Supplementary Materials

Influence of aza-glycine substitution on the internalization of penetratin

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1. Materials

All amino acid derivatives, Fmoc protected amino acids, N, N'- diisopropylcarbodiimide (DIC), and Rink-amide MBHA resin were purchased from IRIS BiotechGmbH (Marktredwitz, Germany). 1.8- diazabicyclo[5.4.0]undec-7-ene (DBU), N,N-diisopropylethylamine (DIEA), ethandithiol (EDT), 1, 1'-carbonyldiimidazole (CDI) and thioanisole were obtained from FLUKA (Buchs, Switzerland), while , 5-(N-Ethyl-N-isopropyl) amiloride (EIPA), Colchicine (COL), Sodium azide (NaN3), Deoxy-D-glucose (DOG), phenol, trifluoroacetic acid(TFA), Ethyl cyano(hydroxyimino)acetate (Oxyma Pure), 5(6)-carboxyfluorescein (Cf), and all other chemicals used for biological studies, were supplied from Sigma Aldrich (Budapest, Hungary) products. Methyl-beta-cyclodextrin (CyD), Fmoc-hydrazide and chlorpromazine (CPZ) were acquired from TCI chemicals. Solvents used for the synthesis and purification were obtained from Molar Chemicals Ltd (Budapest, Hungary).

1.1 RP-HPLC

All samples were dissolved in a small amount of eluant B (0.1% TFA in acetonitrile-water (80:20, v/v)) and injected into the analytical RP-HPLC. This was performed on Exformma (Exformma Technology (ASIA) Co., Ltd, Hong Kong, China) HPLC system. The column used was Hypersil Hypurity C18 column (4.6 mm × 150 mm, 5 μm, 190 Å),and linear gradient elution (0 min 0% B; 2 min 0% B; 22 min 90% B) was applied using eluent A (0.1% TFA in water), and eluant B at flow rate of 1mL/min. The wavelength for the peaks detection is λ= 220 nm, for both analytical and preparative RP-HPLC. The crude samples were dissolved in eluant A and a semi-preparative Phenomenex Jupiter C18 column (250 × 10 mm I.D.) with 10 mm silica (300 Å pore size) (Torrance, CA, USA) was used for the purification. The flow rate was 4 mL/min, and linear gradient elution is applied.

1.2 Mass spectrometry

The determination of the molecular weight of peptides-conjugates, was performed by ESI-MS, using Bruker Amazon SL (Germany). The samples were prepared and dissolved in water-acetonitrile solution (50:50) containing 0.1% of formic acid. The injection of the samples was done directly through a syringe pump. Parameters: capillary voltage: 4 kV, nebulizer gas: 10 psi, dry gas: 4 L/min, heated capillary temperature: 250 ºC.

1.3 Cell Culture

A-431 human skin squamous cancer cells (CRL-1555TM) were used for the in vitro analysis. The cells were cultured in Dulbecco's Modified Eagle Medium (DMEM) Containing 10% heat inactivated foetal calf serum (FCS), nonessential amino acids (NEAA), sodium pyruvate (1mM), L-Glutamine (2 mM), 1% nonessential amino acids and 1% penicillin-streptomycin (from 10,000 units penicillin and 10 mg/ml streptomycin).The cells were maintained in plastic tissue culture dishes under conditions of 37 °C temperature and a humidified atmosphere comprising 5% CO2 and 95% air.

2. Chemical Characterization of Peptides

2.1. RP-HPLC

All samples were dissolved in a small amount of eluant B (0.1% TFA in acetonitrile-water (80:20, v/v)) and injected into the analytical RP-HPLC. This was performed on Exformma (Exformma Technology (ASIA) Co., Ltd, Hong Kong, China) HPLC system. The column used was Hypersil Hypurity C18 column (4.6 mm × 150 mm, 5 μm, 190 Å), and linear gradient elution (0 min 0% B; 2 min 0% B; 22 min 90% B) was applied using eluent A (0.1% TFA in water), and eluant B at flow rate of 1mL/min. The wavelength for the peaks detection is λ= 220 nm. In many chromatograms two main peaks are visible. These two peaks come from the two Cf isomers (5-carboxyfluorescein and 6-carboxyfluorescein), because we used the mixture of them as 5(6)-carboxyfluorescein for the synthesis of the fluorescently labelled peptides.

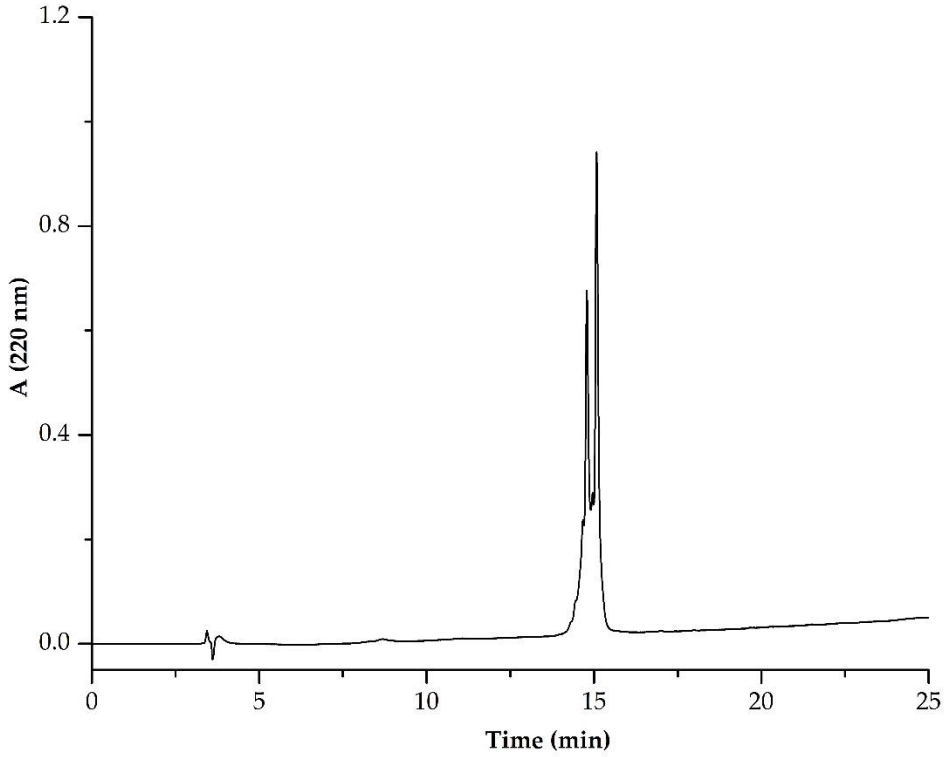

Figure S1. HPLC chromatogram of Cf-RQIKIWFQNRRKWKK-NH_2. Retention time was obtained on Hypersil Hypurity C18 column (4.6 mm x 150 mm, 5 μm, 190 Å). The applied linear gradient elution was 0 min 0% B, 2 min 0% B, 22 min 90% B at 1 mL/min flow rate. The detection was carried on at λ = 220 nm.

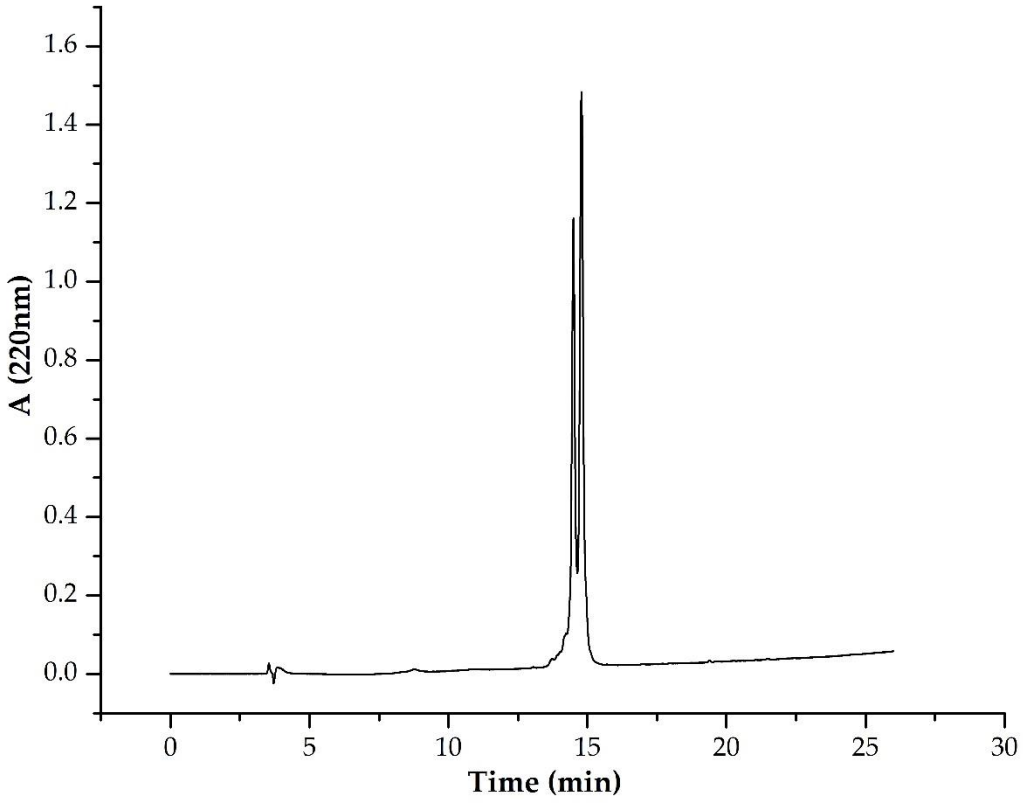

Figure S2. HPLC chromatogram of Cf-RQIKIWFQNRRK-azaGly-KK-NH_2. Retention time was obtained on Hypersil Hypurity C18 column (4.6 mm x 150 mm, 5 μm, 190 Å). The applied linear

gradient elution was 0 min 0% B, 2 min 0% B, 22 min 90% B at 1 mL/min flow rate. The detection was carried on at λ = 220 nm.

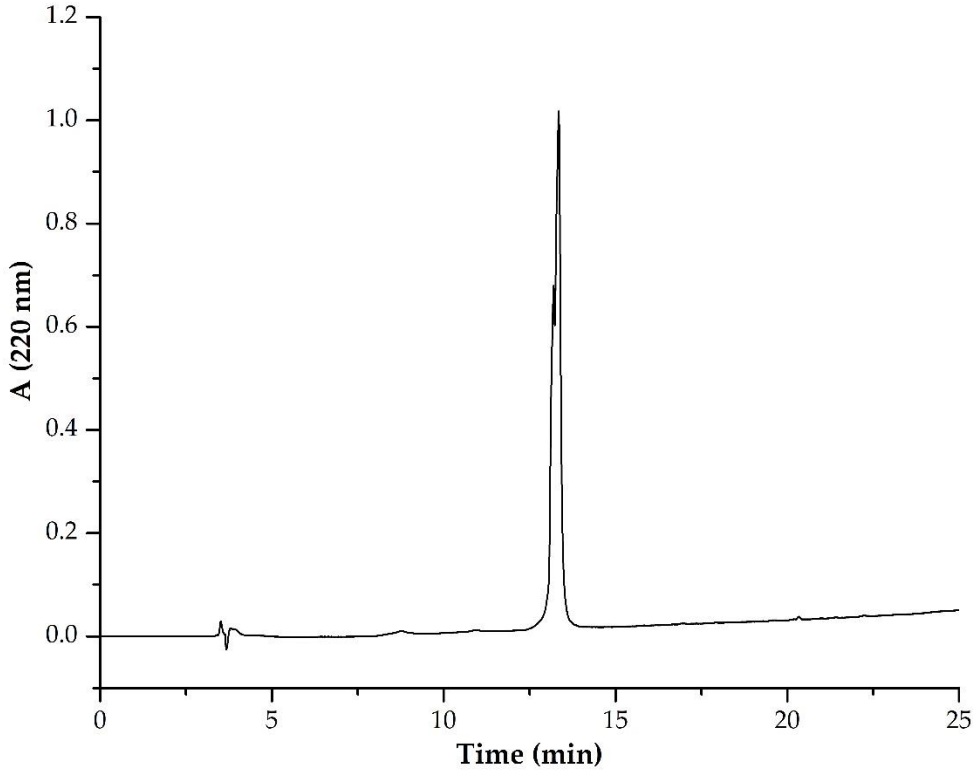

Figure S3. HPLC chromatogram of Cf-RQIKI-azaGly-FQNRRKWKK-*NH*$_2$. Retention time was obtained on Hypersil Hypurity C18 column (4.6 mm x 150 mm, 5 μm, 190 Å). The applied linear gradient elution was 0 min 0% B, 2 min 0% B, 22 min 90% B at 1 mL/min flow rate. The detection was carried on at λ = 220 nm.

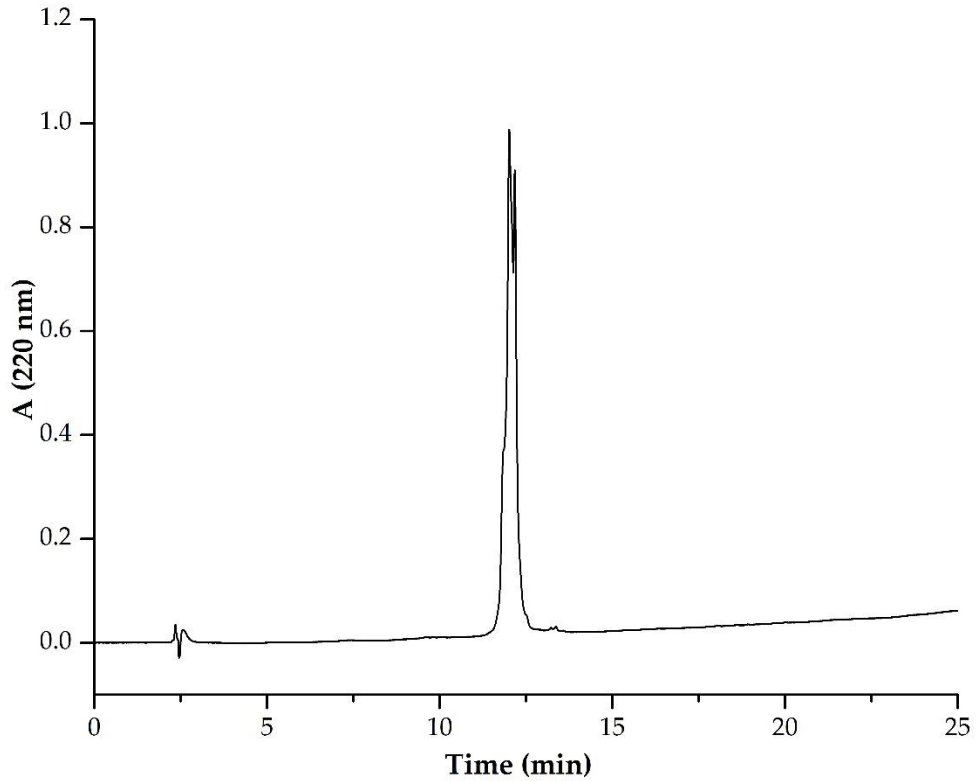

Figure S4. HPLC chromatogram of Cf-RQIKI-azaGly-FQNRRK-azaGly-KK-*NH*$_2$. Retention time was obtained on Hypersil Hypurity C18 column (4.6 mm x 150 mm, 5 μm, 190 Å). The applied linear gradient elution was 0 min 0% B, 2 min 0% B, 22 min 90% B at 1 mL/min flow rate. The detection was carried on at λ = 220 nm.

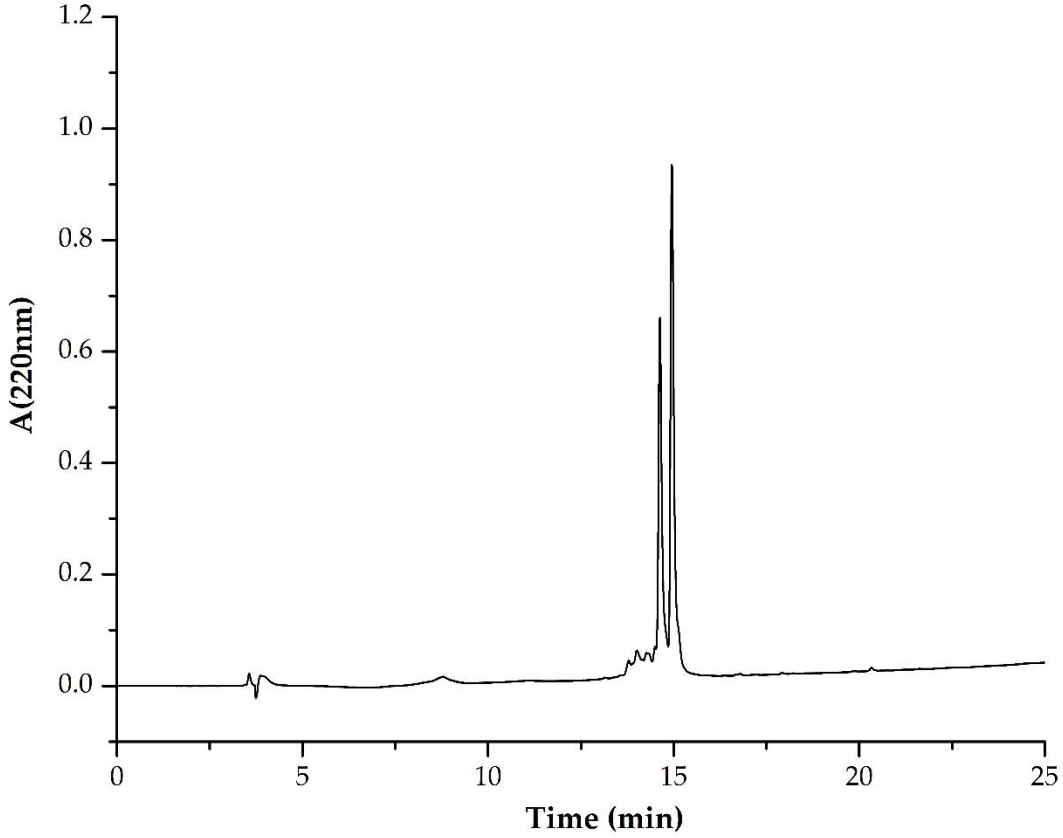

Figure S5. HPLC chromatogram of Cf-RQIKIWFQNRRKGKK-*NH*$_2$. Retention time was obtained on Hypersil Hypurity C18 column (4.6 mm x 150 mm, 5 μm, 190 Å). The applied linear gradient elution was 0 min 0% B, 2 min 0% B, 22 min 90% B at 1 mL/min flow rate. The detection was carried on at λ = 220 nm.

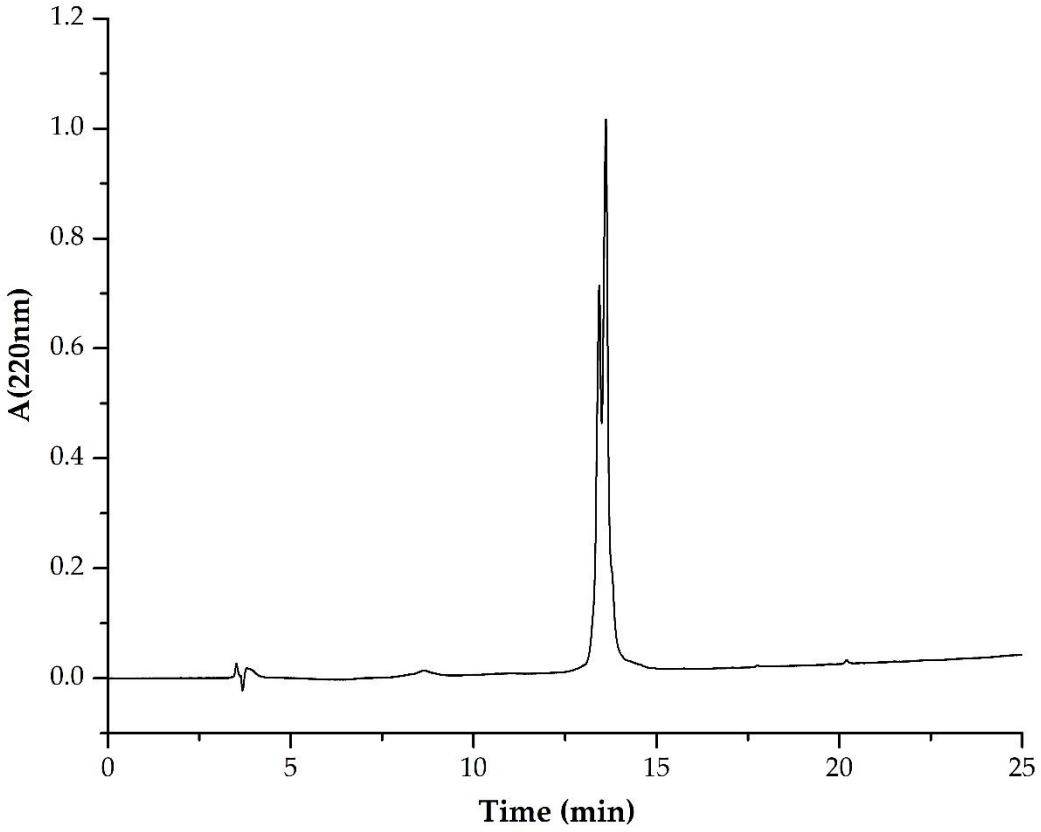

Figure S6. HPLC chromatogram of Cf-RQIKIGFQNRRKWKKNH$_2$. Retention time was obtained on Hypersil Hypurity C18 column (4.6 mm x 150 mm, 5 μm, 190 Å). The applied linear gradient elution was 0 min 0% B, 2 min 0% B, 22 min 90% B at 1 mL/min flow rate. The detection was carried on at λ = 220 nm.

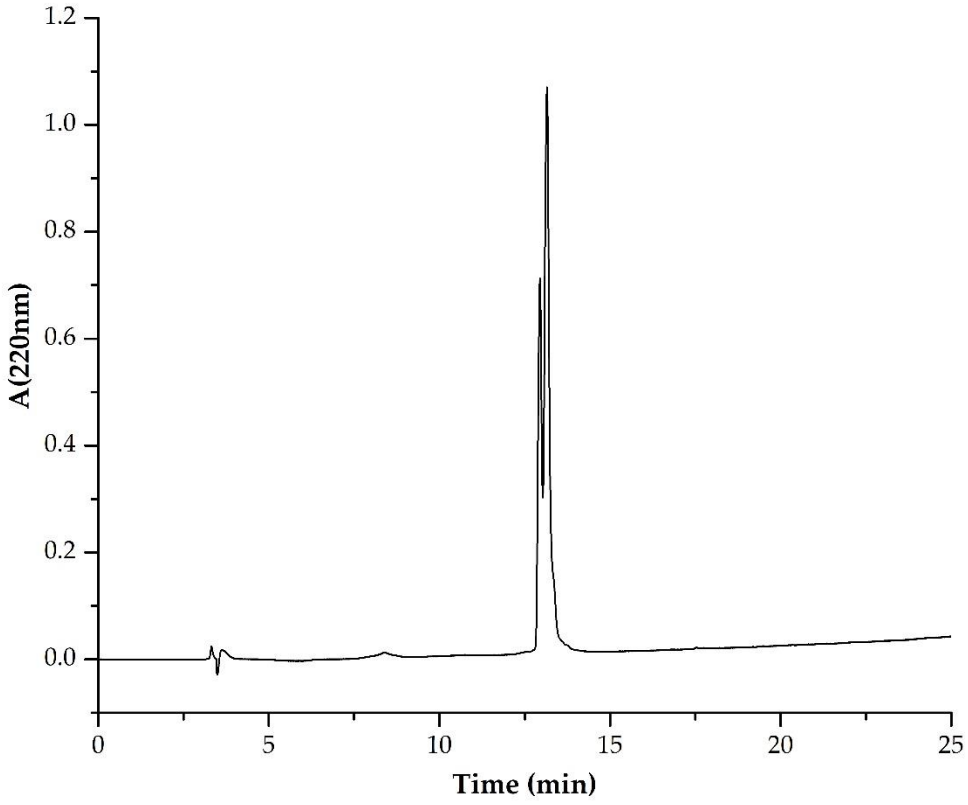

Figure S7. HPLC chromatogram of Cf-RQIKIGFQNRRKGKK-*NH*$_2$. Retention time was obtained on Hypersil Hypurity C18 column (4.6 mm x 150 mm, 5 µm, 190 Å). The applied linear gradient elution was 0 min 0% B, 2 min 0% B, 22 min 90% B at 1 mL/min flow rate. The detection was carried on at λ = 220 nm.

2.2 Mass spectrometry

The determination of the molecular weight of peptides was performed by ESI-MS, using Bruker Amazon SL (Germany). The samples were prepared and dissolved in water-acetonitrile solution (50:50) containing 0.1% formic acid. The injection of the samples was done directly through a syringe pump. Parameters: capillary voltage: 4 kV, nebulizer gas: 10 psi, dry gas: 4 L/min, heated capillary temperature: 250 ºC.

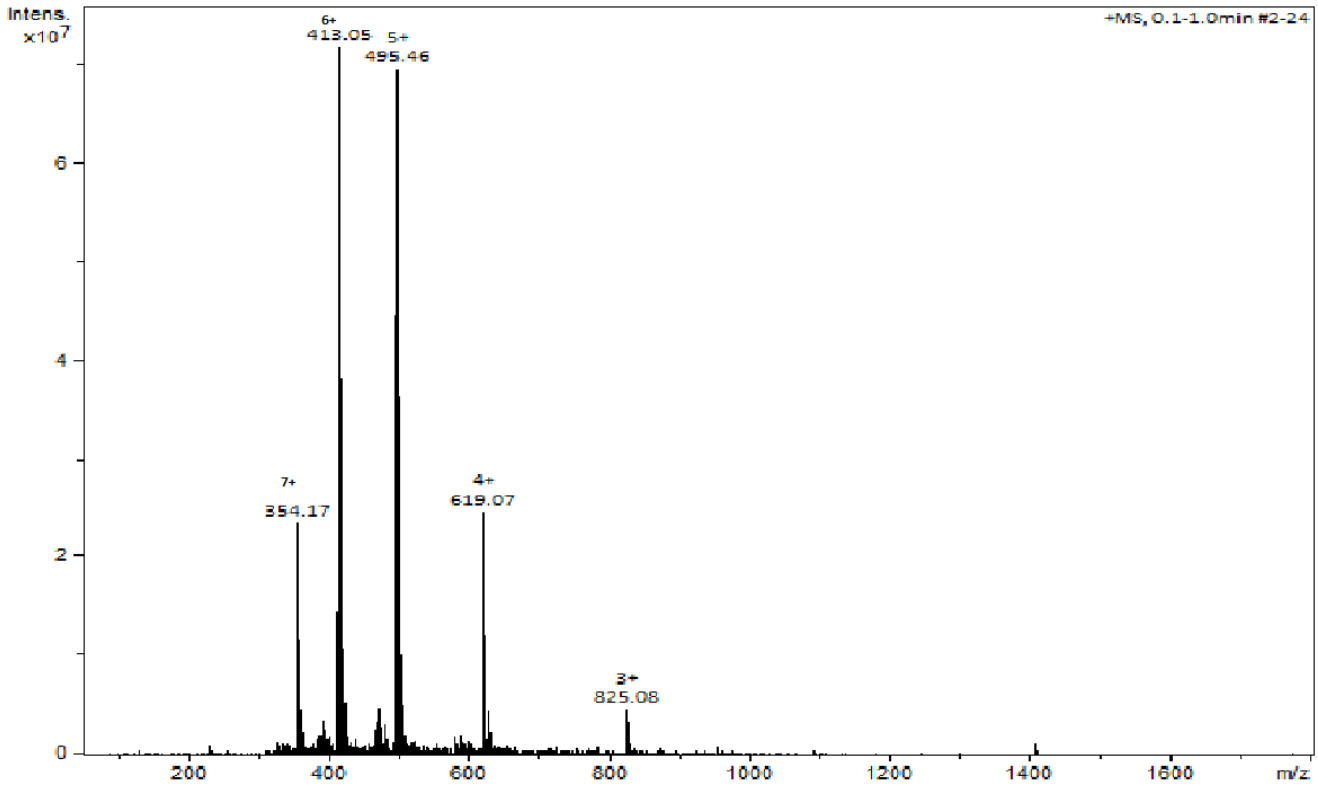

Figure S8. MS Spectrum of Cf-RQIKIWFQNRRKWKK-*NH*$_2$. The identification of the conjugate was determined using Bruker Amazon SL (Germany). The sample is dissolved in water-acetonitrile (50:50) with 0.1% formic acid.

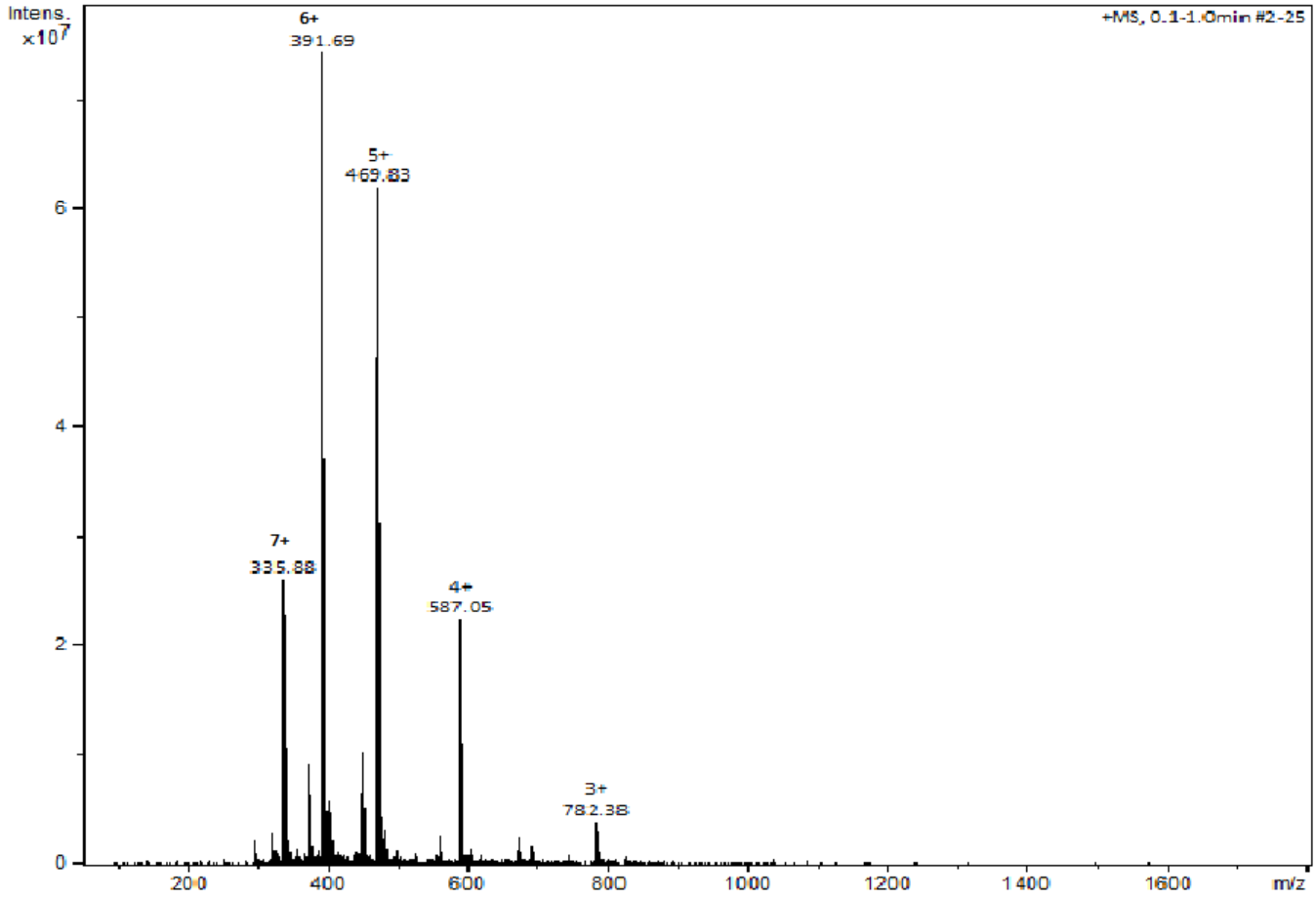

Figure S9. MS Spectrum of Cf-RQIKIWFQNRRK-azaGly-KK-NH_2. The identification of the conjugate was determined using Bruker Amazon SL (Germany). The sample is dissolved in water-acetonitrile (50:50) with 0.1% formic acid.

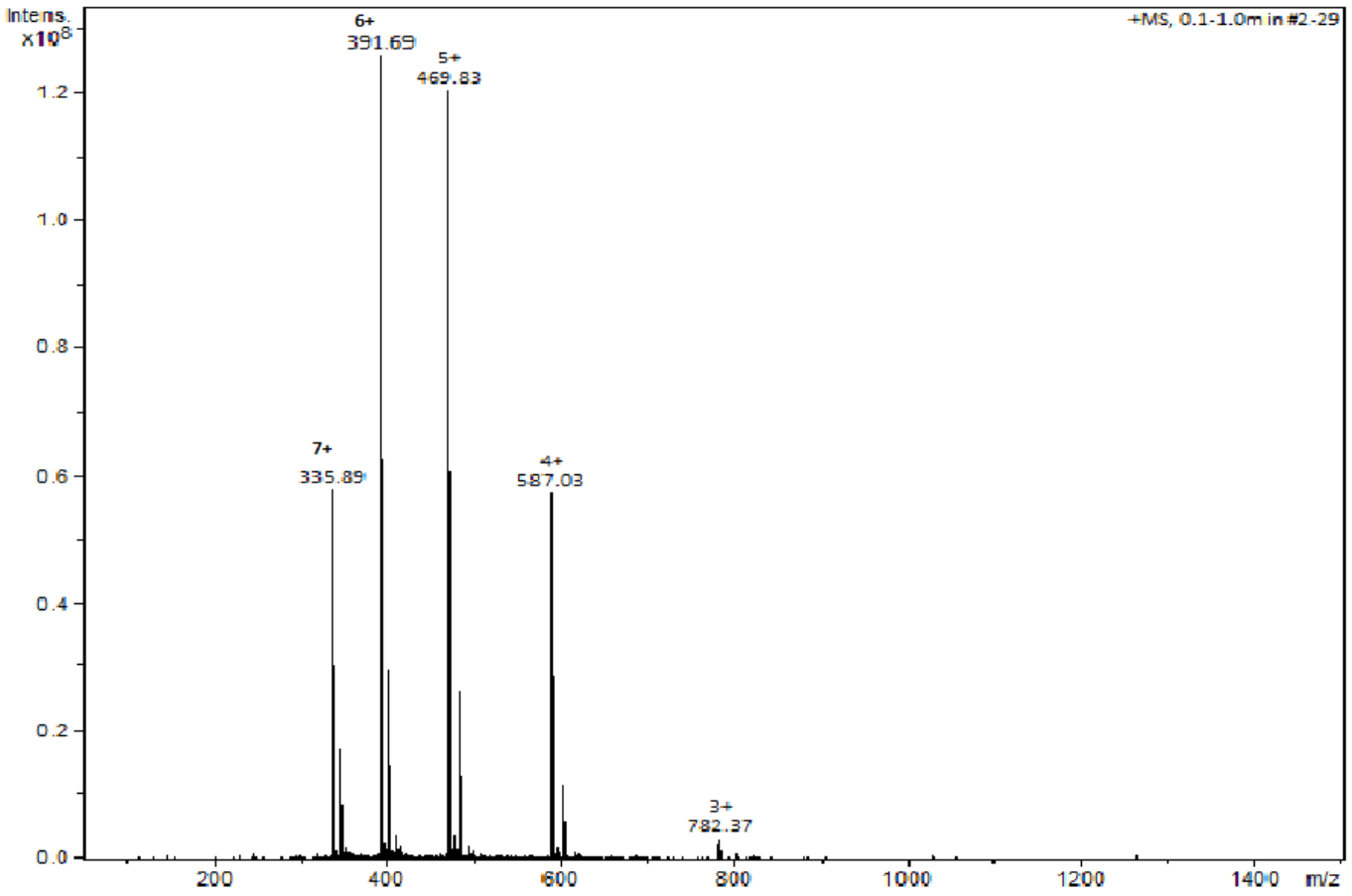

Figure S10. MS Spectrum of Cf-RQIKI-azaGly-FQNRRKWKK-*NH*$_2$. The identification of the conjugate was determined using Bruker Amazon SL (Germany). The sample is dissolved in water-acetonitrile (50:50) with 0.1% formic acid.

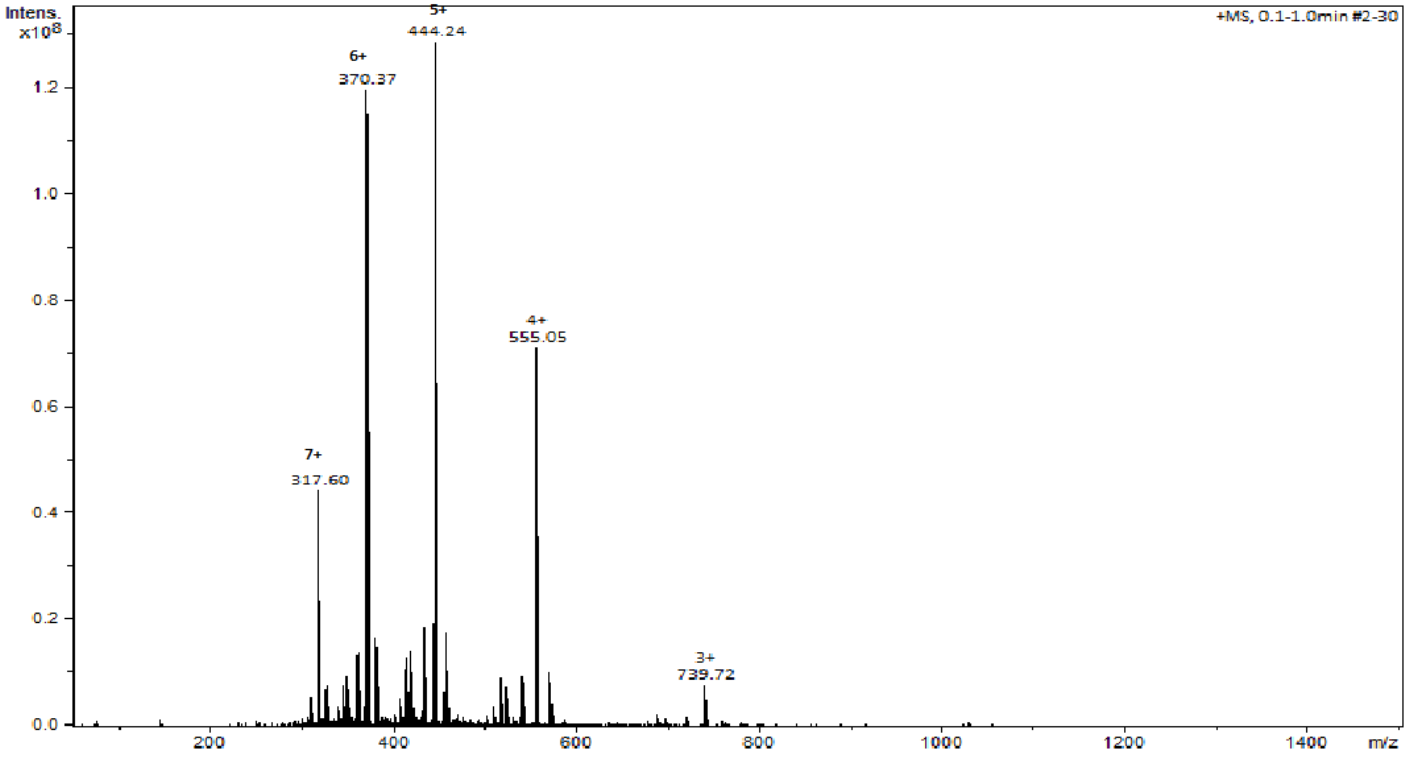

Figure S11. MS Spectrum of Cf-RQIKI-azaGly-FQNRRK-azaGly-KK-*NH*$_2$. The identification of the conjugate was determined using Bruker Amazon SL (Germany). The sample is dissolved in water-acetonitrile (50:50) with 0.1% formic acid.

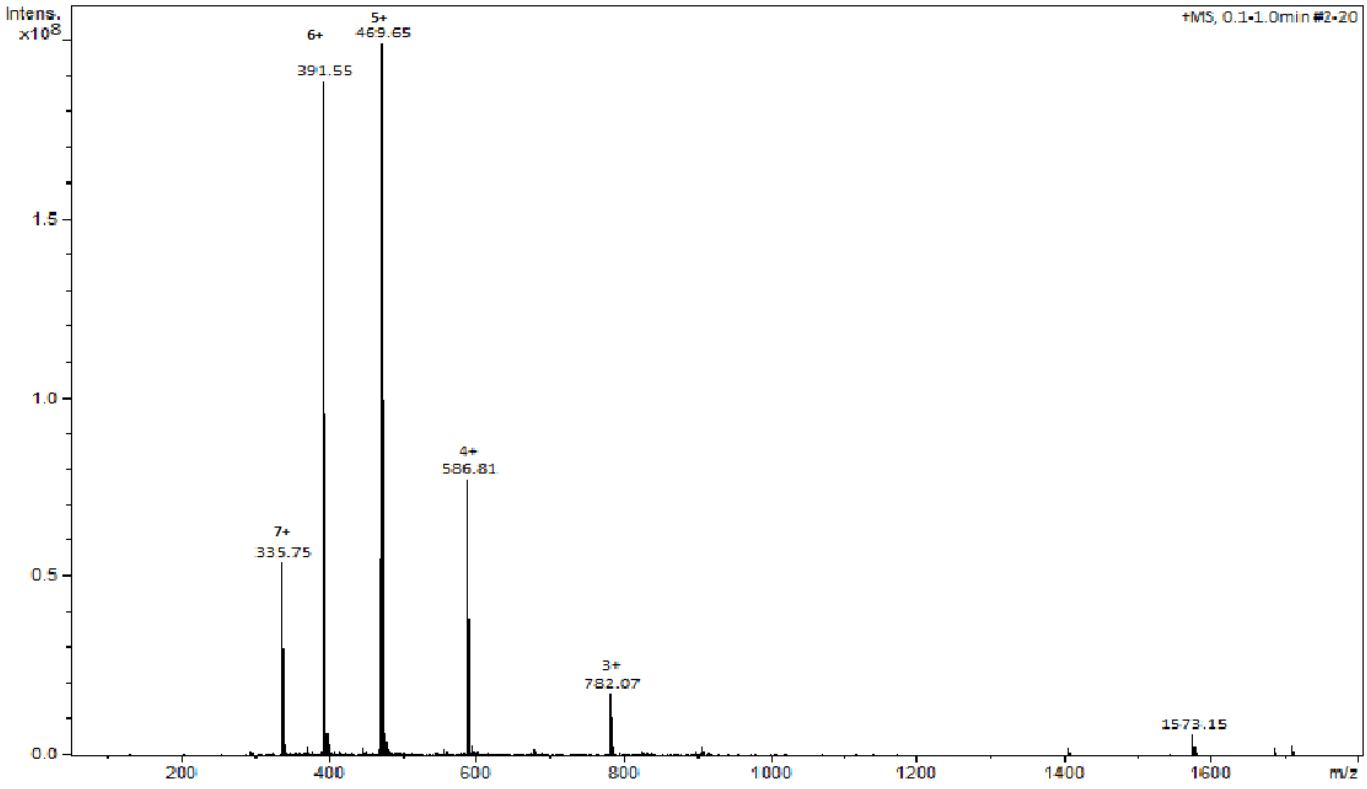

Figure S12. MS Spectrum of Cf-RQIKIWFQNRRKGKK-*NH*$_2$. The identification of the conjugate was determined using Bruker Amazon SL (Germany). The sample is dissolved in water-acetonitrile (50:50) with 0.1% formic acid.

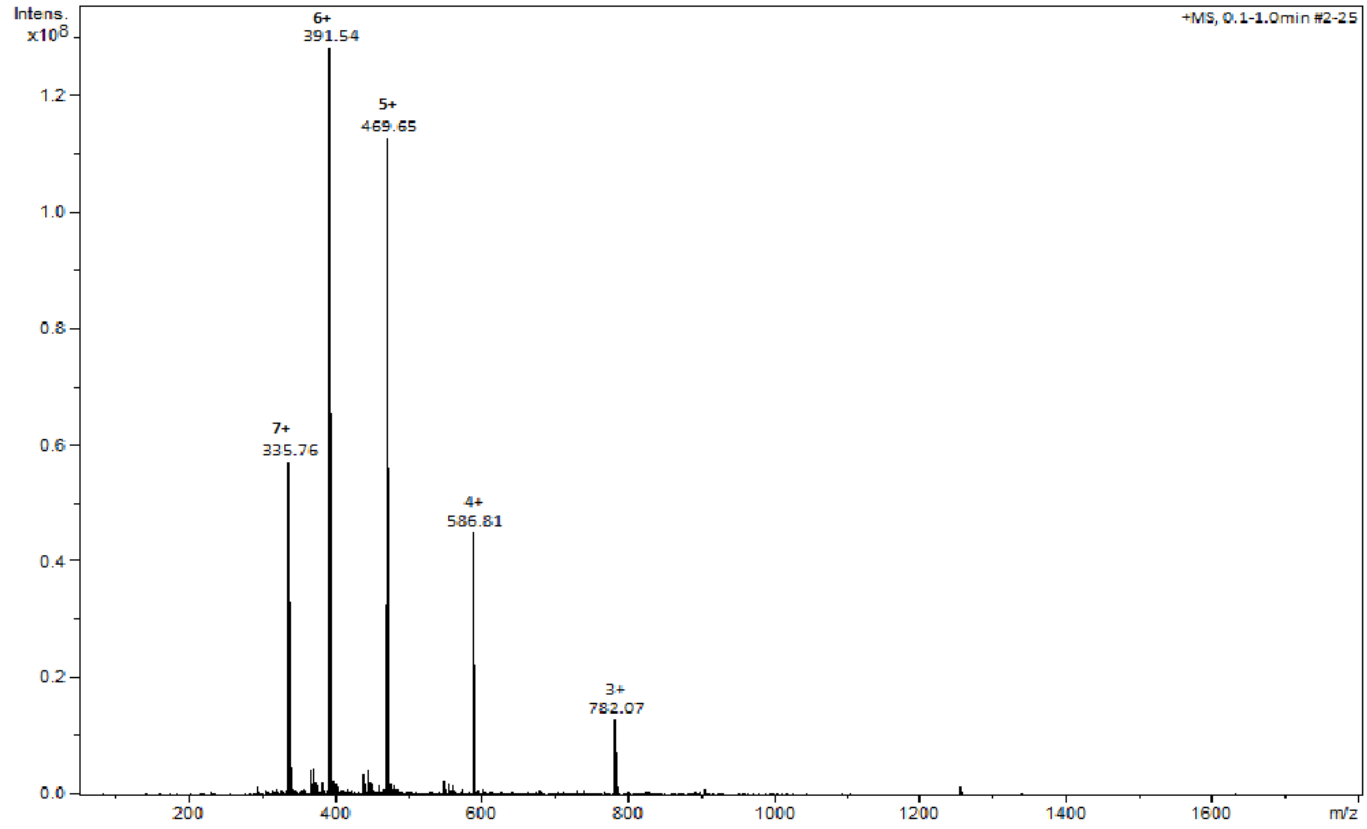

Figure S13. MS Spectrum of Cf-RQIKIGFQNRRKWKK-*NH*$_2$. The identification of the conjugate was determined using Bruker Amazon SL (Germany). The sample is dissolved in water-acetonitrile (50:50) with 0.1% formic acid.

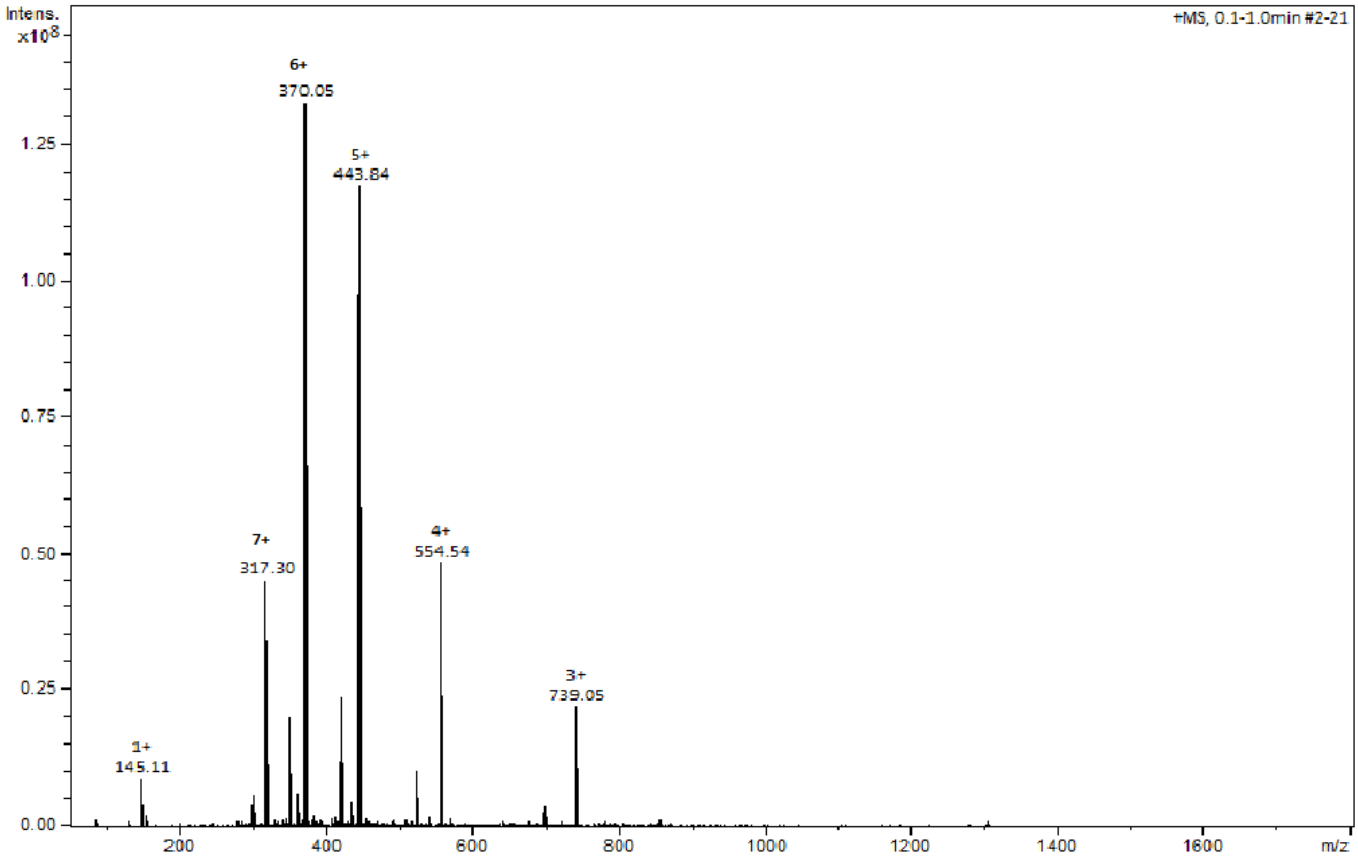

Figure S14. MS Spectrum of Cf-RQIKIGFQNRRKGKK-*NH*$_2$. The identification of the conjugate was determined using Bruker Amazon SL (Germany). The sample is dissolved in water-acetonitrile (50:50) with 0.1% formic acid.

3. Cytotoxicity of Peptide Conjugates

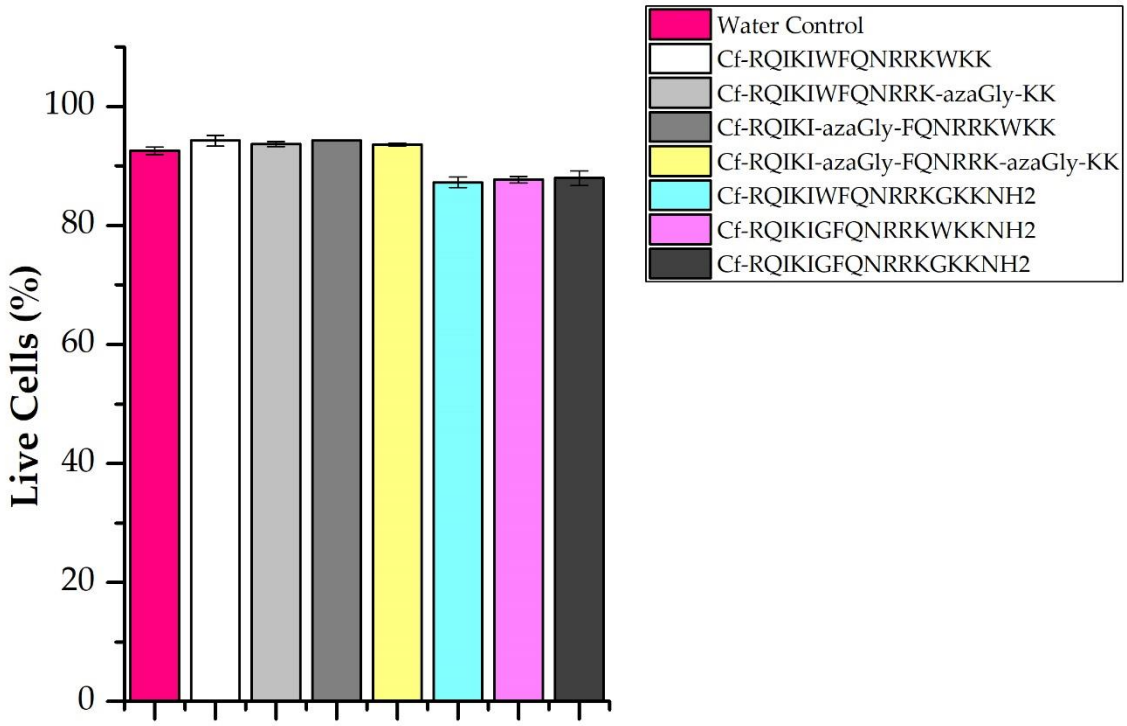

Figure S15. Evaluation of the cytotoxicity of peptides by examining the percentage of live cells by flow cytometry technique. Cells were incubated with 5 μM peptide solution for 90 min at 37°C.

4. ECD measurement

The UV-CD measurements were performed on a JASCO (Tokyo, Japan) J-1500 spectropolarimeter. Each spectrum was the average of five scans collected in the far UV (185-260 nm) range with a 0.1 mm path length quartz cell. The following settings were used throughout the measurements: a temperature control system at room temperature, the bandwidth of 1 nm, 0.2 nm step size, 4 s response time, and a scan rate of 50 nm/min. All spectra were corrected by subtracting the solvent spectrum acquired under identical conditions. All CD data were processed from mDeg to mean residue ellipticity (deg cm^2 $dmol^{-1}$) using the Spectra Analysis function of Jasco Spectra Manager, to account for the concentration differences.

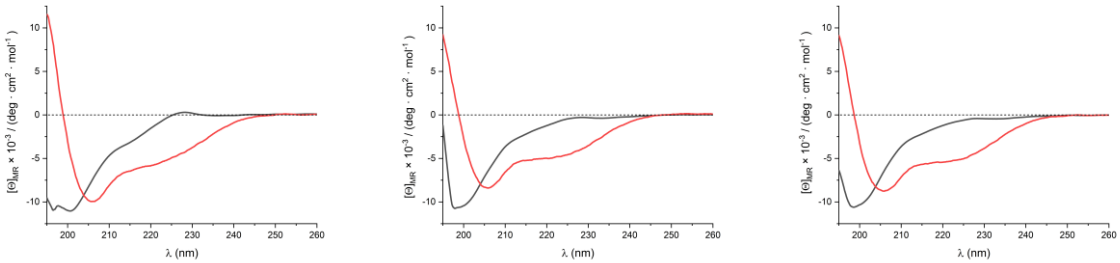

Figure S16. ECD spectra in PBS buffer, pH: 7.3 at 25°C (black) and 50 % TFE in PBS buffer (red) of Pen(desMet) (left panel), Trp56aGlyPen(desMet) (middle panel) and Trp56GlyPen(desMet) (right panel).

5. Calculations

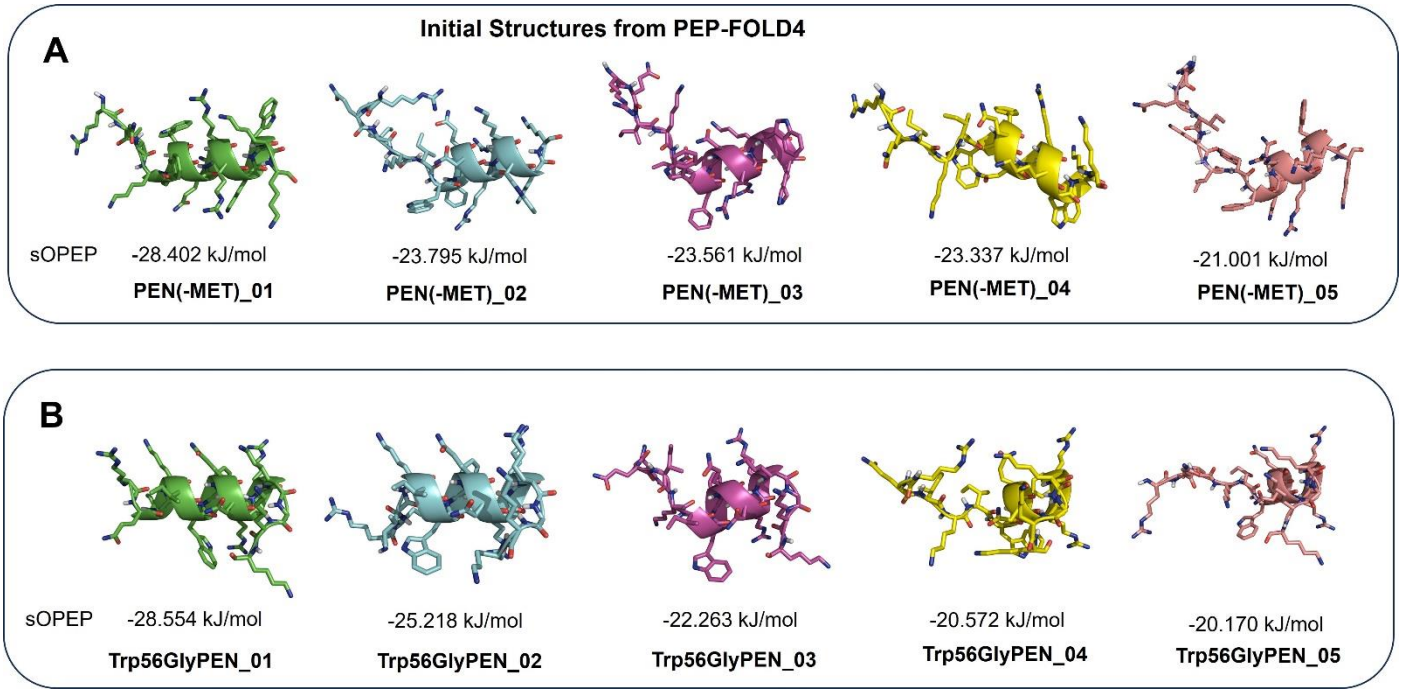

Figure S17. Initial structures of PEN(-Met) and Trp56GlyPen peptide were generated from PEP-Fold4. The best five structures of model peptides were shown with the sOPEP energy for each conformer.

Table S1. The coordinates of optimized structures of model peptides, Pen(-Met), Trp56aGlyPen, and Trp56GlyPen at the wB97XD/3-21G* level of theory.

TITLE Pen(-Met)

REMARK Created by GaussView 6.1.1, E = =-7066.4308708 a.u.

ATOM	1	N	ARG A	1	-14.562	0.239	1.661	N
ATOM	2	CA	ARG A	1	-14.639	-0.989	0.840	C
ATOM	3	C	ARG A	1	-13.569	-0.912	-0.271	C
ATOM	4	O	ARG A	1	-13.555	-1.626	-1.287	O
ATOM	5	CB	ARG A	1	-16.046	-1.261	0.263	C
ATOM	6	CG	ARG A	1	-16.234	-2.701	-0.257	C
ATOM	7	CD	ARG A	1	-17.695	-2.917	-0.692	C
ATOM	8	NE	ARG A	1	-17.912	-4.317	-1.117	N
ATOM	9	CZ	ARG A	1	-19.115	-4.903	-1.173	C
ATOM	10	NH1	ARG A	1	-19.209	-6.225	-1.355	N
ATOM	11	NH2	ARG A	1	-20.227	-4.174	-1.038	N
ATOM	12	H	ARG A	1	-14.722	0.070	2.652	H
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ATOM	15	H03	ARG A	1	-14.356	-1.832	1.481	H
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ATOM	27	CA	GLN A	2	-11.499	0.260	-0.882	C
ATOM	28	C	GLN A	2	-10.285	0.679	-0.046	C
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ATOM	34	OE1	GLN A	2	-12.019	2.862	-4.229	O
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ATOM	40	H05	GLN A	2	-13.612	2.128	-5.995	H
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ATOM	43	N	ILE A	3	-9.679	-0.281	0.678	N
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ATOM	47	CB	ILE A	3	-8.501	-0.984	2.775	C
ATOM	48	CG1	ILE A	3	-9.865	-1.150	3.483	C
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ATOM	51	H	ILE A	3	-10.018	-1.236	0.641	H
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ATOM	53	H02	ILE A	3	-8.859	1.020	2.072	H
ATOM	54	H03	ILE A	3	-8.193	-1.946	2.348	H
ATOM	55	H04	ILE A	3	-10.649	-1.357	2.746	H
ATOM	56	H05	ILE A	3	-7.309	-1.228	4.583	H
ATOM	57	H06	ILE A	3	-10.863	-2.429	4.932	H
ATOM	58	H07	ILE A	3	-10.125	-0.202	3.970	H
ATOM	59	H08	ILE A	3	-7.737	0.451	4.225	H
ATOM	60	H09	ILE A	3	-9.196	-2.062	5.361	H
ATOM	61	H10	ILE A	3	-6.460	-0.383	3.290	H

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ATOM     62  N   LYS A   4      -7.227   1.383   0.184                N
ATOM     63  CA  LYS A   4      -6.141   1.709  -0.737                C
ATOM     64  C   LYS A   4      -4.862   2.108   0.013                C
ATOM     65  O   LYS A   4      -3.769   2.283  -0.582                O
ATOM     66  CB  LYS A   4      -6.624   2.796  -1.718                C
ATOM     67  CG  LYS A   4      -7.720   2.227  -2.651                C
ATOM     68  CD  LYS A   4      -8.590   3.289  -3.356                C
ATOM     69  CE  LYS A   4      -9.426   4.091  -2.343                C
ATOM     70  NZ  LYS A   4     -10.640   4.692  -3.047                N
ATOM     71  H   LYS A   4      -8.115   1.907   0.127                H
ATOM     72  H01 LYS A   4     -11.253   3.888  -3.466                H
ATOM     73  H02 LYS A   4      -5.864   0.809  -1.301                H
ATOM     74  H03 LYS A   4      -5.769   3.147  -2.302                H
ATOM     75  H04 LYS A   4      -8.391   1.589  -2.069                H
ATOM     76  H05 LYS A   4      -9.278   2.766  -4.032                H
ATOM     77  H06 LYS A   4      -8.862   4.914  -1.901                H
ATOM     78  H07 LYS A   4     -10.350   5.299  -3.827                H
ATOM     79  H08 LYS A   4      -7.003   3.640  -1.129                H
ATOM     80  H09 LYS A   4      -7.243   1.599  -3.411                H
ATOM     81  H10 LYS A   4      -7.970   3.959  -3.962                H
ATOM     82  H11 LYS A   4      -9.807   3.437  -1.554                H
ATOM     83  H12 LYS A   4     -11.208   5.253  -2.399                H
ATOM     84  N   ILE A   5      -4.976   2.136   1.347                N
ATOM     85  CA  ILE A   5      -3.799   2.135   2.207                C
ATOM     86  C   ILE A   5      -2.878   1.003   1.767                C
ATOM     87  O   ILE A   5      -1.634   1.113   1.868                O
ATOM     88  CB  ILE A   5      -4.189   1.953   3.698                C
ATOM     89  CG1 ILE A   5      -5.242   3.005   4.115                C
ATOM     90  CG2 ILE A   5      -2.924   2.089   4.568                C
ATOM     91  CD  ILE A   5      -5.691   2.852   5.579                C
ATOM     92  H   ILE A   5      -5.898   2.052   1.754                H
ATOM     93  H01 ILE A   5      -6.033   1.829   5.772                H
ATOM     94  H02 ILE A   5      -3.245   3.068   2.109                H
ATOM     95  H03 ILE A   5      -4.617   0.949   3.814                H
ATOM     96  H04 ILE A   5      -6.136   2.925   3.484                H
ATOM     97  H05 ILE A   5      -2.557   3.120   4.524                H
ATOM     98  H06 ILE A   5      -6.516   3.535   5.797                H
ATOM     99  H07 ILE A   5      -4.817   4.003   3.950                H
ATOM    100  H08 ILE A   5      -2.111   1.442   4.233                H
ATOM    101  H09 ILE A   5      -4.880   3.082   6.274                H
ATOM    102  H10 ILE A   5      -3.155   1.845   5.607                H
ATOM    103  N   TRP A   6      -3.445  -0.121   1.304                N
ATOM    104  CA  TRP A   6      -2.565  -1.237   0.965                C
ATOM    105  C   TRP A   6      -1.622  -0.904  -0.185                C
ATOM    106  O   TRP A   6      -0.469  -1.390  -0.219                O
ATOM    107  CB  TRP A   6      -3.413  -2.497   0.672                C
ATOM    108  CG  TRP A   6      -3.848  -3.068   1.983                C
ATOM    109  CD1 TRP A   6      -5.063  -2.977   2.603                C
ATOM    110  CD2 TRP A   6      -2.947  -3.707   2.908                C
ATOM    111  CE2 TRP A   6      -3.685  -3.981   4.086                C
ATOM    112  CE3 TRP A   6      -1.589  -4.054   2.834                C
ATOM    113  NE1 TRP A   6      -4.975  -3.529   3.874                N
ATOM    114  CZ2 TRP A   6      -3.087  -4.592   5.192                C
ATOM    115  CZ3 TRP A   6      -0.998  -4.655   3.937                C
ATOM    116  CH2 TRP A   6      -1.743  -4.917   5.105                C
ATOM    117  H   TRP A   6      -4.461  -0.255   1.245                H
ATOM    118  H01 TRP A   6      -1.260  -5.400   5.945                H
ATOM    119  H02 TRP A   6      -1.924  -1.443   1.823                H
ATOM    120  H03 TRP A   6      -2.791  -3.220   0.133                H
ATOM    121  H04 TRP A   6      -5.966  -2.529   2.225                H
ATOM    122  H05 TRP A   6      -1.025  -3.881   1.922                H
ATOM    123  H06 TRP A   6      -5.747  -3.654   4.513                H
ATOM    124  H07 TRP A   6      -3.651  -4.816   6.088                H
ATOM    125  H08 TRP A   6       0.043  -4.956   3.899                H
ATOM    126  H09 TRP A   6      -4.265  -2.231   0.039                H
ATOM    127  N   PHE A   7      -2.099  -0.098  -1.148                N
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ATOM    128  CA  PHE A   7      -1.214   0.374  -2.218              C
ATOM    129  C   PHE A   7      -0.083   1.194  -1.596              C
ATOM    130  O   PHE A   7       1.119   1.028  -1.863              O
ATOM    131  CB  PHE A   7      -2.028   1.248  -3.199              C
ATOM    132  CG  PHE A   7      -1.112   2.002  -4.138              C
ATOM    133  CD1 PHE A   7      -0.618   1.390  -5.291              C
ATOM    134  CD2 PHE A   7      -0.721   3.309  -3.840              C
ATOM    135  CE1 PHE A   7       0.250   2.075  -6.137              C
ATOM    136  CE2 PHE A   7       0.146   3.996  -4.685              C
ATOM    137  CZ  PHE A   7       0.633   3.380  -5.836              C
ATOM    138  H   PHE A   7      -2.981   0.392  -1.014              H
ATOM    139  H01 PHE A   7       1.287   3.920  -6.509              H
ATOM    140  H02 PHE A   7      -0.750  -0.469  -2.731              H
ATOM    141  H03 PHE A   7      -2.639   1.944  -2.616              H
ATOM    142  H04 PHE A   7      -0.928   0.381  -5.539              H
ATOM    143  H05 PHE A   7      -1.108   3.791  -2.948              H
ATOM    144  H06 PHE A   7       0.610   1.600  -7.041              H
ATOM    145  H07 PHE A   7       0.419   5.021  -4.462              H
ATOM    146  H08 PHE A   7      -2.701   0.595  -3.764              H
ATOM    147  N   GLN A   8      -0.508   2.115  -0.698              N
ATOM    148  CA  GLN A   8       0.494   2.893   0.016              C
ATOM    149  C   GLN A   8       1.533   1.933   0.621              C
ATOM    150  O   GLN A   8       2.761   2.183   0.621              O
ATOM    151  CB  GLN A   8      -0.102   3.633   1.220              C
ATOM    152  CG  GLN A   8      -1.283   4.575   1.001              C
ATOM    153  CD  GLN A   8      -1.726   5.059   2.388              C
ATOM    154  NE2 GLN A   8      -2.833   5.822   2.417              N
ATOM    155  OE1 GLN A   8      -1.113   4.749   3.435              O
ATOM    156  H   GLN A   8      -1.492   2.189  -0.457              H
ATOM    157  H01 GLN A   8      -3.300   6.126   1.574              H
ATOM    158  H02 GLN A   8       1.025   3.564  -0.664              H
ATOM    159  H03 GLN A   8       0.705   4.215   1.667              H
ATOM    160  H04 GLN A   8      -2.123   4.068   0.511              H
ATOM    161  H05 GLN A   8      -3.134   6.217   3.302              H
ATOM    162  H06 GLN A   8      -0.433   2.876   1.932              H
ATOM    163  H07 GLN A   8      -1.008   5.442   0.389              H
ATOM    164  N   ASN A   9       0.988   0.882   1.243              N
ATOM    165  CA  ASN A   9       1.808  -0.068   1.973              C
ATOM    166  C   ASN A   9       2.812  -0.747   1.059              C
ATOM    167  O   ASN A   9       3.991  -0.910   1.443              O
ATOM    168  CB  ASN A   9       0.915  -1.115   2.638              C
ATOM    169  CG  ASN A   9       0.067  -0.496   3.742              C
ATOM    170  ND2 ASN A   9      -0.871  -1.301   4.251              N
ATOM    171  OD1 ASN A   9       0.247   0.673   4.154              O
ATOM    172  H   ASN A   9      -0.032   0.801   1.322              H
ATOM    173  H01 ASN A   9      -0.994  -2.269   3.948              H
ATOM    174  H02 ASN A   9       2.402   0.440   2.730              H
ATOM    175  H03 ASN A   9       1.542  -1.897   3.081              H
ATOM    176  H04 ASN A   9      -1.440  -0.972   5.022              H
ATOM    177  H05 ASN A   9       0.284  -1.572   1.868              H
ATOM    178  N   ARG A  10       2.378  -1.178  -0.139              N
ATOM    179  CA  ARG A  10       3.406  -1.784  -0.978              C
ATOM    180  C   ARG A  10       4.399  -0.724  -1.461              C
ATOM    181  O   ARG A  10       5.592  -1.026  -1.706              O
ATOM    182  CB  ARG A  10       2.909  -2.662  -2.144              C
ATOM    183  CG  ARG A  10       4.120  -3.513  -2.587              C
ATOM    184  CD  ARG A  10       3.878  -4.459  -3.766              C
ATOM    185  NE  ARG A  10       5.169  -5.119  -4.057              N
ATOM    186  CZ  ARG A  10       5.302  -6.288  -4.687              C
ATOM    187  NH1 ARG A  10       6.493  -6.894  -4.703              N
ATOM    188  NH2 ARG A  10       4.250  -6.859  -5.291              N
ATOM    189  H   ARG A  10       1.393  -1.112  -0.414              H
ATOM    190  H01 ARG A  10       4.298  -7.803  -5.653              H
ATOM    191  H02 ARG A  10       4.000  -2.425  -0.323              H
ATOM    192  H03 ARG A  10       2.530  -2.039  -2.961              H
ATOM    193  H04 ARG A  10       4.464  -4.113  -1.737              H
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ATOM    194  H05 ARG A  10       3.526  -3.904  -4.644                H
ATOM    195  H06 ARG A  10       6.013  -4.649  -3.720                H
ATOM    196  H07 ARG A  10       7.272  -6.520  -4.161                H
ATOM    197  H08 ARG A  10       3.391  -6.352  -5.448                H
ATOM    198  H09 ARG A  10       2.098  -3.303  -1.781                H
ATOM    199  H10 ARG A  10       4.934  -2.831  -2.841                H
ATOM    200  H11 ARG A  10       3.140  -5.222  -3.495                H
ATOM    201  H12 ARG A  10       6.667  -7.707  -5.281                H
ATOM    202  N   ARG A  11       3.974   0.546  -1.585                N
ATOM    203  CA  ARG A  11       5.019   1.534  -1.855                C
ATOM    204  C   ARG A  11       6.044   1.525  -0.700                C
ATOM    205  O   ARG A  11       7.278   1.550  -0.909                O
ATOM    206  CB  ARG A  11       4.436   2.948  -2.034                C
ATOM    207  CG  ARG A  11       5.556   3.886  -2.531                C
ATOM    208  CD  ARG A  11       5.111   5.354  -2.607                C
ATOM    209  NE  ARG A  11       6.234   6.173  -3.124                N
ATOM    210  CZ  ARG A  11       6.112   7.409  -3.620                C
ATOM    211  NH1 ARG A  11       7.137   7.982  -4.259                N
ATOM    212  NH2 ARG A  11       4.959   8.075  -3.486                N
ATOM    213  H   ARG A  11       2.987   0.809  -1.525                H
ATOM    214  H01 ARG A  11       4.788   8.937  -3.990                H
ATOM    215  H02 ARG A  11       5.586   1.239  -2.742                H
ATOM    216  H03 ARG A  11       4.013   3.270  -1.078                H
ATOM    217  H04 ARG A  11       5.868   3.563  -3.530                H
ATOM    218  H05 ARG A  11       4.818   5.705  -1.610                H
ATOM    219  H06 ARG A  11       7.159   5.760  -3.069                H
ATOM    220  H07 ARG A  11       7.950   7.453  -4.547                H
ATOM    221  H08 ARG A  11       4.244   7.768  -2.841                H
ATOM    222  H09 ARG A  11       3.625   2.905  -2.771                H
ATOM    223  H10 ARG A  11       6.422   3.796  -1.864                H
ATOM    224  H11 ARG A  11       4.264   5.450  -3.295                H
ATOM    225  H12 ARG A  11       7.136   8.970  -4.487                H
ATOM    226  N   LYS A  12       5.511   1.541   0.533                N
ATOM    227  CA  LYS A  12       6.378   1.563   1.719                C
ATOM    228  C   LYS A  12       7.358   0.374   1.704                C
ATOM    229  O   LYS A  12       8.555   0.521   2.017                O
ATOM    230  CB  LYS A  12       5.501   1.502   2.991                C
ATOM    231  CG  LYS A  12       4.637   2.771   3.156                C
ATOM    232  CD  LYS A  12       3.456   2.577   4.145                C
ATOM    233  CE  LYS A  12       2.334   3.556   3.775                C
ATOM    234  NZ  LYS A  12       0.996   3.211   4.416                N
ATOM    235  H   LYS A  12       4.494   1.540   0.652                H
ATOM    236  H01 LYS A  12       0.749   2.191   4.238                H
ATOM    237  H02 LYS A  12       7.005   2.458   1.718                H
ATOM    238  H03 LYS A  12       6.153   1.368   3.860                H
ATOM    239  H04 LYS A  12       4.215   3.022   2.180                H
ATOM    240  H05 LYS A  12       3.781   2.710   5.181                H
ATOM    241  H06 LYS A  12       2.176   3.491   2.700                H
ATOM    242  H07 LYS A  12       0.221   3.812   4.019                H
ATOM    243  H08 LYS A  12       4.861   0.620   2.894                H
ATOM    244  H09 LYS A  12       5.263   3.609   3.481                H
ATOM    245  H10 LYS A  12       3.067   1.560   4.043                H
ATOM    246  H11 LYS A  12       2.581   4.585   4.046                H
ATOM    247  H12 LYS A  12       1.032   3.352   5.433                H
ATOM    248  N   TRP A  13       6.784  -0.788   1.341                N
ATOM    249  CA  TRP A  13       7.494  -2.060   1.211                C
ATOM    250  C   TRP A  13       8.759  -1.954   0.382                C
ATOM    251  O   TRP A  13       9.683  -2.773   0.485                O
ATOM    252  CB  TRP A  13       6.518  -3.046   0.497                C
ATOM    253  CG  TRP A  13       7.193  -4.243  -0.096                C
ATOM    254  CD1 TRP A  13       7.537  -5.422   0.507                C
ATOM    255  CD2 TRP A  13       7.713  -4.305  -1.442                C
ATOM    256  CE2 TRP A  13       8.369  -5.560  -1.583                C
ATOM    257  CE3 TRP A  13       7.694  -3.402  -2.516                C
ATOM    258  NE1 TRP A  13       8.238  -6.224  -0.387                N
ATOM    259  CZ2 TRP A  13       9.009  -5.918  -2.776                C
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ATOM    260  CZ3 TRP A  13       8.316  -3.768  -3.706                C
ATOM    261  CH2 TRP A  13       8.976  -5.011  -3.831                C
ATOM    262  H   TRP A  13       5.771  -0.810   1.195                H
ATOM    263  H01 TRP A  13       9.475  -5.258  -4.762                H
ATOM    264  H02 TRP A  13       7.808  -2.459   2.179                H
ATOM    265  H03 TRP A  13       6.076  -2.468  -0.316                H
ATOM    266  H04 TRP A  13       7.356  -5.754   1.516                H
ATOM    267  H05 TRP A  13       7.219  -2.434  -2.401                H
ATOM    268  H06 TRP A  13       8.623  -7.131  -0.166                H
ATOM    269  H07 TRP A  13       9.540  -6.858  -2.868                H
ATOM    270  H08 TRP A  13       8.311  -3.086  -4.549                H
ATOM    271  H09 TRP A  13       5.732  -3.329   1.204                H
ATOM    272  N   LYS A  14       8.822  -0.938  -0.520                N
ATOM    273  CA  LYS A  14      10.066  -0.860  -1.257                C
ATOM    274  C   LYS A  14      11.242  -0.759  -0.278                C
ATOM    275  O   LYS A  14      12.393  -1.200  -0.589                O
ATOM    276  CB  LYS A  14      10.070   0.309  -2.277                C
ATOM    277  CG  LYS A  14      10.416  -0.158  -3.704                C
ATOM    278  CD  LYS A  14      11.825  -0.802  -3.829                C
ATOM    279  CE  LYS A  14      11.830  -2.348  -3.685                C
ATOM    280  NZ  LYS A  14      12.769  -2.778  -2.563                N
ATOM    281  H   LYS A  14       8.110  -0.217  -0.629                H
ATOM    282  H01 LYS A  14      12.618  -3.760  -2.303                H
ATOM    283  H02 LYS A  14      10.207  -1.816  -1.765                H
ATOM    284  H03 LYS A  14      10.793   1.070  -1.963                H
ATOM    285  H04 LYS A  14      10.373   0.710  -4.369                H
ATOM    286  H05 LYS A  14      12.476  -0.364  -3.065                H
ATOM    287  H06 LYS A  14      12.162  -2.837  -4.603                H
ATOM    288  H07 LYS A  14      12.584  -2.114  -1.667                H
ATOM    289  H08 LYS A  14       9.085   0.785  -2.265                H
ATOM    290  H09 LYS A  14       9.653  -0.865  -4.052                H
ATOM    291  H10 LYS A  14      12.254  -0.544  -4.801                H
ATOM    292  H11 LYS A  14      10.843  -2.735  -3.426                H
ATOM    293  H12 LYS A  14      13.750  -2.661  -2.846                H
ATOM    294  N   LYS A  15      11.030  -0.161   0.887                N
ATOM    295  CA  LYS A  15      12.045  -0.263   1.949                C
ATOM    296  C   LYS A  15      11.304  -0.271   3.281                C
ATOM    297  O   LYS A  15      11.488   0.506   4.205                O
ATOM    298  CB  LYS A  15      13.088   0.861   1.905                C
ATOM    299  CG  LYS A  15      14.225   0.584   2.913                C
ATOM    300  CD  LYS A  15      15.308   1.688   2.907                C
ATOM    301  CE  LYS A  15      16.355   1.355   3.976                C
ATOM    302  NZ  LYS A  15      17.462   2.436   4.040                N
ATOM    303  H   LYS A  15      10.076   0.118   1.173                H
ATOM    304  H01 LYS A  15      18.162   2.203   4.763                H
ATOM    305  H02 LYS A  15      12.539  -1.233   1.824                H
ATOM    306  H04 LYS A  15      12.600   1.810   2.144                H
ATOM    307  H05 LYS A  15      14.690  -0.381   2.677                H
ATOM    308  H06 LYS A  15      14.836   2.653   3.129                H
ATOM    309  H07 LYS A  15      16.865   0.413   3.763                H
ATOM    310  H08 LYS A  15      17.054   3.356   4.268                H
ATOM    311  H09 LYS A  15      13.490   0.902   0.888                H
ATOM    312  H10 LYS A  15      13.779   0.526   3.909                H
ATOM    313  H11 LYS A  15      15.777   1.743   1.917                H
ATOM    314  H12 LYS A  15      15.910   1.318   4.972                H
ATOM    315  H13 LYS A  15      17.947   2.512   3.132                H
TER     316      LYS A  15
HETATM  317  O         0      10.411  -1.294   3.318                O
HETATM  318  H         0       9.908  -1.265   4.168                H
END
CONECT  296  317
CONECT  317  296  318
CONECT  318  317
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ATOM 1 N ARG A 1 -10.525 -1.430 -2.573 N
ATOM 2 CA ARG A 1 -11.220 -1.197 -1.266 C
ATOM 3 C ARG A 1 -10.042 -1.186 -0.283 C
ATOM 4 O ARG A 1 -9.519 -0.127 0.120 O
ATOM 5 CB ARG A 1 -12.331 -2.238 -1.046 C
ATOM 6 CG ARG A 1 -13.181 -2.052 0.228 C
ATOM 7 CD ARG A 1 -14.356 -3.053 0.196 C
ATOM 8 NE ARG A 1 -15.240 -2.893 1.369 N
ATOM 9 CZ ARG A 1 -16.506 -3.343 1.413 C
ATOM 10 NH1 ARG A 1 -17.307 -2.984 2.421 N
ATOM 11 NH2 ARG A 1 -16.971 -4.141 0.449 N
ATOM 12 H ARG A 1 -10.766 -0.738 -3.282 H
ATOM 13 H01 ARG A 1 -17.961 -4.346 0.367 H
ATOM 14 H02 ARG A 1 -10.681 -2.372 -2.938 H
ATOM 15 H03 ARG A 1 -11.639 -0.189 -1.260 H
ATOM 16 H04 ARG A 1 -11.905 -3.250 -1.052 H
ATOM 17 H05 ARG A 1 -13.581 -1.033 0.264 H
ATOM 18 H06 ARG A 1 -13.963 -4.077 0.158 H
ATOM 19 H07 ARG A 1 -14.844 -2.481 2.206 H
ATOM 20 H08 ARG A 1 -17.067 -2.234 3.056 H
ATOM 21 H09 ARG A 1 -16.357 -4.619 -0.198 H
ATOM 22 H10 ARG A 1 -12.989 -2.172 -1.921 H
ATOM 23 H11 ARG A 1 -12.564 -2.222 1.119 H
ATOM 24 H12 ARG A 1 -14.952 -2.868 -0.704 H
ATOM 25 H13 ARG A 1 -18.196 -3.444 2.580 H
ATOM 26 N GLN A 2 -9.470 -2.403 -0.100 N
ATOM 27 CA GLN A 2 -8.097 -2.526 0.370 C
ATOM 28 C GLN A 2 -7.107 -1.890 -0.608 C
ATOM 29 O GLN A 2 -5.896 -1.824 -0.263 O
ATOM 30 CB GLN A 2 -7.680 -3.980 0.603 C
ATOM 31 CG GLN A 2 -8.381 -4.678 1.776 C
ATOM 32 CD GLN A 2 -7.381 -5.669 2.404 C
ATOM 33 NE2 GLN A 2 -7.923 -6.743 3.008 N
ATOM 34 OE1 GLN A 2 -6.161 -5.439 2.367 O
ATOM 35 H GLN A 2 -9.908 -3.238 -0.467 H
ATOM 36 H01 GLN A 2 -8.915 -6.934 3.011 H
ATOM 37 H02 GLN A 2 -7.984 -1.966 1.305 H
ATOM 38 H03 GLN A 2 -6.613 -3.978 0.846 H
ATOM 39 H04 GLN A 2 -9.303 -5.183 1.478 H
ATOM 40 H05 GLN A 2 -7.311 -7.406 3.468 H
ATOM 41 H06 GLN A 2 -7.805 -4.555 -0.322 H
ATOM 42 H07 GLN A 2 -8.624 -3.945 2.557 H
ATOM 43 N ILE A 3 -7.554 -1.350 -1.747 N
ATOM 44 CA ILE A 3 -6.615 -0.549 -2.535 C
ATOM 45 C ILE A 3 -5.973 0.525 -1.664 C
ATOM 46 O ILE A 3 -4.840 0.970 -1.936 O
ATOM 47 CB ILE A 3 -7.300 0.116 -3.754 C
ATOM 48 CG1 ILE A 3 -8.381 1.128 -3.304 C
ATOM 49 CG2 ILE A 3 -7.825 -0.967 -4.714 C
ATOM 50 CD ILE A 3 -9.210 1.682 -4.475 C
ATOM 51 H ILE A 3 -8.534 -1.439 -2.067 H
ATOM 52 H01 ILE A 3 -9.877 2.479 -4.133 H
ATOM 53 H02 ILE A 3 -5.795 -1.177 -2.892 H
ATOM 54 H03 ILE A 3 -6.506 0.672 -4.268 H
ATOM 55 H04 ILE A 3 -7.886 1.962 -2.797 H
ATOM 56 H05 ILE A 3 -7.041 -1.697 -4.936 H
ATOM 57 H06 ILE A 3 -9.824 0.904 -4.940 H
ATOM 58 H07 ILE A 3 -9.041 0.656 -2.568 H
ATOM 59 H08 ILE A 3 -8.138 -0.521 -5.661 H
ATOM 60 H09 ILE A 3 -8.559 2.099 -5.250 H
ATOM 61 H10 ILE A 3 -8.679 -1.494 -4.282 H
ATOM 62 N LYS A 4 -6.691 1.006 -0.620 N
ATOM 63 CA LYS A 4 -6.067 2.041 0.200 C
ATOM 64 C LYS A 4 -4.848 1.486 0.956 C

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ATOM     65  O   LYS A   4      -3.850   2.208   1.198                O
ATOM     66  CB  LYS A   4      -7.079   2.642   1.189                C
ATOM     67  CG  LYS A   4      -8.272   3.310   0.461                C
ATOM     68  CD  LYS A   4      -8.948   4.371   1.364                C
ATOM     69  CE  LYS A   4     -10.065   5.091   0.601                C
ATOM     70  NZ  LYS A   4     -10.663   6.241   1.449                N
ATOM     71  H   LYS A   4      -7.626   0.651  -0.402                H
ATOM     72  H01 LYS A   4      -9.935   6.936   1.681                H
ATOM     73  H02 LYS A   4      -5.673   2.828  -0.449                H
ATOM     74  H03 LYS A   4      -6.537   3.386   1.783                H
ATOM     75  H04 LYS A   4      -8.996   2.540   0.169                H
ATOM     76  H05 LYS A   4      -8.188   5.099   1.674                H
ATOM     77  H06 LYS A   4     -10.896   4.424   0.363                H
ATOM     78  H07 LYS A   4     -11.054   5.879   2.334                H
ATOM     79  H08 LYS A   4      -7.438   1.859   1.866                H
ATOM     80  H09 LYS A   4      -7.906   3.800  -0.449                H
ATOM     81  H10 LYS A   4      -9.351   3.888   2.262                H
ATOM     82  H11 LYS A   4      -9.691   5.558  -0.313                H
ATOM     83  H12 LYS A   4     -11.418   6.727   0.936                H
ATOM     84  N   ILE A   5      -4.952   0.214   1.363                N
ATOM     85  CA  ILE A   5      -3.810  -0.466   1.974                C
ATOM     86  C   ILE A   5      -2.743  -0.689   0.912                C
ATOM     87  O   ILE A   5      -1.522  -0.584   1.174                O
ATOM     88  CB  ILE A   5      -4.227  -1.805   2.626                C
ATOM     89  CG1 ILE A   5      -5.377  -1.550   3.624                C
ATOM     90  CG2 ILE A   5      -3.004  -2.419   3.333                C
ATOM     91  CD  ILE A   5      -5.803  -2.827   4.368                C
ATOM     92  H   ILE A   5      -5.673  -0.393   0.976                H
ATOM     93  H01 ILE A   5      -5.921  -3.661   3.668                H
ATOM     94  H02 ILE A   5      -3.378   0.172   2.743                H
ATOM     95  H03 ILE A   5      -4.587  -2.473   1.836                H
ATOM     96  H04 ILE A   5      -6.240  -1.146   3.079                H
ATOM     97  H05 ILE A   5      -3.245  -3.423   3.690                H
ATOM     98  H06 ILE A   5      -6.749  -2.666   4.897                H
ATOM     99  H07 ILE A   5      -5.054  -0.779   4.336                H
ATOM    100  H08 ILE A   5      -2.719  -1.796   4.188                H
ATOM    101  H09 ILE A   5      -5.056  -3.116   5.112                H
ATOM    102  H10 ILE A   5      -2.133  -2.484   2.675                H
ATOM    103  N   TRP A   6      -3.175  -1.016  -0.311                N
ATOM    104  CA  TRP A   6      -2.184  -1.196  -1.368                C
ATOM    105  C   TRP A   6      -1.370   0.090  -1.548                C
ATOM    106  O   TRP A   6      -0.129   0.081  -1.698                O
ATOM    107  CB  TRP A   6      -2.880  -1.585  -2.692                C
ATOM    108  CG  TRP A   6      -1.870  -2.172  -3.622                C
ATOM    109  CD1 TRP A   6      -1.332  -1.645  -4.765                C
ATOM    110  CD2 TRP A   6      -1.202  -3.430  -3.386                C
ATOM    111  CE2 TRP A   6      -0.256  -3.602  -4.426                C
ATOM    112  CE3 TRP A   6      -1.352  -4.426  -2.410                C
ATOM    113  NE1 TRP A   6      -0.356  -2.502  -5.256                N
ATOM    114  CZ2 TRP A   6       0.561  -4.734  -4.487                C
ATOM    115  CZ3 TRP A   6      -0.536  -5.547  -2.470                C
ATOM    116  CH2 TRP A   6       0.418  -5.692  -3.498                C
ATOM    117  H   TRP A   6      -4.160  -1.235  -0.486                H
ATOM    118  H01 TRP A   6       1.028  -6.585  -3.530                H
ATOM    119  H02 TRP A   6      -1.478  -1.975  -1.077                H
ATOM    120  H03 TRP A   6      -3.381  -0.704  -3.103                H
ATOM    121  H04 TRP A   6      -1.573  -0.726  -5.273                H
ATOM    122  H05 TRP A   6      -2.122  -4.341  -1.650                H
ATOM    123  H06 TRP A   6       0.144  -2.380  -6.124                H
ATOM    124  H07 TRP A   6       1.274  -4.871  -5.290                H
ATOM    125  H08 TRP A   6      -0.656  -6.345  -1.747                H
ATOM    126  H09 TRP A   6      -3.648  -2.336  -2.460                H
ATOM    127  N   PHE A   7      -2.089   1.226  -1.527                N
ATOM    128  CA  PHE A   7      -1.413   2.522  -1.572                C
ATOM    129  C   PHE A   7      -0.387   2.611  -0.438                C
ATOM    130  O   PHE A   7       0.797   2.958  -0.622                O
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ATOM    131  CB  PHE A   7      -2.474   3.635  -1.410              C
ATOM    132  CG  PHE A   7      -1.824   4.997  -1.331              C
ATOM    133  CD1 PHE A   7      -1.552   5.727  -2.490              C
ATOM    134  CD2 PHE A   7      -1.452   5.526  -0.092              C
ATOM    135  CE1 PHE A   7      -0.925   6.967  -2.413              C
ATOM    136  CE2 PHE A   7      -0.820   6.764  -0.014              C
ATOM    137  CZ  PHE A   7      -0.556   7.488  -1.175              C
ATOM    138  H   PHE A   7      -3.114   1.195  -1.524              H
ATOM    139  H01 PHE A   7      -0.085   8.462  -1.115              H
ATOM    140  H02 PHE A   7      -0.854   2.653  -2.501              H
ATOM    141  H03 PHE A   7      -3.046   3.428  -0.500              H
ATOM    142  H04 PHE A   7      -1.853   5.331  -3.454              H
ATOM    143  H05 PHE A   7      -1.668   4.966   0.810              H
ATOM    144  H06 PHE A   7      -0.742   7.539  -3.315              H
ATOM    145  H07 PHE A   7      -0.553   7.175   0.953              H
ATOM    146  H08 PHE A   7      -3.159   3.580  -2.263              H
ATOM    147  N   GLN A   8      -0.871   2.285   0.780              N
ATOM    148  CA  GLN A   8       0.037   2.272   1.920              C
ATOM    149  C   GLN A   8       1.276   1.431   1.586              C
ATOM    150  O   GLN A   8       2.426   1.766   1.964              O
ATOM    151  CB  GLN A   8      -0.568   1.551   3.132              C
ATOM    152  CG  GLN A   8      -1.825   2.103   3.796              C
ATOM    153  CD  GLN A   8      -2.226   1.091   4.872              C
ATOM    154  NE2 GLN A   8      -3.405   1.316   5.482              N
ATOM    155  OE1 GLN A   8      -1.521   0.097   5.164              O
ATOM    156  H   GLN A   8      -1.854   2.038   0.905              H
ATOM    157  H01 GLN A   8      -3.958   2.139   5.290              H
ATOM    158  H02 GLN A   8       0.380   3.280   2.166              H
ATOM    159  H03 GLN A   8       0.210   1.525   3.895              H
ATOM    160  H04 GLN A   8      -2.642   2.221   3.075              H
ATOM    161  H05 GLN A   8      -3.692   0.705   6.238              H
ATOM    162  H06 GLN A   8      -0.788   0.531   2.813              H
ATOM    163  H07 GLN A   8      -1.640   3.075   4.270              H
ATOM    164  N   ASN A   9       1.013   0.268   0.990              N
ATOM    165  CA  ASN A   9       2.083  -0.665   0.675              C
ATOM    166  C   ASN A   9       3.111  -0.008  -0.235              C
ATOM    167  O   ASN A   9       4.333  -0.133  -0.010              O
ATOM    168  CB  ASN A   9       1.492  -1.907   0.012              C
ATOM    169  CG  ASN A   9       0.634  -2.694   0.990              C
ATOM    170  ND2 ASN A   9      -0.063  -3.698   0.436              N
ATOM    171  OD1 ASN A   9       0.589  -2.453   2.216              O
ATOM    172  H   ASN A   9       0.043  -0.022   0.816              H
ATOM    173  H01 ASN A   9      -0.014  -3.930  -0.554              H
ATOM    174  H02 ASN A   9       2.626  -0.947   1.575              H
ATOM    175  H03 ASN A   9       2.302  -2.555  -0.340              H
ATOM    176  H04 ASN A   9      -0.621  -4.294   1.037              H
ATOM    177  H05 ASN A   9       0.893  -1.589  -0.848              H
ATOM    178  N   ARG A  10       2.629   0.699  -1.268              N
ATOM    179  CA  ARG A  10       3.588   1.418  -2.100              C
ATOM    180  C   ARG A  10       4.381   2.431  -1.260              C
ATOM    181  O   ARG A  10       5.585   2.674  -1.468              O
ATOM    182  CB  ARG A  10       2.875   2.172  -3.242              C
ATOM    183  CG  ARG A  10       3.941   2.716  -4.216              C
ATOM    184  CD  ARG A  10       3.369   3.691  -5.256              C
ATOM    185  NE  ARG A  10       4.469   4.136  -6.144              N
ATOM    186  CZ  ARG A  10       4.299   4.730  -7.329              C
ATOM    187  NH1 ARG A  10       5.341   4.908  -8.149              N
ATOM    188  NH2 ARG A  10       3.083   5.143  -7.705              N
ATOM    189  H   ARG A  10       1.620   0.742  -1.450              H
ATOM    190  H01 ARG A  10       2.899   5.448  -8.653              H
ATOM    191  H02 ARG A  10       4.329   0.724  -2.506              H
ATOM    192  H03 ARG A  10       2.264   2.966  -2.797              H
ATOM    193  H04 ARG A  10       4.400   1.872  -4.741              H
ATOM    194  H05 ARG A  10       2.921   4.554  -4.749              H
ATOM    195  H06 ARG A  10       5.413   3.987  -5.805              H
ATOM    196  H07 ARG A  10       6.232   4.455  -7.985              H
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ATOM    197  H08 ARG A  10       2.319   5.203  -7.046                H
ATOM    198  H09 ARG A  10       2.208   1.476  -3.762                H
ATOM    199  H10 ARG A  10       4.727   3.213  -3.637                H
ATOM    200  H11 ARG A  10       2.610   3.188  -5.865                H
ATOM    201  H12 ARG A  10       5.278   5.499  -8.969                H
ATOM    202  N   ARG A  11       3.657   3.090  -0.328                N
ATOM    203  CA  ARG A  11       4.347   4.052   0.517                C
ATOM    204  C   ARG A  11       5.431   3.385   1.373                C
ATOM    205  O   ARG A  11       6.470   4.007   1.709                O
ATOM    206  CB  ARG A  11       3.335   4.763   1.441                C
ATOM    207  CG  ARG A  11       4.011   5.792   2.366                C
ATOM    208  CD  ARG A  11       4.625   6.956   1.567                C
ATOM    209  NE  ARG A  11       5.521   7.797   2.377                N
ATOM    210  CZ  ARG A  11       6.850   7.613   2.433                C
ATOM    211  NH1 ARG A  11       7.611   8.589   2.961                N
ATOM    212  NH2 ARG A  11       7.410   6.505   1.959                N
ATOM    213  H   ARG A  11       2.645   2.965  -0.246                H
ATOM    214  H01 ARG A  11       8.413   6.487   1.816                H
ATOM    215  H02 ARG A  11       4.885   4.761  -0.117                H
ATOM    216  H03 ARG A  11       2.852   3.981   2.032                H
ATOM    217  H04 ARG A  11       4.799   5.306   2.946                H
ATOM    218  H05 ARG A  11       3.837   7.598   1.164                H
ATOM    219  H06 ARG A  11       5.109   8.541   2.927                H
ATOM    220  H07 ARG A  11       7.251   9.524   3.107                H
ATOM    221  H08 ARG A  11       6.918   5.590   1.797                H
ATOM    222  H09 ARG A  11       2.570   5.243   0.819                H
ATOM    223  H10 ARG A  11       3.274   6.187   3.073                H
ATOM    224  H11 ARG A  11       5.213   6.583   0.727                H
ATOM    225  H12 ARG A  11       8.578   8.429   3.207                H
ATOM    226  N   LYS A  12       5.172   2.143   1.789                N
ATOM    227  CA  LYS A  12       6.174   1.356   2.519                C
ATOM    228  C   LYS A  12       7.374   1.096   1.586                C
ATOM    229  O   LYS A  12       8.543   1.321   1.927                O
ATOM    230  CB  LYS A  12       5.520   0.043   3.001                C
ATOM    231  CG  LYS A  12       4.423   0.332   4.051                C
ATOM    232  CD  LYS A  12       3.403  -0.827   4.224                C
ATOM    233  CE  LYS A  12       2.064  -0.224   4.673                C
ATOM    234  NZ  LYS A  12       0.880  -1.172   4.537                N
ATOM    235  H   LYS A  12       4.255   1.735   1.594                H
ATOM    236  H01 LYS A  12      -0.025  -0.664   4.750                H
ATOM    237  H02 LYS A  12       6.565   1.937   3.358                H
ATOM    238  H03 LYS A  12       6.291  -0.615   3.413                H
ATOM    239  H04 LYS A  12       3.871   1.213   3.712                H
ATOM    240  H05 LYS A  12       3.767  -1.577   4.932                H
ATOM    241  H06 LYS A  12       1.851   0.618   4.019                H
ATOM    242  H07 LYS A  12       0.968  -1.961   5.190                H
ATOM    243  H08 LYS A  12       5.079  -0.443   2.125                H
ATOM    244  H09 LYS A  12       4.882   0.574   5.015                H
ATOM    245  H10 LYS A  12       3.253  -1.318   3.259                H
ATOM    246  H11 LYS A  12       2.099   0.119   5.709                H
ATOM    247  H12 LYS A  12       0.818  -1.577   3.554                H
ATOM    248  N   GLY A  13       6.985   0.597   0.378                N
ATOM    249  C   GLY A  13       8.925  -0.090  -0.977                C
ATOM    250  O   GLY A  13       9.812   0.261  -1.770                O
ATOM    251  H   GLY A  13       6.001   0.411   0.166                H
ATOM    252  H01 GLY A  13       7.732   1.574  -1.260                H
ATOM    253  N   LYS A  14       8.961  -1.268  -0.284                N
ATOM    254  CA  LYS A  14      10.156  -2.083  -0.375                C
ATOM    255  C   LYS A  14       9.744  -3.543  -0.215                C
ATOM    256  O   LYS A  14       8.587  -3.890   0.045                O
ATOM    257  CB  LYS A  14      11.163  -1.756   0.773                C
ATOM    258  CG  LYS A  14      11.243  -0.248   1.030                C
ATOM    259  CD  LYS A  14      12.088   0.067   2.280                C
ATOM    260  CE  LYS A  14      11.833   1.522   2.669                C
ATOM    261  NZ  LYS A  14      12.612   1.862   3.967                N
ATOM    262  H   LYS A  14       8.157  -1.664   0.185                H
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ATOM    263  H01 LYS A  14      12.309   1.237   4.730                H
ATOM    264  H02 LYS A  14      10.623  -1.887  -1.344                H
ATOM    265  H03 LYS A  14      12.155  -2.137   0.502                H
ATOM    266  H04 LYS A  14      10.231   0.128   1.200                H
ATOM    267  H05 LYS A  14      13.153  -0.108   2.085                H
ATOM    268  H06 LYS A  14      10.770   1.693   2.858                H
ATOM    269  H07 LYS A  14      12.462   2.839   4.258                H
ATOM    270  H08 LYS A  14      10.844  -2.286   1.676                H
ATOM    271  H09 LYS A  14      11.641   0.262   0.147                H
ATOM    272  H10 LYS A  14      11.767  -0.594   3.095                H
ATOM    273  H11 LYS A  14      12.197   2.214   1.906                H
ATOM    274  H12 LYS A  14      13.623   1.715   3.817                H
ATOM    275  N   LYS A  15      10.776  -4.444  -0.292                N
ATOM    276  CA  LYS A  15      10.593  -5.758   0.302                C
ATOM    277  O   LYS A  15      10.542  -4.558   2.454                O
ATOM    278  CB  LYS A  15      11.766  -6.708   0.000                C
ATOM    279  CG  LYS A  15      11.887  -7.091  -1.486                C
ATOM    280  CD  LYS A  15      13.036  -8.113  -1.671                C
ATOM    281  CE  LYS A  15      13.146  -8.556  -3.133                C
ATOM    282  NZ  LYS A  15      14.274  -9.606  -3.296                N
ATOM    283  H   LYS A  15      11.723  -4.107  -0.407                H
ATOM    284  H01 LYS A  15      15.181  -9.210  -3.002                H
ATOM    285  H02 LYS A  15       9.653  -6.186  -0.056                H
ATOM    286  H04 LYS A  15      11.605  -7.607   0.600                H
ATOM    287  H05 LYS A  15      12.073  -6.198  -2.093                H
ATOM    288  H06 LYS A  15      12.836  -8.983  -1.033                H
ATOM    289  H07 LYS A  15      13.404  -7.727  -3.794                H
ATOM    290  H08 LYS A  15      14.357  -9.913  -4.279                H
ATOM    291  H09 LYS A  15      12.700  -6.245   0.344                H
ATOM    292  H10 LYS A  15      10.942  -7.535  -1.820                H
ATOM    293  H11 LYS A  15      13.979  -7.658  -1.345                H
ATOM    294  H12 LYS A  15      12.231  -9.039  -3.480                H
ATOM    295  H13 LYS A  15      14.080 -10.435  -2.712                H
TER     296      LYS A  15
HETATM  297  C         0      10.469  -5.598   1.820                C
HETATM  298  N         0       7.826   0.711  -0.738                N
HETATM  299  O         0      10.264  -6.820   2.381                O
HETATM  300  H         0      10.186  -6.756   3.364                H
END
CONECT  248  298
CONECT  249  298
CONECT  252  298
CONECT  276  297
CONECT  277  297
CONECT  297  276  277  299
CONECT  298  252  248  249
CONECT  299  297  300
CONECT  300  299
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TITLE Trp56GlyPen

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REMARK   Created by GaussView 6.1.1: E =  =-6666.7260931 a.u.
ATOM      1  N   ARG A   1      -9.850  -1.035  -2.673                N
ATOM      2  CA  ARG A   1     -10.572  -0.635  -1.422                C
ATOM      3  C   ARG A   1      -9.429  -0.604  -0.399                C
ATOM      4  O   ARG A   1      -8.857   0.456  -0.070                O
ATOM      5  CB  ARG A   1     -11.757  -1.577  -1.149                C
ATOM      6  CG  ARG A   1     -12.650  -1.201   0.052                C
ATOM      7  CD  ARG A   1     -13.893  -2.118   0.060                C
ATOM      8  NE  ARG A   1     -14.815  -1.775   1.162                N
ATOM      9  CZ  ARG A   1     -16.114  -2.123   1.182                C
ATOM     10  NH1 ARG A   1     -16.929  -1.605   2.105                N
ATOM     11  NH2 ARG A   1     -16.595  -2.978   0.277                N
ATOM     12  H   ARG A   1     -10.030  -0.405  -3.455                H
ATOM     13  H01 ARG A   1     -17.594  -3.115   0.161                H
ATOM     14  H02 ARG A   1     -10.051  -1.998  -2.951                H
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ATOM     15  H03 ARG A   1     -10.922   0.393  -1.527                H
ATOM     16  H04 ARG A   1     -11.401  -2.608  -1.026                H
ATOM     17  H05 ARG A   1     -12.976  -0.159  -0.038                H
ATOM     18  H06 ARG A   1     -13.574  -3.164   0.147                H
ATOM     19  H07 ARG A   1     -14.426  -1.314   1.977                H
ATOM     20  H08 ARG A   1     -16.660  -0.813   2.676                H
ATOM     21  H09 ARG A   1     -15.993  -3.566  -0.285                H
ATOM     22  H10 ARG A   1     -12.371  -1.566  -2.058                H
ATOM     23  H11 ARG A   1     -12.089  -1.316   0.987                H
ATOM     24  H12 ARG A   1     -14.432  -1.987  -0.884                H
ATOM     25  H13 ARG A   1     -17.858  -1.980   2.261                H
ATOM     26  N   GLN A   2      -8.935  -1.830  -0.092                N
ATOM     27  CA  GLN A   2      -7.587  -1.989   0.438                C
ATOM     28  C   GLN A   2      -6.529  -1.503  -0.556                C
ATOM     29  O   GLN A   2      -5.327  -1.473  -0.176                O
ATOM     30  CB  GLN A   2      -7.272  -3.438   0.818                C
ATOM     31  CG  GLN A   2      -8.064  -3.978   2.016                C
ATOM     32  CD  GLN A   2      -7.170  -4.991   2.758                C
ATOM     33  NE2 GLN A   2      -7.818  -5.962   3.429                N
ATOM     34  OE1 GLN A   2      -5.934  -4.866   2.745                O
ATOM     35  H   GLN A   2      -9.410  -2.668  -0.401                H
ATOM     36  H01 GLN A   2      -8.822  -6.068   3.415                H
ATOM     37  H02 GLN A   2      -7.471  -1.352   1.322                H
ATOM     38  H03 GLN A   2      -6.218  -3.481   1.105                H
ATOM     39  H04 GLN A   2      -9.015  -4.431   1.725                H
ATOM     40  H05 GLN A   2      -7.278  -6.631   3.965                H
ATOM     41  H06 GLN A   2      -7.400  -4.087  -0.056                H
ATOM     42  H07 GLN A   2      -8.270  -3.166   2.726                H
ATOM     43  N   ILE A   3      -6.909  -1.040  -1.752                N
ATOM     44  CA  ILE A   3      -5.905  -0.348  -2.563                C
ATOM     45  C   ILE A   3      -5.241   0.759  -1.751                C
ATOM     46  O   ILE A   3      -4.075   1.115  -2.006                O
ATOM     47  CB  ILE A   3      -6.513   0.248  -3.855                C
ATOM     48  CG1 ILE A   3      -7.557   1.344  -3.528                C
ATOM     49  CG2 ILE A   3      -7.062  -0.882  -4.746                C
ATOM     50  CD  ILE A   3      -8.318   1.839  -4.770                C
ATOM     51  H   ILE A   3      -7.882  -1.102  -2.098                H
ATOM     52  H01 ILE A   3      -8.953   2.693  -4.518                H
ATOM     53  H02 ILE A   3      -5.101  -1.038  -2.836                H
ATOM     54  H03 ILE A   3      -5.676   0.722  -4.381                H
ATOM     55  H04 ILE A   3      -7.037   2.194  -3.072                H
ATOM     56  H05 ILE A   3      -6.309  -1.664  -4.881                H
ATOM     57  H06 ILE A   3      -8.955   1.057  -5.193                H
ATOM     58  H07 ILE A   3      -8.263   0.967  -2.781                H
ATOM     59  H08 ILE A   3      -7.321  -0.498  -5.736                H
ATOM     60  H09 ILE A   3      -7.621   2.159  -5.552                H
ATOM     61  H10 ILE A   3      -7.955  -1.331  -4.305                H
ATOM     62  N   LYS A   4      -5.974   1.363  -0.783                N
ATOM     63  CA  LYS A   4      -5.327   2.429  -0.023                C
ATOM     64  C   LYS A   4      -4.176   1.879   0.836                C
ATOM     65  O   LYS A   4      -3.163   2.576   1.087                O
ATOM     66  CB  LYS A   4      -6.342   3.169   0.865                C
ATOM     67  CG  LYS A   4      -7.455   3.851   0.031                C
ATOM     68  CD  LYS A   4      -8.101   5.016   0.823                C
ATOM     69  CE  LYS A   4      -9.133   5.747  -0.044                C
ATOM     70  NZ  LYS A   4      -9.692   6.990   0.692                N
ATOM     71  H   LYS A   4      -6.935   1.077  -0.576                H
ATOM     72  H01 LYS A   4      -8.931   7.654   0.911                H
ATOM     73  H02 LYS A   4      -4.862   3.136  -0.716                H
ATOM     74  H03 LYS A   4      -5.779   3.922   1.427                H
ATOM     75  H04 LYS A   4      -8.212   3.107  -0.241                H
ATOM     76  H05 LYS A   4      -7.310   5.716   1.119                H
ATOM     77  H06 LYS A   4      -9.994   5.117  -0.276                H
ATOM     78  H07 LYS A   4     -10.146   6.719   1.579                H
ATOM     79  H08 LYS A   4      -6.782   2.466   1.580                H
ATOM     80  H09 LYS A   4      -7.016   4.250  -0.892                H
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ATOM     81  H10 LYS A   4      -8.576   4.625   1.731                H
ATOM     82  H11 LYS A   4      -8.688   6.123  -0.968                H
ATOM     83  H12 LYS A   4     -10.389   7.484   0.109                H
ATOM     84  N   ILE A   5      -4.355   0.643   1.319                N
ATOM     85  CA  ILE A   5      -3.276  -0.031   2.040                C
ATOM     86  C   ILE A   5      -2.162  -0.365   1.061                C
ATOM     87  O   ILE A   5      -0.952  -0.259   1.377                O
ATOM     88  CB  ILE A   5      -3.784  -1.302   2.756                C
ATOM     89  CG1 ILE A   5      -4.924  -0.914   3.723                C
ATOM     90  CG2 ILE A   5      -2.609  -1.957   3.503                C
ATOM     91  CD  ILE A   5      -5.457  -2.115   4.524                C
ATOM     92  H   ILE A   5      -5.077   0.035   0.934                H
ATOM     93  H01 ILE A   5      -5.608  -2.982   3.872                H
ATOM     94  H02 ILE A   5      -2.862   0.645   2.786                H
ATOM     95  H03 ILE A   5      -4.181  -1.987   1.999                H
ATOM     96  H04 ILE A   5      -5.744  -0.473   3.142                H
ATOM     97  H05 ILE A   5      -2.940  -2.878   3.987                H
ATOM     98  H06 ILE A   5      -6.406  -1.862   5.009                H
ATOM     99  H07 ILE A   5      -4.553  -0.134   4.401                H
ATOM    100  H08 ILE A   5      -2.216  -1.271   4.263                H
ATOM    101  H09 ILE A   5      -4.756  -2.406   5.310                H
ATOM    102  H10 ILE A   5      -1.791  -2.202   2.819                H
ATOM    103  N   TRP A   6      -2.532  -0.791  -0.158                N
ATOM    104  CA  TRP A   6      -1.442  -1.076  -1.084                C
ATOM    105  C   TRP A   6      -0.658   0.206  -1.366                C
ATOM    106  O   TRP A   6       0.587   0.198  -1.490                O
ATOM    107  CB  TRP A   6      -1.877  -1.737  -2.421                C
ATOM    108  CG  TRP A   6      -0.620  -2.389  -2.926                C
ATOM    109  CD1 TRP A   6       0.424  -1.770  -3.559                C
ATOM    110  CD2 TRP A   6      -0.082  -3.592  -2.331                C
ATOM    111  CE2 TRP A   6       1.307  -3.614  -2.605                C
ATOM    112  CE3 TRP A   6      -0.651  -4.624  -1.570                C
ATOM    113  NE1 TRP A   6       1.587  -2.504  -3.378                N
ATOM    114  CZ2 TRP A   6       2.148  -4.587  -2.062                C
ATOM    115  CZ3 TRP A   6       0.173  -5.634  -1.094                C
ATOM    116  CH2 TRP A   6       1.566  -5.598  -1.315                C
ATOM    117  H   TRP A   6      -3.508  -0.997  -0.385                H
ATOM    118  H01 TRP A   6       2.190  -6.368  -0.879                H
ATOM    119  H02 TRP A   6      -0.744  -1.752  -0.588                H
ATOM    120  H03 TRP A   6      -2.290  -0.981  -3.096                H
ATOM    121  H04 TRP A   6       0.442  -0.827  -4.077                H
ATOM    122  H05 TRP A   6      -1.716  -4.642  -1.371                H
ATOM    123  H06 TRP A   6       2.491  -2.274  -3.760                H
ATOM    124  H07 TRP A   6       3.224  -4.495  -2.134                H
ATOM    125  H08 TRP A   6      -0.253  -6.453  -0.528                H
ATOM    126  H09 TRP A   6      -2.651  -2.485  -2.217                H
ATOM    127  N   PHE A   7      -1.378   1.331  -1.482                N
ATOM    128  CA  PHE A   7      -0.692   2.615  -1.638                C
ATOM    129  C   PHE A   7       0.329   2.788  -0.507                C
ATOM    130  O   PHE A   7       1.513   3.133  -0.705                O
ATOM    131  CB  PHE A   7      -1.747   3.742  -1.587                C
ATOM    132  CG  PHE A   7      -1.098   5.102  -1.700                C
ATOM    133  CD1 PHE A   7      -0.913   5.704  -2.946                C
ATOM    134  CD2 PHE A   7      -0.648   5.761  -0.554                C
ATOM    135  CE1 PHE A   7      -0.295   6.948  -3.045                C
ATOM    136  CE2 PHE A   7      -0.025   7.002  -0.650                C
ATOM    137  CZ  PHE A   7       0.152   7.599  -1.897                C
ATOM    138  H   PHE A   7      -2.403   1.301  -1.528                H
ATOM    139  H01 PHE A   7       0.615   8.575  -1.971                H
ATOM    140  H02 PHE A   7      -0.125   2.659  -2.572                H
ATOM    141  H03 PHE A   7      -2.296   3.649  -0.645                H
ATOM    142  H04 PHE A   7      -1.276   5.207  -3.840                H
ATOM    143  H05 PHE A   7      -0.797   5.299   0.417                H
ATOM    144  H06 PHE A   7      -0.183   7.423  -4.012                H
ATOM    145  H07 PHE A   7       0.305   7.513   0.246                H
ATOM    146  H08 PHE A   7      -2.453   3.579  -2.409                H
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ATOM    147  N   GLN A   8      -0.156   2.532   0.726              N
ATOM    148  CA  GLN A   8       0.753   2.565   1.866              C
ATOM    149  C   GLN A   8       1.980   1.683   1.584              C
ATOM    150  O   GLN A   8       3.139   2.049   1.895              O
ATOM    151  CB  GLN A   8       0.121   1.953   3.124              C
ATOM    152  CG  GLN A   8      -1.149   2.578   3.694              C
ATOM    153  CD  GLN A   8      -1.624   1.667   4.828              C
ATOM    154  NE2 GLN A   8      -2.824   1.969   5.357              N
ATOM    155  OE1 GLN A   8      -0.961   0.686   5.236              O
ATOM    156  H   GLN A   8      -1.138   2.291   0.860              H
ATOM    157  H01 GLN A   8      -3.347   2.784   5.068              H
ATOM    158  H02 GLN A   8       1.123   3.578   2.045              H
ATOM    159  H03 GLN A   8       0.881   1.995   3.903              H
ATOM    160  H04 GLN A   8      -1.937   2.654   2.935              H
ATOM    161  H05 GLN A   8      -3.162   1.432   6.148              H
ATOM    162  H06 GLN A   8      -0.104   0.912   2.895              H
ATOM    163  H07 GLN A   8      -0.962   3.581   4.096              H
ATOM    164  N   ASN A   9       1.707   0.475   1.084              N
ATOM    165  CA  ASN A   9       2.784  -0.471   0.819              C
ATOM    166  C   ASN A   9       3.765   0.073  -0.208              C
ATOM    167  O   ASN A   9       4.998  -0.102  -0.073              O
ATOM    168  CB  ASN A   9       2.206  -1.812   0.366              C
ATOM    169  CG  ASN A   9       1.414  -2.422   1.512              C
ATOM    170  ND2 ASN A   9       0.571  -3.407   1.186              N
ATOM    171  OD1 ASN A   9       1.561  -2.029   2.693              O
ATOM    172  H   ASN A   9       0.736   0.180   0.942              H
ATOM    173  H01 ASN A   9       0.483  -3.782   0.245              H
ATOM    174  H02 ASN A   9       3.369  -0.624   1.723              H
ATOM    175  H03 ASN A   9       3.028  -2.483   0.077              H
ATOM    176  H04 ASN A   9       0.053  -3.870   1.924              H
ATOM    177  H05 ASN A   9       1.573  -1.648  -0.511              H
ATOM    178  N   ARG A  10       3.244   0.773  -1.225              N
ATOM    179  CA  ARG A  10       4.167   1.459  -2.121              C
ATOM    180  C   ARG A  10       5.047   2.425  -1.318              C
ATOM    181  O   ARG A  10       6.279   2.508  -1.513              O
ATOM    182  CB  ARG A  10       3.413   2.246  -3.212              C
ATOM    183  CG  ARG A  10       4.436   2.833  -4.206              C
ATOM    184  CD  ARG A  10       3.809   3.817  -5.206              C
ATOM    185  NE  ARG A  10       4.874   4.328  -6.102              N
ATOM    186  CZ  ARG A  10       4.659   4.938  -7.273              C
ATOM    187  NH1 ARG A  10       5.679   5.180  -8.103              N
ATOM    188  NH2 ARG A  10       3.420   5.302  -7.622              N
ATOM    189  H   ARG A  10       2.227   0.833  -1.351              H
ATOM    190  H01 ARG A  10       3.208   5.615  -8.562              H
ATOM    191  H02 ARG A  10       4.863   0.746  -2.572              H
ATOM    192  H03 ARG A  10       2.811   3.018  -2.721              H
ATOM    193  H04 ARG A  10       4.904   2.014  -4.764              H
ATOM    194  H05 ARG A  10       3.339   4.647  -4.665              H
ATOM    195  H06 ARG A  10       5.829   4.222  -5.779              H
ATOM    196  H07 ARG A  10       6.593   4.766  -7.961              H
ATOM    197  H08 ARG A  10       2.665   5.318  -6.951              H
ATOM    198  H09 ARG A  10       2.731   1.564  -3.732              H
ATOM    199  H10 ARG A  10       5.228   3.342  -3.645              H
ATOM    200  H11 ARG A  10       3.057   3.304  -5.815              H
ATOM    201  H12 ARG A  10       5.578   5.785  -8.909              H
ATOM    202  N   ARG A  11       4.412   3.197  -0.415              N
ATOM    203  CA  ARG A  11       5.216   4.116   0.388              C
ATOM    204  C   ARG A  11       6.247   3.384   1.260              C
ATOM    205  O   ARG A  11       7.310   3.941   1.619              O
ATOM    206  CB  ARG A  11       4.297   4.967   1.293              C
ATOM    207  CG  ARG A  11       5.079   5.921   2.218              C
ATOM    208  CD  ARG A  11       5.934   6.929   1.427              C
ATOM    209  NE  ARG A  11       6.814   7.730   2.295              N
ATOM    210  CZ  ARG A  11       8.098   7.417   2.543              C
ATOM    211  NH1 ARG A  11       8.877   8.326   3.151              N
ATOM    212  NH2 ARG A  11       8.595   6.238   2.183              N
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ATOM    213  H   ARG A  11       3.396   3.153  -0.296                H
ATOM    214  H01 ARG A  11       9.597   6.092   2.210                H
ATOM    215  H02 ARG A  11       5.807   4.742  -0.285                H
ATOM    216  H03 ARG A  11       3.711   4.262   1.890                H
ATOM    217  H04 ARG A  11       5.734   5.348   2.879                H
ATOM    218  H05 ARG A  11       5.293   7.619   0.872                H
ATOM    219  H06 ARG A  11       6.421   8.551   2.738                H
ATOM    220  H07 ARG A  11       8.596   9.294   3.244                H
ATOM    221  H08 ARG A  11       8.020   5.412   1.909                H
ATOM    222  H09 ARG A  11       3.610   5.533   0.654                H
ATOM    223  H10 ARG A  11       4.370   6.468   2.847                H
ATOM    224  H11 ARG A  11       6.573   6.412   0.709                H
ATOM    225  H12 ARG A  11       9.792   8.084   3.508                H
ATOM    226  N   LYS A  12       5.912   2.146   1.644                N
ATOM    227  CA  LYS A  12       6.819   1.297   2.408                C
ATOM    228  C   LYS A  12       7.907   0.653   1.536                C
ATOM    229  O   LYS A  12       8.818  -0.014   2.077                O
ATOM    230  CB  LYS A  12       6.021   0.140   3.054                C
ATOM    231  CG  LYS A  12       4.976   0.641   4.067                C
ATOM    232  CD  LYS A  12       3.932  -0.439   4.454                C
ATOM    233  CE  LYS A  12       2.658   0.264   4.948                C
ATOM    234  NZ  LYS A  12       1.436  -0.647   4.943                N
ATOM    235  H   LYS A  12       4.965   1.815   1.454                H
ATOM    236  H01 LYS A  12       0.540  -0.087   5.041                H
ATOM    237  H02 LYS A  12       7.326   1.896   3.170                H
ATOM    238  H03 LYS A  12       6.743  -0.538   3.518                H
ATOM    239  H04 LYS A  12       4.439   1.469   3.598                H
ATOM    240  H05 LYS A  12       4.327  -1.124   5.211                H
ATOM    241  H06 LYS A  12       2.433   1.067   4.251                H
ATOM    242  H07 LYS A  12       1.484  -1.325   5.713                H
ATOM    243  H08 LYS A  12       5.533  -0.391   2.229                H
ATOM    244  H09 LYS A  12       5.475   1.024   4.964                H
ATOM    245  H10 LYS A  12       3.662  -1.027   3.573                H
ATOM    246  H11 LYS A  12       2.771   0.678   5.952                H
ATOM    247  H12 LYS A  12       1.411  -1.187   4.027                H
ATOM    248  N   GLY A  13       7.766   0.797   0.215                N
ATOM    249  CA  GLY A  13       8.657   0.144  -0.727                C
ATOM    250  C   GLY A  13       8.519  -1.380  -0.752                C
ATOM    251  O   GLY A  13       9.481  -2.095  -1.064                O
ATOM    252  H   GLY A  13       7.027   1.371  -0.183                H
ATOM    253  H01 GLY A  13       9.704   0.341  -0.488                H
ATOM    254  H02 GLY A  13       8.435   0.552  -1.716                H
ATOM    255  N   LYS A  14       7.305  -1.893  -0.380                N
ATOM    256  CA  LYS A  14       7.275  -3.317  -0.092                C
ATOM    257  C   LYS A  14       6.099  -4.074  -0.686                C
ATOM    258  O   LYS A  14       4.972  -3.616  -0.918                O
ATOM    259  CB  LYS A  14       7.324  -3.552   1.448                C
ATOM    260  CG  LYS A  14       8.697  -3.092   1.958                C
ATOM    261  CD  LYS A  14       8.858  -3.085   3.495                C
ATOM    262  CE  LYS A  14      10.067  -2.189   3.782                C
ATOM    263  NZ  LYS A  14      10.467  -2.222   5.278                N
ATOM    264  H   LYS A  14       6.491  -1.302  -0.199                H
ATOM    265  H01 LYS A  14       9.684  -1.906   5.868                H
ATOM    266  H02 LYS A  14       8.202  -3.696  -0.535                H
ATOM    267  H03 LYS A  14       7.114  -4.600   1.679                H
ATOM    268  H04 LYS A  14       8.846  -2.064   1.623                H
ATOM    269  H05 LYS A  14       8.999  -4.101   3.879                H
ATOM    270  H06 LYS A  14       9.822  -1.157   3.513                H
ATOM    271  H07 LYS A  14      11.279  -1.609   5.451                H
ATOM    272  H08 LYS A  14       6.530  -2.946   1.902                H
ATOM    273  H09 LYS A  14       9.486  -3.709   1.513                H
ATOM    274  H10 LYS A  14       7.961  -2.652   3.955                H
ATOM    275  H11 LYS A  14      10.951  -2.523   3.234                H
ATOM    276  H12 LYS A  14      10.719  -3.183   5.560                H
ATOM    277  N   LYS A  15       6.423  -5.394  -0.885                N
ATOM    278  CA  LYS A  15       5.413  -6.427  -1.014                C
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ATOM    279  O   LYS A  15       4.998  -6.016   1.372                O
ATOM    280  CB  LYS A  15       6.037  -7.780  -1.421                C
ATOM    281  CG  LYS A  15       6.696  -7.762  -2.813                C
ATOM    282  CD  LYS A  15       7.291  -9.157  -3.133                C
ATOM    283  CE  LYS A  15       7.935  -9.168  -4.524                C
ATOM    284  NZ  LYS A  15       8.522 -10.566  -4.841                N
ATOM    285  H   LYS A  15       7.354  -5.700  -0.627                H
ATOM    286  H01 LYS A  15       9.243 -10.824  -4.147                H
ATOM    287  H02 LYS A  15       4.661  -6.132  -1.750                H
ATOM    288  H04 LYS A  15       5.236  -8.524  -1.397                H
ATOM    289  H05 LYS A  15       7.483  -7.002  -2.847                H
ATOM    290  H06 LYS A  15       6.489  -9.904  -3.087                H
ATOM    291  H07 LYS A  15       8.769  -8.467  -4.593                H
ATOM    292  H08 LYS A  15       8.958 -10.581  -5.778                H
ATOM    293  H09 LYS A  15       6.778  -8.068  -0.663                H
ATOM    294  H10 LYS A  15       5.943  -7.501  -3.566                H
ATOM    295  H11 LYS A  15       8.040  -9.409  -2.373                H
ATOM    296  H12 LYS A  15       7.208  -8.961  -5.310                H
ATOM    297  H13 LYS A  15       7.781 -11.285  -4.817                H
TER     298      LYS A  15
HETATM  299  C         0      4.730  -6.603   0.340                C
HETATM  300  O         0      3.756  -7.561   0.240                O
HETATM  301  H         0      3.341  -7.737   1.121                H
END
CONECT  278  299
CONECT  279  299
CONECT  299  278  279  300
CONECT  300  299  301
CONECT  301  300
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