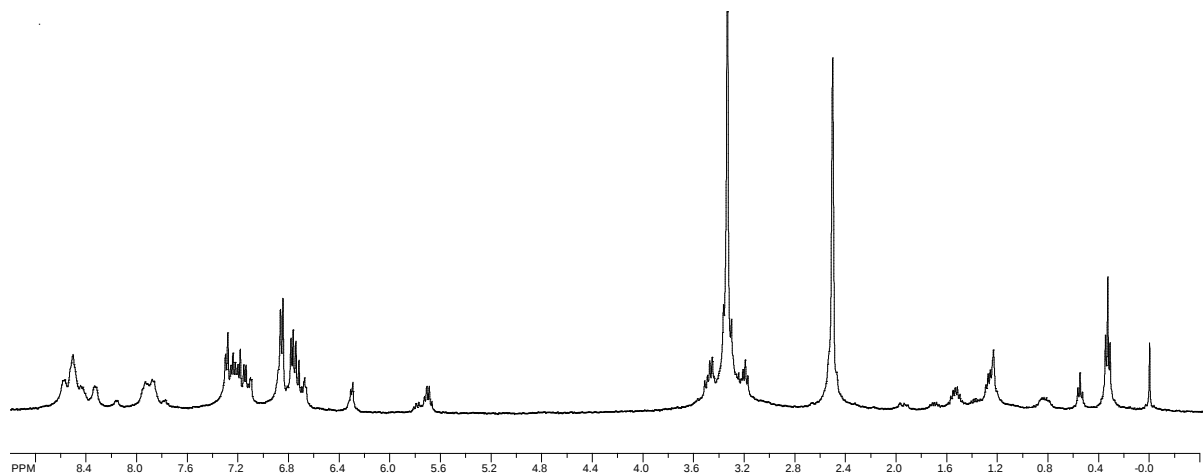
2b ester of (*S*)-2-phenylbutric acid



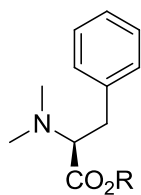
(1*R*,2*S*)-2b-C



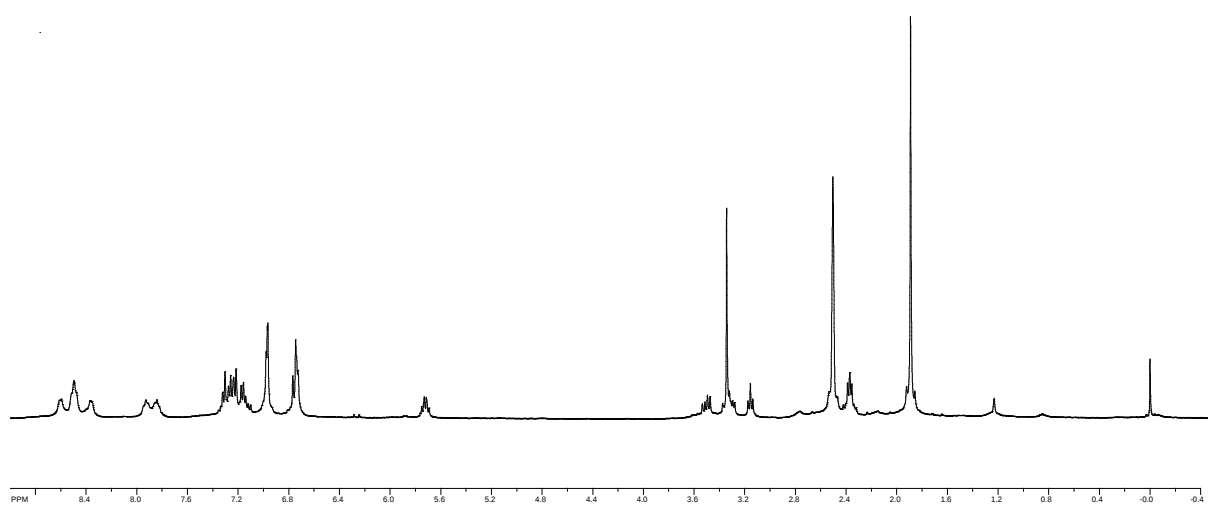
(1*S*,2*R*)-2b-C



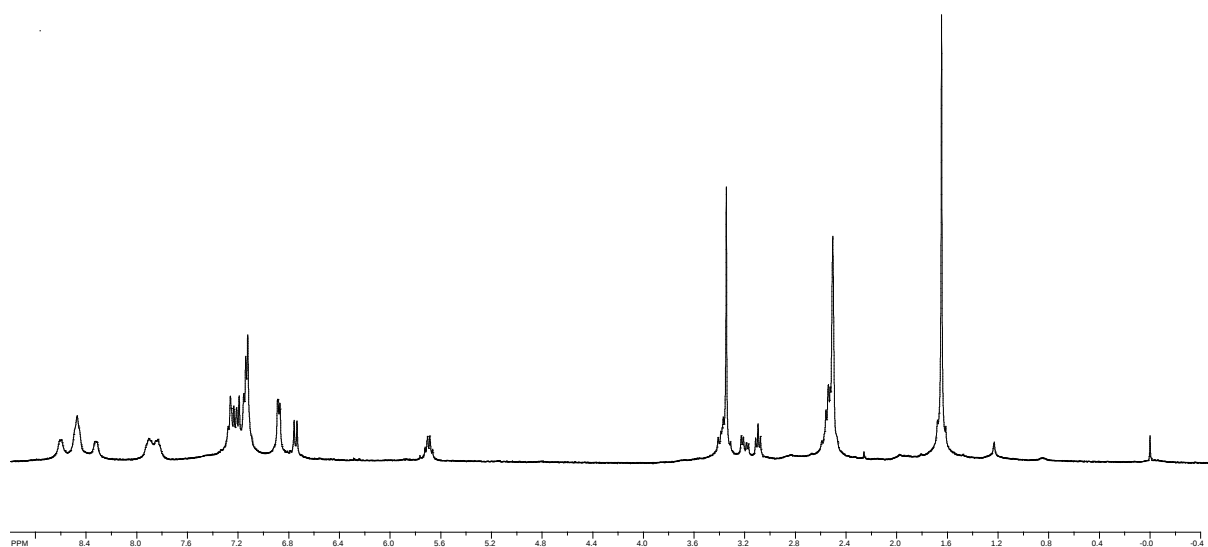
2b ester of *N,N*-dimethyl-L-phenylalanine



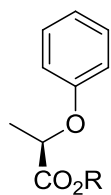
(1*R*,2*S*)-2b-D



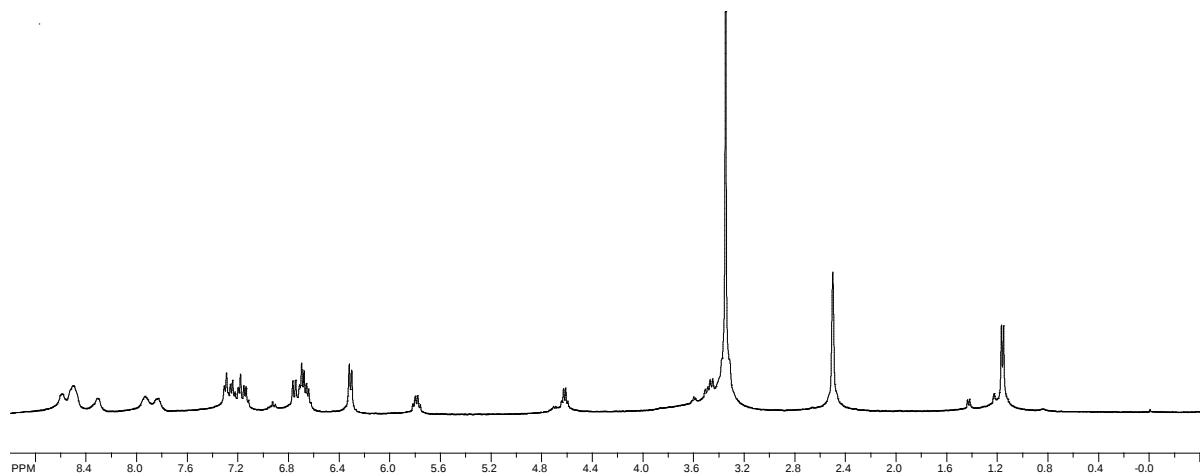
(1*S*,2*R*)-2b-D



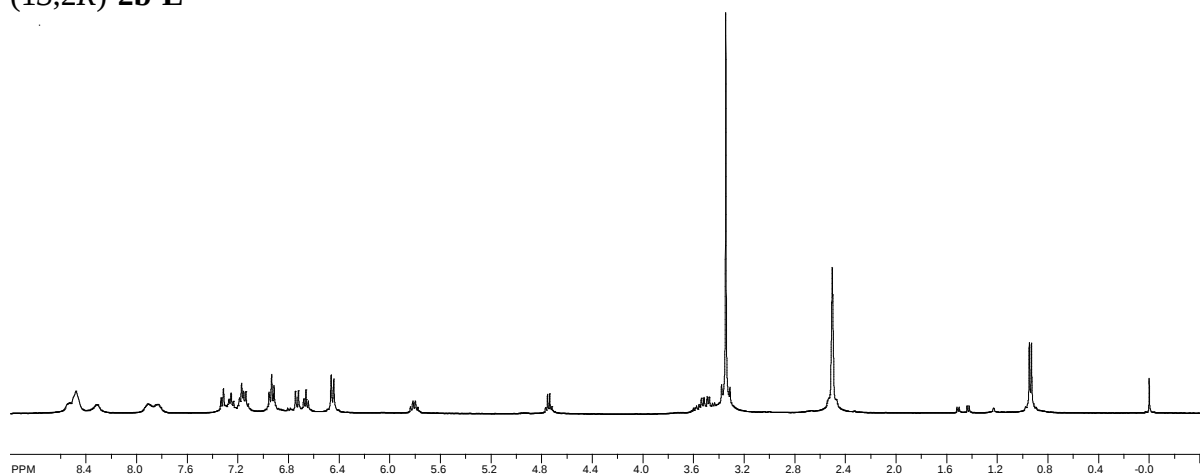
2b ester of (*R*)-2-phenoxypropionic acid



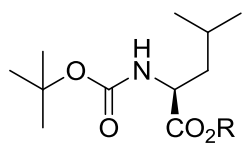
(1*R*,2*S*)-2b-E



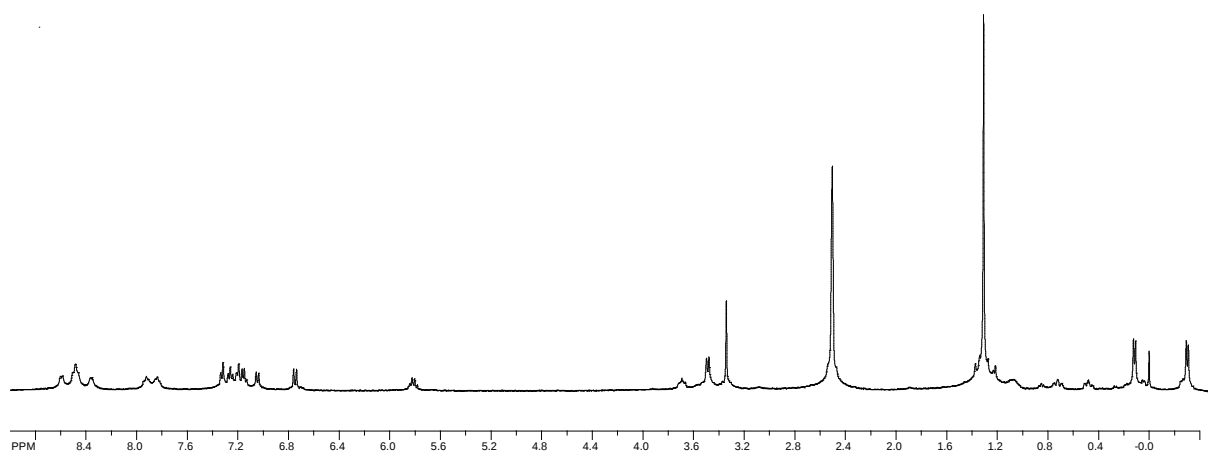
(1*S*,2*R*)-2b-E



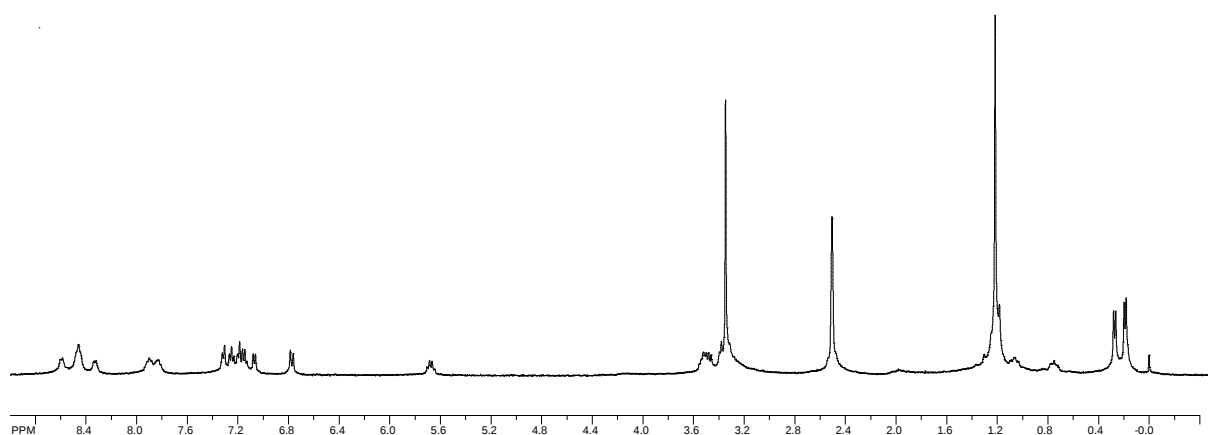
2b ester of Boc-L-leucine



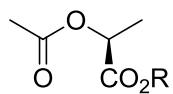
(1R,2S)-2b-F



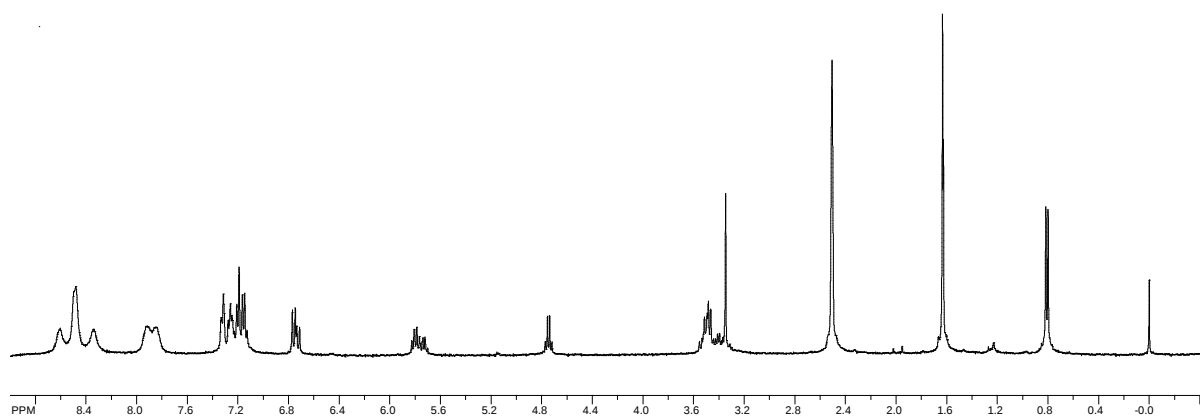
(1S,2R)-2b-F



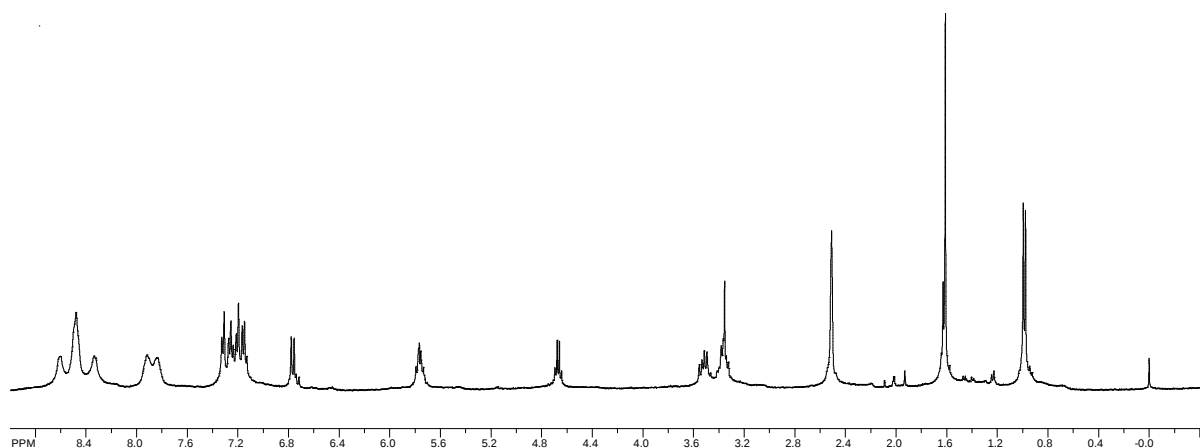
2b ester of (*S*)-2-acetoxypropionic acid



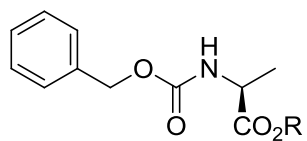
(1*R*,2*S*)-2b-G



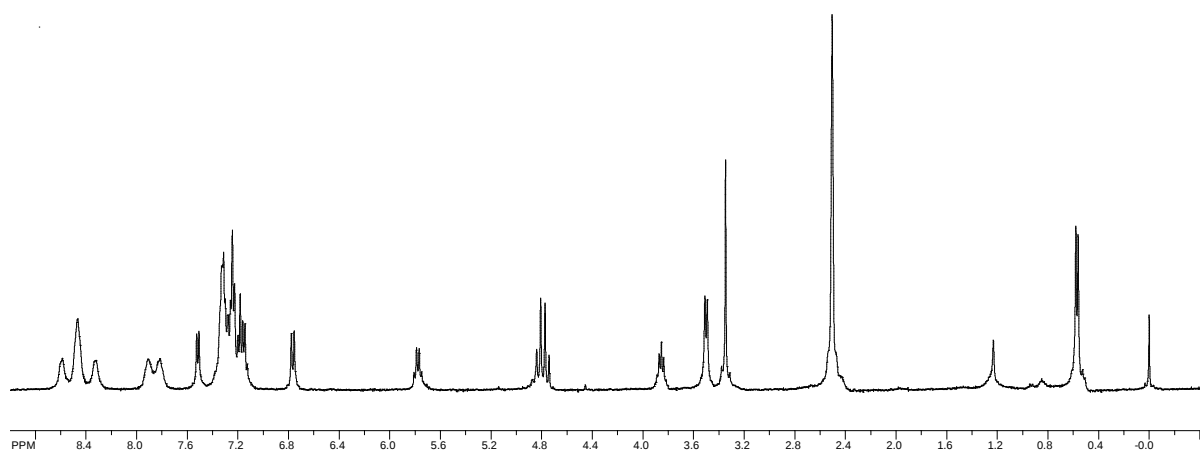
(1*S*,2*R*)-2b-G



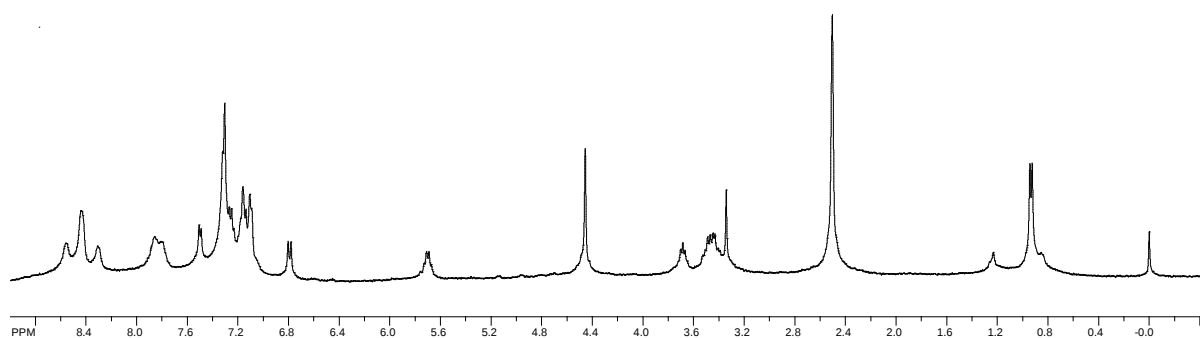
2b ester of Cbz-L-alanine



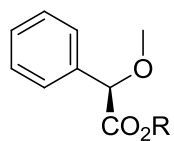
(1R,2S)-2b-H



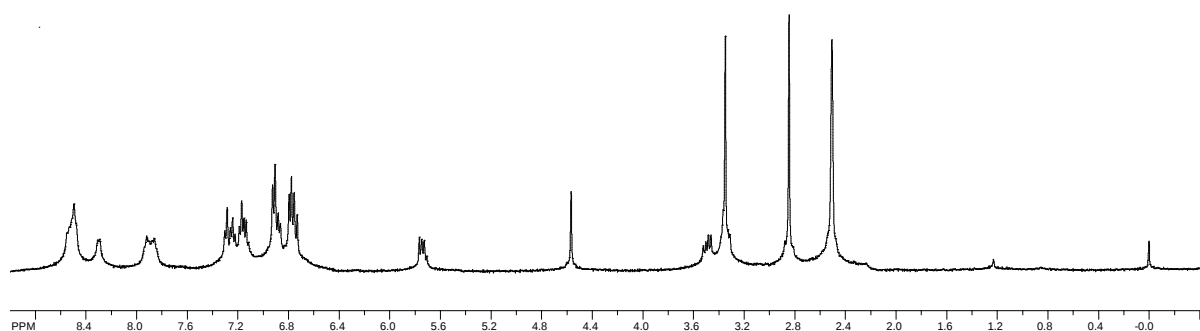
(1S,2R)-2b-H



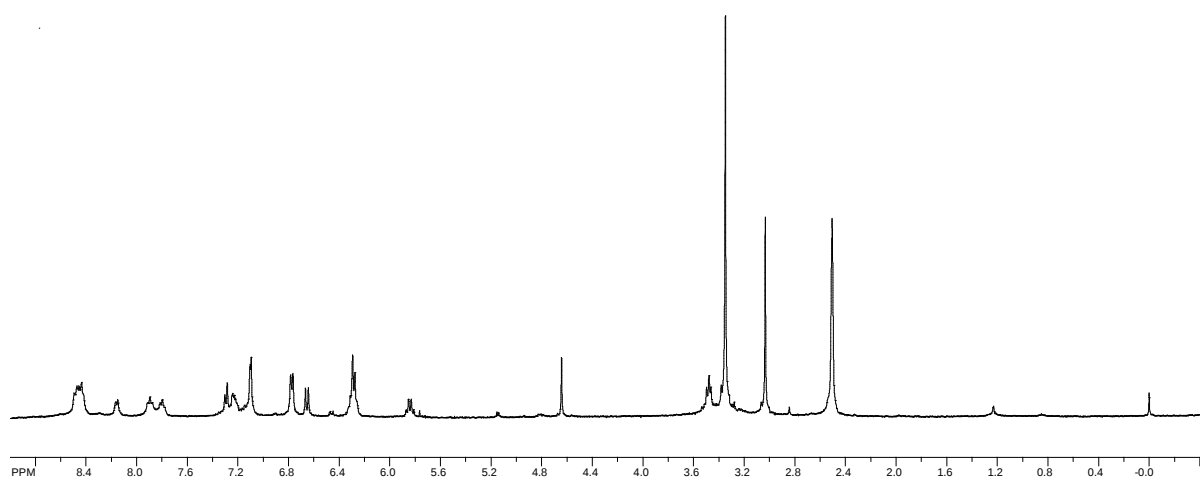
2b ester of (*R*)- α -methoxyphenylacetic acid



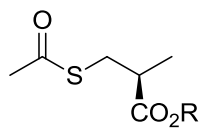
(1*R*,2*S*)-2b-I



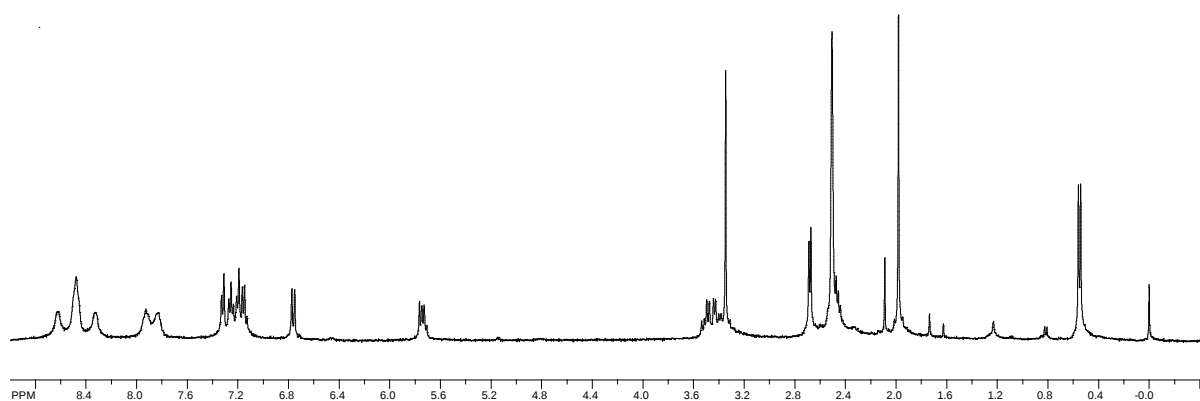
(1*S*,2*R*)-2b-I



2b ester of (*S*)-3-acetylthio-2-methylpropionic acid



(1*R*,2*S*)-2b-J



(1*S*,2*R*)-2b-J

