Supporting Information

Synthesis of Novel Oxazolyl Amino Acids and their Use in the Parallel Synthesis of Di-substituted Oxazole Libraries

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General Information: All the reagents were commercial grade and purified according to the established procedures. Organic extracts were dried over anhydrous sodium sulphate. Solvents were removed in a rotary evaporator under reduced pressure. Silica gel (60-120 mesh size) was used for the column chromatography. Reactions were monitored by TLC on aluminum backed silica G TLC plates w/UV254. NMR spectra were recorded in Chloroform-d, DMSO-d6 for 1H NMR (400 MHz) and 13C NMR (100 MHz). 1H and 13C shifts are expressed in ppm relative to the internal solvent peak of either DMSOD6 or CDCl3. Coupling constants are reported in hertz. LC-MS (ESI) traces were recorded on samples with concentrations of roughly 1 mg/ mL in 50:50 MeCN/ water at both 214 nm and 254 nm using a reverse phase Vydac column with a gradient of 5 % to 95 % formic acid in MeCN. The purity of the
crude samples was estimated based on the UV traces recorded. Hydrofluoric acid cleaves were performed in specially equipped and ventilated hoods with full personal protective equipment.

**Experimental Procedures:**

**Synthesis of 4-methoxybenzyl N2-(tert-butoxycarbonyl)-N4-(3-hydroxy-1-methoxy-1-oxopropan-2-yl)-D-asparaginate (Boc-L-Asp-OBzl-Ser-OMe, 2):** Diisopropylethylamine (DIEA, 10 mmol) was added to a solution of Boc-L-Asp-OBzl (1) (10 mmol) and hydroxybenzotriazole (HOBt, 10 mmol) in dichloromethane solvent (15 mL). The solution was cooled to 0 °C and a solution of DIC (12 mmol) was added. After the solution was stirred at 0 °C for an hour, a solution of L-Ser-OMe.HCl was added and continued stirring at room temperature for another 8 hours. After filtration and removal of the solvent on rotavap, the residue was dissolved in ethylacetate and washed with 10 % citric acid (50 mL) followed by washing with saturated aq. NaHCO₃ solution and water. The organic extract is dried over MgSO₄ and evaporated the solvent to obtain the β-hydroxy peptide product (Boc-L-Asp-OBzl-Ser-OMe) 2 which was used for the next step without any further purification.

**Synthesis of methyl (R)-2-(3-benzyloxy)-2-((tert-butoxycarbonyl)amino)-3-oxopropyl)oxazole-4-carboxylate (Boc-L-Asp-Oxz-OBzl, 3):**

Diethylaminosulfur trifluoride (DAST) (10 mmol) was added dropwise to the solution of β-hydroxy peptide 2 in CH₂Cl₂ at -78 °C (acetone-dryice bath). After completion of cyclization (monitored by TLC), the reaction mixture was allowed to warm to 0 °C and added bromotrichloromethane (BTCM) (10 mmol) dropwise, followed by DBU (10 mmol). The reaction was monitored by TLC till completion and then quenched with saturated aq. NaHCO₃ solution. The reaction mixture was extracted with EtOAc and dried over MgSO₄, filtered, and concentrated on rotavap. Purification of the residue by flash chromatography (5-10 % ethyl acetate in hexane) gave the desired oxazole ester in 62 % overall yield.

**Synthesis of (R)-2-((tert-butoxycarbonyl)amino)-3-(4-(methoxycarbonyl)oxazol-2-yl)propanoic acid (Boc-L-Asp-Oxz-OH, 4):**

The oxazole ester (Boc-L-Asp-Oxz-OBzl, 3) (6 mmol) was dissolved in 1:1 Ethanol and Ethylacetate (20 mL) and added 0.1 equiv of 10% Pd/C catalyst. The resulting mixture was stirred in presence of H₂-gas (1 atm) for 2 hrs. Progress of the reaction was monitored
with TLC. After complete conversion, it was filtered through a pad of celite and washed with ethyl acetate followed by the removal of volatile organic solvents in vacuo. The crude product obtained was washed with hexane to get a white solid (4) in 93 % yield.

**General procedure for the solid-phase parallel synthesis of trifunctional oxazole small molecules [8a(i)-8d(iv), 12a(i)-12d(iv)]:**

**Step-1:** A 16 set of 50 mg sealed polypropylene mesh bags containing p-methylbenzhydramine hydrochloride salt (MBHA) resin (1.15 mequiv/g, 100-200 mesh) were prepared. Reactions were carried out by placing all the bags in plastic reaction bottles. Following neutralization of the resin with 5% diisopropylethylamine (DIEA) in dichloromethane (DCM), Boc-L-Asp-Oxz-OH aminoacid (4) (2 equiv) was coupled using the conventional reagents hydroxybenzotriazole (HOBt, 2 equiv) and diisopropylcarbodiimide (DIC, 2 equiv.) in anhydrous DMF while shaking for overnight. Completion of the coupling was monitored by the Kaiser (ninhydrin) test.

**Step-2:** Following the removal of Boc group with 55% TFA/DCM for 30 min. and neutralization with 5% DIEA/DCM, the free amine group was coupled with four different carboxylic acids which results new amide functionality. The completion of amide coupling process was monitored by the Kaiser (ninhydrin) test.

**Step-3:** After removal of the solvents and multiple washes with DMF and DCM, dioxane (10 mL) solvent and 1N aq. NaOH solution (10 mL) were added and left for shaking overnight to deprotect the methyl ester group. The free carboxylic acid group was coupled with another four different types of amines to obtain new amide functionality.

The resin was then washed with DMF (3X), and DCM (3X) followed by HF cleave provided the desired trifunctional oxazol small molecules. All the products were confirmed by LC-MS and NMR analysis. (Full details provided in supporting information)
Characterization Data

2-((tert-butoxycarbonyl)amino)-3-(4-(methoxycarbonyl)oxazol-2-yl)propanoic acid [4]¹:

![Chemical Structure](image)

¹H NMR (400 MHz, CDCl₃): δ 1.34 (s, 9H), 3.12 (d, 1H, J = 9.2 Hz), 3.24 (d, 1H, J = 5.6 Hz), 3.80 (s, 3H), 4.03 (q, 1H, J = 7.2 Hz), 4.39 (q, 1H, J = 7.6 Hz), 8.76 (s, 1H).

¹³C NMR (100 MHz, CDCl₃): δ 28.5, 30.4, 52.1, 60.1, 78.8, 132.7, 146.0, 155.6, 161.6, 162.6, 172.5.

(R)-2-((tert-butoxycarbonyl)amino)-4-(4-(methoxycarbonyl)oxazol-2-yl)butanoic acid [10]²:

![Chemical Structure](image)

¹H NMR (400 MHz, CDCl₃): δ 1.36 (s, 9H), 2.33 (brs, 2H), 2.89 (q, 1H, J = 8.4 Hz), 3.82 (s, 3H), 4.49 (brs, 1H), 5.45 (d, 1H, J = 6.0 Hz), 8.10 (s, 1H).

¹³C NMR (100 MHz, CDCl₃): δ 23.2, 27.3, 28.5, 51.5, 57.2, 79.1, 131.8, 142.9, 154.7, 160.5, 164.1, 172.6.

(R)-3-(4-(piperidine-1-carbonyl)oxazol-2-yl)-2-propionamidopropanamide [8a(i)]:

S4
\[ \text{H NMR (400 MHz, CDCl}_3\text{): } \delta 0.96 (d, 3H, J = 8.0 \text{ Hz}), 0.98 (d, 3H, J = 8.0 \text{ Hz}), 1.22 (s, 9H), 1.71 (m, 1H), 1.84 (m, 2H), 4.90 (t, 1H, J = 7.0 \text{ Hz}), 5.58 (brs, 1H), 5.86 (brs, 1H), 6.07 (s, 1H), 6.80 (brs, 1H), 8.16 (s, 1H); \text{^13C NMR (100 MHz, CDCl}_3\text{): } \delta 22.3, 22.5, 24.7, 29.6, 34.6, 43.5, 52.1, 98.8, 135.6, 141.6, 162.5, 162.7, 164.7, 166.9; \text{ ESI-MS: 345 (M + Na). HRMS (ESI-TOF) calcd for C}_{15}H_{23}N_4O_4 (M+ H^+), 323.1714; found 323.1712.\]

(R)-2-(3-amino-3-oxo-2-propionamidopropyl)-N-butyloxazole-4-carboxamide [8a(ii)]:

\[ \text{H NMR (400 MHz, CD}_3\text{OD): } \delta 0.95 (t, 3H, J = 7.2 \text{ Hz}), 1.06 (t, 3H, J = 7.2 \text{ Hz}), 1.39 (m, 2H), 1.55 (m, 2H), 2.22 (q, 2H, J = 7.6 \text{ Hz}), 3.14 (dd, 1H, J1=15.6, J2 = 8.8 \text{ Hz}), 3.30-3.35 (m, 5H), 4.89 (t, 1H, J = 7.2 \text{ Hz}), 8.23 (s, 1H); \text{^13C NMR (100 MHz, CD}_3\text{OD): } \delta 10.0, 14.0, 21.0, 29.8, 31.2, 32.6, 39.7, 51.8, 137.3, 142.6, 162.8, 162.9, 174.8, 176.9; \text{ ESI-MS: 334 (M + Na). HRMS (ESI-TOF) calcd for C}_{14}H_{23}N_4O_4 (M+ H^+), 311.1714; found 323.1708.\]
(R)-3-(4-(4-((9H-fluoren-9-yl)acetyl)piperazine-1-carbonyl)oxazol-2-yl)-2-propionamidopropanamide [8a(iii)e]:

![Chemical Structure](image)

$^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 1.12 (brs, 3H), 2.23 (brs, 2H), 2.76 (d, 2H, $J = 5.2$ Hz), 3.23-3.37 (m, 4H), 3.59 – 4.02 (m, 6H), 4.61 (s, 1H), 5.00 (brs, 1H), 5.91 – 6.14 (m, 1H), 6.90 – 6.94 (m, 2H), 7.28 (t, 2H, $J = 7.6$ Hz), 7.36 (t, 2H, $J = 7.2$ Hz), 7.52 (d, 2H, $J = 7.6$ Hz), 7.74 (d, 2H, $J = 7.6$ Hz), 8.07 (s, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 9.6, 29.5, 30.1, 37.6, 42.4, 43.7, 45.3, 46.3, 50.0, 120.0, 124.6, 127.2, 127.5, 136.0, 140.7, 143.6, 146.8, 160.8, 170.4, 172.4, 174.2; ESI-MS: 552 (M + Na). HRMS (ESI-TOF) calcd for C$_{29}$H$_{32}$N$_5$O$_5$ (M+ H$^+$), 530.2398; found 530.2409.

(R)-2-(3-amino-3-oxo-2-propionamidopropyl)-N-benzyloxazole-4-carboxamide [8a(iv)]:

![Chemical Structure](image)

$^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 1.11 (t, 3H, $J = 7.2$ Hz), 2.21 -2.27 (q, 2H, $J = 7.6$ Hz), 3.20 (dd, 1H, $J_1 = 16.0$ Hz, $J_2 = 6.8$ Hz), 3.27 (dd, 1H, $J_1 = 16.0$ Hz, $J_2 = 6.0$ Hz), 4.60 (d, 2H, $J = 6.0$ Hz), 4.94 (q, 1H, $J = 7.2$ Hz), 5.39 (brs, 1H), 6.49 – 6.54 (m, 2H), 7.08 (brs, 1H), 7.29 – 7.37 (m, 5H), 8.15 (s, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 9.5, 29.5, 30.0, 43.1, 50.0, 127.7, 127.9, 128.8, 136.1, 137.8, 141.5, 160.1, 161.2, 171.7, 174.1; ESI-MS: 367 (M + Na). HRMS (ESI-TOF) calcd for C$_{17}$H$_{21}$N$_4$O$_4$ (M+ H$^+$), 345.1557; found 345.1555.
(R)-N-(1-amino-1-oxo-3-(4-(piperidine-1-carbonyl)oxazol-2-yl)propan-2-yl)cyclohexanecarboxamide [8b(i)]:

\[
\begin{align*}
\text{H}_2\text{N} & \quad \text{O} \\
\text{O} & \quad \text{N} \\
\text{O} & \quad \text{N} \\
\text{C} & \quad \text{H}_2
\end{align*}
\]

$^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 1.19 – 1.26 (m, 3H), 1.30 (d, 2H, $J = 12.0$ Hz), 1.41-1.69 (m, 8H), 1.70 – 1.87 (m, 4H), 2.16 (t, 1H, $J = 11.6$ Hz), 3.12 (dd, 1H, $J_1 = 16.4$ Hz, $J_2 = 6.4$ Hz), 3.38 (dd, 1H, $J_1 = 16.4$ Hz, $J_2 = 4.8$ Hz), 3.71 (brs, 4H), 4.95 (q, 1H, $J = 6.4$ Hz), 5.44 (brs, 1H), 6.79 (brs, 1H), 6.95 (d, 1H, $J = 7.2$ Hz), 8.0 (s, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 24.6, 25.6, 25.61, 25.65, 29.4, 29.5, 29.8, 45.2, 49.6, 136.6, 142.2, 160.6, 160.8, 172.1, 176.4; ESI-MS: 399 (M + Na). HRMS (ESI-TOF) calcd for C$_{19}$H$_{29}$N$_4$O$_4$ (M+H$^+$), 377.2183; found 377.2184.

(R)-2-(3-amino-2-(cyclohexanecarboxamido)-3-oxopropyl)-N-butyloxazole-4-carboxamide [8b(ii)]:

\[
\begin{align*}
\text{H}_2\text{N} & \quad \text{O} \\
\text{O} & \quad \text{N} \\
\text{O} & \quad \text{NH}
\end{align*}
\]

$^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 0.97 (t, 3H, $J = 8.0$ Hz), 1.22 – 1.38 (m, 3H), 1.39 – 1.43 (m, 4H), 1.57 (s, 10H), 1.68 (d, 1H, $J = 8.8$ Hz), 1.85 -1.97 (m, 4H), 2.15 (t, 1H, $J = 11.2$ Hz), 3.21 (dd, 1H, $J_1 = 16.0$ Hz, $J_2 = 8.0$ Hz), 3.29 (dd, 1H, $J_1 = 16.0$ Hz, $J_2 = 8.0$ Hz), 3.41 (q, 2H, $J = 8.0$ Hz), 4.95 (q, 1H, $J = 6.8$ Hz), 5.38 (brs, 1H), 6.51-6.58 (m, 2H), 6.75 (brs, 1H), 8.11 (s, 1H); $^{13}$C NMR (100 MHz,


CDCl$_3$: $\delta$ 13.7, 20.1, 25.6, 29.4, 29.6, 29.9, 31.7, 38.8, 45.1, 49.9, 136.3, 141.2, 160.1, 161.1, 171.9, 176.4; ESI-MS: 387 (M + Na).

HRMS (ESI-TOF) calcd for C$_{18}$H$_{29}$N$_4$O$_4$ (M + H$^+$), 365.2183; found 365.2183.

(R)-N-(1-amino-3-(4-(2-(naphthalen-1-yl)acetyl)piperazine-1-carbonyl)oxazol-2-yl)-1-oxopropan-2-y) cyclohexanecarboxamide [8b(iii)f]:

![Chemical Structure](image)

$^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 1.19 – 1.35 (m, 5H), 1.65 – 1.75 (m, 5H), 2.08 (brs, 1H), 3.18 (brs, 2H), 3.52 (brs, 3H), 3.75 (brs, 3H), 3.97 (brs, 1H), 4.19 (s, 2H), 4.94 (brs, 1H), 5.58 – 5.91 (m, 1H), 6.78 (brs, 2H), 7.34 (d, 1H, $J = 8.0$ Hz), 7.43 (t, 1H, $J = 7.6$ Hz), 7.52 (t, 2H, $J = 8.4$ Hz), 7.79 (d, 1H, $J = 8.0$ Hz), 7.88 (d, 1H, $J = 8.0$ Hz), 7.98 (d, 1H, $J = 8.0$ Hz), 8.06 (s, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 25.6, 29.3, 29.5, 30.2, 30.3, 38.4, 42.4, 45.0, 46.2, 49.8, 123.3, 125.4, 126.0, 126.3, 126.5, 128.0, 128.9, 130.9, 131.8, 133.9, 136.1, 143.6, 143.7, 160.8, 170.0, 172.3, 176.3, 176.4; ESI-MS: 568 (M + Na). HRMS (ESI-TOF) calcd for C$_{30}$H$_{36}$N$_5$O$_5$ (M + H$^+$), 546.2711; found 546.2715.

(R)-2-(3-amino-2-(cyclohexanecarboxamido)-3-oxopropyl)-N-benzylazoxazole-4-carboxamide [8b(iv)]:

![Chemical Structure](image)
\(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) 1.18 – 1.26 (m, 3H), 1.32–1.38 (m, 2H), 1.58 (s, 5H), 1.65 – 1.79 (m, 2H), 2.10 (t, 1H, \(J = 10.8\) Hz), 3.20 (dd, 1H, \(J_1 = 16.0\) Hz, \(J_2 = 6.4\) Hz), 3.27 (dd, 1H, \(J_1 = 16.0\) Hz, \(J_2 = 5.6\) Hz), 4.60 (d, 2H, \(J = 5.6\) Hz), 4.92 (t, 1H, \(J = 6.4\) Hz), 5.37 (broad s, 1H), 6.50 – 6.57 (m, 1H), 7.07 (broad s, 1H), 7.29 – 7.33 (m, 5H), 8.16 (s, 1H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\) 25.5, 25.6, 29.3, 29.6, 29.8, 43.1, 45.1, 49.8, 127.7, 127.8, 128.8, 136.1, 137.8, 141.5, 160.1, 161.2, 171.8, 176.5; ESI-MS: 421 (M + Na). HRMS (ESI-TOF) calcd for C\(_{21}\)H\(_{27}\)N\(_4\)O\(_4\) (M+H\(^+\)), 399.2027; found 399.2025.

\((R)^{-2-(2-(3,5-bis(trifluoromethyl)phenyl)acetamido)-3-((4-(piperidine-1-carbonyl)oxazol-2-yl)propanamide [8c(i)]:

![](image1)

\(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) 1.47 (broad s, 3H), 1.52 (s, 2H), 1.68 (broad s, 2H), 4.15 – 4.25 (m, 6H), 4.70 (q, 2H, \(J = 8.0\) Hz), 7.23 (s, 1H), 7.61 (s, 1H), 7.92 – 7.96 (m, 3H), 8.24 (s, 1H), 8.55 (d, 1H, \(J = 8.0\) Hz); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\) 24.3, 30.7, 41.2, 43.2, 51.1, 79.3, 120.6, 122.4, 125.1, 129.9, 130.3, 130.5, 130.6, 136.3, 139.6, 142.7, 160.6, 160.8, 169.6, 172.3; ESI-MS: 543 (M + Na). HRMS (ESI-TOF) calcd for C\(_{22}\)H\(_{22}\)F\(_6\)N\(_4\)O\(_4\) (M+H\(^+\)), 521.1618; found 521.1615.

\((R)^{-2-(3-amino-2-(2-(3,5-bis(trifluoromethyl)phenyl)acetamido)-3-oxopropyl)-N-butyloxazole-4-carboxamide [8c(ii)]:

![](image2)
**13C NMR (100 MHz, CDCl₃):** δ 14.1, 20.0, 30.9, 31.7, 38.4, 41.3, 51.1, 79.6, 120.6, 122.5, 125.2, 130.2, 130.5, 136.6, 139.8, 139.9, 141.7, 160.3, 161.5, 169.5, 172.0; ESI-MS: 531 (M + Na). HRMS (ESI-TOF) calcd for C₁₂H₂₁F₆N₄O₄ (M+ H⁺), 509.1618; found 509.1615.

(R)-2-(2-(3,5-bis(trifluoromethyl)phenyl)acetamido)-3-(4-(4-butyrylpiperazine-1-carbonyl)oxazol-2-yl)propanamide [8c(iii)g]:

![Chemical structure](image)

**1H NMR (400 MHz, CDCl₃):** δ 0.87 (t, 3H, J = 7.2 Hz), 1.28 (q, 2H, J = 7.6 Hz), 1.45 (t, 2H, J = 7.6 Hz), 3.04 (dd, 1H, J₁ = 15.2 Hz, J₂ = 8.0 Hz), 3.17 – 3.24 (m, 3H), 3.74 (s, 1H), 4.68 (q, 1H, J = 6.8 Hz), 7.24 (s, 1H), 7.59 (s, 1H), 7.92 – 7.94 (m, 3H), 8.05 (brs, 1H), 8.33 (s, 1H), 8.59 (d, 1H, J = 8.0 Hz); **13C NMR (100 MHz, CDCl₃):** δ 14.1, 20.0, 30.9, 31.7, 38.4, 41.3, 51.1, 79.6, 120.6, 122.5, 125.2, 130.2, 130.5, 136.6, 139.8, 139.9, 141.7, 160.3, 161.5, 169.5, 172.0; ESI-MS: 614 (M + Na). HRMS (ESI-TOF) calcd for C₂₅H₂₇F₆N₅O₅ (M+ H⁺), 592.1989; found 592.2000.

(R)-2-(3-amino-2-(2-(3,5-bis(trifluoromethyl)phenyl)acetamido)-3-oxopropyl)-N-benzyloxazole-4-carboxamide [8c(iv)]:

![Chemical structure](image)
\(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) 3.05 (dd, 1H, \(J_1 = 15.6\) Hz, \(J_2 = 8.0\) Hz), 3.26 (dd, 1H, \(J_1 = 16.0\) Hz, \(J_2 = 5.6\) Hz), 3.62-3.78 (m, 2H), 4.41 (s, 2H), 4.68 (q, 1H, \(J = 6.8\) Hz), 7.16 – 7.28 (m, 5H), 7.64 (s, 1H), 7.93 (s, 2H), 8.42 (s, 1H), 8.66 (d, 1H, \(J = 8.0\) Hz); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\) 31.2, 40.8, 42.4, 51.1, 120.9, 122.6, 127.3, 128.1, 128.3, 128.7, 130.2, 130.5, 137.3, 139.5, 140.2, 160.2, 163.0, 169.2, 172.5; ESI-MS: 565 (M + Na). HRMS (ESI-TOF) calcd for C\(_{24}\)H\(_{21}\)F\(_6\)N\(_4\)O\(_4\) (M+ H\(^+\)), 543.1462; found 543.1464.

\((3R,5R,7R)\)-N-((R)-1-amino-1-oxo-3-(4-(piperidine-1-carbonyl)oxazol-2-yl)propan-2-yl)adamantane-1-carboxamide [8d(i)]:

\(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) 1.61-1.77 (m, 12H), 1.84 (brs, 6H), 2.00-2.04 (m, 3H), 3.15 (dd, 1H, \(J_1 = 16.0\) Hz, \(J_2 = 6.0\) Hz), 3.36 (dd, 1H, \(J_1 = 16.0\)Hz, \(J_2 = 6.0\)Hz), 3.62 – 3.85 (m, 4H), 4.95 (q, 1H, \(J = 6.0\) Hz), 5.80 (s, 1H), 6.89 (brs, 1H), 7.11 (d, 1H, \(J = 7.2\) Hz), 8.02 (s, 1H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\) 24.6, 25.6, 26.7, 28.0, 29.9, 36.4, 39.0, 40.7, 49.7, 136.6, 142.4, 160.7, 160.8, 172.5, 178.4; ESI-MS: 451 (M + Na). HRMS (ESI-TOF) calcd for C\(_{23}\)H\(_{33}\)N\(_4\)O\(_4\) (M+ H\(^+\)), 429.2496; found 429.2492.

\(2-((R)-2-((3R,5R,7R)-adamantane-1-carboxamido)-3-amino-3-oxopropyl)-N\)-butyloxazole-4-carboxamide [8d(ii)]:

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\( ^1 \)H NMR (400 MHz, CDCl\(_3\)): \( \delta \) 0.94 (t, 3H, \( J = 7.2 \) Hz), 1.39 (q, 2H, \( J = 7.6 \) Hz), 1.56 (t, 2H, \( J = 7.2 \) Hz), 1.67-1.78 (m, 6H), 1.83 (brs, 6H), 2.05 (s, 3H), 3.20 (dd, 1H, \( J_1 = 14.8 \) Hz, \( J_2 = 6.0 \) Hz), 3.28 (dd, 1H, \( J_1 = 15.6 \) Hz, \( J_2 = 6.0 \) Hz), 3.39 (q, 2H, \( J = 6.8 \) Hz), 4.96 (q, 1H, \( J = 6.8 \) Hz), 5.69 (brs, 1H), 6.81 (d, 2H, \( J = 6.4 \) Hz), 6.92 (d, 1H, \( J = 7.6 \) Hz), 8.12 (s, 1H); \( ^{13} \)C NMR (100 MHz, CDCl\(_3\)): \( \delta \) 13.7, 20.1, 28.0, 29.9, 31.7, 36.4, 38.8, 39.1, 40.7, 49.8, 136.3, 141.2, 160.2, 161.2, 172.3, 178.5; ESI-MS: 439 (M + Na).

HRMS (ESI-TOF) calcd for C\(_{22}\)H\(_{33}\)N\(_4\)O\(_4\) (M+ H\(^+\)), 417.2496; found 417.2495.

\((3R,5R,7R)\)-N-((R)-1-amino-1-oxo-3-(4-(4-(2-phenylacetyl)piperazine-1-carbonyloxazol-2-yl)propan-2-yl)adamantane-1-carboxamide [\( ^{8d(iii)h} \)]:

\( ^1 \)H NMR (400 MHz, CDCl\(_3\)): \( \delta \) 1.66 (d, 3H, \( J = 12.0 \) Hz), 1.75 (d, 3H, \( J = 12.8 \) Hz), 1.81 (s, 6H), 2.03 (s, 3H), 3.18 (dd, 1H, \( J_1 = 15.6 \) Hz, \( J_2 = 5.6 \) Hz), 3.28 (brs, 1H), 3.50 (brs, 3H), 3.69 (brs, 3H), 3.77-3.96 (m, 4H), 4.95 (q, 1H, \( J = 6.0 \) Hz), 5.71-5.82 (m, 1H), 6.74 (s, 1H), 6.81-6.93 (m, 1H), 7.23-7.27 (m, 3H), 7.33 (t, 2H, \( J = 7.2 \)Hz), 8.07 (s, 1H); \( ^{13} \)C NMR (100 MHz, CDCl\(_3\)): \( \delta \) 28.0, 30.0, 36.4, 39.0, 40.7, 41.1, 42.3, 46.1, 49.8, 127.1, 128.5, 128.9, 134.6, 136.1, 143.6, 160.7, 160.9, 169.8, 172.3, 178.4; ESI-MS: 570 (M + Na).

HRMS (ESI-TOF) calcd for C\(_{30}\)H\(_{38}\)N\(_5\)O\(_5\) (M+ H\(^+\)), 548.2867; found 548.2871.
2-((R)-2-((3R,5R,7R)-adamantane-1-carboxamido)-3-amino-3-oxopropyl)-N-benzyloxazole-4-carboxamide [8d(iv)]:

\[
\begin{align*}
\text{H}_2\text{N} & \quad \text{O} \\
\text{O} & \quad \text{NH} \\
\text{N} & \quad \text{NH}
\end{align*}
\]

\[\text{adamantane-1-carboxamido-3-amino-3-oxopropyl-N-benzyloxazole-4-carboxamide}\]

\[\delta 1.59 (\text{d, } 3\text{H, } J = 12.0 \text{ Hz}), 1.70 (\text{d, } 3\text{H, } J = 12.4 \text{ Hz}), 1.76 (\text{s, } 6\text{H}), 1.88 (\text{s, } 1\text{H}), 1.95 (\text{brs, } 3\text{H}), 3.15 (\text{dd, } 1\text{H, } J1 = 16 \text{ Hz, } J2 = 5.6 \text{ Hz}), 3.23 (\text{dd, } 1\text{H, } J1 = 16.0 \text{ Hz, } J2 = 6.4 \text{ Hz}), 4.57 (\text{t, } 2\text{H, } J = 5.2 \text{ Hz}), 4.92 (\text{q, } 1\text{H, } J = 6.4 \text{ Hz}), 5.64 (\text{brs, } 1\text{H}), 6.80 (\text{brs, } 1\text{H}), 6.89 (\text{d, } 1\text{H, } J = 7.2 \text{ Hz}), 7.18 (\text{brs, } 1\text{H}), 7.29-7.34 (\text{m, } 5\text{H}), 8.15 (\text{s, } 1\text{H}); \]

\[\text{C NMR (100 MHz, CDCl}_3)\]: \[\delta 27.9, 29.9, 36.3, 39.0, 40.6, 40.7, 43.1, 49.8, 127.6, 127.8, 128.8, 136.0, 137.8, 141.5, 160.2, 161.4, 172.2, 178.4; \]

\[\text{ESI-MS: 473 (M + Na). HRMS (ESI-TOF) calcd for C}_{25}\text{H}_{31}\text{N}_{4}\text{O}_4 (M + H^+), 451.2340; found 451.2345.}\]

(R)-4-(4-(piperidine-1-carbonyl)oxazol-2-yl)-2-propionamidobutanamide [12a(i)]:

\[
\begin{align*}
\text{H}_2\text{N} & \quad \text{O} \\
\text{O} & \quad \text{NH} \\
\text{N} & \quad \text{NH}
\end{align*}
\]

\[\delta 1.14 (\text{t, } 3\text{H, } J = 7.2 \text{ Hz}), 1.62-1.68 (\text{m, } 6\text{H}), 2.09-2.16 (\text{m, } 1\text{H}), 2.25 (\text{q, } 2\text{H, } J = 7.6 \text{ Hz}), 2.29-2.35 (\text{m, } 1\text{H}), 2.84-2.90 (\text{m, } 1\text{H}), 2.95-3.01 (\text{m, } 1\text{H}), 3.67-3.78 (\text{m, } 4\text{H}), 4.63 (\text{q, } 1\text{H, } J = 6.8 \text{ Hz}), 5.80 (\text{brs, } 1\text{H}), 6.71 (\text{brs, } 1\text{H}), 7.00 (\text{brs, } 1\text{H}), \]

\[\text{S13}\]
7.95 (s, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$): δ 9.6, 23.5, 24.5, 24.6, 25.6, 29.5, 29.6, 51.5, 136.3, 141.5, 161.0, 163.3, 173.5, 174.2; ESI-MS: 359 (M + Na). HRMS (ESI-TOF) calcd for C$_{16}$H$_{25}$N$_4$O$_4$ (M+ H$^+$), 337.1870; found 337.1866.

(R)-2-(4-amino-3-(cyclohexanecarboxamido)-4-oxobutyl)-N-butyloxazole-4-carboxamide [12b(ii)]:

![Chemical Structure](image)

$^1$H NMR (400 MHz, CDCl$_3$): δ 0.96 (t, 3H, $J = 7.6$ Hz), 1.21-1.28 (m, 3H), 1.41 (q, 4H, $J = 8.0$ Hz), 1.60-1.68 (m, 2H), 1.81 (t, 4H, $J = 14.8$ Hz), 2.07-2.17 (m, 2H), 2.36 (q, 1H, $J = 7.2$ Hz), 2.78 – 2.86 (m, 1H), 2.89-3.38 (m, 1H), 3.42 (q, 2H, $J = 6.8$ Hz), 4.57 (q, 1H, $J = 7.6$ Hz), 5.39 (brs, 1H), 6.16 (d, 1H, $J = 6.8$ Hz), 6.27 (brs, 1H), 6.83 (brs, 1H), 8.08 (s, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$): δ 14.1, 20.0, 24.6, 25.6, 25.8, 25.9, 29.4, 29.5, 29.9, 31.8, 38.4, 44.2, 51.9, 136.6, 141.6, 160.4, 164.1, 173.7, 175.8; ESI-MS: 401 (M + Na). HRMS (ESI-TOF) calcd for C$_{19}$H$_{31}$N$_4$O$_4$ (M+ H$^+$), 379.2340; found 379.2338.

(R)-3-(4-(piperidine-1-carbonyloxazol-2-yl)-2-propionamidopropanamide [12c(iii)g]:

![Chemical Structure](image)

$^1$H NMR (400 MHz, CDCl$_3$): δ 0.98 (t, 3H, $J = 6.8$ Hz), 1.67 (q, 4H, $J = 7.6$ Hz), 2.07-2.14 (m, 1H), 2.33 (t, 3H, $J = 6.8$ Hz), 2.81-2.88 (m, 1H), 2.93-3.00 (m, 1H), 3.54 (s, 2H), 3.69-4.63 (m, 8H), 4.62 (d, 1H, $J = 6.0$ Hz), 5.83 (brs, 1H), 6.70 (brs, 1H), 7.12 (brs,
1H), 7.76-7.78 (m, 3H), 8.02 (s, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 13.9, 18.6, 24.3, 29.5, 35.2, 42.3, 51.7, 121.3, 121.8, 124.6, 129.5, 131.7, 132.0, 137.0, 142.8, 163.2, 169.4, 171.9, 172.8; ESI-MS: 628 (M + Na). HRMS (ESI-TOF) calcd for C$_{26}$H$_{30}$F$_6$N$_5$O$_5$ (M+H$^+$), 606.2146; found 606.2150.

2-((R)-3-((3R,5R,7R)-adamantane-1-carboxamido)-4-amino-4-oxobutyl)-N-benzyloxazole-4-carboxamide [12d(iv)]:

![Chemical Structure](image)

$^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 1.64-1.74 (m, 9H), 1.80 (s, 6H), 2.01 (s, 3H), 2.10-2.17 (m, 1H), 2.30-2.37 (m, 1H), 2.76-2.82 (m, 1H), 2.85-2.91 (m, 1H), 4.54-4.60 (m, 3H), 5.45 (brs, 1H), 6.30 (d, 1H, $J$ = 7.2 Hz), 6.43 (brs, 1H), 7.21 (brs, 1H), 7.29-7.33 (m, 5H), 8.12 (s, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 24.2, 28.0, 28.7, 36.4, 39.1, 40.7, 43.1, 51.4, 127.6, 127.9, 128.7, 136.0, 137.9, 141.1, 160.4, 163.7, 173.1, 178.6; ESI-MS: 487 (M + Na). HRMS (ESI-TOF) calcd for C$_{26}$H$_{33}$N$_4$O$_4$ (M+H$^+$), 465.2496; found 465.2503.

References:


SPECTRA

2-((tert-butoxycarbonyl)amino)-3-(4-(methoxycarbonyl)oxazol-2-yl)propanoic acid (4): $^1$H NMR (400 MHz, CDCl$_3$)
2-((tert-butoxycarbonyl)amino)-3-(4-(methoxycarbonyl)oxazol-2-yl)propanoic acid (4): $^{13}$C NMR (100 MHz, CDCl$_3$)
(R)-2-((tert-butoxycarbonyl)amino)-4-(4-(methoxycarbonyl)oxazol-2-yl)butanoic acid (10): $^1$H NMR (400 MHz, CDCl$_3$)
(R)-2-((tert-butoxycarbonyl)amino)-4-(4-(methoxycarbonyl)oxazol-2-yl)butanoic acid (10): $^{13}$C NMR (100 MHz, CDCl$_3$)
(R)-3-(4-(piperidine-1-carbonyl)oxazol-2-yl)-2-propionamidopropanamide [8a(i)]: $^1$H NMR (400 MHz, CDCl$_3$)
(R)-3-(4-(piperidine-1-carbonyl)oxazol-2-yl)-2-propionamidopropanamide [8a(i)]: $^{13}$C NMR (100 MHz, CDCl$_3$)
(R)-3-(4-(piperidine-1-carbonyl)oxazol-2-yl)-2-propionamidopropanamide [8a(i)]: LC-MS
(R)-3-(4-(piperidine-1-carbonyl)oxazol-2-yl)-2-propionamidopropanamide [8a(i)]: HR-MS
(R)-2-(3-amino-3-oxo-2-propionamidopropyl)-N-butyloxazole-4-carboxamide [8a(ii)]: $^1$H NMR (400 MHz, CD$_3$OD)
(R)-2-(3-amino-3-oxo-2-propionamidopropyl)-N-butyloxazole-4-carboxamide [8a(ii)]: $^{13}$C NMR (100 MHz, CD$_3$OD)
(R)-2-(3-amino-3-oxo-2-propionamidopropyl)-N-butyloxazole-4-carboxamide [8a(ii)]: LC-MS
(R)-2-(3-amino-3-oxo-2-propionamidopropyl)-N-butyloxazole-4-carboxamide [8a(ii)] : HR-MS
(R)-3-(4-(4-(2-(9H-fluoren-9-yl)acetyl)piperazine-1-carbonyl)oxazol-2-yl)-2-propionamidopropanamide [8a(iii)e]: $^1$H NMR (400 MHz, CDCl$_3$)
(R)-3-(4-(4-(2-(9H-fluoren-9-yl)acetyl)piperazine-1-carbonyl)oxazol-2-yl)-2-propionamidopropanamide [8a(iii)e]: $^{13}$C NMR (100 MHz, CDCl$_3$)
(R)-3-(4-(4-(2-(9H-fluoren-9-yl)acetyl)piperazine-1-carbonyl)oxazol-2-yl)-2-propionamidopropanamide [8a(iii)e]: LC-MS
(R)-3-(4-(4-(2-(9H-fluoren-9-yl)acetyl)piperazine-1-carbonyl)oxazol-2-yl)-2-propionamidopropanamide [8a(iii)e]: HR-MS
(R)-2-(3-amino-3-oxo-2-propionamidopropyl)-N-benzyloxazole-4-carboxamide [8a(iv)]: $^1$H NMR (400 MHz, CDCl$_3$)
(R)-2-(3-amino-3-oxo-2-propionamidopropyl)-N-benzoxazole-4-carboxamide [8a(iv)]: $^{13}$C NMR (100 MHz, CDCl$_3$)
(R)-2-(3-amino-3-oxo-2-propionamidopropyl)-N-benzylloxazole-4-carboxamide [8a(iv)]: LC-MS
(R)-2-(3-amino-3-oxo-2-propionamidopropyl)-N-benzoxazole-4-carboxamide [8a(iv)]: HR-MS
(R)-N-(1-amino-1-oxo-3-(4-(piperidine-1-carbonyl)oxazol-2-yl)propan-2-yl)cyclohexanecarboxamide [8b(i)]: $^1$H NMR (400 MHz, CDCl$_3$)
(R)-N-(1-amino-1-oxo-3-(4-(piperidine-1-carbonyl)oxazol-2-yl)propan-2-yl)cyclohexanecarboxamide [8b(l)]: $^{13}$C NMR (100 MHz, CDCl$_3$)
(R)-N-(1-amino-1-oxo-3-(4-(piperidine-1-carbonyl)oxazol-2-yl)propan-2-yl)cyclohexanecarboxamide [8b(l)]: LC-MS
(R)-N-(1-amino-1-oxo-3-(4-(piperidine-1-carbonyl)oxazol-2-yl)propan-2-yl)cyclohexanecarboxamide [8b(l)]: HR-MS
(R)-2-(3-amino-2-(cyclohexanecarboxamido)-3-oxopropyl)-N-butyloxazole-4-carboxamide [8b(ii)]: $^1$H NMR (400 MHz, CDCl$_3$)
(R)-2-(3-amino-2-(cyclohexanecarboxamido)-3-oxopropyl)-N-butyloxazole-4-carboxamide [8b(ii)]: $^{13}$C NMR (100 MHz, CDCl$_3$)
(R)-2-(3-amino-2-(cyclohexanecarboxamido)-3-oxopropyl)-N-butyloxazole-4-carboxamide [8b(ii)]: LC-MS
(R)-2-(3-amino-2-(cyclohexanecarboxamido)-3-oxopropyl)-N-butyloxazole-4-carboxamide [8b(ii)]: HR-MS
(R)-N-(1-amino-3-(4-(2-(naphthalen-1-yl)acetyl)piperazine-1-carbonyl)oxazol-2-yl)-1-oxopropan-2-yl)cyclohexanecarboxamide [8b(iii)f]: $^1$H NMR (400 MHz, CDCl$_3$)
(R)-N-{1-amino-3-(4-(4-(2-(naphthalen-1-yl)acetyl)piperazine-1-carbonyl)oxazol-2-yl)-1-oxopropan-2-yl)cyclohexanecarboxamide [8b(iii)f]: $^{13}$C NMR (100 MHz, CDCl$_3$)
(R)-N-(1-amino-3-(4-(4-(2-(naphthalen-1-yl)acetyl)piperazine-1-carbonyl)oxazol-2-yl)-1-oxopropan-2-yl)cyclohexanecarboxamide [8b(iii)f]: LC-MS
(R)-N-(1-amino-3-(4-(4-(2-(naphthalen-1-yl)acetyl)piperazine-1-carbonyl)oxazol-2-yl)-1-oxopropan-2-yl)cyclohexanecarboxamide [8b(iii)f]: HR-MS
(R)-2-(3-amino-2-(cyclohexanecarboxamido)-3-oxopropyl)-N-benzyloxazole-4-carboxamide [8b(iv)]: $^1$H NMR (400 MHz, CDCl$_3$)
(R)-2-(3-amino-2-(cyclohexanecarboxamido)-3-oxopropyl)-N-benzyloxazole-4-carboxamide [8b(iv)]: $^{13}$C NMR (100 MHz, CDCl$_3$)
(R)-2-(3-amino-2-(cyclohexanecarboxamido)-3-oxopropyl)-N-benzoxazole-4-carboxamide [8b(iv)]: LC-MS
(R)-2-(3-amino-2-(cyclohexanecarboxamido)-3-oxopropyl)-N-benzyloxazole-4-carboxamide [8b(iv)]: HR-MS
(R)-2-(2-(3,5-bis(trifluoromethyl)phenyl)acetamido)-3-(4-(piperidine-1-carbonyl)oxazol-2-yl)propanamide [8c(i)]: $^1$H NMR (400 MHz, CDCl$_3$)
(R)-2-((3,5-bis(trifluoromethyl)phenyl)acetamido)-3-(4-(piperidine-1-carbonyl)oxazol-2-yl)propanamide [8c(i)]: $^{13}$C NMR (100 MHz, CDCl$_3$)
(R)-2-(2-(3,5-bis(trifluoromethyl)phenyl)acetamido)-3-(4-(piperidine-1-carbonyl)oxazol-2-yl)propanamide [8c(i)]: LC-MS

![Chromatogram](image)

![MS Chromatogram](image)

![MS Spectrum Graph](image)

**S54**
(R)-2-(2-(3,5-bis(trifluoromethyl)phenyl)acetamido)-3-(4-(piperidine-1-carbonyl)oxazol-2-yl)propanamide [8c(i)]: HR-MS
(R)-2-(3-amino-2-(2-(3,5-bis(trifluoromethyl)phenyl)acetamido)-3-oxopropyl)-N-butyloxazole-4-carboxamide [8c(ii)]: $^1$H NMR (400 MHz, CDCl$_3$)
(R)-2-(3-amino-2-(2-(3,5-bis(trifluoromethyl)phenyl)acetamido)-3-oxopropyl)-N-butyloxazole-4-carboxamide [8c(ii)]: $^{13}$C NMR (100 MHz, CDCl$_3$)
(R)-2-(3-amino-2-(2-(3,5-bis(trifluoromethyl)phenyl)acetamido)-3-oxopropyl)-N-butyloxazole-4-carboxamide [8c(ii)]: LC-MS

![Chemical Structure Image]

**Chromatogram**

2283 U/Siva/2283/Pure Final/2283-10.png

1 Det A Ch1 / 214nm
2 Det A Ch2 / 254nm

**MS Chromatogram**

2283 U/Siva/2283/Pure Final/2283-10.png

Segment#1: x(10,000,000)

3.283, 151

**MS Spectrum Graph**

Peak#3: Ret Time: Averaged 5.630-5.637 (Scan#1: 1690-1692)
BG Mode: Calc 5.477c,<6.027c (>6.477c>1809)
Mass Peaks: 59, Base Peak: 508.85 (12727462) MS Stage: Polarity: Pos, Segment 1 - Event 1, Precursor, Cutoff: Ionization Mode: Ionization Mode S

S58
(R)-2-(3-amino-2-(2-(3,5-bis(trifluoromethyl)phenyl)acetamido)-3-oxopropyl)-N-butyloxazole-4-carboxamide [8c(ii)]: HR-MS
(R)-2-(2-(3,5-bis(trifluoromethyl)phenyl)acetamido)-3-(4-(4-butyrylpiperazine-1-carbonyl)oxazol-2-yl)propanamide [8c(iii)g]:

$^1$H NMR (400 MHz, CDCl$_3$)
(R)-2-(2-(3,5-bis(trifluoromethyl)phenyl)acetamido)-3-(4-(4-butyrylpiperazine-1-carbonyl)oxazol-2-yl)propanamide [8c(iii)g]:
$^{13}$C NMR (100 MHz, CDCl$_3$)
(R)-2-(2-(3,5-bis(trifluoromethyl)phenyl)acetamido)-3-(4-(4-butyrylpiperazine-1-carbonyloxadol-2-yl)propanamide [8c(iii)g]: LC-MS
(R)-2-(2-(3,5-bis(trifluoromethyl)phenyl)acetamido)-3-(4-(4-butyrylpiperazine-1-carbonyl)oxazol-2-yl)propanamide [8c(iii)g]: HR-MS
(R)-2-(3-amino-2-(2-(3,5-bis(trifluoromethyl)phenyl)acetamido)-3-oxopropyl)-N-benzoxazole-4-carboxamide \([8c(iv)]\): \(^1\)H NMR (400 MHz, CDCl\(_3\))
(R)-2-(3-amino-2-(2-(3,5-bis(trifluoromethyl)phenyl)acetamido)-3-oxopropyl)-N-benzyloxazole-4-carboxamide [8c(iv)]: $^{13}$C NMR (100 MHz, CDCl$_3$)
(R)-2-(3-amino-2-(2-(3,5-bis(trifluoromethyl)phenyl)acetamido)-3-oxopropyl)-N-benzoyloxazole-4-carboxamide [8c(iv)]: LC-MS
(R)-2-(3-amino-2-(2-(3,5-bis(trifluoromethyl)phenyl)acetamido)-3-oxopropyl)-N-benzyloxazole-4-carboxamide [8c(iv)]: HR-MS
(3R,5R,7R)-N-((R)-1-amino-1-oxo-3-(4-(piperidine-1-carbonyl)oxazol-2-yl)propan-2-yl)adamantane-1-carboxamide [8d(i)]: $^1$H NMR (400 MHz, CDCl$_3$)
(3R,5R,7R)-N-((R)-1-amino-1-oxo-3-(4-(piperidine-1-carbonyl)oxazol-2-yl)propan-2-yl)adamantane-1-carboxamide [8d(i)]: $^{13}$C NMR (100 MHz, CDCl$_3$)
(3R,5R,7R)-N-((R)-1-amino-1-oxo-3-(4-(piperidine-1-carbonyl)oxazol-2-yl)propan-2-yl)adamantane-1-carboxamide [8d(i)]:
LC-MS
(3R,5R,7R)-N-((R)-1-amino-1-oxo-3-(4-(piperidine-1-carbonyl)oxazol-2-yl)propan-2-yl)adamantane-1-carboxamide [8d(i)]: HR-MS
2-((R)-2-((3R,5R,7R)-adamantane-1-carboxamido)-3-amino-3-oxopropyl)-N-butyloxazole-4-carboxamide [8d(ii)]: $^1$H NMR (400 MHz, CDCl$_3$)
2-((R)-2-((3R,5R,7R)-adamantane-1-carboxamido)-3-amino-3-oxopropyl)-N-butyloxazole-4-carboxamide [8d(ii)]: $^{13}$C NMR (100 MHz, CDCl$_3$)
2-((R)-2-((3R,5R,7R)-adamantane-1-carboxamido)-3-amino-3-oxopropyl)-N-butyloxazole-4-carboxamide [8d(ii)]: LC-MS
2-((R)-2-((3R,5R,7R)-adamantane-1-carboxamido)-3-amino-3-oxopropyl)-N-butyloxazole-4-carboxamide [8d(ii)]: HR-MS
(3R,5R,7R)-N-((R)-1-amino-1-oxo-3-(4-(4-(2-phenylacetyl)piperazine-1-carbonyl)oxazol-2-yl)propan-2-yl)adamantane-1-carboxamide [8d(iii)h]: $^1$H NMR (400 MHz, CDCl$_3$)
(3R,5R,7R)-N-((R)-1-amino-1-oxo-3-(4-(4-(2-phenylacetyl)piperazine-1-carbonyl)oxazol-2-yl)propan-2-yl)adamantane-1-carboxamide [8d(iii)h]: $^{13}$C NMR (100 MHz, CDCl$_3$)
(3R,5R,7R)-N-((R)-1-amino-1-oxo-3-(4-(4-(2-phenylacetyl)piperazine-1-carbonyl)oxazol-2-yl)propan-2-yl)adamantane-1-carboxamide [8d(iii)h]: LC-MS
(3R,5R,7R)-N-((R)-1-amino-1-oxo-3-(4-(4-(2-phenylacetyl)piperazine-1-carbonyl)oxazol-2-yl)propan-2-yl)adamantane-1-carboxamide [8d(iii)h]: HR-MS
2-((R)-2-((3R,5R,7R)-adamantane-1-carboxamido)-3-amino-3-oxopropyl)-N-benzyloxazole-4-carboxamide [8d(iv)]: \[^1\text{H}\] NMR (400 MHz, CDCl\textsubscript{3})
2-((R)-2-((3R,5R,7R)-adamantane-1-carboxamido)-3-amino-3-oxopropyl)-N-benzyl-oxazole-4-carboxamide [8d(iv)]: $^{13}$C NMR (100 MHz, CDCl$_3$)
2-((R)-2-((3R,5R,7R)-adamantane-1-carboxamido)-3-amino-3-oxopropyl)-N-benzoxazole-4-carboxamide [8d(iv)]: LC-MS
2-((R)-2-((3R,5R,7R)-adamantane-1-carboxamido)-3-amino-3-oxopropyl)-N-benzyloxazole-4-carboxamide [8d(iv)]: HR-MS
(R)-4-(4-(piperidine-1-carbonyl)oxazol-2-yl)-2-propionamidobutanamide [12a(i)]: $^1$H NMR (400 MHz, CDCl$_3$)
(R)-4-(4-(piperidine-1-carbonyl)oxazol-2-yl)-2-propionamidobutanamide [12a(i)]: $^{13}$C NMR (100 MHz, CDCl$_3$)
(R)-4-(4-(piperidine-1-carbonyl)oxazol-2-yl)-2-propionamidobutanamide [12a(i)]: LC-MS

![Chromatogram](image)

**MS Spectrum Graph**

Peak#1 Ret.Time: Averaged 3.673-3.690/Scan#1:103-1105
BG Mode Calc: 3.527c->4.147(1058c->1245)
Mass Peaks:100 Base Peak 336.90(15316158) MS Stage: Polarity:Pos Segment 1 -> Event1 Precursor: Cutoff: Ionization Mode:Slonization ModeS
(R)-4-(4-(piperidine-1-carbonyl)oxazol-2-yl)-2-propionamidobutanamide [12a(i)]: HR-MS

[Graph showing mass spectrometry data with peaks at different masses]
(R)-2-(4-amino-3-(cyclohexanecarboxamido)-4-oxobutyl)-N-butyloxazole-4-carboxamide [12b(ii)]: $^1$H NMR (400 MHz, CDCl$_3$)
(R)-2-(4-amino-3-(cyclohexanecarboxamido)-4-oxobutyl)-N-butyloxazole-4-carboxamide [12b(ii)]: $^{13}$C NMR (100 MHz, CDCl$_3$)
(R)-2-(4-amino-3-(cyclohexanecarboxamido)-4-oxobutyl)-N-butyloxazole-4-carboxamide [12b(ii)]: LC-MS

[Chemical structure image]
(R)-2-(4-amino-3-(cyclohexanecarboxamido)-4-oxobutyl)-N-butyloxazole-4-carboxamide [12b(ii)]: HR-MS

![HR-MS spectrum of the compound](image)
(R)-3-(4-(piperidine-1-carbonyl)oxazol-2-yl)-2-propionamidopropanamide [12c(iii)g]: $^1$H NMR (400 MHz, CDCl$_3$)
(R)-3-(4-(piperidine-1-carbonyl)oxazol-2-yl)-2-propionamidopropanamide [12c(iii)]: $^{13}$C NMR (100 MHz, CDCl$_3$)
(R)-3-(4-(piperidine-1-carbonyl)oxazol-2-yl)-2-propionamidopropanamide [12c(iii)g]: LC-MS
(R)-3-(4-(piperidine-1-carbonyl)oxazol-2-yl)-2-propionamidopropanamide [12c(iii)g]: HR-MS
2-((R)-3-((3R,5R,7R)-adamantane-1-carboxamido)-4-amino-4-oxobutyl)-N-benzoxazole-4-carboxamide [12d(iv)]: $^1$H NMR (400 MHz, CDCl$_3$)
2-((R)-3-((3R,5R,7R)-adamantane-1-carboxamido)-4-amino-4-oxobutyl)-N-benzoxazole-4-carboxamide [12d(iv)]: $^{13}$C NMR (100 MHz, CDCl$_3$)
2-((R)-3-((3R,5R,7R)-adamantane-1-carboxamido)-4-amino-4-oxobuty1)-N-benzyl oxazole-4-carboxamide [12d(iv)]: LC-MS
2-((R)-3-((3R,5R,7R)-adamantane-1-carboxamido)-4-amino-4-oxobutyl)-N-benzyloxazole-4-carboxamide [12d(iv)]: HR-MS