Supporting Information

Diversity-Oriented Synthesis of Macrocyclic Peptidomimetics

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General Remarks.

Unless otherwise mentioned, all reagents were purchased from commercial sources. Room temperature (r.t.) refers to ambient temperature. Temperatures of 0 °C were maintained using an ice–water bath. Yields refer to chromatographically and spectroscopically pure compounds unless otherwise stated. Where possible, reactions were monitored by thin layer chromatography (TLC) performed on commercially prepared glass plates precoated with Merck silica gel 60 F254 or aluminium oxide 60 F254. Visualisation was by the quenching of UV fluorescence (λ_{max}= 254 nm) or by staining with potassium permanganate. All flash chromatography was carried out using slurry-packed Merck 9325 Keiselgel 60 silica gel unless otherwise stated. Infrared spectra were recorded neat (unless otherwise stated) on a Perkin–Elmer Spectrum One spectrometer with internal referencing. Selected abrorption maxima (λ_{max}) are reported in wavenumbers (cm^{-1}). Melting points

were obtained using a Büchi Melting Point B-545 instrument and are uncorrected. Microwave heating was performed in a C.E.M. Discover S-Class apparatus. ^{1}H NMR were recorded using an internal deuterium lock at ambient probe temperatures on the following instruments: Bruker DPX-400 (400 MHz), Bruker Avance 400 QNP (400 MHz) and Bruker Avance 500 BB ATM (500 MHz). Chemical shifts (δ) are quoted in ppm, to the nearest 0.01 ppm, and are referenced to the residual non-deuterated solvent peak. Coupling constants (*J*) are reported in Hertz (Hz) to the nearest 0.5 Hz. Data are reported as follows: chemical shift, multiplicity (br = broad; s = singlet; d = doublet; t = triplet; m = multiplet), integration and assignment and coupling constant(s). Proton assignments were determined either on the basis of unambiguous chemical shift or coupling pattern, by patterns obrerved in 2D experiments (^{1}H–^{1}H COSY, HSQC) or by analogy to fully interpreted spectra for related compounds. ^{13}C NMR were recorded by broadband proton-spin-decoupling at ambient probe temperatures using an internal deuterium lock on the following instruments: Bruker DPX-400 (100 MHz), Bruker Avance 400 QNP (100 MHz) and Bruker Avance 500 BB ATM (125 MHz). Chemical shifts (δ) are quoted in ppm, to the nearest 0.1 ppm, and are referenced to the residual non-deuterated solvent peak. Assignments were supported by DEPT and 2D experiments (HSQC) or by analogy to fully interpreted spectra for related compounds. Any numbering in selected spectral data does not follow the IUPAC naming system and is used for the assignment of the ^{1}H NMR and ^{13}C NMR spectra. The general numbering used for the compounds is shown in Fig. S1, S2 and S3. High Resolution Masses were measured using a Spectrometer or a Micromass Quadrapole-Time of Flight (Q-ToF) spectrometer. Mass values are reported within the error limits of ±5 ppm mass units. The ionisation technique used was electrospray ionisation (ESI). Optical rotations were recorded on a Perkin–Elmer 343 polarimeter. $[\alpha]^{25}_{D}$ values are reported in 10^{-1} deg cm^{2} g^{-1} at 589 nm, concentration (*c*) is given in g(100mL)$^{-1}$. Full spectral data for all novel compounds are given below, all previously characterized compounds gave spectra consistent with the literature. Other abbreviations used: microwave heating (MW), aromatic (arom.).

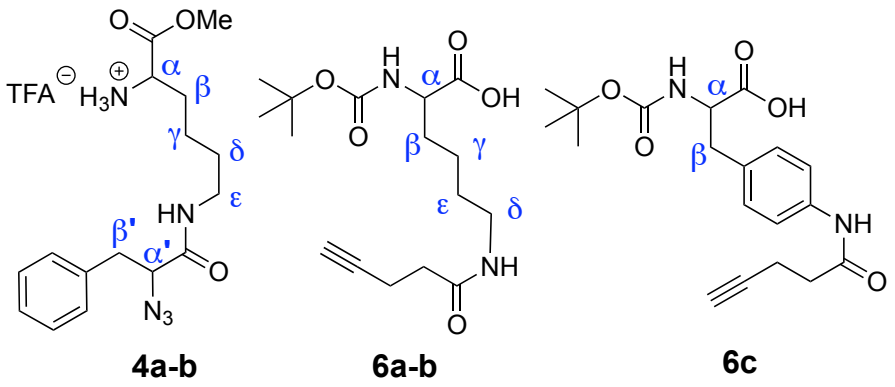


Fig. S1. Nomenclature for ^{1}H NMR assignment of the building blocks.

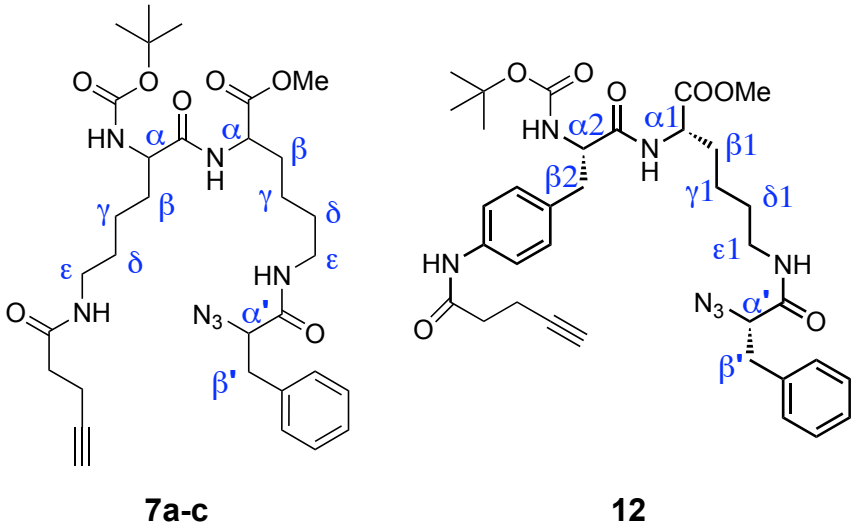


Fig. S2. Nomenclature for ^{1}H NMR assignment of the linear peptidomimetics.

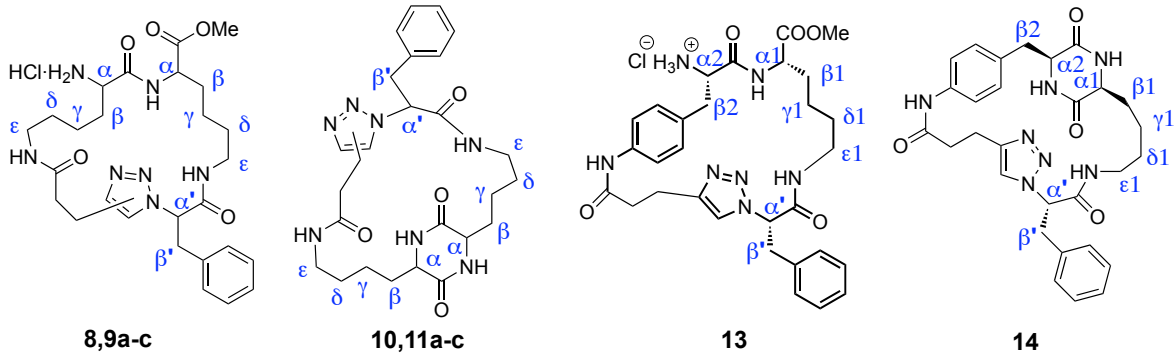


Fig. S3. Nomenclature for ^{1}H NMR assignment of the macrocyclic peptidomimetics.

Synthesis of the building blocks.

(*S*)-2-azido-3-phenylpropanoic acid 1a, **(*R*)-2-azido-3-phenylpropanoic acid 1b, Boc-*L*-Lys(*Z*)-OMe** & **4-pentynoic acid succinimidyl ester 5** were prepared by literature procedures (1-3).

H-*L*- Lys(*L*-N_3-Phe)-OMe·TFA 4a. Boc-*L*-Lys(Z)-OMe (3.90 g, 9.91 mmol) was dissolved in MeOH (40 mL) and hydrogenated overnight over 10% palladium charcoal (200 mg) at room temperature and pressure. The mixture was filtered through a pad of Celite and the solvent was removed under reduced pressure. The slurry was co-evaporated with Et_2O (3x) and petrol ether 40:60 (3x) to yield 2.32 g of Boc-*L*-Lys-OMe (2.32 g) as an oil which was used without further purification. Boc-*L*-Lys-OMe (2.05 g, 8.3 mmol) was dissolved in dry CH_2Cl_2 (25 mL). Triethylamine (2.3 mL, 16.6 mmol), EDC.HCl (1.60 g, 8.3 mmol) and HOBt (1.28 g, 8.3 mmol) were added sequentially. After total dissolution, *(S)*-2-azido-3-phenylpropanoic **1a** (1.59 g, 8.3 mmol) in dry CH_2Cl_2 (25 mL) was added to the solution of **3** and the mixture was stirred overnight at room temperature. Subrequently, the CH_2Cl_2 was removed under reduced pressure and EtOAc (50 mL) was added to the slurry. The organic layer was washed with H_2O (2 x 40 mL) and saturated aqueous $NaHCO_3$ (2 x 40 mL). Extra EtOAc (50 mL) was added to the organic phase and it was washed with 5% citric acid (2 x 40 mL) and H_2O (2 x 40 mL). The organic layer was then dried ($MgSO_4$), evaporated to dryness under reduced pressure performing co-evaporations with CH_2Cl_2 (3x) giving 2.84 g of Boc-*L*-Lys-(N_3-L-Phe)-OMe. The Boc group of the latter was removed upon treatment with TFA (16 mL) in CH_2Cl_2 (16 mL) for 2h at rt. The organic solvent was removed under reduced pressure, the slurry was then co-evaporated with CH_2Cl_2 (3x), Et_2O (3x) and dried at high vacuum to remove all traces of TFA. H-*L*- Lys(L-N_3-Phe)-OMe·TFA was obtained as an brown oil (2.86 g, 73% yield over 3 steps). $[\alpha]^{25}_D$= +39.0 (c 0.5, MeOH). IR: *νmax* (neat)/cm^{-1} 2956, 2117, 1751, 1668; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.37 (br, 3H, NH_3^+), 8.20 (t, 1H, ε-NH, *J*= 5.5 Hz), 7.33-7.23 (m, 5H, CH arom.), 4.05-3.97 (m, 1H, α-CH), 3.94 (dd, 1H, α'-CH, *J*= 8.5 Hz, *J'*= 6.0 Hz), 3.76 (s, 3H, CH_3), 3.10-3.02 (m, 3H, 1H β'-CH_2, ε-CH_2), 2.93 (dd, 1H, β'-CH_2, *J*=

14.0 Hz, *J'*= 8.5 Hz), 1.80-1.68 (m, 2H, β-CH_2), 1.42-1.16 (m, 4H, γ-CH_2, δ-CH_2). ^{13}C NMR (125 MHz, DMSO-d_6) δ 169.9 (C), 168.6 (C), 136.7 (C), 129.0 (CH), 128.3 (CH), 126.6 (CH), 62.5 (CH), 52.7 (CH_3), 51.7 (CH), 38.1 (CH_2), 36.9 (CH_2), 29.6 (CH_2), 28.2 (CH_2), 21.5 (CH_2). HRMS (ESI): *m*/*z* calcd. for $C_{16}H_{24}N_5O_3$ [M + H^+] 334.1879, found 334.1867.

H-Lys-(N_3-D-Phe)-OMe·TFA 4b. A procedure analogous to the one used for the synthesis of **4a** but using *(R)*-2-azido-3-phenylpropanoic **1b** as starting material yielded H-Lys-(N_3-D-Phe)-OMe·TFA as an brown oil(1.4 g, 65% yield over 3 steps). $[\alpha]^{25}_D$= -19.8 (c 0.5, MeOH). IR: ν*max* (neat)/cm^{-1} 2950, 2111, 1751, 1670; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.36 (br, 3H, NH_3^+), 8.19 (t, 1H, ε-NH, *J*= 5.5 Hz), 7.34-7.24 (m, 5H, CH arom.), 4.05-3.97 (m, 1H, α-CH), 3.94 (dd, 1H, α'-CH, *J*= 8.5 Hz, *J'*= 6.0 Hz), 3.76 (s, 3H, CH_3), 3.10-3.02 (m, 3H, 1H β'-CH_2, ε-CH_2), 2. 93 (dd, 1H, β'-CH_2, *J*= 13.5 Hz, *J'*= 8.5 Hz), 1.80-1.68 (m, 2H, β-CH_2), 1.42-1.16 (m, 4H, γ-CH_2, δ-CH_2). ^{13}C NMR (125 MHz, DMSO-d_6) δ 169.9 (C), 168.6 (C), 136.7 (C), 129.0 (CH), 128.3 (CH), 126.6 (CH), 62.5 (CH), 52.7 (CH_3), 51.7 (CH), 39.4 (CH_2), 38.1 (CH_2), 36.9 (CH_2), 29.6 (CH_2), 28.2 (CH_2), 21.4 (CH_2). HRMS (ESI): *m*/*z* calcd. for $C_{16}H_{24}N_5O_3$ [M + $H]^+$ 334.1879, found 334.1883.

Boc-*L*- Lys(*N*-4-Pentynoyl)-OH 6a. To a suspension of Boc-*L*-Lys-OH (4.2 g, 17.05 mmol), in dry DMF (75 mL), was added a first fraction of DIPEA (3.1 mL, 18.76 mmol). A solution of **5** (4.0 g, 20.46 mmol) in dry DMF (30 mL) was then added dropwise over 10 minutes. At the minute 5, a second fraction of DIPEA (3.1 mL, 18.76 mmol) was added and the mixture was stirred at room temperature for 4 hours. The organic solvent was removed under reduced pressure and the slurry was diluted with H_2O (100 mL). The pH was adjusted to 8-9 by addition of saturated Na_2CO_3 and washings with Et_2O (3 x 60 mL) were performed. The aqueous layer was then acidified to pH 2-3 with conc. HCl and extracted with EtOAc (3 x 75 mL). The organic extracts were dried ($MgSO_4$) and evaporated to dryness under reduced pressure. After precipitations in Et_2O, Boc-*L*-Lys(*N*-4-Pentynoyl)-OH was obtained as a white solid in 86% yield (contaminated with 5% by mass of *N*-Hydroxysuccinimide, ^{1}H NMR). $[\alpha]^{25}_D$= +4.8 (c 0.5, $CHCl_3$). mp= 92.0-94.0ºC. IR: ν*max* (neat)/cm^{-1} 3284, 2936, 1738, 1683, 1619, 1545; ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.99 (br, 1H, NH

carbamate), 5.26 (d, 1H, ε-NH, *J*= 7.0 Hz), 4.33-4.23 (m, 1H, α-CH), 3.33-3.23 (m, 2H, ε-CH_2), 2.54 (td, 2H, $\underline{CH_2}CH_2CO$, *J*= 6.5 Hz, *J'*= 2.5 Hz), 2.41 (t, 2H, $CH_2\underline{CH_2}CO$, *J*= 6.5 Hz), 2.04 (t, 1H, CH alkyne, *J*= 2.5 Hz), 1.93-1.79 (m, 1H, β-CH_2), 1.79-1.67 (m, 1H, β-CH_2), 1.62-1.48 (m, 2H, δ-CH_2), 1.45 (s, 9H, CH_3 ^{t}Bu), 1.48-1.35 (m, 2H, γ-CH_2). ^{13}C NMR (100 MHz, $CDCl_3$): 175.3 (C), 172.1 (C), 155.8 (C), 82.8 (CH), 80.1 (C), 69.6 (CH), 53.1 (CH), 39.2 (CH_2), 35.2 (CH_2), 31.9 (CH_2), 28.7 (CH_2), 28.3(CH_3), 22.3 (CH_2), 14.9 (CH_2). HRMS (ESI): *m*/*z* calcd. for $C_{16}H_{26}N_2O_5Na$ $[M + Na]^+$ 349.1739, found 349.1773.

Boc-*D*- Lys(*N*-4-Pentynoyl)-OH 6b. A procedure analogous to the one used for the synthesis of **6a** but using Boc-*D*-Lys-OH as starting material yielded Boc-*D*- Lys(*N*-4-Pentynoyl)-OH (474 mg, 73%) as a white solid. $[\alpha]^{25}_D$= -4.9 (c 0.39, $CHCl_3$), mp= 92.5-95.0ºC. IR, ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (100 MHz, $CDCl_3$) and HRMS data were identical to those of Boc-*L*-Lys(*N*-4-Pentynoyl)-OH. HRMS (ESI): *m*/*z* calcd. for $C_{16}H_{26}N_2O_5Na$ $[M + Na]^+$ 349.1739, found 349.1739.

Boc-*L*-4-amino-phenylalanine(*N*-4-pentynoyl)-OH 6c. A procedure analogous to the one used for the synthesis of **6a** but using Boc-*L*-4-amino-phenylalanine-OH as starting material and extending the reaction time to 15h yielded Boc-*L*-4-amino-phenylalanine(*N*-4-pentynoyl)-OH as a white solid (750 mg, 58% yield) and an estimated purity of 90% (^{1}H NMR). $[\alpha]^{25}_D$= +14.7 (c 0.70, $CHCl_3$). mp= 86-89ºC. IR: ν*max* (neat)/cm^{-1} 3288, 2974, 2935, 1668, 1603, 1540, 1515, 1159; ^{1}H NMR (500 MHz, DMSO): δ= 9.90 (s, 1H, NH aniline), 7.48 (d, 2H, CH aniline, *J*= 8.5 Hz), 7.15 (d, 2H, CH aniline, *J*= 8.5 Hz), 7.06 (d, 1H, , α-NH, *J*= 8.5 Hz), 4.04 (m, 1H, α-CH), 2.96-2.92 (m, 1H, β-CH_2), 2.79 (t, 1H, CH alkyne, *J*= 2.5 Hz), 2.78-2.74 (m, 1H, β-CH_2), 2.52-2.43 (m, 4H, CH_2CH_2CO), 1.32 (s, 9H, CH_3 ^{t}Bu). ^{13}C NMR (125 MHz, DMSO): δ= 173.5 (C), 169.0 (C), 155.3 (C) , 137.3 (C), 132.5 (C), 129.1 (CH), 118.7 (CH), 83.5 (CH), 77.9 (C), 71.3 (CH), 55.1 (CH), 35.7 (CH_2), 35.0 (CH_2), 28.0 (CH_3), 14.0 (CH_2). HRMS (ESI): *m*/*z* calcd. for $C_{19}H_{24}N_2O_5Na$ $[M + Na]^+$ 383.1583, found 383.1596.

Linear peptidomimetics synthesis.

Linear peptidomimetic 7a ***(1S,2S,3S).*** Compound **4a** (1.41 g, 3.25 mmol) was dissolved in dry CH_2Cl_2 (30 mL). Triethylamine (1.13 mL, 8.13 mmol) was added followed by EDC·HCl (748 mg, 3.90 mmol) and HOBt (550 mg, 3.90 mmol). When all products were dissolved, free carboxylic acid **6a** (1.27 g, 3.90 mmol) in dry CH_2Cl_2 (7 mL) was added and the mixture was stirred overnight at room temperature. Most of the organic solvent was removed under reduced pressure without heating. EtOAc (100 mL) was added to the slurry and the resulting suspension was washed with H_2O, saturated aqueous $NaHCO_3$ (2 x 60 mL each). Extra EtOAc (30 mL) was added and washings with 5% citric acid and H_2O (2 x 60 mL each) were performed. The organic phase was dried ($MgSO_4$) and evaporated to dryness under reduced pressure. After purification by flash chromatography on silica gel (1% MeOH in EtOAc), compound **7a** was obtained as a white solid (735 mg, 37% yield). $[\alpha]^{25}{}_D$= +10.9 (c 0.53, $CHCl_3$). mp= 86-89ºC. IR: v*max* (neat)/cm^{-1} 3301, 2935, 2106, 1724, 1640, 1542, 1522; ^{1}H NMR (400 MHz, $CDCl_3$): δ= 7.33-7.24 (m, 5H, CH arom.), 6.83 (d, 1H, α-NH, *J*= 7.5 Hz), 6.48 (t, 1H, ε-NH, *J*= 5.5 Hz), 6.03 (t, 1H, ε-NH, *J*= 5.0 Hz), 5.32 (d, 1H, α-NH, *J*= 6.5 Hz), 4.51 (td, 1H, α-CH, *J*= 8.0 Hz, *J'*=5.0 Hz), 4.15 (dd, 1H, α'-CH, *J*= 8.0 Hz, *J'*= 5.0 Hz), 4.17-4.10 (m, 1H, α-CH), 3.74 (s, 3H, CH_3O), 3.33-3.25 (m, 3H, ε-CH_2 , 1H β'-CH_2), 3.24-3.12 (m, 1H, ε-CH_2), 3.03 (dd, 1H, β'-CH_2, *J*= 14.0 Hz, *J'*= 8.0 Hz), 2.52 (td, 2H, , $\underline{CH_2}CH_2CO$, *J*= 7.0 Hz, *J'*= 2.5 Hz), 2.39 (t, 2H, , $CH_2\underline{CH_2}CO$, *J*= 7.0 Hz), 2.02 (t, 1H, CH alkyne, *J*= 2.5 Hz), 1.92-1.79 (m, 2H, 1H β-CH_2, 1H β-CH_2), 1.69-1.62 (m, 2H, 1H β-CH_2, 1H β-CH_2), 1.59-1.50 (m, 2H, δ-CH_2), 1.48-1.37 (m, 4H, γ-CH_2, δ-CH_2), 1.43 (s, 9H, CH_3 ^{t}Bu), 1.32-1.24 (m, 2H, γ-CH_2). ^{13}C NMR (100 MHz, $CDCl_3$): δ= 172.6 (C), 172.2 (C), 171.2 (C), 168.9 (C), 155.8 (C), 136.2 (C), 129.4 (CH), 128.6 (CH), 127.2 (CH), 83.1 (CH), 80.1 (C), 69.3 (C) 65.3 (CH), 54.2 (CH), 52.4 (CH_3), 51.8 (CH), 38.8 (CH_2), 38.7 (CH_2), 38.4 (CH_2), 35.3 (CH_2), 31.7 (CH_2), 31.5 (CH_2), 28.9 (CH_2), 28.6 (CH_2), 28.3 (CH_3), 22.3 (CH_2), 22.3 (CH_2), 14.9 (CH_2). HRMS (ESI): *m*/*z* calcd. for $C_{32}H_{48}N_7O_7$ $[M + H]^+$ 642.3615, found 642.3597.

Linear peptidomimetic 7b *(1S,2R,3S).* A procedure analogous to the one used for the synthesis of **7a** but using **4a** and **6b** as starting materials yielded **7b** as a white solid (564 mg, 39% yield). $[\alpha]^{25}_{D}$= +32.2 (c 0.50, $CHCl_3$). mp= 91-92ºC. IR: ν*max* (neat)/cm^{-1} 3315, 2934, 2107, 1738, 1642, 1524; ^{1}H NMR (400 MHz, $CDCl_3$): δ= 7.33-7.24 (m, 5H, CH arom.), 6.77 (d, 1H, α-NH, *J*= 7.5 Hz), 6.51 (t, 1H, ε-NH, *J*= 5.0 Hz), 5.97 (t, 1H, ε-NH, *J*= 5.5 Hz), 5.28 (br, 1H, α-NH), 4.54 (td, 1H, α-CH, *J*= 8.0 Hz, *J'*=4.8 Hz), 4.14 (dd, 1H, α'-CH, *J*= 8.0 Hz, *J'*=4.5 Hz), 4.12-4.04 (m, 1H, α-CH), 3.73 (s, 3H, CH_3O), 3.33-3.20 (m, 4H, 3H ε-CH_2, 1H β'-CH_2), 3.18-3.10 (m, 1H, ε-CH_2), 3.01 (dd, 1H, β'-CH_2, *J*= 14.0 Hz, *J'*= 8.0 Hz), 2.52 (td, 2H, $\underline{CH_2}CH_2CO$, *J*= 7.0 Hz, *J'*= 2.5 Hz), 2.38 (t, 2H, $CH_2\underline{CH_2}CO$, *J*= 7.0 Hz), 2.03 (t, 1H, CH alkyne, *J*= 2.5 Hz), 1.90-1.80 (m, 2H, 1H β-CH_2, 1H β-CH_2), 1.70-1.60 (m, 2H, 1H β-CH_2, 1H β-CH_2), 1.56-1.47 (m, 2H, δ-CH_2), 1.47-1.35 (m, 4H, δ-CH_2, γ-CH_2), 1.44 (s, 9H, CH_3 ^{t}Bu), 1.32-1.22 (m, 2H, γ-CH_2). ^{13}C NMR (100 MHz, $CDCl_3$): δ= 172.5 (C), 172.0 (C), 171.3 (C), 168.8 (C), 155.8 (C), 136.3 (C), 129.4 (CH), 128.6 (CH), 127.1 (CH), 83.0 (CH), 80.2 (C), 69.4 (C) 65.3 (CH), 54.5 (CH), 52.4 (CH_3), 51.7 (CH), 39.0 (CH_2), 38.6 (CH_2), 38.5 (CH_2), 35.4 (CH_2), 31.7 (CH_2), 31.3 (CH_2), 29.1 (CH_2), 28.6 (CH_2), 28.3 (CH_3), 22.3 (CH_2), 22.2 (CH_2), 14.9 (CH_2). HRMS (ESI): *m/z* calcd. for $C_{32}H_{48}N_7O_7$ $[M + H]^+$ 642.3615, found 642.3625.

Linear peptidomimetic 7c *(1S,2S,3R).* A procedure analogous to the one used for the synthesis of **7a** but using **4b** and **6a** as starting materials yielded **7c** as a white solid (659 mg, 43% yield). $[\alpha]^{25}_{D}$= -34.9 (c 0.68, $CHCl_3$). mp= 69-71ºC. IR: ν*max* (neat)/cm^{-1} 3312, 2943, 2103, 1738, 1646, 1522; ^{1}H NMR (400 MHz, $CDCl_3$): δ= 7.33-7.26 (m, 5H, CH arom.), 6.87 (d, 1H, α-NH, *J*= 6.0 Hz), 6.48 (br, 1H, ε-NH, *J*= 5.0 Hz), 6.05 (br, 1H, ε-NH), 5.26 (d, 1H, α-NH, *J*= 7.0 Hz), 4.51-4.41 (m, α-CH, 1H,), 4.34-4.28 (m, 1H, α'-CH), 4.12 (d, 1H, α-CH, *J*= 6.0 Hz), 3.74 (s, 3H, CH_3O), 3.34 (dd, 1H, β'-CH_2, *J*= 14.0 Hz, *J'*= 4.5 Hz), 3.30-3.25 (m, 3H, ε-CH_2 Lys), 3.16-3.06 (m, 1H, ε-CH_2 Lys), 3.02 (dd, 1H, β'-CH_2, *J*= 14.0 Hz, *J'*= 8.0 Hz), 2.50 (td, 2H, $\underline{CH_2}CH_2CO$, *J*= 7.0 Hz, *J'*= 2.5 Hz), 2.38 (t, 2H, , $CH_2\underline{CH_2}CO$, *J*= 7.0 Hz), 2.01 (t, 1H, CH alkyne, *J*= 2.5 Hz), 1.88-1.78 (m, 2H, 1H β-CH_2, β-CH_2), 1.75-1.63 (m, 2H, 1H β-CH_2, 1H β-CH_2), 1.60-1.50 (m, 2H, δ-CH_2), 1.50-1.37 (m,

4H, γ-CH_2, δ-CH_2), 1.43 (s, 9H, CH_3 ^{t}Bu), 1.35-1.23 (m, 2H, γ-CH_2). ^{13}C NMR (100 MHz, $CDCl_3$): δ= 172.7 (C), 171.2 (C), 171.2 (C), 169.2 (C), 155.7 (C), 136.1 (C), 129.5 (CH), 128.6 (CH), 127.2 (CH), 83.1 (CH), 80.0 (C), 69.3 (C) 65.2 (CH), 54.1 (CH), 52.4 (CH_3), 52.0 (CH), 38.7 (CH_2), 38.5 (CH_2), 38.3 (CH_2), 35.3 (CH_2), 32.0 (CH_2), 30.9 (CH_2), 28.8 (CH_2), 28.7 (CH_2), 28.3 (CH_3), 22.3 (CH_2), 22.1 (CH_2), 15.0 (CH_2). HRMS (ESI): *m*/*z* calcd. for $C_{32}H_{48}N_7O_7$ $[M + H]^+$ 642.3615, found 642.3627.

Linear peptidomimetic 12. A procedure analogous to the one used for the synthesis of **7a** but using **4a** and Boc-*L*- 4-amino-Phe(*N*-Pentynoyl)-OH as starting materials yielded **12** as a yellowish solid (770 mg, 87% yield). In this case the product was not purified by column chromatography as in our hands it proved to be unstable to silica gel. The estimated purity is more than 80% (^{1}H NMR). $[\alpha]^{25}{}_D$= -2.0 (c 0.5, $CHCl_3$). mp= 145-147ºC. IR: ν*max* (neat)/cm^{-1} 3286, 2929, 2115, 1732, 1684, 1647, 1519; ^{1}H NMR (500 MHz, DMSO-d_6): δ= 9.90 (s, 1H, NH aniline), 8.23 (1H, α1-NH), 8.15 (t, 1H, ε1-NH), 7.47 (d, 2H, CH aniline, *J*= 8.5 Hz), 7.32-7.17 (m, 7H, CH arom.), 6.84 (d, 1H, , α2-NH, *J*= 8.5 Hz), 4.25-4.18 (m, 1H, α1-CH), 4.17-4.13 (m, 1H, α2-CH), 3.92 (d, 1H, α'-CH, *J*= 8.5 Hz, *J*'= 6.5 Hz), 3.61 (s, 3H, CH_3O),3.09-2.88 (m, 5H, β'-CH_2,1H β2-CH_2, ε-CH_2), 2.79 (t, 1H, CH alkyne, *J*= 2.5 Hz), 2.69-2.64 (m, 1H, β2-CH_2) 2.54-2.33 (m, 4H, , CH_2CH_2CO), 1.75-0.80 (m, 6H, β1-CH_2, γ1-CH_2, δ1-CH_2), 1.30 (s, 9H, CH_3 ^{t}Bu). ^{13}C NMR (125 MHz, DMSO- d_6): δ= 172.6 (C), 172.0 (C), 169.2 (C), 168.7 (C), 155.3 (C), 137.4 (C), 136.8 (C), 132.8 (C), 129.5 (CH), 129.2 (CH), 128.4 (CH), 126.8 (CH), 118.8 (CH), 83.7(CH), 78.1 (C), 71.6 (CH), 62.7 (CH), 55.6 (CH), 51.9 (CH_3), 51.9 (CH), 38.4 (CH_2), 37.1 (CH_2), 36.9 (CH_2), 35.3 (CH_2), 30.7 (CH_2), 28.5 (CH_2), 28.3 (CH_3), 22.6 (CH_2), 14.2 (CH_2). HRMS (ESI): *m*/*z* calcd. for $C_{35}H_{45}N_7O_7Na$ $[M + Na]^+$ 698.3278, found 698.3278.

Macrocyclic peptidomimetics synthesis.

Macrocyclic peptidomimetic 8a (*1S,2S,3S*-1,4-triazole). **7a** (310 mg, 0.48 mmol, 1 eq) was suspended in dry THF (400 mL) in a three neck round-bottomed flask, DIPEA (0.24 mL, 1.45 mmol, 3 eq) was added. The reaction mixture was bubbled with Argon for 30 min. At this point CuI (184 mg, 0.97 mmol, 2 eq) was added and the reaction refluxed under N_2 for 15h. The solvent was removed under reduced pressure and the product was purified by column chromatography (CH_2Cl_2-MeOH) yielding 279 mg of a white solid. 156.8 mg of this solid were treated with 1.25M HCl-MeOH (2.75 mL) 24h at rt, the solvent was removed under reduced pressure, co-evaporations with MeOH and CH_2Cl_2 were performed. **8a** was obtained as an off-white solid (141 mg, 90% yield over 2 steps). $[\alpha]^{25}_{D}$= +6.4 (c 0.5, MeOH). mp= 227-228ºC. IR: ν*max* (neat)/cm^{-1} 3240, 3060, 2935, 1735, 1665, 1550, 1438, 1216; ^{1}H NMR (500 MHz, DMSO-d_6): δ= 8.90 (d, 1H, α-NH, *J*= 6.0 Hz), 8.67 (t, 1H, ε-NH, *J*= 5.5 Hz), 8.23 (*d*, 3H, NH_3^+, *J*= 4.5 Hz), 7.84 (t, 1H, ε-NH, *J*= 5.5 Hz), 7.81 (s, 1H, CH triazole), 7.24-7.15 (m, 5H, CH arom.), 5.61 (dd, 1H, α'-CH, *J*= 9.0 Hz, *J'*= 6.5 Hz), 4.12-4.08 (m, 1H, α-CH), 3.96-3.92 (m, 1H, α-CH), 3.60 (s, 3H, CH_3), 3.41 (dd, 1H, β'-CH_2, *J*= 14.0 Hz, *J'*= 6.5 Hz), 3.31 (dd, 1H, β'-CH_2, *J*= 14.0 Hz, *J'*= 9.0 Hz), 3.16-3.07 (m, 1H, 1H ε-CH_2), 3.09-3.01 (m, 2H, ε-CH_2), 3.02-2.94 (m, 1H, ε-CH_2), 2.90-2.79 (m, 2H, $\underline{CH_2}CH_2CO$), 2.38-2.35 (m, 2H, $CH_2\underline{CH_2}CO$), 1.80-1.60 (m, 4H, β-CH_2), 1.55-1.20 (m, 8H, γ-CH_2, δ-CH_2). ^{13}C NMR (125 MHz, DMSO-d_6): 171.4 (C), 170.9 (C), 168.8 (C), 167.2 (C), 145.8 (C), 136.3 (C), 128.8 (CH), 128.2 (CH), 126.6 (CH), 121.2 (CH), 63.6 (CH), 52.4 (CH), 51.8 (CH_3), 51.7 (CH), 38.0 (CH_2), 37.7 (CH_2), 37.1 (CH_2), 34.3 (CH_2), 30.7 (CH_2), 28.8 (CH_2), 28.1 (CH_2), 28.1 (CH_2), 21.8 (CH_2).21.2, (CH_2) 21.0 (CH_2). HRMS (ESI): *m*/*z* calcd. for $C_{27}H_{40}N_7O_5$ $[M + H]^+$ 542.3091, found 542.3095.

Macrocyclic peptidomimetic 8b (*1S,2R,3S*-1,4-triazole). A procedure analogous to the one used for the synthesis of **8a** but using **7b** as starting material afforded **8b** as an off-white solid (167 mg, 81% yield). $[\alpha]^{25}_{D}$= -15.2 (c 0.31, DMSO-d_6). mp= 191-193ºC. IR: ν*max* (neat)/cm^{-1} 3283, 2934, 1718, 1649, 1548; ^{1}H NMR (500 MHz, DMSO-d_6): δ= 8.92 (d, 1H, α-NH, *J*= 8.0 Hz), 8.51 (t, 1H,

ε-NH, *J*= 5.5 Hz), 8.21 (d, 3H, NH_3^+, *J*= 4.5 Hz), 7.83 (s, 1H, CH triazole), 7.81 (t, 1H, ε-NH, *J*= 5.5 Hz), 7.25-7.15 (m, 5H, CH arom.), 5.43 (dd, 1H, α'-CH, *J*= 9.0 Hz, *J'*= 6.5 Hz), 4.40-4.36 (m, 1H, α-CH), 3.86-3.80 (m, 1H, α-CH), 3.66 (s, 3H, CH_3), 3.37 (dd, 1H, β'-CH_2, *J*= 14.0 Hz, *J'*= 6.5 Hz), 3.25 (dd, 1H, β'-CH_2, *J*= 14.0 Hz, *J'*= 9.0 Hz), 3.03-2.86 (m, 4H, ε-CH_2), 2.86-2.81 (m, 2H, $\underline{CH_2}CH_2CO$), 2.39-2.27 (m, 2H, $CH_2\underline{CH_2}CO$), 1.80-1.60 (m, 4H, 2 β-CH_2), 1.40-1.10 (m, 8H, γ-CH_2, δ-CH_2). ^{13}C NMR (125 MHz, DMSO-d_6): 171.8 (C), 170.6 (C), 168.6 (C), 167.1 (C), 145.5 (C), 136.2 (C), 128.8 (CH), 128.2 (CH), 126.6 (CH), 121.0 (CH), 63.6 (CH), 52.0 (CH_3), 51.9 (CH), 51.1 (CH), 38.6 (CH_2), 38.0 (CH_2), 37.8 (CH_2), 34.5 (CH_2), 30.9 (CH_2), 30.5 (CH_2), 28.6 (CH_2), 28.0 (CH_2), 22.2 (CH_2), 21.4, (CH_2) 21.3 (CH_2). HRMS (ESI): *m*/*z* calcd. for $C_{27}H_{40}N_7O_5$ [M + H]$^+$,542.3091, found 542.3116.

Macrocyclic peptidomimetic 8c (*1S,2S,3R*-1,4-triazole). A procedure analogous to the one used for the synthesis of **8a** but using **7c** as starting material afforded **8c** as an off-white solid (47 mg, 68% yield). $[\alpha]^{25}{}_D$= -4.8 (c 0.37, MeOH). mp= 230-231ºC. IR: v*max* (neat)/cm^{-1} 3250, 3040, 2933, 1738, 1663, 1552, 1438, 1213; ^{1}H NMR (500 MHz, DMSO-d_6): δ= 8.74 (t, 1H, ε-NH, *J*= 6.0 Hz), 8.55 (d, 1H, α-NH, *J*= 6.0 Hz), 8.27 (d, 3H, NH_3^+, *J*= 4.0 Hz), 7.84 (s, 1H, CH triazole), 7.81 (t, 1H, ε-NH, *J*= 5.5 Hz), 7.25-7.18 (m, 5H, CH arom.), 5.51 (dd, 1H, α'-CH, *J*= 9.0 Hz, *J'*= 7.0 Hz), 4.02 (dd, 1H, α-CH, *J*= 13.0 Hz, *J'*= 6.0 Hz), 3.92-3.85 (m, 1H, α-CH), 3.58 (s, 3H, CH_3), 3.38 (dd, 1H, β'-CH_2, *J*= 14.0 Hz, *J'*= 7.0 Hz), 3.30 (dd, 1H, β'-CH_2, *J*= 14.0 Hz, *J'*= 9.0 Hz), 3.15-2.98 (m, 4H, ε-CH_2), 2.91-2.80 (m, 2H, $\underline{CH_2}CH_2CO$), 2.45-2.33 (m, 2H, , $CH_2\underline{CH_2}CO$), 1.85-1.65 (m, 4H, 2 β-CH_2), 1.45-1.05 (m, 8H, γ-CH_2, δ-CH_2). ^{13}C NMR (125 MHz, DMSO-d_6): 171.6 (C), 170.9 (C), 168.8 (C), 167.8 (C), 146.1 (C), 136.1 (C), 128.9 (CH), 128.2 (CH), 126.6 (CH), 120.6 (CH), 63.7 (CH), 52.7 (CH), 51.8 (CH_3), 51.8 (CH), 37.7 (CH_2), 37.4 (CH_2), 37.4 (CH_2), 34.5 (CH_2), 30.7 (CH_2), 28.9 (CH_2), 28.3 (CH_2), 28.0 (CH_2), 21.9 (CH_2), 20.9 (CH_2). $C_{27}H_{40}N_7O_5$ [M + H]$^+$ 542.3091, found 542.3107.

Macrocyclic peptidomimetic 9a (*1S,2S,3S*-1,5-triazole). 7a (100 mg, 0.156 mmol, 1 eq) was suspended in dry toluene (125 mL) under Argon. The reaction mixture was heated to 80ºC and

bubbled with Argon for 30 min. $[Cp^*RuCl]_4$ (16.9 mg, 0.016mmol, 0.1 eq) was added and the reaction was refluxed for 20h. Then, it was cooled to rt, filtered through a pad of Celite washing it with CH_2Cl_2 and MeOH. The filtrate was evaporated to dryness under reduced pressure and purified by column chromatography (CH_2Cl_2-MeOH, 95:5) yielding 90.2 mg of a white solid. 87.7 mg of this solid were treated with 1.25M HCl-MeOH (2.75 mL) 24h at rt, the solvent was removed under reduced pressure and co-evaporations with MeOH and CH_2Cl_2 were performed. **9a** was obtained as an off-white solid (78.9 mg, 90% yield over 2 steps). $[\alpha]^{25}{}_D$= +39.8 (c 0.54, MeOH). mp= 233-235ºC. IR: ν*max* (neat)/cm^{-1} 3250, 3060, 2932, 1743, 1672, 1552, 1443, 1218; ^{1}H NMR (500 MHz, DMSO-d_6): δ= 9.03 (d, 1H, α-NH, *J*= 5.5 Hz), 8.83 (t, 1H, ε-NH, *J*= 5.5 Hz), 8.21 (d, 3H, NH_3^+, *J*= 4.0 Hz), 7.96 (t, 1H, ε-NH, *J*= 5.5 Hz), 7.40 (s, 1H, CH triazole), 7.29-7.12 (m, 5H, CH arom.), 5.75 (dd, 1H, α'-CH, *J*= 10.5 Hz, *J'*= 5.0 Hz), 4.18-4.15 (m, 1H, α-CH), 4.12-4.06 (m, 1H, α-CH), 3.62 (dd, 1H, β'-CH_2, *J*= 14.0 Hz, *J'*=10.5 Hz), 3.54 (s, 3H, CH_3), 3.40 (dd, 1H, β'-CH_2, *J*= 14.0 Hz, *J'*= 5.0 Hz), 3.29-3.22 (m, 1H, ε-CH_2), 3.16-3.09 (m, 2H, ε-CH_2), 3.00-2.92 (m, 1H, ε-CH_2), 2.72 (t, 2H, $\underline{CH_2}CH_2CO$, *J*= 8.5 Hz), 2.37-2.26 (m, 2H, , $CH_2\underline{CH_2}CO$), 1.84-1.25 (m, 12H, β-CH_2, γ-CH_2, δ-CH_2). ^{13}C NMR (125 MHz, DMSO-d_6): 171.3 (C), 170.4 (C), 169.1 (C), 167.2 (C), 137.2 (C), 136.9 (C), 130.8 (CH), 129.1 (CH), 127.9 (CH), 126.4 (CH), 61.5 (CH), 52.7 (CH), 51.7 (CH), 51.6 (CH_3), 37.2 (CH_2), 37.1 (CH_2), 36.7 (CH_2), 33.9 (CH_2), 30.6 (CH_2), 28.9 (CH_2), 28.0 (CH_2), 21.2, (CH_2) 21.0 (CH_2), 19.0 (CH_2). $C_{27}H_{40}N_7O_5$ $[M + H]^+$ 542.3091, found 542.3105.

Macrocyclic peptidomimetic 9b (*1S,2R,3S*-1,5-triazole). A procedure analogous to the one used for the synthesis of **9a** but using **7b** as starting material afforded **9b** as an off-white solid (162 mg, 90% yield). $[\alpha]^{25}{}_D$= -55.4 (c 0.36, MeOH). mp= 295-297ºC. IR: ν*max* (neat)/cm^{-1} 3215, 3040, 2935, 1736, 1668, 1552, 1439, 1218; ^{1}H NMR (500 MHz, DMSO-d_6): δ= 8.88 (d, 1H, α-NH, *J*= 7.5 Hz), 8.24-8.17 (m, 4H, NH_3^+ and ε-NH), 8.02 (t, 1H, ε-NH, *J*= 5.5 Hz), 7.39 (s, 1H, CH triazole), 7.19-7.07 (m, 5H, CH arom.), 5.44 (dd, 1H, α'-CH, *J*= 10.0 Hz, *J'*= 5.5 Hz), 4.29-4.24 (m, 1H, α-CH), 3.84-3.77 (m, 1H, α-CH), 3.66 (s, 3H, CH_3), 3.50-3.45 (m, 2H, β'-CH_2), 3.12-2.98 (m, 2H, ε-CH_2), 2.98-2.93 (m, 2H, ε-CH_2), 2.66-2.57 (m, 1H, $\underline{CH_2}CH_2CO$), 2.47-2.42 (m, 1H, $\underline{CH_2}CH_2CO$),

2.37-2.31 (m, 2H, $CH_2\underline{CH_2}CO$), 1.78-1.57 (m, 4H, β-CH_2), 1.42-1.35 (m, 2H, δ-CH_2), 1.30-1.10 (m, 6H, 2 x γ-CH_2, δ-CH_2). ^{13}C NMR (125 MHz, DMSO-d_6): 172.0 (C), 170.7 (C), 168.4 (C), 167.0 (C), 137.5 (C), 136.9 (C), 131.3 (CH), 128.9 (CH), 128.0 (CH), 126.4 (CH), 61.5 (CH), 52.0 (CH_3), 51.9 (CH), 51.7 (CH), 38.3 (CH_2), 38.0 (CH_2), 36.7 (CH_2), 33.6 (CH_2), 30.6 (CH_2), 30.3 (CH_2), 28.8 (CH_2), 27.9 (CH_2), 22.2, (CH_2) 20.8 (CH_2), 17.8 (CH_2). $C_{27}H_{40}N_7O_5$ $[M + H]^+$ 542.3091, found 542.3080.

Macrocyclic peptidomimetic 9c (*1S,2S,3R*-1,5-triazole). A procedure analogous to the one used for the synthesis of **9a** but using **7c** as starting material afforded **9c** as an off-white solid (54 mg, 87% yield). $[\alpha]^{25}{}_D$= +6.4 (c 0.37, MeOH). mp= 251-253ºC. IR: ν*max* (neat)/cm^{-1} 3240, 3040, 2921, 1736, 1666, 1550, 1438, 1213; ^{1}H NMR (500 MHz, DMSO-d_6): δ= 8.60 (d, 1H, α-NH, *J*= 5.5 Hz), 8.35 (t, 1H, ε-NH, *J*= 5.5 Hz), 8.20 (d, 3H, NH_3^+, *J*= 4.5 Hz), 7.97 (t, 1H, ε-NH, *J*= 5.5 Hz), 7.36 (s, 1H, CH triazole), 7.20-7.07 (m, 5H, CH arom.), 5.42 (dd, 1H, α'-CH, *J*= 10.0 Hz, *J'*= 5.5 Hz), 4.10-4.07 (m, 1H, α-CH), 3.75-3.68 (m, 1H, α-CH), 3.61 (s, 3H, CH_3), 3.51 (dd, α'-CH 1H, *J*= 14.0 Hz, *J'*= 5.5 Hz), 3.40 (dd, 1H, β'-CH_2, *J*= 14.0 Hz, *J'*= 10.0 Hz), 3.16-3.02 (m, 4H, ε-CH_2), 2.69-2.63 (m, 1H, $\underline{CH_2}CH_2CO$), 2.57-2.45 (m, 1H, $\underline{CH_2}CH_2CO$), 2.43-2.33 (m, 2H, $CH_2\underline{CH_2}CO$), 1.80-1.60 (m, 4H, β-CH_2), 1.50-1.20 (m, 8H, γ-CH_2, δ-CH_2). ^{13}C NMR (125 MHz, DMSO-d_6): 171.3 (C), 170.7 (C), 168.7 (C), 167.0 (C), 137.5 (C), 136.8 (C), 131.2 (CH), 128.9 (CH), 128.0 (CH), 126.4 (CH), 61.7 (CH), 52.6 (CH), 51.9 (CH_3), 51.8 (CH), 38.4 (CH_2), 37.2 (CH_2), 36.7 (CH_2), 33.3 (CH_2), 30.3 (CH_2), 29.3 (CH_2), 28.2 (CH_2), 28.1 (CH_2), 21.8 (CH_2) 21.0 (CH_2), 18.2 (CH_2). $C_{27}H_{40}N_7O_5$ $[M + H]^+$ 542.3091, found 542.3071.

Macrocyclic Diketopiperazine 10a (*1S,2S,3S*-1,4-triazole). 8a (50 mg, 0.086 mmol) and morpholinomethyl-polystyrene (136.8 mg, 0.48 mmol) were placed in a microwave (MW) tube. 2-butanol (6 mL) was added followed by AcOH (35 μL, 0.61 mmol). The mixture was heated with MW (150ºC) for 3h. Then the resin was filtered and washed with MeOH, CH_2Cl_2. The filtrate was evaporated to dryness under reduced pressure, performing co-evaporations with CH_2Cl_2(3x). Final DKP compound **10a** was obtained as an off-white solid (41.4 mg, 94%). $[\alpha]^{25}$

$_D$= -7.1 (c 0.36, MeOH). mp= 229-230ºC. IR: ν*max* (neat)/cm^{-1} 3250, 3040, 2923, 1666, 1640, 1544, 1454; ^{1}H NMR (500 MHz, DMSO-d_6): δ= 8.34 (t, 1H, ε-NH, *J*= 5.5 Hz), 8.18 (d, 1H, α-NH, *J*= 2.5 Hz), 8.04 (d, 1H, α-NH, *J*= 2.5 Hz), 7.80 (s, 1H, CH triazole), 7.78 (t, 1H, ε-NH, *J*= 5.5 Hz), 7.25-7.11 (m, 5H, CH arom.), 5.44 (dd, 1H, α'-CH, *J*= 9.5 Hz, *J'*= 6.0 Hz), 3.80-3.76 (m, 1H, α-CH), 3.68-3.64 (m, 1H, α-CH), 3.30 (dd, 1H, β'-CH_2, *J*= 14.0 Hz, *J'*= 6.0 Hz), 3.19 (dd, 1H, β'-CH_2, *J*= 14.0 Hz, *J'*= 9.5 Hz), 3.14-2.94 (m, 4H, ε-CH_2), 2.91-2.77 (m, 2H, $\underline{CH_2}CH_2CO$), 2.40-2.30 (m, 2H, $CH_2\underline{CH_2}CO$), 1.75-1.55 (m, 4H, β-CH_2), 1.50-1.10 (m, 8H, γ-CH_2, δ-CH_2). ^{13}C NMR (125 MHz, DMSO-d_6): 170.8 (C), 167.5 (C), 167.3 (C), 167.0 (C), 145.6 (C), 136.1 (C), 128.8 (CH), 128.2 (CH), 126.8 (CH), 121.0 (CH), 63.6 (CH), 54.1 (CH), 53.9 (CH), 38.5 (CH_2), 38.0 (CH_2), 38.0 (CH_2), 34.5 (CH_2), 34.3 (CH_2), 33.1 (CH_2), 29.0 (CH_2), 28.6 (CH_2), 21.6, (CH_2) 21.2 (CH_2), 21.2 (CH_2). $C_{26}H_{36}N_7O_4$ $[M + H]^+$ 510.2829, found 510.2841.

Macrocyclic Diketopiperazine 10b (*1S,2R,3S*-1,4-triazole). A procedure analogous to the one used for the synthesis of **10a** but using **8b** as starting material and increasing the MW heating time to 4h yielded **10b** an off-white solid (41.9 mg, 93% yield). $[\alpha]^{25}$ $_D$= +22.8 (c 0.38, MeOH). mp= 249-251ºC. IR: ν*max* (neat)/cm^{-1} 3260, 2929, 1653, 1547, 1436; ^{1}H NMR (500 MHz, DMSO-d_6): δ= 8.48 (t, 1H, ε-NH, *J*= 6.0 Hz), 8.10 (s, 1H, α-NH), 8.05 (d, 1H, α-NH, *J*= 3.0 Hz), 7.96 (t, 1H, ε-NH, *J*= 5.5 Hz), 7.83 (s, 1H, CH triazole), 7.24-7.16 (m, 3H, CH arom.), 7.09 (d, 2H, CH arom., *J*= 7.0 Hz), 5.45 (dd, 1H, α'-CH, *J*= 10.0 Hz, *J'*= 5.6 Hz), 3.88-3.85 (m, 1H, α-CH), 3.72-3.69 (m, 1H, α-CH), 3.29-3.15 (m, 4H, β'-CH_2, 1H ε-CH_2 , 1H εCH_2), 3.07-2.96 (m, 2H, 1H ε-CH_2, 1H ε-CH_2), 2.92-2.78 (m, 2H, $\underline{CH_2}CH_2CO$), 2.47-2.30 (m, 2H, $CH_2\underline{CH_2}CO$), 1.99-1.91 (m, 1H, β-CH_2), 1.79-1.70 (m, 1H, β-CH_2), 1.65-1.44 (m, 6H, 1H β-CH_2, 1H β-CH_2, γ-CH_2, δ-CH_2), 1.42-1.20 (m, 4H, γ-CH_2, δ-CH_2). ^{13}C NMR (125 MHz, DMSO-d_6): 171.1 (C), 169.8 (C), 168.7 (C), 167.7 (C), 146.1 (C), 136.0 (C), 128.9 (CH), 128.2 (CH), 126.6 (CH), 120.3 (CH), 63.9 (CH), 54.6 (CH), 53.1 (CH), 38.6 (CH_2), 38.5 (CH_2), 37.4 (CH_2), 33.8 (CH_2), 32.3 (CH_2), 31.7 (CH_2), 28.8 (CH_2), 28.3 (CH_2), 23.0, (CH_2) 21.3 (CH_2), 20.9 (CH_2). $C_{26}H_{36}N_7O_4$ $[M + H]^+$ 510.2829, found 510.2818.

Macrocyclic Diketopiperazine 10c (*1S,2S,3R*-1,4-triazole). A procedure analogous to the one used for the synthesis of **10a** but using **8c** as starting material afforded **10c** as an off-white solid (43.8 mg, 90% yield). $[\alpha]^{25}_{D}$= +16.6 (c 0.32, MeOH). mp= 230-231ºC. IR: ν*max* (neat)/cm^{-1} 3284, 2934, 1655, 1544, 1454; ^{1}H NMR (500 MHz, DMSO-d_6): δ= 8.34 (t, 1H, ε-NH, *J*= 5.5 Hz), 8.11 (d, 1H, α-NH, *J*= 2.5 Hz), 8.06 (d, 1H, α-NH, *J*= 2.5 Hz), 7.85 (t, 1H, ε-NH, *J*= 5.5 Hz), 7.74 (s, 1H, CH triazole), 7.25-7.13 (m, 5H, CH arom.), 5.47 (dd, 1H, α'-CH, *J*= 10.0 Hz, *J'*= 6.0 Hz), 3.76-3.74 (m, 1H, α-CH), 3.70-3.66 (m, 1H, α-CH), 3.32 (dd, 1H, β'-CH_2, *J*= 14.0 Hz, *J'*= 6.0 Hz), 3.22 (dd, 1H, β'-CH_2, *J*= 14.0 Hz, *J'*= 10.0 Hz), 3.18-3.12 (m, 1H ε-CH_2), 3.11-3.05 (m, 1H ε-CH_2), 3.04-2.97 (m, 2H, 1H ε-CH_2, 1H ε-CH_2), 2.88-2.79 (m, 2H, $\underline{CH_2}CH_2CO$), 2.35 (t, 2H, $CH_2\underline{CH_2}CO$, *J*= 6.5 Hz), 1.81-1.73 (m, 2H, 1H β-CH_2, 1H β-CH_2), 1.69-1.62 (m, 1H, β-CH_2), 1.58-1.52 (m, 1H, β-CH_2), 1.46-1.38 (m, 2H, δ-CH_2), 1.38-1.30 (m, 4H, γ-CH_2, δ-CH_2), 1.30-1.18 (m, 2H, γ-CH_2). ^{13}C NMR (125 MHz, DMSO-d_6): 170.8 (C), 167.4 (C), 167.3 (C), 167.2 (C), 145.6 (C), 136.1 (C), 128.8 (CH), 128.1 (CH), 126.6 (CH), 120.7 (CH), 63.6 (CH), 54.1 (CH), 54.1(CH), 38.4 (CH_2), 38.0 (CH_2), 37.7 (CH_2), 34.5 (CH_2), 34.1 (CH_2), 33.1 (CH_2), 29.0 (CH_2), 28.7 (CH_2), 21.8, (CH_2) 21.1 (CH_2). $C_{26}H_{36}N_7O_4$ $[M + H]^+$ 510.2829, found 510.2807.

Macrocyclic Diketopiperazine 11a (*1S,2S,3S*-1,5-triazole). A procedure analogous to the one used for the synthesis of **10a** but using **9a** as starting material afforded **11a** as an off-white solid (46.5 mg, 91% yield). $[\alpha]^{25}_{D}$= -44.3 (c 0.54, MeOH). mp= 182-184ºC.IR: ν*max* (neat)/cm^{-1} 3235, 2928, 1663, 1558, 1456. ^{1}H NMR (400 MHz, DMSO-d_6): δ= 8.16 (t, 1H, ε-NH, *J*= 5.5 Hz), 8.00 (d, 1H, α-NH, *J*= 1.5 Hz), 7.93-7.88 (m, 2H, α-NH, ε-NH) 7.38 (s, 1H, CH triazole), 7.21-7.08 (m, 5H, CH arom.), 5.36 (t, 1H, α'-CH, *J*= 7.5 Hz), 3.90-3.86 (m, 1H, α-CH), 3.84-3.79 (m, 1H, α-CH), 3.48 (d, 2H, β'-CH_2, *J*= 7.5 Hz), 3.20-2.80 (m, 4H, ε-CH_2), 2.60-2.30 (m, 4H, CH_2CH_2CO), 1.80-1.50 (m, 4H, β-CH_2), 1.45-1.10 (m, 8H, γ-CH_2, δ-CH_2). ^{13}C NMR (125 MHz, DMSO-d_6): 170.6 (C), 167.0 (C), 167.0 (C), 166.9 (C), 137.5 (C), 136.9 (C), 131.0 (CH), 128.9 (CH), 128.0 (CH), 126.4 (CH), 61.5 (CH), 53.9 (CH), 53.7 (CH), 38.4 (CH_2), 37.8 (CH_2), 36.6 (CH_2), 33.4 (CH_2), 32.6

(CH_2), 31.8 (CH_2), 29.3 (CH_2), 28.6 (CH_2), 20.8, (CH_2) 20.4 (CH_2), 18.0 (CH_2). $C_{26}H_{35}N_7O_4Na$ [M + Na]$^+$ 532.2648, found 532.2650.

Macrocyclic Diketopiperazine 11b (*1S,2R,3S*-1,5-triazole). Compound **9b** was reacted using a procedure analogous to the one used for the synthesis of **6a** but increasing the MW heating time to 6h.**.** After removal of the solvent under reduced pressure, cold MeOH was added to the crude. The resuling white solid was washed with small amounts of cold MeOH and dried to yield **11b** (14.5 mg, 50% yield). $[\alpha]^{25}{}_D$= +24.8 (c 0.43, DMSO-d_6). mp= 191-193ºC. IR: ν*max* (neat)/cm^{-1} 3340, 3322, 3199, 2927, 1658, 1645, 1528, 1450; ^{1}H NMR (500 MHz, DMSO-d_6): δ= 8.23 (dd, 1H, ε-NH, *J*= 7.1 Hz, *J'*= 3.5 Hz), 8.02 (d, 1H, α-NH, *J*= 3.0 Hz), 7.94 (s, 1H, α-NH), 7.86 (t, 1H, *J*= 3.0 Hz, ε-NH), 7.35 (s, 1H, CH triazole), 7.24-7.13 (m, 5H, CH arom.), 5.36 (dd, 1H, α'-CH, *J*= 10.0 Hz, *J'*= 5.0 Hz), 3.80-3.76 (m, 1H, α-CH), 3.70-3.66 (m, 1H, α-CH), 3.60 (dd, 1H, β'-CH_2, *J*= 14.0 Hz, *J'*= 10.0 Hz), 3.49 (dd, 1H, β'-CH_2, *J*= 14.0 Hz, *J'*= 5.0 Hz), 3.37-3.30 (m, 1H, ε-CH_2), 3.28-3.21 (m, 1H, ε-CH_2), 3.02-2.95 (m, 1H, ε-CH_2), 2.91-2.85 (m, 1H, ε-CH_2), 2.71-2.61 (m, 2H, $\underline{CH_2}CH_2CO$), 2.43-2.30 (m, 2H, $CH_2\underline{CH_2}CO$), 1.89-1.82 (m, 1H, β-CH_2), 1.73-1.61 (m, 2H, β-CH_2), 1.48-1.22 (m, 9H, 1H β-CH_2, γ-CH_2, δ-CH_2). ^{13}C NMR (125 MHz, DMSO- d_6): 170.4 (C), 169.0 (C), 168.8 (C), 166.9 (C), 137.3 (C), 136.9 (C), 130.8 (CH), 128.9 (CH), 128.0 (CH), 126.4 (CH), 62.0 (CH), 54.8 (CH), 52.9 (CH), 38.5 (CH_2), 37.2 (CH_2), 36.2 (CH_2), 32.5 (CH_2), 32.3 (CH_2), 31.1 (CH_2), 28.7 (CH_2), 27.6 (CH_2), 22.7 (CH_2), 21.0 (CH_2), 18.6 (CH_2). $C_{26}H_{36}N_7O_4$ [M + H]$^+$ 510.2829, found 510.2838.

Macrocyclic Diketopiperazine 11c (*1S,2S,3R*-1,5-triazole). A procedure analogous to the one used for the synthesis of **10a** but using **9c** as starting material afforded **11c** as an off-white solid (32.5 mg, 91% yield). $[\alpha]^{25}{}_D$= +10.3 (c 0.39, MeOH). mp= 175-177ºC. IR: ν*max* (neat)/cm^{-1} 3284, 2930, 1662, 1553, 1455; ^{1}H NMR (500 MHz, DMSO-d_6): δ= 8.13 (t, 1H, ε-NH, *J*= 5.5 Hz), 7.96 (s, 2H, 2 α-NH), 7.88 (t, 1H, ε-NH, *J*= 6.0 Hz), 7.37 (s, 1H, CH triazole), 7.19-7.08 (m, 5H, CH arom.), 5.42 (dd, 1H, α'-CH, *J*= 9.0 Hz, *J'*= 6.5 Hz), 3.90-3.86 (m, 1H, α-CH), 3.86-3.82 (m,

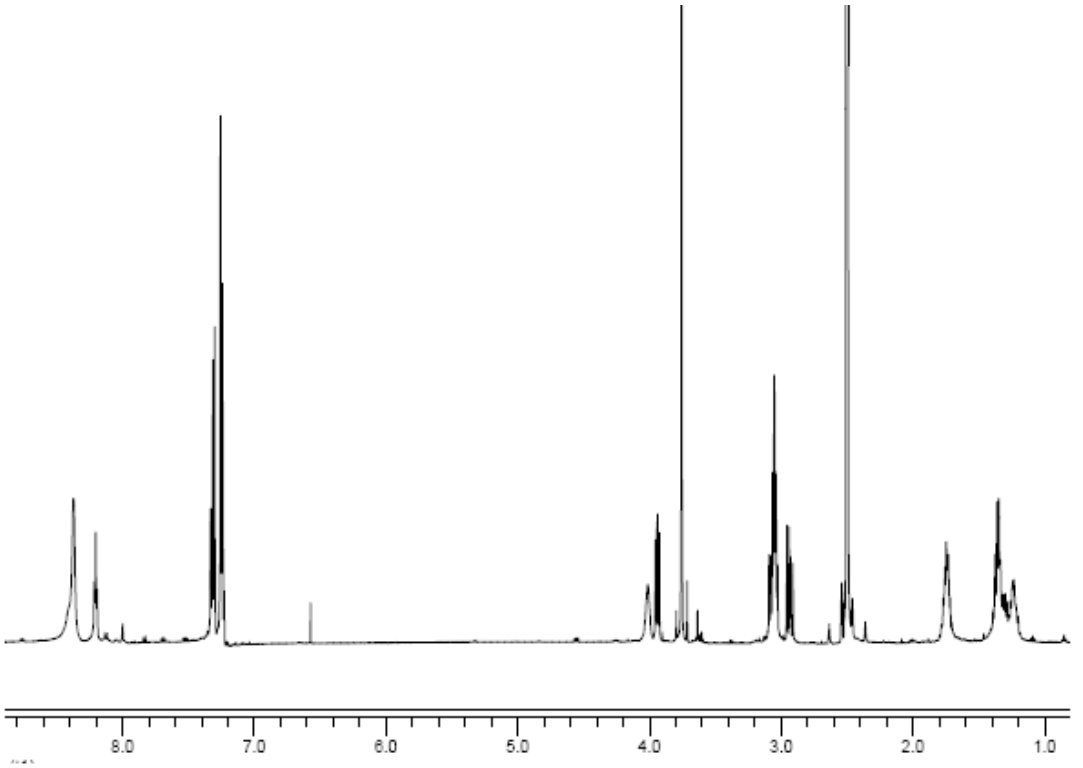
1H, α-CH), 3.48-3.45 (m, 2H, β'-CH_2), 3.18-2.92 (m, 4H, 2 ε-CH_2), 2.60-2.46 (m, 2H, $\underline{CH_2}CH_2CO$), 2.41-2.34 (m, 2H, $CH_2\underline{CH_2}CO$), 1.80-1.68 (m, 2H, β-CH_2), 1.59-1.48 (m, 2H, β-CH_2), 1.45-1.05 (m, 8H, γ-CH_2, δ-CH_2). ^{13}C NMR (125 MHz, DMSO-d_6): 170.6 (C), 167.0 (C), 166.9 (C), 137.6 (C), 137.0 (C), 130.9 (CH), 128.9 (CH), 128.0 (CH), 126.4 (CH), 61.3 (CH), 54.0 (CH), 53.6 (CH), 38.5 (CH_2), 37.7 (CH_2), 36.6 (CH_2), 33.1 (CH_2), 32.6 (CH_2), 31.6 (CH_2), 29.3 (CH_2), 28.3 (CH_2), 20.6, (CH_2) 20.5 (CH_2), 17.8 (CH_2). $C_{26}H_{35}N_7O_4Na$ $[M + Na]^+$ 532.2648, found 532.2654.

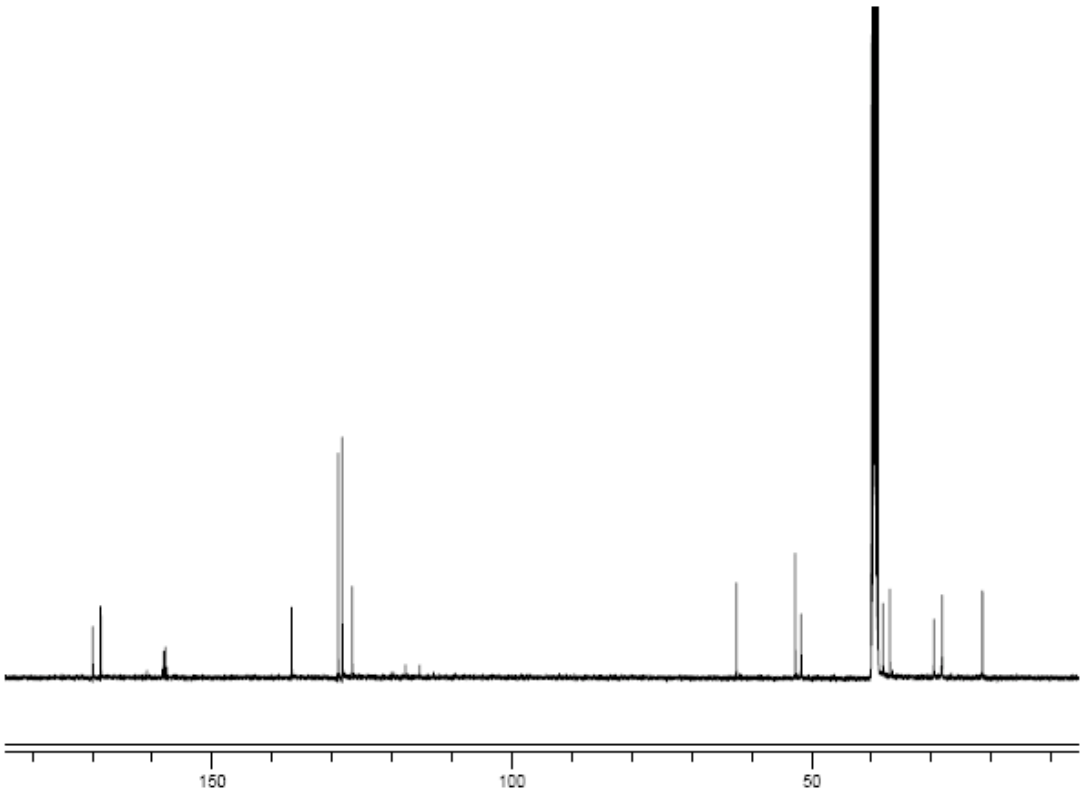
Macrocyclic peptidomimetic 13. 12 (176.8 mg, 0.261 mmol, 1eq) was suspended in dry THF (215 mL) in a three neck round-bottomed flask, DBU (0.117 mL, 0.784 mmol, 3 eq) was added. The reaction mixture was bubbled with Argon for 30 min. At that point CuI (99.5 mg, 0.523 mmol, 2 eq) was added and the reaction refluxed under N_2 for 15h. The solvent was removed under reduced pressure. The reaction mixture was filtered and 79.6 mg of a white solid were obtained. 60 mg of this solid were treated with 1.25M HCl-dioxane (2.75 mL) 16h at rt, the solvent was removed under reduced pressure and co-evaporations with MeOH and CH_2Cl_2 were performed. **8a** was obtained as a brownish solid (54.4 mg, 45% yield over 2 steps). The product was not purified by column chromatography due to its instability to silica gel. The estimated purity is more than 90% (low molecular weight impurities present, ^{1}H NMR) $[\alpha]^{25}_D$= +30.2 (c 0.39, DMSO-d_6). mp>300ºC. IR: ν*max* (neat)/cm^{-1} 3295, 2923, 1724, 1661, 1521, 1455; ^{1}H NMR (500 MHz, DMSO-d_6): δ= 9.89 (s, 1H, NH aniline), 8.50-8.42 (m, 3H, NH_3^+), 8.35-8.30 (m, 2H, ε-NH, α1-NH), 7.87 (s, 1H, CH triazole), 7.44 (d, 2H, CH aniline, *J*=8.4 Hz), 7.25-7.11 (m, 7H, CH arom.), 5.38 (t, 1H, α'-CH, *J*= 7.5 Hz), 4.00-3.92 (m, 1H, α2-CH), 3.73-3.67 (m, α1-CH), 3.54 (s, 3H, CH_3), 3.50-3.30 (m, 1H, β'-CH_2), 3.22 (dd, 1H, β'-CH_2, *J*= 14.0 Hz, *J'*= 9.0 Hz), 3.14-3.05 (m, 2H, 1H β2-CH_2, 1H ε-CH_2), 2.98-2.86 (m, 2H, $\underline{CH_2}CH_2CO$), 2.82 (dd, 1H, β2-CH, *J*= 13.0 Hz, *J'*= 11.5 Hz), 2.78-2.70 (m, 1H, ε1-CH_2), 2.70-2.58 (m, 2H, $CH_2\underline{CH_2}CO$), 1.62-0.86 (m, 6H, β1-CH_2, γ1-CH_2, δ1-CH_2). ^{13}C NMR (125 MHz, DMSO-d_6): δ= 170.8 (C), 169.7 (C), 167.1 (C), 166.6 (C), 145.7 (C), 137.8 (C), 136.2 (C), 129.4 (CH), 129.2 (C), 128.8 (CH), 128.1 (CH), 126.6 (CH), 120.7 (CH), 119.2 (CH), 63.8 (CH) , 53.2 (CH), 52.7 (CH), 51.6 (CH_3), 37.9, 37.7 (CH_2), 37.5 (CH_2), 36.1 (CH_2), 35.0 (CH_2),

29.6, 28.6 (CH_2), 28.2, 28.0 (CH_2), 21.7 (CH_2), 20.8 (CH_2). $C_{30}H_{38}N_7O_5$ $[M + H]^+$ 576.2934, found 576.2947.

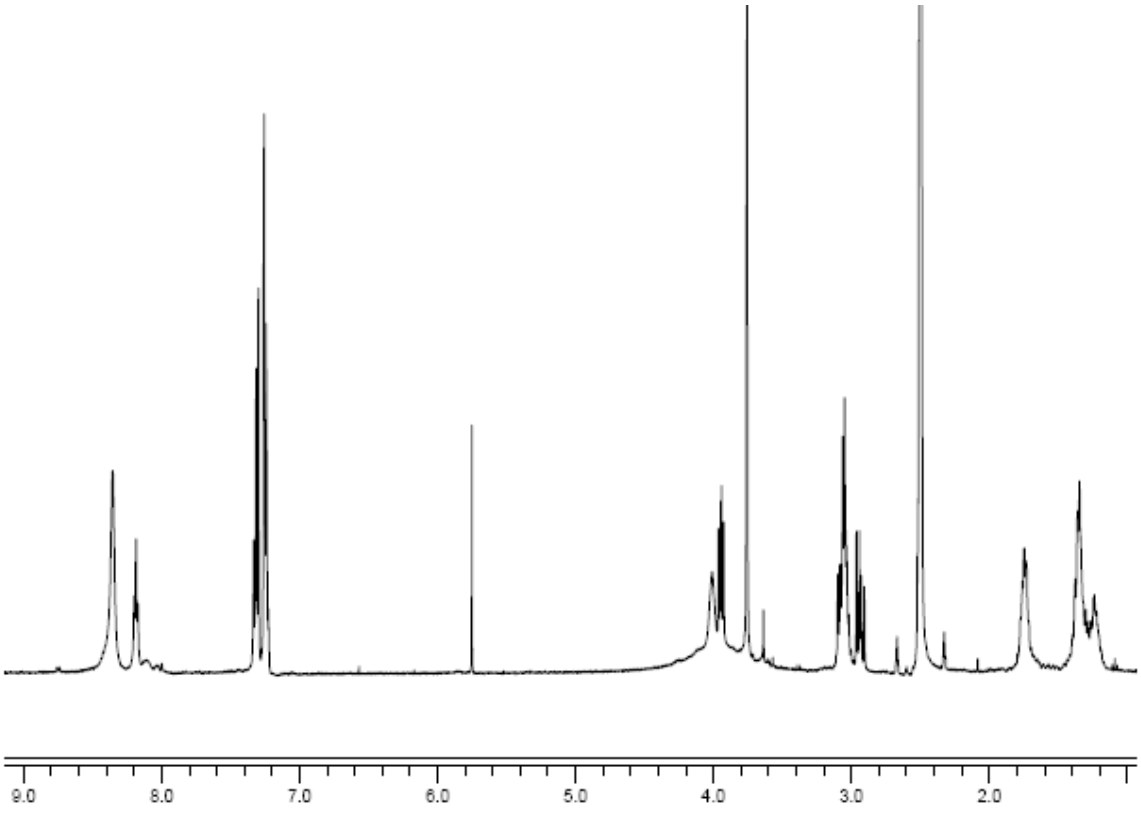
Macrocyclic DKP 14. Compound **13** was reacted using a procedure analogous to the one used for the synthesis of **10a** but increasing the MW heating time to 9h. Then the resin was filtered and washed with DMSO-DMF (1:1) and DMF. The final DKP compound **14** was obtained as a brownish solid (8.7 mg, 40% yield). The product was not purified by column chromatography due to its instability to silica gel. The estimated purity is more than 90% (low molecular weight impurities present, ^{1}H NMR). $[\alpha]^{25}_D$= +10.6 (c 0.51, DMSO-*d*$_6$). mp>300ºC. IR: *νmax* (neat)/cm^{-1} 2928, 1666, 1517, 1454, 1411; ^{1}H NMR (500 MHz, DMSO-*d*$_6$): δ= 9.79 (s, 1H, NH aniline), 8.16-8.11 (m, 2H, α-NH, ε-NH), 7.97 (d, 1H, α-NH, *J*= 1.8 Hz), 7.77 (s, 1H, CH triazole), 7.45 (d, 2H, CH arom., *J*= 8.5 Hz), 7.25-7.14 (m, 5H, CH arom.), 7.45 (d, 2H, CH arom., *J*= 8.5Hz), 5.29 (t, 1H, α'-CH, *J*= 7.7 Hz), 4.14-4.11 (m, 1H, α2-CH), 3.42-3.24 (m, 3H, β'-CH_2, α1-CH), 3.11-3.04 (m, 2H, 1H β2-CH_2, 1H ε-CH_2), 2.95-2.87 (m, 2H, $\underline{CH_2}CH_2CO$), 2.73-2.58 (m, 3H, 1H β2-CH, $CH_2\underline{CH_2}CO$), 2.56-2.44 (m, 1H, ε-CH_2), 1.80-0.10 (m, 6H, β1-CH, γ1-CH_2, δ1-CH_2). ^{13}C NMR (125 MHz, DMSO-*d*$_6$): δ= 169.6 (C), 166.9 (C), 166.5 (C), 165.8 (C), 146.3 (C), 138.3 (C), 136.6 (C), 130.8 (CH), 130.2 (C), 129.1 (CH), 128.4 (CH), 126.7 (CH), 120.5 (CH), 118.3 (CH), 103.1 (CH), 64.1 (CH), 55.5 (CH), 53.4 (CH), 38.1 (CH_2), 37.7 (CH_2), 36.9 (CH_2), 35.2 (CH_2), 33.7 (CH_2), 31.9 (CH_2), 27.9 (CH_2), 23.2 (CH_2), 21.2 (CH_2), 20.4 (CH_2). $C_{29}H_{34}N_7O_4$ $[M + H]^+$ 544.2672, found 544.2697.

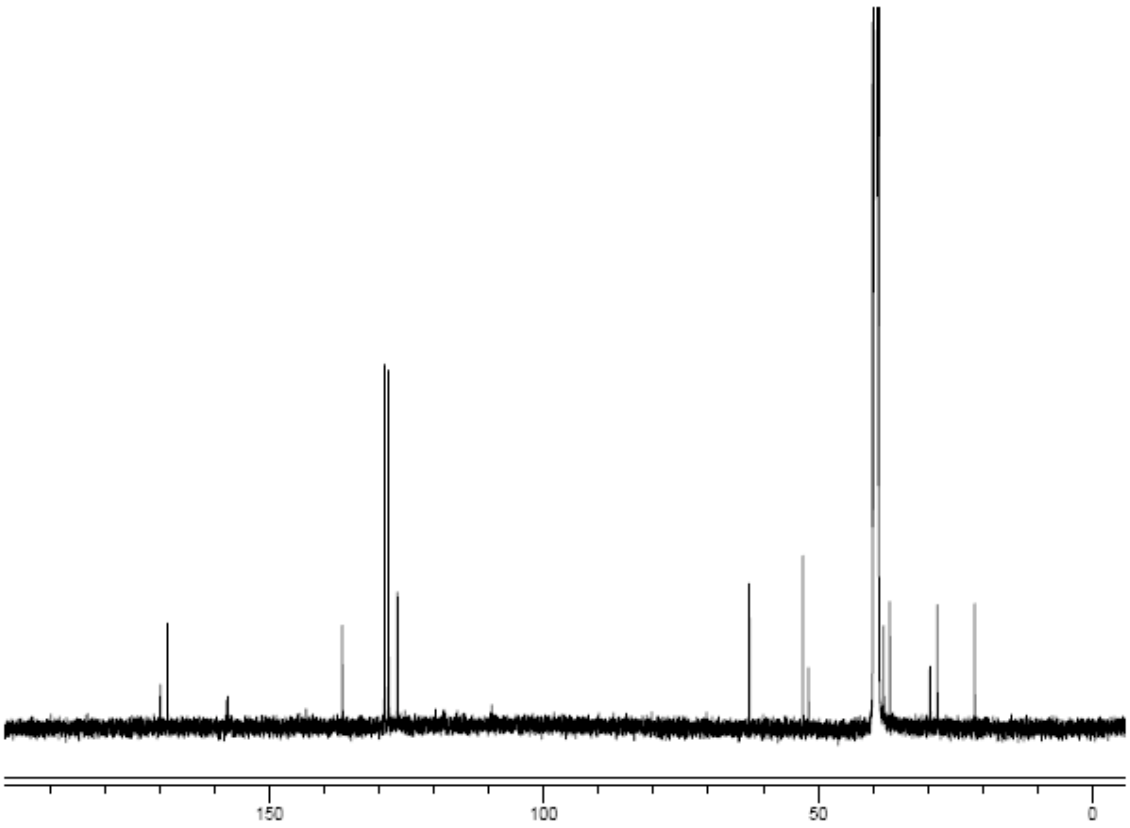
H-L- Lys(L-N_3-Phe)-OMe·TFA 4a.



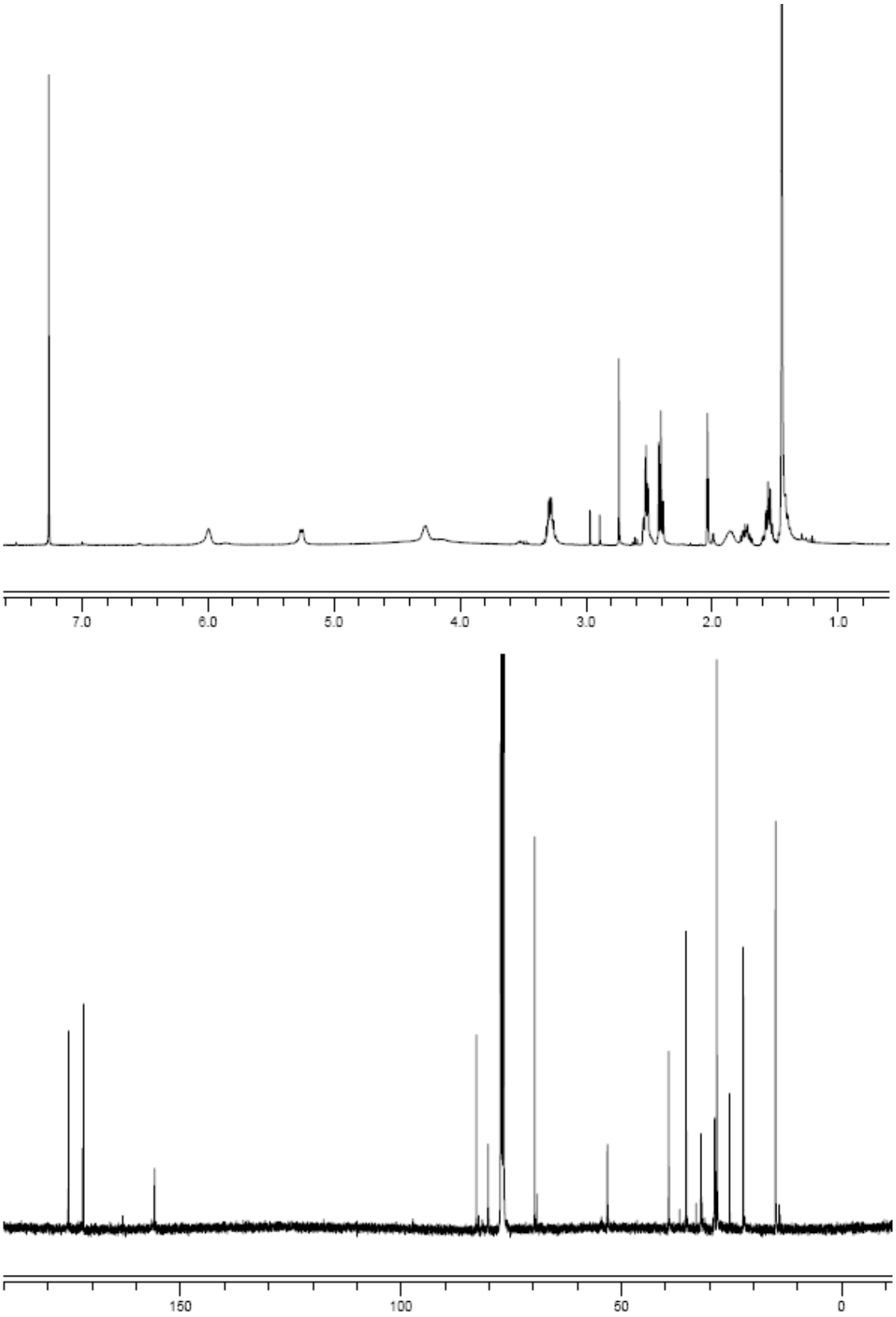


H-L- Lys(D-N_3-Phe)-OMe·TFA 4b.

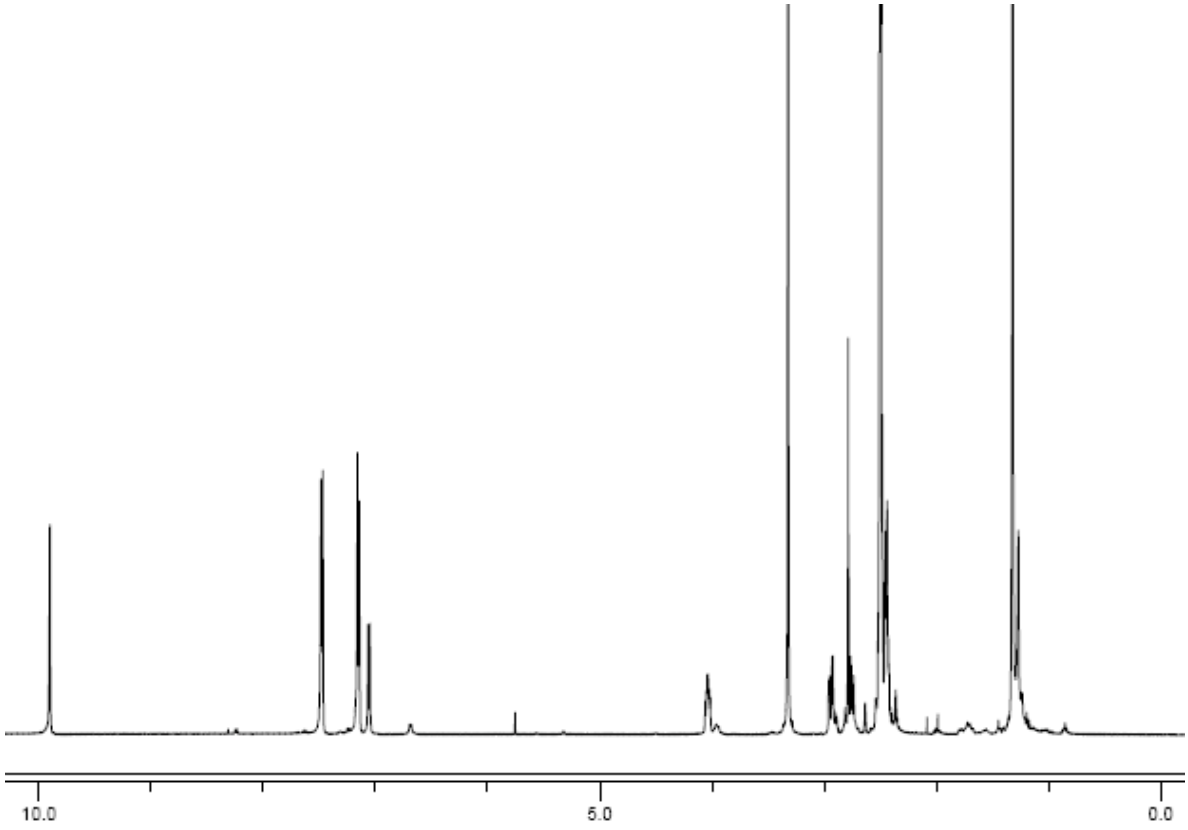


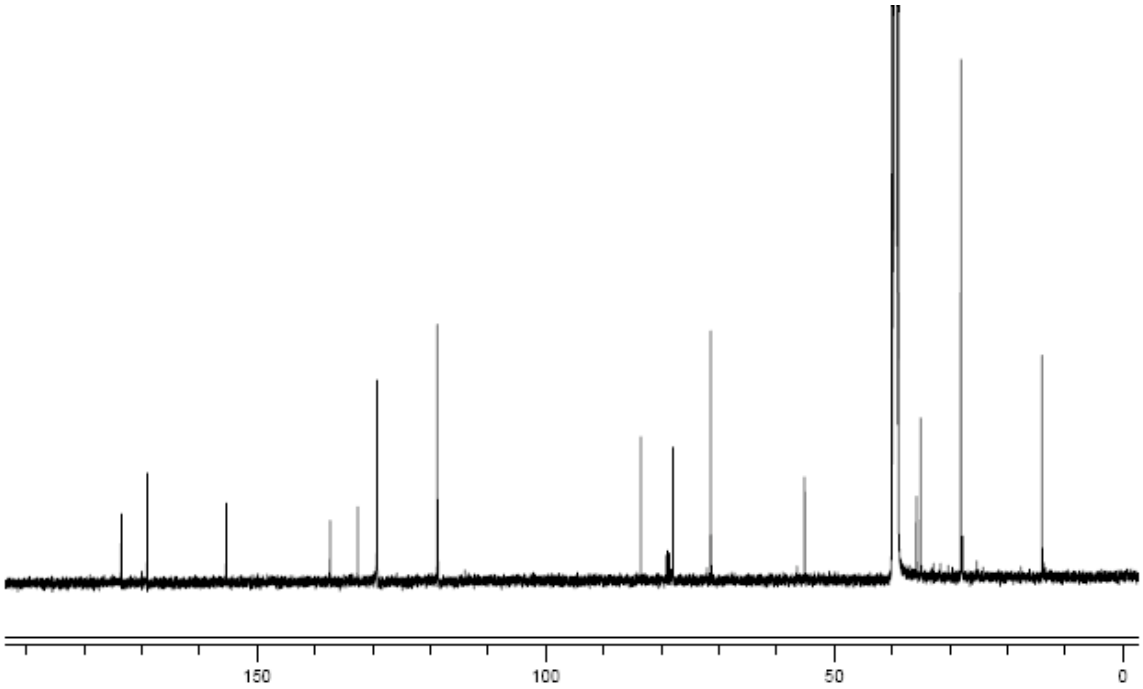


Boc-*L*- Lys(*N*-4-Pentynoyl)-OH 6a.

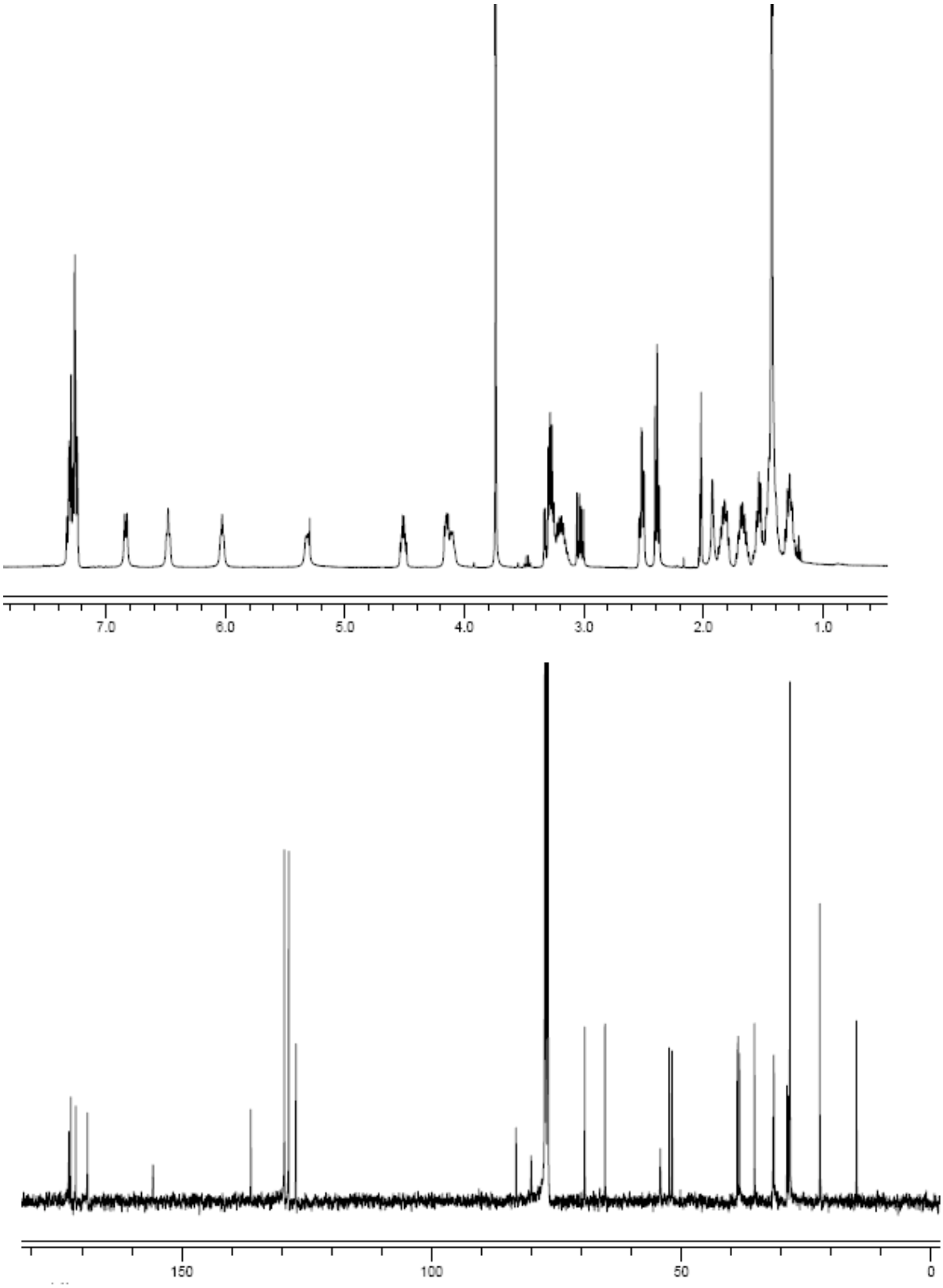


Boc-*L*-4-amino-phenylalanine(*N*-4-pentynoyl)-OH 6c.





Linear peptidomimetic 7a *(1S,2S,3S).*



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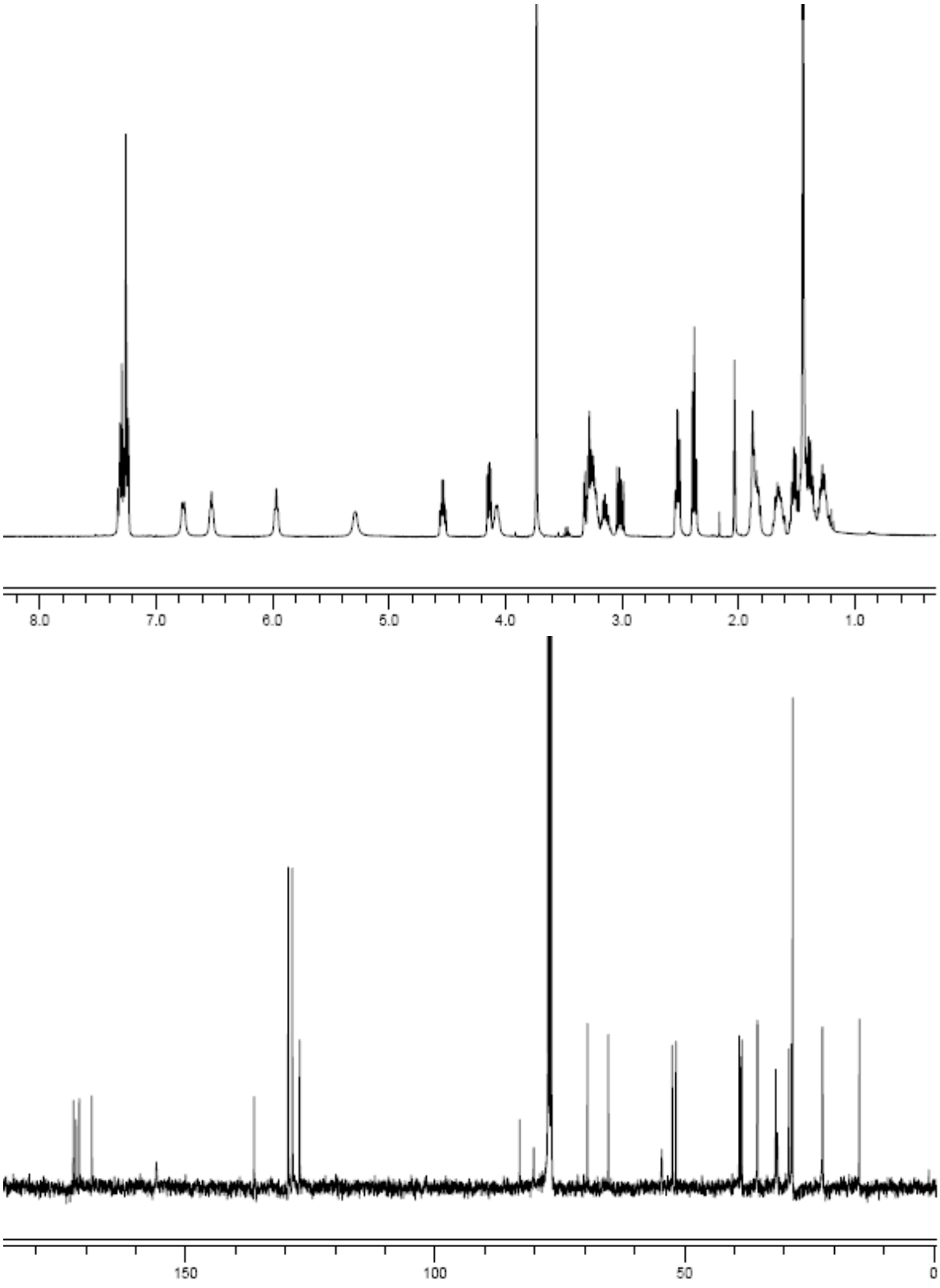
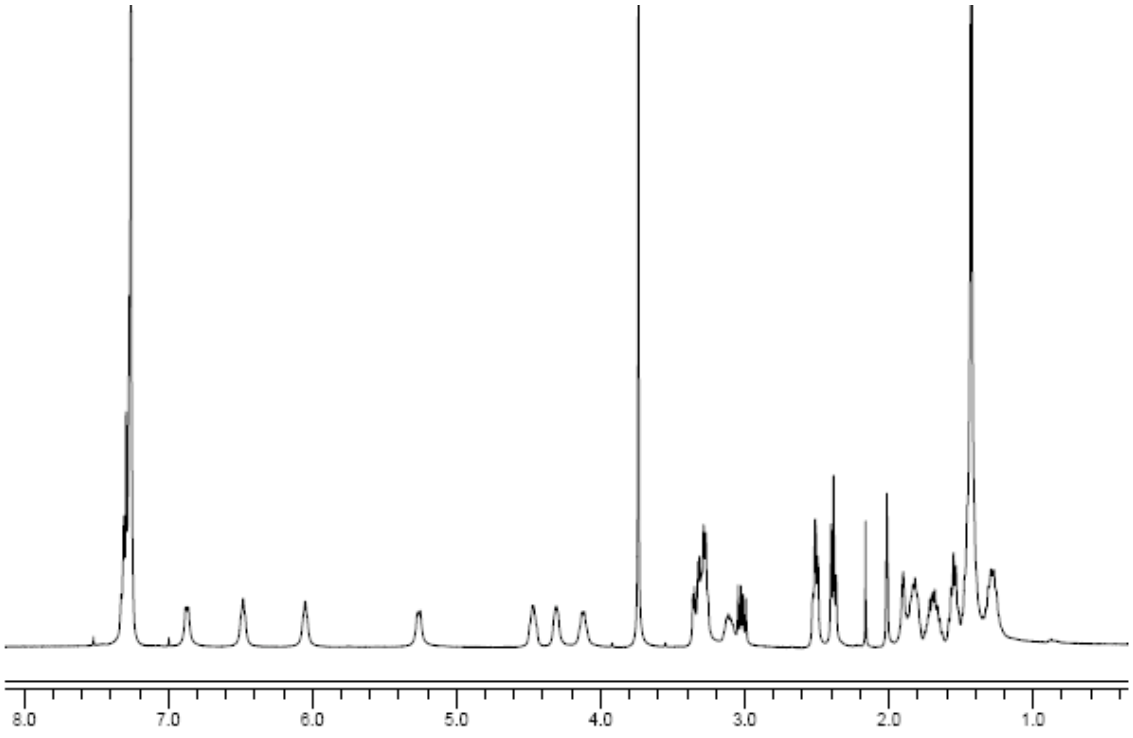
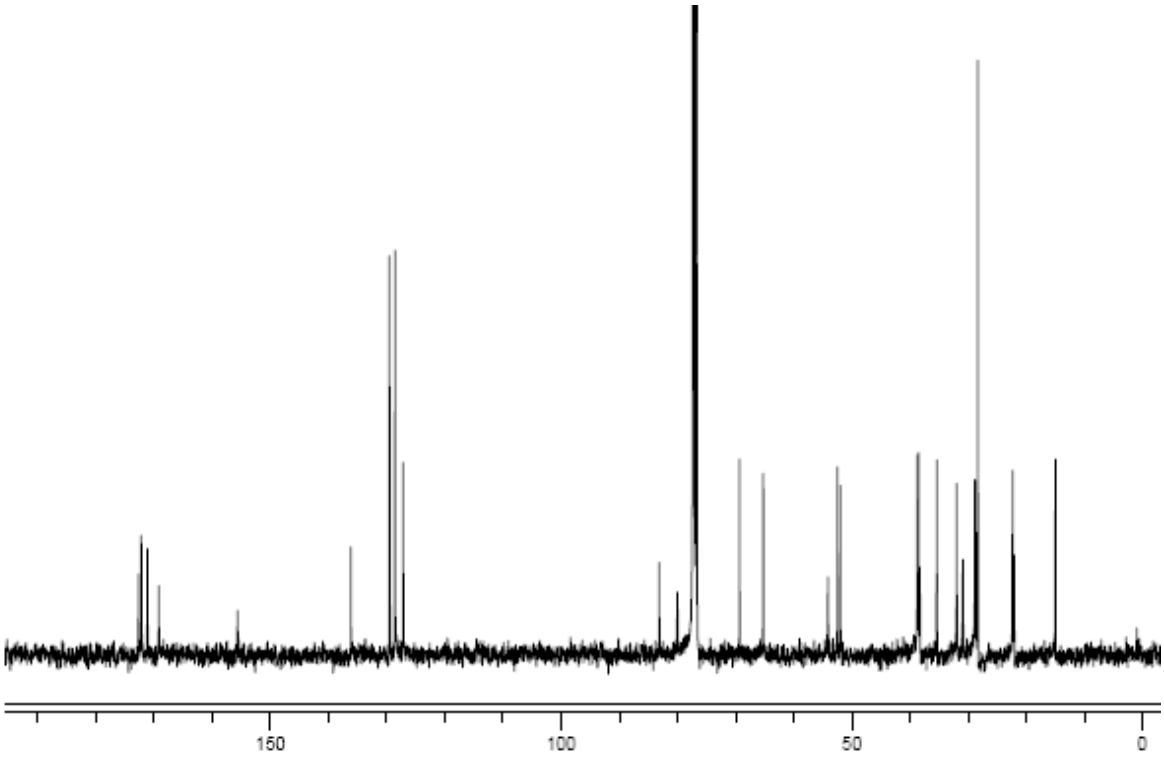
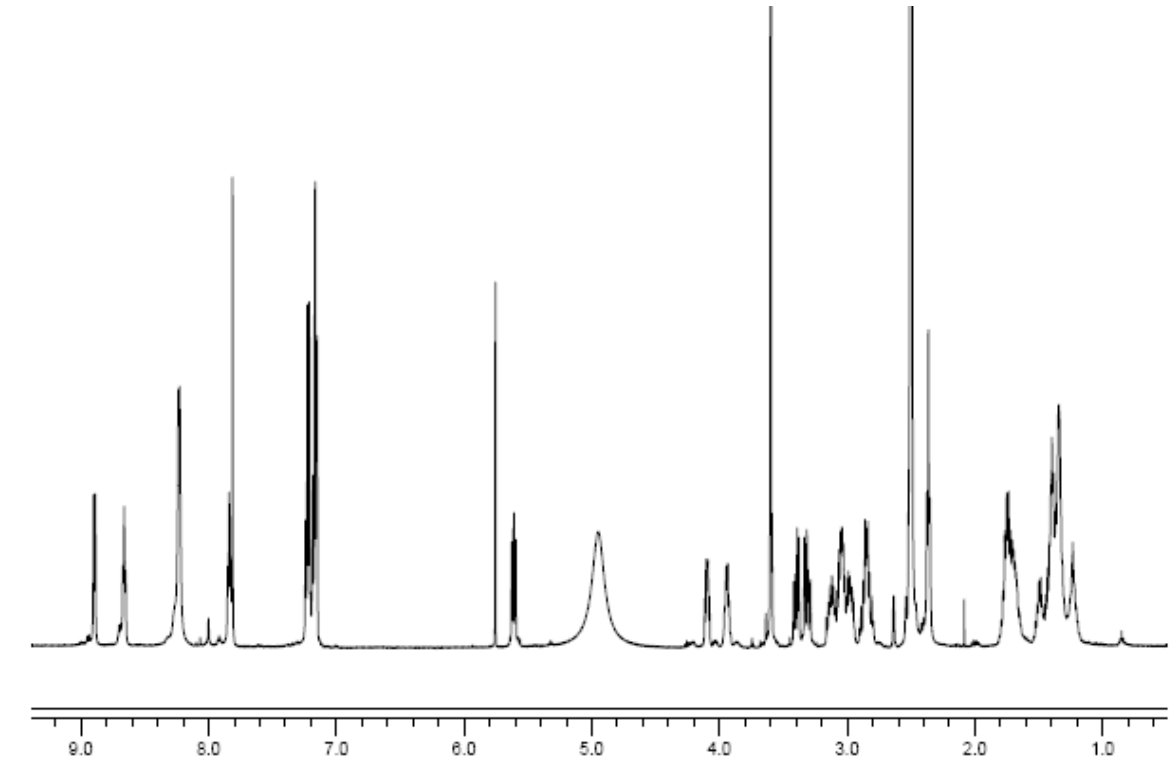


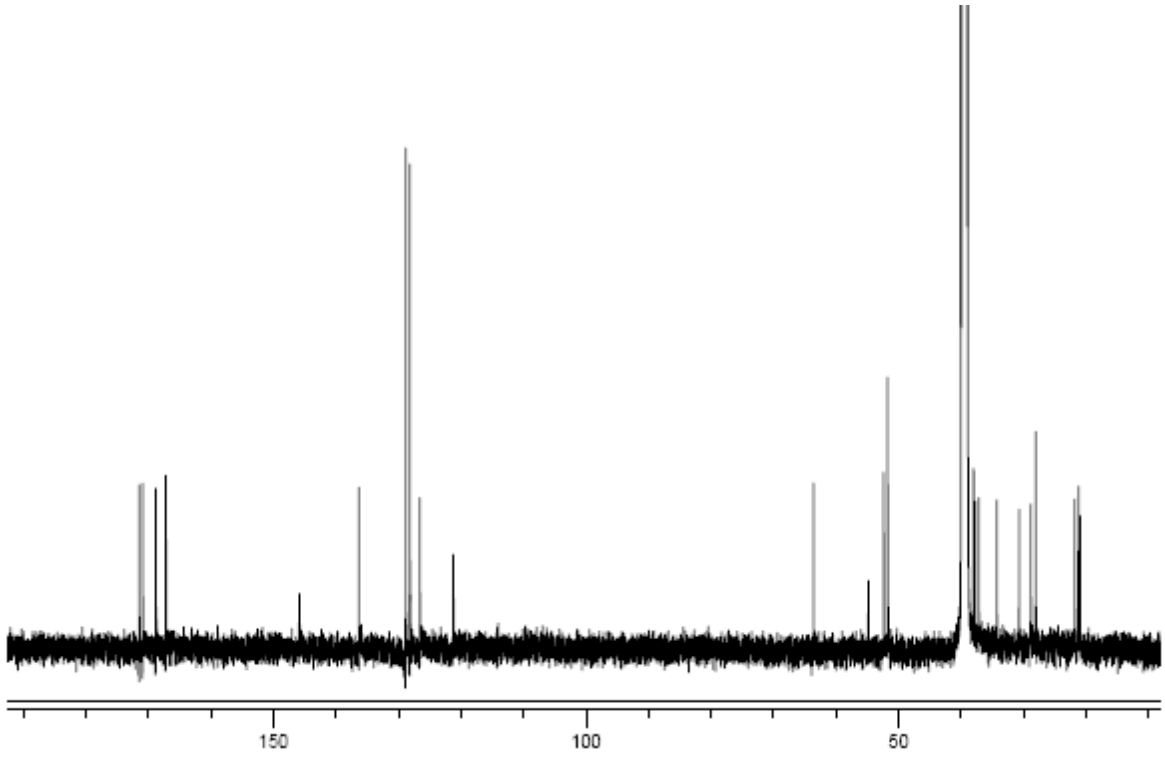
Linear peptidomimetic 7c *(1S,2S,3R).*



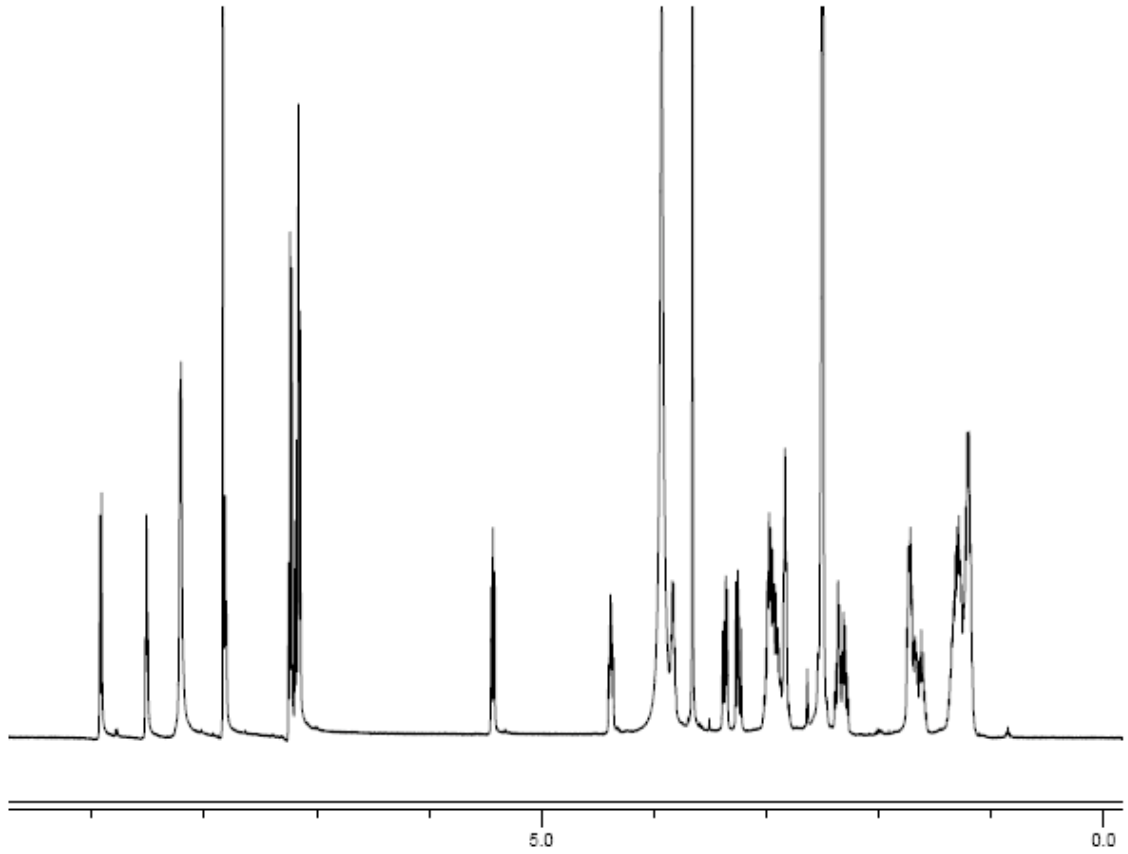


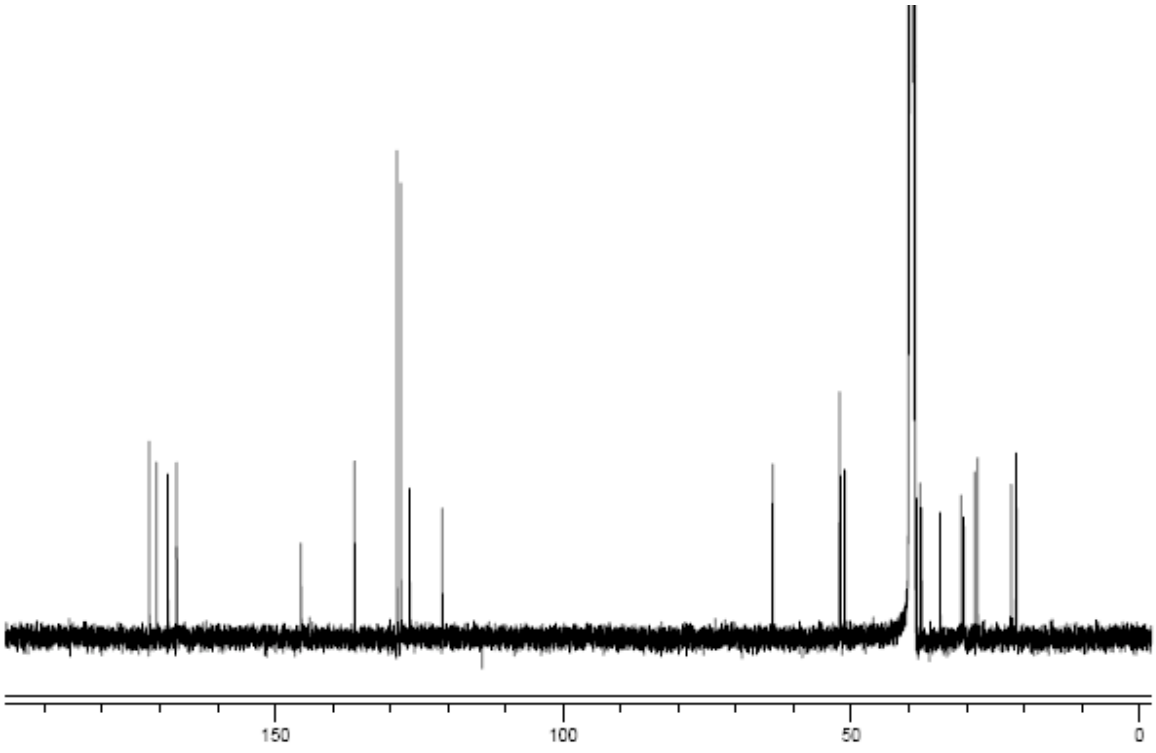
Macrocyclic peptidomimetic 8a (*1S,2S,3S*-1,4-triazole).



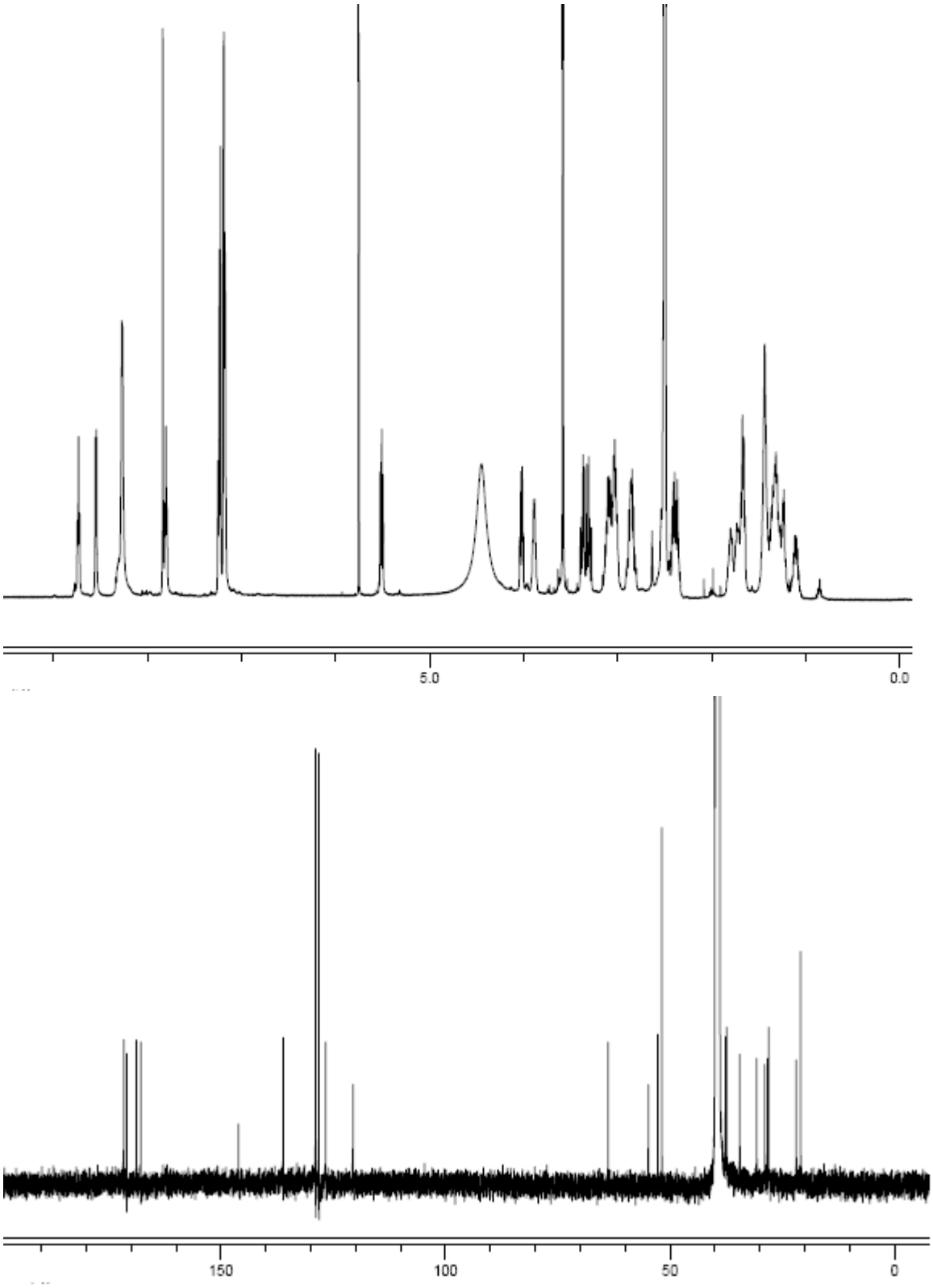


Macrocyclic peptidomimetic 8b (*1S,2R,3S*-1,4-triazole).

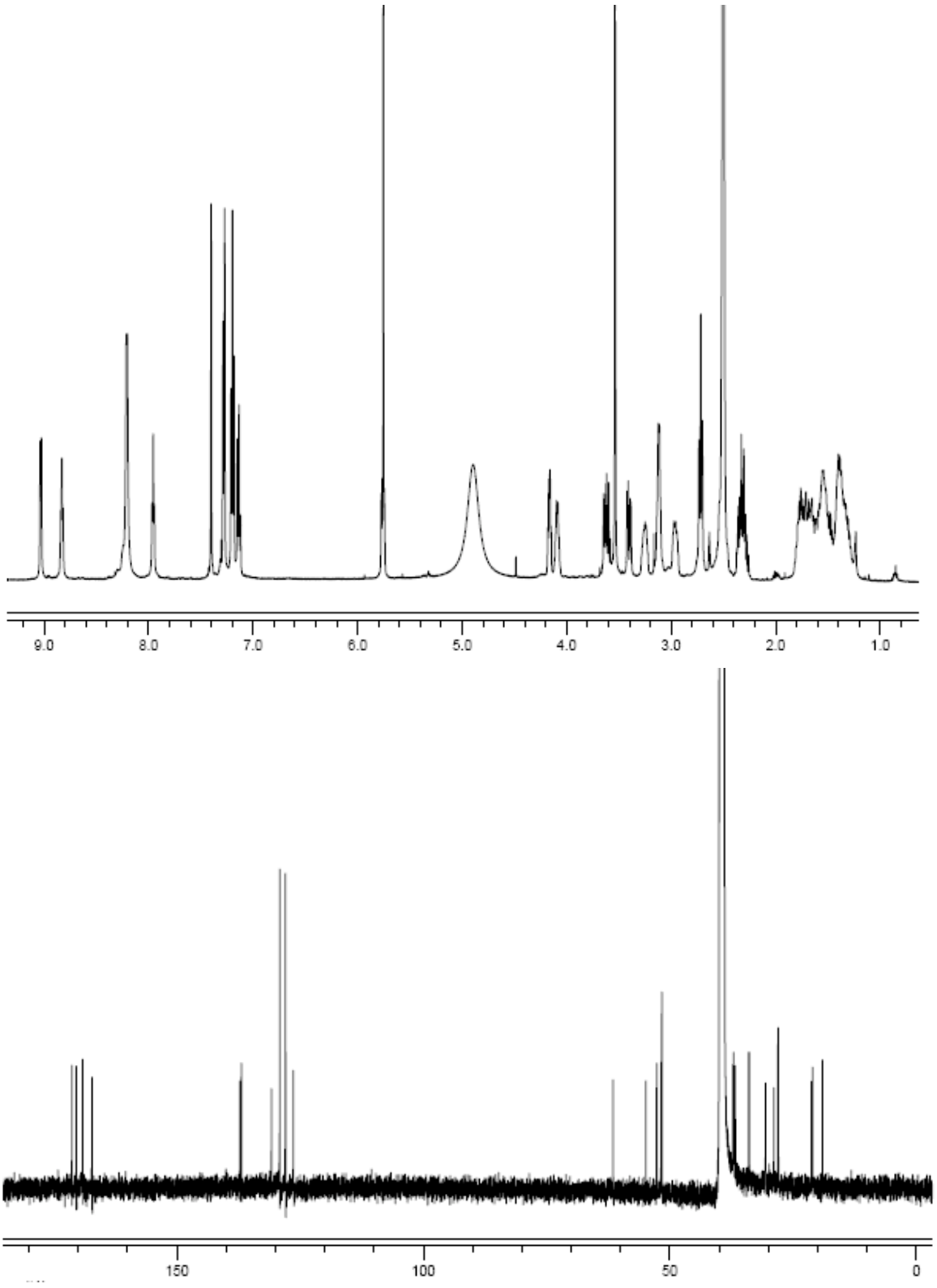




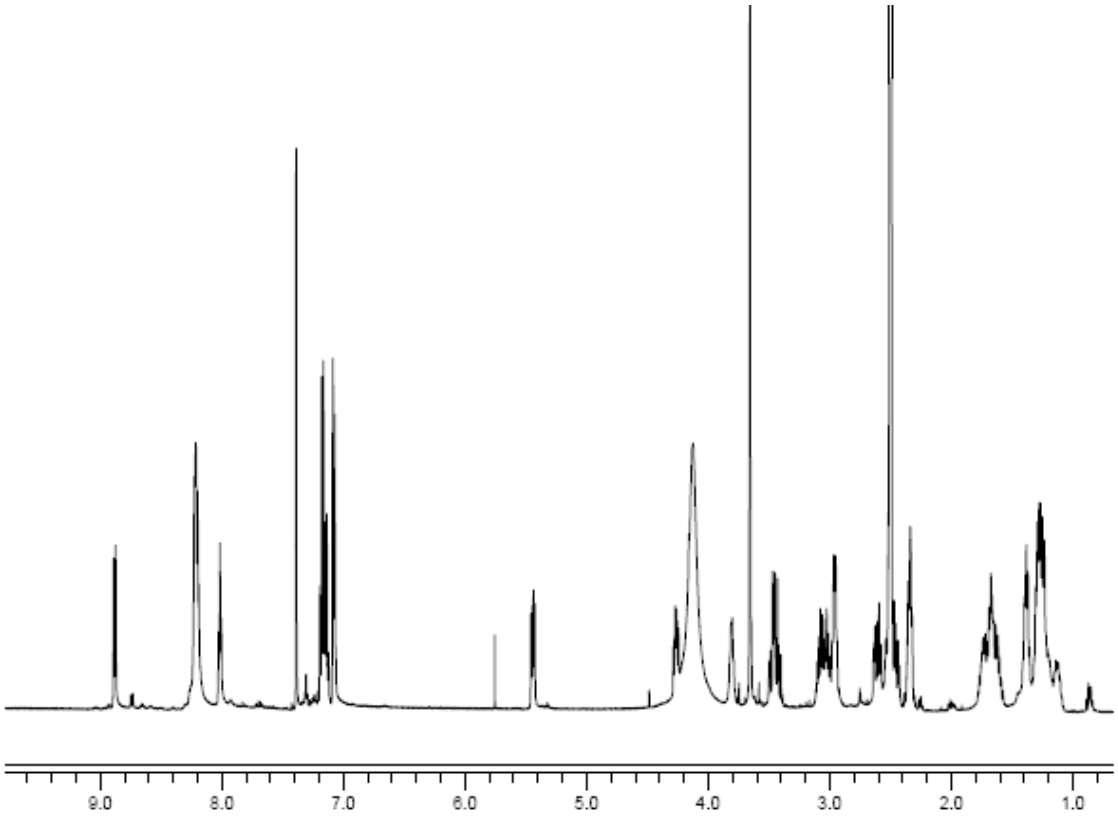
Macrocyclic peptidomimetic 8c (*1S,2S,3R*-1,4-triazole).

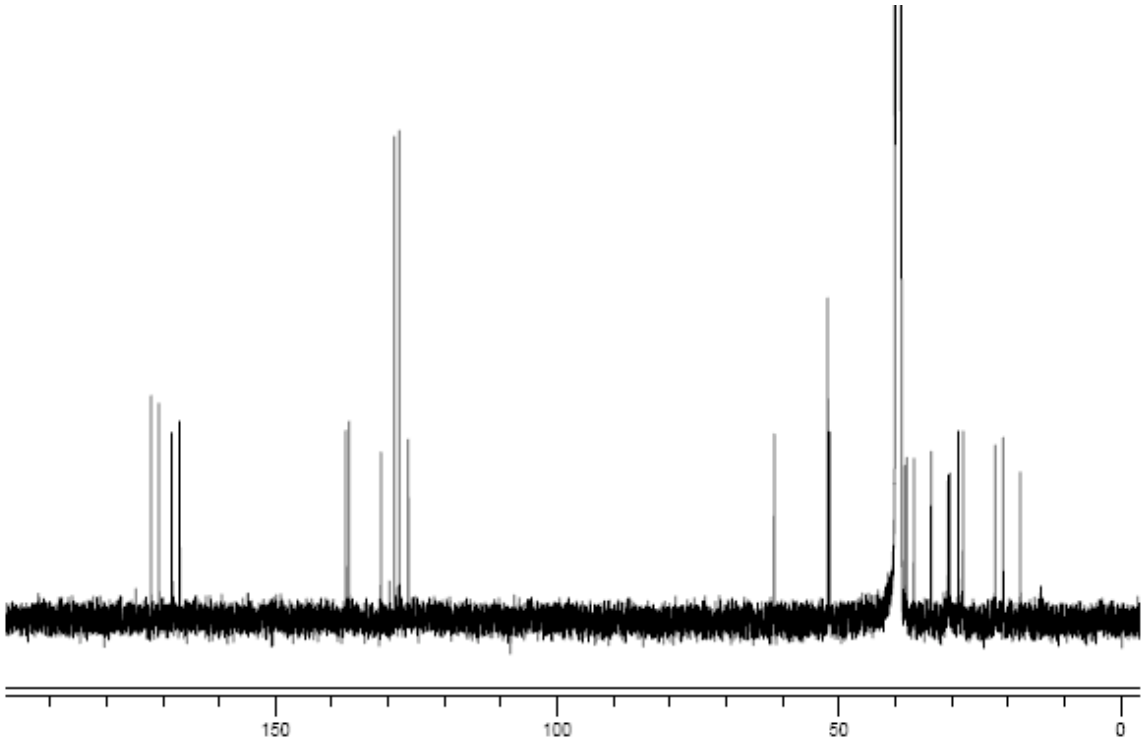


Macrocyclic peptidomimetic 9a (*1S,2S,3S*-1,5-triazole).

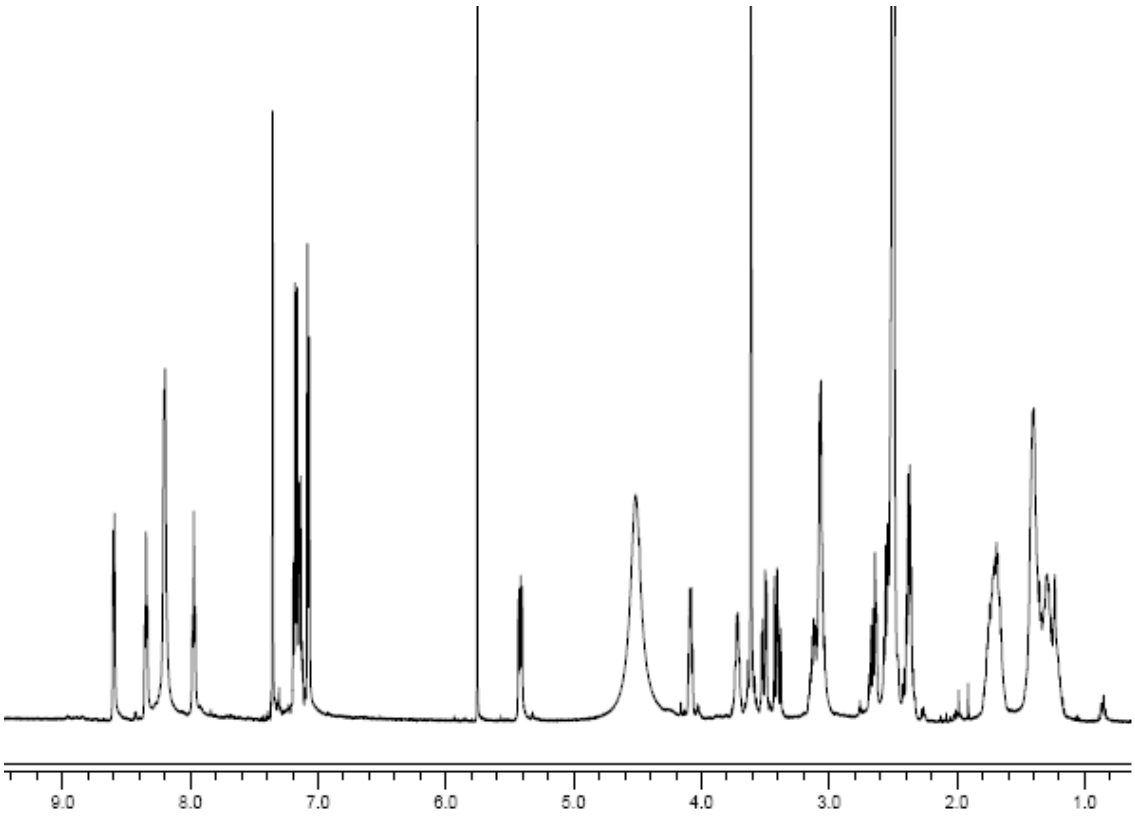


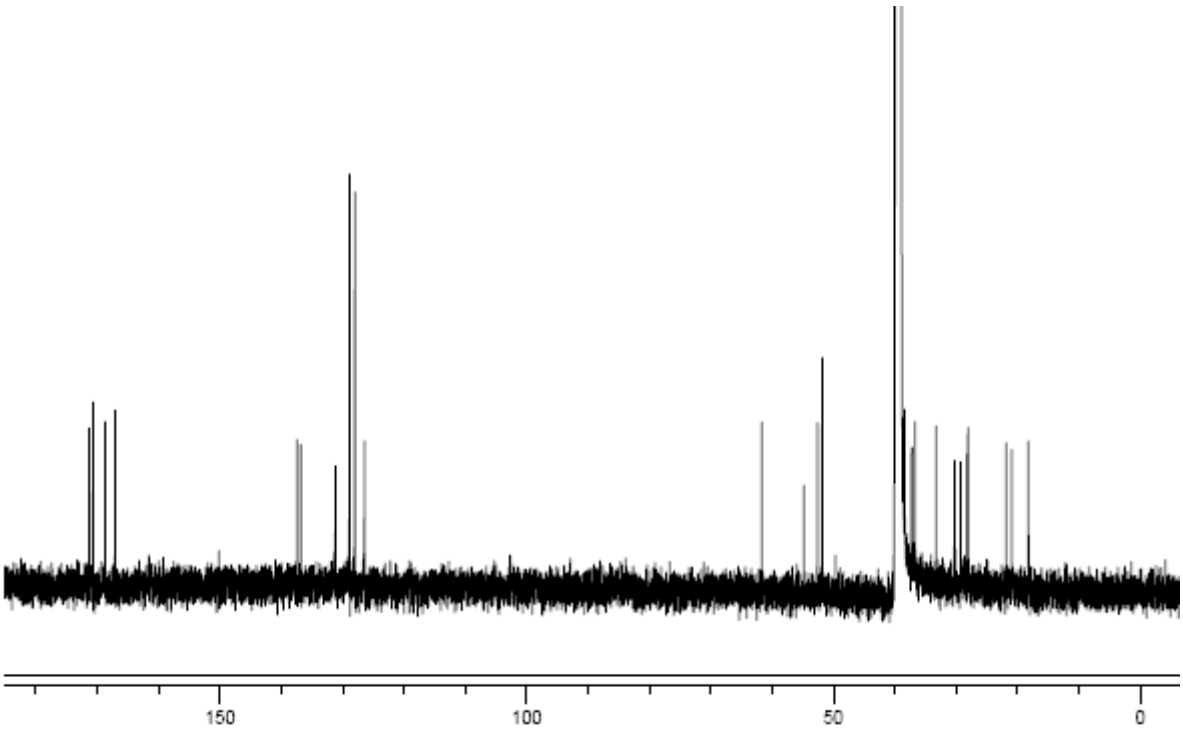
Macrocyclic peptidomimetic 9b (*1S,2R,3S*-1,5-triazole).



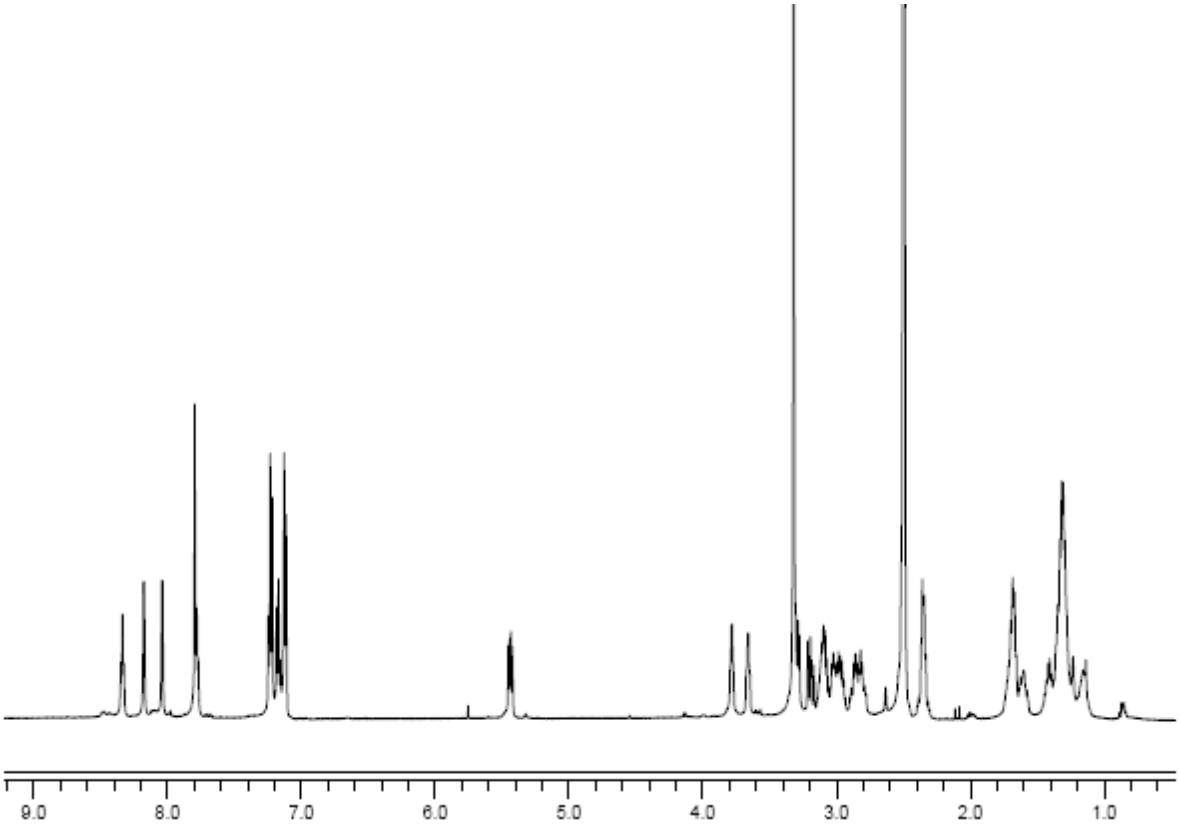


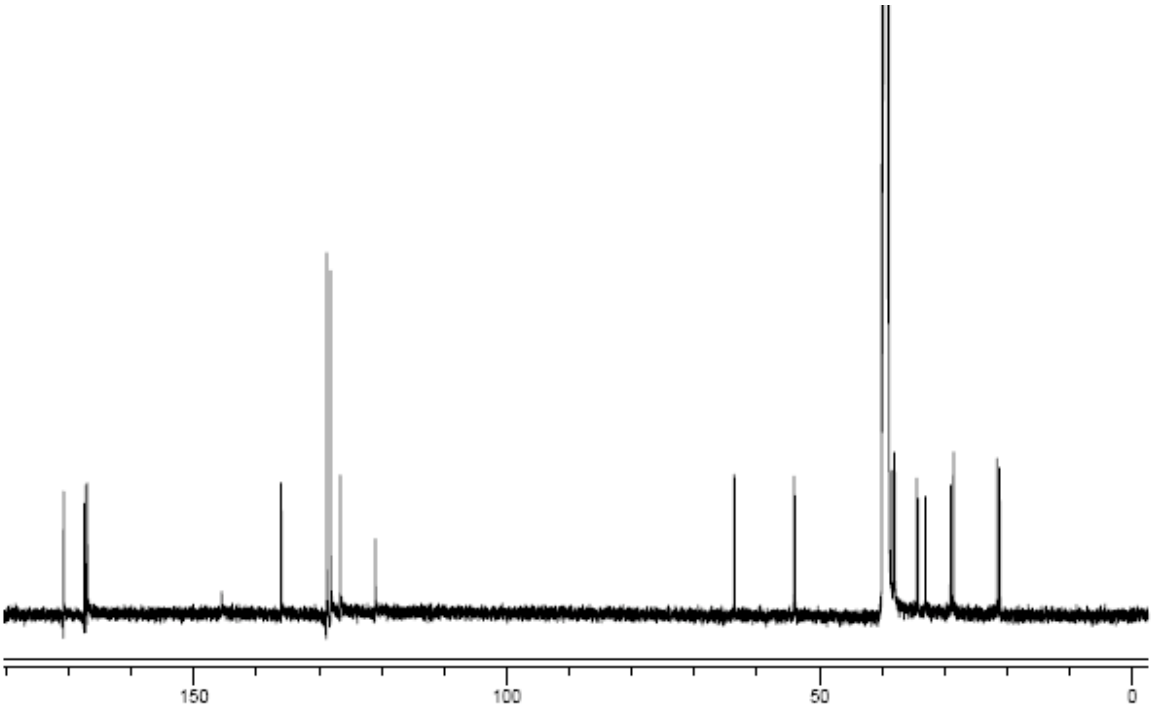
Macrocyclic peptidomimetic 9c (*1S,2S,3R*-1,5-triazole).



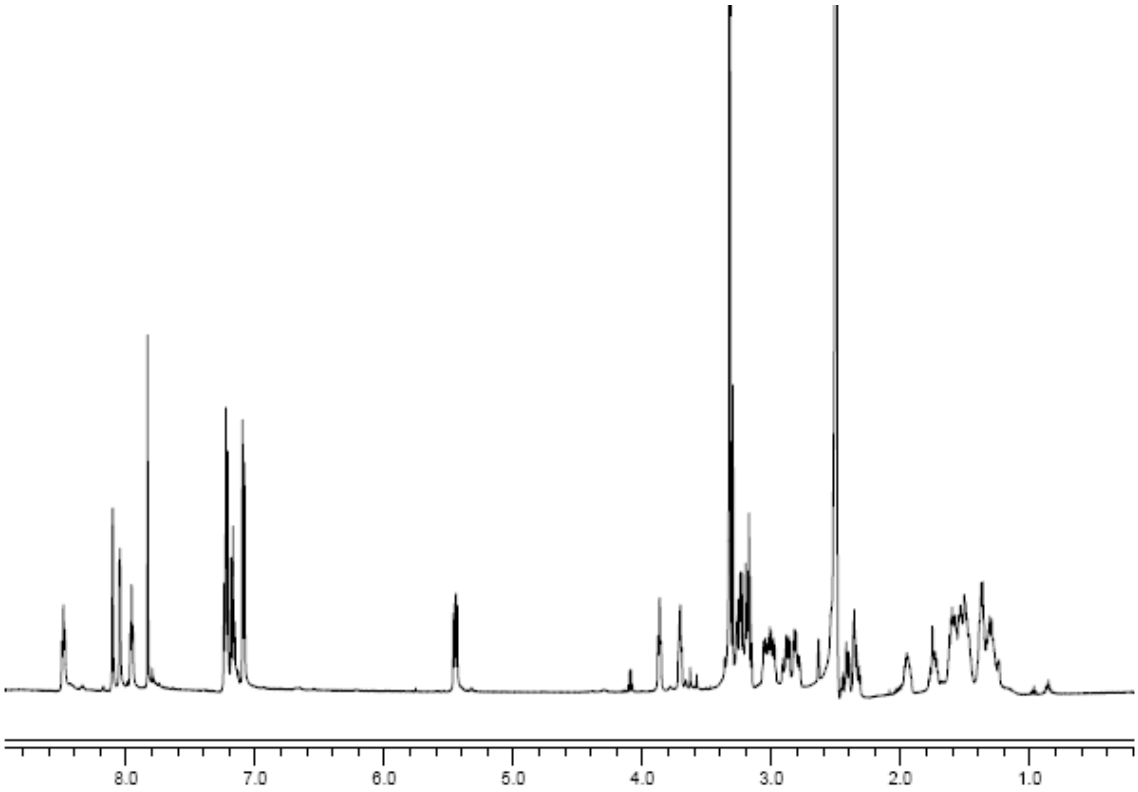


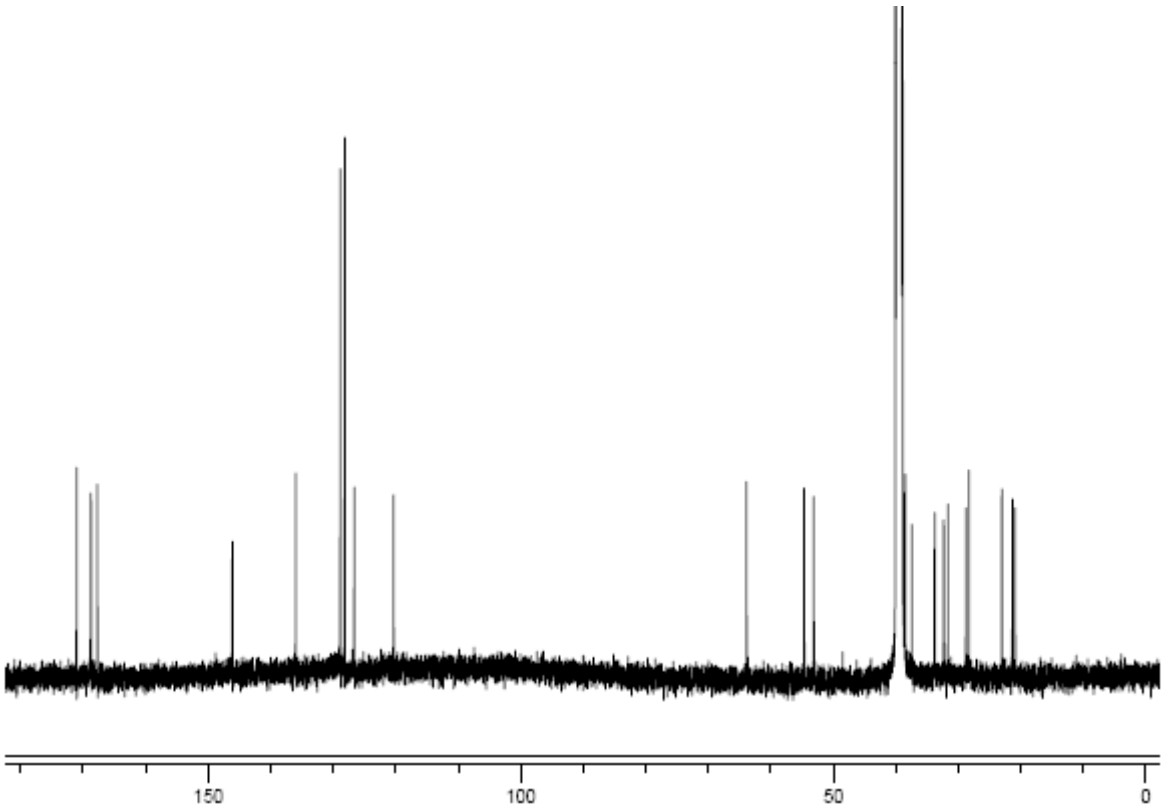
Macrocyclic Diketopiperazine 10a (*1S,2S,3S*-1,4-triazole).



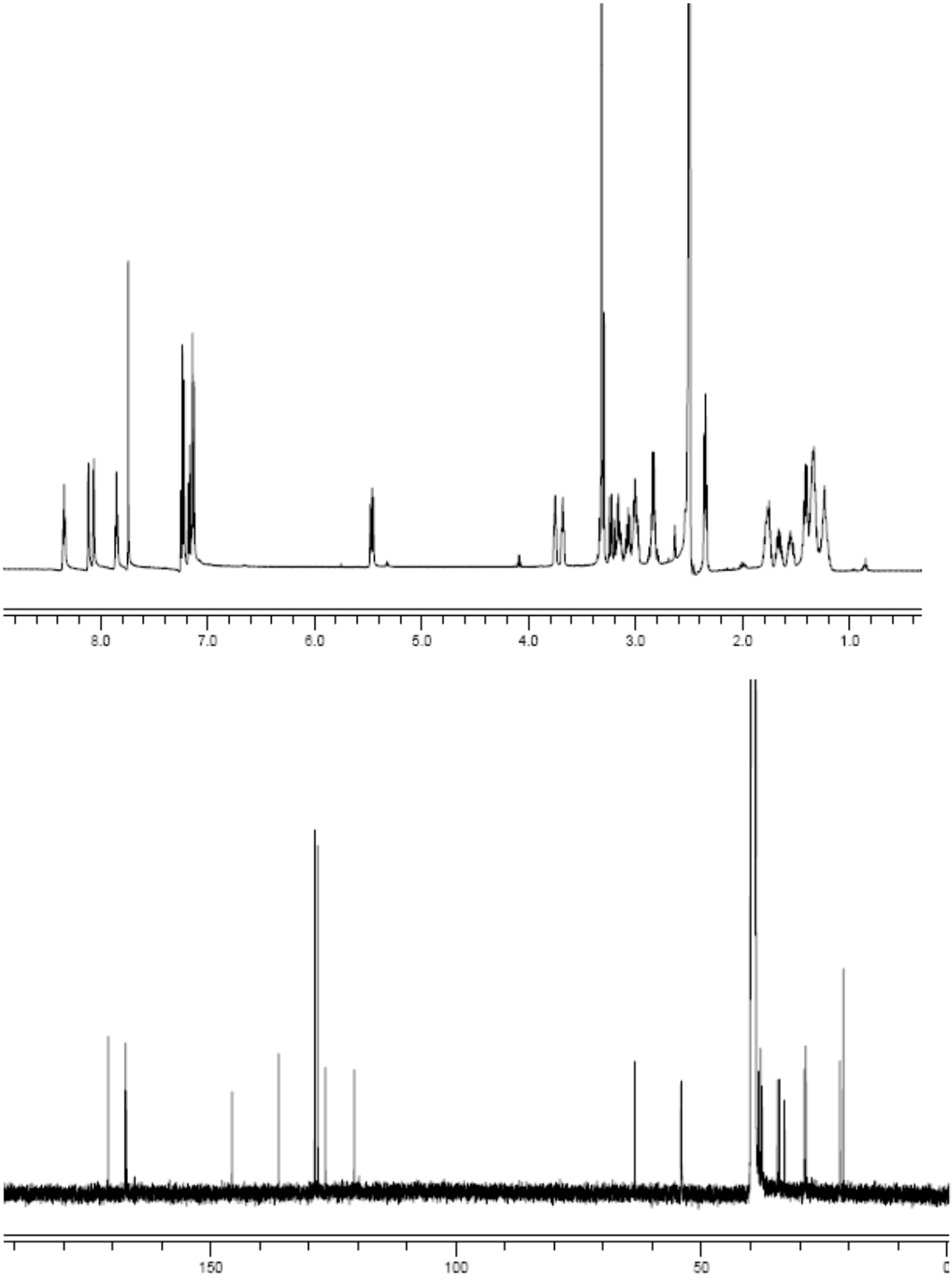


Macrocyclic Diketopiperazine 10b (*1S,2R,3S*-1,4-triazole).

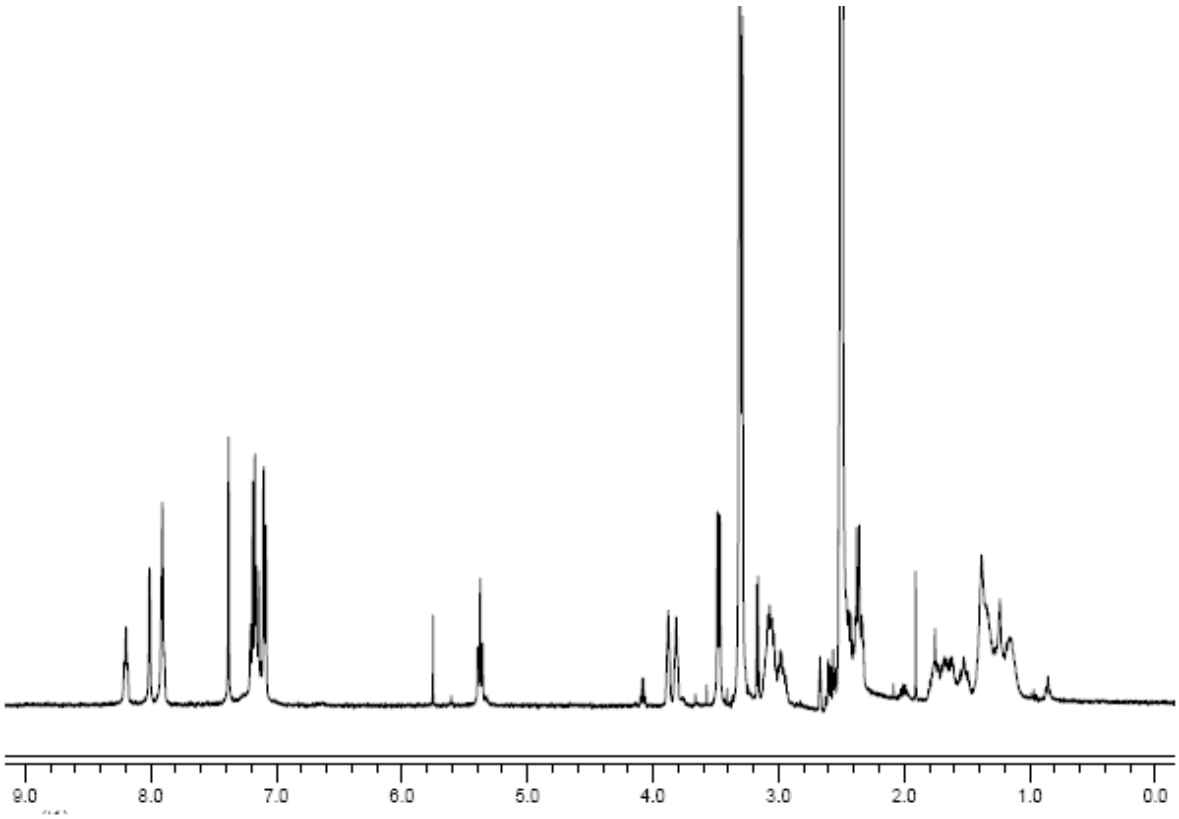


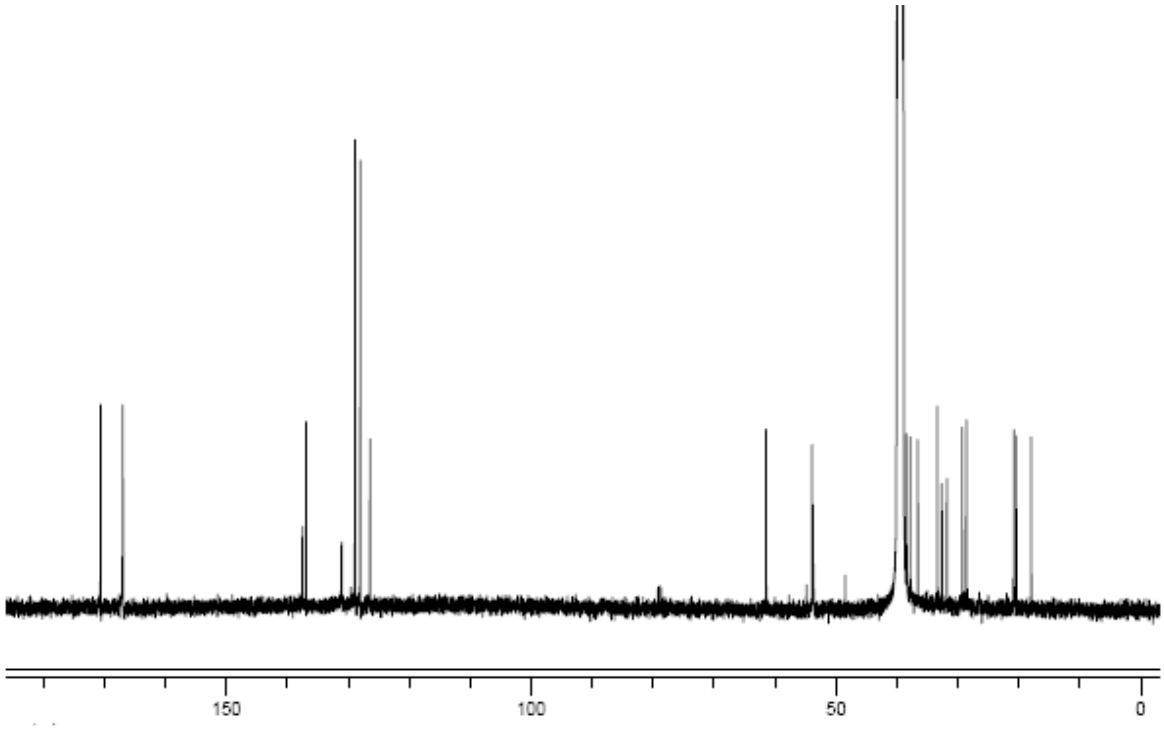


Macrocyclic Diketopiperazine 10c (*1S,2S,3R*-1,4-triazole).

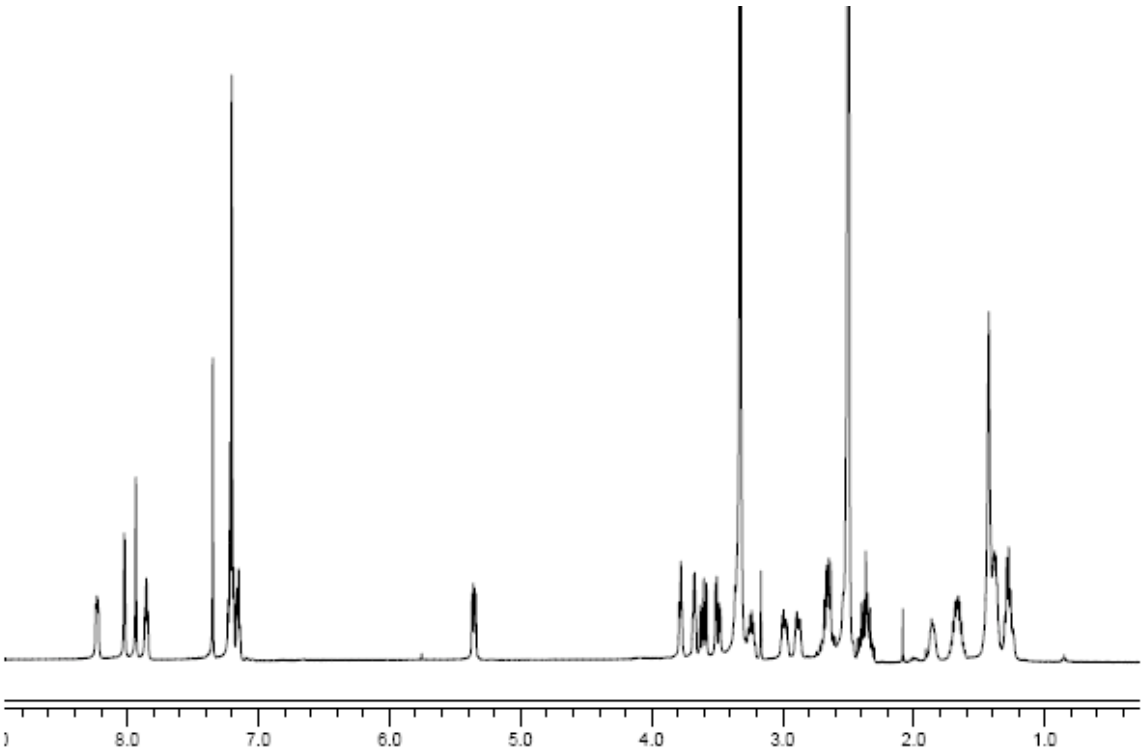


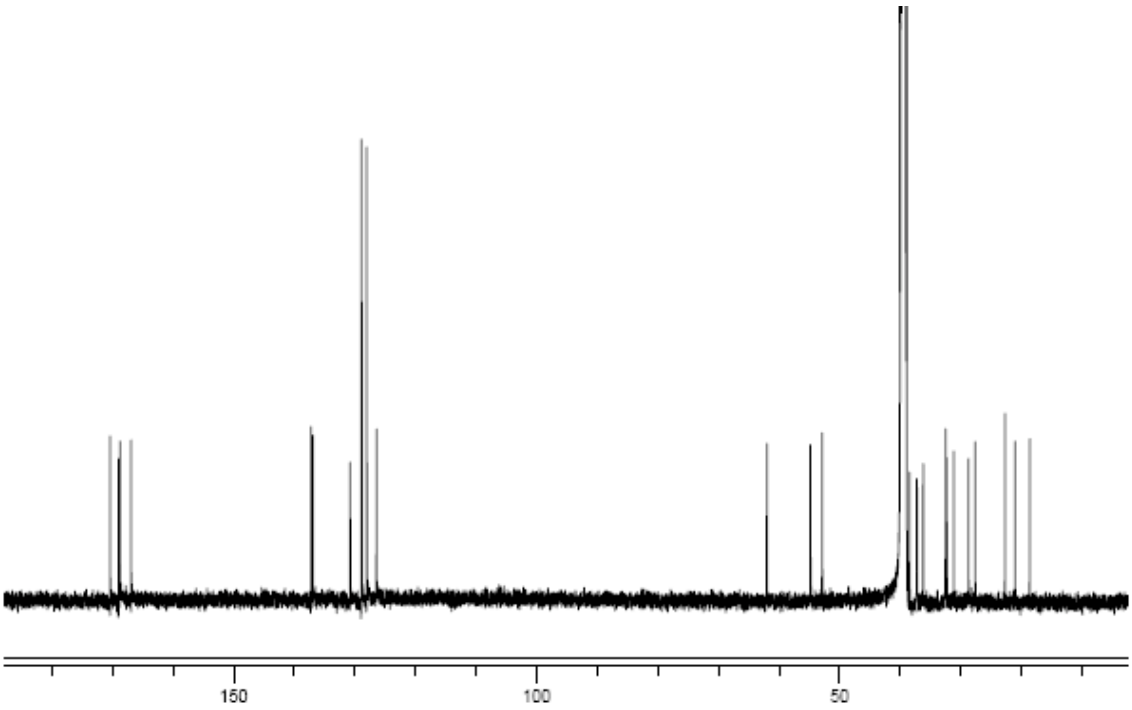
Macrocyclic Diketopiperazine 11a (*1S,2S,3S*-1,5-triazole).



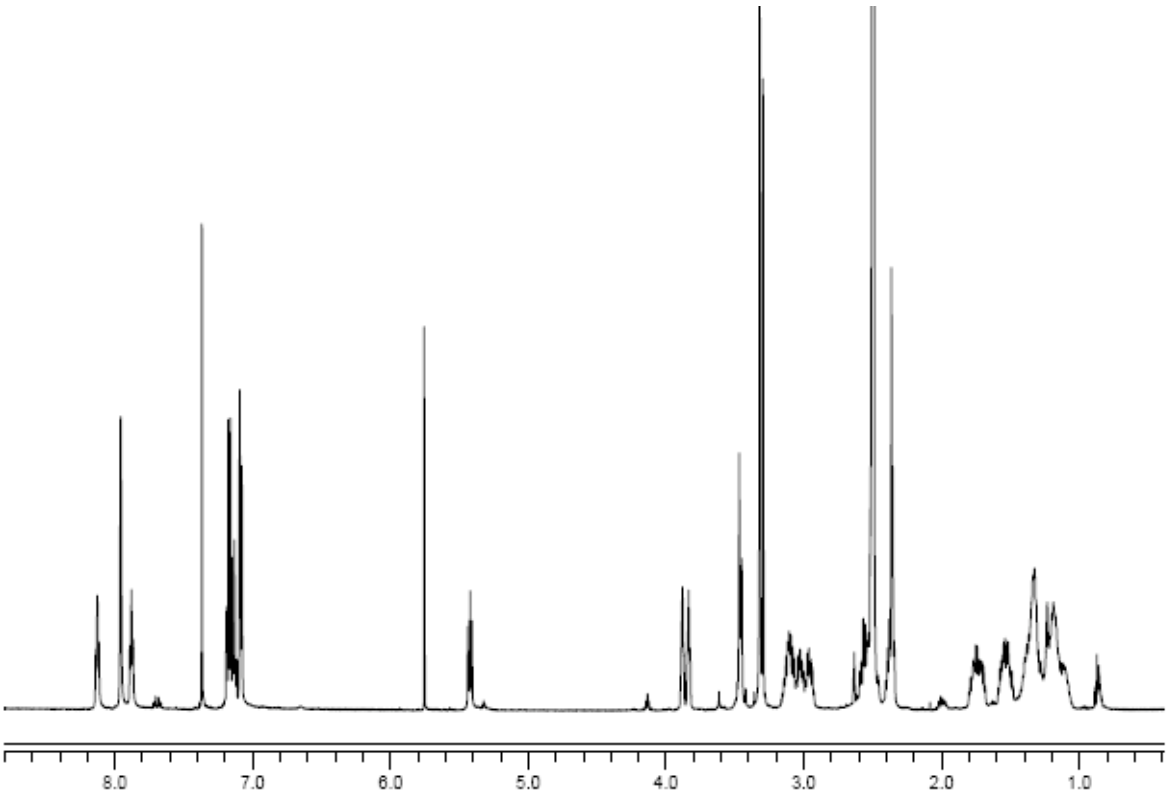


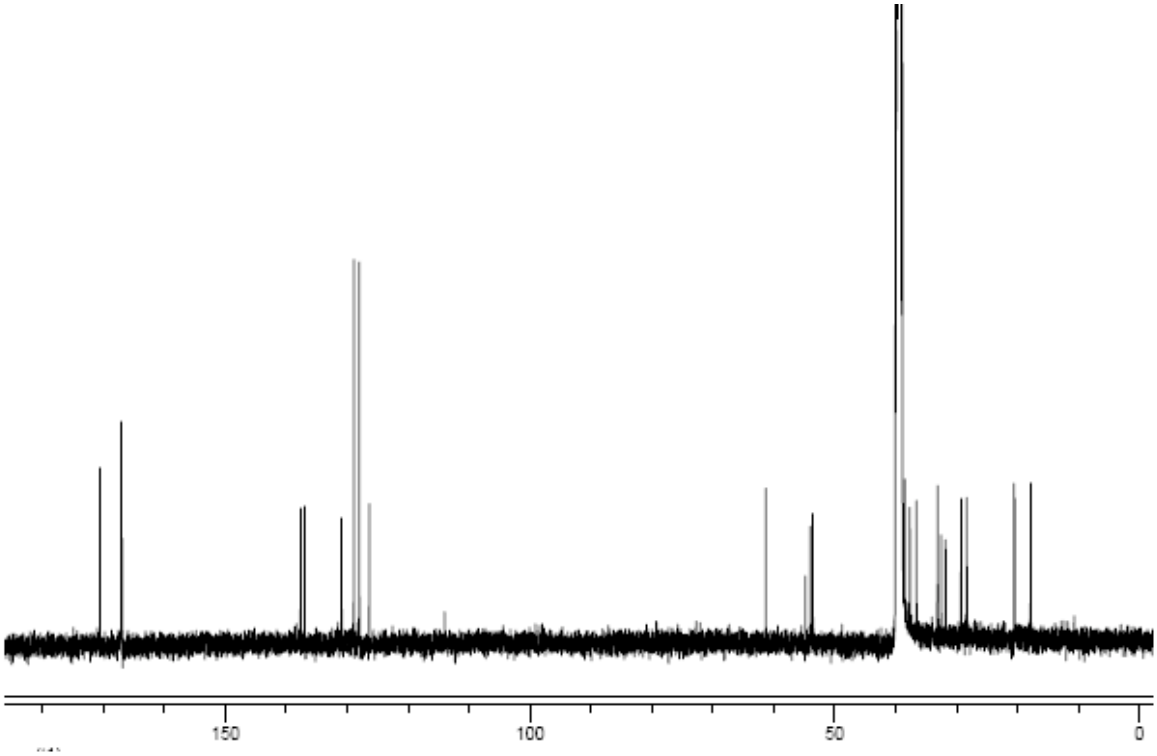
Macrocyclic Diketopiperazine 11b (*1S,2R,3S*-1,5-triazole).



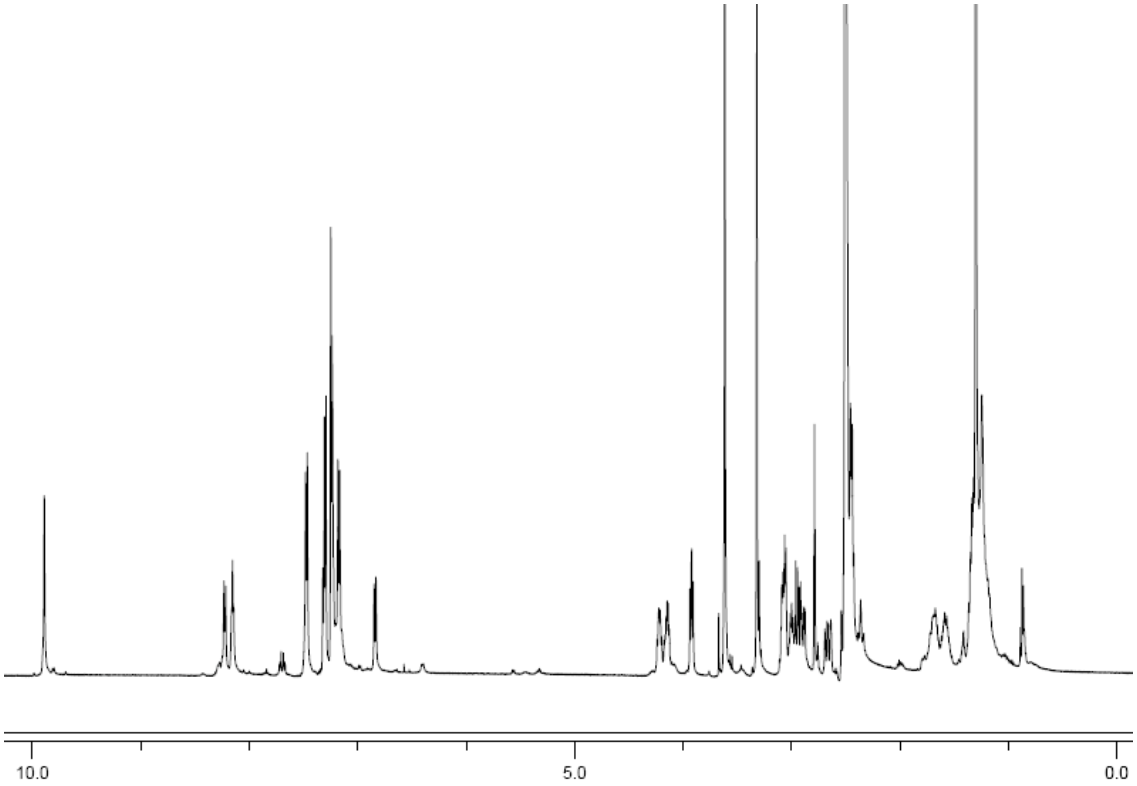


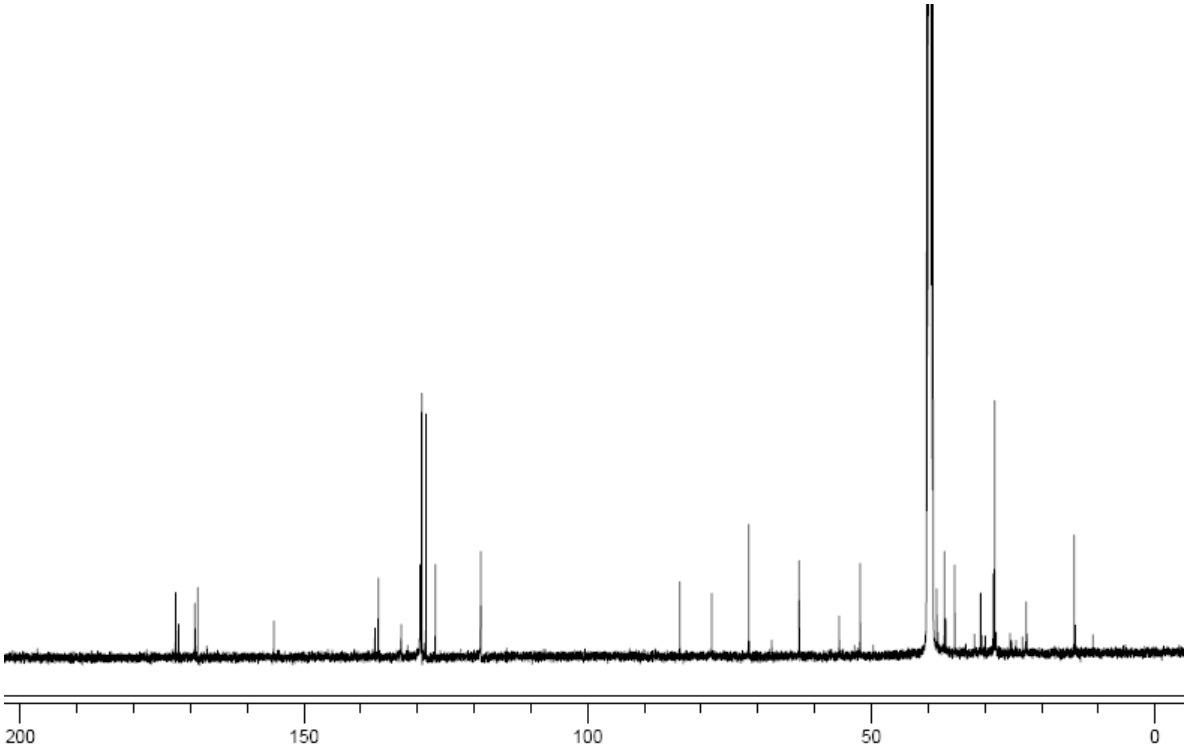
Macrocyclic Diketopiperazine 11c (*1S,2S,3R*-1,5-triazole).



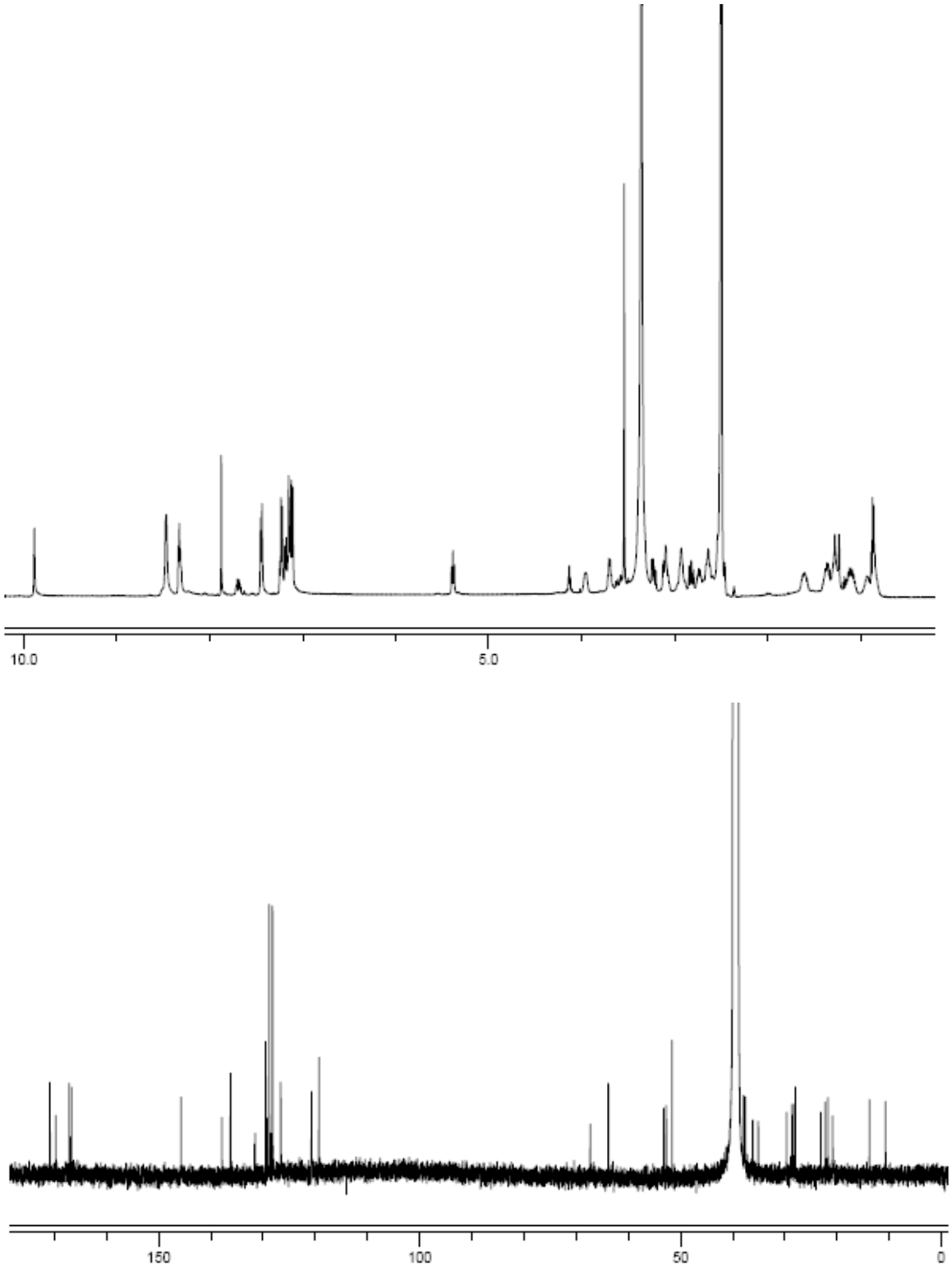


Linear peptidomimetic 12

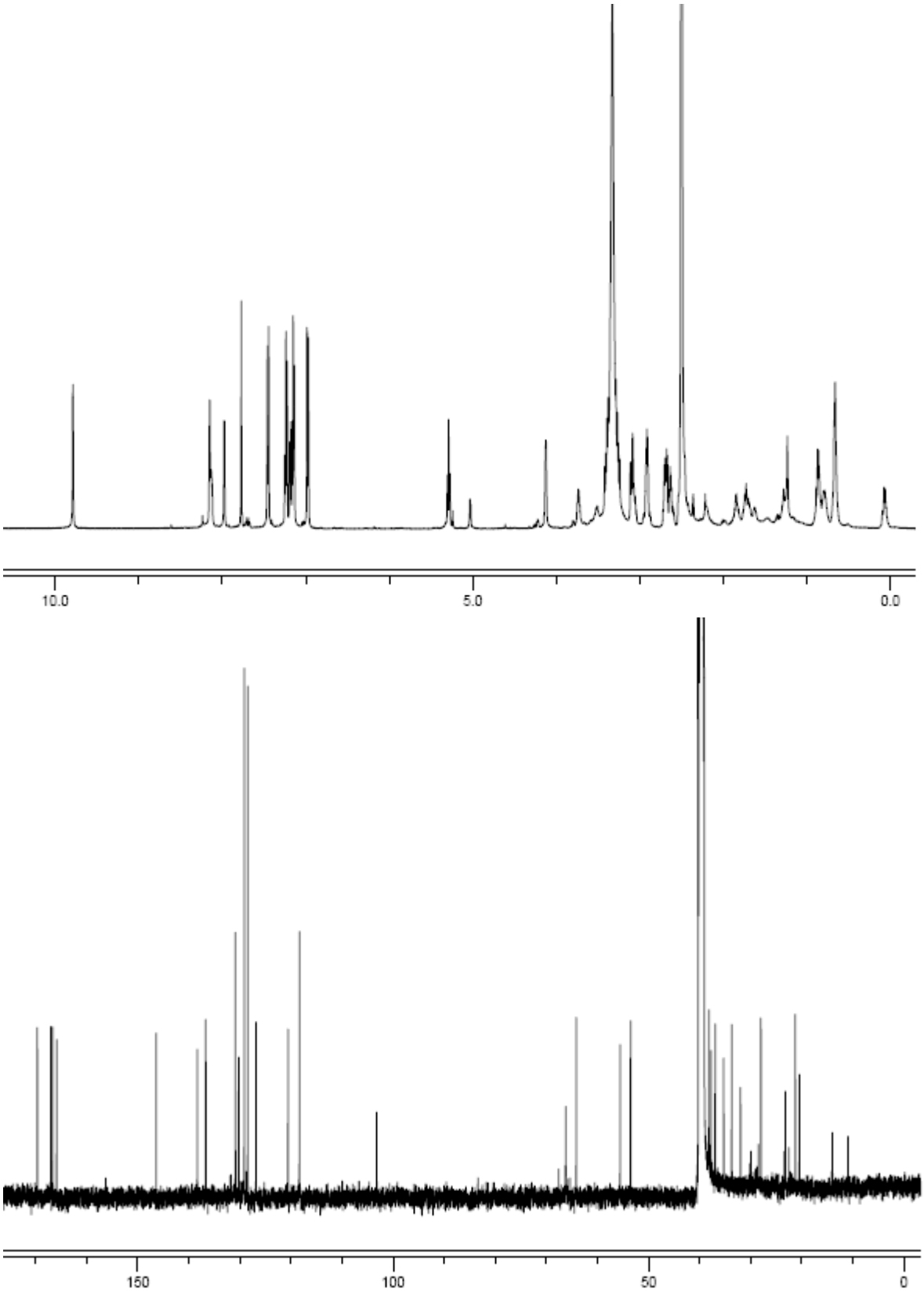




Macrocyclic peptidomimetic 13.



Macrocyclic DKP 14.



1. Lundquist JT & Pelletier JC (2001) Improved Solid-Phase Peptide Synthesis Method Utilizing α-Azide-Protected Amino Acids. *Org Lett* 3:781-783.
2. Talaga P, Benezra C & Stampf J-L (1990) Stereochemistry of the michael addition of lysine derivatives to [alpha]-methylene-[gamma]-butyrolactones. *Bioorg Chem* 18:199-206.
3. Galibert M, Dumy P & Boturyn D (2009) One-Pot Approach to Well-Defined Biomolecular Assemblies by Orthogonal Chemoselective Ligations. *Angew Chem Int Ed* 48:2576-2579.

Analysis of Chemical Space Coverage

We analyzed the chemical diversity of the 14 macrocyclic compounds reported in this work as follows.

Firstly, in order to put the diversity of compounds into context to other typical chemical libraries we randomly selected a set of 657 approved drugs from DrugBank[1] and 746 compounds from the Chembridge screening library, as downloaded from ZINC[2] (all structures are given as well in the supplementary material). For both libraries as well as our newly synthesized structures TAE/RECON)[3] electrostatic potential (RECON_EP1 to RECON_EP9) and electrostatic potential autocorrelation descriptors (RA_EP1 to RA_EP9) were calculated as implemented in the Molecular Operating Environment (MOE). These descriptors capture the diversity of chemical structures with respect to their electrostatic surface properties which are of crucial importance to binding, but implicitly and partially (due to the autocorrelation descriptors) also information about the shape of the molecule. The resulting 20-dimensional descriptor space was subject to principal component analysis (PCA) in the same program and the first two resulting principle components were displayed in Figure 5 in the manuscript.

[1] DrugBank: a knowledgebase for drugs, drug actions and drug targets. Wishart DS, Knox C, Guo AC, Cheng D, Shrivastava S, Tzur D, Gautam B, Hassanali M. Nucleic Acids Res. 2008; 36: D901-6.

[2] ZINC - A Free Database of Commercially Available Compounds for Virtual Screening. Irwin JJ, Shoichet BK. J. Chem. Inf. Model. 2005; 45: 177-82.

[3] New developments in PEST shape/property hybrid descriptors. Breneman CM, Sundling CM, Sukumar N, Shen L, Embrechts MJ. J. Comp.-Aided Mol. Des. 2003; 17: 231 – 240.

SMILES of FDA-Approved Drugs

```
P(OCc1cnc(C)c(O)c1C=O)(=O)([O-])[O-]
O=C1N=C(NC=2NCC(NC1=2)CNc1ccc(cc1)C(=O)N[C@@H](CCC(=O)[O-])C(=O)[O-])N
O=C([O-])[C@@H]([NH3+])Cc1[nH]cnc1
O=C(C(=O)[O-])C
OCC[N+](C)(C)C
O=C([O-])[C@@H]([NH3+])CCCC[NH3+]
O=C([O-])[C@@H]([NH3+])CCC[NH+]=C(N)N
[NH2+](CCCC[NH2+]CCC[NH3+])CCC[NH3+]
O=C([O-])[C@@H]([NH3+])CCC[NH3+]
O=C(N)CC[C@H]([NH3+])C(=O)[O-]
P(OC[C@H]1O[C@@H](n2c3ncnc(N)c3nc2)[C@H](O)[C@@H]1O)(=O)([O-])[O-]
OC1CC(C)(C)C(\C=C\C(=C\C=C\C(=C\C=C\C=C(\C=C\C=C(\C=C\C2C(CC(O)C=C2C)(C)C)/C)/C)\C)\C)=C(C1)
C
O=C1NC(=O)N=C2N(c3cc(C)c(cc3N=C12)C)C[C@@H](O)[C@@H](O)[C@@H](O)CO
O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H](NC(=O)C)C1O
O=C([O-])CC[C@H]([NH3+])C(=O)[O-]
P(OC[C@H]([NH3+])C(=O)[O-])(OC[C@H](OC(=O)CCC)COC(=O)CC)(=O)[O-]
O[C@H]1C\C(=C\C=C/2\C3CC[C@H]([C@@H](CCCC(O)(C)C)C)[C@]3(CCC\2)C)\C(CC1)=C
O=C([O-])CN(C(=[NH2+])N)C
O=C([O-])C([NH3+])CC(C)C
O=C([O-])[C@@H]([NH3+])Cc1c2c([nH]c1)cccc2
SC[C@H]([NH3+])C(=O)[O-]
s1c[n+](Cc2cnc(nc2N)C)c(C)c1CCO
O=C([O-])[C@@H]([NH3+])CCCNC(=O)N
O=C([O-])[C@@H]([NH3+])[C@H](O)C
P(OC[C@H]1O[C@@H](N2C=C(CC=C2)C(=O)N)[C@H](O)[C@@H]1O)(OP(OC[C@H]1O[C@@H](n2c3ncnc(N)c3nc2)[
C@H](O)[C@@H]1O)(=O)[O-])(=O)[O-]
O=C1N=C(Nc2ncc(nc12)CNc1ccc(cc1)C(=O)N[C@@H](CCC(=O)[O-])C(=O)[O-])N
O=C([O-])[C@@H]([NH3+])C
O=C1c2c(cccc2)C(=O)C=C1C
O=C([O-])[C@H]1[NH2+]CCC1
[nH]1c2c(ncnc2N)nc1
O=C(N)C[C@H]([NH3+])C(=O)[O-]
FC(F)(F)c1ccc(cc1)C(=NOCC[NH3+])CCCCOC
O=C(N([C@@H](C(C)C)C(=O)[O-])Cc1ccc(cc1)-c1ccccc1-c1n[n-]nn1)CCCC
O(CC)C(=O)[C@@H]([NH2+][C@H](C(=O)N1[C@@H]2[C@H](C[C@H]1C(=O)[O-])CCC2)C)CCc1ccccc1
Oc1cc(ccc1O)C[C@H]([C@H](Cc1cc(O)c(O)cc1)C)C
Clc1ccc(cc1)C(CC(=O)[O-])C[NH3+]
[NH+]1(CCCC1c1cccnc1)C
S1C[C@@]2(O[C@H]1C)C1CC[NH+](C2)CC1
Clc1ccccc1C1=NC(O)C(=O)Nc2c1cc(Cl)cc2
O(CC(O)C[NH2+]C(C)C)c1ccc(cc1)CCC(OC)=O
ClC=CC(O)(CC)C#C
[NH3+]C(Cc1ccccc1)(C)C
O=C(N)C1(c2c(-c3c1cccc3)cccc2)CCC[NH2+]C(C)C
O(C)c1cc(ccc1)[C@@]1(O)CCCC[C@@H]1C[NH+](C)C
O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H]1n1c2ncnc(N)c2nc1
O(CC(O)C[NH2+]C(C)C)c1ccc(cc1)CCOCC1CC1
Fc1cc(F)ccc1C(O)(Cn1ncnc1)Cn1ncnc1
O(C(CC)CC)[C@@H]1C=C(C[C@H]([NH3+])[C@H]1NC(=O)C)C(OCC)=O
O(C(=O)CCC(OCC[N+](C)(C)C)=O)CC[N+](C)(C)C
S(=O)(=O)(N1CC[NH+](CC1)C)c1cc(C2=NC(=O)c3n(nc(c3N2)CCC)C)c(OCC)cc1
S(=O)(=O)(Nc1ccc(cc1)CC[NH+](CCOc1ccc(NS(=O)(=O)C)cc1)C)C
Clc1ccc(cc1)-c1c(nc(nc1N)N)CC
O(C)c1c(OC)cc(cc1OC)C(O[C@@H]1C[C@H]2[C@H](C[C@H]3[NH+](CCc4c5c([nH]c34)cc(OC)cc5)C2)[C@H](C
(OC)=O)[C@H]1OC)=O
O1[C@H](CC)[C@](O)(C)[C@H](O)[C@H]([NH+](C[C@@H](C[C@](O)(C)[C@H](O[C@@H]2O[C@@H](C[C@H]([NH
+](C)C)[C@H]2O)C)C(C)[C@H](O[C@@H]2O[C@@H](C)[C@H](O)[C@](OC)(C2)C)[C@@H](C)C1=O)C)C)C
Clc1ccccc1C[NH+]1CCc2sccc2C1
O(C)c1ccc(cc1C12CC3CC(C1)CC(C2)C3)-c1cc2c(cc(cc2)C(=O)[O-])cc1
S(=O)([O-])(=NC(=O)NC(C)C)c1c[nH+]ccc1Nc1cc(ccc1)C
Oc1cc2C[C@H](/[N+](/c2cc1O)=C\C=C/1\C=C(N[C@@H](C\1)C(=O)[O-])C(=O)[O-])C(=O)[O-]
S(=O)([O-])(=NC(=O)NC1CCC(CC1)C)c1ccc(cc1)CCNC(=O)N1CC(C)=C(CC)C1=O
F[C@@]12[C@H]([C@@H]3C[C@H](C)[C@](OC(=O)C)(C(=O)COC(=O)C)[C@]3(C[C@@H]1O)C)C[C@H](F)C1=CC(=
O)C=C[C@@]12C
O1C(COC12CCCCC2)C[NH+]=C(N)N
O1[C@@H](C[C@@H](O)CC1=O)CC[C@@H]1[C@@H]2C(=C[C@@H](C[C@@H]2OC(=O)[C@H](CC)C)C)C=C[C@@H]1C
```

ClC(F)C(F)(F)OC(F)F
s1cc(nc1N)CC(=O)N[C@H]1[C@H]2SCC(CSc3nnnn3CC[NH+](C)C)=C(N2C1=O)C(=O)[O-]
O=C([O-])C[C@H](CC(C)C)C[NH3+]
Clc1cc2c(N(C)C(=O)C(O)N=C2c2ccccc2)cc1
Clc1cc2NC(N(S(=O)(=O)c2cc1S(=O)(=O)N)C)CCl
Oc1cc(N)ccc1C(=O)[O-]
O1CC[NH2+]C[C@H]1[C@@H](Oc1ccccc1OCC)c1ccccc1
BrCCC(=O)N1CCN(CC1)C(=O)CCBr
O=C1NC(=O)NC(=O)C1(C(CC)C)CC
O=C1Nc2c(nccc2C)N(c2ncccc12)C1CC1
Clc1nc(N)c2ncn(c2n1)[C@@H]1O[C@H](CO)[C@@H](O)C1
Oc1ccc(N)cc1C(=O)[O-]
O(C(c1ccccc1)c1ccccc1)C1C[C@@H]2[NH+]([C@@H](C1)CC2)C
S(=O)(=O)(c1ccc(N)cc1)c1ccc(N)cc1
Clc1cc(Cl)ccc1[C@@]1(O[C@H](CO1)COc1ccc(N2CC[NH+](CC2)C(C)C)cc1)Cn1ncnc1
O=C1NC(=O)NC1(c1ccccc1)c1ccccc1
Oc1c2c(ccc1)[C@@H]([C@@H]1C(C(=O)[C@@]3(O)[C@H]([C@H]([NH+](C)C)C(=O)/C(=C(/[O-
])\N)/C3=O)[C@H]1O)=C2[O-])C
Oc1ccc(cc1)C(=C(CC)c1ccc(O)cc1)CC
Clc1ccccc1C(n1ccnc1)(c1ccccc1)c1ccccc1
Clc1c2CN3CC(=O)N=C3Nc2ccc1Cl
O=C(N(CC)c1ccccc1C)C=CC
O1c2c(cccc2)C(=O)C(CC=2C(=O)c3c(OC=2[O-])cccc3)=C1[O-]
Ic1c(C(=O)[O-])c(I)c(NC(=O)C)c(I)c1NC(=O)C
S(=O)(=O)(Nc1cc(OC)c(Nc2c3c([nH+]c4c2cccc4)cccc3)cc1)C
O=C1N(C)C(=O)N(c2nc[nH]c12)C
O=C(N)C(CC[NH+](C(C)C)C(C)C)(c1ccccc1)c1ncccc1
O=C(Nc1c(cccc1C)C)C[NH+](CC)CC
P(=O)([O-])([O-])C(P(=O)([O-])[O-])(O)CC[NH3+]
Clc1ccc(cc1)[C@@](OCC[C@@H]1[NH+](CCC1)C)(C)c1ccccc1
S(Oc1cc2CC[C@H]3[C@@H]4CCC(=O)[C@]4(CC[C@@H]3c2cc1)C)(=O)(=O)[O-]
O(C(=O)c1n(cnc1)C(C)c1ccccc1)CC
O1[C@@H]2[C@]34[C@H]([C@H]([NH+](CC3)C)Cc3c4c1c(O)cc3)C=C[C@@H]2O
S([C@H]1C[C@H]([NH2+]C1)C(=O)Nc1cc(ccc1)C(=O)[O-])C=1[C@@H]([C@H]2N(C=1C(=O)[O-
])C(=O)[C@@H]2[C@H](O)C)C
O=C1N(C)C(=O)N(C)C(=O)C1(C(CC)C)CC=C
S(=O)(=O)(Nc1ccc(cc1)C(O)CCC[NH+](CCCCCCC)CC)C
O(C)c1cc2N([C@@H]3[C@@]4([C@H]5[NH+](CC=C[C@@]5(CC)[C@@H](O)[C@]3(O)C(=O)N)CC4)c2cc1[C@@]1(c
2[nH]c3c(c2CC[NH+]2C[C@@](O)(C[C@H](C1)C2)CC)cccc3)C(OC)=O)C
s1c2cc(OCC)ccc2nc1S(=O)(=O)N
O1C[C@H](NC1=O)Cc1cc2c([nH]cc2CC[NH+](C)C)cc1
Clc1cc(Nc2ncnc3c2cc(OCCC[NH+]2CCOCC2)c(OC)c3)ccc1F
O1[C@@H]2[C@]34[C@H]([C@H]([NH+](CC3)C)Cc3c4c1c(OC)cc3)C=C[C@@H]2O
S1[C@H]2N([C@@H](C(=O)[O-])C1(C)C)C(=O)[C@H]2NC(=O)[C@H](NC(=O)N1CCN(CC)C(=O)C1=O)c1ccccc1
O1[C@](NC(=O)[C@@H]2C[C@H]3[C@H]([NH+](C2)C)Cc2c4c3cccc4[nH]c2)(C)C(=O)N2[C@@H](Cc3ccccc3)C(
=O)N3[C@@H](CCC3)[C@]12O
[NH+](CCC=C1c2c(CCc3c1cccc3)cccc2)(C)C
F[C@@]12[C@H]([C@@H]3CC[C@](O)(C(=O)C)[C@]3(C[C@@H]1O)C)C[C@@H](C1=CC(=O)C=C[C@@]12C)C
O=[N-]
OCC([NH2+]CC[NH2+]C(CC)CO)CC
[NH+](=C(N)N)C(=[NH2+])N(C)C
O(CC(O)C[NH2+]C(C)C)c1ccc(cc1)CC(=O)N
O=C(N)c1nccnc1
[NH2+](CCCC1c2c(C=Cc3c1cccc3)cccc2)C
O1CCCC1C(=O)NCCCN(C)c1nc(N)c2cc(OC)c(OC)cc2n1
FC(F)(F)c1cc([N+](=O)[O-])c(cc1)C(=O)C1C(=O)CCCC1=O
ON1C(N)=CC(=NC1=N)N1CCCCC1
O=C1CC[C@@]2([C@@H]3[C@H]([C@@H]4CC[C@](O)(C(=O)C)[C@]4(CC3)C)C=C(C2=C1)C)C
Clc1cc2NC(Oc2cc1)=O
O=C1NC(=O)CCC1(CC)c1ccc(N)cc1
S(=O)(=O)(Nc1ncccn1)c1ccc(N)cc1
Clc1cc2NC(N3CC[NH+](CC3)C)=C3C(=Nc2cc1)C=CC=C3
O(C(C)(c1ccccc1)c1nccccc1)CC[NH+](C)C
S1c2c(N(c3c1cccc3)CCC[NH+]1CC[NH+](CC1)C)cc(SCC)cc2
[NH2+](CC[NH2+]CC[NH3+])CC[NH2+]CC[NH3+]
OC(CC[NH+]1CCCCC1)(C1CCCCC1)c1ccccc1
O=C1NC(=O)C[NH+](C1)C[C@@H]([NH+]1CC(=O)NC(=O)C1)C
Clc1ccccc1C1C(C(OCC)=O)=C(NC(C)=C1C(OC)=O)COCC[NH3+]
[nH+]1c2c(CCCC2)c(N)c2c1cccc2
FC(F)(F)C(=O)NC1CC(OC(C)C1O)O[C@@H]1c2c(C[C@](O)(C1)C(=O)COC(=O)CCCC)c(O)c1c(C(=O)c3c(cccc3O
C)C1=O)c2O

OC(CC[NH+]1CCCC1)(C1CCCCC1)c1ccccc1
O1CC(=CC1=O)C1CC[C@]2(O)[C@H]3[C@H](C[C@@H](O)[C@]12C)[C@@]1([C@@H](C[C@@H](O[C@@H]2O[C@H](C
)[C@@H](O[C@@H]4O[C@H](C)[C@@H](O[C@@H]5O[C@H](C)[C@@H](O)[C@@H](O)C5)[C@@H](O)C4)[C@@H](O)C
2)CC1)CC3)C
S(=O)(=O)(N)c1cc(C(=O)NCC2[NH+](CCC2)CC)c(OC)cc1
O(C(=O)C=1C(C(C(OCCOC)=O)=C(NC=1C)C)c1cc([N+](=O)[O-])ccc1)C(C)C
Cl[C@@]12[C@H]([C@@H]3C[C@H](C)[C@](O)(C(=O)CO)[C@]3(C[C@@H]1O)C)CCC1=CC(=O)C=C[C@@]12C
O[C@H]([C@H]([NH3+])C)c1ccccc1
Clc1ccc(nc1)N1[C@@H](OC(=O)N2CC[NH+](CC2)C)c2nccnc2C1=O
Clc1cc2c(-n3c(nnc3C)CN=C2c2ccccc2)cc1
Brc1ccc(cc1)[C@H](CC[NH+](C)C)c1ncccc1
[N+](C)(C)=C1C=CC(C=C1)=C(c1ccc(N(C)C)cc1)c1ccc(N(C)C)cc1
Clc1cc2c(Oc3c(N=C2N2CC[NH+](CC2)C)cccc3)cc1
O(CC[N+](C)(C)C)C(=O)N
S(=O)([O-])(=NC(=O)NC1CCCCC1)c1ccc(cc1)C(=O)C
O1c2cc(C[C@H]3[N+](CCc4cc(OC)c(OC)c(Oc5ccc(C[C@@H]6[N+](CCc7cc(OC)c1cc67)(C)C)cc5)c34)(C)C)c
cc2OC
S1[C@H]2N([C@@H](C(=O)[O-])C1(C)C)C(=O)[C@H]2NC(=O)COc1ccccc1
O=C1NC(=O)NC(=O)C1([C@@H](CCC)C)CC=C
S1c2c(N(c3c1cccc3)CCC[NH+](C)C)cccc2
O(CC(O)COC(=O)N)c1ccccc1OC
O(C(=O)[C@H](CO)c1ccccc1)C1CC2[NH+](C(C1)CC2)C
O=C(N(C)C)Cc1n2C=C(C=Cc2nc1-c1ccc(cc1)C)C
[NH+]1(CCCC1)C\C=C(/c1ccc(cc1)C)\c1ncccc1
O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H](NC(=O)N(N=O)C)[C@H]1O
O[C@H]1C[C@@H](O)[C@H](\C=C\[C@@](O)(CCCCC)C)[C@H]1C\C=C\CCCC(=O)[O-]
ClC1C(Cl)C(Cl)C(Cl)C(Cl)C1Cl
FC(F)(F)C1=CN([C@@H]2O[C@H](CO)[C@@H](O)C2)C(=O)NC1=O
Clc1cc2N(c3c(Sc2cc1)cccc3)CCC[NH+]1CC[NH+](CC1)C
O(C)c1c(OC)cc(cc1OC)Cc1cnc(nc1N)N
FC1(F)[C@H](O)[C@H](O[C@H]1N1C=CC(=NC1=O)N)CO
O=C1N=C(Nc2n(cnc12)[C@H]1C[C@H](O)[C@@H](CO)C1=C)N
s1cccc1C1OC[C@H]2O[C@@H](O[C@H]3[C@@H]4[C@@H]([C@@H](c5c3cc3OCOc3c5)c3cc(OC)c(O)c(OC)c3)C(OC
4=O)[C@H](O)[C@@H](O)[C@@H]2O1
O1[C@@H](C)[C@H](O)[C@@H]([NH3+])C[C@@H]1O[C@@H]1c2c(C[C@](O)(C1)C(=O)CO)c(O)c1c(C(=O)c3c(cc
cc3OC)C1=O)c2O
ClC(Cl)C(=O)NC(C(O)c1ccc([N+](=O)[O-])cc1)CO
S(=O)(Cc1nccc(OCC(F)(F)F)c1C)c1[nH]c2c(n1)cccc2
Fc1ccc(cc1)C(=O)CCC[NH+]1CCC(N2c3c(NC2=O)cccc3)=CC1
Ic1cc(cc(I)c1Oc1cc(I)c(O)c(I)c1)C[C@H]([NH3+])C(=O)[O-]
Clc1c2c(C([O-])=C3[C@H](C[C@@H]4[C@@](O)(C(=O)\C(=C(/[O-
])\NCO)\C(=O)[C@H]4[NH+](C)C)C3=O)[C@@]2(O)C)c(O)cc1
O(C(=O)C1(CC[NH+](CC1)C)c1ccccc1)CC
Clc1cc2c(cc1)C(c1ncccc1CC2)=C1CCN(CC1)C(OCC)=O
s1cccc1CC(=O)N[C@H]1[C@H]2SCC(COC(=O)C)=C(N2C1=O)C(=O)[O-]
o1cccc1C(=O)N1CCN(CC1)c1nc(N)c2cc(OC)c(OC)cc2n1
[NH+](CCCN1c2c(CCc3c1cccc3)cccc2)(C)C
O(C)c1cc(C)c(\C=C\C(=C\C=C\C(=C/C(=O)[O-])\C)\C)c(C)c1C
O(C(=O)C1=CC=C2C3=NC(=Cc4[nH]c(C=C5N=C(C=c6[nH]c(=C3)c(C)c6C=C)C(C)=C5CCC(=O)[O-
])c(CCC(OC)=O)c4C)[C@]2(C)[C@@H]1C(OC)=O)C
O(C)c1cc2c(cc(cc2)CCC(=O)C)cc1
O1C2[C@H]3OC(=O)[C@@]45O[C@@H]4C[C@@](O)(C([C@@H]2C(O)(C)C)C1=O)[C@@]35C
Fc1cc2c(nc1N1CC[NH2+]CC1)N(C=C(C(=O)[O-])C2=O)CC
O(C)c1cc2c(nccc2[C@@H](O)[C@H]2[NH+]3C[C@@H](C(C2)CC3)C=C)cc1
O1c2c([C@H]3[C@@H](CCC(=C3)C)C1(C)C)c(O)cc(c2)CCCCC
Clc1cc2nc(ccc2cc1)\C=C\c1cc(ccc1)[C@H](SCC1(CC1)CC(=O)[O-])CCc1ccccc1C(O)(C)C
O(C(=O)c1ccccc1)C(C[NH2+]C1CCCCC1)C
O=C1N(C)C(=O)NC(=O)C1(C(C#CCC)C)CC=C
s1cccc1[C@@H](Oc1c2c(ccc1)cccc2)CC[NH2+]C
O=C1NC(=O)CCC1N1Cc2c(cccc2N)C1=O
s1c2c(ccc(O)c2)c(C(=O)c2ccc(OCC[NH+]3CCCCC3)cc2)c1-c1ccc(O)cc1
S(=O)(=O)(N)c1ccc(-n2nc(cc2-c2ccc(cc2)C)C(F)(F)F)cc1
O(CC[NH+](CC)CC)c1c(OCC[NH+](CC)CC)cccc1OCC[NH+](CC)CC
Brc1c2nccnc2ccc1NC1=[NH+]CCN1
Clc1cccc(Cl)c1-c1noc(C)c1C(=O)N[C@H]1[C@H]2SC(C)(C)[C@@H](N2C1=O)C(=O)[O-]
Fc1cc2c(N(C=C(C(=O)[O-])C2=O)CC)cc1N1CC[NH+](CC1)C
n1c(nc(nc1N(C)C)N(C)C)N(C)C
S(=O)(=O)(Nc1ccc(cc1)C(O)C[NH2+]C(C)C)C
O=C1N(CCCC[NH+]2CCN(CC2)c2ncccn2)C(=O)CC2(C1)CCCC2
O1[C@H](CO)[C@@H](N=[N+]=[N-])C[C@@H]1N1C=C(C)C(=O)NC1=O
O1CCc2cc(ccc12)CC[NH+]1C[C@@H](CC1)C(C(=O)N)(c1ccccc1)c1ccccc1

OC(CC[N+](CC)(CC)CC)(C1CCCCC1)c1ccccc1
O=C1CC[C@@H]2[C@@H]3[C@H]([C@@H]4CC[C@@](O)(C#C)[C@]4(CC3)CC)CCC2=C1
O1CC(=CC1=O)[C@H]1CC[C@]2(O)[C@H]3[C@H](CC[C@]12C)[C@@]1([C@@H](CC(O[C@@H]2O[C@H](C)[C@@H](O
[C@@H]4O[C@H](C)C(O[C@@H]5O[C@H](C)[C@@H](O)[C@@H](OC(=O)C)C5)[C@@H](O)C4)[C@@H](O)C2)CC1)CC
3)C
O(C)c1cc2[C@]34[C@@H]([C@H]([NH+](CC3)C)Cc2cc1)CCCC4
[AlH2-](O[AlH2-]O)O
S(CCC)c1cc2[nH]c(nc2cc1)NC(OC)=O
O=C([O-])\C=C(\C=C\C=C(\C=C\C=1C(CCCC=1C)(C)C)/C)/C
Clc1cc2NC(N(c3ccccc3C)C(=O)c2cc1S(=O)(=O)N)C
S=C(Oc1cc2c(cc1)cccc2)N(C)c1cc(ccc1)C
O(CCCC)c1nc2c(cccc2)c(c1)C(=O)NCC[NH+](CC)CC
O(C(=O)C=1C(C(C(OC)=O)=C(NC=1C)C)c1cc([N+](=O)[O-
])ccc1)C(C[NH+](CCC(c1ccccc1)c1ccccc1)C)(C)C
P(=O)([O-])([O-])C(=O)[O-]
Fc1cc2c(N(C=C(C(=O)[O-])C2=O)C2CC2)cc1N1CC[NH2+]CC1
ClCC\C(=C(\c1ccc(OCC[NH+](C)C)cc1)/c1ccccc1)\c1ccccc1
O(C)c1cc2N([C@@H]3[C@@]4([C@H]5[NH+](CC=C[C@@]5(CC)[C@@H](OC(=O)C)[C@]3(O)C(OC)=O)CC4)c2cc1[
C@@]1(c2[nH]c3c(c2CC[NH+]2C[C@@](O)(C[C@H](C1)C2)CC)cccc3)C(OC)=O)C=O
O(C(=O)N(C)C)c1ccc[n+](c1)C
F[C@@]12[C@H]([C@@H]3C[C@@H](C)[C@H](C(=O)CO)[C@]3(C[C@@H]1O)C)CCC1=CC(=O)C=C[C@@]12C
O=C([O-])CCCCCCCC(=O)[O-]
S=C1NC(=CC(=O)N1)CCC
O1c2c(C=CC1=O)cc1c(occ1)c2OC
S1(=O)(=O)N(C)\C(=C(\[O-])/Nc2nccccc2)\C(=O)c2c1cccc2
FC(F)(C(F)(F)F)C(F)(F)F
Clc1ccc(cc1)C([NH+]1CC[NH+](CC1)CCOCCO)c1ccccc1
O1[C@@H]([C@H](O)[C@H](O)CO)[C@H](NC(=O)C)[C@@H]([NH+]=C(N)N)C=C1C(=O)[O-]
S(=O)(=O)(Nc1nc(nc(OCCO)c1Oc1ccccc1OC)-c1ncccn1)c1ccc(cc1)C(C)(C)C
Oc1c2c(C[C@@H]3C(C(=O)[C@@]4(O)[C@@H](C3)[C@H]([NH+](C)C)C)C(=O)/C(=C(/[O-])\N)/C4=O)=C2[O-
])c(N(C)C)cc1NC(=O)C[NH2+]C(C)(C)C
O1CC[NH+](CC1)CCC1CN(CC)C(=O)C1(c1ccccc1)c1ccccc1
S1[C@H]2N(C(C(=O)[O-])=C(C1)C)C(=O)[C@H]2NC(=O)[C@H]([NH3+])c1ccccc1
O(C)c1cc2N([C@@H]3[C@@]4([C@H]5[NH+](CC=C[C@@]5(CC)[C@@H](OC(=O)C)[C@]3(O)C(OC)=O)CC4)c2cc1[
C@@]1(c2[nH]c3c(c2CC[NH+]2C[C@@](O)(C[C@@H](C1)C2)CC)cccc3)C(OC)=O)C
O(CC(O)C[NH2+]C(C)C)c1c2c(ccc1)cccc2
O(c1cc(ccc1)C(C(=O)[O-])C)c1ccccc1
Clc1cccc(Cl)c1NC1=[NH+]CCN1
O=C1N=C(Nc2n(cnc12)COCCOC(=O)[C@@H]([NH3+])C(C)C)N
Clc1ccc(cc1)C1(O)N2C(=NCC2)c2c1cccc2
Fc1cc(F)ccc1[C@](O)([C@@H](C)c1ncncc1F)Cn1ncnc1
O=C([O-])C[C@@H](O)C[N+](C)(C)C
O(CC)C(=O)[C@H]([NH2+][C@H](C(=O)N1CCC[C@H]1C(=O)[O-])C)CCc1ccccc1
s1cc(nc1\C=C\c1cc(NC(=O)CC(CC)(CC)C(=O)[O-])ccc1)C1CCC1
O1c2c(OCC1C(=O)N1CCN(CC1)c1nc(N)c3cc(OC)c(OC)cc3n1)cccc2
[NH2+]1CC[NH2+]CC1
Oc1ccc(cc1C(=O)N)C(O)C[NH2+]C(CCc1ccccc1)C
O(Cc1ccccc1)c1ccc(O)cc1
O=C1CC[C@@]2([C@@H]3[C@H]([C@@H]4CC[C@](O)(C(=O)C)[C@]4(CC3)C)C[C@@H](C2=C1)C)C
Clc1cc(C(=O)NC2CC[NH+](CC2OC)CCCOc2ccc(F)cc2)c(OC)cc1N
S(=O)(C)c1ccc(cc1)C=C1c2c(cc(F)cc2)C(CC(=O)[O-])=C1C
S1[C@H]2N([C@@H](C(=O)[O-])C1(C)C)C(=O)[C@H]2NC(=O)c1c2c(ccc1OCC)cccc2
S=C(N)c1cc(ncc1)CC
O(CC(O)C[NH2+]C(C)C)c1ccc(cc1)COCCOC(C)C
Clc1cc2[nH+]ccc(Nc3cc(C[NH+](CC)CC)c(O)cc3)c2cc1
O1CCN(N=Cc2oc([N+](=O)[O-])cc2)C1=O
F[C@@]12[C@H]([C@@H]3C[C@@H](O)[C@](O)(C(=O)CO)[C@]3(C[C@@H]1O)C)CCC1=CC(=O)C=C[C@@]12C
O1C[C@]2([C@H](CC1=O)CC[C@H]1[C@@H]3CC[C@@](O)(C)[C@]3(CC[C@@H]12)C)C
S1c2c(N(c3c1cccc3)CCC[NH+]1CC[NH+](CC1)CCO)cc(cc2)C(F)(F)F
O=C1CC[C@@]2([C@@H]3[C@H]([C@@H]4CC[C@H](O)[C@]4(CC3)C)CCC2=C1)C
Clc1cc2c(NC(O[C@]2(C#CC2CC2)C(F)(F)F)=O)cc1
Clc1cc2c(NC(=O)C(N=C2c2ccccc2)C(=O)[O-])cc1
OCCCCCCCCCCCCCCCCCCCCCCC
[nH]1cncc1C(C)c1cccc(C)c1C
S(=O)([O-])(=NC(=O)C)c1ccc(N)cc1
Fc1ccc(cc1)Cn1c2c(nc1NC1CC[NH+](CC1)CCc1ccc(OC)cc1)cccc2
Clc1cccc(Cl)c1SC(CCc1ccc(Cl)cc1)Cn1ccnc1
O1[C@H](CO)[C@@H](O)[C@@H](O)[C@@H]1n1c2ncnc(N)c2nc1
O1[C@@H](C[C@@H](O)CC1=O)CC[C@@H]1[C@@H]2C(=C[C@@H](C[C@@H]2OC(=O)C(CC)(C)C)C)C=C[C@@H]1C
O=C1N=C(Nc2[nH]cc(c12)CCc1ccc(cc1)C(=O)N[C@H](CCC(=O)[O-])C(=O)[O-])N
O(C(=O)Nc1[nH]c2cc(ccc2n1)C(=O)c1ccccc1)C

O(CCCC)c1ccc(cc1)C(=O)CC[NH+]1CCCCC1
O1C(C)C(C)C(O)C(\C=C\C=C\CC\C=C\C=C\C=C\C=C\C(OC2O[C@H](C)[C@@H](O)[C@H]([NH3+])[C@@H]2O)CC(
O)C(C(=O)[O-])C(O)CC(=O)CC(O)C(O)CCC(O)CC(O)CC(O)CC1=O)C
O(C(Cc1ccccc1)(C(C[NH+](C)C)C)c1ccccc1)C(=O)CC
O1[C@@H](C=C[C@@H]1N1C=C(C)C(=O)NC1=O)CO
O=C1N(C)C(=O)N(c2ncn(c12)CC(O)CO)C
O[C@@H]1C[C@H](O)[C@H](C\C=C\CCCC(OC(C)C)=O)[C@H]1CC[C@@H](O)CCc1ccccc1
O(C)c1cc(ccc1OC)C(C(C)C)(CCC[NH+](CCc1cc(OC)c(OC)cc1)C)C#N
O(C)c1c(OC)cc(cc1OC)C(=O)NCc1ccc(OCC[NH+](C)C)cc1
FC(F)(F)c1cc(N2C(=O)C(NC2=O)(C)C)ccc1[N+](=O)[O-]
Oc1cc(ccc1O)[C@@H](O)C[NH2+]C
O=C1Nc2cccnc2N(c2c1cccc2)C(=O)C[NH+]1CC[NH+](CC1)C
Fc1ccc(cc1)[C@H]1[NH+](CCO[C@H]1O[C@H](C)c1cc(cc(c1)C(F)(F)F)C(F)(F)F)CC1=NC(=O)[N-]N1
O(CC[NH+](C)C)c1ccc(cc1)\C(=C(\CC)/c1ccccc1)\c1ccccc1
Clc1nc(n(Cc2ccc(cc2)-c2ccccc2-c2n[n-]nn2)c1CO)CCCC
S1c2c(N(c3c1cccc3)CCC1[NH+](CCCC1)C)cc(SC)cc2
S1c2c(N(c3c1cccc3)C(=O)CC[NH+]1CCOCC1)cc(NC(OCC)=O)cc2
O1[C@@H](C)[C@H](C)[C@H](O)[C@H](C=CC=CC=CC=CC=CC=C[C@H](O[C@@H]2O[C@H](C)[C@@H](O)[C@H](
[NH3+])[C@@H]2O)C[C@@H]2O[C@@](O)(C[C@H](O)[C@H]2C(=O)[O-
])C[C@@H](O)C[C@@H](O)[C@H](O)CC[C@@H](O)C[C@@H](O)CC1=O)C
Clc1cc2c(-n3c(CN=C2c2ccccc2F)cnc3C)cc1
Fc1cc(F)ccc1N1C=C(C(=O)[O-])C(=O)c2cc(F)c(nc12)N1C[C@@H]2[C@H](C1)C2[NH3+]
S1[C@H]2N(C(C(=O)[O-])=C(C1)COC(=O)C)C(=O)[C@H]2NC(=O)[C@H]([NH3+])c1ccccc1
O(C)c1cc2C[C@H](N(Cc2cc1OC)C(=O)[C@@H]([NH2+][C@@H](CCc1ccccc1)C(OCC)=O)C)C(=O)[O-]
O1[C@@H](C)[C@@H](O)[C@@H]([NH3+])C[C@@H]1O[C@@H]1c2c(C[C@](O)(C1)C(=O)C)c(O)c1c(C(=O)c3c(cc
cc3OC)C1=O)c2O
S1\C(=N/C(=O)C)\N(N=C1S(=O)(=O)N)C
S(=O)(=O)(N)c1cc(ccc1OC)C[C@H]([NH2+]CCOc1ccccc1OCC)C
S1C[C@H](O[C@H]1CO)N1C=CC(=NC1=O)N
O=C(N(CC)CC)N1CC[NH+](CC1)C
Fc1cc(ccc1-c1ccccc1)C(C(=O)[O-])C
S1[C@H]2N([C@@H](C(=O)[O-])C1(C)C)C(=O)[C@H]2NC(=O)c1c(noc1C)-c1ccccc1
Fc1ccc(cc1)[C@@H]1CC[NH2+]C[C@H]1COc1cc2OCOc2cc1
P(OCOC(=O)C(C)(C)C)(OCOC(=O)C(C)(C)C)(=O)COCCn1c2ncnc(N)c2nc1
[NH+]1(CCC(CC1)=C1c2c(CCc3c1nccc3)cccc2)C
ClC(Cl)(P(=O)([O-])[O-])P(=O)([O-])[O-]
O(C)c1ccc(OC)cc1C(O)C([NH3+])C
n1c2c(c3n(cnc3c1N)CC(C)C)cccc2
O(C(=O)C(O)c1ccccc1)C1CC2[N+](C(C1)CC2)(C)C
O([N+](=O)[O-])C(CO[N+](=O)[O-])CO[N+](=O)[O-]
O1CC[NH+](CC1)[C@H]1C[C@]2([C@H](C[C@@H]1O)CC[C@H]1[C@@H]3C[C@H]([N+]4(CCCC4)CC=C)[C@H](OC(=
O)C)[C@]3(CC[C@@H]12)C)C
[N+]1(CCC(CC1)=C(c1ccccc1)c1ccccc1)(C)C
O=C(N[C@@H](Cc1ccccc1)C(=O)[O-])C1CCC(CC1)C(C)C
O=[NH+]\C=C/1\N(C=CC=C\1)C
S(=O)(Cc1ncc(C)c(OC)c1C)c1[nH]c2cc(OC)ccc2n1
Clc1ccc(cc1)C([NH+]1CC[NH+](CC1)Cc1cc(ccc1)C)c1ccccc1
O(CCCCCOc1ccc(cc1)C(=[NH2+])N)c1ccc(cc1)C(=[NH2+])N
S1[C@H]2N([C@@H](C(=O)[O-])C1(C)C)C(=O)[C@H]2N1C(=O)[C@H]([NH2+]C1(C)C)c1ccccc1
s1c2cc(OC(F)(F)F)ccc2nc1N
O=C1CC[C@@]2([C@@H]3[C@H]([C@@H]4CC[C@](O)(C(=O)CO)[C@]4(C[C@@H]3O)C)CCC2=C1)C
O1C2C3[NH+](C(CC(OC(=O)C(CO)c4ccccc4)C3)C12)C
O1CCc2c([nH]c3c2cccc3CC)C1(CC(=O)[O-])CC
O=C(Nc1ccccc1C)C([NH2+]CCC)C
ClC(OC(F)F)C(F)(F)F
O=C1N(CC)C(=O)NC1c1ccccc1
O=C([O-])C=C(C=CC=C(C=CC=1C(CCCC=1C)(C)C)C)C
O1CC2=C(C=C3N(Cc4c3nc3c(cc(OC(=O)N5CCC([NH+]6CCCCC6)CC5)cc3)c4CC)C2=O)[C@@](O)(CC)C1=O
S=C1NC=CN1C
Cl[C@@]12C([C@@H]3C[C@@H](C)[C@](O)(C(=O)CC1)[C@]3(C[C@@H]1O)C)CCC1=CC(=O)C=C[C@@]12C
O\1[C@H]2N([C@@H](C(=O)[O-])/C/1=C/CO)C(=O)C2
O=C1C[C@@H](O)[C@H](C=C[C@@H](O)CCCCC)[C@H]1CCCCCCC(=O)[O-]
O1C[C@H]2[C@@H]([C@@H](c3c(cc4OCOc4c3)[C@H]2O[C@@H]2O[C@H]3[C@@H](O[C@@H](OC3)C)[C@H](O)[C@H
]2O)c2cc(OC)c(O)c(OC)c2)C1=O
S(=O)(=O)(N)c1cc2S(=O)(=O)NCNc2cc1C(F)(F)F
S1c2c(N(c3c1cccc3)CC([NH+](C)C)C)cc(cc2)C(=O)CC
O1[C@H](CC)[C@](O)(C)[C@H](O)[C@@H](C)C(=NOCOCCOC)[C@@H](C[C@](O)(C)[C@H](O[C@@H]2O[C@@H](C[
C@H]([NH+](C)C)[C@H]2O)C)[C@@H](C)[C@H](O[C@@H]2O[C@@H](C)[C@H](O)[C@](OC)(C2)C)[C@@H](C)C1=
O)C
O=C1c2ccc(nc2N(C=C1C(=O)[O-])CC)C
O=C(N[C@@H](C(C)(C)C)C(=O)NC)[C@@H]([C@H](O)C(=O)N[O-])CC(C)C

O(C)c1cc2c(cc(cc2)C(C(=O)[O-])C)cc1
O=C([O-])C[NH+](CC[NH+](CC(=O)[O-])CC(=O)[O-])CC[NH+](CC(=O)[O-])CC(=O)[O-]
O(CC)C(=O)[C@@H]([NH2+][C@H](C(=O)N1[C@@H]2[C@H](C[C@H]1C(=O)[O-])CCCC2)C)CCC
[NH+](CCN(Cc1ccccc1)c1ncccc1)(C)C
IC#CCOc1cc(Cl)c(Cl)cc1Cl
S(=O)(=O)(Nc1ncccc1)c1ccc(N\N=C/2\C=C(C(=O)[O-])C(=O)C=C\2)cc1
O1C(OC2C(O)C(OC3OCC(O)(C)C([NH2+]C)C3O)C([NH3+])CC2[NH3+])C([NH3+])CCC1C([NH2+]C)C
Clc1c2c(cc(O)c1O)C(C[NH2+]CC2)c1ccc(O)cc1
Clc1cc2c(N(CC(F)(F)F)C(=O)CN=C2c2ccccc2)cc1
O=C1N(N=NN1CC)CC[NH+]1CCC(N(C(=O)CC)c2ccccc2)(CC1)COC
O1CC[NH+](CC1)CCNc1nnc(cc1C)-c1ccccc1
O(CCC)c1ccc(cc1N)C(OCC[NH+](CC)CC)=O
OC(CC[NH+]1CCCCC1)(C1C2CC(C1)C=C2)c1ccccc1
Oc1cc(cc(O)c1)C(O)C[NH2+]C(C)C
Clc1cc2c3c([nH]c2cc1)cc(cc3)C(C(=O)[O-])C
O(C(=O)C)[C@]1(CC[C@H]2[C@H]3[C@@H]([C@@H]4C(=C[C@@H](OC(=O)C)CC4)CC3)CC[C@]12C)C#C
O[C@@H]1C[C@@H](CC[C@H]1C(C)C)C
O1c2c(OC1)cc1N(N=C(C(=O)[O-])C(=O)c1c2)CC
Clc1cc2c(N(C)C(=O)CN=C2c2ccccc2)cc1
O=C1N(C)C(=O)CC1c1ccccc1
ClC=1CS[C@H]2N(C=1C(=O)[O-])C(=O)[C@H]2NC(=O)C([NH3+])c1ccccc1
O=C1CCC2=C3[C@H]([C@@H]4CC[C@@](O)(C#CC)[C@]4(C[C@@H]3c3ccc(N(C)C)cc3)C)CCC2=C1
Clc1ccc(cc1)C1(O)CC[NH+](CC1)CCC(C(=O)N(C)C)(c1ccccc1)c1ccccc1
Cl[C@@]12[C@H]([C@@H]3C[C@@H](C)[C@H](C(=O)COC(=O)C(C)(C)C)[C@]3(C[C@@H]1O)C)C[C@H](F)C1=CC(
=O)C=C[C@@]12C
S(=O)([O-])(=NC(=O)[N-]N1CCCCCC1)c1ccc(cc1)C
Oc1cc(ccc1O)CC[NH2+]C(CCc1ccc(O)cc1)C
Clc1cc2c(NC(=O)C(O)N=C2c2ccccc2)cc1
F[C@@H]1C2=CC(=O)CC[C@@]2([C@@H]2[C@H]([C@@H]3C[C@H]4OC(O[C@@]4(C(=O)CO)[C@]3(C[C@@H]2O)C)(C
)C)C1)C
SCC[NH3+]
Clc1cc2N(c3c(Sc2cc1)cccc3)CCC[NH+]1CC[NH+](CC1)CCO
O=C(N)C/1=NC=N\C\1=N/NN(C)C
O[C@H]([C@@H]([NH2+]C)C)c1ccccc1
[NH+](Cc1c2c(ccc1)cccc2)(CC=CC#CC(C)(C)C)C
O=C1C=C2CC[C@@H]3[C@@H]([C@]2(C=C1)C)[C@@H](O)C[C@]1([C@H]3CC[C@]1(O)C(=O)CO)C
S(=O)(=O)(N1CC[NH+](CC1)CC)c1cc(C2=NC(=O)c3n(N2)c(nc3C)CCC)c(OCC)cc1
O1[C@H](C(=C[C@H]2C[C@@H](OC)[C@H](O)CC2)C)[C@H](C)[C@@H](O)CC(=O)[C@@H](C=C(C[C@@H](C[C@H](
OC)[C@H]2O[C@](O)([C@@H](C[C@@H]2OC)C)C(=O)C(=O)N2[C@@H](CCCC2)C1=O)C)C)CC=C
Oc1ccc(cc1)CC[NH2+][C@H]([C@H](O)c1ccc(O)cc1)C
O(C(=O)c1ccc(NCCCC)cc1)CCOCCOCCOCCOCCOCCOCCOCCOCCOC
s1c2S(=O)(=O)C(CC([NH2+]CC)c2cc1S(=O)(=O)N)C
Oc1cc(cc(O)c1)C(O)C[NH2+]C(C)(C)C
O=C(N1CCc2[nH]c(nc2-c2c1cccc2)C)c1ccc(NC(=O)c2ccccc2-c2ccccc2)cc1
ClCOC(=O)[C@@]1(OC(OCC)=O)CC[C@H]2[C@H]3[C@@H]([C@@]4(C(=CC(=O)C=C4)CC3)C)[C@@H](O)C[C@]12C
O(CC(O)CO)c1ccccc1OC
S1c2c(cc(cc2)C(F)(F)F)C(c2c1cccc2)=CCC[NH+]1CC[NH+](CC1)CCO
s1cccc1CC(=Cc1n(Cc2ccc(cc2)C(=O)[O-])c(nc1)CCCC)C(=O)[O-]
Clc1ccc(N\C(=[NH+]\C(=[NH+]\CCCCCC\[NH+]=C(\[NH+]=C(\Nc2ccc(Cl)cc2)/N)/N)\N)\N)cc1
S1C[C@H](O[C@H]1CO)N1C=C(F)C(=NC1=O)N
Cl\C(=C(/c1ccc(OCC[NH+](CC)CC)cc1)\c1ccccc1)\c1ccccc1
O1[C@H]2[C@H](OC[C@@H]2O[N+](=O)[O-])[C@H](O[N+](=O)[O-])C1
ClCC[NH+](CCCl)C
O=C(NC1CC2[NH+](C(C1)CCC2)C)c1nn(c2c1cccc2)C
S(=O)(=O)(Nc1ncccc1)c1ccc(N)cc1
O(CCCC)c1cc(ccc1N)C(OCC[NH+](CC)CC)=O
O1[C@@]2([C@H]([C@H]3[C@H](CC2)[C@@]2(C(=CC(=O)C=C2)CC3)C)CCC1=O)C
O=C1C=C2CCC3C([C@]2(C=C1)C)[C@@H](O)C[C@]1(C3C[C@@H](C)[C@@]1(C(=O)CC)C)C
O(C(=O)C1(N(C(=O)CC)c2ccccc2)CC[NH+](CC1)CCC(OC)=O)C
O1[C@@H](CC[C@@H]1n1c2NC=NC(=O)c2nc1)CO
S1c2c(N(c3c1cccc3)CC1CC[NH+](C1)C)cccc2
Clc1c(Cl)c(OCC(=O)[O-])ccc1C(=O)C(CC)=C
O[C@H]1C[C@@H](O)[C@H](\C=C\[C@@H](O)CCc2ccccc2)[C@H]1C\C=C/CCCC(=O)NCC
s1ccc(C)c1C(=CCC[NH+]1C[C@@H](CCC1)C(=O)[O-])c1sccc1C
O(C(=O)c1ccccc1)[C@H]1CC2[NH+](C(CC2)[C@H]1C(OC)=O)C
O(C)c1cc2c(nccc2[C@H](O)[C@@H]2[NH+]3C[C@@H]([C@H](C2)CC3)C=C)cc1
S(=O)(=O)(N)Cc1noc2c1cccc2
S(=O)(=O)(CCn1c(ncc1[N+](=O)[O-])C)CC
O(CC)c1cc(ccc1C(=O)[O-])CC(=O)N[C@@H](CC(C)C)c1ccccc1N1CCCCC1
[NH+](=C(\[NH+]=C(N)N)/N)/CCc1ccccc1
OCCn1c(ncc1[N+](=O)[O-])C

O=C1C[C@@H](O)[C@H](\C=C\[C@@H](O)CCCCC)[C@H]1C\C=C/CCCC(=O)[O-]
S(=O)(=O)(N1CCCC1)Cc1cc2c([nH]cc2CC[NH+](C)C)cc1
O1[C@H]2[C@H](O[C@@H]3O[C@@H](CC(=O)[C@]13O)C)[C@@H](O)[C@H]([NH2+]C)[C@H](O)[C@@H]2[NH2+]C
O=C1NN=C([C@@H](C1)C)c1ccc(NN=C(C#N)C#N)cc1
ClCC[NH+](Cc1ccccc1)C(COc1ccccc1)C
s1cc(nc1[NH+]=C(N)N)CSCCC(N)=NS(=O)(=O)N
Oc1c2c(ccc1)C([C@@H]1C(C(=O)[C@@]3(O)[C@H]([C@H]([NH+](C)C)C(=O)/C(=C(/[O-
])\N)/C3=O)[C@H]1O)=C2[O-])=C
[NH2+](CCCC12CCC(c3c1cccc3)c1c2cccc1)C
Oc1ccccc1C(=O)[O-]
Oc1ccc(cc1CO)C(O)C[NH2+]CCCCCCOCCCCc1ccccc1
O1c2c(cccc2)C(c2c1cccc2)C(OCC[N+](CC)(CC)C)=O
O(C(=O)N(CCCCCCCCCCN(C(Oc1cc([N+](C)(C)C)ccc1)=O)C)C)c1cc([N+](C)(C)C)ccc1
O1c2c(cccc2)C(=O)C(C(CC)c2ccccc2)=C1[O-]
S1[C@H]2N([C@@H](C(=O)[O-
])C1(C)C)C(=O)[C@H]2NC(=O)[C@H](NC(=O)N1CCN(S(=O)(=O)C)C1=O)c1ccccc1
O(CC(COC(=O)N)c1ccccc1)C(=O)N
O=C(NN)c1ccncc1
O1[C@H](CC)[C@@](O)(C2O[C@@H]([NH2+][C@H]([C@@H]2C)[C@@H](C[C@](O)(C)[C@H](O[C@@H]2O[C@@H](C
[C@H]([NH+](C)C)[C@H]2O)C)[C@@H](C)[C@H](O[C@@H]2O[C@@H](C)[C@H](O)[C@](OC)(C2)C)[C@@H](C)C1
=O)C)COCCOC)C
O(C(=O)C)[C@]1(CC[C@H]2[C@H]3[C@@H]([C@@H]4C(=C/C(=N/O)/CC4)CC3)CC[C@]12CC)C#C
O=C([O-])C1(CCC1)C(=O)[O-]
O=C1C=C2[C@@]([C@@H]3[C@H]([C@@H]4CC[C@](O)(C(=O)CO)[C@]4(C[C@@H]3O)C)C[C@@H]2C)(C=C1)C
O=C(Nc1c(cccc1C)C)C1[NH+](CCCC1)C
Brc1ccc(cc1)C(=O)c1cccc(CC(=O)[O-])c1N
Clc1cc(N)cc(Cl)c1NC1=[NH+]CCN1
O=C1N(CCc2n(c3c(c12)cccc3)C)Cc1nc[nH]c1C
Clc1ccc(cc1)CC1=NN(C2CCC[NH+](CC2)C)C(=O)c2c1cccc2
Fc1ccc(cc1)[C@@H](O)CC[C@@H]1[C@H](N(C1=O)c1ccc(F)cc1)c1ccc(O)cc1
OCCN(CCO)c1nc(N2CCCCC2)c2nc(nc(N3CCCCC3)c2n1)N(CCO)CCO
Fc1c2N(C=C(C(=O)[O-])C(=O)c2cc(F)c1N1CC([NH2+]CC1)C)CC
OC1(CCCC1)C(C(OCC[NH+](C)C)=O)c1ccccc1
O=C([O-])C=C(C=CC=C(C=CC=1C(CCCC=1C)(C)C)C)C
O(C)c1ccc(cc1)CC([NH2+]CC(O)c1cc(NC=O)c(O)cc1)C
O=C1CC[C@@H]2[C@@H]3[C@H]([C@@H]4CC[C@H](OC(=O)CCc5ccccc5)[C@]4(CC3)C)CCC2=C1
O(C(c1ccccc1)c1ccccc1)CC[NH+](C)C
O(C(=O)C(O)(C1CCCC1)c1ccccc1)C1CC[N+](C1)(C)C
O=C1CC[C@H]2[C@H]3[C@H](CC[C@]12C)[C@@]1(C(=CC(=O)C=C1)C(C3)=C)C
o1c(c(nc1CCC(=O)[O-])-c1ccccc1)-c1ccccc1
O(C(=O)CCC(=O)C[NH3+])C
S(c1n(cnc1[N+](=O)[O-])C)c1ncnc2nc[nH]c12
[S-]C1OC(COC(=O)C)C(OC(=O)C)C(OC(=O)C)C1OC(=O)C
O=C([O-])CC1(CCCCC1)C[NH3+]
O1[C@@H](C)[C@@H](O)[C@@H]([NH3+])C[C@@H]1O[C@@H]1c2c(C[C@](O)(C1)C(=O)CO)c(O)c1c(C(=O)c3c(c
ccc3OC)C1=O)c2O
Oc1ccc(cc1CO)C(O)C[NH2+]C(C)(C)C
Clc1cc(Cl)ccc1C(OCc1ccsc1Cl)Cn1ccnc1
S(OCCCCOS(=O)(=O)C)(=O)(=O)C
O=C(c1cc(ccc1)C(C(=O)[O-])C)c1ccccc1
Oc1cc([N+](CC)(C)C)ccc1
O=C1C=C/C(=N/Nc2ccc(cc2)C(=O)NCCC(=O)[O-])/C=C1C(=O)[O-]
S(=O)([O-])(=Nc1noc(c1)C)c1ccc(N)cc1
Clc1cccc(Cl)c1CC(=O)N=C(N)N
O(C(C[N+](C)(C)C)C)C(=O)N
O1[C@H]2[C@H](OC[C@@H]2O)[C@H](O[N+](=O)[O-])C1
O=C1c2c(cccc2)C(=O)C(C)=C1CC=C(CCCC(CCCC(CCCC(C)C)C)C)C
O1Cc2c(c(O)c(C\C=C(\CCC(=O)[O-])/C)c(OC)c2C)C1=O
O1c2c(cc(cc2)C(C)C)C(=O)c2cc(C(=O)[O-])c(nc12)N
Clc1cc(Cl)ccc1[C@]1(O[C@@H](CO1)COc1ccc(N2CCN(CC2)C(=O)C)cc1)Cn1ccnc1
ClC(Cl)C(F)(F)OC
O(C(=O)N)C1(CCCCC1)C#C
S(=O)(=O)(N(CCC)CCC)c1ccc(cc1)C(=O)[O-]
S=C1N=CNc2nc[nH]c12
O=C(NCC[NH+](CC)CC)c1ccc(N)cc1
Oc1ccc(cc1[C@@H](CC[NH+](C(C)C)C(C)C)c1ccccc1)C
[NH+]([C@@H](Cc1ccccc1)C)(CC#C)C
Clc1ccc(cc1)C(=O)c1ccc(OC(C(OC(C)C)=O)(C)C)cc1
O=C/1C=C(C=C\C\1=C\C=C1C=CC(C=C1)=C(N)N)C(N)=N
O=C1NC(=O)CCC1N1C(=O)c2c(cccc2)C1=O
ClCCN(CCCl)c1ccc(cc1)CC([NH3+])C(=O)[O-]

Fc1cc2c(N(C=C(C(=O)[O-])C2=O)C2CC2)c(OC)c1N1CC([NH2+]CC1)C
FC(F)(CCCC)[C@@]1(O[C@H]2[C@H](CC1)[C@H](CCCCCCC(=O)[O-])C(=O)C2)O
OC[C@@H]1CC(n2c3nc(nc(NC4CC4)c3nc2)N)C=C1
O1C(NC(=O)C2CC3C([NH+](C2)C)Cc2c4c3cccc4[nH]c2)(C(C)C)C(=O)N2C(C(CC)(C)C)C(=O)N3C(CCC3)C12O
O=C([O-])C(C)c1ccc(cc1)CC(C)C
O(C(=O)C=1C(C(C(OC)=O)=O)=C(NC=1C)C)c1cc([N+](=O)[O-])ccc1)CC
S1[C@H]2N([C@@H](C(=O)[O-])C1(C)C)C(=O)[C@H]2NC(=O)[C@H]([NH3+])c1ccc(O)cc1
Oc1cc(ccc1O)C(O)C[NH2+]C(C)C
S(=O)([O-])(=NC(=O)NC1CCCCC1)c1ccc(cc1)CCNC(=O)c1ncc(nc1)C
Clc1ccccc1C1=NCC(=O)Nc2c1cc([N+](=O)[O-])cc2
OC1C\C(=C\C=C/2\C3CCC(C(\C=C\C(C(C)C)C)C)C3(CCC\2)C)\C(CC1)C
S1c2c(N(c3c1cccc3)CC1C3CC[NH+](C1)CC3)cccc2
O(C(=O)N[C@@H](C(C)(C)C)C(=O)N[C@H]([C@@H](O)CN(NC(=O)[C@@H](NC(OC)=O)C(C)(C)C)Cc1ccc(cc1)-
c1ncccc1)Cc1ccccc1)C
O(C(c1ccccc1)c1ccccc1)CC[NH+](C)C
O1CC(=CC1=O)[C@H]1CC[C@]2(O)[C@H]3[C@@H](C[C@@H](O)[C@]12C)[C@@]1([C@@H](C[C@@H](O[C@@H]2O[C
@H](C)[C@@H](O[C@@H]4O[C@H](C)[C@@H](O[C@@H]5O[C@H](C)[C@@H](O[C@@H]6O[C@H](CO)[C@@H](O)[C@H
](O)[C@H]6O)[C@@H](O)C5)[C@@H](O)C4)[C@@H](O)C2)CC1)CC3)C
O=C([O-])CCC([NH3+])C=C
O(C(=O)C1(CC[NH+](CC1)CCC(C#N)(c1ccccc1)c1ccccc1)c1ccccc1)CC
O(CCn1c2c(nc1N1CCC[NH+](CC1)C)cccc2)CC
O1C[C@H](Cc2n(cnc2)C)[C@H](CC)C1=O
O1CC(=CC1=O)[C@H]1CC[C@]2(O)[C@H]3[C@@H]([C@]4(CO)[C@@](O)(C[C@@H](O[C@@H]5O[C@@H](C)[C@H](O
)[C@@H](O)[C@H]5O)C[C@H]4O)CC3)[C@H](O)C[C@]12C
O1c2c(C(=O)C[C@H]1c1cc(O)c(OC)cc1)c(O)cc(O)c2
Fc1ccc(cc1)-c1c2c(n(C(C)C)c1\C=C\[C@H](O)C[C@H](O)CC(=O)[O-])cccc2
OCc1cc2CCC(Nc2cc1[N+](=O)[O-])C[NH2+]C(C)C
S(=O)(=O)(N(C)c1nc(-c2ccc(F)cc2)c(\C=C\[C@H](O)C[C@@H](O)CC(=O)[O-])c(n1)C(C)C)C
FC1=CN([C@@H]2O[C@H](C)[C@@H](O)[C@H]2O)C(=O)N=C1NC(OCCCCC)=O
Oc1cc(ccc1O)[C@@H](O)C[NH2+]CCCCc1ccc(O)cc1
Clc1cc2[nH+]c3c(cc(OC)cc3)c(NC(CCC[NH+](CC)CC)C)c2cc1
Clc1cc(Cl)ccc1C(OCc1ccc(Cl)cc1Cl)Cn1ccnc1
S1[C@H]2N(C(C(=O)[O-])=C(C1)COC(=O)N)C(=O)[C@H]2NC(=O)\C(=N\OC)\c1occc1
Ic1cc(cc(I)c1OCC[NH+](CC)CC)C(=O)c1c2c(oc1CCCC)cccc2
Clc1cc2S(=O)(=O)N=C(Nc2cc1)C
O=C(NC(=O)N)Cc1ccccc1
Clc1ccccc1C[N+](CCNC(=O)C(=O)NCC[N+](Cc1ccccc1Cl)(CC)CC)(CC)CC
O(C)c1ccc(cc1)C1C(=O)c2c(cccc2)C1=O
FC(F)(F)c1ccc(cc1NC(=O)[C@H]1CC[C@H]2[C@H]3C(CC[C@]12C)[C@@]1([C@H](NC(=O)C=C1)CC3)C)C(F)(F)
F
Clc1cc(Cl)ccc1C(OCc1ccc(Cl)cc1)Cn1ccnc1
S(=O)(=O)(C[C@](O)(C(=O)Nc1cc(C(F)(F)F)c(cc1)C#N)C)c1ccc(F)cc1
O(C(OCC)=O)C1(CCC2C3C(C4(C(=CC(=O)C=C4)CC3)C)C(O)CC12C)C(=O)COC(=O)CC
O(CC[NH2+]CC(O)COc1c2c3c([nH]c2ccc1)cccc3)c1ccccc1OC
S1[C@H]2N(C(C(=O)[O-])=C(C1)COC(=O)C)C(=O)[C@H]2NC(=O)CSc1ccncc1
O1c2c(cccc2C(OCC[NH+]2CCCCC2)=O)C(=O)C(C)=C1c1ccccc1
S1[C@H]2N(C(C(=O)[O-])=C(C1)\C=C\C)C(=O)[C@H]2NC(=O)[C@H]([NH3+])c1ccc(O)cc1
[NH2+](CCCN1c2c(CCc3c1cccc3)cccc2)C
Clc1cc(Cl)ccc1C(OCc1c2c(sc1)c(Cl)ccc2)Cn1ccnc1
S=C1NC(=O)C(C(CCC)C)(CC=C)C(=O)N1
Fc1cc2c(nc1N1CC(C[NH3+])/C(=N\OC)/C1)N(C=C(C(=O)[O-])C2=O)C1CC1
O[C@H]1C[C@@H](O)[C@H](\C=C\[C@@H](O)CCCCC)[C@H]1C\C=C/CCCC(=O)[O-]
Clc1cc(N)ccc1C(OCC[NH+](CC)CC)=O
S1[C@H]2N([C@@H](C(=O)[O-])C1(C)C)C(=O)[C@H]2\N=C\N1CCCCCC1
Fc1cc2c3N(C=C(C(=O)[O-])C2=O)C(COc3c1N1CC[NH+](CC1)C)C
Clc1cc(Cl)ccc1[C@@]1(O[C@H](CO1)COc1ccc(N2CCN(CC2)c2ccc(N3C=NN(C(CC)C)C3=O)cc2)cc1)Cn1ncnc1
O1[C@H](C[NH3+])[C@@H](O)[C@H](O)[C@@H](O)[C@H]1O[C@H]1[C@H](O)[C@@H](O[C@H]2O[C@H](CO)[C@@H
](O)[C@H]([NH3+])[C@H]2O)[C@H]([NH3+])C[C@@H]1[NH3+]
O=C1NC(=O)NC(=O)C1(CC)c1ccccc1
Fc1ccc(cc1)[C@@]1(OCc2cc(ccc12)C#N)CCC[NH+](C)C
O1[C@@H](C)[C@@H](O)[C@@H]([NH3+])C[C@@H]1O[C@@H]1c2c(C[C@](O)(C1)C(=O)C)c(O)c1c(C(=O)c3c(cc
cc3)C1=O)c2O
Clc1ccc(cc1)C1S(=O)(=O)CCC(=O)N1C
O(C)c1c(OC)cc(cc1OC)C=CC(O[C@@H]1C[C@H]2[C@H](C[C@H]3[NH+](CCc4c5c([nH]c34)cc(OC)cc5)C2)[C@H
](C(OC)=O)[C@H]1OC)=O
O1[C@@H]2[C@]34CC[NH+]([C@H](Cc5c3c1c(O)cc5)[C@]4(O)CCC2=O)CC=C
F[C@@]12[C@H]([C@@H]3CC[C@@](O)(C)[C@]3(C[C@@H]1O)C)CCC1=CC(=O)CC[C@@]12C
S(C[C@@H]1C[C@H]2[C@H]([NH+](C1)CCC)Cc1c3c2cccc3[nH]c1)C
Ic1ccccc1C(CCCCCCCCC(OCC)=O)C
O1[C@@H]2[C@]34CC[NH+]([C@H](Cc5c3c1c(O)cc5)[C@]4(O)CCC2=O)C
O(CC(O)C[NH2+]C(C)C)c1ccc(NC(=O)CCC)cc1C(=O)C

SC[C@H](C(=O)N1CCC[C@H]1C(=O)[O-])C
Brc1[nH]c2c3c1C[C@H]1[NH+](C[C@@H](C=C1c3ccc2)C(=O)N[C@@]1(O[C@]2(O)N([C@@H](CC(C)C)C(=O)N3[
C@H]2CCC3)C1=O)C(C)C)C
ClCCN(N=O)C(=O)NC1CCCCC1
FC(F)(F)c1cc(ccc1)\C(=N/OCCCCC(=O)[O-])\c1cccnc1
Fc1c(N2C[C@H]([NH2+][C@H](C2)C)C)c(F)c2N(C=C(C(=O)[O-])C(=O)c2c1N)C1CC1
O1[C@@H](CC)[C@](O)(C)[C@H](O)[C@H](C)C(=O)[C@@H](C[C@](OC)(C)[C@H](O[C@@H]2O[C@@H](C[C@H]([
NH+](C)C)[C@H]2O)C)[C@@H](C)[C@H](O[C@@H]2O[C@@H](C)[C@H](O)[C@](OC)(C2)C)[C@@H](C)C1=O)C
O(C(=O)C)c1c(C)c(C)c(OCC(O)C[NH2+]C(C)C)cc1C
O=C1N[C@@H]2CC[C@H]3[C@@H]4CC[C@H](C(=O)NC(C)(C)C)[C@]4(CC[C@@H]3[C@]2(C=C1)C)C
n1cn(nc1)Cc1cc(cc(c1)C(C#N)(C)C)C(C#N)(C)C
o1c(ccc1C=NN1CC(=O)NC1=O)-c1ccc([N+](=O)[O-])cc1
O1[C@@]2([C@H](O[C@@H]1CCC)C[C@H]1[C@H]3[C@@H]([C@@]4(C(=CC(=O)C=C4)CC3)C)[C@@H](O)C[C@@]12C
)C(=O)CO
O=C1N(C)C(=O)N(c2nc[nH]c12)C
O([C@H](C(C[C@@H]([NH+](C)C)C)C)(c1ccccc1)c1ccccc1)CC)C(=O)C
FC(F)(F)C(OCF)C(F)(F)F
Clc1c(N2CC[NH+](CC2)CCCCOc2cc3NC(=O)CCc3cc2)cccc1Cl
S1c2c(N(c3c1cccc3)CC(C[NH+](C)C)C)cccc2
o1nc(cc1C)C(=O)NNCc1ccccc1
S(=O)([O-])(=NC(=O)NC1CCCCC1)c1ccc(cc1)CCN1C(=O)C(c2c(cc(OC)cc2)C1=O)(C)C
OC[C@@H](NC(=O)[C@@H]1C=C2[C@H]([NH+](C1)C)Cc1c3c2cccc3[nH]c1)C
Clc1cccc(C)c1NC(=O)c1sc(nc1)Nc1nc(nc(N2CC[NH+](CC2)CCO)c1)C
Clc1cc(Nc2ncnc3c2cc(cc3)-c2oc(cc2)C[NH2+]CCS(=O)(=O)C)ccc1OCc1cc(F)ccc1
O1[C@@]2([C@H](OC1(C)C)C[C@H]1[C@H]3[C@@H]([C@@]4(C(=CC(=O)C=C4)CC3)C)[C@@H](O)C[C@@]12C)C(=
O)CO
O(C)c1ccc(cc1)C[C@H]([NH2+]C[C@H](O)c1cc(NC=O)c(O)cc1)C
S1C[C@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](N(C)C(=O)CCC1)Cc1ccc(O)cc1)[C@H
](CC)C)CCC(=O)N)CC(=O)N)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CC(C)C)C(=O)NCC(=O)N
Clc1cccc(F)c1Nc1ccc(cc1CC(=O)[O-])C
Oc1ccc(nc1CO)C(O)C[NH2+]C(C)(C)C
[BiH]1OC(=O)c2c(O1)cccc2
O(C)c1cc(ccc1OC)CC[NH2+]CC(O)COc1cc(ccc1)C
O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H]([NH3+])C1O
S(=O)(=O)(Nc1ncnc(OC)c1OC)c1ccc(N)cc1
Oc1c2c(ccc1)[C@@](O)([C@@H]1C(C(=O)[C@@]3(O)[C@@H](C1)[C@H]([NH+](C)C)C)C(=O)/C(=C(/[O-
])\NC[NH+]1CCCC1)/C3=O)=C2[O-])C
O=C1N(C)C([O-])=C2N=CN=C2N1C
S(=O)(=O)(N(CC(C)C)C[C@@H](OP(=O)([O-])[O-])[C@@H](NC(O[C@H]1CCOC1)=O)Cc1ccccc1)c1ccc(N)cc1
O1[C@@H](C\C=C\C=C\[C@H](O)[C@@H](C[C@H](CC=O)[C@H](O[C@@H]2O[C@H](C)[C@@H](O[C@@H]3O[C@@H](
C)[C@H](OC(=O)CC(C)C)[C@](O)(C3)C)[C@H]([NH+](C)C)[C@H]2O)[C@@H](OC)[C@H](OC(=O)C)CC1=O)C)C
Clc1cc2NC(N(S(=O)(=O)c2cc1S(=O)(=O)N)C)CSCC(F)(F)F
Clc1cc2NC(NC(=O)c2cc1S(=O)(=O)N)CC
S1[C@H]2N(C(C(=O)[O-])=C(C1)CSc1nnnn1C)C(=O)[C@H]2NC(=O)[C@H](O)c1ccccc1
S1[C@H]2N(C(C(=O)[O-
])=C(C1)CSc1nnnn1C)C(=O)[C@H]2NC(=O)C(NC(=O)N1CCN(CC)C(=O)C1=O)c1ccc(O)cc1
S1C(SC1=C(C(=O)N)C(=O)[O-])C(=O)N[C@@]1(OC)C2SCC(CSc3nnnn3C)=C(N2C1=O)C(=O)[O-]
s1cc(nc1N)/C(=N/OC)/C(=O)N[C@H]1[C@H]2SCC=C(N2C1=O)C(=O)[O-]
O1c2cc(C[C@H]3[N+](CCc4cc(OC)c(OC)c(Oc5ccc(C[C@@H]6[N+](CCc7cc(OC)c1cc67)(C)C)cc5)c34)(C)C)c
cc2OC
O(C(=O)C)[C@@H]1[C@@]2([C@H]([C@H]3[C@H](CC2)[C@@]2([C@H](C[C@H](OC(=O)C)[C@@H]([N+]4(CCCCC4
)C)C2)CC3)C)C[C@@H]1[N+]1(CCCCC1)C)C
O(C(=O)C)[C@@H]1[C@@]2([C@H]([C@H]3[C@H](CC2)[C@@]2([C@H](C[C@H](OC(=O)C)[C@@H]([NH+]4CCCCC4
)C2)CC3)C)C[C@@H]1[N+]1(CCCCC1)C)C
Brc1c2cc(ccc2oc1-c1ccccc1NS(=O)(=O)C(F)(F)F)Cn1c(C(=O)N)c(nc1CC)C1CC1
S1CCSC12C[C@H](N(C2)C(=O)[C@@H]([NH2+][C@@H](CCc1ccccc1)C(OCC)=O)C)C(=O)[O-]
O=C1NC(=O)NC(=O)C1(CCC(C)C)CC
O=C1NC([O-])=NC(=O)C1(C(C)C)CC=C
O=C1NC(=O)NC(=O)C1(CCCC)CC
O=C1N(C)C(=O)NC(=O)C1(C)C=1CCCCC=1
[Li+]
O(C)c1cc2CC[C@H]3[C@@H]4CC[C@@](O)(C#C)[C@]4(CC[C@@H]3c2cc1)C
O(C[C@@H](O)C[NH2+]C(C)(C)C)c1ccccc1C1CCCC1
O1[C@H](C)[C@H](C)[C@H](OC(=O)C)[C@@H](C)C(=O)[C@@]2(OC2)C[C@H](C)[C@H](O[C@@H]2O[C@@H](C[C@
H]([NH+](C)C)[C@H]2OC(=O)C)C)[C@@H](C)[C@H](O[C@@H]2O[C@@H](C)[C@H](OC(=O)C)[C@@H](OC)C2)[C@
@H](C)C1=O
Ic1c(C(=O)NCC(O)CO)c(I)c(N(C(=O)C)CC(O)CO)c(I)c1C(=O)NCC(O)CO
O[C@@H]([C@@H]([NH2+]C)C)c1ccccc1
Oc1c2NC(=O)C=Cc2c(cc1)[C@@H](O)[C@@H]([NH2+]C(C)C)CC
[NH2+](CC#C)[C@@H]1CCc2c1cccc2
[MgH2-]O

S(=O)(=O)(Nc1ncc(OCCOC)cn1)c1ccccc1
F[C@@H]1C2=CC(=O)C=C[C@@]2([C@@H]2[C@H]([C@@H]3C[C@@H](C)[C@](O)(C(=O)CO)[C@]3(C[C@@H]2O)C)C
1)C
O=C([O-])[O-]
O1[C@]2([C@@H]3[C@H]([C@H]4[C@H]5[C@H](CC[C@]24C)[C@]2(CCC(=O)C=C2[C@H]2[C@@H]5C2)C)C3)CCC1=
O
O1CC(=CC1=O)[C@H]1CC[C@]2(O)[C@H]3[C@H](CC[C@]12C)[C@@]1([C@@H](C[C@@H](O[C@@H]2O[C@H](C)[C@
@H](O[C@@H]4O[C@H](C)[C@@H](O[C@@H]5O[C@H](C)[C@@H](O)[C@@H](O)C5)[C@@H](O)C4)[C@@H](O)C2)CC
1)CC3)C
O(C(=O)c1ccccc1O)c1ccccc1C(=O)[O-]
O(C(=O)N(C)C)c1cc([N+](C)(C)C)ccc1
[BiH]1OC(=O)c2c(O1)cccc2
S1c2c(N(c3c1cccc3)C[C@@H](C[NH+](C)C)C)cc(OC)cc2
O1[C@@]2([C@H](OC1C1CCCCC1)C[C@H]1[C@H]3[C@@H]([C@@]4(C(=CC(=O)C=C4)CC3)C)[C@@H](O)C[C@@]12C
)C(=O)COC(=O)C(C)C
O1c2c(cccc2)C(=O)C(C(CC(=O)C)c2ccc([N+](=O)[O-])cc2)=C1[O-]
O=C1CC[C@@]2([C@@H]3[C@H]([C@@H]4CC[C@H](OC(=O)CC)[C@]4(CC3)C)CCC2=C1)C
O1[C@@H](C[NH3+])[C@@H](O)[C@H](O)[C@@H]([NH3+])[C@H]1O[C@H]1[C@@H](O)[C@@H](O[C@@H]1CO)O[C@
H]1[C@H](O[C@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2[NH3+])[C@@H]([NH3+])C[C@@H]([NH3+])[C@@H]1
O
O=C1N(N(C)C(C)=C1N(C)C)c1ccccc1
O(C)c1cc2n[nH]nc2cc1C(=O)NCC1[NH+](CCC1)CC=C
O(C)c1cc(O)c(cc1)C(=O)c1ccccc1
O[C@]1(CC[C@H]2[C@H]3[C@@H]([C@@H]4C(CC3)=CCCC4)CC[C@]12C)CC=C
O(C(C(CC([NH+](C)C)C)C)(c1ccccc1)c1ccccc1)CC)C(=O)C
O[C@H]1C[C@H](O)C\C(=C\C=C/2\[C@@H]3CC[C@H]([C@@H](CCCC(C)C)C)[C@]3(CCC\2)C)\C1=C
O=C1NC(=O)CCC1(CC)c1ccccc1
n1c(N)c(N=Nc2ccccc2)ccc1N
Fc1ccccc1C1=NCC(=O)N(c2c1cc([N+](=O)[O-])cc2)C
Brc1cc2c(NC(=O)CN=C2c2ncccc2)cc1
Clc1ccccc1C1=NCC(=O)N(c2sc(cc12)CC)C
O1CC[NH+](C)C(C)C1c1ccccc1
O(CC(O)C[NH2+]C(C)C)c1ccccc1OCC=C
S(=O)(=O)(Nc1nc(cc(n1)C)C)c1ccc(N)cc1
Clc1cc2c(N(C)C(=O)CN3C2(OC(=CC3=O)C)c2ccccc2)cc1
O1[C@@H](CC(=O)[C@@H](\C=C(\C)/[C@@H](O)[C@@H](OC)C(=O)[C@@H](C[C@@H](\C=C\C=C/C=C(/C)\[C@@H
](OC)C[C@H]2O[C@](O)([C@@H](CC2)C)C(=O)C(=O)N2[C@@H](CCCC2)C1=O)C)C)[C@@H](C[C@H]1C[C@@H](
OC)[C@H](OCCO)CC1)C
[Zn]
S(C(Sc1cc(C(C)(C)C)c(O)c(c1)C(C)(C)C)(C)C)c1cc(C(C)(C)C)c(O)c(c1)C(C)(C)C
O(CC(=O)N[C@H]([C@@H](O)C[C@@H](NC(=O)[C@@H](N1CCCNC1=O)C(C)C)Cc1ccccc1)Cc1ccccc1)c1c(cccc1C
)C
S1[C@H]2N([C@@H](C(OCOC(=O)C(C)(C)C)=O)C1(C)C)C(=O)[C@H]2NC(=O)[C@H]([NH3+])c1ccccc1
S1[C@H]2N(C(C(OCOC(=O)C(C)(C)C)=O)C1(C)C)C(=O)[C@H]2\N=C\N1CCCCCC1
O=C/1C=CC=C\C\1=C/1\N\C(\NN\1c1ccc(cc1)C(=O)[O-])=C\1/C=CC=CC/1=O
O=C1N=C(Nc2n(cnc12)COC(COC(=O)[C@@H]([NH3+])C(C)C)CO)N
Clc1cc2[nH+]ccc(NC(CCC[NH+](CCO)CC)C)c2cc1
O([N+](=O)[O-])C(C(O[N+](=O)[O-])CO[N+](=O)[O-])CO[N+](=O)[O-]
S1c2c(N(c3c1cccc3)CCC[NH+](C)C)cc(cc2)C(=O)C
S1c2c(N(c3c1cccc3)CC([NH+](C)C)C)cc(cc2)C(=O)C
[NH+](CCC(c1ccccc1)c1ncccc1)(C)C
S1c2c(cc(S(=O)(=O)N(C)C)cc2)\C(\c2c1cccc2)=C/CC[NH+]1CC[NH+](CC1)C
Clc1cc\2c(Sc3c(cccc3)/C/2=C/CC[NH+]2CC[NH+](CC2)CCO)cc1
O=C(N)C(CC[N+](C(C)C)(C(C)C)C)(c1ccccc1)c1ccccc1
S(C)[C@H]1O[C@H]([C@H](NC(=O)C2[NH+](C[C@@H](C2)CCC)C)[C@H](O)C)[C@H](O)[C@H](O)[C@H]1O
Clc1cc(c(nc1)-c1ccc(nc1)C)-c1ccc(S(=O)(=O)C)cc1
S(=O)(=O)(CC[NH+](CC)CC)C1C2N(CC1)C(=O)c1nc(oc1)CC(=O)CC(O)\C=C(/C=C\CNC(=O)\C=C/C(C)C(OC2=O
)C(C)C)\C
O=C(Nc1ccccc1)CCCCCCC(=O)N[O-]
O(C(=O)C)[C@H]/1C[C@]2([C@@H](C[C@@H](O)[C@@H]3[C@@]2(CC[C@H]2[C@H](C)[C@H](O)CC[C@@]23C)C)\
C\1=C(/CCC=C(C)C)\C(=O)[O-])C
S(CC=1CO[C@H]2N(C=1C(=O)[O-])C(=O)[C@@]2(OC)NC(=O)C(C(=O)[O-])c1ccc(O)cc1)c1nnnn1C
Oc1cc2CC[C@H]3[C@@H]4C[C@@H](O)[C@H](O)[C@]4(CC[C@@H]3c2cc1)C
S(Oc1cc2CC[C@H]3[C@@H]4CCC(=O)[C@]4(CC[C@@H]3c2cc1)C)(=O)(=O)[O-]
O(C1CCCC1)c1cc2CC[C@H]3[C@@H]4CC[C@@](O)(C#C)[C@]4(CC[C@@H]3c2cc1)C
n1ccn(c1)C(c1ccc(cc1)-c1ccccc1)c1ccccc1
Clc1ccccc1C(O)(CC[NH+](C)C)c1ccccc1
ClC=1C2=CC(=O)[C@H]3[C@H](C3)[C@@]2([C@@H]2[C@H]([C@@H]3CC[C@](O)(C(=O)C)[C@]3(CC2)C)C=1)C
Fc1ccc(cc1)C(CCC[NH+]1CCC2(N(CNC2=O)c2ccccc2)CC1)c1ccc(F)cc1
s1cc(nc1C)\C=C(/C)\[C@H]1NC(=O)C[C@@H](O)C(C)(C)C(=O)[C@@H](C)[C@@H](O)[C@H](CCC[C@]2(O[C@H]
2C1)C)C

Fc1cc2CCC(Oc2cc1)C(O)C[NH2+]CC(O)C1Oc2c(cc(F)cc2)CC1
FC(F)(F)c1cc(NC(=O)c2cc(Nc3nc(ccn3)-c3cccnc3)c(cc2)C)cc(-n2cc(nc2)C)c1
OC12CC3([NH2+]CC(=O)N4CCC[C@H]4C#N)CC(C1)CC(C3)C2
S(C)c1ccc(cc1)C(=O)C=1NC(=O)NC=1C
O(C(=O)C[NH2+][C@@H](C(=O)N1CC[C@H]1C(=O)NCc1ccc(cc1)/C(=N/O)/N)C1CCCCC1)CC
ClC(Cl)=CC1C(C)(C)C1C(OCc1cc(Oc2ccccc2)ccc1)=O
O=C(Nc1cc2c(cc1)C(CCC2(C)C)(C)C)c1ccc(cc1)C(=O)[O-]
Clc1cccc(Cl)c1OC(C)C1=[NH+]CCN1
S(=O)([O-])(=Nc1ncccn1)c1ccc(N)cc1
O=C1N(C)C(=O)CC1(C)c1ccccc1
O=[N+]([O-])[O-]
S(=O)(=O)([O-])c1cc2c(cc1C(C)C)CC[C@H]1[C@@](CCC[C@@]12C)(C(=O)[O-])C
O=C(C(C)C)c1c2n(nc1C(C)C)C=CC=C2
[Cl+]([O-])[O-]
ClC12C(C3CC(C)C(O)(C(=O)CO)C3(CC1O)C)CCC1=CC(=O)C=CC12C
Fc1cccc(F)c1Cn1nnc(c1)C(=O)N
S([C@H]1C[C@H]([NH2+]C1)CNS(=O)(=O)N)C=1[C@@H]([C@H]2N(C=1C(=O)[O-])C(=O)[C@@H]2[C@H](O)C)C
O=C(N(C1CC[NH+](CC1)CCc1ccccc1)c1ccccc1)CC
P(=O)([O-])([O-])C(P(=O)([O-])[O-])[NH2+]C1CCCCCC1
Oc1cc(ccc1O)[C@H](O)[C@@H]([NH3+])C(=O)[O-]
Clc1cc(Cl)ccc1Cn1nc(c2c1cccc2)C(=O)[O-]
S(=O)(=O)(NCCC1[NH+](CCC1)C)c1cc(C2=NC(=O)c3n(nc(c3N2)CCC)C)c(OCCC)cc1
o1cccc1CNC(=O)c1ccccc1N(C(=O)COc1ccccc1)C

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O=C1N(CC(C1)c1ccccc1)CC(=O)N1[C@@H]2[C@H](CCC1)C[NH+](CC2)CCc1ccccc1
S(CC(=O)N1CCC([NH+]2CCC(CC2)C(=O)NCCc2ccccc2)CC1)C
o1nc(cc1COc1ccc(cc1)C(=O)C)C(=O)N1CCCC1
S(=O)(=O)(C)c1ncc(n1CCCOC)C[NH+]1CC(OCc2ncccc2)CCC1
Fc1ccccc1C[NH+]1CCC(CC1)CN(CC1OCCC1)C(=O)CCn1nnnc1
s1c(ccc1C)-c1cc(OCC2CCC[NH+](C2)C)c2OCCN(Cc2c1)C(=O)C1CCC1
O(C)c1cccc(C[NH+]2CC([NH+](CC2)Cc2ccccc2)CCO)c1O
Fc1cc(F)ccc1\C=C\C(=O)N1CCC2(CC2C(=O)NC2CCN(CC2)C(OCC)=O)CC1
Oc1cc(ccc1)C[NH+]1CCC(CC1)C1(NC(=O)N(CC#CC)C1=O)CCc1ccccc1
O=C1N(CC(CC1)C(=O)NCCCc1cccnc1)C1CCCCC1
O(CCNC(=O)c1cc2c(nccc2)cc1)c1cccnc1
o1c(ccc1C[NH+]1CC(CCC1)c1[nH]ncc1-c1ccc(cc1)C)CC
FC(F)(F)C(NC(=O)c1cnn(c1C)-c1nc2-c3c(CCCc2cn1)cccc3)c1cccnc1
O(C)c1nc(OC)ccc1C(=O)N1CCc2n(CC1)cnn2
Fc1cc(ccc1)CC[NH+]1CC(CCC1)C[NH+](Cc1ccc(NC(=O)C)cc1)CC
s1cc(c2c1cccc2)-c1cc(OCC)c2OCCN(Cc2c1)C(=O)c1occc1
O(C)c1ccc(cc1)CN1C(CC)=C(C(=O)N2CCN(CC2)c2ncccc2)C(=O)C=C1C
s1cc2c(CCCC2)c1C(=O)N1CCC2(CC2C(=O)N2CC[NH+](CC2)Cc2cc(F)ccc2)CC1
Clc1ccccc1C[NH+]1CCc2n(CC1)c(nn2)CNC(=O)c1cc(oc1C)C
o1nc(nc1C[NH+]1CC[NH+](CC1)Cc1cc2OCOc2cc1)-c1ccccc1
Fc1ccc(OC)cc1C[NH+]1Cc2cc(ccc2OCC1)C[NH+]1CCC(Oc2cccnc2)CC1
Fc1cc(ccc1)-c1nc(nnc1)NCCC=1CCCCC=1
s1c(cnc1N(C)C)C[NH+](CC1CCC[NH+](C1)CCc1cc(F)ccc1)CC
O=C(NC(C(C)(C)C)Cn1ccnc1)c1nnn(c1)C\C=C\c1ccccc1
O1C(CCC12CCN(CC2)C(=O)C1CC1)CNC(=O)c1ccc(cc1)C=C
S(=O)(=O)(Nc1cc(cc(c1)C(OC)=O)CNC(=O)Cc1[nH]nc(n1)C)c1ccc(F)cc1
o1c(nnc1CCC(=O)N(Cc1ccccc1)CCc1ccccc1)-c1noc(c1)C
O=C(N1CCc2c(C1)cccc2)c1nn(c2c1CC([NH2+]CC=C)CC2)C
o1c(ccc1C)C[NH+]1CC([NH+](CC1)C1CCCC1)CCO
o1cccc1CNC(=O)C1=C2N(CC[NH+](CC2)Cc2cc(OC)c(OC)cc2)C(=O)C=C1OC
s1cc(cc1C(=O)C)C(=O)N1CC(CCC1)C(=O)c1cc2c(cc(OC)cc2)cc1
O=C1N(CC[NH+](C)C)C(=O)NC1(CCC(C)C)C1CCN(CC1)C(=O)c1[nH]c2c(c1)cccc2
ClC1=NN(CC(=O)N(CC2CC[NH+](CC2)C2CCCC2)CC2OCCC2)C(=O)C=C1
[NH+](CC1CC[NH+](CC1)Cc1ccccc1C)(Cc1cccnc1)CCC
s1c(ccc1C[NH+]1CCC(CC1)C(=O)Nc1ccc(cc1)-c1cc(ccc1)C)C#CCO
Fc1ccc(OCc2occ(n2)C(=O)NC(Cc2nccnc2)C)cc1
s1cccc1\C=C\C(=O)NCC1Oc2c(C1)cccc2-c1ccc(S(=O)(=O)C)cc1
s1cc(nc1C)C(=O)N1[C@H]2[C@H](CCC1)CN(CC2)C(=O)Cc1cc(OC)ccc1
Clc1cc(ccc1)-c1oc(C)c(n1)C[NH+]1CC[NH+](CC1)Cc1cccnc1
O1CCC(CC1)C(=O)N(CC1CC[NH+](CC1)C1CCCC1)Cc1cccnc1
s1cc(cc1)CC([NH2+]C1CCN(CC1)c1nc(c2c(n1)cc(OC)cc2)C)C
Fc1ccc(N2CCN(CC2)C(=O)C2=CN3CCc4c3c(ccc4)C2=O)cc1
O1CC[NH+](Cc2cc(ccc12)C[NH+]1CCC(O)(CC1)c1cccnc1)Cc1cc(OC)cc(OC)c1
s1c2c(cc1C(=O)N1CC([NH+]3CCN(CC3)c3ccccc3)CCC1)cccc2
O1C(CCC12CC[NH+](CC2)Cc1ccc(cc1)C(C)C)CNC(=O)c1nn(cc1)C
FC(F)(F)c1cc(N2CC[NH+](CC2)[C@@H]2CC[NH+](C[C@@H]2CCC(=O)NCc2ccc(OC)cc2)Cc2ccccc2)ccc1
Fc1cc2N(CC[NH+]3CCCCC3)C(=O)C(=Cc2cc1)C[NH2+]Cc1ccc(OC)cc1
s1cc(cc1)[C@H]1[NH+]2[C@]3([C@@H](C1)CN(Cc1cc(OC)ccc1)C3=O)CCC2
O(CC)c1ccccc1C[NH+]1CC[NH+](CC1CCO)Cc1cc(OC)ccc1OC
Clc1cc2C=C(COc2cc1)CNc1nn(nn1)CC
S(C)c1nnc(n1-c1ccc(OC)cc1)CCNC(=O)c1ccoc1
s1cc(cc1)CNC(=O)CCc1oc(nn1)CCc1ccccc1
o1c(ccc1COC)C(=O)N1CCC(CC1)C(N(C(=O)Cn1nccc1)C)Cc1ccccc1C
Clc1ccc(cc1)C1(CC1)C(=O)N(Cc1cc2c(nc1N(C)C)c(OC)ccc2OC)CCCN1CCCC1=O
O=C(NC(C)c1cnn(c1C)-c1c2c(ccc1)cccc2)CCn1nnnc1
S1CCN(CC1)C(=O)C1=C2N(CC[NH+](CC2)Cc2n3C=CSc3nc2C)C(=O)C=C1OC
s1cccc1C[NH+]1C[C@H](n2nnc(c2)C(OC)=O)C[C@H]1C(=O)NCCc1ccc(F)cc1
Fc1cc(OC)c(cc1)C[NH+]1CCC(n2nccc2NC(=O)c2cccnc2)CC1
O=C1N([C@@H]2[C@H](CC1)C[NH+](CC2)Cc1cc(ccc1)C)CCCC
O(C(=O)C1(CCN(CC1)C(=O)c1cccnc1C)CCCc1ccccc1)CC
s1cc(nc1C[NH+]1CCc2n(CC1)c(nn2)CCc1ccccc1)-c1ccccc1
o1nc(nc1-c1ccccc1N1CCC(=O)NC1=O)C(C)(C)C
S1C=C(n2cc(nc12)-c1ccc(cc1)C)C(=O)N1CCCCCCC1
O(C)c1cc(ccc1OC)C(=O)N(Cc1ccc(OCc2ncccc2)cc1)[C@H]1CCCCNC1=O
s1c2CC([NH2+]Cc3cc(ccc3)C)CCc2c2c1N=CN(CC[NH+](C)C)C2=O
O(C(=O)c1n(c2ncc(NC3CCN(CC3)C(=O)C)cc2c1NC(=O)COC)C)C
Fc1ccc(cc1)-c1nn(cc1C[NH+](C)C1CCOCC1)-c1ccc(cc1)C

O(C)c1c(cc(cc1C)C(=O)C1CCCN(C1)C(=O)c1cc(-n2nccc2)ccc1)C
S(CC(=O)NCc1nc(oc1C)-c1ccccc1NC(=O)C1CCC1)c1nccccc1
S(CCOc1ccccc1)c1nnc(n1-c1cc(ccc1)C(F)(F)F)CNC(=O)C(C)C
s1c2CC[NH+](Cc2cc1)Cc1cc(OC)c(OCC(O)C[NH+](CC)CC)cc1
Clc1cc2[nH]c(nc2cc1)CNC(=O)C1=CN(C=C(C(=O)NCC2CCCCC2)C1=O)C1CC1
Clc1ccccc1CNC(=O)C1=CC=C(NC1=O)C[NH+](CC(O)c1ccccc1)C
s1cccc1C(=O)NCC1CCC[NH+](C1)Cc1[nH]nc(c1)C
O=C1N(CCC[NH+](C)C)C(=O)NC1(Cc1ccccc1C)C1CCN(CC1)C(=O)c1ccccc1C
o1nc(C)c(CCC(=O)N2Cc3c(n(nc3C(OCC)=O)CC(C)C)CC2)c1C
O(C)c1ccccc1C[NH+]1CCC(CC1)C[NH+](Cc1nccn1C)CC(C)C
O1CCC(NC(=O)C2CCN(CC2)c2nc(nc3c2CCC3)-c2ccccc2)CC1(C)C
O1CCC(CC1)CN1CC(OCc2nccccc2)C[NH+](CC1=O)C(Cc1ccccc1OC)C
O(C)c1ccccc1CCNC(=O)[C@H]1[NH+](C[C@@H](n2nnnc2)C1)Cc1ccc(OCc2ccccc2)cc1
S(=O)(=O)(N1CCCC1)c1cc(cc(NCc2[nH]cnc2C)c1)C(=O)NCc1ccc(OC)cc1
O1c2cc(ccc2OC1)C(CC(=O)NCc1[nH]c(nn1)C)c1ccccc1
O(Cc1nnn(c1)CC1CCN(CC1)c1nc(NC)ccn1)C
[NH3+]CCn1c2c(cc1C)cccc2
S(C(CC([NH+]1CCC(CC1)CCC(=O)NC1CC1)C)(C)C)C
O=C1N(Cc2cccnc2)C(=O)CC1(CC(=O)N1CCN(CC1)c1ccccc1)c1ccccc1
Fc1cc(F)ccc1Cc1nc(on1)-c1ocnc1C
O(C)c1cc(ccc1)CC(=O)NC1CCC[NH+](C1)CC1CCCCC1
[NH2+](C1CC[NH+](CC1)CC)C1CCCc2n(ncc12)-c1cc(C)c(cc1)C
O=C1N(CCc2ccccc2)C(=O)N(C)C12CC[NH+](CC2)Cc1cccnc1
[nH]1c2c(nc1C(C)c1ccccc1)n(nc2C(C)C)C
Fc1cc(ccc1F)CN1CCCC(O)(C[NH+]2CC[NH+](CC2)C(C)C)C1=O
S(CC(=O)N[C@@H]1c2c(cccc2)C2(CC[NH+](CC2)Cc2cc(OC)c3OCOc3c2)[C@H]1OC)C
o1nc(cc1CC1(O)CC[NH+](CC1)CC=C(C)C)-c1ccccc1
Fc1cc2cc([nH]c2cc1)C(=O)N1CCC(=O)N(CC1)Cc1cc(OC)ccc1
o1cccc1\C=C\C[NH+]1Cc2cc(ccc2OCC1)C[NH+]1CCC(O)CC1
O1CC[NH+](CC1)CCCN1CC(CCC1=O)C(=O)N1CCC(CC1)C(=O)c1ccccc1
O(C)c1ccccc1CC[NH+]1CCC(CC1)CN(C(=O)c1ncccc1)C
O(CC)c1ccc(cc1)C[NH+](CC1CC[NH+](CC1)C1CCCC1)Cc1cccnc1
Clc1ccc(cc1)CCN1CC(CCC1=O)C(=O)NC(CC)CC
O1c2cc(ccc2OC1)-c1n[nH]cc1C[NH+]1CCc2nc[nH]c2C1c1ncccc1
O(C)c1cc(ccc1)-c1nn(cc1C[NH+]1CCC([NH+]2CCCC2)CC1)-c1ccccc1
[NH2+](CC(C)C)C1CCCc2n(ncc12)-c1ncccc1
O(C)c1cc(cc(OC)c1)C[NH+]1CCNC(=O)C1CC(=O)NCC1CC1
Clc1cc(C)c(OC(C(=O)N2[C@@H]3[C@H](CCC2)CN(CC3)C(=O)C)C)cc1
S1CCN(CC1)c1nc2nonc2nc1N1CCC([NH+]2CCCC2)CC1
O1c2cc(ccc2OC1)C(CC(=O)NCC(C)=C)c1ccccc1
s1cc(nc1C(=O)N(Cc1cn(nc1)C)C(C)C)C(C)C
s1cccc1C[NH+]1CC[NH+](CC1CCO)Cc1ccc(Oc2ncccn2)cc1
O=Cc1cc2C3c4c(C(c2cc1)c1c3cccc1)cccc4
BrC=1C(Oc2c(cccc2)C=1[O-])=O
O(C)c1ccc(cc1)C(=O)NC(Cc1c2c([nH]c1)cccc2)C
O(C)c1ccc(OC)cc1N\N=C\1/CCCNC/1=O
Brc1c2oc(C(OCC[NH+](CC)CC)=O)c(c2cc(Br)c1OC)C
O(C)c1cc(N(N=O)C)ccc1
Clc1ccccc1N1C(=O)C(=O)N(c2cc3c(cc2)cccc3)C1=O
O=C(Nc1ccccc1)c1ccccc1NC(=O)C[NH+](CC)CC
Oc1ccccc1\C=N\NC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Ic1ccccc1C(=O)Nc1ccccc1C#N
O=C(N1C=Cc2c(cccc2)C1c1c2c([nH]c1)cccc2)C
Clc1ccc(cc1)C1(O)CC[NH+](CC1)Cc1onc(n1)-c1nccnc1
O(Cc1ccccc1)c1ccc(cc1OC)C(O)C[N+](=O)[O-]
Clc1cc([N+](=O)[O-])ccc1N1CCCC1
Fc1ccc(cc1)C(=O)NCCc1ccc(OC)cc1
O=C1Nc2c(ccc3c2cccc3)C(C1)c1ccc([N+](=O)[O-])cc1
S(=O)(=O)(CC1CC1)c1ncc(n1CC1CCCCC1)C[NH+]1CCC[C@H]1C(=O)N
ClC(Cl)(Cl)C(NC(=O)CCC)NC(=S)Nc1ccccc1OC
S(C(F)(F)F)c1ccc(NC(=O)\C(=C\c2ccc(OC)cc2)\C#N)cc1
S1CC(=O)N(N2C(=O)C3C(C4CC3C=C4)C2=O)C1=S
O=[N+]([O-])c1c2nc(-n3nc(cc3C)C)ccc2ccc1
O=C1N(CC2N(CCc3c2cccc3)C(=O)N(CC)CC)C(=O)c2c1cccc2
O1CC[NH+](CC1)Cc1nnnn1CCC(=O)N(CC1CCC[NH+](C1)CC)C
s1cc(cc1)CN1C(=O)c2c(cccc2N2CC[NH+](CC2)Cc2c(F)cccc2F)C1=O
o1c(ccc1COC)C[NH+]1CCC(Oc2cc(OC)ccc2C(=O)N2CCCC2)CC1
S(=O)(=O)(N1CCOCC1)c1cc(ccc1)C(=O)Nc1cc(O)ccc1
Oc1cc(ccc1O)-c1nc2c(c3c1CCC3)c1c(cc2)cccc1
S1\C(=C\c2ccc(OC)cc2OC)\C(=O)N(CC(=O)[O-])C1=S
Oc1ccc(cc1)C(=O)NNC(=O)CCC(=O)[O-]

O1C2(C3C(C1c1ccc(cc1)C)C(=O)N(C1CCCCC1)C3=O)C(=O)c1c(cccc1)C2=O
s1cccc1C1N(c2c(N1C)cccc2)C
Brc1cc(cnc1)C(=O)N\N=C/c1c2c(ccc1O)cccc2
Brc1cc(cnc1)C(=O)N\N=C\c1cc([N+](=O)[O-])c(O)c(OC)c1
Brc1cc(Br)cc(CNC(=O)c2ccccc2Cl)c1OC(=O)C
FC(F)(F)C(NC(OC(C(C)(C)C)(C)C)=O)C(F)(F)F
S(CCOC(=O)C=1C(NC(=O)NC=1C)c1ccc(OC)cc1)c1ccccc1
o1c2c(nc1-c1cc(N)c(cc1)C)cc(cc2)C
Clc1cc(Cl)ccc1OCC(=O)N1CCCC1
o1cccc1C[NH+]1CCC[NH+](CC1)C
Clc1ccccc1C(Oc1cc2OC(=O)C=C(c2cc1)C)=O
Clc1ccccc1N1CC[NH+](CC1)Cc1ccccc1C(F)(F)F
s1c2CC([NH2+]CCCOC(C)C)CCc2c2c1N=CN(CC(C)C)C2=O
O(CC)c1ccccc1N1CC[NH+](CC1)Cc1cc([N+](=O)[O-])c(O)c(OC)c1
Brc1ccc(\N=C\c2cc([N+](=O)[O-])ccc2Cl)cc1
O1C(=CC=2OC(N)=C(C#N)C(C=2C1=O)c1cc(C)c(OC)cc1)C
Clc1ccccc1NC(=O)c1cc(NC(=O)C(c2ccccc2)c2ccccc2)ccc1
Fc1cccc(F)c1CNc1ncc(cc1)C(=O)NCc1nc(on1)C(C)C
S=C(N)N1NC(=CC1=O)c1ccccc1
O(C)c1cc(OC)ccc1C1Nc2c(NC3=C1C(=O)CC(C3)(C)C)cccc2
Fc1ccccc1C(O\N=C(/N)\c1cc([N+](=O)[O-])ccc1)=O
Fc1ccc(cc1)CN1CCCC(O)(C[NH+](Cc2onc(c2)C)C)C1=O
Clc1cc([N+](=O)[O-])ccc1C(=O)NCC#N
Ic1ccc(NC(NC(=O)c2sccc2)C(Cl)(Cl)Cl)cc1
P(OCCCC)(OCCCC)(=O)CC(=O)N
Clc1cc2OCOc2cc1\C=C/1\SC(NC\1=O)=N
O=C\1N(c2ccccc2C)C(=O)NC(=O)/C/1=C/NCCCn1ccnc1
[NH+]1(CCN(CC1)c1ncccc1)CCC(C)c1ccccc1
Fc1ccccc1N1CC[NH+](CC1)Cc1ccc(OCCCCCC)cc1
o1nc(nc1C[NH+]1CCCCC1c1ncccc1)-c1ccc(OC)c(OC)c1OC
Clc1ccc(N=Nc2cc(\C=N\c3c4c(ccc3)cccc4)c(O)cc2)cc1
o1c(ccc1[N+](=O)[O-])\C=N\NC(=O)c1ccoc1C
Oc1ccc(cc1)C[NH+]1Cc2c(n(nc2C(=O)NCc2ncccc2)CCc2ccccc2)CC1
FC(F)Oc1ccccc1C(=O)Nc1ccc(NC(=O)C)cc1
O(CC)c1ccc(cc1)C(=O)NC1CC1
Fc1cc2nc(N3CCN(CC3)c3ccccc3)cc(c2cc1)C
o1cccc1C[NH2+]CCc1cc(OC)c(OC)cc1
Fc1ccc(OC)cc1C[NH+]1CC2(CCC1)CCN(C2)C(=O)c1[nH]c(cc1C)C
Clc1ccccc1C(=O)Nc1sc2c(CCCCC2)c1C(=O)N1CCOCC1
Fc1ccccc1CN1CCCC(O)(C[NH2+]CC(C)C)C1=O
S1\C(=C\C=C\c2ccccc2)\C(=O)N(C)C1=S
Brc1cc(NS(=O)(=O)c2cc(OC)c(OC)cc2)ccc1
S(=O)(=O)(N(CC(=O)Nc1cccnc1)c1cc(cc(c1)C)C)c1cc(OC)c(OC)cc1
S(=O)(=O)(N\N=C\c1c2c(ccc1OC)cccc2)c1ccccc1
Oc1ccc(cc1[N+](=O)[O-])C1NC(=O)NC(C)=C1C(OCCC)=O
O1c2cc(ccc2OC1)C1C2=C(NC(C)=C1C(OCCOC)=O)CC(CC2=O)(C)C
S(CC(=O)NCCc1cc(OC)c(OC)cc1)c1nnnn1-c1ccccc1
s1c(ccc1C)C1C2=C(OC(N)=C1C#N)CC(CC2=O)(C)C
[nH]1nc(-c2ccccc2)c(c1)\C=N\Nc1nc(nc(n1)Nc1cccc(C)c1C)N1CCC(CC1)C
s1cc(cc1)C[NH+](Cc1n(CC(C)C)c(S(=O)(=O)Cc2ccccc2)nc1)C
O=C(Nc1cc(cc(c1)C)C)C(=O)NCCCn1ccnc1
O(C(=O)Cn1nc(C)c([N+](=O)[O-])c1C)CC
s1c2c(CC(OC2)(C)C)c2c1N=C(SCC)N(CC)C2=O
O(C)c1cc(C2CC([O-])=C3C(=CC(CC3=O)(C)C)C2(C#N)C#N)c([N+](=O)[O-])cc1OC
s1c(ccc1C)-c1nc2c(cccc2)c(c1)C(=O)Nc1cc(C)c(cc1)C
Clc1sc(cc1)-c1nc2c(cccc2)c(c1)C(=O)NCCc1ccc(OC)cc1
s1c2c(CCCCCC2)c(C(OC)=O)c1NC(=O)c1ccccc1F
Clc1cc(ccc1Cl)-c1nc(sc1)NC(=O)c1cccnc1
s1c2c(CCCCCC2)c(C(OCC)=O)c1NC(=O)c1ccccc1[N+](=O)[O-]
s1c(C)c(CC)c(C(OC)=O)c1NC(=O)C1CC1
Brc1cc(F)c(NC(=O)c2cc(nc3c2cccc3)-c2cc(Br)ccc2)cc1
O=C1NC(=O)N(c2nc(n(c12)CCC(C)C)N1CCCCC1)C
Clc1cc(Cl)ccc1\C=C\1/N(C)C(NC/1=O)=N
S1SC2=C(c3c(N(C(=O)COc4sc5c(n4)cccc5)C2(C)C)cccc3)C1=S
Clc1ccc(cc1)C1CC(=O)C2=C(NC(C)=C(C(OCCOC)=O)C2c2cc(F)ccc2)C1
Clc1ccccc1CSCCNC(=O)\C=C\c1ccc(OC)cc1
O=C(CC1=NC(Cc2c1cccc2)(C)C)C
O(C(=O)c1ccc(NC(=O)CC(c2ccccc2)c2ccccc2)cc1)C
O=C/1N(c2c(cccc2)\C\1=N\NC(=O)c1cccnc1)CC(OCC)=O
O=C(c1cc(NC(=O)c2cc([N+](=O)[O-])c(cc2)C)ccc1)c1ccccc1
o1nc(-c2ccccc2)c(C(=O)NCc2cccnc2)c1C

O(C)c1cc(OC)ccc1\C=N\n1c(nnc1C)C
Fc1ccc(cc1)C=NN1CCN(CC1)c1ncccc1
Oc1c(cccc1\C=N\NC(=O)c1[nH]nc(c1)C1CC1)CC=C
Brc1cc(ccc1N(C)C)\C=C\1/C(=NN(C/1=O)c1ccccc1)C
O1CCCC1COC(=O)C=1C(C2=C(NC=1C)CC(CC2=O)(C)C)c1cc(OCc2ccccc2)ccc1
Fc1cc(ccc1)-c1[nH]c2c(n1)cccc2
S(CC#C)c1nc(cc(C)c1C#N)C
O(C)c1cc(OC)ccc1\C=C/1\C(=O)N(c2cc(ccc2)C)C(=O)NC\1=O
Clc1ccc(cc1)C1(CCC1)C(=O)N1CCC2(CC2C(=O)Nc2cc(F)ccc2)CC1
Clc1ccc(-n2c(C)c(cc2C)\C=C(\C(=O)N)/C#N)cc1
S(=O)(=O)(NC)c1cc(cc(NCC(C)C)c1)C(=O)Nc1cc2CCCc2cc1
Clc1ccc(cc1NC(=O)COc1ccccc1)-c1sc2c(n1)cccc2
Brc1ccc(OCC(=O)Nc2cc(NC(=O)c3ccc(Cl)cc3Cl)ccc2)cc1
Fc1ccc(NC(=O)\C(=C\c2cc(n(c2C)C2CCCCC2)C)\C#N)cc1
S(=O)(=O)(N(CC(=O)Nc1cc(cc(c1)C)C)c1ccccc1)C
S([C@@H]1C[C@H]([NH+](C1)C\C(=C\C)\C)C(=O)NCc1ccccc1OC)c1[nH]c2c(n1)cccc2
s1c2c(CCCC2)c(C(OCC)=O)c1-n1c(C)c(cc1C)\C=C(\C(=O)Nc1ccc(F)cc1)/C#N
OCc1nnn(c1)CC1CC[NH+](CC1)C1CCN(C1)c1ccccc1
S1\C(=C/c2oc(cc2)-c2cc([N+](=O)[O-])ccc2C)\C(=O)N(c2ccc(OC)cc2)C1=S
S(=O)(=O)(N(CCc1ccccc1)CC(=O)Nc1ccc(F)cc1)c1cc(OC)c(OC)cc1
Clc1ccc(NC(=O)\C(=C/c2occc2)\C#N)cc1
O1CCOc2c1cc(cc2)C(=O)N1CC(Nc2ccc(cc2)C(C)C)CCC1
Clc1cccc(NC(=O)\C(=C\c2oc(cc2)-c2cc(C(=O)[O-])c(Cl)cc2)\C#N)c1C
Clc1cc(ccc1)C(=O)NC(COC)C
O(CC)c1cc(cc([N+](=O)[O-])c1O)\C=C\1/C(=O)N(c2cc(ccc2)C)C(=O)NC/1=O
O(C)c1ccc(cc1)C1N(CCCC(=O)[O-])C(=O)C([O-])=C1C(=O)c1ccccc1
Clc1cc(C)c(cc1)C(=O)C1CCC[NH+](C1)Cc1sc(nc1)C
Clc1ccc(Cl)cc1OCC12OC3(C(C1)CN(CC=C)C3=O)C=C2
O(C)c1cc2c(n(C)c(C)c2\C=C\C2=Nc3c(cccc3)C(=O)N2C)cc1
Clc1c(cccc1Cl)Cc1sc(nc1)N1C(=O)c2c(cccc2)C1=O
O=C(N1CCCC1)C(=O)NC1CCCC1
O(CC)c1ccc(NC(=O)\C(=C/c2c3c(n(c2)CC#C)cccc3)\C#N)cc1
o1c2c(nc1-c1ccc(OCC)cc1)cc(NC(=O)c1cccc([N+](=O)[O-])c1C)cc2
S(=O)(=O)(N)c1ccc(NC(=O)Cc2ccccc2OC)cc1
O(C)c1cc(ccc1OC)CCNC(=O)c1cc([N+](=O)[O-])c(cc1)C
Clc1cc(NC(=O)C2=Cc3c(OC2=O)c(ccc3)CC=C)ccc1C
s1cc(nc1NC(=O)\C=C\c1cc([N+](=O)[O-])ccc1)C
O(CC(=O)N1CC[NH+](CC1)Cc1ccccc1C)c1cc(ccc1)C
Brc1ccc(OCC(=O)NCC=C)cc1
O(C)c1ccc(cc1)CC[NH2+]C1CC(=O)N(C1=O)c1ccc(cc1)C(OCC)=O
O=C1N(CC(CC1)C(=O)NCc1[nH]c2c(c1)cccc2)CC1CCCCC1
Brc1ccc(N2C(=O)\C(=C\c3cc(O)ccc3)\C(=O)NC2=O)cc1C
S(Cc1ccc([N+](=O)[O-])cc1)c1nnc(n1-c1ccccc1)C1Oc2c(OC1)cccc2
Clc1ccc(cc1)C1(O)N(N=C(C1)C)C(=O)c1ccc([N+](=O)[O-])cc1
Clc1ccc(cc1)\C=C(\NC(=O)c1occc1)/C(=O)N1CCOCC1
O1c2c(ccc(OCC=C)c2)C(C)=C(CC)C1=O
O(C)c1ccc(cc1)Cc1nn2c(NC(=CC2=O)c2ccc([N+](=O)[O-])cc2)c1-c1ccccc1
o1c(nnc1COc1ccc(cc1)C(C)(C)C)-c1ccccc1
o1c2c(nc1-c1cc(NC(=O)COc3ccc([N+](=O)[O-])cc3)ccc1)cccc2
O1c2c(cc([N+](=O)[O-])c(O)c2C)C(=CC1=O)C
O=C(CC(=O)NC1C2CC3CC1CC(C2)C3)C
Clc1cc(ccc1)CCNC(=O)c1cccnc1
Clc1c(cc(OCC(O\N=C(/N)\c2cccnc2)=O)cc1C)C
Clc1cc(NC(=O)NCC(C)C)ccc1
Clc1cc(ccc1)C1CC(=O)C=C(Nc2ccccc2)C1
Clc1cc(ccc1)C(=O)NCc1cc(cc(NS(=O)(=O)c2sccc2)c1)C(OC)=O
s1cc(nc1C([NH+](Cc1nc(oc1C)-c1cc(C)c(OC)cc1)C)C)C
Fc1cc(ccc1)-c1nn2c(N=C(C=C2C)C)c1
S(=O)(=O)(Nc1ncccn1)c1ccc(NC(=O)\C=C\c2cc(OC)c(OCCC)cc2)cc1
Brc1c(OC)c(OC)c(OC)cc1C(=O)Nc1c(cccc1C(C)C)C(C)C
O(CC(=O)Nc1cc(ccc1)C(OCCCC)=O)c1cccc(C)c1C
S(=O)(=O)(N(CC(=O)Nc1cc(C)c(cc1)C)c1cc(OC)ccc1)c1ccc(cc1)C
S(C)c1cc(OC)c(cc1)C(=O)NCc1ccccc1
ClC(Cl)(Cl)C(=O)Nc1ccc(OC)cc1OC
Clc1cc(N(S(=O)(=O)c2ccccc2)CC(=O)Nc2cc(ccc2C)C)ccc1Cl
S(C1CC[NH+](CC1)Cc1nc(oc1C)-c1cccc(OC)c1OC)c1ccc(F)cc1
S(=O)(=O)(N(C)C)N1CCC(CC1)C(OCC)=O
Clc1ccc(SCC(=O)NCCCOC)cc1
s1c(ccc1C)CCNC(=O)c1noc(c1)C[NH+]1CCC(O)CC1
O(C)c1cc(ccc1)-c1nc(ncc1)-n1ncc(C(=O)N2CCN(CC2)C=O)c1C1CC1
Brc1ccc(cc1)C(=O)NC(=S)Nc1c(cccc1C)C

o1c2c(nc1-c1cc(NC(=O)C(C)(c3ccccc3)c3ccccc3)ccc1O)cccc2
Fc1ccc([N+](=O)[O-])cc1NC(=O)COc1ccc(cc1)C(C)(C)C
O=C1C(=CN(C=C1C(=O)NC)C1CCCCC1)C(=O)NCCc1ccccc1
S=C1NC(C(C(OCC)=O)=C(N1)C)c1cc2c(cc1)cccc2
S1\C(=C/c2ccc(OCCOc3cc(cc(c3)C)C)cc2)\C(=O)NC1=N
Brc1cc2-c3nnc(SCCCC)nc3OC(Nc2cc1)C(=O)c1ccccc1
S(CC=C)c1nc2OC(N(c3c(-c2nn1)cccc3)C(=O)C)c1ccc(N(C)C)cc1
s1cc(nc1-n1ncc(C(OCC)=O)c1C[NH+]1C2CC(CC2)C1)-c1ccc(OC)cc1
Clc1ccc(NC(=O)COc2cc3c(cc2)cccc3)cc1-c1oc2cc(ccc2n1)C
Clc1ccc(cc1)C(=O)NC(=S)Nc1c2c3c(CCc3ccc2)cc1
S(C(C(=O)Nc1ccc(cc1)CC#N)C)c1ccccc1
O1CCN(CC1)c1ccc(NC(=O)CC2Nc3cc(C)c(cc3NC2=O)C)cc1
S(Cc1ccc(cc1)C)CCNC(=O)CN(S(=O)(=O)C)c1cc(ccc1OC)C
O=C(NCc1cccnc1N(C)C1CCCCC1)C(n1nccc1)C
S(=O)(=O)(N1CC[NH+](CC1)C)c1ccc(cc1C)C
Clc1ccc(SCCC(=O)NCCSCc2ccccc2)cc1
O(C)c1cc(ccc1OC)C(=O)c1nc2CCCCc2n1O
Clc1ccc(OCCCCOc2c3ncccc3ccc2)cc1
S(=O)(=O)(N(CC(=O)Nc1ccccc1C(=O)[O-])c1cc(ccc1)C(F)(F)F)C
Clc1c2c(nccc2)c(OS(=O)(=O)c2cc([N+](=O)[O-])ccc2)cc1
O=C(NCc1nccccc1)C1CCC[NH+](C1)C1CCN(CC1)C(=O)NCCC
S1\C(=C\c2ccc(OC)cc2)\C(=O)N(c2c3c(ccc2)cccc3)C1=S
s1cc(nc1NC(=S)NC(=O)c1ccc(cc1)C(C)(C)C)-c1cc([N+](=O)[O-])ccc1
S(Cc1ccc(F)cc1)c1[nH]c2c(n1)cc(OC)cc2
Oc1ccc(Nc2nnc(c3c2cccc3)-c2ccc(cc2)C(=O)N)cc1
Clc1cc(cc(Cl)c1O)\C=C/1\C(N2N=C(SC2=NC\1=O)CCCC)=N
O(C)c1cc(OC)ccc1C[NH+]1CCC(CC1)C(=O)N1CCCCC1
Brc1cc(cnc1)C(=O)NC(=S)Nc1ccc(OC)cc1OC
Clc1ccc(cc1)\C=C\C(=O)NC(=S)Nc1cc(OC)ccc1
O=C(N(CC1CC[NH+](CC1)CCc1ccccc1C)C1CCCC1)CCn1ncnc1
Sc1nnc(n1N=Cc1cccc(OCC)c1O)-c1ccc(cc1)C
O=C1C(=CN(C=C1C(=O)NC(C)C)C1CCCC1)C(=O)N1CCCCCCC1
O=C1N(CC(=O)Nc2c(cc(cc2C)C)C)C(=O)C2C1C1c3c(C2c2c1cccc2)cccc3
O1c2c(-c3c(cc(OC)cc3)C1=O)ccc(OCc1cc(OC)ccc1)c2C
Brc1cc(Cl)c(OCC(=O)NCCCc2ccccc2)cc1
O(CC)c1ccccc1NC(=O)CCCc1ccccc1
o1c2c(cccc2)c(NC(=O)c2ccc(OC)cc2)c1C(=O)c1ccc(OC)cc1
Brc1cc2C=C(C(=O)NC=3SCCN=3)C(Oc2cc1)=O
O=C1N(CCC(OCC=C)=O)C(=O)c2c1cc([N+](=O)[O-])cc2
O(C(=O)c1ccccc1NC(=O)CCC(C)(C)C1CCCCC1)C
s1c2CC(CCc2c(C(OCC)=O)c1NC(=O)COc1ccc(F)cc1F)CC
s1cccc1-c1scc(n1)C(=O)N
Fc1ccc(cc1)C1[NH+](CCCC1)Cc1onc(n1)CC1CC1
O=C1C2=C(N(N(C)C)C(N)=C(C#N)C2c2cc([N+](=O)[O-])ccc2)CC(C1)(C)C
S=C(Nc1ccccc1F)N1CCN(CC1)C(=O)C1OCCC1
Clc1cc(Cl)ccc1\C=C\C(=O)Nc1cc(NC(=O)CC)ccc1
s1cccc1-c1nn(cc1C1NC(=O)NC(C)=C1C(OC(C)C)=O)-c1ccccc1
Clc1ccc(SCC(=O)Nc2ccc(S(=O)(=O)Nc3c4c(ccc3)cccc4)cc2)cc1
Clc1cc(cc(OCC)c1OS(=O)(=O)c1ccc(cc1)C)C(=S)N1CCOCC1
O=C1N(CC(C1)C(=O)[O-])Cc1ccccc1
n1c(cc(nc1NCc1ccccc1)Nc1ccc(cc1C)C)C
Clc1cc(ccc1C)-c1oc2c(n1)cc(NC(=O)c1ccccc1F)cc2
O(C)c1ccc(OC)cc1C[NH+]1CCC([NH+]2CC[NH+](CC2)CCO)CC1
Clc1cccnc1NC(=O)C1Oc2c(OC1)cccc2
O(CC)c1ccc(cc1)C[NH+]1CCC([NH+]2CCCCCC2)CC1
Fc1ccccc1NC(=O)c1ccc(OCc2ccccc2)cc1
Clc1cc(NC(=O)CN(S(=O)(=O)c2ccccc2)c2cccc(C)c2C)ccc1
S(Cc1occc1)CCNC(=O)CN(S(=O)(=O)C)c1ccc(cc1)C(C)C
Brc1cc2c(NC(=O)C2(O)CC(=O)c2c(cc(cc2C)C)C)cc1
Clc1cc2c(nc(C)c(C[NH+]3CCCC3)c2O)cc1
Brc1cc(ccc1OC)C(=O)Nc1ccc(NC(=O)c2sccc2)cc1
s1cc(cc1)C[NH2+]C1CCN(CC1)c1ccc(cc1)C(=O)NC(C)c1ccccc1
Clc1ccccc1\C=C\C(=O)Nc1sc(nn1)C(C)(C)C
Clc1cc([N+](=O)[O-])c(cc1)C(=O)Nc1ccc(S(=O)(=O)N2CCOCC2)cc1
O(C)c1cc(OC)ccc1CNC(=O)CCC1CCC[NH+](C1)Cc1nccn1C
S1/C(=C\C=C\c2ccccc2)/C(=O)N(CCC(=O)Nc2ncccc2)C1=S
S1c2c(N(c3c1cccc3)C(O\N=C(/N)\c1ccc(cc1)C)=O)cccc2
S(=O)(=O)(N(Cc1ccccc1)CC(=O)Nc1cc(ccc1OC)C)c1ccc(F)cc1
Clc1cccc(NC(=S)NCc2ccccc2)c1C
Clc1cc(ccc1)CSc1nnc(n1C)CCNC(=O)c1cccc(OC)c1OC
s1cccc1C(=O)C=1C(N(CC[NH+]2CCOCC2)C(=O)C=1[O-])c1ccc(OCC)cc1

Clc1ccc(cc1C(=O)[O-])-c1oc(cc1)\C=C/1\C(=O)N(NC\1=O)c1cc(C)c(cc1)C
Clc1cc2c(OC(=O)C=C2CCCC)cc1OC(=O)c1ccccc1
O1c2cc(ccc2OC1)C1N(CC[NH+](CC)CC)C(=O)C([O-])=C1C(=O)c1ccc(OC(C)C)cc1
O(C(=O)C=1C(n2ncnc2NC=1c1ccccc1)c1cccnc1)CC
Fc1ccc(cc1)C1C2=C(NC=3NC(=O)NC(=O)C1=3)CCCC2=O
Oc1c2cc(ccc2nc(C)c1C[NH+]1CC[NH+](CC1)C)CC
Clc1cc(NC(=O)\C=C\c2ccc(OCCC)cc2)ccc1C
O=C1CC2(CCC1(C)C2(C)C)C(=O)Nc1c2c(ccc1)cccc2
Oc1c2c(nc(C)c1C[NH+](C)C)c(C)c(cc2)C
O(CCCC(=O)Nc1ccc(OCC)cc1)c1ccc(OC)cc1
s1cccc1C(=O)CSc1nnc(n1Cc1ccccc1)-c1ccccc1
O=C(N1CCC(CC1)C(=O)NC1CCCCCC1)c1ccccc1C
S(=O)(=O)(NC(C)C)c1cc(cc(NCC2CCC=CC2)c1)C(=O)N(Cc1nonc1C)C
S(CC(=O)Nc1ccccc1Oc1ccccc1)c1nnnn1Cc1ccccc1
Clc1cc(NC(=O)C)c(OS(=O)(=O)c2ccc(OC)cc2)cc1
Brc1ccc(O)cc1C=C1C(=O)N(C)C(=O)N(C)C1=O
O=C(NCc1cccnc1N(Cc1ccccc1)C)C[C@H]1[C@H]2C=C[C@@H](C1)C2
Brc1cc(OCC[NH+]2CCCC2)ccc1
S(=O)(=O)(N1CCC(CC1)C(=O)N1CCC(CC1)C(OCC)=O)c1ccc(OC)cc1
O(C(=O)c1ccccc1NC(=O)C1CCN(CC1)C(=O)Cc1ccccc1)C
Fc1ccc(cc1)C(=O)COC(=O)CCC(=O)Nc1ccccc1CC
s1cccc1C1NC(=S)NC(C)=C1C(=O)N(C)C
S(CCCN1c2c(NC1=O)cccc2)c1nc2n(c3c(c2nn1)cccc3)CCc1ccccc1
Clc1cc(ccc1Cl)CN(S(=O)(=O)c1ccccc1)CC(=O)NCc1occc1
OC1(c2c(N(CC(=O)N)C1=O)cccc2)CC(=O)c1ccc([N+](=O)[O-])cc1
S(=O)(=O)(N1CCC(CC1)(Cc1ccc(OC)cc1)CO)Cc1ccccc1
Clc1cc(ccc1Cl)C(=O)COC(=O)c1cc(OC)ccc1
s1cccc1-c1csc(NC(=O)c2ccccc2OC(=O)C)c1C(OCC)=O
Clc1ccc(cc1)-c1nc-2n(n1)C=Nc1sc3c(CC([NH2+]C3(C)C)(C)C)c1-2
S(=O)(=O)(N(CC(=O)Nc1cccc(C)c1C)c1cc([N+](=O)[O-])ccc1)C
s1c2ncnc(NC3CCOC3)c2c(C)c1C(=O)NC1CCCCC1
s1c2CCCc2c2c1N=C1N(N=C(N3CCCCC3)c3c1cccc3)C2=O
Brc1ccc(OCC(O)C[NH+]2CC[NH+](CC2)C)cc1
Clc1cc(\C=C\2/SC(=NC/2=O)NC(=O)C)c(OCc2ccc(F)cc2)cc1
O(N=C(C)C)c1nc(nc(n1)NCC)N(C)C
S(CC(=O)Nc1c2c(ccc1)cccc2)c1nc(N)cc(n1)N
O=C(NC(CCc1ccccc1)C)c1ccccc1C(=O)NC(CCc1ccccc1)C
Clc1cc(ccc1)CCNS(=O)(=O)c1ccccc1
Clc1cc(C(=O)NC23CC4CC(C2)CC(C3)C4)c([N+](=O)[O-])cc1
Clc1cc(ccc1Cl)\C=C\C(=O)Nc1cc([N+](=O)[O-])ccc1OC
S(=O)(=O)(NC1CCC(NS(=O)(=O)CC)CC1)CC
S1C=Cn2cc(nc12)C(=O)N1CCc2c(C1)cnc(C)c2CNC(=O)c1ccoc1C
S(=O)(=O)(NCC(OC(C(=O)c1ccccc1)CC)=O)c1ccc(cc1)C
Clc1ccccc1C[NH+]1C[C@H]([NH2+]Cc2cc(ccc2C)C)C[C@H]1C(=O)NCC
FC(F)(F)c1nc2c(n1C(C)c1ccccc1)cccc2
Brc1cc(cnc1)C(=O)NC(=S)Nc1cc(ccc1)C1OC(C)(C)C(O1)(C)C
O(C)c1ccccc1C[NH+]1CCC(CC1)CN(C(=O)c1ccc(N(C)C)cc1)CCOC
S1\C(=C\c2c3c(n(c2)C)cccc3)\C(=O)N(CC=C)C1=O
FC(F)(F)c1cc(N2N=C(C)\C(=C\c3cc(OC)c(OCC(=O)N)cc3)\C2=O)ccc1
S(=O)(=O)(N(C(=O)C)c1cc2c(oc(C)c2C(OCC)=O)cc1)c1ccc(F)cc1
Ic1cc(ccc1C)C(=O)Nc1cc([N+](=O)[O-])ccc1OC
Brc1cc(\C=C\C(=O)NC(=S)Nc2cc(C(=O)[O-])c(Cl)cc2)c(OC)cc1
S=C1NC(=O)/C(=C\c2ccc(N3CCOCC3)cc2C)/C(=O)N1c1ccccc1
Brc1cc2c(n(cc2\C=C/2\C(=O)N(C)C(=S)NC\2=O)CC(=O)N(CC)CC)cc1
Clc1ccccc1OCC(=O)Nc1ccc(S(=O)(=O)N2CCCCC2)cc1
S(CC(=O)Nc1ccc(OC(=O)C)cc1)c1ccccc1
Clc1cc(C)c(NC(=S)N2CCN(CC2)C(=O)C2OCCC2)cc1
o1c(ccc1COc1c2c(ccc1)cccc2)C(=O)NCc1occc1
s1c(nnc1SC(CC)C(=O)NC(C)c1ccccc1)N
Clc1cc(NC(=O)c2sc3nc(C)c(CC=C)c(c3c2N)C)ccc1
Clc1ccccc1OCc1cc(ccc1)C(=O)N1CC(OC(C1)C)C
Brc1ccc(S(=O)(=O)N(Cc2ccc(Cl)cc2)CC(=O)N)cc1
Clc1cc(Cl)c(Cl)cc1NC(=O)CN(S(=O)(=O)c1ccccc1)C
O(C)c1cc(ccc1)-c1nc(nnc1)NCCc1nc(cc(n1)C)C
S(=O)(=O)(NCC(=O)Nc1ccccc1F)c1ccc(cc1)C
S(=O)(=O)(N1CCN(CC1)c1ccccc1OCC)c1ccc(cc1)C1CCCCC1
S(=O)(=O)(Nc1nc(nc(c1)C)C)C)c1ccc(NC(=O)c2c(cc(cc2C)C)C)cc1
Clc1cc(ccc1Cl)COc1ccc(cc1OCC)CO
s1c(C(OCC)=O)c(nc1NC(=O)CCN1C(=O)c2c(cccc2)C1=O)C
S(=O)(=O)(N1CCC(CC1)C(=O)N1CC[NH+](CC1)Cc1cc2OCOc2cc1)C
S(=O)(=O)(N(CC(=O)Nc1ccccc1C(=O)NCC=C)c1cc(C)c(cc1)C)c1ccccc1

Fc1ccc(cc1)CN1C=C(C(OCC)=O)C(C(=C1)C(OCC)=O)c1cc2OCOc2cc1
Clc1cc(NC(=O)CCCC)ccc1N1CCN(CC1)C(=O)CCC
Brc1cc(\C=C\c2nc3c(cc2)cccc3OC(=O)CC)c(OC)cc1
Clc1ccc(cc1)/C(=N/OC(=O)CSc1ccccc1)/N
Oc1c(cc(cc1-c1[nH]c2c(n1)cccc2)C(C)(C)C)-c1[nH]c2c(n1)cccc2
s1cccc1CNC(=O)CSc1nc(cc(n1)C(F)(F)F)-c1occc1
S(=O)(=O)(N1CCc2c(C1)cccc2)c1cc(C)c(OC)cc1C
N(CCCNc1ccccc1)c1ccccc1
Fc1cc(F)ccc1N\C=C\C(=O)c1occc1
Clc1cc2c(OC(=O)C=C2CC)cc1OCC(=O)c1cc(Cl)c(Cl)cc1
O1CCc2c(cccc2)C1CNC(=O)C1=CN(C=C(C(=O)NCC(C)C)C1=O)C(C)C
O1c2cc(OC(=O)CCN3C(=O)c4c5c(cccc5ccc4)C3=O)ccc2OC1
O1c2c(ccc(OCc3ccccc3OC)c2)C(=CC1=O)c1cc([N+](=O)[O-])ccc1
S(=O)(=O)(NCC1OCCC1)c1ccc(cc1)C(=O)N1CCN(CC1)c1ccccc1F
Clc1cc2nn(nc2cc1NC(=O)C(Cl)(Cl)Cl)-c1ccccc1
S(Cc1occc1)CCNC(=O)c1ccc(cc1)-c1ccccc1
O(CCn1ncnc1)c1ccccc1-c1ccccc1
O=C1N(CCN(C1)C(=O)C=1NC(=O)c2c(N=1)cccc2)Cc1cc(ccc1)C
S(=O)(=O)(NCCC)c1cc2c(cc1)cccc2
Clc1cc(ccc1OCC)C(=O)C=1C(N(CC[NH+](C)C)C)C(=O)C=1[O-])c1ccc(F)cc1
S(=O)(=O)(NC(CC)C)c1ccc(OCC(=O)NCC2OCCC2)cc1
Ic1cc2c(N=C(SCC=C)N(CC=C)C2=O)cc1
Clc1ccc(N2C3=C(C=C(C(=O)Nc4ccc(cc4)C(OCC)=O)C2=O)C(=O)CCC3)cc1
S(CC=1NC(=NC(=O)C=1)Nc1nc(c2cc(ccc2n1)C)C)c1nnnn1-c1ccccc1
Brc1oc(cc1)C(=O)N1CCN(CC1)c1ccc(OC)cc1
O(CCC)c1ccc(cc1OC)C(=O)N
S(CC(=O)Nc1cc(ccc1)C(F)(F)F)C=1NC2=C(C(C=1C#N)c1ccc(OC)cc1)C(=O)CC(C2)(C)C
s1cccc1C1=NN(C(=O)C)C(C1)c1occc1
s1ccnc1NC(=O)C(Sc1nnnn1-c1ccccc1)CC
S(=O)(=O)(C(S(=O)(=O)c1ccccc1)=CNc1ccc(OC)cc1)c1ccccc1
O(C)c1c(OC)cc(cc1OC)CNc1nc2c(n1CC[NH+](CC)CC)cccc2
O(C)c1cc(OC)ccc1C1C(=CN(C=C1C(OC)=O)Cc1cc(OC)c(OC)cc1)C(OC)=O
O(C)c1ccccc1NC(=O)C(=O)NCC1[NH+](CCC1)CC
S(CC(=O)NCc1ccccc1)c1nnc(n1C)CNC(=O)c1ccccc1F
O=C(NC(CCc1ccccc1)C)c1ccc(NC(=O)CCCC)cc1
S(CC(=O)Nc1cccc(C)c1C)c1[nH]c(c(n1)-c1ccccc1)-c1ccccc1
s1c(nnc1NC(=O)c1cc(C)c([N+](=O)[O-])cc1)CCCC
o1ccc(C(=O)N[N-]C(=O)Nc2cc(ccc2OC)C)c1C
S(=O)(=O)(N1CCCC1)c1ccc(NC(=O)CN(S(=O)(=O)C)c2ccc(Oc3ccccc3)cc2)cc1
S(=O)(=O)(Nc1nc(cc(n1)C)C)c1ccc(NC(=O)COc2c(cccc2C)C)cc1
S(c1ccc([N+](=O)[O-])cc1C=O)c1oc(nn1)-c1ccccc1
S(=O)(=O)(N1C(CCC1=O)C(=O)Nc1ccccc1C(=O)N)c1ccc(cc1)C
S(C)c1ccccc1NC(=O)CN(S(=O)(=O)C)c1ccccc1CC
Clc1cc(NC(=O)N2CCCCCC2)c(OC)cc1
S(=O)(=O)(Nc1nc(nc(c1)C)C)c1ccc(NC(=O)COC)cc1
Clc1cc(NC(=O)Nc2ccc(cc2)C(F)(F)F)c(OC)cc1
Brc1ccc(S(=O)(=O)NC(C(=O)Nc2cc(ccc2)C(=O)C)C)cc1
s1c2CC(CCc2c2c1ncnc2SCC(=O)NCC1OCCC1)C
n1c2c(n(CC=C)c1NCc1c3c(ccc1)cccc3)cccc2
S(=O)(=O)(NC1CC(=O)N(C1)CCc1ccc(F)cc1)CC
Ic1cc2c(N=C(N(c3ccc(cc3C)C)C2=O)\C=C\c2ncccc2)cc1
s1c2c(nc(nc2NC(Cc2ccccc2)C)C)c2cc3c(nc12)CC(OC3)(C)C
O=C(NCc1ccccc1)c1nc(NCc2ccccc2)c2c(n1)cccc2
Clc1cccc(NC(=O)c2cc3c(cc2)C(=O)N(Cc2cccnc2)C3=O)c1C
Brc1ccc(cc1)C(=O)CN(N1C(=O)c2c(cccc2)C1=O)C(=O)c1ccc([N+](=O)[O-])cc1
Clc1ccc(OCCCN2C=Nc3c(cccc3)C2=O)cc1CC
O=C1NC(=O)c2c1cc(NC(=O)CCC(=O)[O-])cc2
S(CCC([NH+]1CCC(Oc2ccc(cc2)C(=O)NCc2ncccc2)CC1)C)C
FC(F)(F)C1(NC(=O)N(CCc2cc(OC)c(OC)cc2)C1=O)NC(=O)c1ccccc1
S(=O)(=O)(NC1(C2=C(NC1=O)N(c1ccc(cc1)C)C(=O)NC2=O)C(F)(F)F)c1ccc(cc1)C
Brc1ccc(cc1)C(=O)C(C(C)C)C1C(C(OCC)=O)C(OC1(C)C)=O
s1c(SCc2c3c(ccc2)cccc3)nnc1SCc1ccc(OC)cc1
O1CCN(CC1)c1ccc(NC(=O)NC(C)(C)c2cc(ccc2)C(C)=C)cc1
O1CCOc2c1cc(cc2)\C=C(\C#N)/c1[nH]c2c(n1)cc(cc2)C
Clc1cc(Cl)cc(C[NH2+]CCc2cc(OC)c(OC)cc2)c1OC
O=C(NCc1ccccc1)c1cccnc1NCc1ccccc1
s1c(nnc1SCC(=O)Nc1scc(n1)C)C
Clc1ccc(cc1S(=O)(=O)Nc1cc(ccc1C)C)C(=O)NCCOC
s1c2c(CCC2)c(C(=O)NCc2occc2)c1NC(=O)c1oc2c(ccc(c2)C)c1C
s1c(C)c(CC)c(C#N)c1NC(=O)c1cc(nc2c1ccc(C)c2C)-c1cccnc1
O(C)c1cc2c(n(C)c(C)c2\C=C\C2=Nc3c(cccc3)C(=O)N2CCc2ccccc2)cc1

Brc1ccc(cc1)C(=O)COc1cc2OC(=O)C(=Cc2cc1)c1ccc(OC)cc1
Clc1ccc(NC(=O)c2ccccc2)cc1C(=O)[O-]
s1cc(c2c1N=C(SCC(=O)c1c3c([nH]c1C)cccc3)N(C2=O)c1ccccc1)-c1occc1
O=C(NCC(=O)NNC(=O)c1ccc(cc1)-c1ccccc1)C1CCCCC1
Clc1cc(cc(OCC)c1OCc1ccccc1C#N)\C=C(\C#N)/c1ccc(F)cc1
Brc1cc(NC(=O)c2ccc(N(S(=O)(=O)c3ccc(Cl)cc3)C)cc2)ccc1
S1c2c(N(c3c1cccc3)C(=O)CSc1nnc(n1C)-c1occc1)cccc2
Clc1cc(C[NH+]2CCN(CC2)c2ncccc2)c(O)c2ncccc12
Clc1ccc(cc1)-c1nc(on1)CN(C(C)C)C(=O)COc1ccccc1
o1cccc1-c1n2N=C(c3c(-c2nn1)cccc3)C
O1c2cc(ccc2OC1)C(=O)NC(CC)(CC)C#C
o1c(ccc1C)C(=O)Nc1cc(OC)c(OC)cc1
S(=O)(=O)(Nc1ccccc1C)c1cc(ccc1C)C(=O)NCCc1cc(OC)c(OC)cc1
s1c2c(nc1C)cc(S(=O)(=O)NC1CCCCCCC1)cc2
Ic1cc(S(=O)(=O)N2CCc3c(C2)cccc3)ccc1OC
S(=O)(=O)(Nc1ccccc1C(=O)NCc1ccccc1C)C
s1c2CCCCc2c2-c3nc(nn3C=Nc12)COc1cc2c(cc1)cccc2
O(C)c1cc(ccc1)CNC(=O)CCC1CCCN(C1)C(=O)CCCc1ccccc1
O(C)c1ccc(NC(=O)c2ccccc2NC(=O)c2ccc(NC(=O)C)cc2)cc1
S(=O)(=O)(NCCCOCC)c1ccc(NC(=O)Cn2c3c(nc2)N(C)C(=O)N(C)C3=O)cc1
S(CC(=O)Nc1ccccc1)c1nnc(n1-c1ccccc1)-c1ccc(cc1)C(C)(C)C
s1c(cnc1NC(=O)COc1cc(C)c(cc1)C)Cc1cc(ccc1)C(F)(F)F
S(=O)(=O)(NCC)c1ccc(NC(=O)C(CC)c2ccccc2)cc1
s1c(C(=O)NC(C)c2ccccc2)c(C)c(C(OC)=O)c1NC(=O)c1ccccc1F
Clc1c2c(ccc1)c(ccc2)-c1oc2c(n1)cc(NC(=O)c1oc([N+](=O)[O-])cc1)cc2
Clc1cc(NC(=O)COc2cc3c(OC(=CC3=O)c3ccccc3)cc2)ccc1Cl
Clc1ccc(S(=O)(=O)N(C)c2ccc(cc2)C(=O)N2CC[NH+](CC2)Cc2ccccc2)cc1
o1c2cc(NCc3ccc(OC)cc3OC)ccc2c2c1cccc2
Fc1ccc(cc1)C(Oc1cc2c(OC(=CC2=O)c2ccccc2)cc1)=O
Ic1ccccc1C(=O)Nc1ccc(S(=O)(=O)Nc2cc(OC)ccc2OC)cc1
Clc1cc(ccc1NC(=O)Cn1ncc([N+](=O)[O-])c1)C(F)(F)F
Fc1ccc(cc1)Cn1c2c(nc1C[NH+]1CCCCC1)N(C)C(=O)N(C)C2=O
Clc1cc2c(occ2CC(=O)N)cc1C
s1ccc(C)c1C1C2=C(NC=3N(C)C(=O)N(C)C(=O)C1=3)CCCC2=O
ClC(F)C(F)(F)Oc1ccc(N2C(=O)C(Sc3ncccc3C(=O)[O-])CC2=O)cc1
Clc1cc([N+](=O)[O-])ccc1C(=O)Nc1ccc(cc1)C(F)(F)F
O=C1N(Cc2cccnc2)C(=O)c2c1c(N1CCN(CC1)C(=O)C(C)C)ccc2
s1cc(nc1)CC(=O)N1Cc2cc(ccc2OCC1)C(O)(CCn1nccc1)C
s1c2ncnc(NCCc3ccccc3F)c2c(C)c1C(=O)N(C(C)C)C
Clc1ccccc1S(=O)(=O)N1Cc2c(OCC1)c(OCCC1[NH+](CCC1)C)cc(c2)-c1cccnc1
s1c(ccc1C(=O)NCCNC=1NC(=O)C=C(N=1)C)C1[NH2+]CCC1
Fc1ccccc1CNC(=O)c1nn(c2c1CC([NH+](CCOC)C)CC2)C
FC(F)(F)c1cc(N2CC[NH+](CC2)C2CCC[NH+](C2)CCC)ccc1
O=C(NCc1cccnc1)c1nn(c2c1C[NH+](CC2)C(CCc1c2c([nH]c1)cccc2)C)C
O1CC[NH+](CC1)CC(C)(C)c1[nH]c2c(n1)n(nc2C)C1CCCCC1
Oc1cc2c(n(C)c(C)c2C(=O)N2Cc3c(n(nc3C(=O)NC3CCCC3)CC(C)C)CC2)cc1
o1nc(nc1C[NH+](Cc1n2c(nc1C)C=CC=C2)C)-c1cc2OCOc2cc1
Oc1nc(ccc1C[NH+]1CCCCC1CCCO)C
O=C1NCCN(C1)C(=O)c1nn(c2c1C[NH+](CC2)C(C)C)CCCc1ccccc1
O(C)c1c2c(cccc2)c(cc1)C[NH+](CCn1nnc(c1)C(=O)N1CC[NH+](CC1)C)C
Clc1cc(ccc1)CCNC(=O)[C@H]1[NH+](C[C@H](n2nnnc2)C1)Cc1ccc(OCc2ccccc2)cc1
FC(F)(F)c1ccccc1C[NH+]1CC(CCC1)(Cc1cc(OC)ccc1)CO
O(c1ccccc1C(=O)N(CC=C)CC=C)C1CCN(CC1)C(=O)COC
Clc1cc(F)ccc1CC(=O)N1[C@@H]2[C@H](CCC1)CN(CC2)C(=O)c1ccccc1
S1CC(Nc2ncc(cc2)C(=O)N2CCC(Oc3cccnc3)CC2)CC1
Clc1ccc(cc1)CN1C=C(C(OCC)=O)C(C(=C1)C(OCC)=O)c1cc2OCOc2cc1
O=C1C2=C(NC(=O)CC2c2cc([N+](=O)[O-])c(cc2)C)CCC1
Clc1ccc([N+](=O)[O-])cc1C(=O)N1CCN(CC1)c1ccc(OCc2ccccc2)cc1
s1cc(c2CCC(Cc12)C)C(=O)N\N=C\c1ncccc1
Brc1cc2c(nc(cc2C(=O)Nc2ccc(cc2)C(=O)N2CCCC2)-c2ccc(cc2)CCCC)cc1
O1c2c(C=C(C(=O)NCC(OCC)=O)C1=O)cccc2OCC
Brc1cc2nc(cc(c2cc1)C(=O)[O-])-c1cc(Cl)c(Cl)cc1
s1c2N=C(S)N(NC(=O)c3ccoc3C)C(=O)c2c(C)c1C(=O)[O-]
Clc1cc(F)ccc1CSCC(=O)NN
O=C(NNC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Clc1cccc(F)c1CC(=O)N[N-]C(=S)Nc1cc2OCCOc2cc1
Clc1ccccc1OCC(=O)Nc1sc(C)c(C)c1C(OC(C)C)=O
O(C)c1cc(ccc1OC)-c1nc2c(cccc2)c(c1)C(=O)N\N=C(/C)\c1ccc(NC(=O)C)cc1
s1c2c(CCC2)c(C(OC(C)C)=O)c1NC(=O)c1ccccc1
Clc1ccc(Cl)cc1S(=O)(=O)N\N=C(\C)/c1cc(NC(=O)c2sc(cc2)C)ccc1
s1ccc(C)c1C(=O)N\N=C\c1c(cc(cc1C)C)C

O1C2CCC1C(C(=O)[O-])C2C(=O)N(CCCCC)CCCCC
Brc1cn(nc1[N+](=O)[O-])Cc1oc(cc1)C(=O)N\N=C/C(=C/c1ccccc1)/C
FC(F)(COCc1cc(ccc1OC)\C=C(\C(=O)C(C)(C)C)/C#N)C(F)F
Clc1ccc(Cl)cc1S(=O)(=O)N\N=C/c1c[nH]nc1-c1ccc(cc1)CC
S(=O)(=O)(N\N=C/c1c[nH]nc1-c1cc(OC)c(OC)cc1)c1ccc(cc1)CCC
s1cc(-c2nnc(SCc3cc(OC)ccc3)n2C)c(C)c1C
Brc1ccc(cc1)-c1nc(sc1)NC(=O)CSc1nnc(n1C)-c1cccnc1
s1cc(-c2nnc(SCC(=O)Nc3ccccc3C(F)(F)F)n2CC)c(C)c1C
Clc1c2c(sc1C(=O)N\N=C(/C)\c1cc(NC(=O)C(F)(F)F)ccc1)cc(cc2)CC
Clc1ccc(cc1)-c1nc(nnc1)NCc1c(F)c(ccc1F)C
s1ccc(C(OCC)=O)c1NC(=O)\C(=C\c1ccccc1OCCCCC)\C#N
S(C)c1cc(NC(=O)NCc2ccncc2)ccc1
Clc1cccc(Cl)c1C[NH+]1CCN(CC1)C(=O)Nc1cc(SC)ccc1
O(C)c1cc([N+](=O)[O-])ccc1NC(=O)N1CC[NH+](CC1)Cc1cccnc1
Clc1cc(ccc1Cl)Cn1nc(NC(=S)Nc2cc(ccc2C)C)c(Cl)c1
o1c2c(cccc2)c(C)c1C(=O)NC(C)c1ccc(cc1C)C
Clc1cc(NC(=S)Nc2nn(cc2)Cc2ccc(Cl)cc2)ccc1C
Clc1sc(cc1)C(NC(=O)NCC1OCCC1)C
S(=O)(=O)(N1CCc2c1cccc2)c1ccc(NC(=S)Nc2ccc(cc2)C(CC)C)cc1
O1c2c(cc(OCC)cc2)C(=CC1=O)C[NH+]1CC[NH+](CC1)CC(=O)Nc1ccc(cc1)C
Clc1cc(NC(=O)CN2C(=O)c3cccnc3N(c3ccccc3)C2=O)c(cc1)C
Brc1ccc(cc1)C(=O)CSC=1NC(C)=C(C(=O)C)C(CCC)C=1C#N
O1c2c(C(=O)Nc3c1cccc3)c(OCCC)cc([N+](=O)[O-])c2
O1c2c(C(=O)Nc3c1cccc3)c(Oc1cc(ccc1)C)cc([N+](=O)[O-])c2
O1c2c(C(=O)Nc3c1cccc3)c(Oc1ccc(NC(=O)C)cc1)cc([N+](=O)[O-])c2
ClC(Cl)(Cl)Cc1c2c(n(c1C)-c1ccc(OC(F)(F)F)cc1)CC(CC2=O)(C)C
FC(F)(F)COc1nc(nc(n1)NC(CC)C)N1CC[NH+](CC1)C12CC3CC(C1)CC(C2)C3
S(=O)(=O)(NCCc1cc(OCC)c(OCC)cc1)c1ccc([N+](=O)[O-])cc1
O1C(C)(C)C(O)(N(CC(=O)Nc2ccc(cc2)C)C1=O)C
s1c(ccc1C(=O)NC(CCCC)C(=O)[O-])C#CC(O)(C)C
O(C)c1cc(C#N)c(NC(=O)C[NH+]2CCCCC2CCO)cc1OC
S=C(Nc1nccc(c1)C)C(=O)N
s1c2c(CCCC2)c(C(OCC)=O)c1NC(=O)C[NH+]1CCC(CC1)Cc1ccccc1
Clc1cc(N2NC3(NC2=S)CCCCC3)c(OC)cc1
O(C)c1cc(ccc1)C=1N(c2n(c3c(n2)N(C)C(=O)N(C)C3=O)C=1)CC(O)c1ccccc1
s1cccc1C1CC(=O)C2=C(NC(C)=C(C(=O)Nc3cc(F)ccc3)C2c2ccc(F)cc2)C1
s1c2nc(cc(c2c(NC(=O)CC(C)C)c1C(OCC)=O)COC)C
S/1CC(=O)N\C\1=N\N=C/1\CC(N2N=C(N(CC)C2=S)Cn2nc(nn2)-c2ccc(cc2)C)C2OC\1OC2
O=C1N(C)C(=O)N(c2nc3n(c12)C(C)=C(N3c1ccc(cc1)CC)c1ccccc1)C
Clc1cc(Cl)ccc1Cn1nc(NC(=O)c2ccc(F)cc2)cc1
OC=1N2CC(=O)C=C2C=C(C)C=1C#N
O=C1N(C)C(=O)N(c2nc3n(c12)C=C(N3c1cc(cc(c1)C)C)c1ccc(cc1)CCCCCCC)C
O(C)c1cc(C(OC)=O)c(NC(=O)c2cc3c(n(Cc4ccccc4)c(C)c3C)cc2)cc1OC
FC(F)(F)C1n2nc(cc2NC(C1)c1ccc(cc1)C)C(=O)NCc1cn(nc1C)C
FC(F)(F)C(NC(ON=C(C)C)=O)C(F)(F)F
o1c(ccc1Cn1nc(cc1C)C)C(=O)Nc1ccc(OC)cc1OC
s1c(C(=O)C)c(C)c(C(OCC)=O)c1NC(=O)\C=C\c1cn(nc1)C
Clc1cccc(F)c1Cn1nc(N)cc1
Fc1c(Cn2nc(C)c(NC(=O)c3c(nn(c3C)-c3ccccc3)-c3ccccc3)c2C)c(F)c(F)c(F)c1F
Clc1ccc(S(=O)(=O)N(Cc2cn(nc2C)C)C)cc1
Brc1ccccc1OCc1cc(ccc1OC)C(=O)Nc1nn(cc1)C12CC3CC(C1)CC(C2)C3
O(C)c1cc(NC(=O)Cn2nnnc2)cc(-n2nnnc2)c1
Brc1c(n(nc1C)C)C(=O)NC1C2SCC(COC(=O)C)=C(N2C1=O)C(=O)[O-]
Clc1cc(Cl)ccc1C(=O)\C=C\c1cn(nc1C)C
O(Cn1nc(cc1)C(=O)[O-])c1ccc(OC)cc1
S(=O)(=O)(N(Cc1nn(cc1)CC)C)c1cnn(CC)c1C
[S-]C1=NC(=O)c2c(nc(cc2C(F)(F)F)C2CC2)N1c1ccccc1OCC
[S-]C1=NC(=O)c2c(nc(cc2C(F)(F)F)CC)N1c1cc(ccc1)C
Fc1c(NC(=O)c2n(nc(c2)C(=O)N(CC)CC)C)c(F)c(F)c(F)c1F
s1c2CC(CCc2c(C(OCC)=O)c1NC(=O)c1c2n(nc1)C(=CC=N2)c1occc1)CC
S(C)c1[nH]nc(n1)N1Cc2c(c(OC)c(OC)cc2)C1=O
O(C(=O)C=1n2nc(cc2N=C(C=1)c1nn(cc1)CC)-c1ccccc1)C
FC(F)(F)C1(O)N(N=C(C1)C)C(=O)C(n1nc(cc1)C)C
Clc1cccc(NC(=O)c2nn(cc2)COc2cc(Cl)ccc2)c1C
Brc1c(n(nc1C(F)(F)F)C(C(=O)Nc1cnn(C)c1C(=O)Nc1cnn(C)c1C)C)C
Brc1cn(nc1[N+](=O)[O-])Cc1cc(ccc1)C(=O)N1CC2[NH+](CCC2)CC1
S(=O)(=O)(N1CC(CCC1)C(=O)Nc1cn(nc1)Cc1ccc(F)cc1)C
Clc1cnn(CC)c1CN(C(=O)c1n(ncc1)COc1ccc(Cl)cc1)C
Clc1ccc(cc1)C(=O)\C=C\Nc1scc(n1)-c1ccc(OC(F)F)cc1
S=C(Nc1cnn(CC)c1C)[N-]NC(=O)CC12CC3(CC(C1)CC(C3)C2)c1c(noc1C)C
Clc1ccc(cc1)Cn1ncc(NC(=S)N2CCCC2)c1

S(=O)(=O)(Nc1nn(cc1)Cc1ccccc1C)c1cn(nc1)C
Sc1nnc(n1\N=C\c1cc(OC)c(OCn2ncc([N+](=O)[O-])c2)cc1)C(F)(F)F
O=C(NCCCn1nccc1C)CCn1ncc([N+](=O)[O-])c1C
Brc1ccc(nc1)NC(=O)c1nn(cc1C(=O)[O-])C
s1c(ccc1C)-c1nc2N(c3cc(ccc3)C)C([S-])=NC(=O)c2c(c1)C(F)F
O(C(=O)c1ccc(NC(=O)c2n(ncc2C(=O)[O-])C)cc1)CC
Clc1ccccc1NC(=O)c1nn(cc1)CC(=O)Nc1ccccc1Cl
o1nc(-c2cn(nc2C)C)c(C)c1-c1cn(nc1C)C
Ic1cn(nc1C(=O)Nc1cc(OC)ccc1)C
Sc1nnc(n1C1CC1)COc1ccc(OC)cc1
Clc1ccccc1OCc1oc(cc1)C(=O)NCc1cc(Cl)c(Cl)cc1
O=C1N(c2ccccc2C)C(=O)C2N=NN(C12)CC(=O)Nc1ccc(cc1)C(OCC)=O
o1c2c(cc1-c1nn(cc1C[NH+](CCn1ccnc1)C)Cc1ccccc1)cccc2
S(=O)(=O)(NCC=C)c1ccc(NC(=O)Cc2c3c(ccc2)cccc3)cc1
O(CC(=O)Nc1ccccc1C)c1ccc(cc1OC)C#N
S1(=O)(=O)N(c2c3c(ccc2)cccc13)CCCCC#N
Brc1ccc(S(=O)(=O)Nc2cc(F)cc(F)c2)cc1
Clc1ccc(N2C(=O)C(NNC(=O)c3ncccc3)CC2=O)cc1
FC(F)(F)c1cc(Oc2ccc(cc2OC)CO)c([N+](=O)[O-])cc1
O=C1N(Cc2cccnc2)C(=O)N(CCOC)C12CC[NH+](CC2)Cc1ccccc1
O1C(CN(CC1C)C(=O)c1ccc(OCc2ccccc2)cc1)C
s1cc(nc1N(Cc1ccccc1)C)-c1ccccc1O
Clc1cc(ccc1OC)C(=O)Nc1ccccc1OC
O(C(=O)C)c1ccccc1C(=O)N(C(C)C)C(C)C
s1cccc1C(=O)NCCOc1cc(ccc1)C
Clc1cc(S(=O)(=O)N2CC(CCC2)C(=O)NCCO)c(OC)cc1
O(CC=C)c1ccc(cc1OC)C[NH2+]CCOC
O(CCC[NH+]1CCC(CC1)C(OCC)=O)c1cc2CCCc2cc1
O(CC)c1c(cccc1OC)C[NH2+]C(C)c1ccccc1
Clc1cc(S(=O)(=O)N(CC(=O)N2CC[NH+](CC2)C)C)ccc1OCC
O=C(Nc1cccc(C)c1C)C[NH+]1CC[NH+](CC1)C
Clc1cc(NC(=O)CSc2nnc(n2CC)-c2ccncc2)ccc1OC
O=C1N(C)C(=O)N=C2N(N=C(N=C12)c1ccc(cc1)CC)CC
S(CC(=O)Nc1cc2OCCOc2cc1)c1nnc(n1CC=C)-c1ccncc1
Clc1ccc(cc1)-c1oc(C)c(c1)C(=O)N1CCOCC1
o1nc(nc1CN(CC)C(=O)NCC)-c1ccccc1
S(=O)(=O)(N1CCOCC1)c1cc(C)c(OCC(=O)N)cc1
S(=O)(=O)(N(Cc1ccccc1)C)c1ccc(NC(=O)c2cccnc2)cc1
Clc1ccc(S(=O)(=O)N2CCCC2C(=O)N(C)C)cc1
FC(F)Oc1ccccc1NC(=O)c1ccc(OC)cc1OC
O(C)c1ccc(N2CC(CC2=O)C(=O)Nc2cc(ccc2C)C)cc1
S(=O)(=O)(N(C)c1ccc(cc1)C(=O)NC1CCCC1)CC
S(=O)(=O)(N1CCCCCC1)c1cc(ccc1C)C(=O)N1CC[NH+](CC1)C
O(C)c1c(OC)cc(cc1OC)C(=O)Nc1ccc(cc1)Cc1ncccc1
o1nc(NC(=O)Cc2ccccc2C)cc1
Clc1cc(F)ccc1C[NH+]1CCN(S(=O)(=O)c2cn(nc2C)C)CC1
S(=O)(=O)(N1CC[NH+](CC1)CC(=O)Nc1ccccc1CC)c1ccc(F)cc1
Clc1cc(F)c(NS(=O)(=O)c2cn(nc2)CC)cc1
S(=O)(=O)(N(C)C)c1ccc(NC(=O)Cc2ccccc2OC)cc1
O=C(Nc1ncc(cc1)C)C1CCN(CC1)C(=O)C
O(C)c1cc(N2CC[NH+](CC2)CC(=O)Nc2c(cccc2CC)CC)ccc1
Fc1ccc(N2CCN(CC2)C(=O)NCCCC)cc1
S1c2n(N=C1c1sccc1)c(nn2)COc1ccc(F)cc1
S(CC(=O)Nc1ncccc1)c1nnc(n1C)-c1ccccc1OC
s1c(nnc1NC(=O)C1CC(=O)N(C1)c1cc(C)c(cc1)C)C(F)(F)F
S(CC(=O)Nc1ccc(N2CCN(S(=O)(=O)C)CC2)cc1)c1nccn1C
O(CCOC)c1ccc(cc1)C(=O)N(C)c1ccccc1
o1nc(nc1CN(C(C)C)C(=O)NCC)-c1ccc(OC)cc1
Brc1ccc(NC(=O)CC2Nc3c(OC2=O)cccc3)cc1
O1c2c(CC1C)cc(cc2)C(=O)Nc1ccc(cc1C)C
O(CC(O)C[NH+]1CC(CC(C1)C)C)C1CCCCC1
Clc1cc(ccc1Cl)C(=O)Nc1cc(OC)ccc1N1CCOCC1
O=C1N(CCOCC)C(=O)N(c2nc3n(c12)C=C(N3c1cc(ccc1)C)C)C
Clc1c2c(sc1C(=O)N1CCN(CC1)c1nccccc1)cc(F)cc2
Fc1cc(ccc1)C(=O)NCC[NH+]1CCCCC1
O1CCC([NH+]2CCC(CC2)C(=O)Nc2ccc(-n3nnnc3)cc2)CC1
S(=O)(=O)(NCc1ccccc1)c1ccc(NC(=O)C2OCCC2)cc1
s1cccc1C(=O)NC1CC[NH+](CC1)C(C)C
s1c(C(=O)N(C)C)c(nc1NC(=O)CC12CC3CC(C1)CC(C2)C3)C
O(C)c1ccccc1C(=O)Nc1ccccc1C(C)(C)C
Clc1cc(ccc1)C[NH+]1C[C@@H]([NH2+]Cc2ccc(OC)c(C)c2C)C[C@H]1C(=O)NCCc1ccccc1F

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Clc1ccccc1CC(=O)NCc1cc(Cl)ccc1
O1c2cc(ccc2OC1)C[NH+]1CCN(CC1)C(=O)CCNC(=O)c1ccccc1
O=C1N(C)C(=O)N(c2nc3n(c12)C(C)C(=NN3Cc1ccccc1)C)C
O(CCn1c2c(nc1CCO)cccc2)c1ccc(cc1)C
Clc1cc(C)c(NC(=O)C[NH+]2CCC(CC2)C)cc1
Clc1ccc(cc1)-c1oc(cc1)C(=O)Nc1nn(nn1)C
O1CC[NH+](CC1)C\C=C\COc1ccccc1C
s1cc(nc1-c1ccc(cc1)C)Cn1c2c(nc1C#N)cccc2
s1cc(cc1)C(=O)Nc1cc(OC)c(OC)cc1
Clc1cccc(F)c1C[NH+]1CC([NH+](CC1)CCC(C)C)CCO
s1ccnc1NC(=O)C(Sc1nnc(n1CC)-c1ccc(OC)cc1)C
O=C1N2C(=Nc3n(CCCOC)c(cc13)C(=O)NCCCO)C=CC=C2
S(C(C)C)c1ccccc1C(=O)Nc1cc2OCCOc2cc1
O(C\C=C\Cn1ccnc1)c1ccc(cc1)C(C)(C)C
[NH2+]1CC(CCC1)c1[nH]c2c(n1)cccc2
o1c(ccc1COC)C(=O)Nc1cc([nH+]c2c1cccc2OC)C
Clc1cc(-n2nnc(C(=O)NCc3occc3)c2N)ccc1
[NH+]1(CCN(CC1)C=1n2nc3nc(cc(c3c2N=C(C=1)C)C)C)CC(C)=C
Clc1cc2c(oc(C(OCC)=O)c2C[NH+]2CC[NH+](CC2)C)cc1
S(=O)(=O)(N(C)C)N1CCC(CC1)C(=O)N1CCN(CC1)c1cccc(C)c1C
O(CC)c1ccccc1C(=O)Nc1ccc(cc1)C(=O)NCCC
Clc1ccc(SCC(=O)NCC[NH+](C)C)cc1
S(=O)(=O)(Nc1ccc(cc1)C(=O)NCCC[NH+]1CCCCC1)CC
O=C(Nc1ccc(cc1)C)c1nnn(c1N)-c1ccccc1
O=C(NCC[NH+]1CCCCC1)c1n(c2c(cc(cc2)CC)c1C)C
Fc1ccc(cc1)-c1nn(cc1C[NH+]1CCC(CC1)CN1CCCC1=O)-c1ccc(cc1)C
O=C(NCC(C)=C)C1CC[NH+](CC1)C1CC[NH+](CC1)Cc1ccccc1C
Fc1cc(ccc1F)CNC(=O)c1nnn(c1)C1CCCCC1
S(CCCNC(=O)c1noc(c1)COc1c(F)cccc1F)C
O(C)c1cc(ccc1OC)CNC(=O)c1cc(cc(-n2nnnc2)c1)-c1cc(ccc1)C
O(C)c1cc(ccc1OC)C(=O)C1CCC[NH+](C1)Cc1cnc(nc1)N
Clc1cc(F)ccc1C[NH+]1CCNC(=O)C1CC(=O)N1CCOCC1
s1ccc(C)c1C(=O)NCc1nnc(SCC2OCCC2)n1-c1cc(ccc1)C(F)(F)F
O(C)c1c(cccc1OC)C[NH+]1CC([NH+](CC1)Cc1ccccc1C)CCO
o1nc(c2c1CCN(C2)C(=O)CCOC)-c1ccc(cc1)-c1ccccc1
Clc1cc(ccc1)C(=O)N(CCOc1ccc(cc1)C[NH+](Cc1nc(sc1)C)C)C
s1c(C)c(nc1CCNC(=O)C1OCCC1)C
s1cc(cc1C(=O)C)C(=O)N1CC[C@@H]2N(CCC[C@@H]2C1)C(=O)c1cc2nccnc2cc1
Fc1c(cccc1F)CN1CCCC(O)(C[NH2+]Cc2ncccc2)C1=O
s1c2CC([NH2+]Cc3cccnc3)CCc2c2c1N=CN(Cc1ccc(F)cc1)C2=O
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