Supporting information

Rational design of mimetic peptides based on aldo-ketoreductase enzyme as asymmetric organocatalyst in aldol reactions

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General

All chemicals were purchased and used without further purification. Recombinant Human AKR1A1 aldehyde reductase (Homo sapiens, freeze-dried CFE, in 20 mM sodium phosphate, cat.no. = Pro-E0601) was purchased from Prozomix company to employ as a control promiscuous asymmetry biocatalyst in the aldol reaction. Analytical thin layer chromatography (TLC) was performed using Merck 60 F\textsubscript{254} precoated silica gel plate (0.2 mm thickness). Flash chromatography was performed using Merck silica gel 60 (70-230 mesh). Fourier transforms infrared spectroscopy (FTIR); Perkin Elmer Spectrum 100 was used for identification of functional groups. NMR data were recorded on 700
MHz (Bruker), 500 MHz (JEOL) for $^1$HNMR and 127 MHz (Bruker) 100 MHz (JEOL JNM ECA) for $^{13}$C NMR spectrometer. The relative and absolute configurations (dr) of the Aldol reactions were determined by comparison with $^1$H NMR spectroscopic analysis. Mass spectra (MS) were measured with a spectrometer (DIMS QP5050A SHIMADZU). Optical rotations were measured on a JASCO P-2000 Polarimeter. Enantioselectivity were determined by HPLC (Waters 1525 Binary Pump and UV-Water 2489) analysis employing a Daicel ChiralCel OD-H, and ChiralPak AD-H columns (4.6mm×250mm). CD spectra were measured on a JASCO J-810 automatic recording spectropolarimeter.

- Experimental method

**Characterizations of peptide 8aa**

**IR** (neat) $\nu = 3280, 3103, 2966, 2902, 1635, 1546, 1195, 1139, \text{cm}^{-1}$; **$^1$HNMR** (700 MHz, $\delta = \text{ppm}$); $\delta = 8.71$ (d, $J = 7.09$ Hz, 1H), 8.6 (s, 2H), 8.48 (d, $J = 8.17$, 1H), 8.33 (d, $J = 7.0$ Hz, 1H), 8.19 (d, $J = 7.45$ Hz, 1H), 8.28 (d, $J = 7.19$ Hz, 1H), 8.26 (d, $J = 6.84$ Hz, 1H), 7.97 (d, $J = 7.89$ Hz, 1H), 7.53 (bs, 1H), 7.33 (m, 3H), 7.29 (m, 2H), 7.23 (d, $J = 7.70$ Hz, 3H), 7.18 (s, 1H), 4.63 (m, 2H), 4.40 (t, $J = 7.14$ Hz, 1H), 4.33 (m, 2H), 4.25 (m, 3H), 4.02 (t, $J = 7.50$ Hz, 1H), 3.04 (m, 2H), 3.28 (dd, $J = 15.48$, 5.78 Hz, 1H), 3.16 (dd, $J = 15.50$, 8.90 Hz, 1H), 3.09 (dd, $J = 14.16$, 6.55 Hz, 1H), 3.00 (m, 4H), 2.45 (m,
2H), 2.39 (m, 2H), 2.34 (m, 2H), 1.99 (m, 6H), 1.79 (m, 1H), 1.70 (m, 3H), 1.58 (m, 1H), 1.5 (m, 2H), 1.45 (m, 2H), 0.89 (d, J = 5.00 Hz, 12 H), 0.83 (d, J = 6.23 Hz, 6H). $^{13}$CNMR (125.70 MHz, D$_2$O, 25°C) $\delta$ = 20.52, 20.96, 23.27, 23.56, 24.60, 24.70, 24.79, 26.36, 26.85, 26.93, 28.87, 28.91, 32.50, 32.78, 34.06, 39.58, 42.11, 42.39, 42.58, 54.95, 55.25, 55.80, 56.15, 57.64, 62.09, 62.26, 118.13, 119.80, 120.04, 121.50, 129.75, 131.31, 131.35, 131.81, 136.25, 138.81, 156.50, 165.70, 167.60, 172.3, 175.14, 175.33, 176.27, 176.57, 176.67, 177.10, 179.80. MS (Accurate Q-TOF LC/HRMS): m/z (%): 981.5887 (100) [M+H].

Spectroscopic data of peptide PH16aa

IR (neat) $\nu$ = 3262, 3046, 2925, 2856, 1624, 1523, 1170, 1130, cm$^{-1}$; $^1$HNMR (700 MHz, $\delta$ = ppm); $\delta$ = 8.48 (s, 2H), 8.45 (s, 2H), 8.40 (d, J = 6.15 Hz, 1H), 8.38 (d, J = 6.15 Hz, 1H), 8.26 (d, J = 6.50 Hz, 1H), 8.20 (d, J = 6.50 Hz, 1H), 8.19 (d, J = 6.55 Hz, 1H), 8.15 (d, J = 7.55 Hz, 1H), 8.12 (m, 2H), 7.97 (d, J = 7.55 Hz, 1H), 7.89 (d, J = 7.29 Hz, 1H), 7.53 (bs, 1H), 7.32 (t, J = 7.15 Hz, 3H), 7.27 (d, J = 7.00 Hz, 2H), 7.26 (bs, 2H), 7.22 (m, 3H), 7.17 (bs, 1H), 4.41 (t, J = 7.06 Hz, 1H), 4.35 (m, 4H), 4.24 (m, 3H), 4.17 (dd, J = 14.75, 5.70 Hz, 1H), 4.13 (t, J = 7.50 Hz, 1H), 3.97 (m, 2H), 3.94 (d, J = 5.00 Hz, 2H), 3.89 (dd, J = 12, 5.22 Hz, 1H), 3.84 (dd, J = 11.5, 4.80 Hz, 1H), 3.68 (q, J = 9.25 Hz, 1H), 3.39 (m, 2H), 3.26 (d, J = 5.40 Hz, 1H), 3.24 (t, J = 6.54 Hz, 1H), 3.18 (dd, J = 15.00, 8.00 Hz, 1H), 3.00 (s, 3H), 2.89 (d, J = 6.98 Hz, 3H), 2.78 (d, J = 6.98 Hz, 3H), 2.17 (m, 2H), 1.84 (m, 2H), 1.78 (m, 1H), 1.62 (m, 1H), 1.37 (d, J = 6.15 Hz, 3H), 1.20 (d, J = 6.15 Hz, 3H), 1.09 (d, J = 6.15 Hz, 3H), 0.96 (s, 3H), 0.91 (s, 3H), 0.87 (s, 3H).
3.11 (m, 2H), 3.03 (dd, \( J = 13.50, 8.00 \) Hz, 1H), 2.99 (t, \( J = 7.74 \) Hz, 3H), 2.90 (t, \( J = 8.00 \) Hz, 1H), 2.43 (m, 1H), 2.58 (m, 3H), 1.99 (m, 11H), 1.79 (m, 2H), 1.69 (t, \( J = 7.55 \) Hz, 2H), 1.52 (m, 4H), 1.44 (m, 4H), 1.38 (d, \( J = 7.00 \) Hz, 7H), 1.36 (d, \( J = 7.02 \) Hz, 3H), 1.17 (m, 2H), 0.96 (d, \( J = 7.01 \) Hz, 3H), 0.91 (d, \( J = 6.86 \) Hz, 7H), 0.90 (d, \( J = 7.50 \) Hz, 5H), 0.88 (d, \( J = 6.20 \) Hz, 12H), 0.85 (d, \( J = 7.16 \) Hz, 4H), 0.82 (m, 8H).

\(^{13}\text{CNMR} \) (125.70 MHz, \( \text{D}_2\text{O}, 25^\circ\text{C} \)) \( \delta = 13.00, 17.53, 17.71, 19.18, 19.40, 20.28, 20.83, 21.05, 21.07, 21.80, 23.30, 23.67, 24.67, 24.80, 24.88, 26.89, 26.96, 27.26, 27.48, 28.89, 29.17, 32.08, 32.49, 32.86, 32.93, 33.15, 38.79, 39.45, 40.87, 42.18, 42.44, 44.95, 50.13, 50.99, 52.44, 55.44, 56.46, 57.13, 58.42, 61.00, 63.93, 118.21, 120.08, 129.87, 131.49, 131.84, 136.30, 138.86, 165.59, 172.42, 174.27, 175.84, 176.98.

\textbf{MS} \ (\text{Accurate Q-TOF LC/HRMS}): \( m/z \) (%): 1842.9947 (100) \([\text{M+H}]^+\)

\textbf{Spectroscopic data of peptide 8aa(z)}

\textbf{IR} (neat) \( \nu = 3270, 3153, 2956, 2922, 1726, 1655, 1556, 1205, 1142, \text{cm}^{-1}; \) \( ^1\text{HNMR} \) (700 MHz, \( \delta = \text{ppm} \)); \( \delta = 8.75 \) (d, \( J = 7.02 \) Hz, 1H), 8.65 (s, 2H), 8.48 (d, \( J = 8.15 \) Hz, 1H), 8.35 (d, \( J = 7.02 \) Hz, 1H), 8.21 (d, \( J = 7.41 \) Hz, 1H), 8.28 (d, \( J = 7.15 \) Hz, 1H), 8.23 (d, \( J = 7.04 \) Hz, 1H), 7.93 (d, \( J = 7.81 \) Hz, 1H), 7.57 (bs, 1H), 7.32 (m, 4H), 7.29 (m, 2H), 7.23 (m, 5H), 7.16 (m, 1H), 5.06 (s, 2H), 4.63 (m, 2H), 4.41
(t, $J = 7.12$ Hz, 1H), 4.35 (m, 2H), 4.23 (m, 3H), 4.02 (t, $J = 7.52$ Hz, 1H), 3.08 (m, 2H), 3.27 (dd, $J = 15.48$, 5.78 Hz, 1H), 3.14 (dd, $J = 15.50$, 8.91 Hz, 1H), 3.10 (dd, $J = 14.12$, 6.65 Hz, 1H), 3.06 (m, 4H), 2.42 (m, 2H), 2.32 (m, 2H), 2.31 (m, 2H), 1.94 (m, 6H), 1.71 (m, 1H), 1.72 (m, 3H), 1.58 (m, 1H), 1.53 (m, 2H), 1.43 (m, 2H), 0.85 (d, $J = 5.00$ Hz, 12.00 H), 0.81 (d, $J = 6.20$ Hz, 6H).

$^{13}$CNMR (125.7 MHz, CD$_3$OD, 25°C) $\delta = 18.29$, 19.78, 21.63, 22.15, 22.77, 23.55, 24.31, 24.36, 26.39, 26.65, 27.91, 28.15, 28.17, 30.62, 31.03, 31.55, 32.21, 38.18, 41.29, 41.69, 47.57, 53.59, 54.03, 54.54, 54.66, 55.86, 57.45, 61.06, 61.92, 67.44, 118.73, 128.08, 128.82, 129.09, 129.58, 129.72, 130.38, 131.39, 134.87, 138.10, 138.58, 169.99, 173.93, 174.33, 174.39, 174.90, 175.19, 176.44.

**MS** (Accurate Q-TOF LC/HRMS): $m/z$ (%): 1115.6262 (100) [M+H]$^+$

**Spectroscopic data of PELFV-NH$_2$ (5aa)**

**IR** (neat) $\nu = 3342$, 3125, 3085, 2975, 2846, 1665, 1546, 1187, 1135, cm$^{-1}$; $^1$HNMR (700 MHz, $\delta = ppm$); $\delta = 8.74$ (s, 1H), 8.35 (d, $J = 7.01$ Hz, 1H), 8.33 (d, $J = 7.50$ Hz, 1H), 7.99 (d, $J = 8.32$ Hz, 1H), 7.35 (t, $J = 7.50$ Hz, 2H), 7.29 (t, $J = 7.92$ Hz, 1H), 7.25 (d, $J = 7.60$ Hz), 7.16 (bs, 1H), 6.90 (bs, 1H), 4.30 (m, 2H), 4.03 (t, $J = 7.78$ Hz, 2H), 3.70 (s, 1H), 3.41 (m, 3H), 3.06 (m, 3H), 3.06 (dd, $J = 13.52$, 7.50 Hz, 3H), 2.40 (m, 1H), 2.23 (m, 1H), 2.01 (m, 3H), 1.87 (m, 1H), 1.50 (m, 1H), 1.46 (m, 1H), 1.16 (dd, $J = 6.25$, 0.50 Hz, 2H), 0.89 (d, $J = 6.50$ Hz, 6H), 0.87 (d, $J = 6.72$ Hz, 3H), 0.83 (d, $J = 6.23$ Hz, 3H).

$^{13}$CNMR (125.7 MHz, D$_2$O, 25°C) $\delta = 18.51$, 19.78, 22.17, 23.42, 25.00, 25.30, 25.80, 28.55, 31.07, 31.60, 32.05, 38.62, 42.31, 47.55, 52.35, 53.16, 54.46, 56.04, 59.71, 61.01, 64.81, 66.95, 127.85, 129.54, 130.43, 138.32, 169.80, 173.04, 173.24, 174.25, 174.82, 175.71, 176.71.

**MS** (Accurate Q-TOF LC/HRMS): $m/z$ (%): 603.3515 (100) [M+H]$^+$
General procedure for aldol reaction catalyzed by peptide

To H$_2$O (0.6 mL) was added the corresponding catalyst (0.005 mmol, 5 mg), NMM (1 drop), and iPrOH (0.4 mL). The reaction mixture was stirred for 20 min followed by addition of the corresponding ketone (0.168 mmol, 1.2 eq). Then, the requisite aldehyde (0.14 mmol, 1 eq) was added to the reaction mixture. The resulting mixture was stirred at RT for 24 h. The reaction was monitored by TLC. Then treated with saturated ammonium chloride solution and the mixture was extracted with ethyl acetate (3×2mL). The combined organic extract was washed with brine, dried (Na$_2$SO$_4$), and concentrated in vacuo. After NMR analysis to determine diastereomeric ratio, the residue was purified by flash column chromatography with hexanes/ethyl acetate (3:1) to afford the aldol products that were subjected to chiral HPLC analysis to determine enantiomeric excesses.

1- (R)-2-((S)-hydroxy(4-nitrophenyl)methyl)cyclohexanone

The resulting pure product was examined by $^1$H NMR to determine the dr. The chromatography purified aldol products were then examined by HPLC to determine their ee. OD-H ChiralCel Column (4.6 ×250mm), yield: 97%; The ee was determined by chiral HPLC (Chiral OD-H, iPrOH/n-hexane 5/95, flow rate = 0.8 mL/min, $\lambda$ = 254 nm): tmajor= 35.488 min, tminor= 47.551 min, ee = 97%, dr = 90:10 (anti/syn).

FT-IR (cm$^{-1}$): 3510, 2938, 2901, 2875, 1686, 1603, 1507, 1339; $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ (ppm) = 1.26-1.35 (m, 1H), 1.44-1.65 (m, 4H), 1.77 (d, J= 13.7 Hz, 1H), 2.06-2.11 (m, 1H), 2.30-2.37 (td, J= 13.75Hz, J = 6.9 Hz, 1H), 2.54-2.62 (m, 1H), 4.83 (d, J= 8 Hz, 1H), 7.44 (d, J = 9.15 Hz, 2H), 8.15 (d, J = 9.15 Hz, 2H)
$^{13}$C NMR (100 MHz, CDCl$_3$) δ = 24.62, 27.59, 30.69, 42.62, 57.12, 73.74, 123.40, 123.52, 126.56, 127.86, 147.49, 148.30, 214.78
DEPT$^{90}$ and $^{135}$ deg show four methylene groups (negative) and 6 methine groups (positive) which in the aromatic area two of CH groups have been overlapped together.
MS (DI) = 249

2 (R)-2-((S)-hydroxy(phenyl)methyl)cyclohexanone

![Chemical Structure 1](image1.png)

FT-IR (cm$^{-1}$): 3508, 3112, 2935, 2862, 1692, 1510, 1338; $^1$H NMR (500 MHz, CDCl$_3$): δ (ppm) 1.73- 1.79 (m, 3H), 1.89-1.94 (m, 3H), 2.51- 2.55 (t, J = 6.85 Hz, 2H), 2.83 (td, J = 12.2Hz, J = 5.4 Hz, 1H) - 2.91- 2.94 (m, 1H), 4.78 (d, J = 9.2 Hz, 1H), 7.4, (m, 5H)

$^{13}$C NMR (100 MHz, CDCl$_3$) δ = 23.86, 28.4, 28.92, 40.29, 60.48, 74.54, 128.32, 128.47, 129.2, 130.19, 130.29, 133.78, 215.18
MS(DI) = 204

3 2-(XXXhydroxyl(4-nitrophenyl)methyl)cycloheptanone

![Chemical Structure 2](image2.png)

2-(hydroxy(4-nitrophenyl)methyl)cycloheptanone
FT-IR (cm$^{-1}$): 3100, 2928, 2860, 1704, 1603, 1346, 1117; $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ (ppm) = 1.20-1.45 (m, 4H), 1.65-1.92 (m, 4H), 2.40-2.59 (m, 2H), 2.98 (m, 1H), 3.74 (d, $J=4.8$ Hz, 1H), 4.92 (dd, $J=6.9$, $J=5.2$ Hz, 1H), 7.53 (d, $J=8.1$ Hz, 2H), 8.21(d, $J=9.1$Hz, 2H).

4  $S$-2-((S)-(2-chlorophenyl)(XXXhydroxyl)methyl)cyclohexanone

The resulting pure product was examined by $^1$H NMR to determine the dr. The chromatography purified aldol products were then examined by HPLC to determine their ee. OD-H ChiralCel Column (4.6 $\times$250mm), yield: 95%; The ee was determined by chiral HPLC (Chiral OD-H, $^t$PrOH/n-hexane 5/95, flow rate = 0.8 mL/min, $\lambda = 254$ nm): $t_{major}= 13.055$ min, $t_{minor}= 15.552$ min, ee = 99.9%, dr = 96:4 (anti/syn).

FT-IR (cm$^{-1}$): 3437, 2940, 2864, 1696, 1438, 1030, 756; 1H NMR (500 MHz, CDCl$_3$): $\delta$ (ppm) = 1.54-1.64 (m, 5H), 1.79-1.81 (m, 1H), 2.04-2.08 (m, 1H), 2.29-2.35 (td, $J=13.75$ Hz, $J=6.85$ Hz 1H), 2.43-2.46 (m, 1H), 2.63-2.68 (m, 1H), 5.33 (d, $J=8$ Hz, 1H), 7.19 (dd, $J=8$, $J=5.7$ Hz, 1H), 7.27-7.31 (m, 2H), 7.52 (dd, $J=8$, $J=2.3$ Hz, 1H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta = 24.89$, 27.79, 30.37, 42.71, 57.56, 70.43, 127.23, 128.20, 128.73, 129.19, 132.94, 139.02, 215.32.

DEPT$^{90}$ and $^{135}$ deg demonstrate four methylene groups (negative) and 6 methine groups (positive).

MS(DI) = 238

5  $S$-2-((S)-(4-chlorophenyl)(XXXhydroxyl)methyl)cyclohexanone
The resulting pure product was examined by $^1$H NMR to determine the dr. The chromatography purified aldol products were then examined by HPLC to determine their ee. OD-H ChiralCel Column (4.6 ×250mm). Yield: 95%; The ee was determined by chiral HPLC (Chiral OD-H, $^i$PrOH/n-hexane 5/95, flow rate = 0.8 mL/min, $\lambda = 254$ nm): $t_{major} = 13.831$ min, $t_{minor} = 17.452$ min, ee = 96.54 %, dr = 93:7 (anti/syn).

FT-IR (cm$^{-1}$): 2828, 2663, 2552, 1678, 1418, 1284, 926; $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ (ppm) = 1.25-1.27 (m, 2H), 1.52-1.55 (m, 2H), 1.56-1.60 (m, 1H), 1.60-1.63 (m, 1H), 2.07-2.08 (m, 1H), 2.31-2.37 (td, $J = 13.7$ Hz, $J = 6.8$ Hz, 1H), 2.46-2.53 (m, 1H), 2.54-2.55 (m, 1H), 4.76 (d, $J = 9.15$ Hz, 1H), 7.25 (d, $J = 9.15$ Hz, 2H), 7.32 (d, $J = 9.15$ Hz, 2H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta = 24.67$, 27.71, 30.74, 42.64, 57.30, 74.15, 128.48, 128.54, 129.26, 130.19, 133.79, 171.97, 215.44.

DEPT$^{90}$ and $^{135}$deg demonstrate four methylene groups (negative) and 6 methine groups (positive).

MS (DI) = 238

6 2-[Hydroxy-(4-cyano-phenyl)-methyl]-cyclohexanone

The resulting pure product was examined by $^1$H NMR to determine the dr. The chromatography purified aldol products were then examined by HPLC to determine their ee. OD-H ChiralCel Column (4.6 ×250mm), yield: 95%; The ee was determined by chiral HPLC (Chiral OD-H, $^i$PrOH/hexane 5/95, flow rate = 0.8 mL/min, $\lambda = 254$ nm): $t_{major} = 18.801$ min, $t_{minor} = 26.323$ min, ee = 86 %, dr = 99:1 (anti/syn).

FT-IR (cm$^{-1}$): 3425, 3356, 2932, 2860, 1688, 1481, 1053, 824; $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ (ppm) = 1.61-1.71(m, 3H), 1.89-1.99 (m, 2H), 2.06-2.13 (m, 2H), 2.16-2.24 (m, 1H), 2.29-2.43 (m, 1H), 4.75 (d, $J = 9.15$ Hz, 1H), 5.31 (d, $J = 2.3$ Hz, 1H) 7.41 (dd, $J = 2.3$, $J = 8$ Hz, 2H), 7.58 (dd, $J = 4.6$, $J = 8$ Hz, 2H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta = 20.25$, 22.24, 26.66, 38.94, 55.97, 74.43, 110.82, 118.71, 126.19, 127.17, 132.11, 148.30, 219.91.
DEPT\textsuperscript{90} and 135 deg demonstrate four methylene groups (negative) and 6 methine groups (positive).

MS(DI) = 229

7 \textit{(R)-2-((S)-hydroxy(2-nitrophenyl)methyl)cyclohexanone}

![Chemical structure of (R)-2-((S)-hydroxy(2-nitrophenyl)methyl)cyclohexanone]

The resulting pure product was examined by \textsuperscript{1}H NMR to determine the dr. The chromatography purified aldol products were then examined by HPLC to determine their \textit{ee}. OD-H ChiralCel Column (4.6 $\times$ 250mm). yield: 95\%; The \textit{ee} was determined by chiral HPLC (Chiral OD-H, \textsuperscript{1}PrOH/n-hexane 5/95, flow rate = 0.8 mL/min, $\lambda$ = 254 nm): \text{t}_{\text{major}}= 11.508 min, \text{t}_{\text{minor}}= 16.098 min, \textit{ee} = 88.8 \%, \text{dr} = 98: 2 (anti/syn).

FT-IR (cm$^{-1}$): 3411, 2942, 2866, 1703, 1524, 1349; \textsuperscript{1}H NMR (500 MHz, CDCl$_3$): $\delta$ (ppm) = 1.57-1.75 (m, 5H), 1.80-1.83 (m, 1H), 2.04-2.09 (m, 1H), 2.27-2.34 (td, $J$ = 13.75 Hz, $J$ = 5.75 Hz, 1H), 2.40-2.43 (m, 1H), 5.42 (d, $J$ = 6.85 Hz, 1H), 7.40 (t, $J$ = 8 Hz, 1H), 7.60 (t, $J$ = 8 Hz, 1H), 7.74 (d, $J$ = 8 Hz, 1H), 7.81 (d, $J$ = 8 Hz, 1H)

\textsuperscript{13}C NMR (100 MHz, CDCl$_3$) $\delta$ = 24.93, 27.72, 31.06, 42.78, 57.24, 69.70, 124.04, 128.36, 128.95, 133.05, 136.54, 148.67, 214.96.

DEPT\textsuperscript{90} and 135 deg demonstrate four methylene groups (negative) and 6 methine groups (positive).

MS(DI) = 249

8 \textit{(R)-2-((S)-(4-bromophenyl)(hydroxy)methyl)cyclohexanone}

![Chemical structure of (R)-2-((S)-(4-bromophenyl)(hydroxy)methyl)cyclohexanone]
The resulting pure product was examined by \(^1\)H NMR to determine the dr. The chromatography purified aldol products were then examined by HPLC to determine their ee. OD-H ChiralCel Column (4.6 × 250 mm). Yield: 95%; The ee was determined by chiral HPLC (Chiral OD-H, iPrOH/n-hexane 5/95, flow rate = 0.8 mL/min, \(\lambda = 254\) nm): \(t_{\text{major}} = 22.316\) min, \(t_{\text{minor}} = 29.783\) min, ee = 85.8 %, dr = 90: 10 (anti/syn).

FT-IR (cm\(^{-1}\)): 2941, 2833, 2659, 2550, 1678, 1415, 1281, 925; \(^1\)H NMR (500 MHz, CDCl\(_3\)): \(\delta\) (ppm) = 1.24-1.32 (m, 1H), 1.49-1.70 (m, 4H), 1.77-1.85 (m, 1H), 2.06-2.11 (m, 1H), 2.31-2.37 (td, \(J = 13.7\) Hz, \(J = 5.7\) Hz, 1H), 2.43-2.48 (m, 1H), 2.51-2.57 (m, 1H), 4.74 (d, \(J = 9.2\) Hz, 1H), 7.19 (d, \(J = 8\) Hz, 2H), 7.46 (d, \(J = 8\) Hz, 2H).

\(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta = 24.68, 27.69, 30.73, 42.64, 57.29, 74.14, 121.70, 127.50, 128.71, 131.24, 131.47, 139.95, 215.30.

DEPT\(^{90}\) and \(^{135}\) deg demonstrate four methylene groups (negative) and 6 methine groups (positive).

MS(DI) = 282

9 (R)-2-((S)-(4-(trifluoromethyl)phenyl)(hydroxy)methyl)cyclohexanone

The resulting pure product was examined by \(^1\)H NMR to determine the dr. The chromatography purified aldol products were then examined by HPLC to determine their ee. OD-H ChiralCel Column (4.6 × 250 mm). Yield: 95%; The ee was determined by chiral HPLC (Chiral OD-H, iPrOH/n-hexane 5/95, flow rate = 0.8 mL/min, \(\lambda = 254\) nm): \(t_{\text{major}} = 13.407\) min, \(t_{\text{minor}} = 15.682\) min, ee = 79.5 %, dr = 92: 8 (anti/syn).

FT-IR (cm\(^{-1}\)): 3065, 2828, 2663, 2552, 1678, 1418, 1285, 928; \(^1\)H NMR (500 MHz, CDCl\(_3\)): \(\delta\) (ppm) = 1.25-1.31 (m, 2H), 1.49-1.53 (m, 2H), 1.55-1.64 (m, 1H), 1.73-1.75 (m, 1H), 2.00-2.06 (m, 1H), 2.26-2.32 (td, \(J = 5.7\) Hz, \(J = 13.7\) Hz, 1H), 2.40-2.43 (m, 1H), 2.50-2.55 (m, 1H), 4.77 (d, \(J = 8\) Hz, 1H), 7.37 (d, \(J = 8\) Hz, 2H), 7.53 (d, \(J = 8\) Hz, 2H).

\(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta = 24.70, 27.69, 30.74, 42.66, 57.24, 74.26, 125.58, 125.32, 127.35, 129.94, 130.20, 144.93, 215.12.

DEPT\(^{90}\) and \(^{135}\) deg demonstrate four methylene groups (negative) and 6 methine groups (positive).
10 (R)-2-((S)-hydroxy(pyridin-4-yl)methyl)cyclohexanone

The resulting pure product was examined by $^1$H NMR to determine the dr. The chromatography purified aldol products were then examined by HPLC to determine their $ee$. AD-H ChiralPak Column (4.6 ×250mm). Yield: 95%; The ee was determined by chiral HPLC (Chiral AD-H, iPrOH/n-hexane 5/95, flow rate = 0.8 mL/min, $\lambda$ = 254 nm): $t_{major}$= 12.228 min, $t_{minor}$= 16.668 min, ee = 98 %, dr = 99:1 (anti/syn).

FT-IR (cm⁻¹):  3100, 2928, 2860, 1704, 1603, 1413, 1117; $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ (ppm) = 1.66-1.71 (m, 2H), 1.93- 2.02 (m, 2H), 2.09-2.16 (m, 1H), 2.3- 2.40 (m, 1H), 4.38 (bs, 1H), 5.29 (d, $J = 2.3$ Hz 1H), 7.28 (d, $J = 4.55$ Hz, 2H), 7.43 (d, $J = 4.55$ Hz, 2H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ (ppm) 20.38, 22.14, 39.01, 55.67, 69.50, 120.83, 129.06, 153.18, 219.51.

DEPT$^{90}$ and DEPT$^{135}$ deg demonstrate four methylene groups (negative) and 6 methine groups (positive two overlapped). MS(DI) = 272

11 (S)-4-hydroxy-4-(4-nitrophenyl)butan-2-one

The resulting pure product was examined by $^1$H NMR to determine the dr. The chromatography purified aldol products were then examined by HPLC to determine their $ee$. AD-H ChiralPak Column
The ee was determined by chiral HPLC (Chiral AD-H, iPrOH/n-hexane 10/90, flow rate = 0.8 mL/min, λ = 254 nm).

FT-IR (cm\(^{-1}\)): 3430, 3068, 2922, 1700, 1414, 1281. \(^1\)H NMR (500 MHz, CDCl\(_3\)): \(\delta\) (ppm) = 2.14 (s, 3H), 2.78 (d, \(J = 5.7\) Hz, 2H), 3.96 (bs, 1H), 5.19 (dd, \(J = 6.9, 5.7\) Hz, 1H), 7.46 (d, \(J = 8\) Hz, 2H), 8.11 (d, \(J = 8\) Hz, 2H).

\(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) = 30.61, 51.48, 68.50, 123.66, 126.36, 128.36, 130.01, 147.4, 150.04, 208.44.

DEPT\(^{90}\) and \(^{135}\) deg demonstrate one methylene groups (negative) and five methine groups (positive).

\(12\) (S)-4-(4-chlorophenyl)-4-hydroxybutan-2-one

\begin{center}
\includegraphics[width=0.2\textwidth]{structure.png}
\end{center}

The resulting pure product was examined by \(^1\)H NMR to determine the dr. The chromatography purified aldol products were then examined by HPLC to determine their ee. AD-H ChiralPak Column (4.6 \(\times\) 250mm). The ee was determined by chiral HPLC (Chiral AD-H, iPrOH/n-hexane 10/90, flow rate = 0.5 mL/min, λ = 254 nm).

FT-IR (cm\(^{-1}\)): 3425, 3077, 2919, 1703, 1515, 1340. \(^1\)H NMR (500 MHz, CDCl\(_3\)): \(\delta\) (ppm) = 2.17 (s, 3H), 2.78 (d, \(J = 4.6\) Hz, 2H), 3.36 (bs, 1H), 5.10 (dd, \(J = 8.9, 3.7\) Hz, 1H), 7.27-7.30 (m, 4H).

\(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) = 30.74, 51.76, 69.15, 127.00, 128.65, 133.32, 141.14, 208.93.

DEPT\(^{90}\) and \(^{135}\) deg demonstrate one methylene groups (negative) and five methine groups (positive).

\(13\) (S)-4-(4-(trifluoromethyl)phenyl)-4-hydroxybutan-2-one

\begin{center}
\includegraphics[width=0.2\textwidth]{structure.png}
\end{center}

The resulting pure product was examined by \(^1\)H NMR to determine the dr. The chromatography purified aldol products were then examined by HPLC to determine their ee. AD-H ChiralPak Column
The ee was determined by chiral HPLC (Chiral AD-H, iPrOH/n-hexane 10/90, flow rate = 1 mL/min, λ = 254 nm).

FT-IR (cm⁻¹): 3420, 3078, 2914, 1705, 1515, 1341. ¹H NMR (500 MHz, CDCl₃): δ (ppm) = 2.17 (s, 3H), 2.81 (d, J = 4.55 Hz, 2H), 3.54 (bs, 1H), 5.18 (dd, J = 7.4, 3.45 Hz, 1H), 7.44 (d, J = 8 Hz, 2H), 7.57 (d, J = 9.15 Hz, 2H).

¹⁳C NMR (100 MHz, CDCl₃) δ = 30.65, 51.45, 68.80, 125.45, 125.87, 129.61, 129.94, 146.94, 208.79. DEPT⁹₀ and ¹³⁵ deg demonstrate one methylene groups (negative) and five methine groups (positive).

14 (S)-4-hydroxy-4-(2-nitrophenyl)butan-2-one

![Formula](image)

The resulting pure product was examined by ¹H NMR to determine the dr. The chromatography purified aldol products were then examined by HPLC to determine their ee. AD-H ChiralPak Column (4.6 ×250mm). The ee was determined by chiral HPLC (Chiral AD-H, iPrOH/n-hexane 5/95, flow rate = 0.5 mL/min, λ = 254 nm)

FT-IR (cm⁻¹): 3418, 3077, 2922, 1706, 1520, 1344. ¹H NMR (500 MHz, CDCl₃): δ (ppm) = 2.21 (s, 3H), 2.70 (dd, J = 17.7, 10.3 Hz, 2H), 3.7 (bs, 1H), 5.65 (dd, J = 9.15, 2.3 Hz, 1H), 7.41 (d, J = 8 Hz, 2H), 7.64 (t, J = 8 Hz, 1H), 7.86 (d, J = 8 Hz, 1H), 7.93 (d, J = 8 Hz, 1H)

¹³C NMR (100 MHz, CDCl₃) δ = 30.41, 51.04, 65.57, 124.41, 128.15, 128.25, 133.80, 138.37, 147.11, 208.80.

DEPT⁹₀ and ¹³⁵ deg demonstrate one methylene groups (negative) and five methine groups (positive).

15 (S)-4-(4-bromophenyl)-4-hydroxybutan-2-one

![Formula](image)
The resulting pure product was examined by $^1$H NMR to determine the dr. The chromatography purified aldol products were then examined by HPLC to determine their ee. AD-H ChiralPak Column (4.6 ×250mm). The ee was determined by chiral HPLC (Chiral AD-H, 'PrOH/n-hexane 10/90, flow rate = 1 mL/min, $\lambda = 254$ nm).

FT-IR (cm$^{-1}$): 3418, 2921, 2855, 1705, 1490, 1352. $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ (ppm) = 2.18 (s, 3H), 2.81 (d, $J = 4.55$ Hz, 2H), 3.69 (bs, 1H), 5.22 (dd, $J = 7.4$, 3.45 Hz, 1H), 7.49 (d, $J = 8$ Hz, 2H), 8.15(d, $J = 9.15$ Hz, 2H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ = 30.65, 51.45, 68.80, 123.68, 126.36, 147.21, 150.01, 208.47. DEPT$^{90}$ and DEPT$^{135}$ deg demonstrate one methylene groups (negative) and five methine groups (positive).

- **NMR spectra of corresponding aldol compounds**
HPLC of corresponding aldol compounds Catalyzed by 8aa taken by chiral column
2-(hydroxy(4-nitrophenyl)methyl)cycloheptanone

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2-(hydroxy(4-nitrophenyl)methyl)cycloheptanone

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Racemate
\[\text{(R)-2-((S)-hydroxy(4-methoxyphenyl)methyl)cyclohexanone cat. 8aa}\]
1) (R)-2-((S)-hydroxy(4-nitrophenyl)methyl)cyclohexanone catalyzed by cat.8aa(z)
2) (R)-2-((S)-hydroxy(4-nitrophenyl)methyl)cyclohexanone catalyzed by cat.5aa
3) (R)-2-((S)-hydroxy(4-nitrophosphyl)methyl)cyclohexanone catalyzed by cat.3aa
Aldol reaction Catalyzed by Fmoc-3aa-Resin
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![Chemical Structure Diagram]

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[Graphical Representation of the chromatogram with peaks at RT 7.496 and 7.844 minutes]
**SAMPLE INFORMATION**

Sample Name: 2Nitrobenz + acetone(8aa)ADH  
Sample Type: Unknown  
Vial: 1  
Injection #: 2  
Injection Volume: 0.00 ul  
Run Time: 60.00 Minutes  

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**Chemical Structure:**  
![Chemical Structure Image]
4) **Octapeptide purity:**

Pro-Glu-Leu-Phe-Val-Lys-Leu-His-NH₂

Octapeptide Mass:

\[ [\alpha]^{20}_{\text{Na}589} = +2.86 \text{ (c= 5 mg/25ml H}_2\text{O)} \]

Pro-Glu-Leu-Phe-Val-Lys-Leu-His-NH₂

Theory Mol. Wt. calculated by Chemoffice software:

\[ C_{48}H_{76}N_{12}O_{10} \]

Exact Mass: 980.58

Mol. Wt.: 981.19

m/e: 980.58 (100.0%), 981.58 (56.7%), 982.59 (13.9%), 982.58 (4.4%), 983.59 (3.5%)
And experimental LC- Mass:

Integration Peak List

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m/z | z | Abund  
---|---|--------
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328.2025 | 3 | 1918582  
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328.8709 | 3 | 168530  
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491.8 | 2 | 1076452  
492.3018 | 2 | 336858  
981.5887 | 1 | 290675  
982.5915 | 1 | 172135  

+ESI Scan (8.399-9.604 min, 76 scans) Frag=175.0V Octapeptide-50ppm-Pos-MS-15_30.d Subtract
Backbone Amide H,
Lysine Side Chain NH2,
Phenyl group

Alpha
DMSO
-CH2-
Methy
2- Aldol reaction catalyzed by PE-16aa

1-1 (R)-2-((S)-hydroxy(4-nitrophenyl)methyl)cyclohexanone Catalyzed by PE-16aa
(S)-2-((S)-(4-chlorophenyl)(XXXhydroxyl)methyl)cyclohexanone

Sample Information

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Graph showing chromatographic analysis with peaks at RT 21.565 and 33.594 minutes.
1-3 2-[Hydroxy-(4-cyano-phenyl)-methyl]-cyclohexanone
1-4 (R)-2-((S)-hydroxy(2-nitrophenyl)methyl)cyclohexanone

SAMPLE INFORMATION

Sample Name: 2.NitroBenz+Cyhex  
Sample Type: Unknown  
Vial: 1  
Injection #: 5  
Injection Volume: 10.00 ul  
Run Time: 50.00 Minutes

Acquired By: Breeze  
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AU

Minutes
1-5  \((R)-2-((S)-(4\text{-bromophenyl})(\text{hydroxy})\text{methyl})\text{cyclohexanone}\)
1-6  (R)-2-((S)-(4-(trifluoromethyl)phenyl)(hydroxy)methyl)cyclohexanone
2 - Aldol reaction catalyzed by PH-18aa

2-1 (R)-2-((S)-hydroxy(4-nitrophenyl)methyl)cyclohexanone

![Chemical Structure of 2-1](image)

**SAMPLE INFORMATION**

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<td>143461</td>
<td>88.51</td>
</tr>
<tr>
<td>4 anti2</td>
<td>29.783</td>
<td>399522</td>
<td>6.76</td>
<td>8472</td>
<td>5.23</td>
</tr>
</tbody>
</table>

**Chromatogram**

- **syn1** - 17.657 min
- **syn2** - 19.322 min
- **anti2** - 29.783 min

**Additional Notes:**

- The sample set includes additional peaks that may be relevant for further analysis.
- The chromatogram shows clear separation of the peaks under the specified conditions.
2-2 (R)-2-((S)-hydroxy(4-nitrophenyl)methyl)cyclohexanone (in 1% SDS/iPrOH)
(S)-2-((S)-(4-chlorophenyl)(XXXhydroxyl)methyl)cyclohexanone
(S)-2-((S)-(2-chlorophenyl)(hydroxyl)methyl)cyclohexanone

SAMPLE INFORMATION

Sample Name: 2-ChloroBenz-Cyclohexane (P.H-16aa)
Sample Type: Unknown
Vial: 1
Injection #: 3
Injection Volume: 10.00 ul
Run Time: 20.00 Minutes

Acquired By: Breeze
Date Acquired: 10/17/2012 2:31:46 PM MST
Acq. Method: Saadi
Date Processed: 10/17/2012 2:53:44 PM MST
Channel Name: W2489 ChB
Sample Set Name:

<table>
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<th>RT (min)</th>
<th>Area (μV*sec)</th>
<th>% Area</th>
<th>Height (μV)</th>
<th>% Height</th>
</tr>
</thead>
<tbody>
<tr>
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<td>19742</td>
<td>0.12</td>
<td>1357</td>
</tr>
<tr>
<td>2</td>
<td>7.040</td>
<td>13837720</td>
<td>85.37</td>
<td>1001204</td>
</tr>
<tr>
<td>3</td>
<td>8.385</td>
<td>2352012</td>
<td>14.51</td>
<td>161310</td>
</tr>
</tbody>
</table>
2-5 2-[Hydroxy-(4-cyano-phenyl)-methyl]-cyclohexanone

SAMPLE INFORMATION

<table>
<thead>
<tr>
<th>Sample Name:</th>
<th>4CN.Ben-Cyhex(P.H-16aa,aq)</th>
<th>Acquired By:</th>
<th>Breeze</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample Type:</td>
<td>Unknown</td>
<td>Date Acquired:</td>
<td>10/12/2012 5:29:09 PM MYT</td>
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<tr>
<td>Vial:</td>
<td>1</td>
<td>Acq. Method:</td>
<td>Saadi</td>
</tr>
<tr>
<td>Injection #:</td>
<td>9</td>
<td>Date Processed:</td>
<td>10/15/2012 2:55:34 PM MYT</td>
</tr>
<tr>
<td>Injection Volume:</td>
<td>10.00 ul</td>
<td>Channel Name:</td>
<td>W2489 ChA</td>
</tr>
<tr>
<td>Run Time:</td>
<td>40.00 Minutes</td>
<td>Sample Set Name:</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>RT (min)</th>
<th>Area (µV×sec)</th>
<th>% Area</th>
<th>Height (µV)</th>
<th>% Height</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>14.608</td>
<td>0.19</td>
<td>935</td>
<td>0.40</td>
</tr>
<tr>
<td>2</td>
<td>15.348</td>
<td>0.20</td>
<td>881</td>
<td>0.38</td>
</tr>
<tr>
<td>3</td>
<td>19.815</td>
<td>89.99</td>
<td>212660</td>
<td>91.42</td>
</tr>
<tr>
<td>4</td>
<td>27.389</td>
<td>9.62</td>
<td>18131</td>
<td>7.79</td>
</tr>
</tbody>
</table>

AU

Minutes

0.00

0.02

0.12

0.24

0.40

14.608

15.348

19.815

27.389

8.889
2-6 \((R)-2-((S)\text{-hydroxy}(2\text{-nitrophenyl})methyl)cyclohexanone\)
2-7 (R)-2-((S)-(4-bromophenyl)(hydroxy)methyl)cyclohexanone

SAMPLE INFORMATION

Sample Name: 4Br.Ben-Cyhex(P.H-16aa.aq)  Acquired By: Breeze
Sample Type: Unknown  Date Acquired: 10/12/2012 3:29:47 PM MYT
Vial: 1  Acq. Method: Saadi
Injection #: 4  Date Processed: 10/15/2012 2:48:10 PM MYT
Injection Volume: 10.00 ul  Channel Name: W2489 ChB
Run Time: 17.00 Minutes  Sample Set Name:

<table>
<thead>
<tr>
<th>RT (min)</th>
<th>Area (µV*sec)</th>
<th>% Area</th>
<th>Height (µV)</th>
<th>% Height</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4.851</td>
<td>0.82</td>
<td>8077</td>
<td>2.16</td>
</tr>
<tr>
<td>2</td>
<td>7.508</td>
<td>0.31</td>
<td>2474</td>
<td>0.66</td>
</tr>
<tr>
<td>3</td>
<td>12.286</td>
<td>90.89</td>
<td>332692</td>
<td>88.92</td>
</tr>
<tr>
<td>4</td>
<td>15.647</td>
<td>7.97</td>
<td>30894</td>
<td>8.26</td>
</tr>
</tbody>
</table>

AUC

Minutes

0.00  2.00  4.00  6.00  8.00  10.00  12.00  14.00  16.00

4.851  7.508  15.647
2-8 (R)-2-((S)-(4-(trifluoromethyl)phenyl)(hydroxy)methyl)cyclohexanone
2-9  (R)-2-((S)-hydroxy(phenyl)methyl)cyclohexanone
2-10  (S)-4-hydroxy-4-(4-nitrophenyl)butan-2-one
2-11 \((S)-4-(4\text{-chlorophenyl})\text{-4-hydroxybutan-2-one}\)
2-12  (S)-4-(4-(trifluoromethyl)phenyl)-4-hydroxybutan-2-one

```
\begin{align*}
\text{Sample Name:} & \quad 4\text{CF3Ben+acetone} \\
\text{Sample Type:} & \quad \text{Unknown} \\
\text{Vial:} & \quad 1 \\
\text{Injection #:} & \quad 3 \\
\text{Injection Volume:} & \quad 0.00 \text{ ul} \\
\text{Run Time:} & \quad 60.00 \text{ Minutes}
\end{align*}
```

**Sample Information**

<table>
<thead>
<tr>
<th>RT (min)</th>
<th>Area ((\mu V)sec)</th>
<th>% Area</th>
<th>Height ((\mu V))</th>
<th>% Height</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6.844</td>
<td>215786</td>
<td>69.56</td>
<td>70.84</td>
</tr>
<tr>
<td>2</td>
<td>7.359</td>
<td>94451</td>
<td>30.44</td>
<td>29.16</td>
</tr>
</tbody>
</table>
2-13 (S)-4-(4-bromophenyl)-4-hydroxybutan-2-one
2-14 (S)-4-hydroxy-4-(2-nitrophenyl)butan-2-one
HPLC of peptide (PH16aa)

**Sample Information**

- **Sample Name:** P-H-16aa (0.5mmol/gr resin)
- **Sample Type:** Unknown
- **Vial:** 1
- **Injection #:** 4
- **Injection Volume:** 10.00 ul
- **Run Time:** 70.00 Minutes
- **Acquired By:** Breeze
- **Date Acquired:** 9/10/2012 4:03:07 PM MYT
- **Acq. Method:** Saadi RP
- **Date Processed:** 9/18/2012 12:39:52 PM MYT
- **Channel Name:** W2489 ChB
- **Sample Set Name:**

**Table:**

<table>
<thead>
<tr>
<th>RT (min)</th>
<th>Area (µV*sec)</th>
<th>% Area</th>
<th>Height (µV)</th>
<th>% Height</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>30.396</td>
<td>30716</td>
<td>1.14</td>
<td>4681</td>
</tr>
<tr>
<td>2</td>
<td>31.854</td>
<td>2499062</td>
<td>92.91</td>
<td>203067</td>
</tr>
<tr>
<td>3</td>
<td>33.212</td>
<td>36601</td>
<td>1.36</td>
<td>6589</td>
</tr>
<tr>
<td>4</td>
<td>33.397</td>
<td>41688</td>
<td>1.55</td>
<td>8103</td>
</tr>
<tr>
<td>5</td>
<td>34.636</td>
<td>81693</td>
<td>3.04</td>
<td>11116</td>
</tr>
</tbody>
</table>

**Graph:**

- **AU** on the y-axis, **Minutes** on the x-axis, with peaks at RT values 30.396, 31.854, 33.212, 33.397, and 34.636.
').

LC-Mass spectra of PH16aa

![LC-Mass spectra of PH16aa]

<table>
<thead>
<tr>
<th>RT (min)</th>
<th>Area (µV/sec)</th>
<th>% Area</th>
<th>Height (µV)</th>
<th>% Height</th>
</tr>
</thead>
<tbody>
<tr>
<td>26.809</td>
<td>498190</td>
<td>90.33</td>
<td>473699</td>
<td>88.80</td>
</tr>
<tr>
<td>27.774</td>
<td>341839</td>
<td>6.59</td>
<td>398456</td>
<td>7.24</td>
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<tr>
<td>28.693</td>
<td>100169</td>
<td>3.09</td>
<td>21152</td>
<td>3.96</td>
</tr>
</tbody>
</table>
FT-IR and CD spectrum of PH16aa
- FT-IR and CD spectrum of 16aa

CD spectra in 1% SDS
- Helix (%): 34.1
- Beta (%): 13.8
- Turn (%): 12.5
- Random (%): 32.7
- Sum (%): 93.2

CD spectra in water
- Helix (%): 18.5
- Beta (%): 29.5
- Turn (%): 12.5
- Random (%): 38.5
- Sum (%): 99.0
Characterization of PE16aa

- HPLC of PE16aa

---

**SAMPLE INFORMATION**

- Sample Name: Pro-Glu-16AA, HPLC
- Sample Type: Unknown
- Vial: 1
- Injection #: 2
- Injection Volume: 10.00 ul
- Run Time: 90.00 Minutes
- Acquired By: Breeze
- Date Acquired: 7/5/2012 4:28:55 PM MYT
- Acq. Method: Saadi RP
- Date Processed: 9/18/2012 12:28:44 PM MYT
- Channel Name: W2489 ChB
- Sample Set Name: 

---

**Graph**

**Table**

<table>
<thead>
<tr>
<th>RT (min)</th>
<th>Area (μV/sec)</th>
<th>% Area</th>
<th>Height (μV)</th>
<th>% Height</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>16.308</td>
<td>100.00</td>
<td>8391</td>
<td>100.00</td>
</tr>
</tbody>
</table>
- Spectroscopes data of PE-16aa
CD spectra in 1% SDS
- Helix (%): 36.5
- Beta (%): 11.5
- Turn (%): 12.5
- Random (%): 32.1

CD spectra in water
- Helix (%): 19.1
- Beta (%): 22.9
- Turn (%): 12.5
- Random (%): 38.6
HPLC analysis of 5aa

**SAMPLE INFORMATION**

<table>
<thead>
<tr>
<th>Sample Name:</th>
<th>PELFV, NH2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample Type:</td>
<td>Unknown</td>
</tr>
<tr>
<td>Vial:</td>
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</tr>
<tr>
<td>Injection #:</td>
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</tr>
<tr>
<td>Injection Volume:</td>
<td>20.00 ul</td>
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<tr>
<td>Run Time:</td>
<td>66.00 Minutes</td>
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<td>Acquired By:</td>
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<tr>
<td>Date Acquired:</td>
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<td>Channel Name:</td>
<td>W2489 ChA</td>
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<td>Sample Set Name:</td>
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</tbody>
</table>

**CHROMATOGRAM**

<table>
<thead>
<tr>
<th>RT (min)</th>
<th>Area (μV*sec)</th>
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<th>Height (μV)</th>
<th>% Height</th>
</tr>
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<tbody>
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<td>165183</td>
<td>95.41</td>
</tr>
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<td>4885</td>
<td>2.96</td>
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109
HPLC analysis of 8aa(z)