Biomimetic prebiotic synthesis of homochiral peptides via a potential 5'-aa-AMP precursor

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Supporting Information

Contents

1 Materials and methods

Materials: D-Isoleucine (D-Ile), D-Leucine (D-Leu), D-Alanine (D-Ala), D-Valine (D-Val), D-Proline (D-Pro), and L-Phenylalanine (L-Phe) were obtained from Shanghai Macklin Biochemical Co., Ltd. (China). L-^{15}N-Isoleucine (L-^{15}N-Ile), L-^{15}N-Leucine (L-^{15}N-Leu), L-^{15}N-Alanine (L-^{15}N-Ala), L-^{15}N-Valine (L-^{15}N-Val), L-^{15}N-Proline (L-^{15}N-Pro) were obtained from Shanghai Research Institute Industry Co., Ltd. (China). 2'-Fluoro-2'-deoxyadenosine was purchased from Shanghai yuanye Bio-Technology Co., Ltd. (China). Trimetaphosphate (P_3m) was obtained from Sigma Aldrich. (China). Acetonitrile (AR) was obtained from m Sinopharm Chemical Reagent Co., Ltd. (China). Ultrapure water (18.2 MΩ cm) from a Milli-Q water purification system (Millipore, Bedford, MA) was used to prepare solutions and the mobile phase. A reversed-phase semi-preparative liquid chromatograph purchased from Agilent for the separation and purification of *N*-L-Phe-F-AMP. Reagents were obtained and verified by MS spectra.

The purpose of isotope labeling: The use of ^{15}N-labeled L-amino acids ((M+1) Da) was facilitated the differentiation of peptides generated from D-amino acids (M Da) in our mass spectrometry analysis. By incorporating ^{15}N into specific amino acids, we were able to distinguish these labeled peptides from their unlabeled counterparts based on their distinct mass signatures.

The synthesis of *N*-L-Phe-F-AMP: 100 mM Phe (16.52 mg) was mixed with 100 mM sodium P_3m (30.59 mg) and 100 mM 2'-Fluoro-2'-deoxyadenosine (26.92 mg) in 1 mL water and the pH was adjusted to 11 using 10 M NaOH. The reactants were placed at 60 ℃ for 5 hours.

The synthesis of different chiral dipeptides:

1) Mother liquor configuration: Solution 1: 2 mL 10 mM *N*-L-Phe-F-AMP (10.54 mg) ; Solution 2: 500 μL 100 mM L-^{15}N-Ile (6.60 mg) and 100 mM D-Ile (6.55 mg); Solution 3: 500 μL 50 mM L-^{15}N-Leu (3.30 mg) and 50 mM D-Leu (3.26 mg); Solution 4: 500 μL 400 mM L-^{15}N-Ala (18.21 mg) and 400 mM D-Ala (18.01 mg); Solution 5: 500 μL 200 mM L-^{15}N-Val (11.81 mg) and 200 mM D-Val (11.71 mg); Solution 6: 500 μL 200 mM L-^{15}N-Pro (11.61 mg) and 200 mM D-Pro (11.51 mg);

2) Reaction solution configuration: reaction solution A (racemic isoleucine and *N*-L-Phe-F-AMP): 300 μL solution 1 and 300 μL solution 2 were mixed with 10 M NaOH to adjust the pH to 9, and it was equally divided into three parts as a parallel control experiment; reaction solution B (racemic leucine and *N*-L-Phe-F-AMP): 300 μL solution 1 and 300 μL solution 3 were mixed with 10 M NaOH to adjust the pH to 9, and it was equally divided into three parts as a parallel control experiment; reaction solution C (racemic alanine and *N*-L-Phe-F-AMP): 300 μL solution 1 and 300 μL solution 4 were mixed with 10 M NaOH to adjust the pH to 9, and it was equally divided into three parts as a parallel control experiment; reaction solution D (racemic valine and *N*-L-Phe-F-AMP): 300 μL solution 1 and 300 μL solution 5 were mixed with 10 M NaOH to adjust the pH to 9, and it was equally divided into three parts as a parallel control experiment; reaction solution E (racemic proline and *N*-L-Phe-F-AMP): 300 μL solution 1 and 300 μL solution 6 were mixed with 10 M NaOH to adjust the pH to 9, and it was equally divided into three parts as a parallel control experiment.

The above five reaction mixed solutions were sealed and placed at 37 ℃ for 3 days.

NMR Methods: The ^{31}P, ^{1}H, ^{13}C and F spectrum measurements were performed on Bruker 500 MHz spectrometer at ambient temperature. Bruker AVANCE 500 MHz dodel was used with an BBFO intelligent detector, experimental temperature constant value of 298 K, Bruker VT-200

thermostat control, and temperature control accuracy 0.1.

HPLC method of purifying *N*-L-Phe-F-AMP: The HPLC was performed on Agilent 1260 Infinity system equipped with an Agilent TC-C18 column (5 μm particle size, dimension 10 mm × 250 mm). The column temperature was kept at room temperature. The HPLC flow rate was 5 mL• min^{-1} with TC-C18.Solvent A was water with 5 mM Ammonium acetate aqueous solution and solvent B was acetonitrile. A 25 min gradient method was used: 0∼5 min, 5% B; 5∼15 min, 5%–85% B; 15∼17 min, 85% B; 17∼19 min, 85∼5% B; 19∼25 min, 5% B. The detection wavelength was 210 nm.

HPLC-MS Methods: The MS was conducted in positive ionization mode using Thermo Scientific™ Q Exactive Plus™ system. The instrument parameters were set as follows: The capillary voltage was set to 3800 V, the atomizer pressure was 2 bar, the dry gas flow rate to 3 L•min^{-1}, and the dry temperature was 320 °C. Mass spectra were acquired over a scan range from m/z = 50 to 700. For ESI-MS analysis, approximately 1/10 of the LC eluent was introduced through a splitting T valve. To enable online detection of reaction products by HPLC-MS, we configured the divert valve of the MS instrument according: this valve allows for direct switching of HPLC flows to the MS when positioned at the source location. For online detection of reaction products by HPLC-MS, the diverter T valve was utilized to cleverly switch the HPLC eluent to achieve online desalting and detection. Specifically: during the first two minutes, the diverter valve switches the HPLC eluent to the waste liquid; After 2 minutes, the diverter valve switches the HPLC eluent to MS.

The HPLC was performed on Agilent 1260 Infinity system equipped with a Luna-C18 column (5 μm particle size, dimension 4.6 mm × 250 mm). The column temperature was kept at room temperature. The HPLC flow rate was 1 mL• min^{-1} with Luna-C18. Solvent A was water with 0.1% formic acid and solvent B was acetonitrile. A 25 min gradient method was used: 0∼5 min, 1% B; 5∼15 min, 1%–60% B; 15∼17 min, 60% B; 17∼19 min, 60∼1% B; 19∼25 min, 1% B. The detection wavelength was 210 nm and the sample size was 3 μL.

Enantiomeric excess calculations: In our study, the enantiomeric excess (ee) of the synthesized peptides was determined using liquid chromatography-mass spectrometry (LC-MS) to separate and quantify the peak areas of the two enantiomers. The ee value, which is a measure of the chiral purity of the products, was calculated using the formula:

$$ee = \left(\frac{A_{major} - A_{minor}}{A_{major} + A_{minor}}\right) \times 100\%$$

A_{major} represents the peak areas of the major and A_{minor} represents minor enantiomers.

Computational Details: Density functional theory (DFT) calculations were carried out using the Gaussian 16 suite of programs. The spin-unrestricted RB3LYP-D3(BJ) functional corrected with Grimme 10's dispersion using the Becke-Johnson dumpling scheme was employedthe 6-31G* basis set for the all atoms. This basis set is denoted as B1 and was used to optimize transition states (TS) and minima. All calculations including the optimization was performed within solvation using the conductor-like polarizable continuum model (CPCM) is employed as the solvent in the self-consistent reaction field (SCRF) calculations. The experimental reaction temperature 298.15 K was adopted in the free energy calculations. Transition states were ascertained by vibrational frequency analysis to possess a single mode along the reaction coordinate with a sole imaginary frequency.

2 Hydrolysis diagram of *N*-aa-AMP

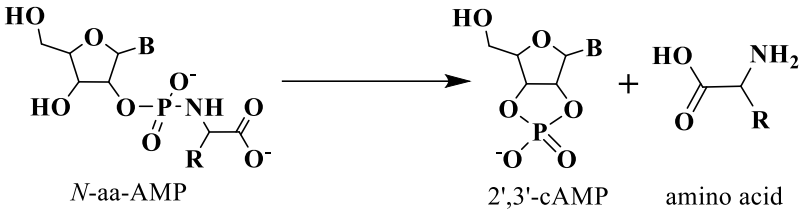


Figure S1. Hydrolysis diagram of *N*-aa-AMP.

3 Spectra of *N*-L-Phe-F-AMP

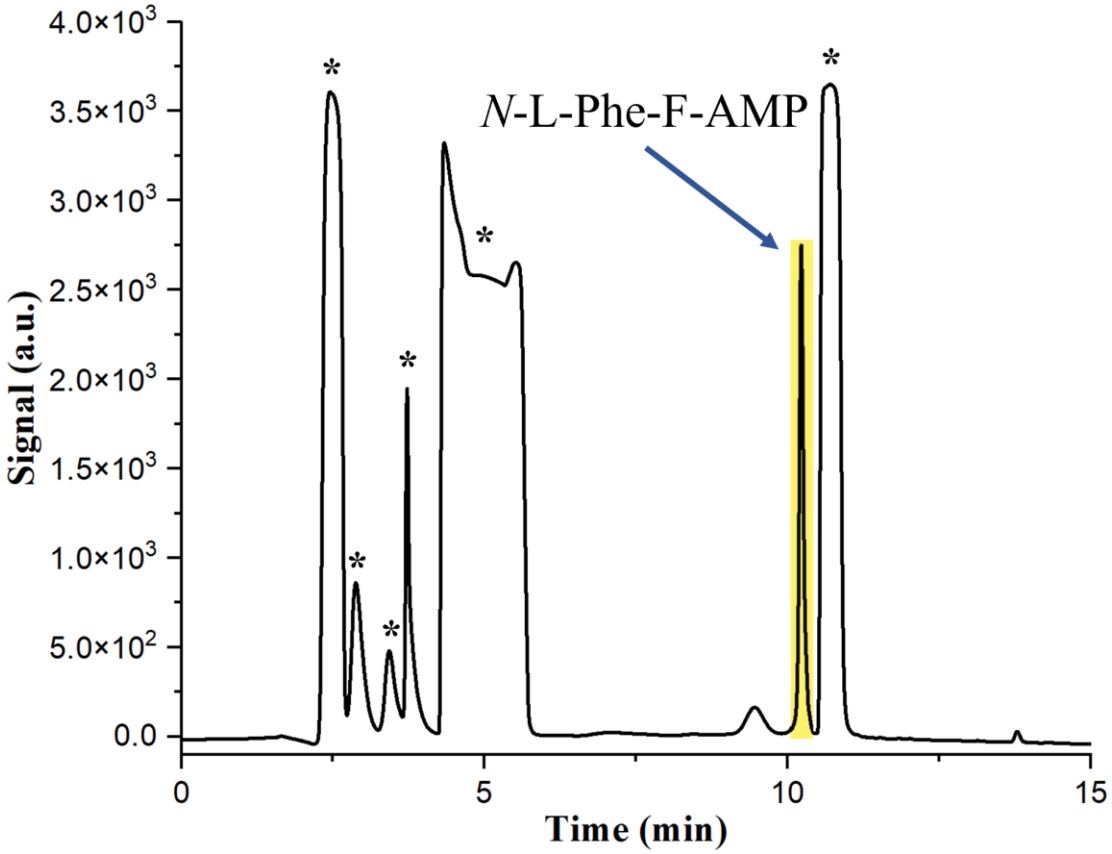


Figure S2. HPLC spectra of purifing *N*-L-Phe-F-AMP. The yellow peak is *N*-L-Phe-F-AMP and its Rt is 10.2 min. "*" represents the peak of unknown compounds.

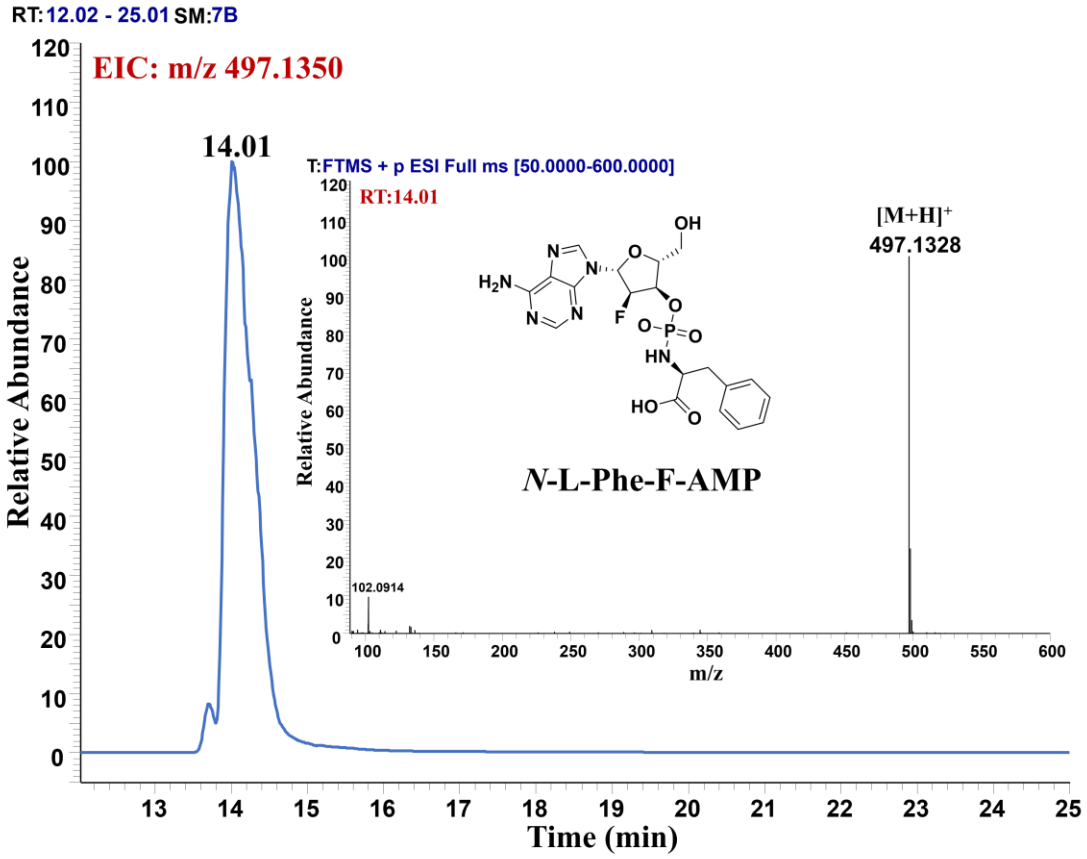


Figure S3. HPLC-MS-EIC spectra of $[M+H]^+$ for *N*-L-Phe-F-AMP. Its Rt is 14.01 min.

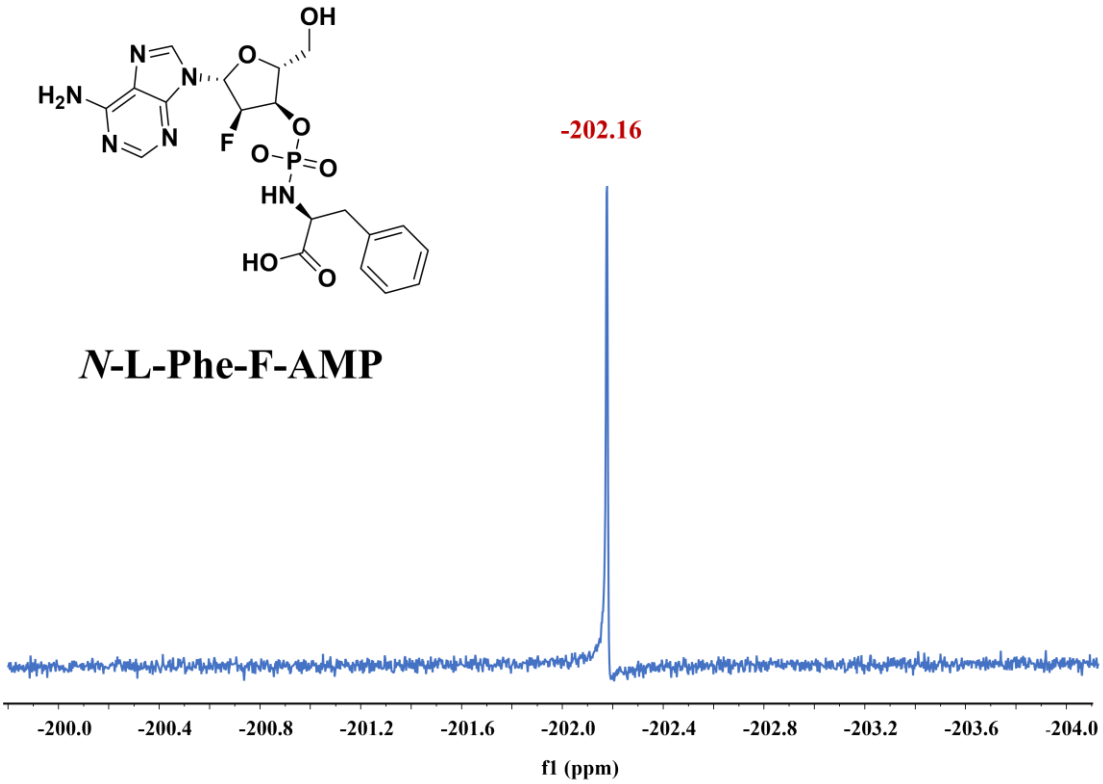
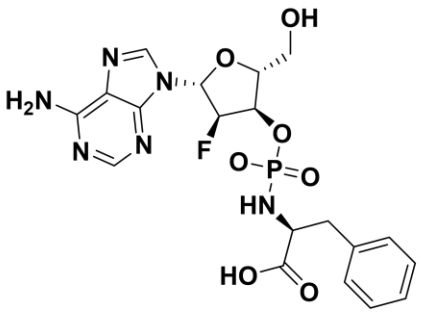


Figure S4. ^{19}F NMR spectrum of *N*-L-Phe-F-AMP. Its ^{19}F-NMR spectrum shift is -202.16 ppm.



***N*-L-Phe-F-AMP**

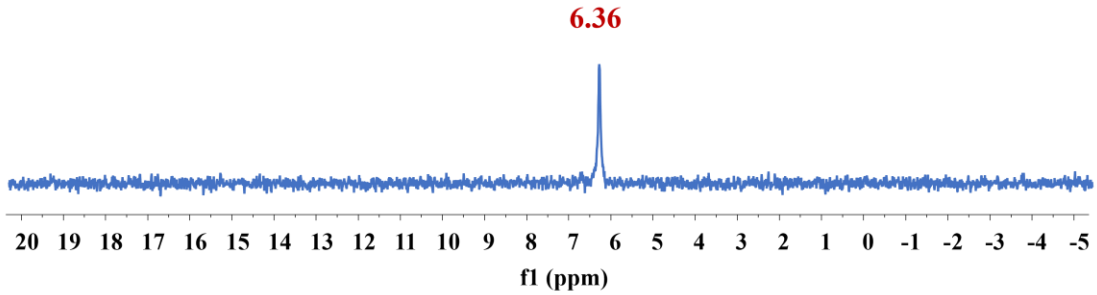


Figure S5. ^{31}P NMR spectrum of *N*-L-Phe-F-AMP. Its ^{31}P-NMR spectrum shift is 6.36 ppm.

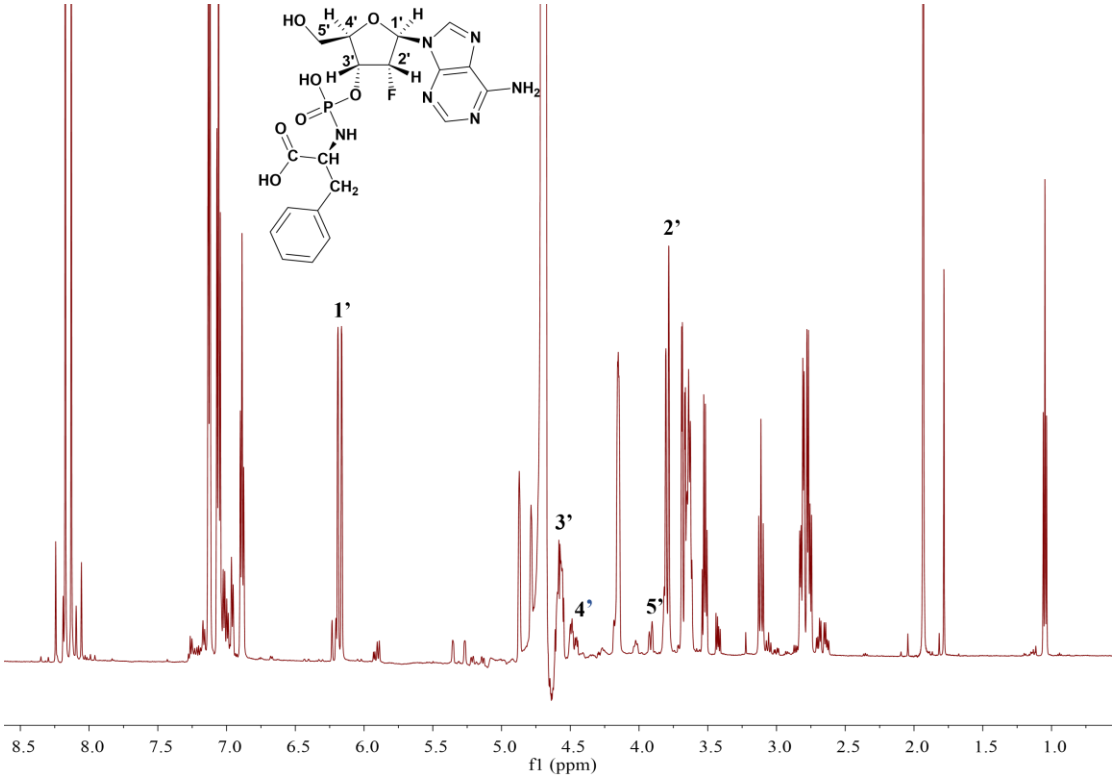


Figure S6. ^{1}H NMR spectrum of intermediate *N*-L-Phe-F-AMP.

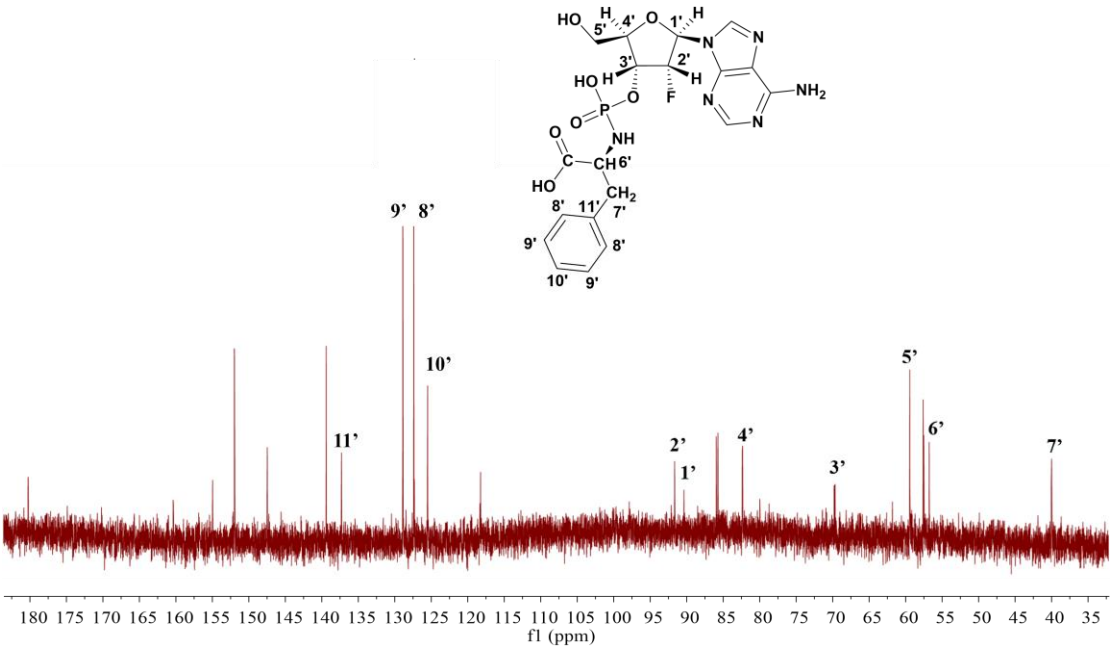
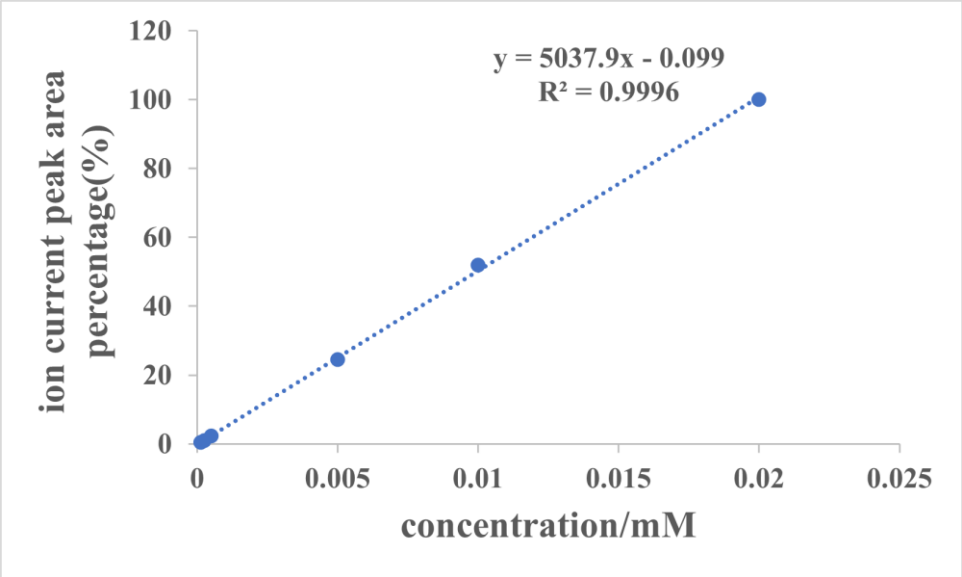


Figure S7. ^{13}C NMR spectrum of intermediate *N*-L-Phe-F-AMP.

4 Measurement of concentration of L-Phe-Ile



Sample	ion current peak area percentage	concentration/mM	yield
1[a]	3.78%	0.00077	0.154‰

Figure S8. A liner plot of concentration of L-Phe-Ile ion current peak area (converted to a percentage) can be obtained as a calibration curve, which was used to measure the concentration of Phe-Ile in the actual sample.

[a] the yield of Phe-Ile formed by the reaction of Ile and *N*-L-Phe-F-AMP.

5 Spectra of initial different chiral amino acids (Ile, Leu, Ala, Val, Pro)

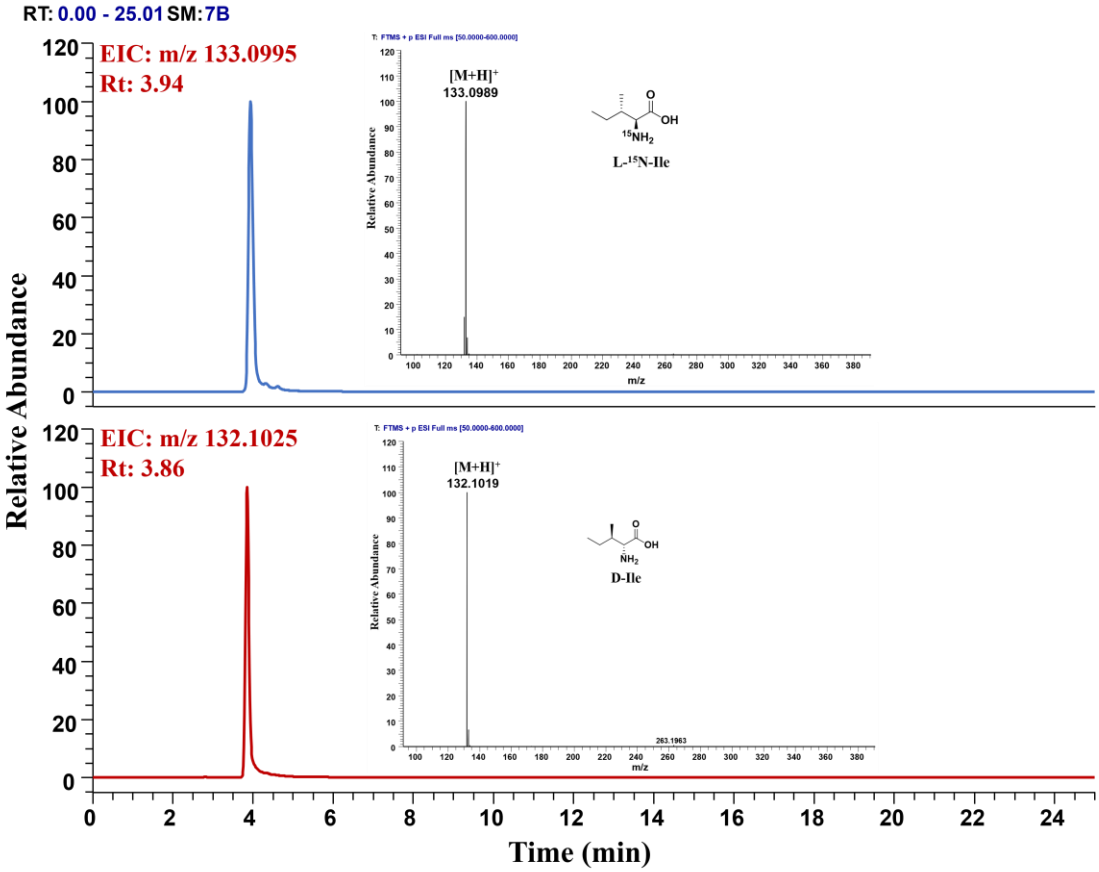


Figure S9. HPLC-MS-EIC spectra of $[M+H]^+$ of racemic isoleucine. The above picture is L-Ile, the below picture is D-Ile. The Rt of L-Ile is 3.94 min, and the Rt of D-Ile is 3.86 min. According to the EIC integral area, the contents of L-Ile and D-Ile in the initial reaction solution are basically equal, and the ratio of L-Ile: D-Ile = 0.99:1.

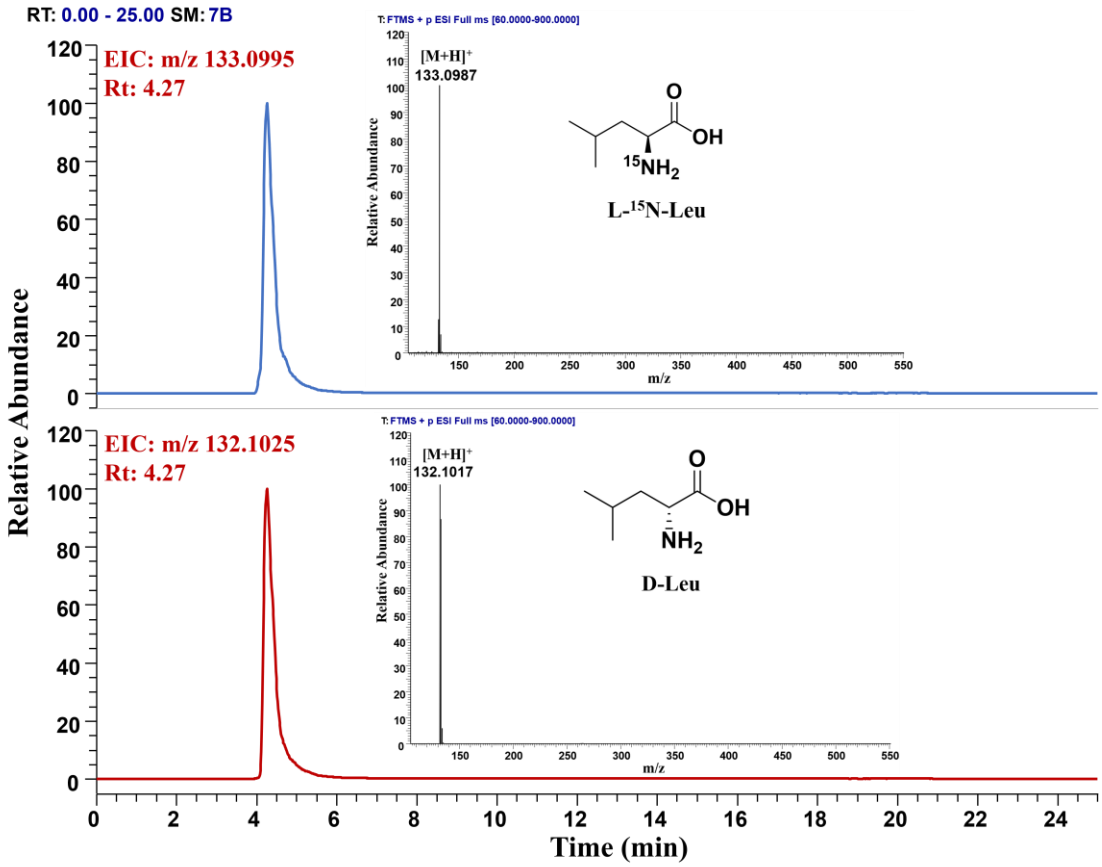


Figure S10. HPLC-MS-EIC spectra of $[M+H]^+$ of racemic leucine. The above picture is L-Leu, the below picture is D-Leu. The Rt of L-Leu is 4.27 min, and the Rt of D-Leu is 4.27 min. According to the EIC integral area, the contents of L-Leu and D-Leu in the initial reaction solution are basically equal, and the ratio of L-Leu: D-Leu = 0.95:1.

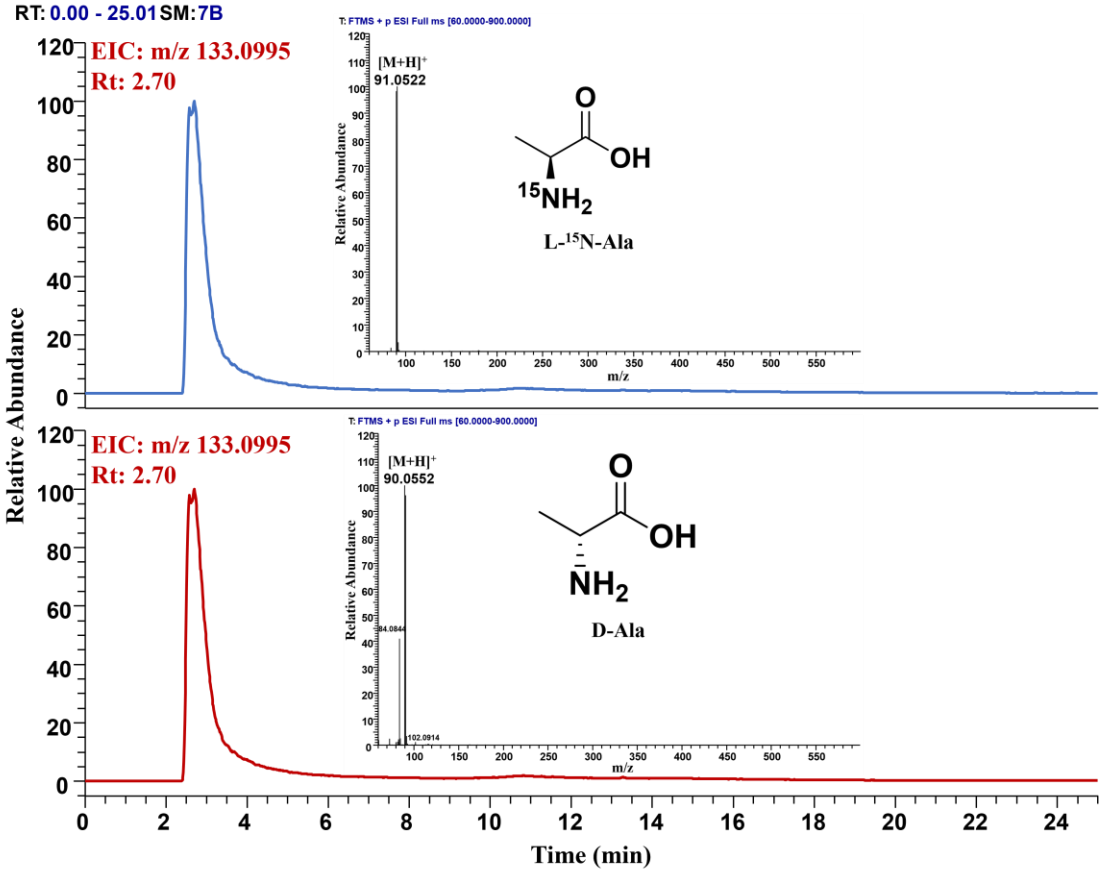


Figure S11. HPLC-MS-EIC spectra of $[M+H]^+$ of racemic alanine. The above picture is L-Ala, the below picture is D-Ala. The Rt of L-Ala is 2.70 min, and the Rt of D-Ala is 2.70 min. According to the EIC integral area, the contents of L-Ala and D-Ala in the initial reaction solution are basically equal, and the ratio of L-Ala: D-Ala = 1.03:1.

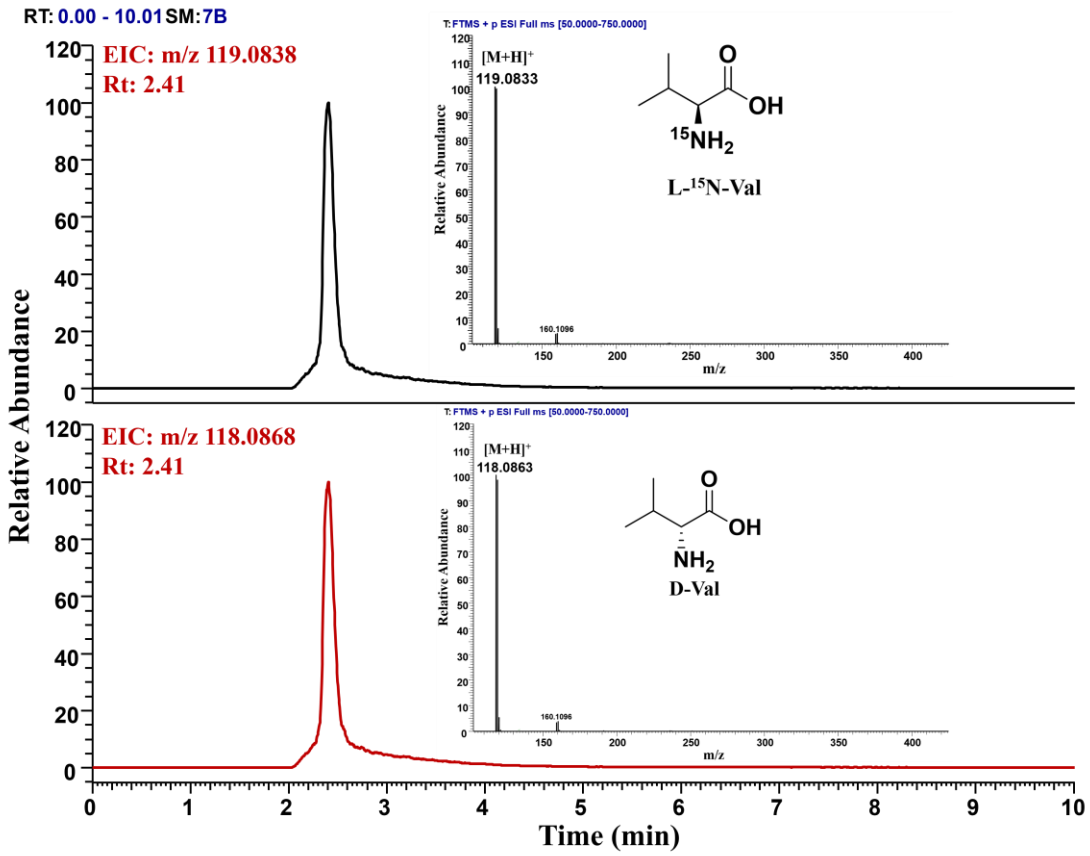


Figure S12. HPLC-MS-EIC spectra of $[M+H]^+$ of racemic valine. The above picture is L-Val, the below picture is D-Val. The Rt of L-Val is 2.41 min, and the Rt of D-Val is 2.41 min. According to the EIC integral area, the contents of L-Val and D-Val in the initial reaction solution are basically equal, and the ratio of L-Val: D-Val = 0.95:1.

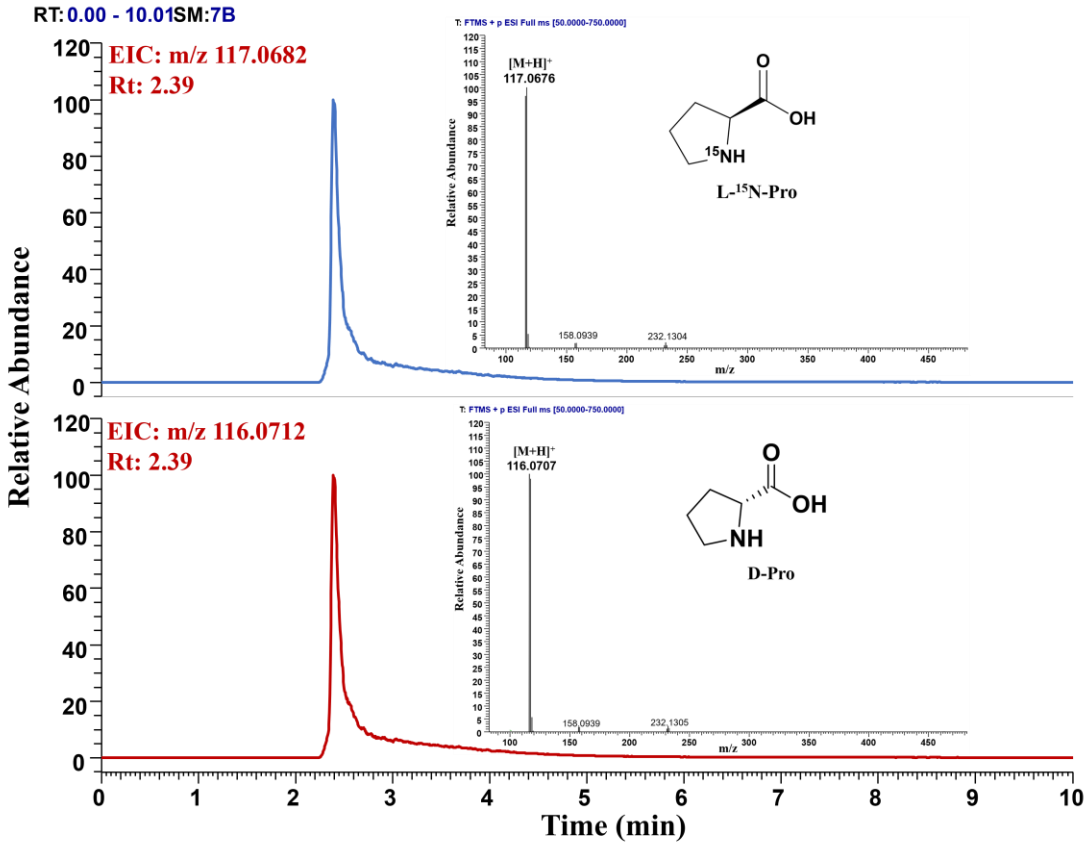


Figure S13. HPLC-MS-EIC spectra of $[M+H]^+$ of racemic proline. The above picture is L-Pro, the below picture is D-Pro. The Rt of L-Pro is 2.39 min, and the Rt of D-Pro is 2.39 min. According to the EIC integral area, the contents of L-Pro and D-Pro in the initial reaction solution are basically equal, and the ratio of L-Pro: D-Pro = 1.05:1.

6 Information of different chiral peptides (Leu, Ala, Val, Pro) produced by reactions with *N*-L-Phe-F-AMP

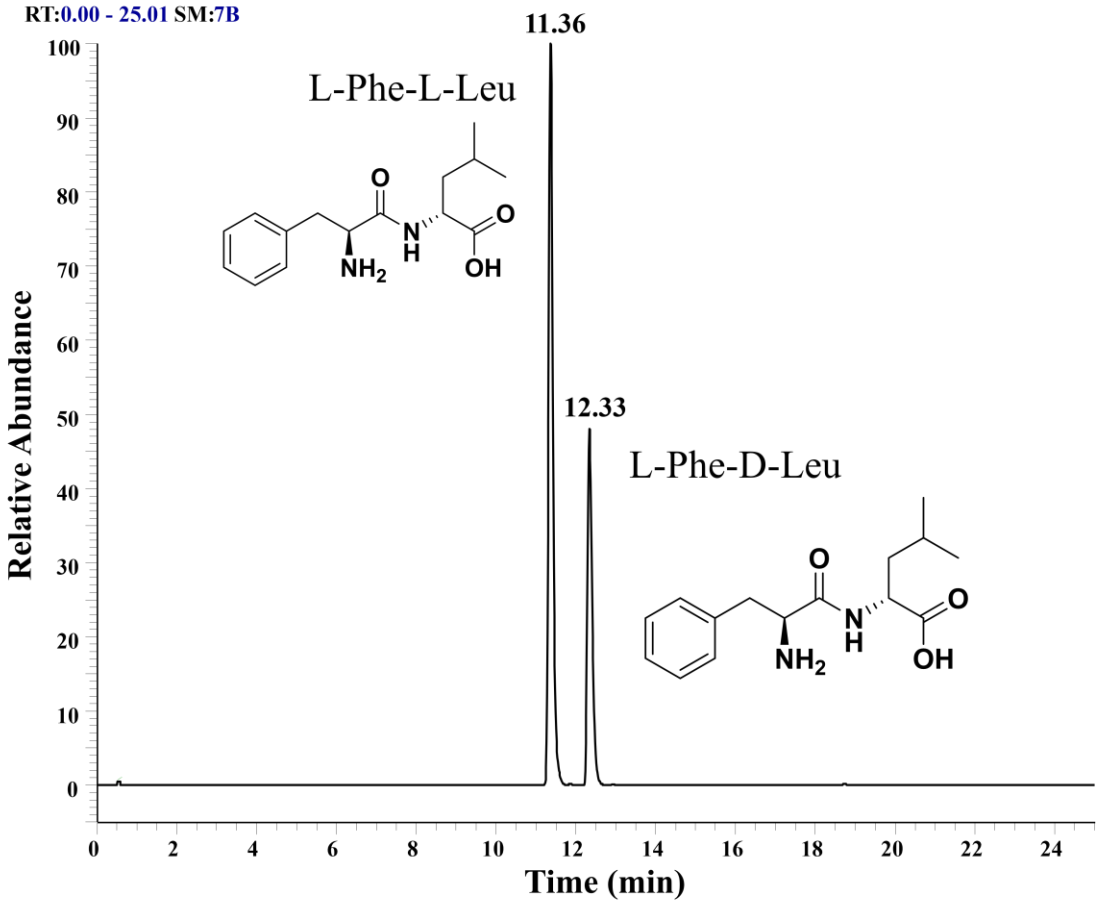


Figure S14. HPLC-MS-EIC spectra of $[M+H]^+$ for the product of racemic Leu with *N*-L-Phe-F-AMP. The retention time 11.36 min was L-Phe-L-Leu. The retention time 12.33 min was L-Phe-D-Leu. According to the EIC integral area, more L-Phe-L-Leu is generated, and its ratio of L-Phe-L-Leu: L-Phe-D-Leu = 1.47:1.

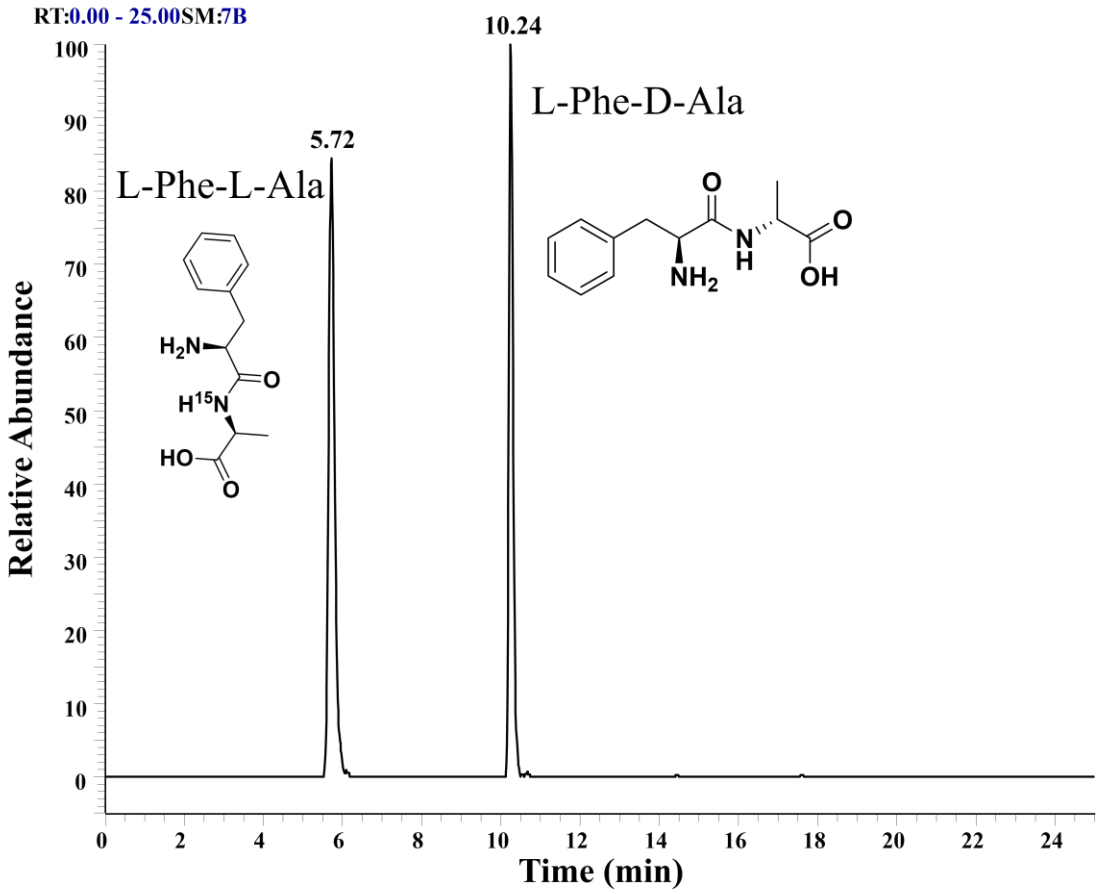


Figure S15. HPLC-MS-EIC spectra of $[M+H]^+$ for the product of racemic Ala with *N*-L-Phe-F-AMP. The retention time 5.72 min was L-Phe-L-Ala. The retention time 10.24 min was L-Phe-D-Ala. Although the peak of L-Phe-L-Ala does not appear to be as high as the peak of L-Phe-D-Ala, the peak of L-Phe-L-Ala is wider than the peak of L-Phe-D-Ala and therefore corresponds to a larger peak area of L-Phe-L-Ala. According to the EIC integral area, more L-Phe-L-Ala is generated, and its ratio of L-Phe-L-Ala: L-Phe-D-Ala = 1.27:1.

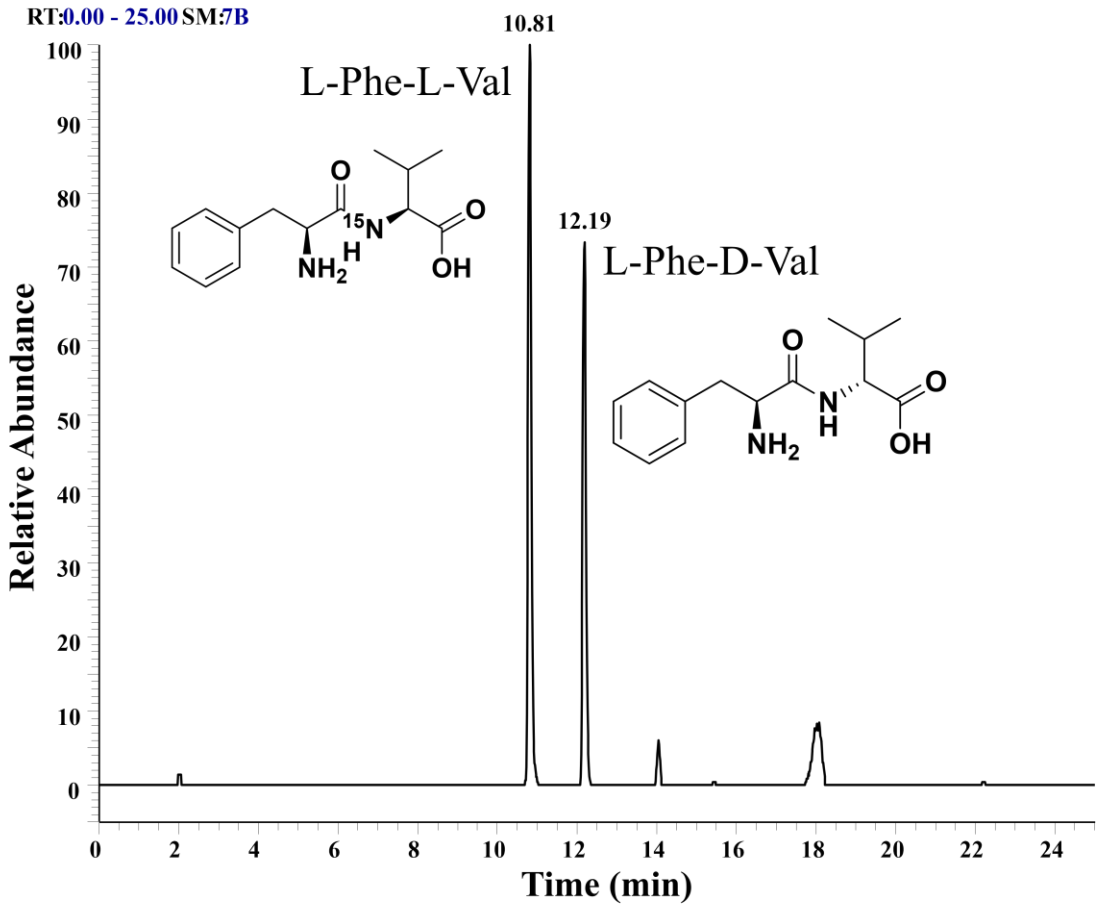


Figure S16. HPLC-MS-EIC spectra of $[M+H]^+$ for the product of racemic Val with *N*-L-Phe-F-AMP. The retention time 10.81 min was L-Phe-L-Val. The retention time 12.91 min was L-Phe-D-Val. According to the EIC integral area, more L-Phe-L-Val is generated, and its ratio of L-Phe-L-Val: L-Phe-D-Val = 1.27:1.

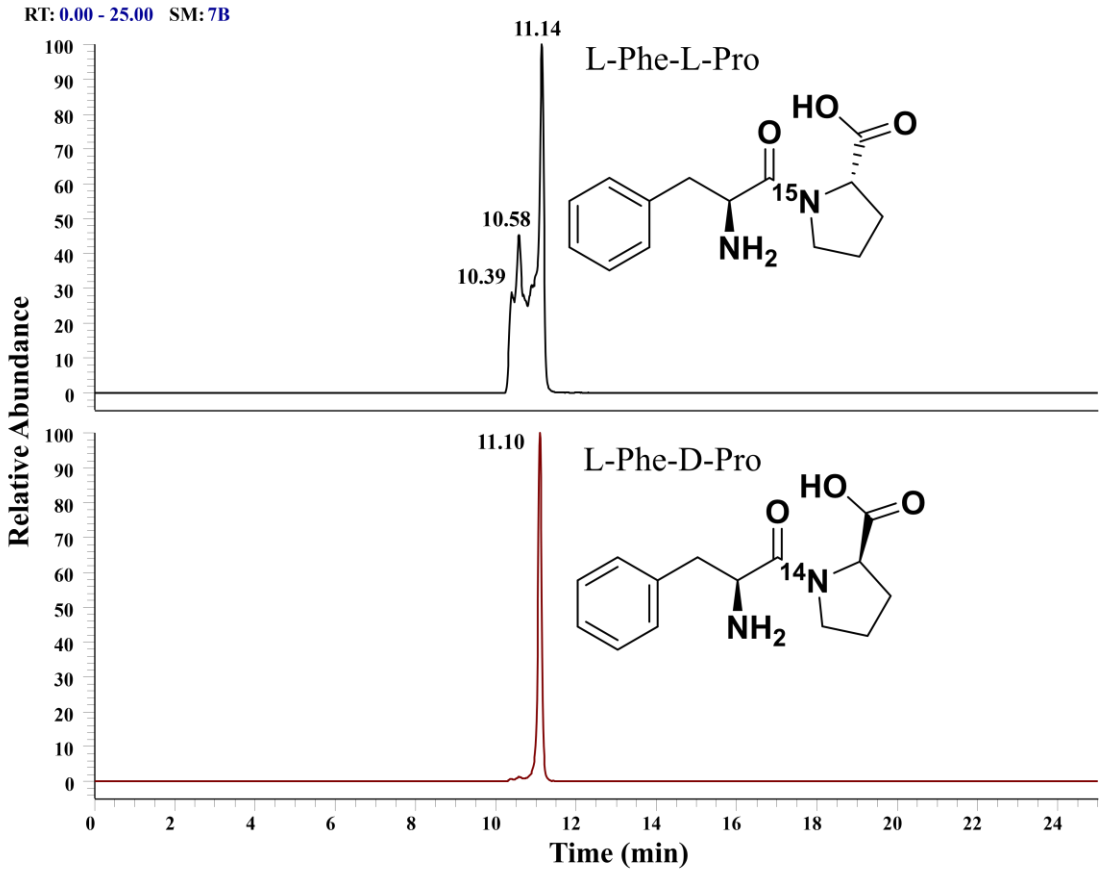


Figure S17. HPLC-MS-EIC spectra of $[M+H]^+$ for the linear Phe-Pro products of racemic Pro with *N*-L-Phe-F-AMP. The retention time 10.39 min, 10.58 min, and 11.14 min were L-Phe-L-Pro. The retention time 11.10 min was L-Phe-D-Pro. The Rt of 10.39 min, 10.58 min, and 11.14 min all correspond to m/z of 264.1366, indicating that the corresponding substances are L-Phe-L-Pro. L-Phe-L-Pro is not unimodal for unknown reasons, but it can be seen from the EIC integration area that more L-Phe-L-Pro is generated, and its ratio of L-Phe-L-Pro: L-Phe-D-Pro = 3.44:1.

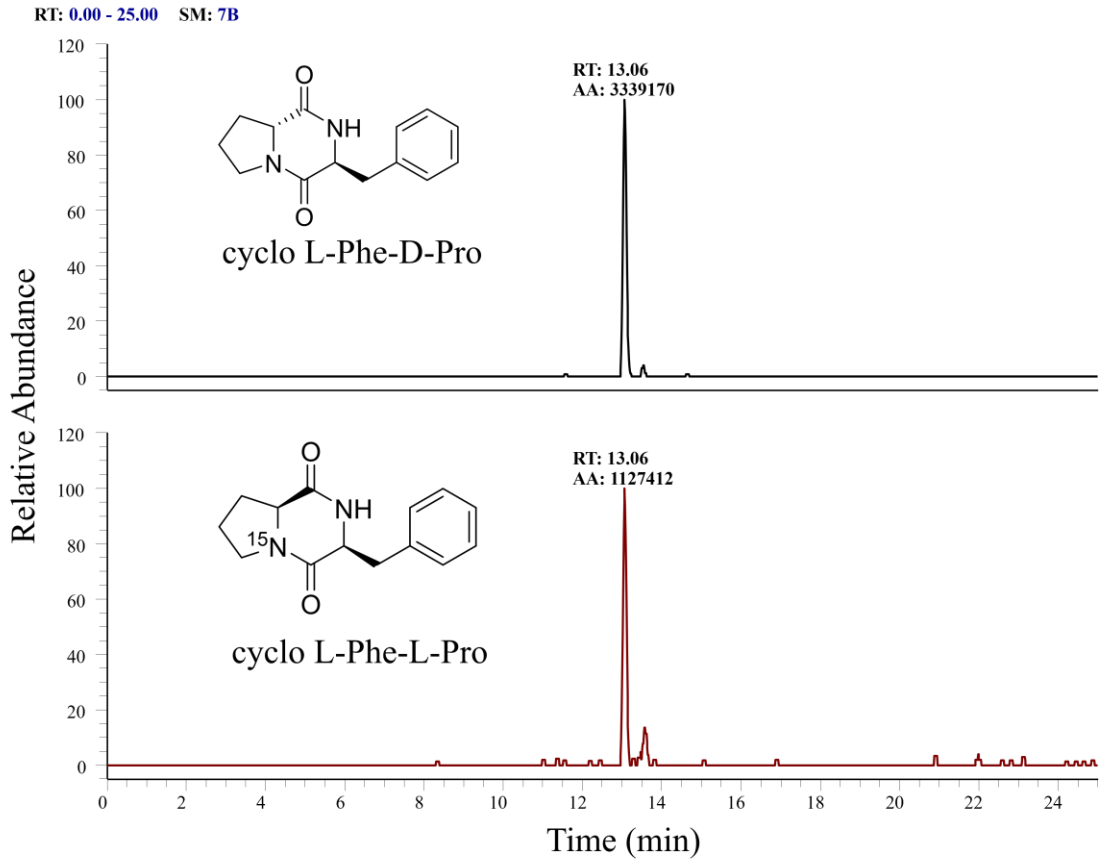


Figure S18. HPLC-MS-EIC spectra of the cycle Phe-Pro products of racemic proline and *N*-L-Phe-F-AMP. "AA" is the area of integration. The AA of cyclo L-Phe-D-Pro is larger than that of cyclo L-Phe-L-Pro, indicating that more cyclo L-Phe-D-Pro is formed than cyclo L-Phe-L-Pro.

Table S1. Initial L-aa:D-aa ratio (five amino acids), homochiral dipeptide: heterochiral dipeptide ratio (EIC peak area) and the enantiomeric excess (ee) of major peptides.

	Ile	Leu	Ala	Val	Pro
L-aa/D-aa	0.99	0.95	1.03	0.95	1.05
L, L-dipeptide/L, D-dipeptide [a]	1.96	1.47	1.27	1.27	3.44
(ee) [b]	(32.42%)	(19.14%)	(5.09%)	(12.04%)	(64.51%)
D, D-dipeptide/D, L-dipeptide [c]	1.63	/	/	/	2.56
(ee) [d]	(24.31%)				(65.62%)

[a] Ratio of L, L-dipeptide to L, D-dipeptide based on EIC peak area in the reaction of L/ D-amino acid with **1**.

[b] The ee of L, L-dipeptide in the reaction of L/ D-amino acid with **1**.

[c] Ratio of D, D-dipeptide to D,L-dipeptide based on EIC peak area in the reaction of L/ D-amino acid with **2**.

[d] The ee of D, D-dipeptide in the reaction of D/ L-amino acid with **1**.

Table S2. The LC-MS assay results of peptide

Dipeptide	[M+H] $^{+}$	*Cal.* [a]	*Exp.* [b]	*Δ ppm* [c]
Phe-L-Ile	[M+H] $^{+}$	280.1679	280.1671	2.8
Phe-D-Ile	[M+H] $^{+}$	279.1709	279.1700	3.2
Phe-L-Leu	[M+H] $^{+}$	280.1679	280.1665	5.0
Phe-D-Leu	[M+H] $^{+}$	279.1709	179.1695	5.0
Phe-L-Ala	[M+H] $^{+}$	238.1210	238.1197	5.5
Phe-D-Ala	[M+H] $^{+}$	237.1239	237.1227	5.1
Phe-L-Val	[M+H] $^{+}$	266.1523	266.1511	4.5
Phe-D-Val	[M+H] $^{+}$	265.1552	265.1541	4.1
Phe-L-Pro	[M+H] $^{+}$	264.1366	264.1356	3.8
Phe-D-Pro	[M+H] $^{+}$	263.1396	263.1385	4.2

[a] *Cal.*: The calculated value of the compound [M+H] $^{+}$.

[b] *Exp.*: The experimental value the compound [M+H] $^{+}$.

[c] *Δ ppm*: The relative error between calculated value and experimental value. Most of *Δ ppm* are less than 6 ppm.

7 Spectra of *N*-D-Phe-F-AMP

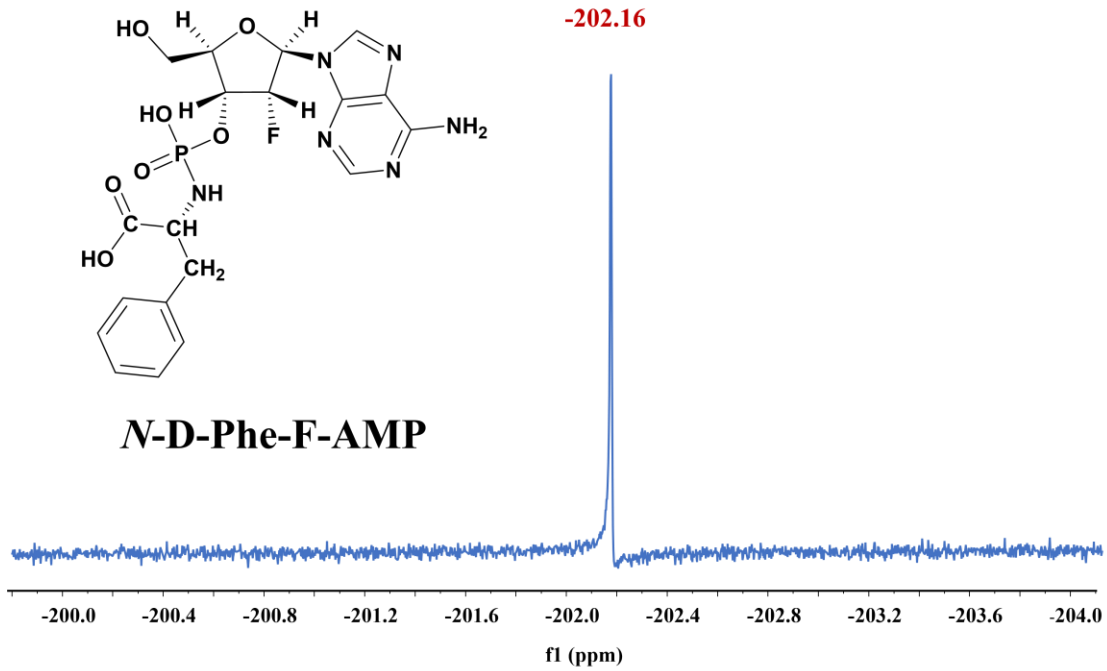


Figure S19. ^{19}F NMR spectrum of *N*-D-Phe-F-AMP. Its ^{19}F-NMR spectrum shift is -202.16 ppm.

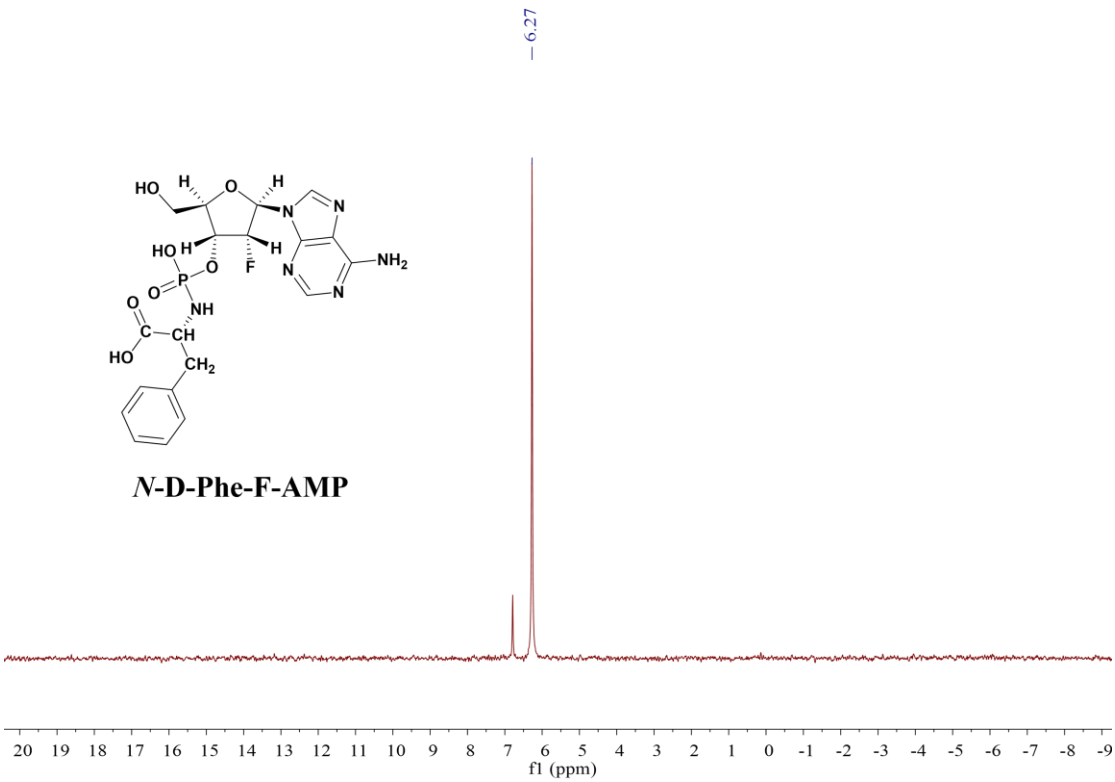


Figure S20. ^{31}P NMR spectrum of *N*-D-Phe-F-AMP. Its ^{31}P-NMR spectrum shift is 6.27 ppm.

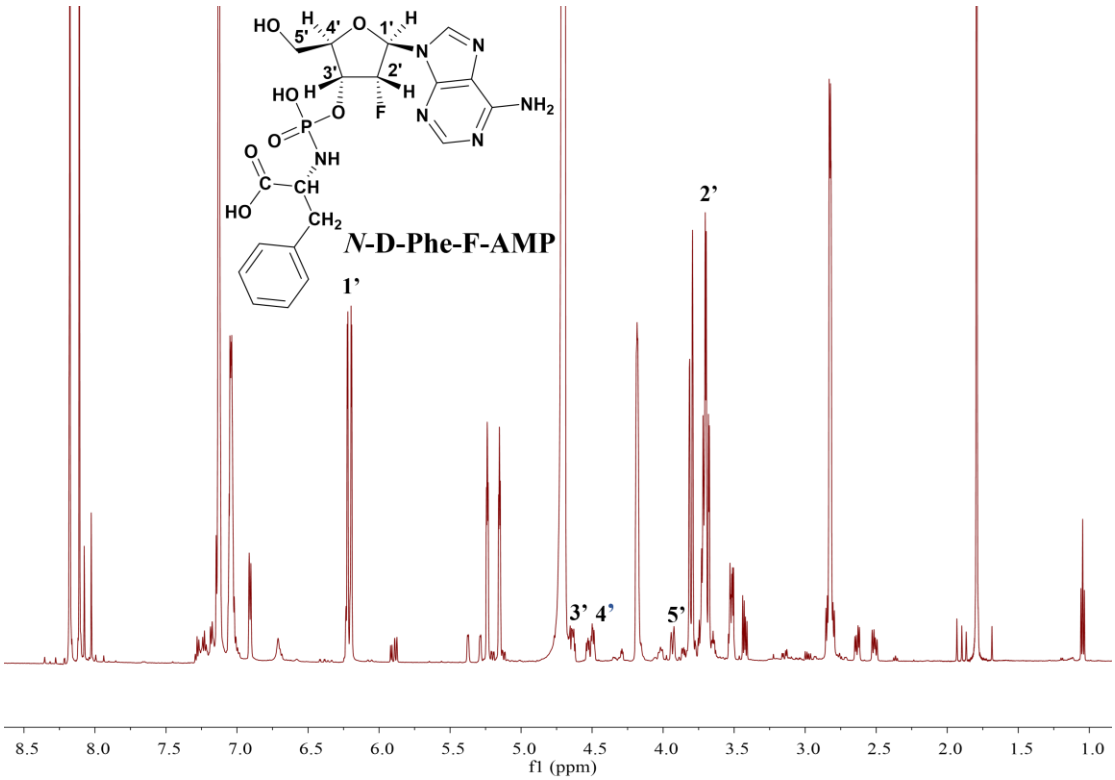


Figure S21. ^{1}H NMR spectrum of intermediate *N*-D-Phe-F-AMP.

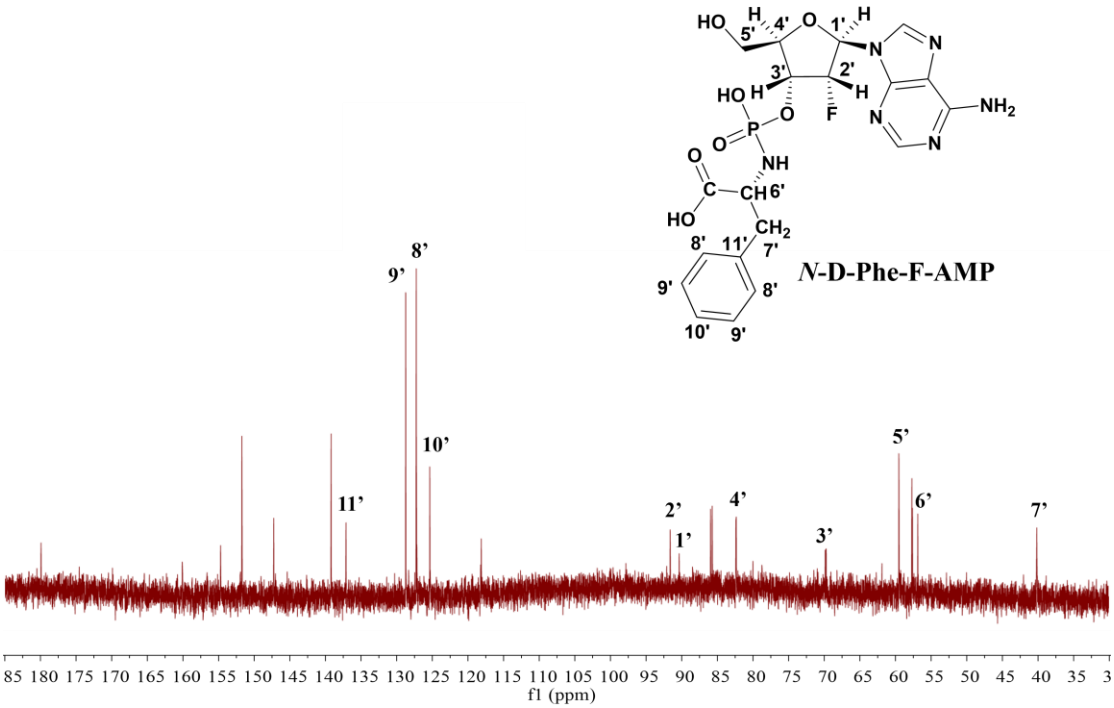


Figure S22. ^{13}C NMR spectrum of intermediate *N*-D-Phe-F-AMP.

8 Information of different chiral peptides (Ile and Pro) produced by reactions with *N*-D-Phe-F-AMP

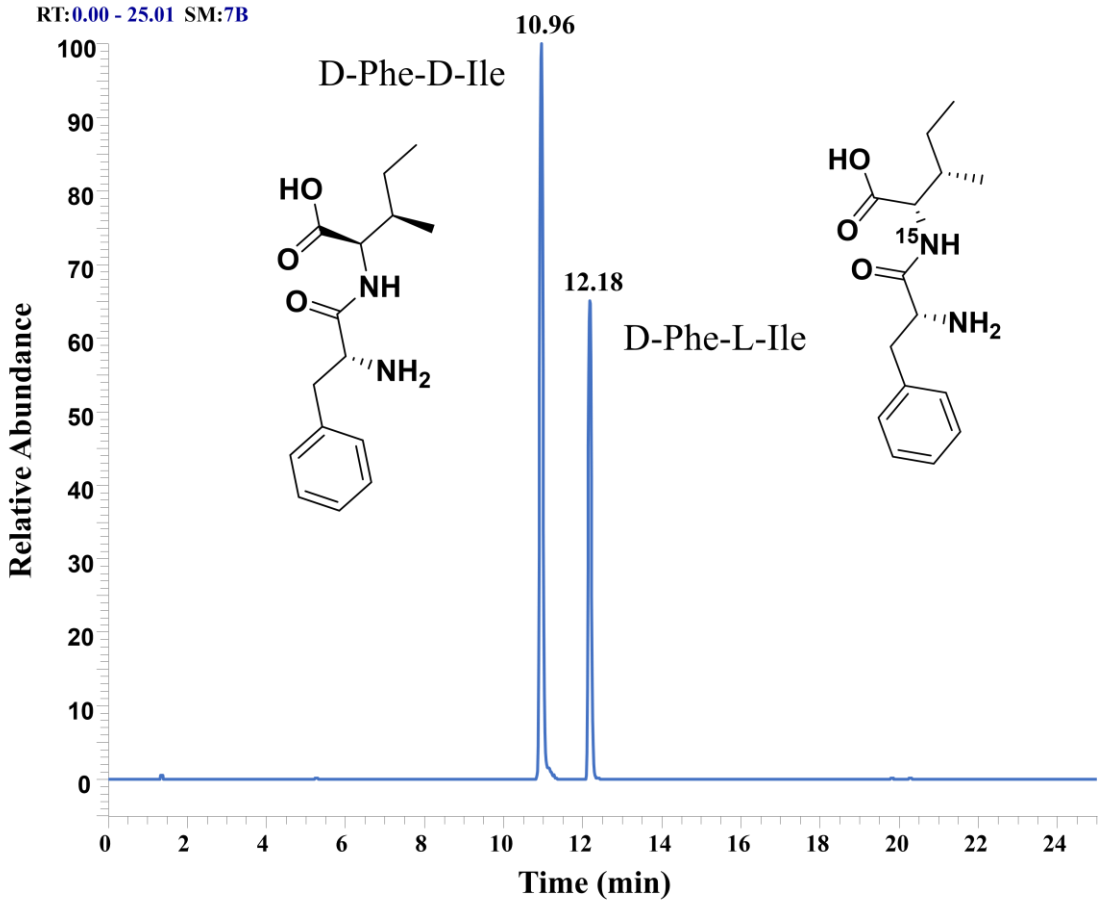


Figure S23. HPLC-MS-EIC spectra of $[M+H]^+$ for the product of racemic Ile with *N*-D-Phe-F-AMP. The retention time 10.96 min was D-Phe-D-Ile. The retention time 12.18 min was D-Phe-L-Ile. According to the EIC integral area, more D-Phe-D-Ile is generated, and its ratio of D-Phe-D-Ile: D-Phe-L-Ile = 1.63:1.

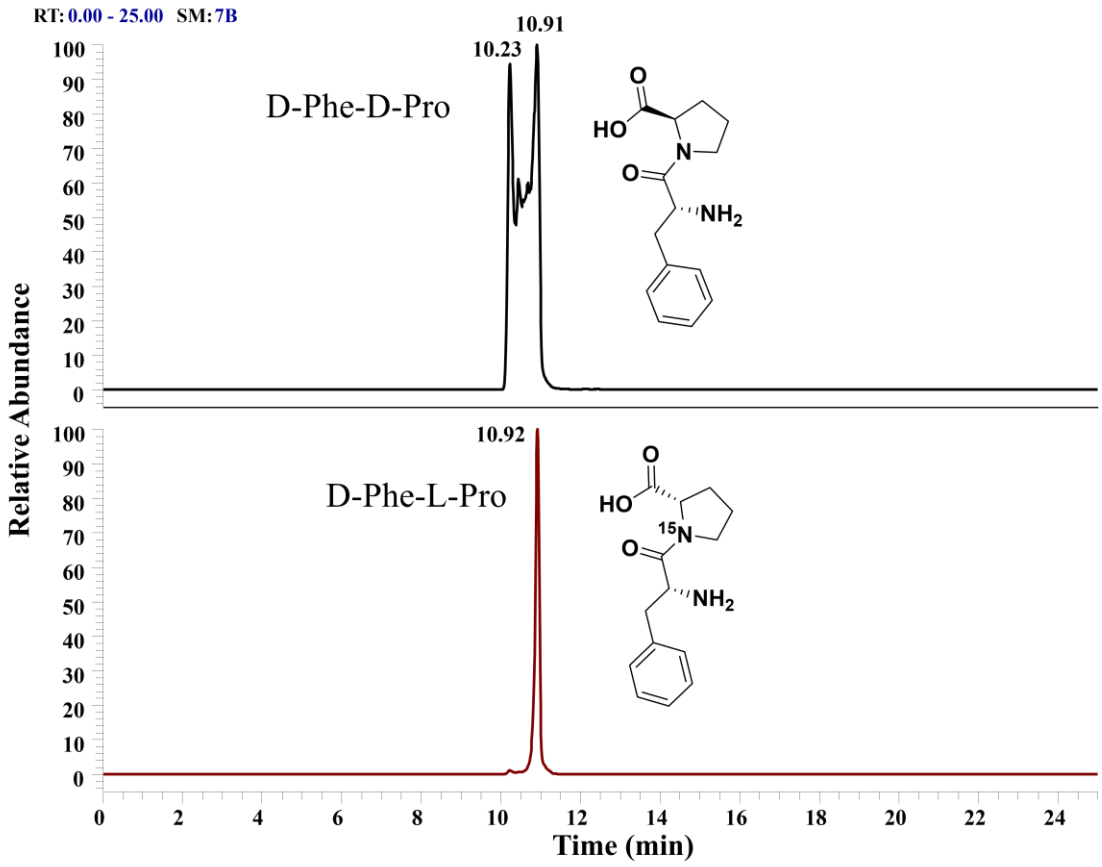


Figure S24. HPLC-MS-EIC spectra of $[M+H]^+$ for the product of racemic Pro with *N*-D-Phe-F-AMP. The retention time 10.23 min and 10.91 min were D-Phe-D-Pro. The retention time 10.92 min was D-Phe-L-Pro. The Rt of 10.23 min and 10.91 min all correspond to m/z of 263.1396, indicating that the corresponding substances are D-Phe-D-Pro. D-Phe-D-Pro is not unimodal for unknown reasons, but it can be seen from the EIC integration area that more D-Phe-D-Pro is generated, and its ratio of D-Phe-D-Pro: D-Phe-L-Pro = 5.26:1.

9 Density functional theory (DFT) calculations

Table S3. Various SCF and Gibbs free energies of the formation of dipeptides with CAPA and L-Ile. Calculations were done at the RB3LYP-D3(BJ)/B1 level in solvent.

	OPT/B1	*ΔE*	OPT/B1+ZPE	*ΔE*	*G*	*ΔG*
RC	-2399.078259	**0.0**	-2398.474857	**0.0**	-2398.546255	**0.0**
TS1	-2399.036003	**26.5**	-2398.438137	**23.0**	-2398.510481	**22.4**
IM1	-2399.068382	**6.2**	-2398.467220	**4.8**	-2398.544562	**1.1**
TS2	-2399.055593	**14.2**	-2398.452771	**13.9**	-2398.526929	**12.1**
IM2	-2399.062548	**9.9**	-2398.458504	**10.3**	-2398.533640	**7.9**
TS3	-2399.047548	**19.3**	-2398.448067	**16.8**	-2398.522541	**14.9**
PC	-2399.087407	**-5.7**	-2398.482439	**-4.8**	-2398.557572	**-7.1**

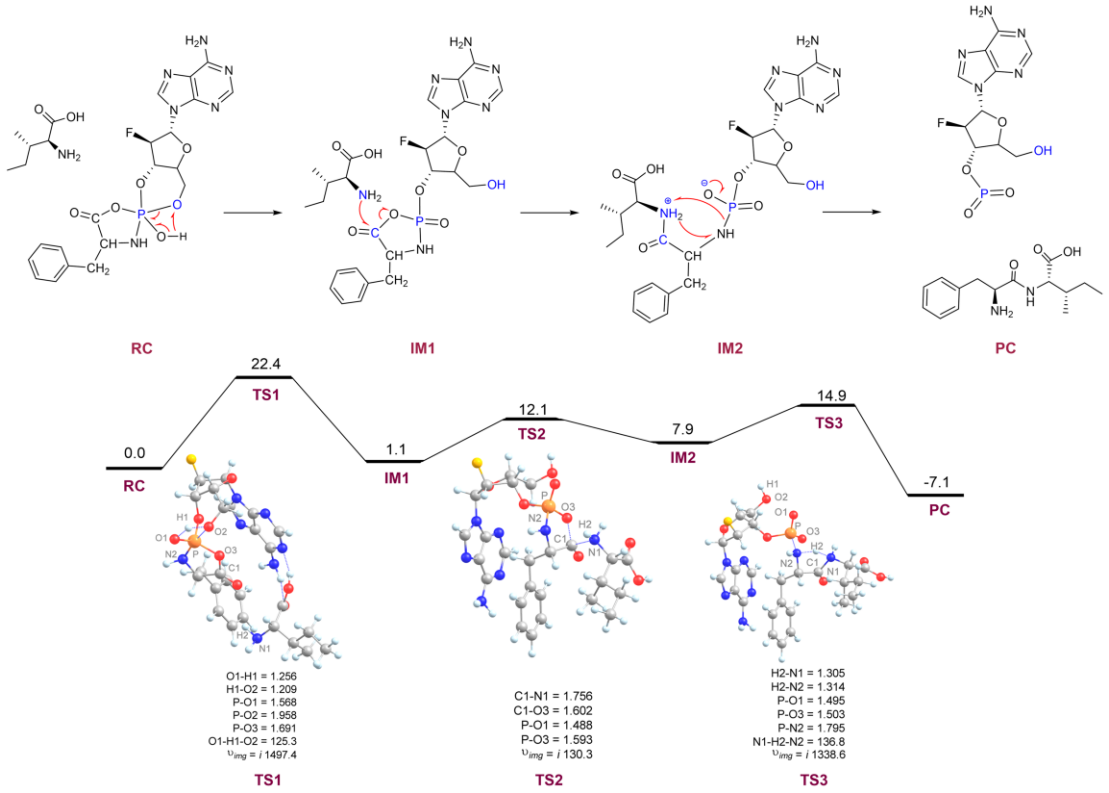


Figure S25. The energy profile (in kcal mol^{-1}) for the formation of dipeptides with CAPA and L-Ile. The curved arrow represents the direction of the atom attack, and lengths are in Å units, the relative energies are in kcal mol^{-1} units. The red arrows do not represent the direction of electron flow but rather the direction of atomic attack.

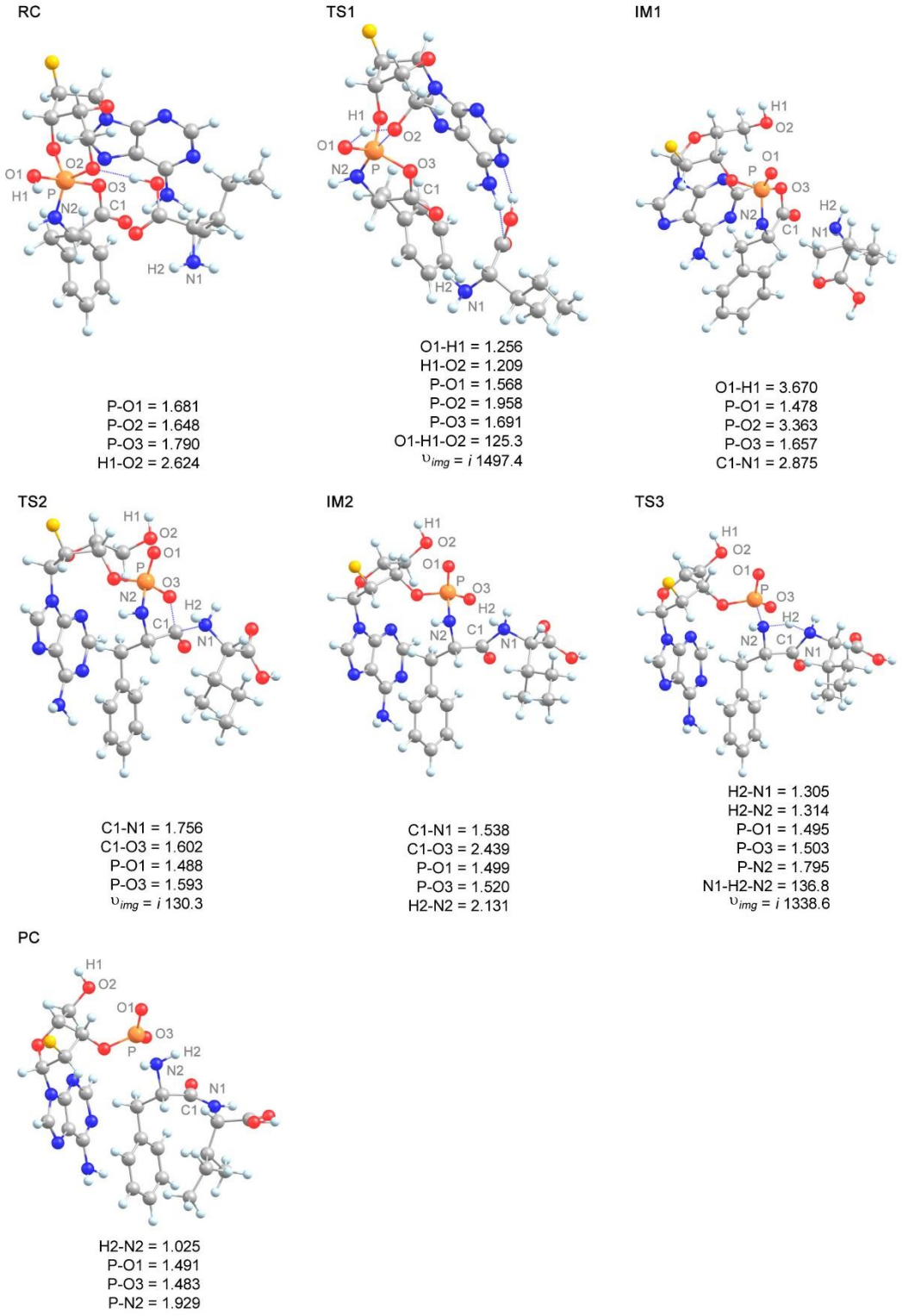


Figure S26. Optimized structures of the formation of dipeptides with CAPA and L-Ile. Calculations were done at the RB3LYP-D3(BJ)/B1 level in solvent. Lengths are in Å units, angles are in degree units and imaginary frequencies are in cm^{-1} units.

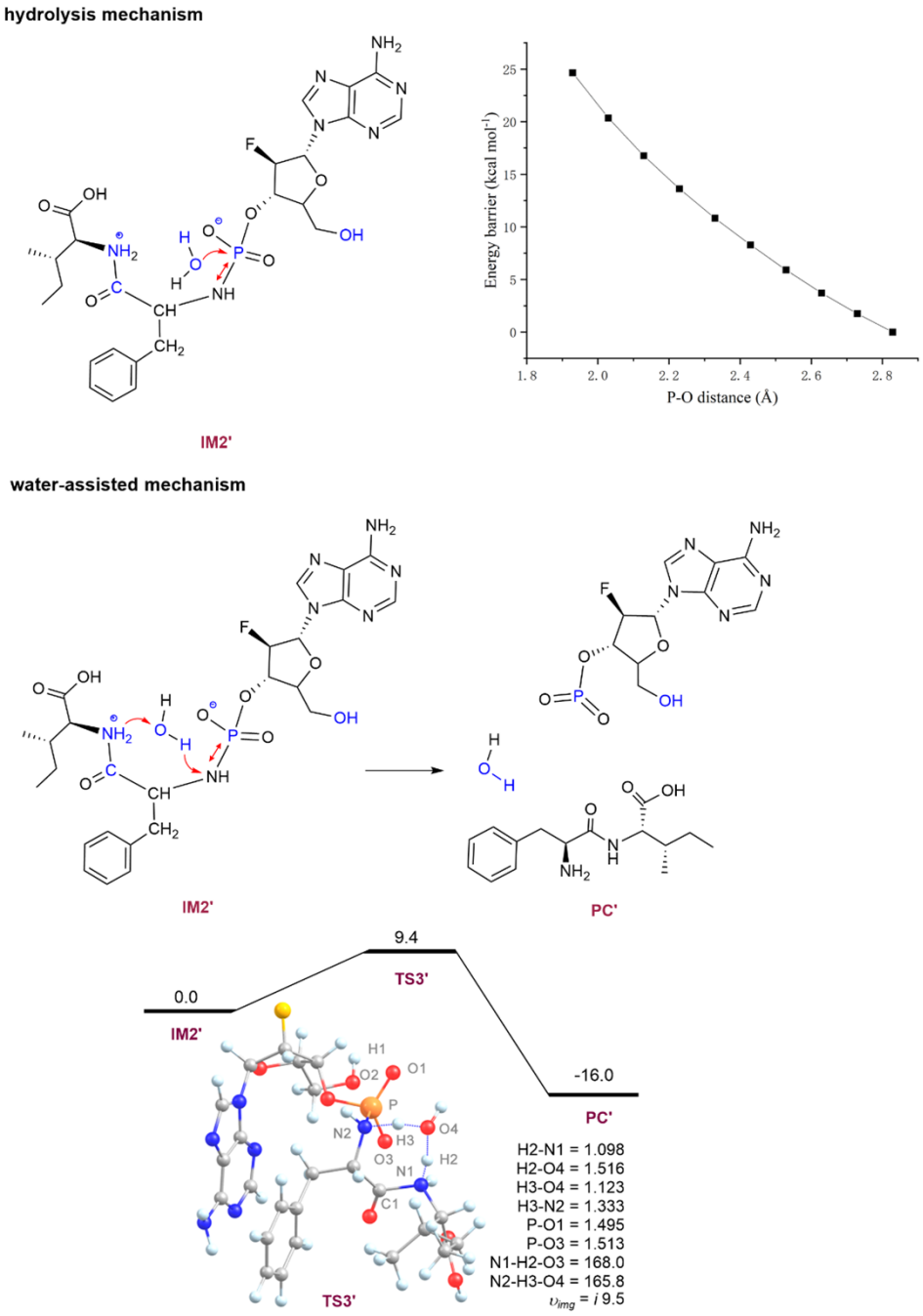


Figure S27. Two pathways involving water molecules: hydrolysis and a water-assisted mechanism.

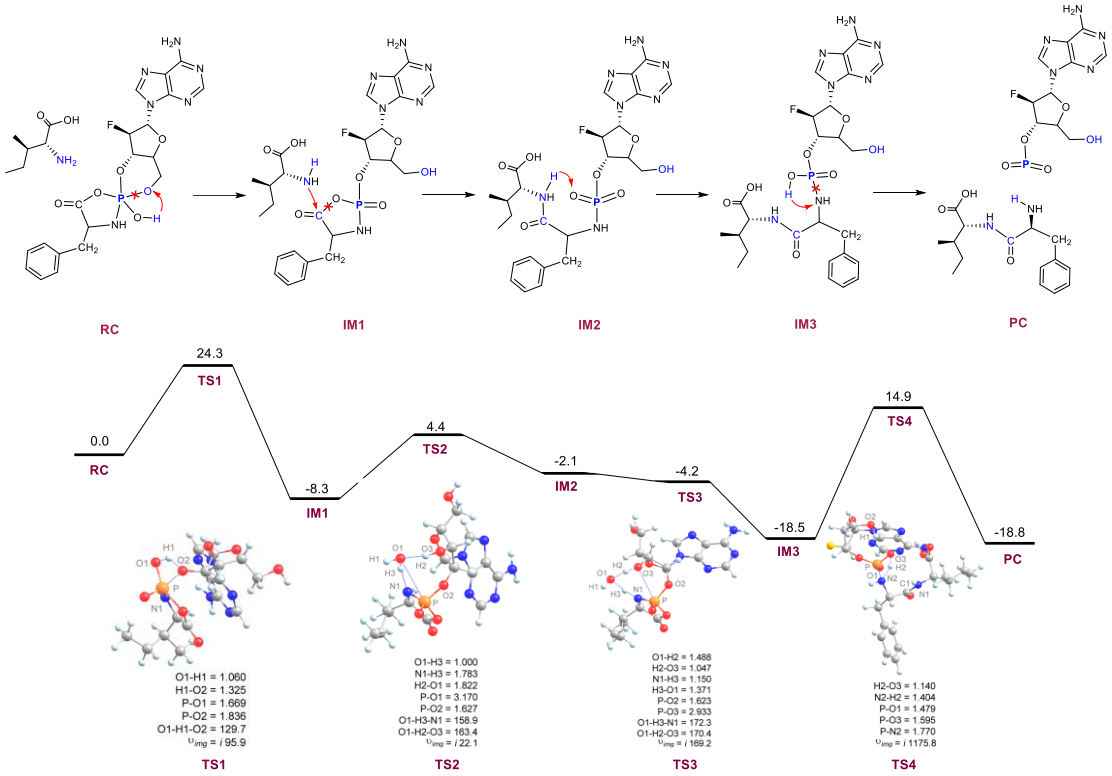


Figure S28. The energy profile (in kcal mol^{-1}) for the formation of dipeptides with CAPA and D-Ile. The curved arrow represents the direction of the atom attack, and the "x" represents the broken bond, Lengths are in Å units, the relative energies are in kcal mol^{-1} units.

Table S4. Various SCF and Gibbs free energies of the formation of dipeptides with CAPA and D-Ile. Calculations were done at the RB3LYP-D3(BJ)/B1 level in solvent.

	OPT/B1	*ΔE*	OPT/B1+ZPE	*ΔE*	*G*	*ΔG*
RC'	-2399.079252	**0.0**	-2398.475693	**0.0**	-2398.549274	**0.0**
TS1'	-2399.036995	**26.5**	-2398.438066	**23.6**	-2398.510487	**24.3**
IM1'	-2399.088471	**-5.8**	-2398.486596	**-6.8**	-2398.562563	**-8.3**
TS2'	-2399.071893	**4.6**	-2398.468756	**4.4**	-2398.542337	**4.4**
IM2'	-2399.084906	**-3.5**	-2398.480767	**-3.2**	-2398.552614	**-2.1**
TS3'	-2399.08223	**-1.9**	-2398.483168	**-4.7**	-2398.555998	**-4.2**
IM3'	-2399.106826	**-17.3**	-2398.504339	**-18.0**	-2398.578783	**-18.5**
TS4'	-2399.050514	**18.0**	-2398.451011	**15.5**	-2398.525543	**14.9**
PC'	-2399.10981	**-19.2**	-2398.504518	**-18.1**	-2398.57923	**-18.8**

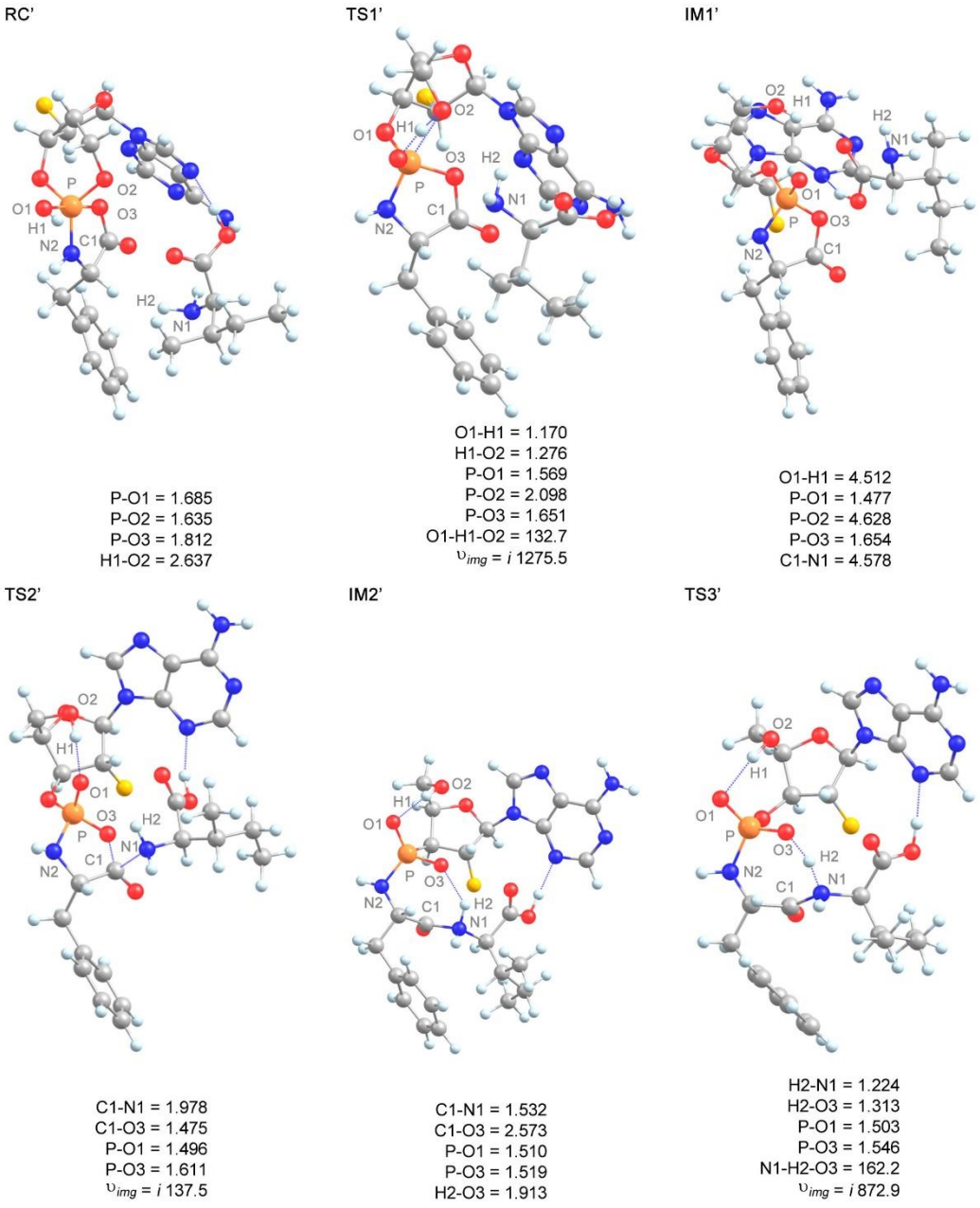


Figure S29. Optimized structures of the formation of dipeptides with CAPA and D-Ile. Calculations were done at the RB3LYP-D3(BJ)/B1 level in solvent. Lengths are in Å units, angles are in degree units and imaginary frequencies are in cm^{-1} units.

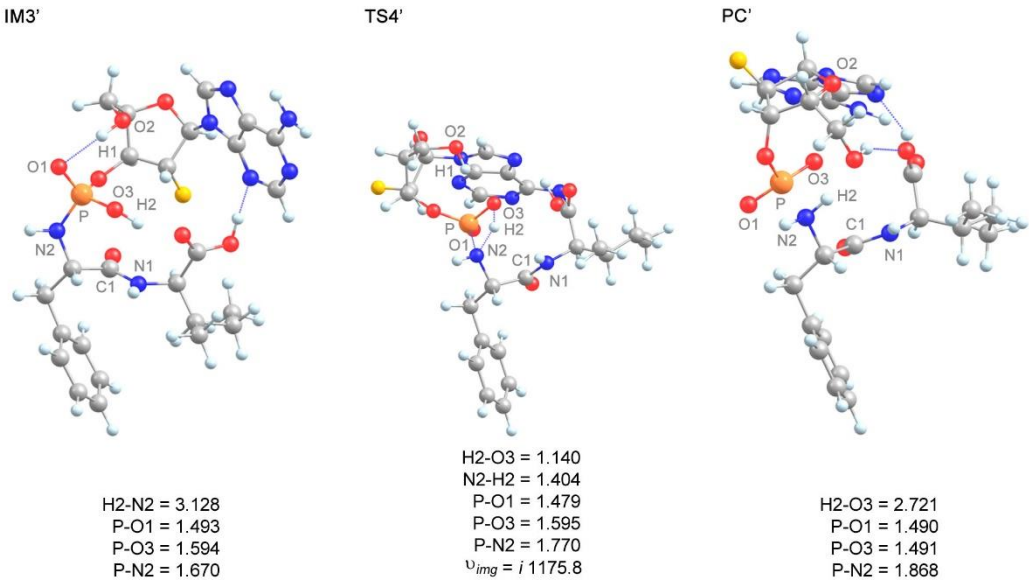


Figure S30. Optimized structures of the formation of dipeptides with CAPA and D-Ile. Calculations were done at the RB3LYP-D3(BJ)/B1 level in solvent. Lengths are in Å units, angles are in degree units and imaginary frequencies are in cm^{-1} units.

10 Cartesian coordinates

Part I the formation of dipeptides with CAPA and L-Ile

RC

O	-6.554384000	0.538751000	-1.207402000
C	-6.432105000	1.376112000	-2.380039000
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C	-4.062429000	0.453960000	-2.899192000
O	-4.149855000	-0.467789000	-1.793613000
C	-2.702370000	1.132399000	-2.736380000
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C	-2.970620000	2.129538000	-1.595018000
O	-4.368023000	2.416030000	-1.660378000
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C	-5.501165000	-2.394080000	1.023191000
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C	-4.272811000	-3.333686000	1.152367000
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C	-3.784582000	-4.088000000	4.501472000	H	-6.817624000	0.404550000	5.002279000
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C	-2.063686000	0.594394000	2.471620000	H	-5.815767000	0.159352000	9.189040000
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H	-4.524251000	2.648646000	-3.616604000	C	-3.952054000	1.886181000	-3.058745000
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H	-1.061149000	1.985587000	-2.757652000	C	-2.808599000	-0.185346000	-2.959930000
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O	-6.346921000	-0.123819000	0.271510000	C	-6.347612000	1.655794000	7.762808000
C	-3.208741000	-2.740193000	2.150234000	C	-6.640572000	2.010206000	9.223080000
P	-6.065843000	-0.709499000	-1.255496000	C	-5.622675000	-0.758729000	8.177530000
O	-7.120905000	-0.536902000	-2.274757000	O	-4.153433000	-0.228353000	5.473541000
C	-1.861523000	-3.136130000	2.143430000	O	-5.293141000	1.464132000	4.526494000
C	-1.218369000	-3.511209000	3.321160000	H	-7.709426000	-1.697734000	5.917232000
C	-1.919138000	-3.509531000	4.532336000	H	-6.896383000	-1.501490000	4.518364000
C	-3.259238000	-3.129852000	4.546155000	H	-7.291763000	0.649769000	5.456265000
C	-3.899629000	-2.745112000	3.364743000	H	-7.605487000	-0.080399000	7.718962000
N	-3.333004000	1.520092000	2.694500000	H	-5.308930000	1.924994000	7.524195000
C	-3.798165000	2.130910000	1.588351000	H	-6.981618000	2.271977000	7.111363000
N	-3.378298000	1.996826000	0.336712000	H	-6.528603000	3.086742000	9.392803000
C	-2.349480000	1.137694000	0.233889000	H	-7.666556000	1.733107000	9.495087000
C	-1.728274000	0.478317000	1.306616000	H	-5.962461000	1.494862000	9.911193000
C	-2.292594000	0.660422000	2.590168000	H	-5.793431000	-0.692343000	9.256555000
N	-1.678013000	0.689223000	-0.893204000	H	-5.773035000	-1.796814000	7.870065000
C	-0.701286000	-0.180561000	-0.435983000	H	-4.579462000	-0.496680000	7.976178000
N	-0.697571000	-0.334913000	0.867096000	H	-4.436145000	1.564978000	3.987551000
N	-1.847464000	0.033065000	3.699679000	TS2			
H	-5.048765000	2.580471000	-1.350919000	O	-6.118238000	2.878073000	-2.217871000
H	-4.542812000	3.860311000	-2.467865000	C	-4.757761000	2.707076000	-1.834427000
H	-3.910892000	2.076110000	-4.139763000	C	-4.038431000	1.801138000	-2.826100000
H	-4.890571000	-0.012372000	-3.630398000	C	-4.586706000	0.373290000	-2.909957000
H	-2.693499000	-1.171349000	-2.507766000	O	-5.066033000	-0.078686000	-1.640547000
H	-0.968352000	0.949458000	-2.821270000	C	-3.329984000	-0.428326000	-3.240012000
H	-5.357736000	-2.940072000	-1.330015000	F	-3.067733000	-0.275267000	-4.599841000
H	-5.792155000	-3.136796000	1.202061000	C	-2.233209000	0.335923000	-2.482247000
H	-3.450130000	-2.966405000	0.047517000	O	-2.639816000	1.672133000	-2.464836000
H	-3.426832000	-1.303396000	0.566944000	N	-6.578697000	-1.922034000	-0.511941000
H	-6.165489000	3.070601000	-3.910267000	C	-6.402446000	-1.612367000	0.912358000
H	-1.310003000	-3.127165000	1.208419000	C	-7.285414000	-0.366968000	1.145282000
H	-0.173837000	-3.808766000	3.293877000	C	-4.939245000	-1.330674000	1.325229000
H	-1.420776000	-3.799851000	5.452801000	O	-7.236812000	0.362056000	2.121134000
H	-3.813231000	-3.100148000	5.477919000	O	-7.166900000	0.416494000	-0.247229000
H	-4.930198000	-2.419161000	3.414403000	C	-4.668130000	-1.578826000	2.789408000
H	-4.634696000	2.806194000	1.749766000	P	-6.624031000	-0.512167000	-1.421547000

O	-7.373844000	-0.564282000	-2.705242000	O	-10.211084000	1.079517000	2.052142000
C	-4.337555000	-2.868503000	3.225033000	O	-10.522345000	-0.101481000	3.944686000
C	-4.076791000	-3.125986000	4.571962000	H	-8.863738000	-1.714941000	0.171119000
C	-4.141012000	-2.088323000	5.504980000	H	-9.340857000	-0.139504000	0.361284000
C	-4.471947000	-0.798660000	5.080083000	H	-10.719359000	-1.637095000	1.568989000
C	-4.735615000	-0.548240000	3.733171000	H	-8.719911000	-3.118370000	2.158939000
N	-2.060258000	1.088780000	2.731363000	H	-10.986044000	-2.622360000	4.125002000
C	-2.404858000	1.927261000	1.740812000	H	-11.083549000	-3.535830000	2.623145000
N	-2.462330000	1.698937000	0.425235000	H	-10.853226000	-5.117204000	4.484776000
C	-2.105351000	0.441912000	0.115315000	H	-9.362743000	-5.172082000	3.528863000
C	-1.721805000	-0.540964000	1.043496000	H	-9.395836000	-4.311023000	5.076250000
C	-1.720105000	-0.171647000	2.403462000	H	-7.658663000	-2.935872000	4.289558000
N	-2.052439000	-0.197376000	-1.115699000	H	-7.510565000	-1.308620000	3.618508000
C	-1.643576000	-1.493904000	-0.855168000	H	-8.744838000	-1.647218000	4.833525000
N	-1.443806000	-1.744653000	0.418558000	H	-10.825198000	0.773453000	4.257997000
N	-1.357292000	-1.035860000	3.392673000	IM2			
H	-4.759708000	2.245061000	-0.848581000	O	-5.779993000	3.096781000	-2.862586000
H	-4.225748000	3.664650000	-1.765679000	C	-4.461316000	2.824355000	-2.396981000
H	-4.072978000	2.244387000	-3.829529000	C	-3.888893000	1.598135000	-3.094443000
H	-5.357018000	0.256711000	-3.671239000	C	-4.631109000	0.285454000	-2.819203000
H	-3.408862000	-1.490055000	-3.003735000	O	-5.156477000	0.244172000	-1.499259000
H	-1.274475000	0.258907000	-3.003016000	C	-3.503321000	-0.735238000	-2.941732000
H	-6.029666000	-2.700288000	-0.863056000	F	-3.293024000	-0.986607000	-4.300667000
H	-6.788687000	-2.444184000	1.505817000	C	-2.268818000	0.029820000	-2.438130000
H	-4.301207000	-1.988837000	0.726693000	O	-2.518880000	1.386962000	-2.663957000
H	-4.680281000	-0.305745000	1.049889000	N	-6.690599000	-1.615551000	-0.356919000
H	-6.134930000	3.379344000	-3.049215000	C	-6.334158000	-1.520193000	1.053547000
H	-4.273731000	-3.675727000	2.498986000	C	-7.353667000	-0.623635000	1.735033000
H	-3.816737000	-4.131506000	4.890487000	C	-4.886715000	-1.082856000	1.381921000
H	-3.933668000	-2.282394000	6.553452000	O	-7.222189000	0.092377000	2.681089000
H	-4.522123000	0.014499000	5.798945000	O	-7.301219000	0.820679000	-0.230202000
H	-4.996462000	0.450487000	3.404870000	C	-4.393102000	-1.590333000	2.718133000
H	-2.680955000	2.931288000	2.056672000	P	-6.749097000	-0.152829000	-1.259312000
H	-1.502086000	-2.206431000	-1.656784000	O	-7.408097000	-0.409084000	-2.580654000
H	-1.719413000	-0.806047000	4.310974000	C	-3.721556000	-2.818269000	2.783336000
H	-1.428259000	-2.019164000	3.162256000	C	-3.257713000	-3.319782000	4.000914000
C	-10.152493000	0.033813000	2.665803000	C	-3.463466000	-2.596928000	5.178218000
N	-8.916889000	-0.939857000	0.836488000	C	-4.127731000	-1.369241000	5.124127000
C	-9.772531000	-1.288624000	2.004518000	C	-4.584987000	-0.869698000	3.903834000
C	-9.228210000	-2.453036000	2.871288000	N	-2.342908000	1.500804000	2.630146000
C	-10.410027000	-3.262411000	3.446324000	C	-2.803071000	2.131726000	1.535952000
C	-9.977788000	-4.535538000	4.176901000	N	-2.773302000	1.735429000	0.260911000
C	-8.222226000	-2.056880000	3.964359000	C	-2.188998000	0.535180000	0.118053000

C	-1.657580000	-0.233880000	1.166854000	H	-10.140115000	-4.559589000	4.965904000
C	-1.757768000	0.299683000	2.466774000	H	-8.433332000	-3.139216000	4.791458000
N	-1.976852000	-0.231389000	-1.018733000	H	-7.804339000	-1.626961000	4.153970000
C	-1.347327000	-1.387007000	-0.590225000	H	-9.343586000	-1.640481000	5.026536000
N	-1.142871000	-1.433558000	0.705891000	H	-11.367193000	0.669035000	4.265678000
N	-1.251537000	-0.344492000	3.555337000	TS3			
H	-4.526815000	2.628971000	-1.328592000	O	-5.572186000	3.044882000	-2.920911000
H	-3.788130000	3.677964000	-2.555349000	C	-4.251295000	2.644723000	-2.571178000
H	-3.868266000	1.760149000	-4.180839000	C	-3.920797000	1.283133000	-3.168696000
H	-5.418912000	0.094187000	-3.547533000	C	-4.800699000	0.124384000	-2.686280000
H	-3.693551000	-1.678758000	-2.427567000	O	-5.202885000	0.295897000	-1.327881000
H	-1.385782000	-0.286864000	-3.002545000	C	-3.835151000	-1.053072000	-2.767387000
H	-6.271739000	-2.416928000	-0.818706000	F	-3.791004000	-1.477376000	-4.097297000
H	-6.499704000	-2.515675000	1.494424000	C	-2.467998000	-0.421218000	-2.457953000
H	-4.257630000	-1.487800000	0.585879000	O	-2.556939000	0.924987000	-2.827168000
H	-4.821418000	0.005544000	1.315761000	N	-6.987695000	-1.161478000	0.017942000
H	-5.719148000	3.352997000	-3.797004000	C	-6.443659000	-1.144842000	1.402311000
H	-3.545386000	-3.376857000	1.867845000	C	-7.456662000	-0.294732000	2.176927000
H	-2.734608000	-4.271486000	4.028811000	C	-4.978953000	-0.727090000	1.589482000
H	-3.103309000	-2.983187000	6.127328000	O	-7.278202000	0.341115000	3.175390000
H	-4.284485000	-0.794631000	6.032838000	O	-7.030187000	1.377040000	0.115538000
H	-5.086626000	0.089675000	3.865999000	C	-4.409827000	-1.216308000	2.903672000
H	-3.269161000	3.097945000	1.718193000	P	-6.798867000	0.339650000	-0.947761000
H	-1.061274000	-2.156085000	-1.295822000	O	-7.647739000	0.149173000	-2.162938000
H	-1.643839000	-0.051954000	4.441838000	C	-3.855924000	-2.500164000	2.984304000
H	-1.155408000	-1.348802000	3.464783000	C	-3.331198000	-2.979367000	4.185889000
C	-10.297761000	0.041943000	2.848035000	C	-3.355559000	-2.175795000	5.328240000
N	-8.773274000	-0.853528000	1.190383000	C	-3.900506000	-0.891507000	5.255951000
C	-9.848752000	-1.246858000	2.162871000	C	-4.421272000	-0.416106000	4.051790000
C	-9.490840000	-2.488033000	3.024072000	N	-2.003340000	1.540814000	2.419655000
C	-10.778835000	-3.298637000	3.291989000	C	-2.469561000	2.111188000	1.295632000
C	-10.526429000	-4.658535000	3.946890000	N	-2.572217000	1.592205000	0.069533000
C	-8.719475000	-2.195550000	4.320827000	C	-2.129632000	0.326168000	0.017051000
O	-10.049338000	1.142908000	2.404720000	C	-1.605825000	-0.391714000	1.104613000
O	-11.061740000	-0.191944000	3.917163000	C	-1.560312000	0.271856000	2.346817000
H	-8.674481000	-1.527427000	0.415720000	N	-2.079459000	-0.565296000	-1.046061000
H	-8.991686000	0.057268000	0.752828000	C	-1.539969000	-1.735533000	-0.539829000
H	-10.689706000	-1.526651000	1.517547000	N	-1.248155000	-1.678258000	0.738552000
H	-8.857159000	-3.114265000	2.379910000	N	-1.051848000	-0.317341000	3.464267000
H	-11.454349000	-2.703548000	3.916727000	H	-4.207687000	2.575213000	-1.486153000
H	-11.292981000	-3.458062000	2.335356000	H	-3.501638000	3.375180000	-2.904753000
H	-11.458853000	-5.229899000	4.002469000	H	-3.984271000	1.325826000	-4.264494000
H	-9.805527000	-5.248212000	3.367698000	H	-5.672254000	-0.028092000	-3.321833000

H	-4.099320000	-1.897177000	-2.128556000	O	-5.088227000	0.676381000	-1.567476000
H	-1.693502000	-0.921926000	-3.047713000	C	-4.097659000	-1.036243000	-2.902116000
H	-6.793904000	-2.028288000	-0.482005000	F	-4.094296000	-1.495247000	-4.219785000
H	-6.567424000	-2.166401000	1.787418000	C	-2.627493000	-0.808016000	-2.507158000
H	-4.414223000	-1.162565000	0.762700000	O	-2.307224000	0.494784000	-2.905646000
H	-4.900074000	0.357607000	1.497307000	N	-7.340395000	0.108795000	-0.345385000
H	-5.603007000	3.173109000	-3.882783000	C	-7.019140000	-0.371290000	1.057126000
H	-3.819205000	-3.121698000	2.093432000	C	-7.797722000	0.481596000	2.074957000
H	-2.901975000	-3.976342000	4.228316000	C	-5.513722000	-0.329078000	1.338126000
H	-2.947112000	-2.544640000	6.264615000	O	-7.452520000	1.633941000	2.321726000
H	-3.916413000	-0.256490000	6.137296000	O	-6.172685000	2.602316000	-0.268680000
H	-4.838795000	0.582665000	3.998345000	C	-5.199537000	-1.045216000	2.630571000
H	-2.816183000	3.136920000	1.403656000	P	-6.441104000	1.542566000	-1.270393000
H	-1.384859000	-2.595143000	-1.178626000	O	-7.333042000	1.626290000	-2.462382000
H	-1.345470000	0.102956000	4.337427000	C	-4.851301000	-2.401158000	2.616366000
H	-1.068092000	-1.330065000	3.473197000	C	-4.596338000	-3.083767000	3.807069000
C	-10.502379000	-0.166839000	3.215955000	C	-4.694594000	-2.416754000	5.030889000
N	-8.779162000	-0.439236000	1.501466000	C	-5.037528000	-1.063127000	5.053743000
C	-9.870822000	-1.145122000	2.224809000	C	-5.286200000	-0.382190000	3.861269000
C	-9.447383000	-2.540829000	2.756761000	N	-2.199634000	1.100476000	2.390531000
C	-10.651080000	-3.506434000	2.733010000	C	-2.375464000	1.740566000	1.221882000
C	-10.272623000	-4.962151000	3.016673000	N	-2.451038000	1.232591000	-0.010142000
C	-8.756715000	-2.517747000	4.129908000	C	-2.325047000	-0.102946000	-0.016351000
O	-10.293896000	1.027541000	3.202572000	C	-2.104276000	-0.899371000	1.119043000
O	-11.371933000	-0.765192000	4.041616000	C	-2.056741000	-0.237771000	2.363258000
H	-8.211852000	-0.991558000	0.463552000	N	-2.377394000	-1.004722000	-1.071898000
H	-9.083126000	0.507126000	1.255256000	C	-2.181408000	-2.257384000	-0.514645000
H	-10.638784000	-1.309647000	1.459437000	N	-2.018169000	-2.241509000	0.787285000
H	-8.734804000	-2.925279000	2.013944000	N	-1.842123000	-0.902376000	3.531989000
H	-11.401275000	-3.168509000	3.455672000	H	-3.466367000	2.607150000	-1.741464000
H	-11.119933000	-3.449098000	1.742052000	H	-2.490327000	3.097004000	-3.142359000
H	-11.141493000	-5.614499000	2.879878000	H	-3.472388000	1.207294000	-4.457253000
H	-9.484706000	-5.305646000	2.335254000	H	-5.538581000	0.453469000	-3.584394000
H	-9.915109000	-5.101291000	4.041752000	H	-4.628268000	-1.752136000	-2.272537000
H	-8.354054000	-3.507185000	4.360192000	H	-1.996460000	-1.530343000	-3.034629000
H	-7.925794000	-1.811517000	4.179537000	H	-7.236406000	-0.689226000	-0.978118000
H	-9.470741000	-2.251208000	4.914823000	H	-7.353366000	-1.407939000	1.086359000
H	-11.774688000	-0.073203000	4.602431000	H	-4.993885000	-0.810333000	0.508076000
PC				H	-5.197047000	0.714638000	1.372818000
O	-4.563836000	3.381021000	-3.268226000	H	-4.527488000	3.445821000	-4.236319000
C	-3.435703000	2.633445000	-2.829274000	H	-4.762655000	-2.919260000	1.666245000
C	-3.486199000	1.206218000	-3.358802000	H	-4.321013000	-4.133986000	3.778710000
C	-4.690070000	0.369295000	-2.905732000	H	-4.499251000	-2.946720000	5.958328000

H	-5.110249000	-0.535664000	6.000320000
H	-5.550790000	0.670219000	3.879894000
H	-2.477213000	2.821426000	1.293499000
H	-2.169276000	-3.143665000	-1.135408000
H	-2.122412000	-0.402168000	4.366531000
H	-2.089870000	-1.884308000	3.536406000
C	-10.840916000	-1.377755000	3.030829000
N	-8.877357000	-0.081681000	2.668971000
C	-9.377520000	-1.450115000	2.614278000
C	-8.564616000	-2.417039000	3.532852000
C	-8.951531000	-3.886648000	3.297027000
C	-7.965686000	-4.876969000	3.924076000
C	-8.644675000	-2.002781000	5.005368000
O	-11.302207000	-0.505672000	3.739559000
O	-11.553687000	-2.406293000	2.551777000
H	-8.331691000	0.360741000	-0.406427000
H	-9.358682000	0.521084000	3.329778000
H	-9.345115000	-1.825659000	1.588759000
H	-7.524420000	-2.293702000	3.210590000
H	-9.959307000	-4.072224000	3.686489000
H	-9.002072000	-4.070127000	2.215377000
H	-8.245927000	-5.906933000	3.678224000
H	-6.948569000	-4.704155000	3.556063000
H	-7.943177000	-4.792250000	5.015598000
H	-7.941103000	-2.587918000	5.602273000
H	-8.379880000	-0.949122000	5.134345000
H	-9.650468000	-2.158540000	5.412739000
H	-12.463540000	-2.326482000	2.900575000

Part II the formation of dipeptides with CAPA and D-ILe

RC’			
O	-5.546926000	1.413110000	-0.211817000
C	-5.720130000	2.207160000	-1.409005000
C	-4.535407000	2.051687000	-2.353291000
C	-4.013932000	0.595840000	-2.546436000
O	-4.769294000	-0.444849000	-1.904405000
C	-2.532634000	0.637475000	-2.129465000
F	-1.749259000	0.521878000	-3.277788000
C	-2.303762000	2.045929000	-1.555726000
O	-3.409863000	2.833241000	-1.899236000
N	-5.981938000	-1.391304000	0.558915000
C	-5.075170000	-1.918784000	1.561210000
C	-3.826505000	-1.070340000	1.402775000
C	-4.792765000	-3.427099000	1.351000000
O	-2.827892000	-1.169460000	2.089865000
O	-3.947528000	-0.226694000	0.386185000
C	-4.126209000	-4.077217000	2.540572000
P	-5.534693000	-0.198865000	-0.487597000
O	-7.029435000	-0.261654000	-1.262658000
C	-2.734374000	-4.207723000	2.616056000
C	-2.133263000	-4.785266000	3.734813000
C	-2.917203000	-5.241818000	4.796968000
C	-4.306505000	-5.121673000	4.730363000
C	-4.903733000	-4.545832000	3.607824000
N	0.460145000	0.173978000	2.349120000
C	0.581608000	0.051463000	1.019732000
N	-0.174044000	0.595237000	0.058589000
C	-1.148769000	1.353460000	0.579814000
C	-1.394515000	1.590236000	1.933128000
C	-0.540349000	0.932559000	2.845275000
N	-2.134977000	2.039372000	-0.100865000
C	-2.919350000	2.646849000	0.843954000
N	-2.507966000	2.410056000	2.073181000
N	-0.655836000	1.046672000	4.189609000
H	-5.787215000	3.243651000	-1.076465000
H	-6.643872000	1.926136000	-1.916991000
H	-4.824748000	2.471760000	-3.320509000
H	-4.044351000	0.328498000	-3.602347000
H	-2.266992000	-0.161476000	-1.441167000
H	-1.400195000	2.475544000	-1.996460000
H	-6.870107000	-1.851927000	0.410021000
H	-5.481173000	-1.750494000	2.561759000
H	-5.758078000	-3.911220000	1.164875000
H	-4.191363000	-3.551924000	0.444064000
H	-7.741405000	0.023837000	-0.665256000
H	-2.120543000	-3.842941000	1.798682000
H	-1.051713000	-4.878873000	3.776960000
H	-2.448796000	-5.691151000	5.667920000
H	-4.926128000	-5.479051000	5.547904000
H	-5.986599000	-4.462718000	3.555849000
H	1.402626000	-0.577029000	0.681166000
H	-3.774693000	3.242984000	0.575900000
H	-0.089289000	0.428901000	4.754608000
H	-1.525169000	1.389104000	4.584976000
C	-4.406820000	0.800384000	4.381800000

N	-3.488792000	-1.306899000	5.256522000	C	-5.016997000	-4.584880000	4.985377000
C	-4.310785000	-0.130119000	5.590690000	C	-5.308014000	-4.254201000	3.661478000
C	-5.680866000	-0.536980000	6.172063000	N	-0.082265000	0.258545000	2.641658000
C	-6.549587000	0.689481000	6.508315000	C	0.047674000	-0.095701000	1.354944000
C	-5.888602000	1.717319000	7.432964000	N	-0.628201000	0.356495000	0.291904000
C	-6.460770000	-1.522451000	5.293342000	C	-1.545350000	1.266272000	0.651311000
O	-5.140014000	0.635113000	3.419814000	C	-1.818440000	1.718618000	1.946304000
O	-3.518524000	1.807973000	4.454831000	C	-1.017041000	1.175848000	2.970383000
H	-3.827052000	-1.744939000	4.400950000	N	-2.420690000	1.948563000	-0.166391000
H	-2.544267000	-0.998539000	5.027710000	C	-3.165989000	2.766624000	0.658239000
H	-3.765235000	0.413647000	6.365595000	N	-2.844112000	2.655590000	1.930907000
H	-5.440081000	-1.049943000	7.114083000	N	-1.104727000	1.571659000	4.267015000
H	-6.854543000	1.177823000	5.572978000	H	-5.890336000	3.398429000	-1.666370000
H	-7.473794000	0.325983000	6.975511000	H	-6.682717000	1.931539000	-2.276644000
H	-6.605782000	2.490971000	7.728434000	H	-4.763182000	2.374807000	-3.655826000
H	-5.512952000	1.242444000	8.347772000	H	-4.211958000	0.123700000	-3.679665000
H	-5.046079000	2.222017000	6.947800000	H	-2.658092000	-0.350132000	-1.347408000
H	-7.369713000	-1.847878000	5.812257000	H	-1.460715000	2.108574000	-2.000786000
H	-5.870544000	-2.416628000	5.072727000	H	-6.634508000	-2.434329000	-0.305042000
H	-6.756672000	-1.058053000	4.348661000	H	-5.897646000	-2.149799000	1.945119000
H	-3.371957000	2.210642000	3.535257000	H	-5.395346000	-4.427485000	0.888489000
TS1’				H	-3.741196000	-3.877804000	0.632512000
O	-5.617821000	1.729176000	-0.489172000	H	-6.728217000	1.198674000	-0.151673000
C	-5.782319000	2.312969000	-1.771606000	H	-2.166855000	-4.295936000	2.378336000
C	-4.581926000	2.010457000	-2.641000000	H	-1.642846000	-4.908564000	4.719952000
C	-4.227967000	0.506960000	-2.661106000	H	-3.467162000	-5.080108000	6.402475000
O	-5.184278000	-0.363186000	-2.012145000	H	-5.821046000	-4.659887000	5.711879000
C	-2.792997000	0.413650000	-2.110264000	H	-6.340293000	-4.079465000	3.367270000
F	-1.944655000	0.121489000	-3.177244000	H	0.808347000	-0.846562000	1.150992000
C	-2.451492000	1.835237000	-1.626625000	H	-3.933163000	3.407195000	0.259166000
O	-3.405113000	2.704018000	-2.169350000	H	-0.611622000	1.000021000	4.940204000
N	-5.704471000	-2.044500000	-0.179427000	H	-1.962740000	2.001520000	4.595535000
C	-5.154025000	-2.329646000	1.154751000	C	-4.949326000	1.794322000	5.004294000
C	-4.090315000	-1.265846000	1.353456000	N	-5.636434000	0.654338000	2.929728000
C	-4.615231000	-3.764462000	1.280748000	C	-4.842501000	0.536162000	4.153908000
O	-3.142191000	-1.271403000	2.084497000	C	-5.268597000	-0.730253000	4.948600000
O	-4.322326000	-0.182332000	0.506850000	C	-4.409979000	-1.004864000	6.194085000
C	-4.286990000	-4.145403000	2.707304000	C	-2.919751000	-1.207651000	5.911836000
P	-5.639128000	-0.369260000	-0.471730000	C	-6.758557000	-0.722093000	5.308152000
O	-7.091665000	0.087625000	-0.093242000	O	-5.955067000	2.460851000	5.140738000
C	-2.968116000	-4.385370000	3.106556000	O	-3.785740000	2.116664000	5.625261000
C	-2.673055000	-4.725678000	4.427741000	H	-6.555138000	1.026946000	3.164891000
C	-3.696511000	-4.822672000	5.372570000	H	-5.198851000	1.345666000	2.320992000

H	-3.800703000	0.412409000	3.857335000	N	-0.646341000	3.795598000	0.460507000
H	-5.095819000	-1.553441000	4.246032000	N	0.148339000	4.871825000	3.208740000
H	-4.545623000	-0.198654000	6.928201000	H	-4.557955000	3.254672000	-1.823137000
H	-4.807081000	-1.913980000	6.662679000	H	-6.032293000	2.415755000	-1.308532000
H	-2.395017000	-1.532095000	6.817651000	H	-4.654090000	0.956390000	-2.667651000
H	-2.768993000	-1.973959000	5.145089000	H	-4.493678000	-0.990900000	-1.274344000
H	-2.444210000	-0.286159000	5.568037000	H	-3.908817000	0.692537000	1.165711000
H	-7.028775000	-1.668611000	5.788879000	H	-1.611534000	-0.034943000	-0.602620000
H	-7.388713000	-0.613574000	4.419660000	H	-6.754081000	-3.026485000	-1.176555000
H	-7.002208000	0.090553000	6.001689000	H	-6.171215000	-4.451441000	0.682056000
H	-3.950580000	2.916138000	6.163419000	H	-4.394811000	-4.491675000	-1.019094000
IM1’				H	-3.599766000	-3.106201000	-0.271650000
O	-4.592555000	2.826552000	0.156171000	H	-8.296076000	0.666764000	4.558535000
C	-4.945000000	2.466421000	-1.170110000	H	-2.053198000	-3.400862000	1.513515000
C	-4.336803000	1.143797000	-1.638823000	H	-0.771074000	-4.912300000	3.004614000
C	-4.628945000	-0.054238000	-0.728278000	H	-1.411381000	-7.308599000	3.195660000
O	-5.968806000	0.023884000	-0.229613000	H	-3.327494000	-8.181843000	1.871512000
C	-3.557004000	0.076967000	0.346791000	H	-4.587611000	-6.671710000	0.367432000
F	-3.185023000	-1.165946000	0.870225000	H	-1.911215000	1.331131000	4.757661000
C	-2.385551000	0.714082000	-0.412354000	H	-1.209684000	2.991114000	-1.432969000
O	-2.893172000	1.160590000	-1.654033000	H	0.235858000	5.231053000	4.148861000
N	-6.232958000	-2.630578000	-0.403081000	H	0.305955000	5.504174000	2.437546000
C	-5.552357000	-3.563614000	0.506192000	C	-5.198317000	0.603417000	3.451877000
C	-5.460589000	-2.833050000	1.846120000	N	-7.578627000	0.703945000	3.836480000
C	-4.181689000	-4.003910000	-0.061590000	C	-6.319942000	0.193769000	4.384470000
O	-4.987749000	-3.239646000	2.868616000	C	-6.019992000	0.649086000	5.849483000
O	-6.048083000	-1.581093000	1.777239000	C	-4.897903000	-0.140070000	6.548302000
C	-3.405664000	-4.932193000	0.840613000	C	-5.077652000	-1.661235000	6.543625000
P	-6.779956000	-1.248463000	0.331594000	C	-5.760602000	2.157737000	5.937027000
O	-8.221279000	-0.929889000	0.388728000	O	-5.296019000	1.523245000	2.645526000
C	-2.325004000	-4.450045000	1.589008000	O	-4.087227000	-0.102578000	3.627655000
C	-1.608743000	-5.300279000	2.431838000	H	-7.459183000	1.684298000	3.589373000
C	-1.968215000	-6.645530000	2.539742000	H	-5.154233000	2.353611000	0.796399000
C	-3.045001000	-7.135502000	1.796869000	H	-6.359461000	-0.898186000	4.369790000
C	-3.755914000	-6.283472000	0.950891000	H	-6.951272000	0.429904000	6.393584000
N	-0.929628000	3.006889000	4.081064000	H	-3.933224000	0.115105000	6.095560000
C	-1.607920000	1.877782000	3.868092000	H	-4.853828000	0.214038000	7.586932000
N	-1.977668000	1.329279000	2.700163000	H	-4.328516000	-2.139347000	7.184809000
C	-1.590053000	2.065193000	1.639419000	H	-6.067941000	-1.944300000	6.922542000
C	-0.885514000	3.273424000	1.718981000	H	-4.967963000	-2.081630000	5.539069000
C	-0.552567000	3.738949000	3.008706000	H	-5.695597000	2.476304000	6.982779000
N	-1.775685000	1.848884000	0.290316000	H	-6.560674000	2.734148000	5.460777000
C	-1.186937000	2.921168000	-0.356143000	H	-4.815307000	2.425845000	5.449031000

H	-3.328031000	0.310789000	3.110119000
TS2’			
O	-4.537411000	2.594906000	-0.811118000
C	-4.170479000	2.121315000	-2.092846000
C	-2.820390000	1.409522000	-2.109382000
C	-2.681649000	0.200394000	-1.171198000
O	-3.815241000	-0.688578000	-1.225056000
C	-2.297187000	0.835683000	0.169316000
F	-1.458451000	-0.001066000	0.894892000
C	-1.513610000	2.083785000	-0.277612000
O	-1.751156000	2.271615000	-1.653409000
N	-5.712031000	-2.266084000	-0.238632000
C	-5.584632000	-3.211776000	0.889579000
C	-4.492210000	-2.639289000	1.830972000
C	-5.208261000	-4.622534000	0.393146000
O	-3.756195000	-3.312429000	2.521519000
O	-3.892295000	-1.466573000	1.168168000
C	-5.421311000	-5.703024000	1.428719000
P	-4.841063000	-0.881292000	0.004666000
O	-5.632909000	0.358728000	0.273935000
C	-4.342395000	-6.372354000	2.016756000
C	-4.554079000	-7.370506000	2.968746000
C	-5.853193000	-7.710370000	3.352547000
C	-6.938106000	-7.048661000	2.773103000
C	-6.721054000	-6.056228000	1.816472000
N	-1.992336000	4.469284000	4.330277000
C	-1.706520000	3.200672000	4.027546000
N	-1.622385000	2.624356000	2.818274000
C	-1.875366000	3.496241000	1.821693000
C	-2.201465000	4.847769000	1.993212000
C	-2.252729000	5.327514000	3.318607000
N	-1.887643000	3.297005000	0.457602000
C	-2.215941000	4.513864000	-0.109151000
N	-2.413601000	5.466858000	0.773357000
N	-2.523444000	6.615697000	3.612711000
H	-4.089948000	2.987306000	-2.759031000
H	-4.926267000	1.445270000	-2.514942000
H	-2.577218000	1.136878000	-3.139888000
H	-1.827333000	-0.402300000	-1.488574000
H	-3.145768000	1.101407000	0.798493000
H	-0.444948000	1.908738000	-0.119153000
H	-6.643333000	-2.166985000	-0.626737000
H	-6.533505000	-3.265096000	1.430017000
H	-5.841260000	-4.819400000	-0.479800000
H	-4.171642000	-4.613340000	0.043572000
H	-6.215092000	-2.122979000	3.554142000
H	-3.330795000	-6.099428000	1.731828000
H	-3.703922000	-7.881003000	3.412801000
H	-6.019091000	-8.485952000	4.094850000
H	-7.953022000	-7.308798000	3.060697000
H	-7.571903000	-5.554422000	1.360834000
H	-1.529065000	2.541011000	4.873703000
H	-2.293169000	4.615328000	-1.179750000
H	-2.699186000	6.865195000	4.575848000
H	-2.880002000	7.225207000	2.890934000
C	-3.831125000	0.170922000	3.448455000
N	-5.527724000	-1.524880000	3.095183000
C	-4.540464000	-1.025770000	4.072420000
C	-5.159191000	-0.673126000	5.451101000
C	-4.085270000	-0.233233000	6.463872000
C	-2.972312000	-1.255408000	6.713180000
C	-6.277989000	0.371679000	5.360063000
O	-4.431444000	1.079004000	2.896833000
O	-2.509757000	0.124926000	3.593244000
H	-6.018979000	-0.741964000	2.656909000
H	-5.029281000	1.874000000	-0.357033000
H	-3.816110000	-1.831580000	4.200095000
H	-5.594590000	-1.614117000	5.819015000
H	-3.646290000	0.719289000	6.136971000
H	-4.598815000	-0.019883000	7.409506000
H	-2.335733000	-0.934597000	7.544837000
H	-3.388940000	-2.236914000	6.970563000
H	-2.329978000	-1.377564000	5.836087000
H	-6.720354000	0.527656000	6.349466000
H	-7.080708000	0.056332000	4.685116000
H	-5.894654000	1.331362000	5.000852000
H	-2.112797000	0.941138000	3.160369000
IM2’			
O	-4.185062000	2.164108000	-1.854822000
C	-3.049524000	1.805145000	-2.627533000
C	-1.906616000	1.252922000	-1.789365000
C	-2.265132000	0.105430000	-0.822897000
O	-3.228642000	-0.815631000	-1.304771000
C	-2.552490000	0.814880000	0.494525000
F	-2.115694000	0.008809000	1.553700000
C	-1.700548000	2.084321000	0.421283000

O	-1.330724000	2.269311000	-0.924448000	H	-4.481882000	7.163857000	4.214175000
N	-5.119988000	-2.510655000	-0.951065000	H	-4.518332000	7.200355000	2.480251000
C	-5.478379000	-2.954887000	0.390612000	C	-3.761254000	0.090327000	3.601542000
C	-4.386047000	-2.497730000	1.354817000	N	-4.946441000	-1.750214000	2.568468000
C	-5.584629000	-4.491260000	0.513055000	C	-3.959609000	-1.423179000	3.652158000
O	-3.214520000	-2.705079000	1.286362000	C	-4.461271000	-1.953653000	5.013659000
O	-5.176868000	-0.274541000	0.329250000	C	-3.365226000	-1.900492000	6.092337000
C	-5.787574000	-4.871612000	1.964584000	C	-2.082291000	-2.655034000	5.733311000
P	-4.866717000	-0.819696000	-1.053917000	C	-5.735211000	-1.239791000	5.484126000
O	-5.533141000	-0.224727000	-2.271329000	O	-4.591908000	0.823576000	3.089614000
C	-4.736219000	-5.416389000	2.713220000	O	-2.628529000	0.479682000	4.155136000
C	-4.888781000	-5.669205000	4.078292000	H	-5.303378000	-0.859396000	2.145958000
C	-6.093131000	-5.367428000	4.717437000	H	-4.857542000	1.464127000	-2.024481000
C	-7.147766000	-4.819617000	3.982407000	H	-3.027489000	-1.910276000	3.370795000
C	-6.996381000	-4.575551000	2.615590000	H	-4.693807000	-3.013169000	4.843661000
N	-3.264268000	4.980928000	4.472141000	H	-3.131178000	-0.855938000	6.327373000
C	-2.681603000	3.781865000	4.429470000	H	-3.799949000	-2.334008000	7.000918000
N	-2.327137000	3.057963000	3.355066000	H	-1.423859000	-2.727478000	6.605012000
C	-2.626047000	3.680671000	2.194914000	H	-2.303902000	-3.674199000	5.393983000
C	-3.253545000	4.928684000	2.095174000	H	-1.519335000	-2.148209000	4.942525000
C	-3.572799000	5.585220000	3.302355000	H	-6.100988000	-1.709306000	6.401954000
N	-2.409123000	3.284805000	0.890560000	H	-6.548143000	-1.286949000	4.750208000
C	-2.919334000	4.292632000	0.090945000	H	-5.542098000	-0.182934000	5.697628000
N	-3.432395000	5.292148000	0.772328000	H	-2.447224000	1.434220000	3.852394000
N	-4.148809000	6.802552000	3.331552000	TS3’			
H	-2.677657000	2.694796000	-3.151823000	O	-4.136200000	2.177539000	-1.671867000
H	-3.310444000	1.054579000	-3.382563000	C	-3.041494000	1.773662000	-2.481936000
H	-1.104516000	0.951194000	-2.470311000	C	-1.877912000	1.231685000	-1.668331000
H	-1.360206000	-0.486587000	-0.651243000	C	-2.209103000	0.144201000	-0.626952000
H	-3.604335000	1.026387000	0.651113000	O	-3.155687000	-0.848134000	-1.003947000
H	-0.811276000	1.973272000	1.051138000	C	-2.495793000	0.934754000	0.641083000
H	-5.743496000	-2.883294000	-1.660863000	F	-2.069648000	0.186320000	1.743662000
H	-6.424718000	-2.517512000	0.733159000	C	-1.629186000	2.186493000	0.488479000
H	-6.423832000	-4.821740000	-0.108550000	O	-1.250533000	2.270098000	-0.865707000
H	-4.668757000	-4.937514000	0.116449000	N	-5.067944000	-2.511109000	-0.730528000
H	-5.747796000	-2.283418000	2.930173000	C	-5.493043000	-3.041002000	0.568508000
H	-3.791407000	-5.636729000	2.224671000	C	-4.381491000	-2.759637000	1.590039000
H	-4.063826000	-6.094094000	4.642213000	C	-5.754247000	-4.556702000	0.558702000
H	-6.209229000	-5.555302000	5.780350000	O	-3.283368000	-3.244780000	1.595835000
H	-8.088390000	-4.583881000	4.470614000	O	-5.162125000	-0.206343000	0.509211000
H	-7.825169000	-4.159859000	2.048006000	C	-6.109330000	-4.981896000	1.969163000
H	-2.474882000	3.320793000	5.392346000	P	-4.793383000	-0.839841000	-0.852417000
H	-2.876647000	4.217094000	-0.982359000	O	-5.436514000	-0.238227000	-2.069779000

C	-5.161311000	-5.607589000	2.789018000	O	-2.676992000	0.644030000	4.295094000
C	-5.440680000	-5.865626000	4.132567000	H	-4.907976000	-0.807082000	1.648399000
C	-6.673147000	-5.497255000	4.675196000	H	-4.831279000	1.497400000	-1.811630000
C	-7.630232000	-4.883250000	3.863747000	H	-2.804227000	-1.642339000	3.213746000
C	-7.349714000	-4.629240000	2.520759000	H	-4.145452000	-3.191343000	4.561413000
N	-3.542066000	5.180361000	4.319574000	H	-2.973125000	-0.979056000	6.309325000
C	-2.980680000	3.970447000	4.355804000	H	-3.287800000	-2.643716000	6.773948000
N	-2.519202000	3.225917000	3.338343000	H	-0.903497000	-2.460298000	6.284288000
C	-2.675796000	3.837603000	2.144481000	H	-1.621070000	-3.399873000	4.965807000
C	-3.259616000	5.098006000	1.961336000	H	-1.200599000	-1.692714000	4.724049000
C	-3.700262000	5.776616000	3.117038000	H	-5.664728000	-2.364452000	6.357263000
N	-2.332016000	3.418871000	0.872942000	H	-6.308125000	-1.951583000	4.779162000
C	-2.725712000	4.428256000	0.012764000	H	-5.506390000	-0.705529000	5.754588000
N	-3.283761000	5.448495000	0.623315000	H	-2.567765000	1.599837000	3.986125000
N	-4.247741000	7.006826000	3.066901000	IM3’			
H	-2.675755000	2.637911000	-3.050705000	O	-4.145204000	2.272113000	-1.510169000
H	-3.347560000	1.003567000	-3.198817000	C	-3.144186000	1.815155000	-2.411423000
H	-1.106065000	0.885345000	-2.361788000	C	-1.972628000	1.172496000	-1.691047000
H	-1.290192000	-0.415506000	-0.428780000	C	-2.300810000	0.115818000	-0.615380000
H	-3.544465000	1.174310000	0.781149000	O	-3.360274000	-0.800385000	-0.869992000
H	-0.741312000	2.104317000	1.124024000	C	-2.401274000	0.911576000	0.674355000
H	-5.606732000	-2.890318000	-1.503444000	F	-1.894819000	0.145956000	1.724812000
H	-6.408351000	-2.546421000	0.918421000	C	-1.503541000	2.126170000	0.426554000
H	-6.570433000	-4.762329000	-0.142154000	O	-1.192296000	2.146339000	-0.945518000
H	-4.857434000	-5.071240000	0.203317000	N	-5.361036000	-2.330737000	-0.692941000
H	-5.693615000	-1.806992000	2.856276000	C	-5.603478000	-2.938439000	0.622493000
H	-4.193361000	-5.876356000	2.376163000	C	-4.435579000	-2.634499000	1.576676000
H	-4.693127000	-6.349157000	4.754556000	C	-5.738064000	-4.469646000	0.496723000
H	-6.888248000	-5.689952000	5.721983000	O	-3.272989000	-2.918800000	1.304765000
H	-8.594385000	-4.600618000	4.275987000	O	-5.475030000	0.084367000	0.414757000
H	-8.097852000	-4.148124000	1.895455000	C	-5.975598000	-5.077380000	1.860203000
H	-2.892150000	3.520718000	5.341924000	P	-4.974159000	-0.715965000	-0.869138000
H	-2.561803000	4.339797000	-1.048187000	O	-5.553485000	-0.106611000	-2.103334000
H	-4.675027000	7.384274000	3.900870000	C	-4.906950000	-5.583172000	2.610920000
H	-4.510423000	7.399388000	2.174496000	C	-5.103550000	-6.030909000	3.918210000
C	-3.786068000	0.175895000	3.732341000	C	-6.375671000	-5.979135000	4.492541000
N	-4.744004000	-1.671627000	2.498693000	C	-7.449962000	-5.485085000	3.748834000
C	-3.781849000	-1.343979000	3.586189000	C	-7.249134000	-5.037996000	2.442302000
C	-4.109144000	-2.138175000	4.872343000	N	-3.591367000	5.070705000	4.204700000
C	-2.997682000	-2.007146000	5.929337000	C	-3.120897000	3.822900000	4.232191000
C	-1.603398000	-2.412659000	5.443471000	N	-2.606686000	3.095451000	3.227412000
C	-5.473564000	-1.761488000	5.464516000	C	-2.596018000	3.771948000	2.057799000
O	-4.705100000	0.866251000	3.328499000	C	-3.066879000	5.080141000	1.886349000

C	-3.579768000	5.734079000	3.026929000	H	-5.832297000	-1.815370000	6.610720000
N	-2.158070000	3.387128000	0.805091000	H	-6.407597000	-1.692724000	4.950198000
C	-2.384349000	4.463649000	-0.032892000	H	-5.533295000	-0.335825000	5.688334000
N	-2.927942000	5.493765000	0.573720000	H	-2.678095000	1.478152000	3.823058000
N	-4.034916000	7.000439000	2.988726000	TS4’			
H	-2.754570000	2.664130000	-2.987187000	O	-6.098764000	2.979063000	-0.470405000
H	-3.558038000	1.087480000	-3.116422000	C	-6.173313000	2.700282000	-1.855672000
H	-1.291154000	0.763381000	-2.441814000	C	-4.868335000	2.197973000	-2.485650000
H	-1.425044000	-0.527664000	-0.503986000	C	-4.441891000	0.748035000	-2.195193000
H	-3.411620000	1.214764000	0.926147000	O	-5.087043000	0.222770000	-1.015747000
H	-0.582218000	2.035199000	1.009956000	C	-2.909553000	0.846397000	-2.177449000
H	-6.024547000	-2.638199000	-1.397814000	F	-2.513419000	0.716708000	-3.509377000
H	-6.531606000	-2.547486000	1.059963000	C	-2.623613000	2.304555000	-1.773797000
H	-6.569171000	-4.691658000	-0.182553000	O	-3.775345000	3.045676000	-2.063394000
H	-4.818079000	-4.854577000	0.047861000	N	-5.740669000	-1.277834000	1.046769000
H	-5.792671000	-1.813380000	2.859641000	C	-5.276138000	-2.439206000	1.861775000
H	-3.912783000	-5.603232000	2.173975000	C	-4.568987000	-1.904978000	3.128946000
H	-4.263530000	-6.418525000	4.487641000	C	-4.398050000	-3.420987000	1.072902000
H	-6.529624000	-6.324620000	5.510697000	O	-3.396362000	-2.151259000	3.383363000
H	-8.443602000	-5.446477000	4.186112000	O	-3.131435000	-0.338225000	0.647157000
H	-8.087106000	-4.647997000	1.869371000	C	-4.284425000	-4.766681000	1.754714000
H	-3.165904000	3.321709000	5.196207000	P	-4.576048000	-0.075620000	0.472496000
H	-2.118474000	4.410936000	-1.076208000	O	-5.391172000	0.932829000	1.402048000
H	-4.508301000	7.375795000	3.798237000	C	-3.124071000	-5.139014000	2.442742000
H	-4.160876000	7.461883000	2.099650000	C	-3.039101000	-6.379982000	3.075989000
C	-3.785126000	-0.029274000	3.546367000	C	-4.118292000	-7.265267000	3.034763000
N	-4.818276000	-2.052132000	2.741626000	C	-5.281880000	-6.903062000	2.352267000
C	-3.875246000	-1.544728000	3.718419000	C	-5.360450000	-5.663838000	1.715870000
C	-4.241758000	-2.015778000	5.150508000	N	0.749374000	1.057253000	1.874712000
C	-3.136096000	-1.755417000	6.188403000	C	0.802247000	0.979262000	0.536780000
C	-1.761981000	-2.315190000	5.812195000	N	-0.112477000	1.373497000	-0.357249000
C	-5.579893000	-1.429345000	5.617931000	C	-1.165724000	1.939082000	0.245575000
O	-4.543973000	0.594610000	2.802907000	C	-1.348744000	2.129353000	1.618121000
O	-2.820076000	0.553878000	4.224491000	C	-0.335761000	1.612810000	2.454604000
H	-5.071679000	0.039891000	1.326593000	N	-2.310784000	2.428489000	-0.348777000
H	-4.927756000	1.711973000	-1.681404000	C	-3.121351000	2.889840000	0.663912000
H	-2.901481000	-1.951048000	3.437683000	N	-2.577068000	2.734341000	1.855724000
H	-4.356675000	-3.103518000	5.051436000	N	-0.385236000	1.670231000	3.812255000
H	-3.056450000	-0.680044000	6.381613000	H	-6.425112000	3.648626000	-2.338091000
H	-3.469837000	-2.215227000	7.127252000	H	-6.970209000	1.983300000	-2.093888000
H	-1.069542000	-2.237331000	6.657188000	H	-4.961946000	2.292941000	-3.574355000
H	-1.827039000	-3.373117000	5.529426000	H	-4.746821000	0.076966000	-2.996554000
H	-1.317368000	-1.766844000	4.975064000	H	-2.396289000	0.102715000	-1.571424000

H	-1.764893000	2.678244000	-2.338282000	F	-2.513419000	0.716708000	-3.509377000
H	-6.371962000	-1.593059000	0.308204000	C	-2.623613000	2.304555000	-1.773797000
H	-6.193781000	-2.946294000	2.177199000	O	-3.775345000	3.045676000	-2.063394000
H	-4.857494000	-3.549474000	0.085876000	N	-5.740669000	-1.277834000	1.046769000
H	-3.413917000	-2.971758000	0.926706000	C	-5.276138000	-2.439206000	1.861775000
H	-6.008083000	-0.008566000	1.583079000	C	-4.568987000	-1.904978000	3.128946000
H	-2.293025000	-4.443382000	2.490962000	C	-4.398050000	-3.420987000	1.072902000
H	-2.129718000	-6.654490000	3.603437000	O	-3.396362000	-2.151259000	3.383363000
H	-4.052783000	-8.230623000	3.528581000	O	-3.131435000	-0.338225000	0.647157000
H	-6.125332000	-7.586532000	2.310285000	C	-4.284425000	-4.766681000	1.754714000
H	-6.265353000	-5.391351000	1.177059000	P	-4.576048000	-0.075620000	0.472496000
H	1.701486000	0.522417000	0.129653000	O	-5.391172000	0.932829000	1.402048000
H	-4.097527000	3.302566000	0.452178000	C	-3.124071000	-5.139014000	2.442742000
H	0.291448000	1.089919000	4.292383000	C	-3.039101000	-6.379982000	3.075989000
H	-1.300975000	1.710461000	4.244896000	C	-4.118292000	-7.265267000	3.034763000
C	-4.655526000	1.100850000	4.429041000	C	-5.281880000	-6.903062000	2.352267000
N	-5.365241000	-1.135132000	3.921592000	C	-5.360450000	-5.663838000	1.715870000
C	-4.837629000	-0.310916000	5.008386000	N	0.749374000	1.057253000	1.874712000
C	-5.698855000	-0.386164000	6.283499000	C	0.802247000	0.979262000	0.536780000
C	-5.157259000	0.559752000	7.372130000	N	-0.112477000	1.373497000	-0.357249000
C	-3.672550000	0.373813000	7.703511000	C	-1.165724000	1.939082000	0.245575000
C	-7.193379000	-0.136327000	6.038941000	C	-1.348744000	2.129353000	1.618121000
O	-5.516225000	1.958078000	4.380450000	C	-0.335761000	1.612810000	2.454604000
O	-3.431173000	1.238887000	3.906209000	N	-2.310784000	2.428489000	-0.348777000
H	-6.317997000	-0.963540000	3.629079000	C	-3.121351000	2.889840000	0.663912000
H	-6.108991000	2.154282000	0.049069000	N	-2.577068000	2.734341000	1.855724000
H	-3.845683000	-0.711107000	5.214120000	N	-0.385236000	1.670231000	3.812255000
H	-5.582229000	-1.417283000	6.645635000	H	-6.425112000	3.648626000	-2.338091000
H	-5.341537000	1.597505000	7.067391000	H	-6.970209000	1.983300000	-2.093888000
H	-5.753157000	0.395569000	8.278326000	H	-4.961946000	2.292941000	-3.574355000
H	-3.390071000	0.986077000	8.566478000	H	-4.746821000	0.076966000	-2.996554000
H	-3.448743000	-0.672051000	7.946869000	H	-2.396289000	0.102715000	-1.571424000
H	-3.024551000	0.669082000	6.870526000	H	-1.764893000	2.678244000	-2.338282000
H	-7.740311000	-0.207530000	6.985231000	H	-6.371962000	-1.593059000	0.308204000
H	-7.627443000	-0.881072000	5.362167000	H	-6.193781000	-2.946294000	2.177199000
H	-7.361189000	0.857301000	5.616248000	H	-4.857494000	-3.549474000	0.085876000
H	-3.376635000	2.018614000	3.274636000	H	-3.413917000	-2.971758000	0.926706000
O	-6.098764000	2.979063000	-0.470405000	H	-6.008083000	-0.008566000	1.583079000
C	-6.173313000	2.700282000	-1.855672000	H	-2.293025000	-4.443382000	2.490962000
C	-4.868335000	2.197973000	-2.485650000	H	-2.129718000	-6.654490000	3.603437000
C	-4.441891000	0.748035000	-2.195193000	H	-4.052783000	-8.230623000	3.528581000
O	-5.087043000	0.222770000	-1.015747000	H	-6.125332000	-7.586532000	2.310285000
C	-2.909553000	0.846397000	-2.177449000	H	-6.265353000	-5.391351000	1.177059000

H	1.701486000	0.522417000	0.129653000
H	-4.097527000	3.302566000	0.452178000
H	0.291448000	1.089919000	4.292383000
H	-1.300975000	1.710461000	4.244896000
C	-4.655526000	1.100850000	4.429041000
N	-5.365241000	-1.135132000	3.921592000
C	-4.837629000	-0.310916000	5.008386000
C	-5.698855000	-0.386164000	6.283499000
C	-5.157259000	0.559752000	7.372130000
C	-3.672550000	0.373813000	7.703511000
C	-7.193379000	-0.136327000	6.038941000
O	-5.516225000	1.958078000	4.380450000
O	-3.431173000	1.238887000	3.906209000
H	-6.317997000	-0.963540000	3.629079000
H	-6.108991000	2.154282000	0.049069000
H	-3.845683000	-0.711107000	5.214120000
H	-5.582229000	-1.417283000	6.645635000
H	-5.341537000	1.597505000	7.067391000
H	-5.753157000	0.395569000	8.278326000
H	-3.390071000	0.986077000	8.566478000
H	-3.448743000	-0.672051000	7.946869000
H	-3.024551000	0.669082000	6.870526000
H	-7.740311000	-0.207530000	6.985231000
H	-7.627443000	-0.881072000	5.362167000
H	-7.361189000	0.857301000	5.616248000
H	-3.376635000	2.018614000	3.274636000
PC’			
O	-6.258964000	0.619124000	0.627503000
C	-6.602471000	1.342984000	-0.548307000
C	-5.432249000	1.958272000	-1.307255000
C	-4.391117000	1.062586000	-2.017993000
O	-4.333455000	-0.309577000	-1.628413000
C	-3.071032000	1.841575000	-1.855990000
F	-2.734644000	2.431698000	-3.073203000
C	-3.386186000	2.976184000	-0.854984000
O	-4.702531000	2.787022000	-0.390355000
N	-5.085568000	-1.777125000	0.228174000
C	-5.064394000	-2.745297000	1.378656000
C	-4.413618000	-2.053738000	2.590158000
C	-4.352761000	-4.048950000	1.008201000
O	-3.232583000	-2.223114000	2.875304000
O	-2.597122000	-2.008479000	-0.778253000
C	-4.595582000	-5.113124000	2.055682000
P	-3.522389000	-0.926047000	-0.339045000
O	-3.221772000	0.124562000	0.675780000
C	-3.643984000	-5.381104000	3.046784000
C	-3.889283000	-6.346338000	4.024842000
C	-5.093025000	-7.053894000	4.026772000
C	-6.049659000	-6.792574000	3.043033000
C	-5.799871000	-5.829470000	2.064955000
N	1.293399000	2.041310000	1.212339000
C	0.884829000	2.058662000	-0.064914000
N	-0.326238000	2.354733000	-0.551437000
C	-1.189676000	2.657879000	0.427689000
C	-0.910466000	2.690589000	1.798391000
C	0.405723000	2.358875000	2.178438000
N	-2.528573000	2.990897000	0.323609000
C	-2.980652000	3.206171000	1.596979000
N	-2.048856000	3.039257000	2.514239000
N	0.826336000	2.378948000	3.466422000
H	-7.291418000	2.155391000	-0.287219000
H	-7.131224000	0.648498000	-1.206032000
H	-5.867614000	2.600773000	-2.086307000
H	-4.623674000	1.020455000	-3.082655000
H	-2.235332000	1.219740000	-1.545486000
H	-3.294884000	3.932955000	-1.383579000
H	-5.483179000	-2.248227000	-0.589857000
H	-6.114346000	-2.954720000	1.603740000
H	-4.742059000	-4.385051000	0.040072000
H	-3.288671000	-3.845729000	0.884996000
H	-5.707416000	-0.957031000	0.434857000
H	-2.715969000	-4.818991000	3.053899000
H	-3.139543000	-6.544968000	4.785609000
H	-5.283999000	-7.805100000	4.787812000
H	-6.987225000	-7.341233000	3.034173000
H	-6.544468000	-5.634889000	1.296298000
H	1.640620000	1.794793000	-0.801252000