SUPPORTING INFORMATION

A Facile synthesis of thioacids from $N$-Acylbenzotriazoles

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1. General Information S2
2. Experimental Procedures and Characterization of compounds 2a–h and 4a–d S2
3. Copy of $^1$H, $^{13}$C NMR and CHN/HRMS spectra for compounds 2a–h and 4a–d S15
General Information. All commercial materials (Aldrich, Fluka) were used without further purification. All solvents were reagent grade or HPLC grade (Fisher Solvents were dried using standard protocols kept under a dry atmosphere of nitrogen. Melting points were determined on a capillary point apparatus equipped with a digital thermometer and are uncorrected. $^1$H NMR and $^{13}$C NMR spectra were recorded in CDCl$_3$ or DMSO-$d_6$ or CD$_3$OD using a 300 MHz spectrometer (with TMS as an internal standard) at ambient temperature unless otherwise stated. Chemical shifts are reported in parts per million relative to residual solvent CDCl$_3$ ($^1$H, 7.26 ppm; $^{13}$C, 77.23 ppm), DMSO-$d_6$ ($^1$H, 2.50 ppm; $^{13}$C, 39.51 ppm). All $^{13}$C NMR spectra were recorded with complete proton decoupling. The data have been reported in order to provide the maximum amount of information regarding coupling constants, which has necessarily led to integrals reported following a group of peaks in some instances. High-resolution and high-performance liquid chromatography mass spectral analyses were performed by the University of Florida chemistry department facility staff. Reactions were carried out in oven-dried glassware under an argon or nitrogen atmosphere unless otherwise noted. Analytical TLC was performed on E. Merck silica gel 60 F254 plates and visualized by UV and potassium permanganate staining. Flash column chromatography was performed on E. Merck silica gel 60 (40–63 mm). Yields refer to chromatographically and spectroscopically pure compounds. Mass spectrometry was done with electro spray ionization (ESI).

Experimental Section

General procedure for the preparation of N-protected amino thioacids 2a–h and N-protected di- and tripeptide thioacids 4a–d

H$_2$S was bubbled through precooled (0 °C) solution of N-protected-$\alpha$-aminoacylbenzotriazole (1.0 mmol), NMM (1 mmol) in THF (10 mL) for 5 min. The reaction mixture was allowed to
warm at r.t. and stirred additional for 1 h, diluted with ether (25 mL) and washed several times with 2N HCl. The organic layer was dried (MgSO₄), the solvent was removed, and the residue was crystallized from pentane-ether to give the desired thio acids.

**(S)-2-(((Benzyloxy)carbonyl)amino)propanethioic S-acid (Cbz-L-Ala-SH, 2a)**

White microcrystals (92%); mp 77–78 °C; [α]D²⁰ -11.1 (c 1.0 in MeOH); ¹H NMR (CDCl₃, 300 MHz) δ 7.31–7.39 (m, 5H), 5.49–5.25 (m, 1H), 5.15 (br s, 2H), 4.36–4.49 (m, 1H), 1.41 (d, J = 7.2 Hz, 3H); ¹³C NMR (CDCl₃, 75 MHz) δ 200.1, 155.8, 135.9, 128.6, 128.3, 128.2, 67.4, 57.6, 18.2; Found: C, 55.58; H, 5.57; N, 5.84. Calcd for C₁₀H₁₃NO₃S: C, 55.21; H, 5.48; N, 5.85%.

**2-(((Benzyloxy)carbonyl)amino)propanethioic S-acid (Cbz-DL-Ala-SH, 2a+2a')**

White microcrystals (93%); mp 65–66 °C; ¹H NMR (CDCl₃, 300 MHz) δ 7.28–7.40 (m, 5H), 5.15 (br s, 2H), 5.44–5.30 (m, 1H), 4.36–4.50 (m, 1H), 1.42 (d, J = 7.1 Hz, 3H); ¹³C NMR (CDCl₃, 75 MHz) δ 200.2, 155.7, 136.1, 128.7, 128.4, 128.3, 77.2, 67.4, 57.7, 18.2; Found: C, 55.58; H, 5.11; N, 5.62. Calcd for C₁₀H₁₃NO₃S: C, 55.21; H, 5.48; N, 5.85%.

**2-(((Benzyloxy)carbonyl)amino)ethanethioic S-acid (Cbz-Gly-SH, 2b)**

Colorless needles (91%); mp 97–98.5 °C; ¹H NMR (CDCl₃, 300 MHz) δ 7.29–7.40 (m, 5H), 5.48–5.32 (m, 1H), 5.15 (br s, 2H), 4.12 (d, J = 5.9 Hz, 2H); ¹³C NMR (CDCl₃, 75 MHz)
MHz) δ 196.5, 136.5, 129.2, 128.92, 128.7, 77.6, 68.1, 52.4; Found: C, 53.32; H, 4.98; N, 6.24.
Calcd for C<sub>10</sub>H<sub>11</sub>NO<sub>3</sub>S: C, 53.32; H, 4.92; N, 6.22%.

(S)-2-(((Benzyloxy)carbonyl)amino)-3-methylbutanethioic S-acid (Cbz-L-Val-SH, 2c)

![Chemical structure of S)-2-(((Benzyloxy)carbonyl)amino)-3-methylbutanethioic S-acid (Cbz-L-Val-SH, 2c)](attachment)

Gum (78%); [α]<sub>D</sub> <sup>20</sup> -13.1 (c 2.1 in MeOH); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 7.30–7.41 (m, 5H), 5.32–5.41 (m, 1H), 5.15 (br s, 2H), 4.30–4.40 (m, 1H), 2.21–2.38 (m, 1H), 1.02 (d, J = 6.8 Hz, 3H), 0.91 (d, J = 6.8 Hz, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 199.6, 156.3, 136.1, 128.7, 128.4, 128.2, 77.2, 67.5, 66.8, 30.8, 19.5, 16.8; HRMS (ESI<sup>-</sup>) calcd for C<sub>13</sub>H<sub>16</sub>NO<sub>3</sub>S [M-H]<sup>-</sup> 266.0856, found: 266.0866.

(S)-2-(((Benzyloxy)carbonyl)amino)-5-(2-nitroguanidino)pentanethioic S-acid (Cbz-L-Agr(NO<sub>2</sub>)-SH, 2d)

White microcrystals (84%); mp 153–155°C; [α]<sub>D</sub> <sup>20</sup> -9.0 (c 0.5 in MeOH); <sup>1</sup>H NMR (DMSO-<sup>d<sub>6</sub></sup>, 300 MHz) δ 8.47 (s, 1H), 8.14–7.79 (m, 3H), 7.30–7.42 (m, 5H), 5.04–5.21 (m, 2H), 4.28–4.41 (m, 1H), 3.07–3.22 (m, 3H), 1.51–1.82 (m, 5H); <sup>13</sup>C NMR (DMSO-<sup>d<sub>6</sub></sup>, 75 MHz) δ 196.3, 159.4, 156.3, 136.7, 128.5, 128.0, 127.8, 66.1, 63.6, 60.9, 32.5, 28.0; Found: C, 45.85; H, 5.15; N, 18.62. Calcd for C<sub>14</sub>H<sub>19</sub>N<sub>5</sub>O<sub>5</sub>S: C, 45.52; H, 5.18; N, 18.96%.
(S)-2-(((Benzyloxy)carbonyl)amino)-3-(1H-indol-3-yl)propanethioic S-acid (Cbz-L-Trp-SH, 2e)

White microcrystals (86%); mp 114–115°C; [α]_D^{20} -44.5 (c 0.2 in MeOH); ^1H NMR (CDCl₃, 300 MHz) δ 8.09 (br s, 1H), 7.57 (d, J = 7.7 Hz, 1H), 7.29–7.39 (m, 6H), 7.19–7.25 (m, 1H), 7.01–7.06 (m, 1H), 5.21–5.31 (m, 1H), 5.11 (br s, 2H), 4.67–4.79 (m, 1H), 3.31 (d, J = 5.6 Hz, 2H); ^13C NMR (CDCl₃, 75 MHz) δ 200.5, 156.0, 136.3, 128.6, 128.4, 128.2, 123.4, 122.5, 120.0, 118.7, 114.6, 111.5, 109.1, 68.1, 67.4, 62.2, 27.7, 25.7; Found: C, 64.62; H, 5.23; N, 7.70.

Calcd for C₁₉H₁₈N₂O₃S: C, 64.39; H, 5.12; N, 7.90%.

(S)-2-(((Benzyloxy)carbonyl)amino)-3-phenylpropanethioic S-acid (Cbz-L-Phe-SH, 2f)

White microcrystals (91%); mp 92.5–93.5 °C; [α]_D^{20} -36.8 (c 0.5 in MeOH); ^1H NMR (CDCl₃, 300 MHz) δ 7.28–7.34 (m, 8H), 7.11–7.21 (m, 2H), 5.14–5.25 (m, 1H), 5.04–5.13 (m, 2H), 4.57–4.75 (m, 1H), 2.97–3.23 (m, 2H). ^13C NMR (CDCl₃, 75 MHz) δ 199.5, 155.8, 135.2, 129.4, 129.0, 128.7, 128.5, 128.2, 127.5, 77.2, 67.5, 62.5, 37.8; Found: C, 65.05; H, 5.59; N, 4.41. Calcd for C₁₇H₁₇NO₃S: C, 64.74; H, 5.43; N, 4.44%.
(S)-2-((((9H-Fluoren-9-yl)methoxy)carbonyl)amino)propanethioic S-acid (Fmoc-L-Ala-SH, 2g)

Colorless crystals (88%); mp 118–120 °C; $[\alpha]^{20}_D$ -6.1 (c 0.2 in MeOH); $^1$H NMR (CDCl$_3$, 300 MHz) $\delta$ 7.73–7.81 (m, 2H), 7.56–7.65 (m, 2H), 7.37–7.45 (m, 2H), 7.29–7.36 (m, 2H), 5.17–5.32 (m, 1H), 4.49–4.60 (m, 1H), 4.32–4.48 (m, 2H), 4.20–4.29 (m, 1H), 1.43 (d, $J = 7.0$ Hz, 3H); $^{13}$C NMR (CDCl$_3$, 75 MHz) $\delta$ 200.2, 155.7, 143.7, 141.5, 127.9, 127.2, 125.1, 120.2, 77.2, 67.3, 57.7, 47.3, 18.3; Found: C, 65.81; H, 5.54; N, 4.27. Caled for C$_{18}$H$_{17}$NO$_3$S: C, 66.03; H, 5.23; N, 4.28%.

(S)-2-((((9H-Fluoren-9-yl)methoxy)carbonyl)amino)-3-phenylpropanethioic S-acid (Fmoc-L-Phe-SH, 2h)

White microcrystals (85%); mp 88.5–90 °C; $[\alpha]^{20}_D$ -40.9 (c 1.0 in MeOH); $^1$H NMR (CDCl$_3$, 300 MHz) $\delta$ 7.73–7.78 (m, 2H), 7.47-7.56 (m, 2H), 7.35-7.43 (m, 2H), 7.25–7.34 (m, 5H), 7.12–7.19 (m, 2H), 5.14–5.25 (m, 1H), 4.59–4.72 (m, 1H), 4.35–4.49 (m, 2H), 4.18 (t, $J = 6.8$ Hz, 1H), 3.21–2.96 (m, 2H); $^{13}$C NMR (CDCl$_3$, 75 MHz) $\delta$ 199.4, 155.7, 143.7, 141.4, 135.2, 129.4, 129.0, 127.9, 127.6, 127.2, 125.1, 120.1, 77.2, 67.3, 62.5, 47.2, 37.7; Found: C, 71.73; H, 5.12; N, 3.90. Caled for C$_{18}$H$_{17}$NO$_3$S: C, 71.44; H, 5.25; N, 3.47%.
(S)-2-(2-(((Benzyloxy)carbonyl)amino)propanamido)ethanethioic S-acid (Cbz-L-Ala-Gly-SH, 4a)

White microcrystals (87%); mp 100–102 °C; \( ^1H \) NMR (CD\(_3\)OD, 300 MHz) \( \delta \) 7.23–7.40 (s, 5H), 5.01–5.16 (m, 2H), 4.14–4.25 (m, 1H), 3.99–4.13 (m, 1H), 1.37 (d, \( J = 7.2 \) Hz, 3H); \( ^13C \) NMR (CD\(_3\)OD, 75 MHz) \( \delta \) 176.1, 171.6, 138.1, 129.4, 129.0, 128.9, 111.4, 67.7, 51.9, 41.8, 18.3; HRMS (DART) calcd. for C\(_{13}\)H\(_{17}\)N\(_2\)O\(_4\)S [M+H]\(^+\) 297.0904, found: 297.0891.

(S)-2-(2-(((Benzyloxy)carbonyl)amino)-3-methylbutanamido)ethanethioic S-acid (Cbz-L-Val-Gly-SH, 4b)

White microcrystals (73%); mp 159–161 °C; \([\alpha]\)\(^{20}\) \(D -25.2 \) (c 0.5 in MeOH); \( ^1H \) NMR (CDCl\(_3\), 300 MHz) \( \delta \) 7.27–7.45 (m, 5H), 6.80–6.90 (m, 1H), 5.35–5.50 (m, 1H), 5.05–5.16 (m, 2H), 4.11–4.24 (m, 2H), 2.11–2.25 (m, 1H), 0.99 (d, \( J = 6.8 \) Hz, 3H), 0.95 (d, \( J = 6.8 \) Hz, 3H); \( ^13C \) NMR (CDCl\(_3\), 75 MHz) \( \delta \) 195.1, 172.0, 156.8, 136.2, 128.7, 128.4, 128.2, 67.4, 60.5, 50.4, 30.8, 19.5, 17.9; HRMS (ESI-) calcd. for C\(_{15}\)H\(_{19}\)N\(_2\)O\(_4\)S [M-H]\(^-\) 323.1086, found: 323.1071.
(S)-2-((S)-2-(((Benzyloxy)carbonyl)amino)propanamido)-3-phenylpropanethioic S-acid

(Cbz-L-Ala-L-Phe-SH, 4c)

White microcrystals (79%); mp 107–109°C; \([\alpha]_D^{20} -17.9\ (c\ 0.14\ \text{in}\ \text{MeOH})\);

\[^1\text{H}\] NMR (CDCl\(_3\), 300 MHz) \(\delta\ 7.20–7.41\ (m, 10H), 7.10–7.19\ (m, 2H), 5.04–5.18\ (m, 2H), 4.10–4.27\ (m, 1H), 3.12–3.24\ (m, 1H), 2.97–3.17\ (m, 1H), 1.31\ (d, \(J = 7.1\ \text{Hz}, 3H)\); HRMS (ESI\(^-\)) calcd. for C\(_{20}\)H\(_{21}\)N\(_2\)O\(_4\)S [M-H\(^-\)] 385.1228, found: 385.1247.

(5S,8S)-8-Benzyl-5-methyl-3,6,9-trioxo-1-phenyl-2-oxa-4,7,10-triazadodecane-12-thioic S-acid (Cbz-L-Ala-L-Phe-Gly-SH, 4d)

White microcrystals (69%); mp 162–163°C; \([\alpha]_D^{20} -31.4\ (c\ 0.5\ \text{in}\ \text{MeOH})\);

\[^1\text{H}\] NMR (CD\(_3\)OD, 300 MHz) \(\delta\ 7.13–7.42\ (m, 10H), 5.00–5.14\ (m, 5H), 4.61–4.70\ (m, 1H), 4.00–4.13\ (m, 3H), 3.17–3.29\ (m, 1H), 2.91–3.03\ (m, 1H), 1.21\ (d, \(J = 7.2\ \text{Hz}, 3H)\); \(^{13}\text{C}\) NMR (CD\(_3\)OD, 75 MHz) \(\delta\ 175.5, 173.7, 138.4, 138.0, 130.3, 129.5, 129.4, 129.0, 128.9, 127.7, 67.9, 55.8, 52.3, 51.4, 49.0, 38.3, 17.9\); HRMS (ESI\(^-\)) calcd. for C\(_{22}\)H\(_{24}\)N\(_3\)O\(_5\)S [M-H\(^-\)] 442.1442, found: 442.1455.
EAGER 200 Stripchart

Sample Ident. 22 2195-L-AlaOH Filename 2200723
Analyzed 09-06-13 10:10:10 Printed 09-06-2010 13:20:11

2a

EAGER 200 Peak Integration Report

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CbzGlySH_06Jun2013_H_CDCl3_Ravi

2b
Theoretical [M-H] = 266.0856
[M-2H+Na] = 288.0676
Theoretical [2M-2H+Na]^+ = 555.1605
new experiment

![Chemical Structure](image)
EAGER 200 Stripchart

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EAGER 200 Peak Integration Report

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Figure S36: 

The graph shows the 1H NMR spectrum of compound 2h. The chemical shifts are indicated at various ppm values, with peaks at 77.16, 71.4, 128.4, 129.0, 129.0, 127.2, 126.2, and 126.1 ppm. The structure of 2h is also depicted, showing the chemical bondings and substituents in the molecule.
Theoretical [M+H]^+ = 297.0904
[M+NH4]^+ = 314.1169
\( 4b \)
Theoretical [M-H] = 323.1071
[2M-2H+Na] = 669.2034
Theoretical $[\text{M-H}]^+ = 385.1228$

$[2\text{M-2H+Na}]^+ = 793.2347$