Solid-Phase Synthesis of N-Substituted Pyrrolidinone Tethered N-substituted Piperidines *via* Ugi Reaction

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Supporting Information

General Experiment

^{1}H NMR spectra were recorded in DMSO-d_6 with TMS for 1H NMR (500 MHz), 13C NMR (125 MHz) as the internal reference solvent. NMR chemical shifts are expressed in ppm relative to internal solvent peak and coupling constant were calculated in hertz. LC-MS (ESI) was recorded at both 214 nm and 254 nm using a reverse phase column (C18, 3 μm, 100Å, 3 × 250 mm). The samples were dissolved in the 50% of ACN in water at the concentration of about 1 mg/ml. As must be the typical dictate when handling hazardous materials, appropriate gloves, goggles, fume

hoods et cetera must be employed when handling aqueous or anhydrous hydrogen fluoride. Anhydrous hydrogen fluoride is an exceedingly acidic material that above and beyond its acidity is penetrating and highly destructive to tissue and toxic in its own right. One should always have readily at hand a slurry of calcium gluconate for immediate application following any skincontact.

Procedure for the synthesis of polymer supported glutamic acid 2

A 100 mg sample of p-methylbenzhydrylamine hydrochloride (MBHA·HCl) resin (CHEM-IMPEX INTERNATIONAL 1.15 mequiv/g, 100-200 mesh, 1% DVB) was contained within a sealed polypropylene mesh bag. 30 bags (30 X 100 mg resin, 3.45 mmol) were put in a polyethylene bottle. Following the neutralization of resin with 300 ml of 5% diisopropylethylamine (DIEA) in dichloromethane (DCM), L Fmoc-Glu(^{t}Bu)-OH (8.8 g, 20.7 mmol) was coupled using the conventional reagents hydroxybenzotriazole (HOBt, 3.2 g, 20.7 mmol) and diisopropylcarbodiimide (DIC, 3.3 ml, 20.7 mmol) in 100 ml anhydrous DMF for 2 h at room temperature. Completion of the coupling was monitored by the ninhydrin test. Following removal of ^{t}-Butyl group with 150 ml 55% TFA/DCM and washing with 150 ml DCM (3 ×), the Fmoc group was deprotected with 150 ml 20% piperidine in DMF (2×10min). The resin was then washed with 150 ml DMF (3×), 150 ml ^{i}PrOH (3×), 150 ml DCM (3×).

General procedure for the solid-phase Ugi reaction

One bag of resin **2** (100 mg, 0.115 mmol) was put into a small glass vial, and immersed with solution of ketone (0.23 mmol) in 2 ml acetonitrile/methanol (4:1)

for 1 h at 65 ^{o}C, then isocyanide (0.23 mmol) was added. After allowing the mixture to react at 65 ^{o}C for 24 h, the resin was washed with 10 ml MeOH (3×), 10 ml DMF (3×), 10 ml DCM (3×), dried and cleaved with condensed HF for 1.5 h at 0 ^{o}C. The HF was evaporated with nitrogen and trapped. The desired product were extracted with acetic/water (95/5) and lyophilized (2 x 5 ml). The completeness of the reaction was verified by analysis with LC-MS.

General procedure for the synthesis of compounds 8a-8c

One bag of Resin **5a** (100 mg, 0.115 mmol) was shaken in 10 ml 55% TFA/DCM for removal of Boc group. Following neutralization with 10 ml 5% DIEA/DCM (3×), the resin was coupled with different carboxylic acids (0.69 mmol) using conventional reagents HOBt (0.69 mmol) and DIC (0.69 mmol) in 10 ml anhydrous DMF overnight. The resin was then washed with 15 ml DMF (3×), 15 ml DCM (3×), dried and cleaved with HF for 1.5 h at 0 ^{o}C. The desired products were extracted with acetic acid/water (95/5) and lyophilized. All samples were purified by preparative HPLC and characterized by LC-MS and 1H-NMR.

General procedure for the synthesis of compounds 8d-8i

One bag of Resin **5a** (100 mg, 0.115 mmol) was shaken in 10 ml 55% TFA/DCM for removal of Boc group. Following neutralization with 10 ml 5% DIEA/DCM (3×), the resin was treated with DIEA (1.15 mmol) and corresponding reagents, such as sulfonyl chloride, isocyanate or thioisocyanate (1.15 mmol) in 10 ml anhydrous DMF overnight. The resin was then washed with 15 ml DMF (3×), 15 ml DCM (3×), dried and cleaved by HF for 1.5 h at 0 ^{o}C. The desired product were extracted with acetic/water (95/5) and lyophilized. All samples were purified by preparative HPLC and characterized.

Notes:

*The solid support was chosen for its compatibility for both Fmoc and Boc chemistries.

*All the LC-MS of the purified compounds show an hydrophobic peak at 10.7 min due to a problem with the column.

Purification

*HPLC Preparative:

The column is Phenomenex (Luna 5u C18(2) 100Å AX, 150 × 21.20 mm 5 micron)

Solvent A: 0.1 % Formic acid in H_2O

Solvent B: 0.1 % Formic acid in ACN

Flow rate: 15 ml/min

Duration: 30 min

Wavelength: 214

Gradient: vary for different compounds.

Gradient for purification **5a**: Start %B: 0, 0/0, 2/0, 8/1.5, 24/10, 30/95

The products were run on a gradients: 0% B for 2 min, 0% to 1.5% B for 6 min and 1.5 % to 10% B for 16 min and 10% to 95% solvent B for 6 min.
Solvent B (0.1% formic acid in ACN).

Analytic HPLCs:

The purified products were run on a Vydac column, gradients 5 to 95% solvent B (0.1% formic acid in ACN) in 6 min, followed by isocratic 95% solvent B for 2 min, followed by 95% to 5% solvent B for 2 min, followed by 5% to 5% solvent B for 2 min.
The purity was estimated on analytical traces at λ= 214 nm and 254 nm.

4: ^{1}H NMR (DMSO d_6): δ 1.30-1.86 (m, 10H, H on cyclohexane ring); 2.12-2.29 (m, 4H, H on pyrrolidine ring); 4.24 (m, 2H, H on benzyl group); 4.56 (m, 1H, H on pyrrolidine ring); 7.08-7.18 (m, 5H, H on benzyl group); 7.49 (s, 1H, H on amide group); 7.98 (s, 1H, H on amide group); 9.00 (t, 1H, J= 5.8 Hz, H on amide group)
^{13} C NMR (DMSO d_6): δ 21.69 (C on piperidine ring), 22.12 (C on piperidine ring), 24.75 (C on pyrrolidine ring), 25.20 (C on piperidine ring), 29.64 (C on pyrrolidine ring), 31.00 (C on piperidine ring), 32.44 (C on piperidine ring), 42.18 (C on benzyl group), 58.24 (C on piperidine ring), 61.79 (C on pyrrolidine ring), 126.40 (C on benzyl group), 126.80 (2C, C on benzyl group), 128.03 (2C, C on benzyl group), 139.66 (C on benzyl group), 173.12 (C on amide group), 174.64 (C on amide group), 176.81 (C on amide group)
ESI-MS: 343 (MH^+)

5a: ^{1}H NMR (DMSO d_6): δ 1.71-1.89 (m, 4H, H on piperidine ring); 2.15-2.34 (m, 3H, H on piperidine ring); 2.76-2.89 (m, 2H, H on piperidine ring); 3.02-3.23 (m, 4H, m, 4H, H on pyrrolidine ring); 4.28 (m, 2H, H on benzyl group); 4.52 (m, 1H, H on pyrrolidine ring); 7.19-7.30 (m, 5H, H on benzyl group); 7.53 (s, 1H, H on amide group); 8.06 (s, 1H, H on amide group); 9.18 (t, 1H, J= 5.7 Hz, H on amide group)
ESI-MS: 345 (MH^+)

5b: ^{1}H NMR (DMSO d_6): δ 1.11-1.86 (m, 20H, H on tow piperidine rings); 2.08-2.28 (m, 4H, H on pyrrolidine ring); 3.48 (m, 1H, H on piperidine ring); 4.53 (m, 1H, H on pyrrolidine ring); 7.52 (s, 1H, H on amide group); 7.93 (s, 1H, H on amide group); 8.47 (m, 1H, H on amide group)
ESI-MS: 336 (MH^+)

5c: ^{1}H NMR (DMSO d_6): δ 0.84 (t, 3H, J= 7.3 Hz, H on the n-butyl group); 1.23-1.86 (m, 14H, H on the n-butyl group and cyclohexane ring); 2.09-2.28 (m, 4H, H on pyrrolidine ring); 2.99 (q, 2H, J= 6.5 Hz, H on the n-butyl group); 4.53 (m, 1H, H on pyrrolidine ring); 7.50 (s, 1H, H on amide group); 7.96 (s, 1H, H on amide group); 8.48 (m, 1H, H on amide group)
ESI-MS: 310 (MH^+)

5d: ^{1}H NMR (DMSO d_6): δ 1.28-1.86 (m, 10H, H on cyclohexane ring); 2.07-2.31 (m, 10H, H on 2-morpholinethyl group and pyrrolidine ring); 3.11 (m, 2H, H on 2-morpholinethyl group); 3.53 (t, 4H, J= 4.6 Hz, H on 2-morpholinethyl group); 4.51 (m, 1H, H on pyrrolidine ring); 7.44 (m, 1H, H on amide group); 7.92 (m, 1H, H on amide group); 8.47 (t, 1H, J= 5.5 Hz, H on amide group)
ESI-MS: 367 (MH^+)

8a: ^{1}H NMR (DMSO d_6): δ 1.75-2.32 (m, 8H, H on piperidine ring); 3.46 (m, 4H, H on pyrrolidine ring); 4.28 (m, 2H, H on benzyl group); 4.57 (m, 1H, H on pyrrolidine ring); 7.20-7.28 (m, 5H, H on benzyl group); 7.37-7.39 (m, 2H, H on benzoyl group); 7.42-7.45 (m, 3H, H on benzoyl group); 7.53 (m, 1H, H on amide group); 7.96 (m, 1H, H on amide group); 9.11 (m, 1H, H on amide group)
ESI-MS: 449 (MH^+)

8b: ^{1}H NMR (DMSO d_6): δ 1.70-2.37 (m, 8H, H on piperidine ring); 3.40 (m, 4H, H on pyrrolidine ring); 3.67 (m, 2H, H on 2-phenylacetyl group); 4.26 (m, 2H, H on benzyl group); 4.48 (m, 1H, H on pyrrolidine ring); 7.19-7.23 (m, 6H, H on benzyl group and 2-phenylacetyl group); 7.26-7.32 (m, 4H, H on 2-phenylacetyl group); 7.52 (m, 1H, H on amide group); 7.95 (m, 1H, H on amide group); 9.12 (t, 1H, J= 5.7 Hz, H on amide group)
ESI-MS: 463 (MH^+)

8c: ^{1}H NMR (DMSO d_6): δ 1.58-2.31 (m, 25H, H on piperidine ring and adamaneacetyl group); 3.40 (m, 4H, H on pyrrolidine ring); 4.27 (m, 2H, H on benzyl group); 4.51 (m, 1H, H on pyrrolidine ring); 7.19-7.30 (m, 5H, H on benzyl group); 7.50 (m, 1H, H on amide group); 7.94 (s, 1H, H on amide group); 9.07-9.13 (m, 1H, H on amide group)
ESI-MS: 521 (MH^+)

8d: ^{1}H NMR (DMSO d_6): δ 1.64-2.40 (m, 11H, H on piperidine ring and tosyl group); 3.41 (m, 4H, H on pyrrolidine ring); 4.15 (m, 2H, H on benzyl group); 4.49 (m, 1H, H on pyrrolidine ring); 7.13-7.26 (m, 5H, H on benzyl group); 7.44 (d, 2H, J= 8.3 Hz, H on tosyl group); 7.50 (s, 1H, H on amide group); 7.59 (d, 2H, J= 8.3 Hz, H on tosyl group); 7.94 (s, 1H, H on amide group); 8.98 (t, 1H, J= 5.7 Hz, H on amide group)
ESI-MS: 499 (MH^+)

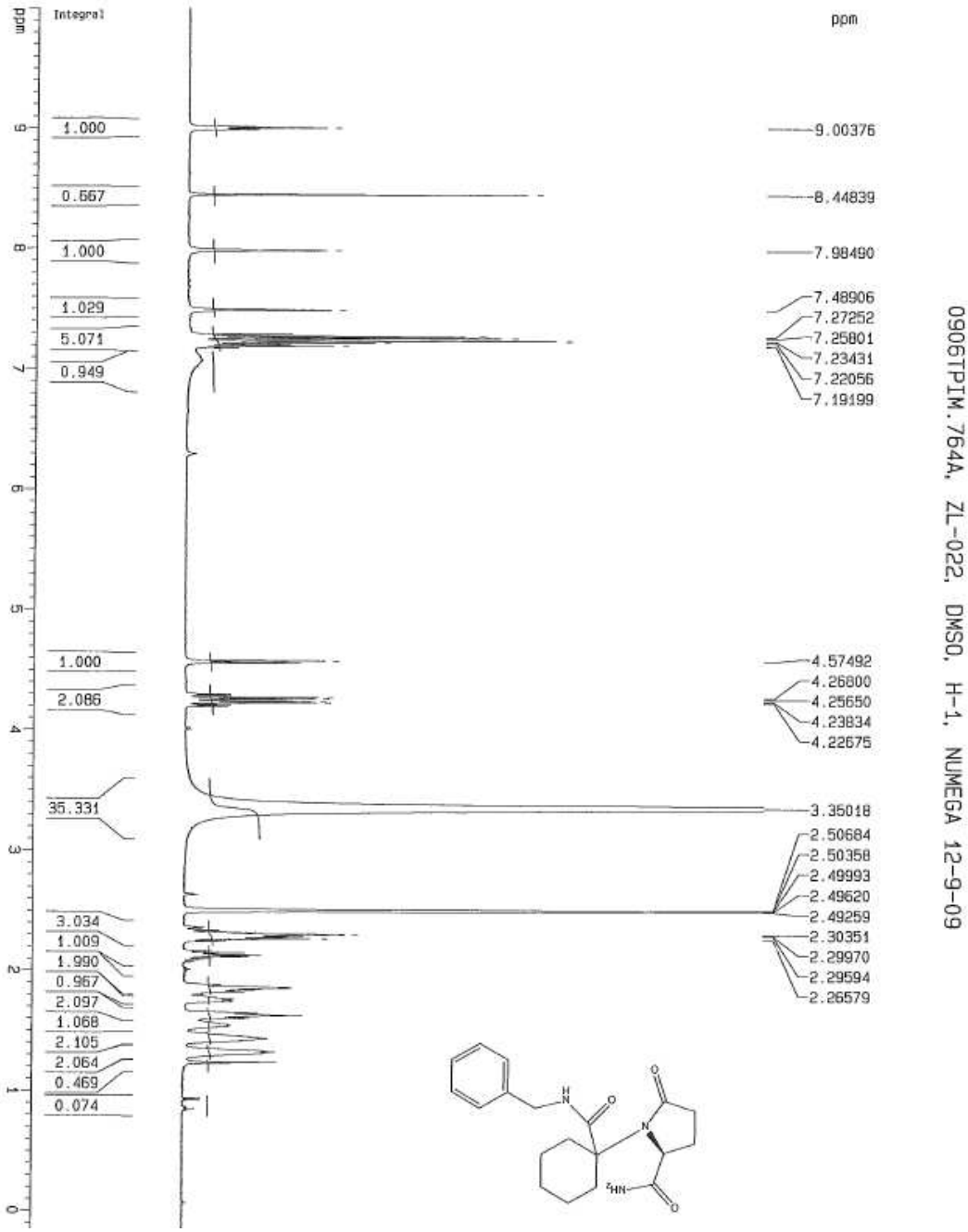
8e: ^{1}H NMR (DMSO d_6): δ 1.66-2.28 (m, 8H, H on piperidine ring); 3.49 (m, 4H, H on pyrrolidine ring); 4.09 (m, 2H, H on benzyl group); 4.49 (m, 1H, H on pyrrolidine ring); 7.07-7.20 (m, 5 H, H on benzyl group); 7.50 (s, 1H, H on amide group); 7.69-7.76 (m, 3H, H on naphthalene-2-ylsulfonyl); 7.94 (s, 1H, H on amide group); 8.08 (d, 1H, J= 8.0 Hz, H on naphthalene-2-ylsulfonyl); 8.17 (d, 1H J= 8.8 Hz, H on naphthalene-2-ylsulfonyl); 8.21 (d, 1H, J= 8.2 Hz, H on naphthalene-2-ylsulfonyl); 8.41 (s, 1H, H on naphthalene-2-ylsulfonyl); 8.95 (t, 1H, J= 5.6 Hz, H on amide group)
ESI-MS: 535 (MH^+)

8f: ^{1}H NMR (DMSO d_6): δ 1.04 (d, 6H, J= 6.5, H on the isopropyl group); 1.58-2.37 (m, 8H, H on piperidine ring); 3.44 (m, 4H, H on pyrrolidine ring); 3.73 (m, 1H, H on the isopropyl group); 4.27 (m, 2H, H on benzyl group); 4.51 (m, 1H, H on pyrrolidine ring); 6.86 (s, 1H, H on urea); 7.19-7.30 (m, 5H, H on benzyl group); 7.52 (s, 1H, H on amide group); 7.96 (s, 1H, H on amide group); 9.09 (t, 1H, J= 5.7Hz, H on amide group)
ESI-MS: 430 (MH^+)

8g: ^{1}H NMR (DMSO d_6): δ 1.24-2.34 (m, 8H, H on piperidine ring); 3.58 (m, 4H, H on pyrrolidine ring); 4.29 (m, 2H, H on benzyl group); 4.54 (m, 1H, H on pyrrolidine ring); 7.20-7.30 (m, 7H, H on benzyl group and phenyl group); 7.44 (m, 2H, H on phenyl group); 7.53 (s, 1H, H on amide group); 7.96 (s, 1H, H on amide group); 8.47 (s, 1H, H on urea); 9.13 (t, 1H, J= 5.8 Hz, H on amide group)
ESI-MS: 464 (MH^+)

8h: ^{1}H NMR (DMSO d_6): δ 1.08 (t, 3H, J= 7.2 Hz, H on ethyl group); 1.23-2.38 (m, 8H, H on piperidine ring); 3.41-3.48 (m, 6H, H on pyrrolidine ring and ethyl group); 4.28 (m, 2H, H on benzyl group); 4.50 (m, 1H, H on pyrrolidine ring); 6.87 (s, 1H, H on thiourea); 7.19-7.30 (m, 5H, H on benzyl group); 7.54 (s, 1H, H on amide group); 7.97 (s, 1H, H on amide group); 9.15 (t, 1H, J= 5.7 Hz, H on amide group)
ESI-MS: 432 (MH^+)

8i: ^{1}H NMR (DMSO d_6): δ 1.23-2.38 (m, 8H, H on piperidine ring); 3.50-3.89 (m, 4H, H on pyrrolidine ring); 4.30 (m, 2H, H on benzyl group); 4.56 (m, 1H, H on pyrrolidine ring); 7.09 (m, 1H, H on benzyl group); 7.28 (m, 9H, H on benzyl group and phenyl group); 7.56 (s, 1H, H on amide group); 8.00 (s, 1H, H on amide group); 9.19 (t, 1H, J= 5.7 Hz, H on amide group); 9.28 (s, 1H, H on thiourea)
ESI-MS: 480 (MH^+)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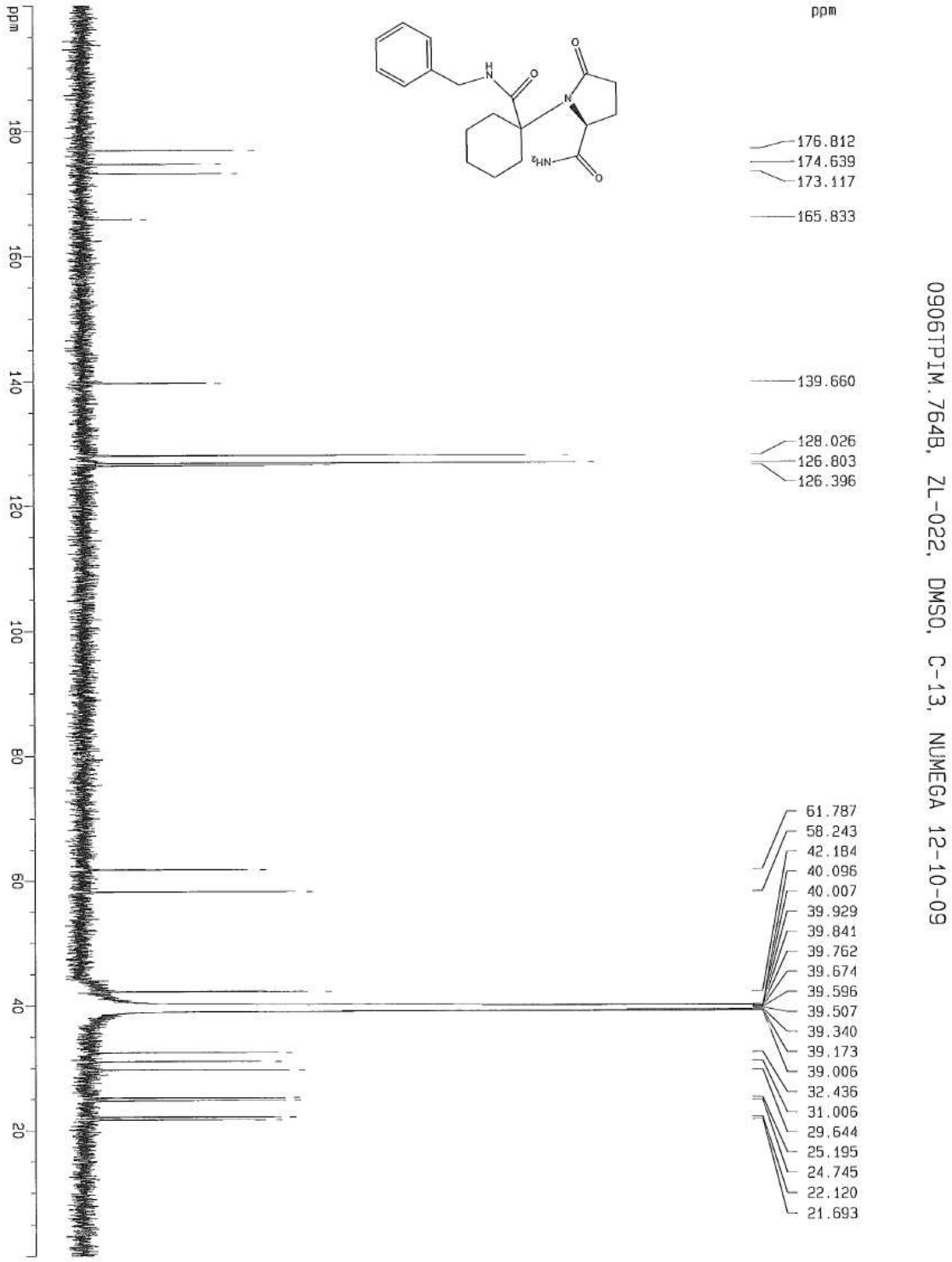
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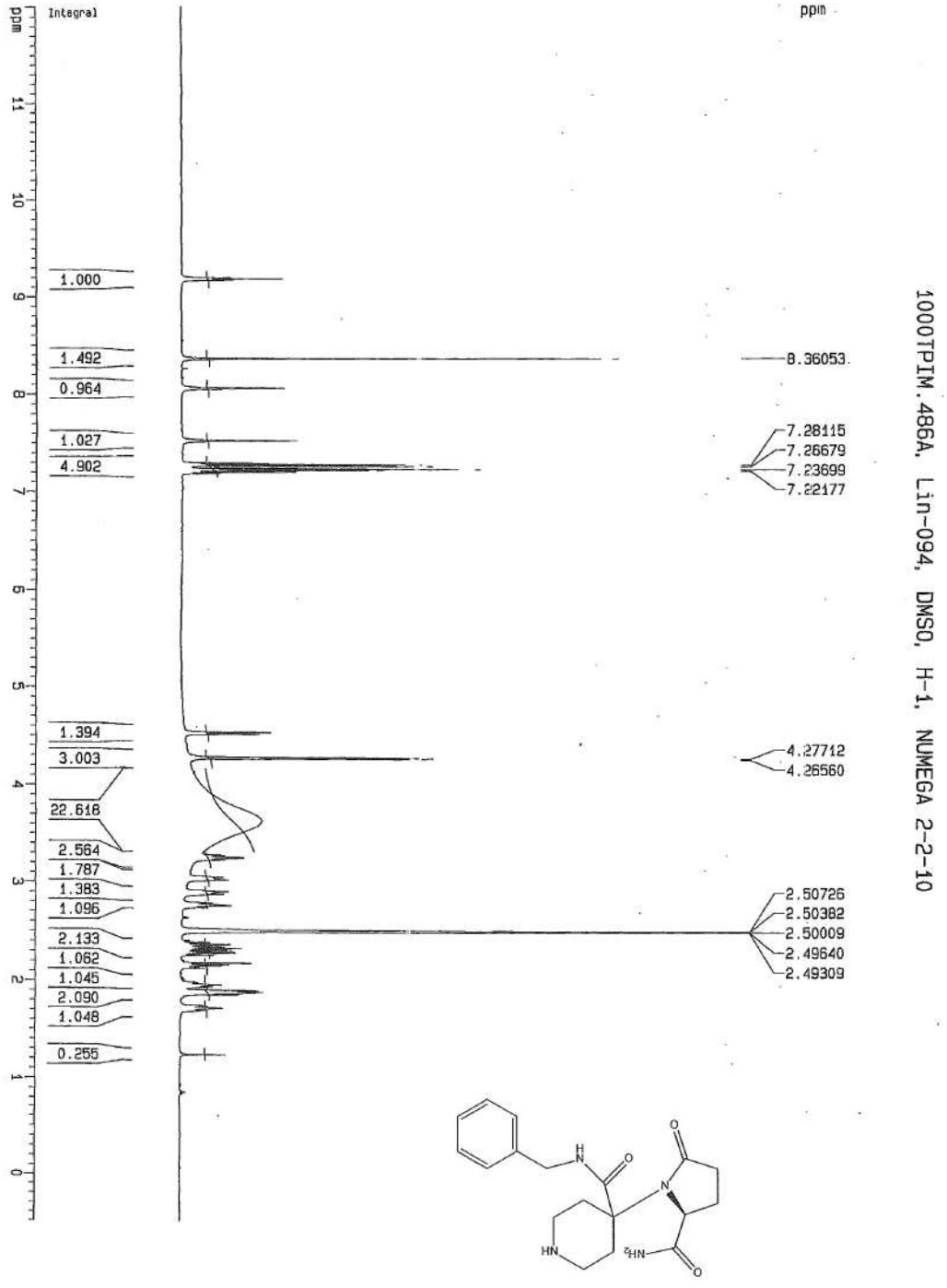
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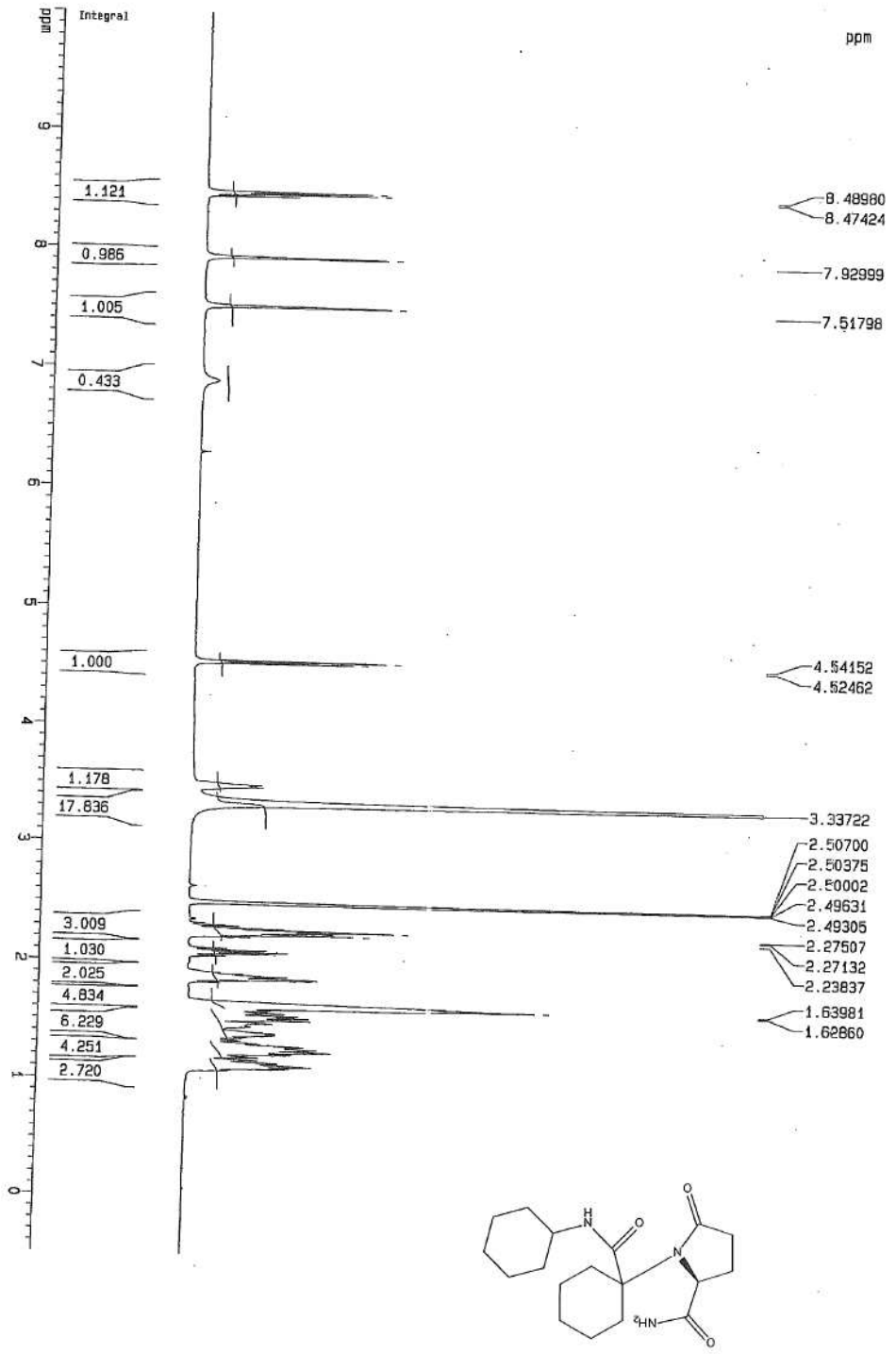

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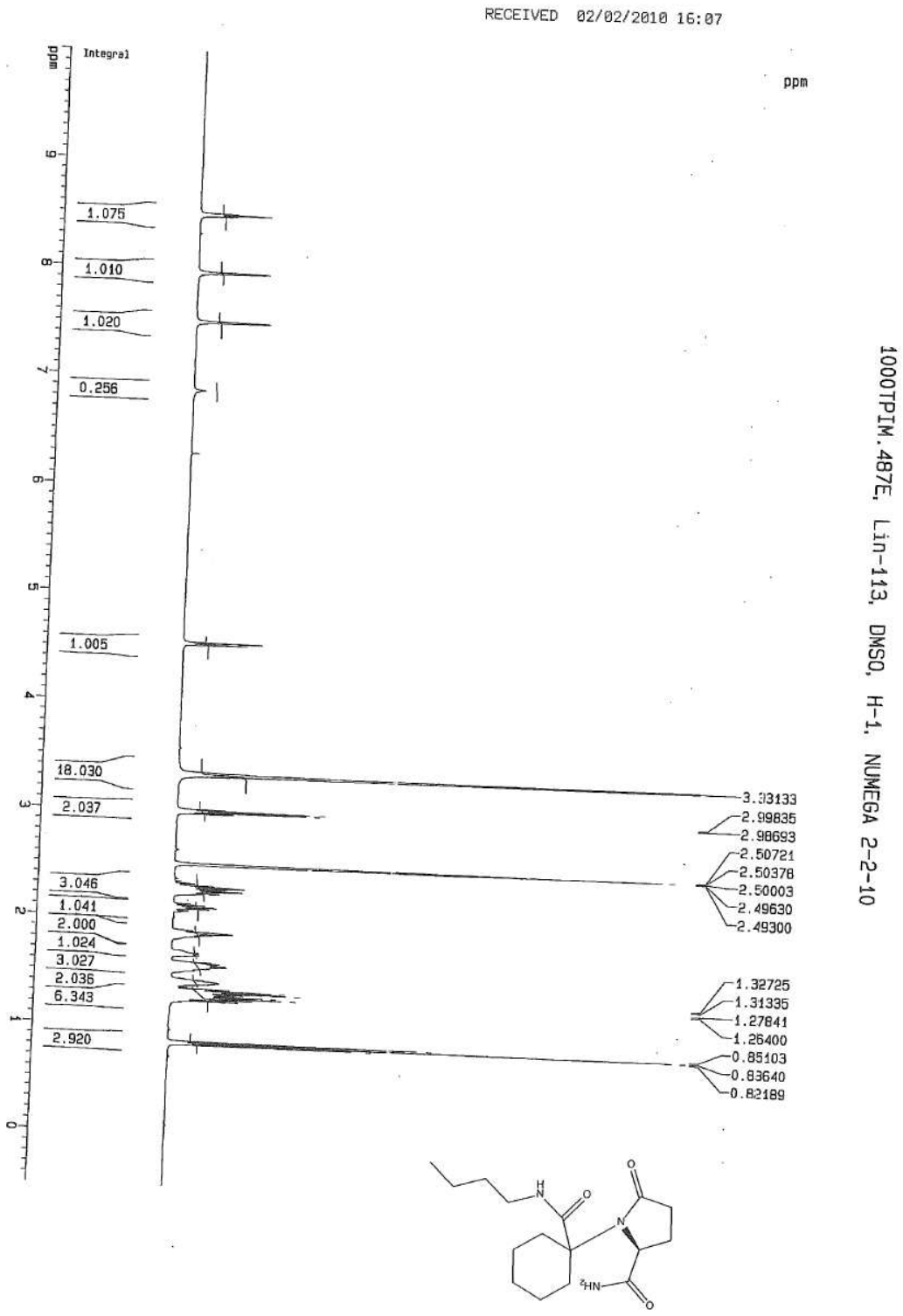
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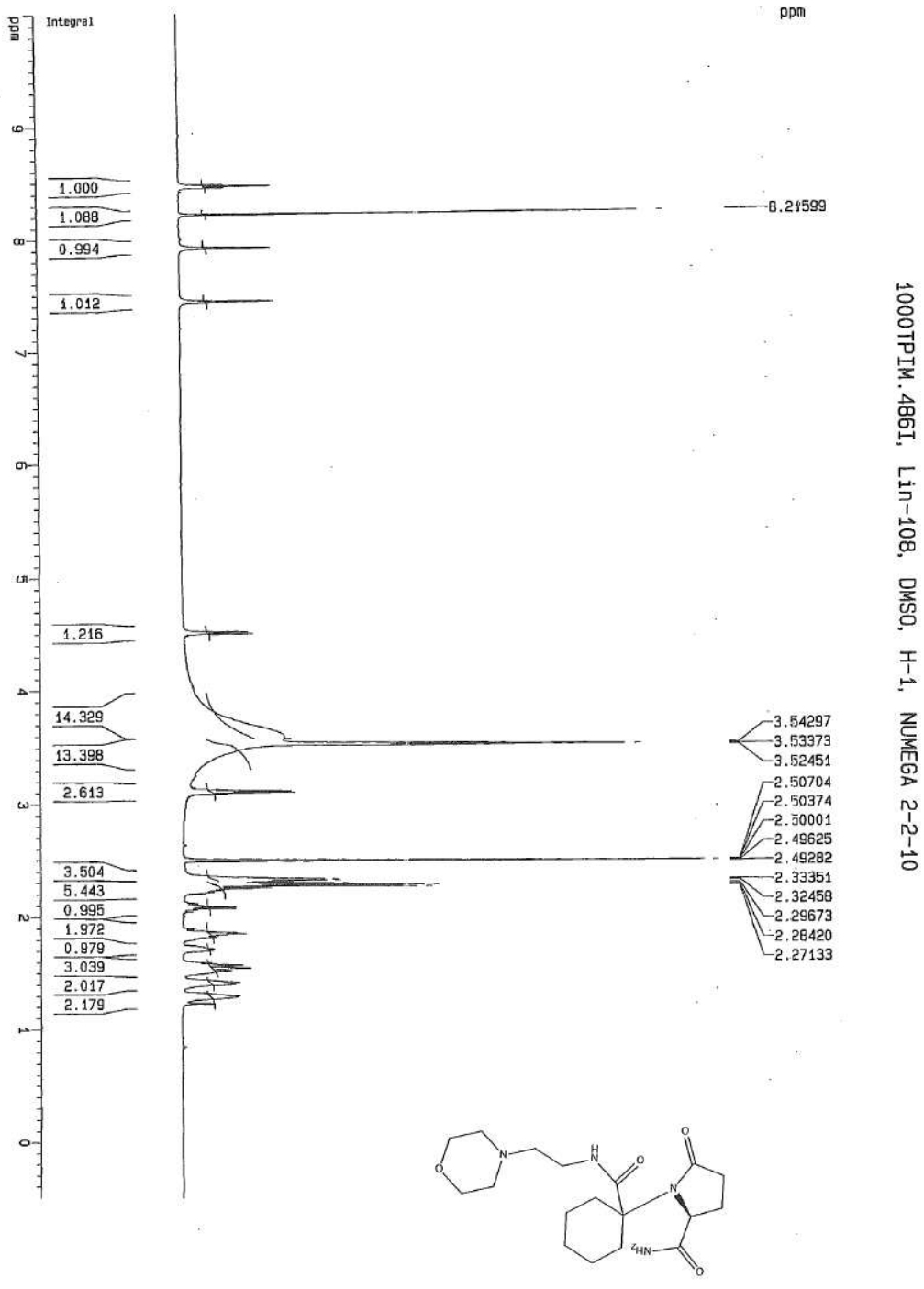

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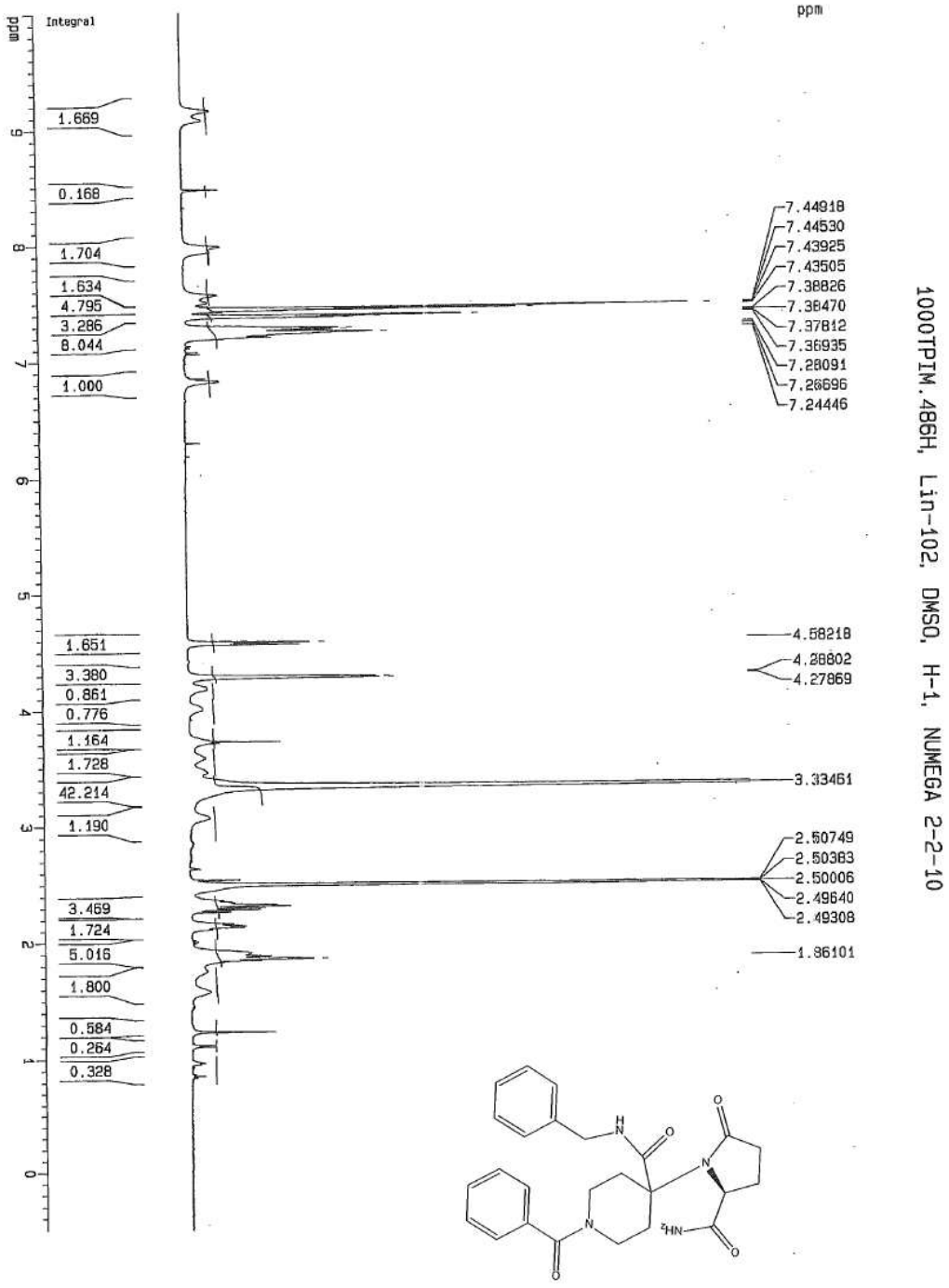

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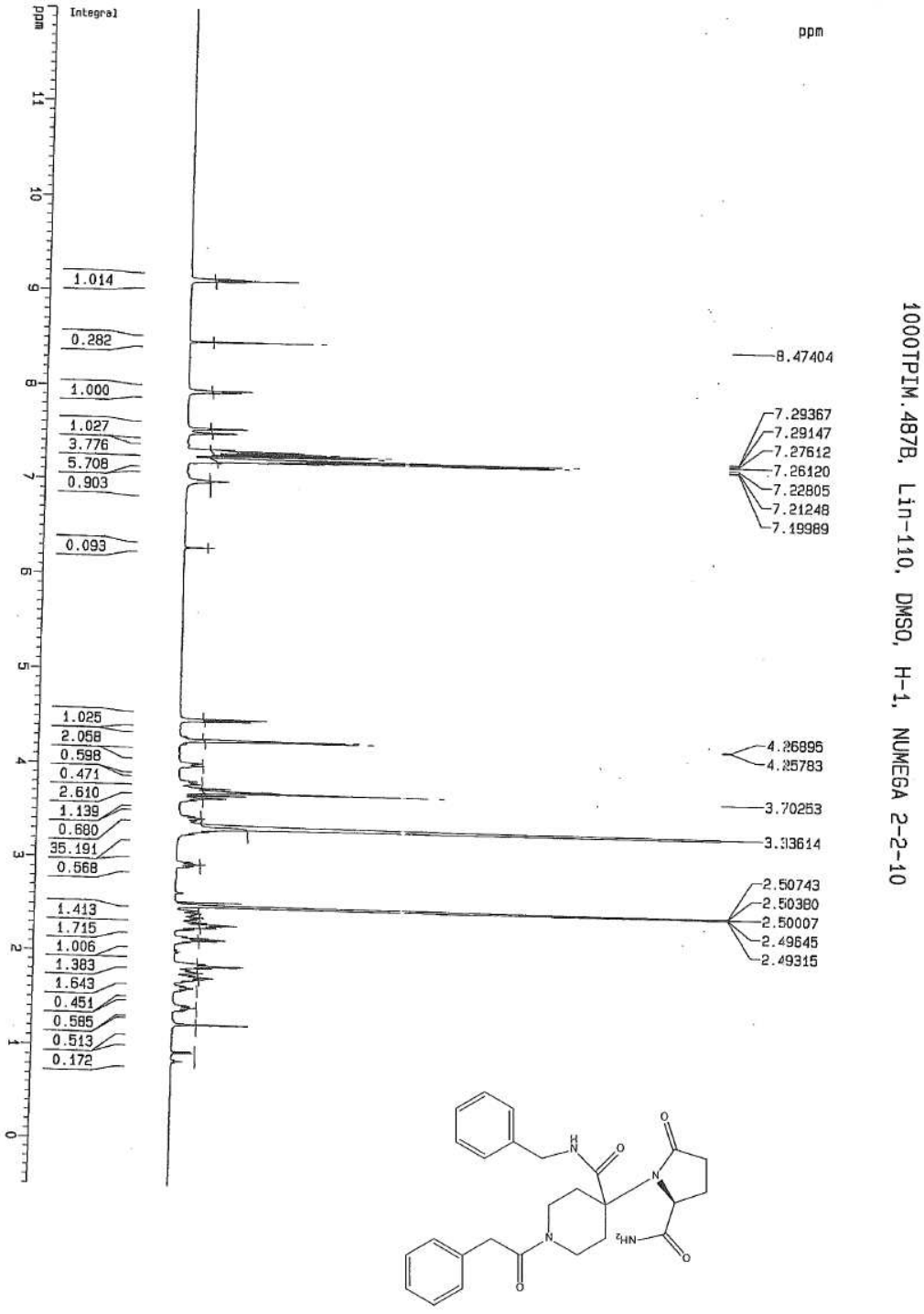
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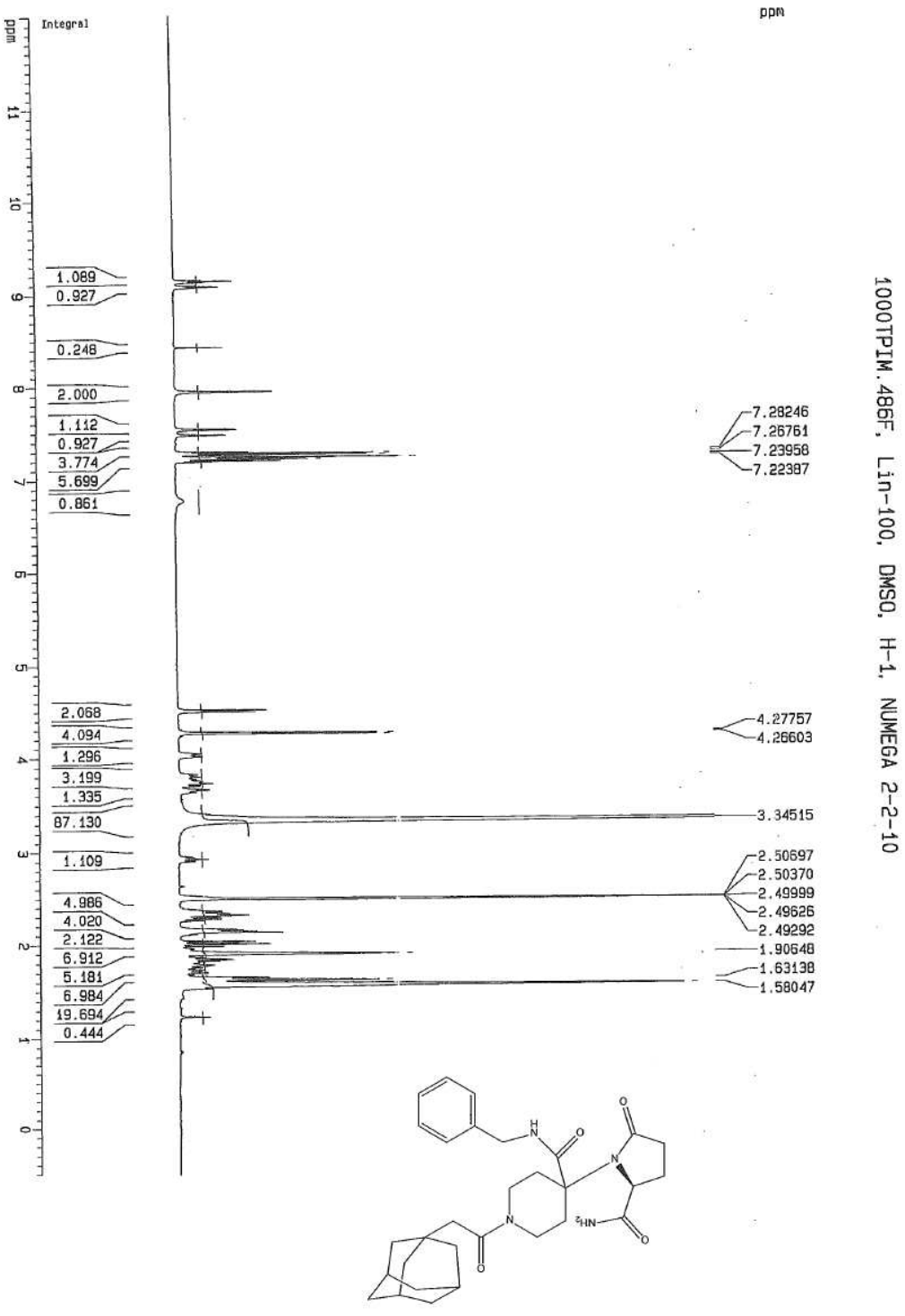

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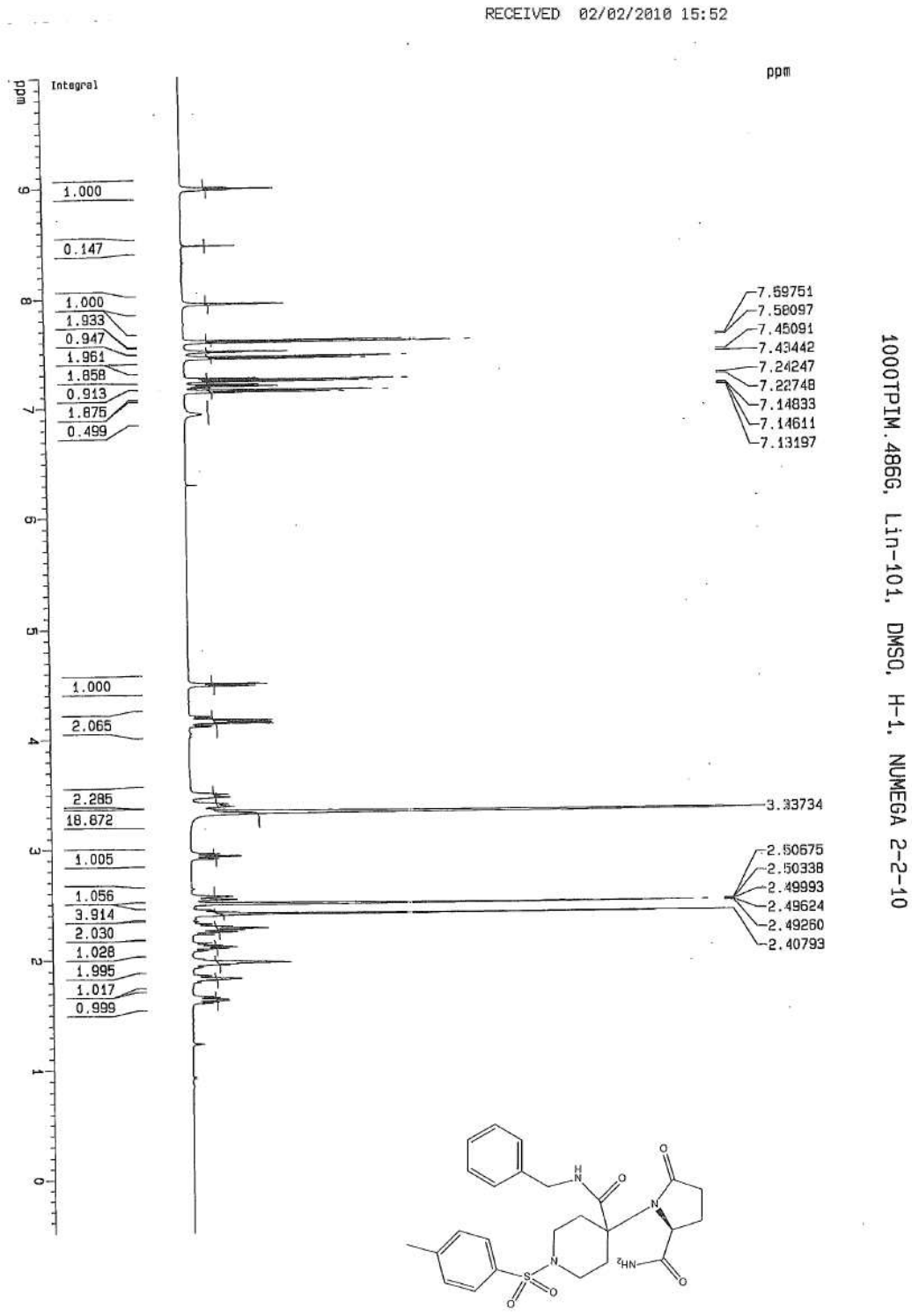
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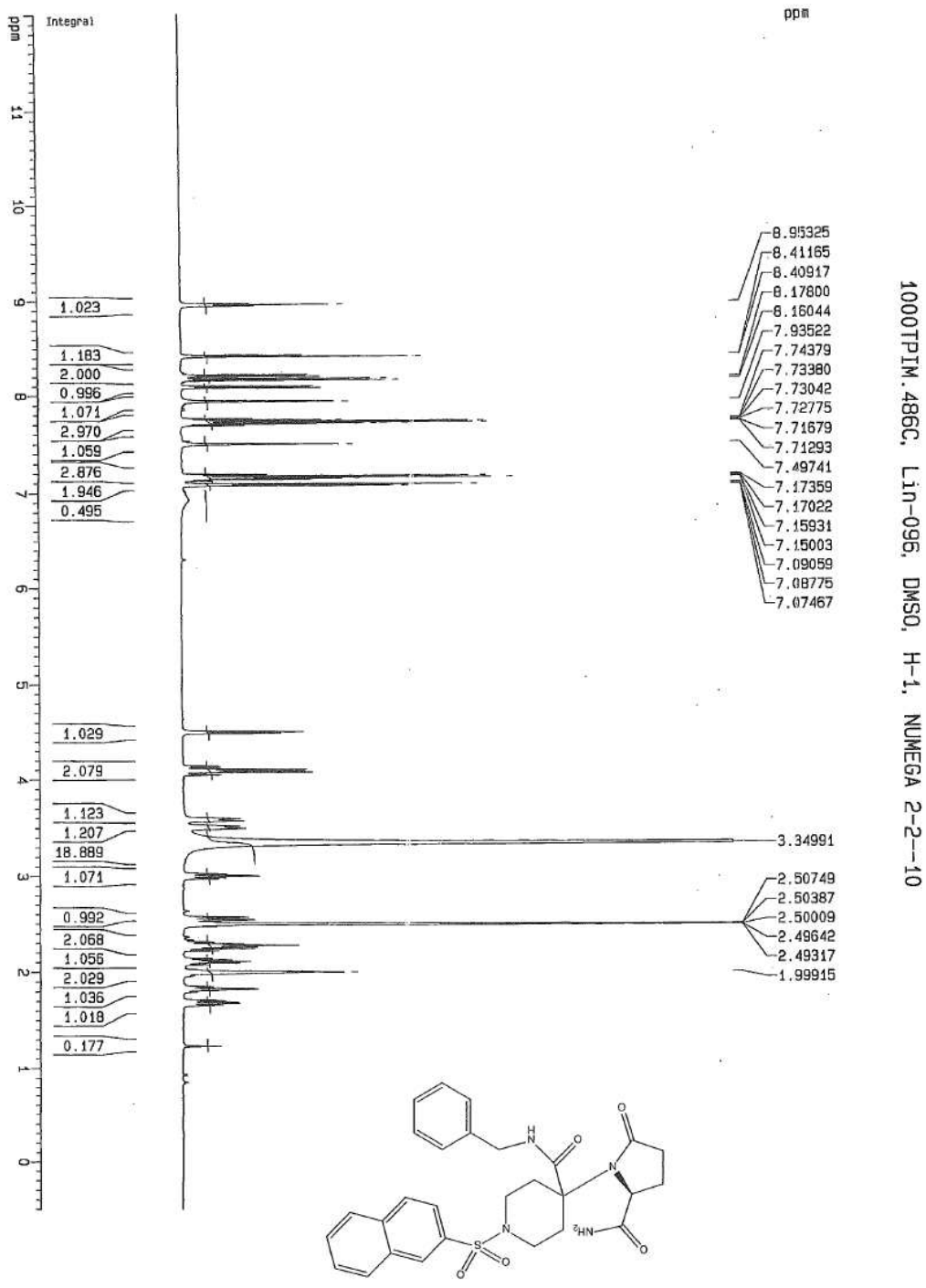

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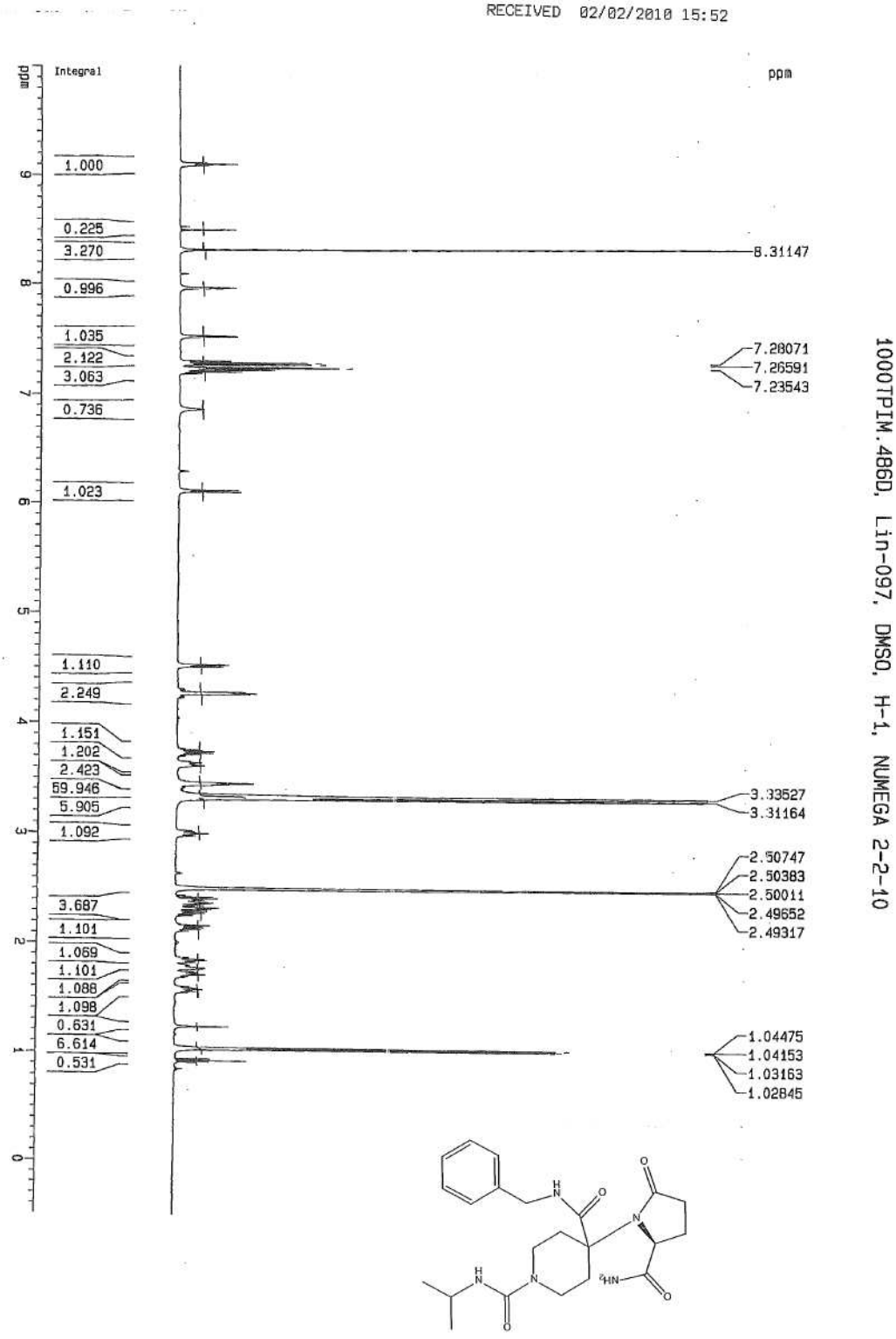
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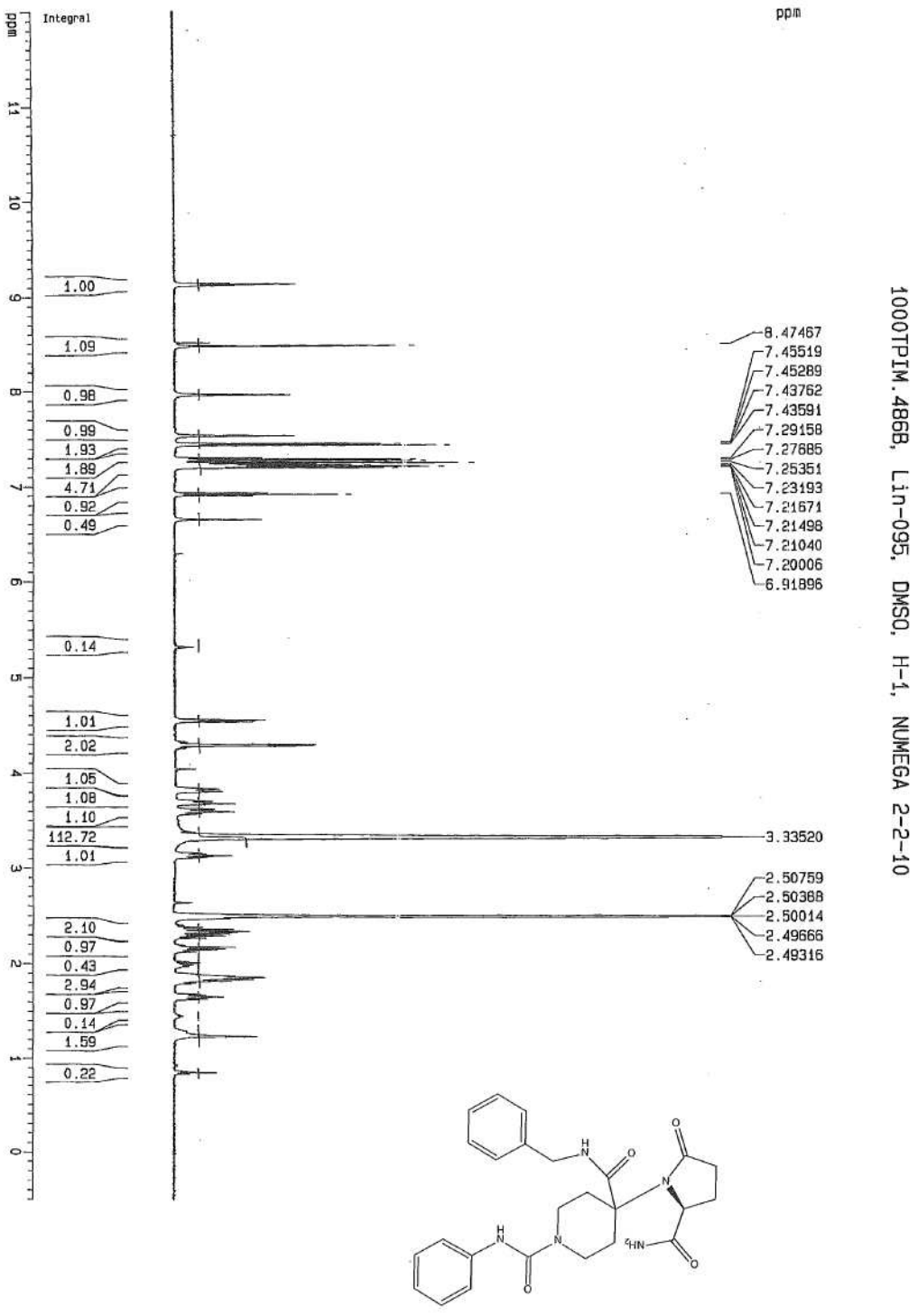
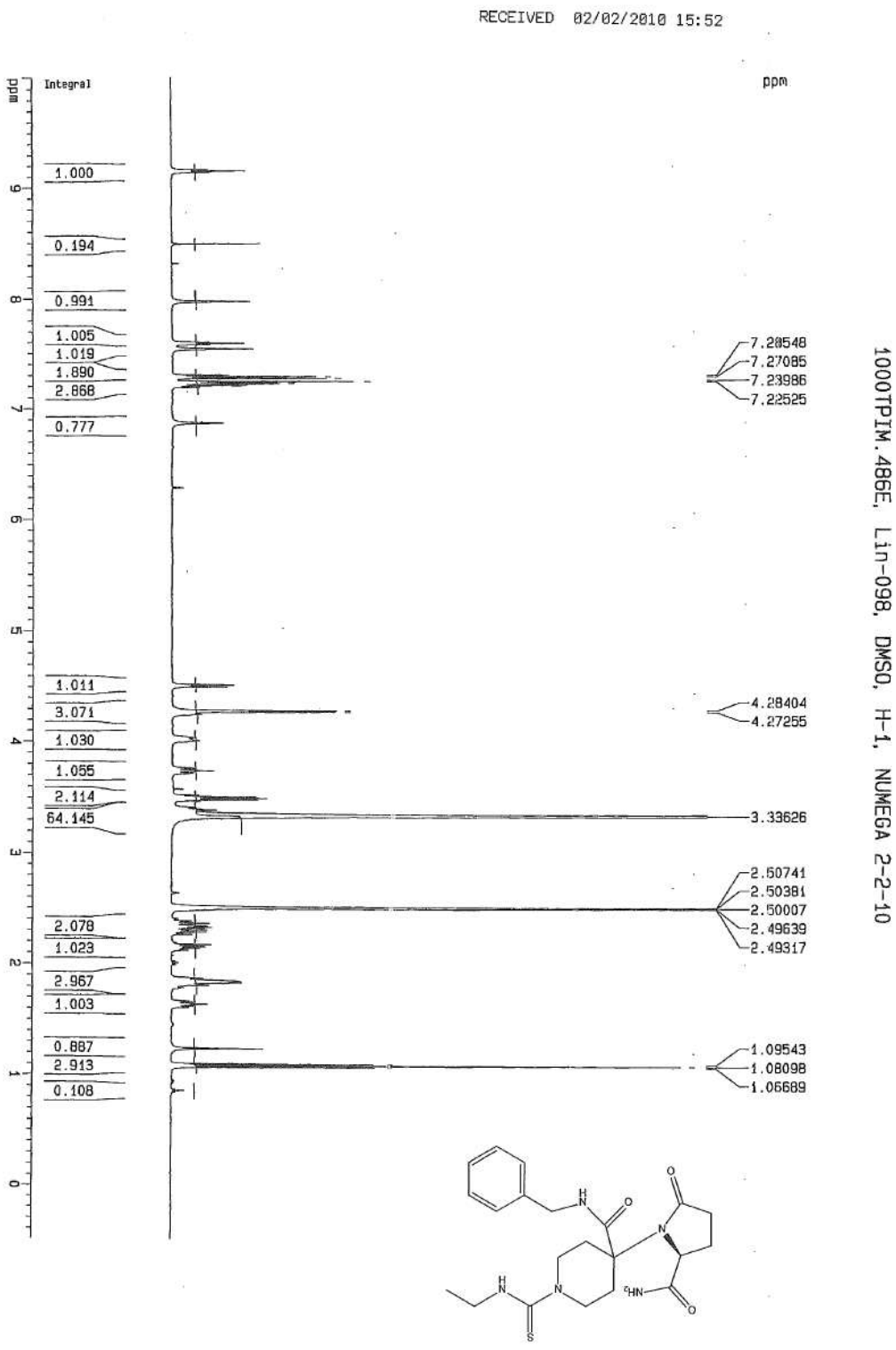


8 g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1.030
1.055
2.114
64.145
2.078
1.023
2.967
1.003
0.887
2.913
0.108
7.28548
7.27085
7.23986
7.22525
4.28404
4.27255
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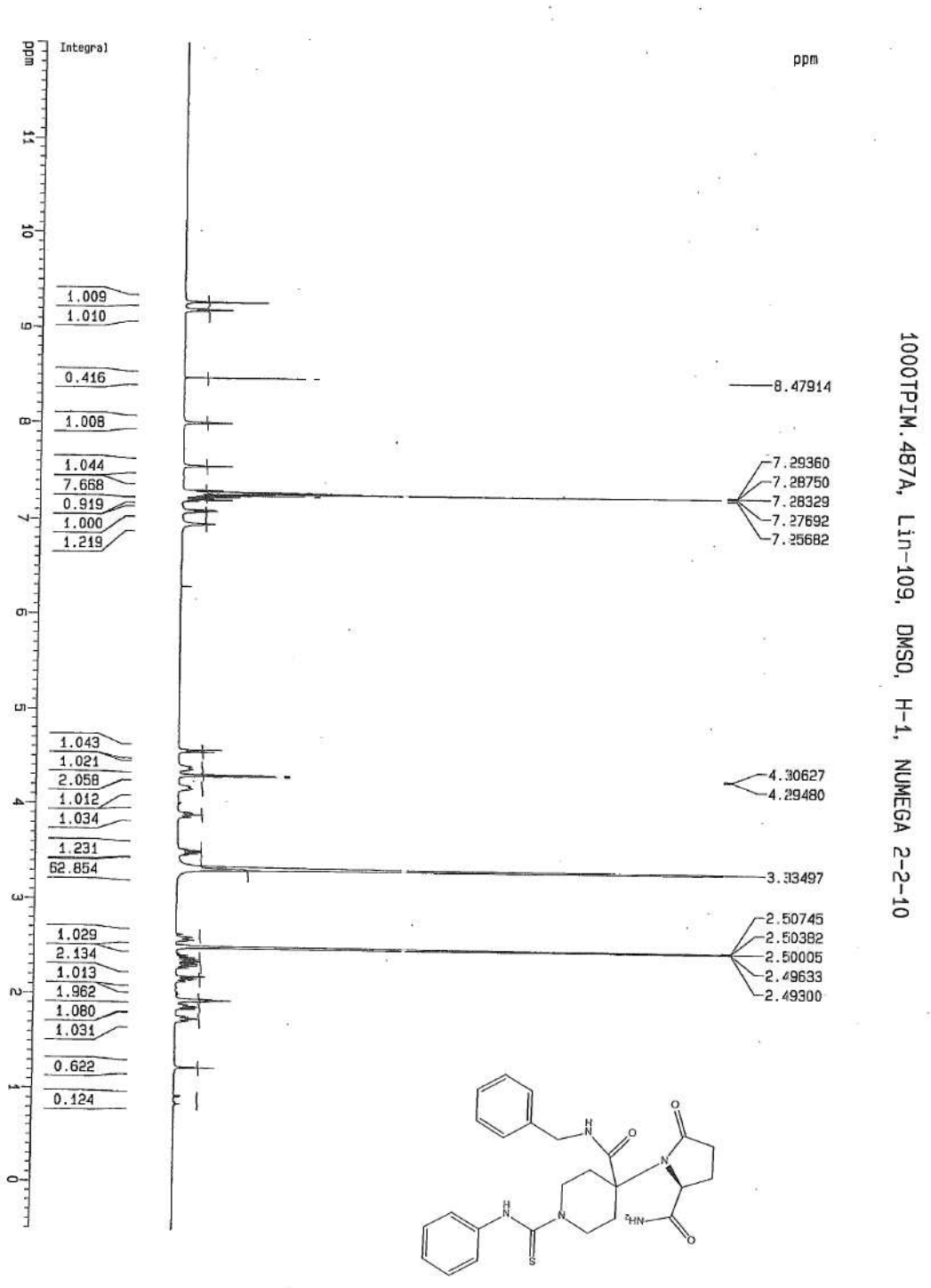
8 h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2.50005
2.49633
2.49300
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1.010
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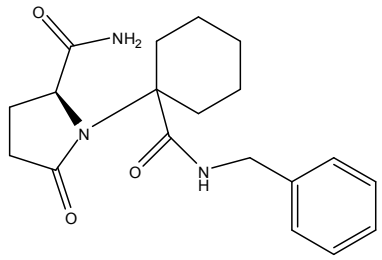
8 i



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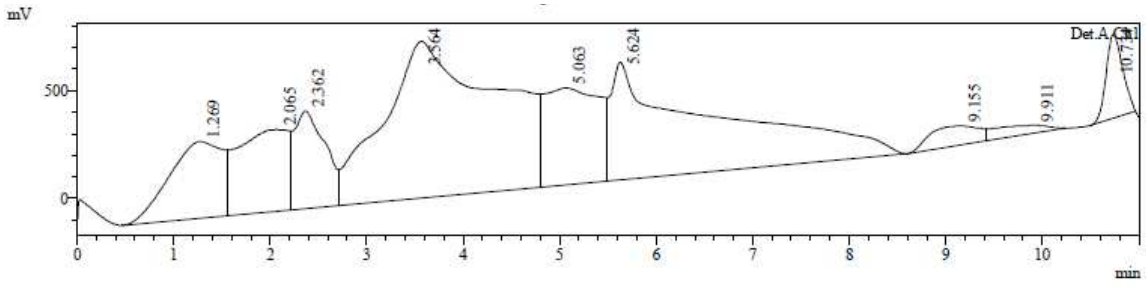
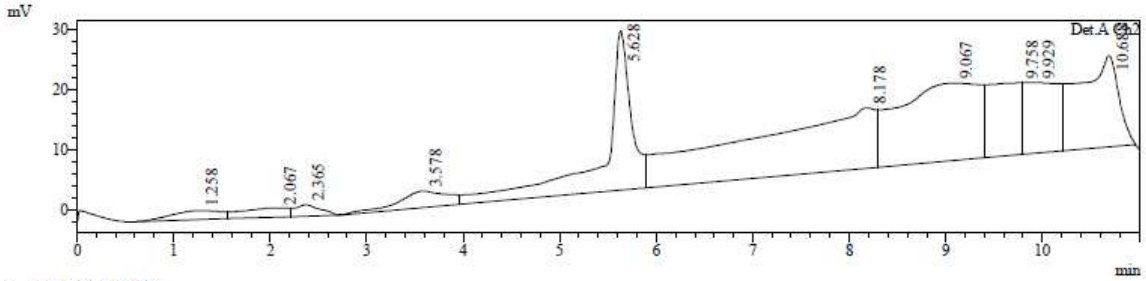
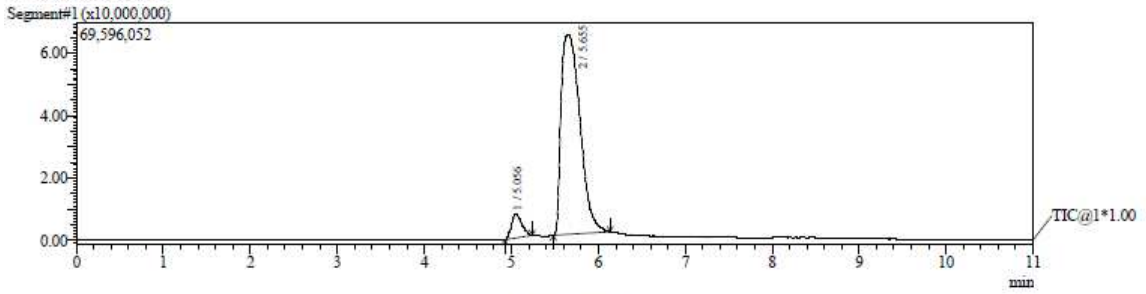


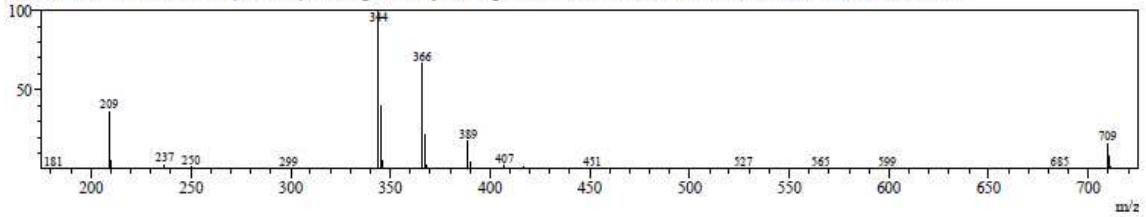


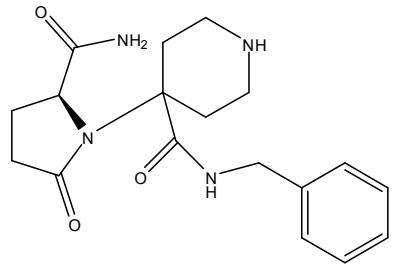
1 Det.A Ch1 / 214nm
2 Det.A Ch2 / 254nm



MS Spectrum Graph

Peak#:2 Ret.Time:Averaged 5.650-5.657(Scan#:1696-1698)
BG Mode:Calc 5.487<->6.140(1647<->1843)
Mass Peaks:77 Base Peak:344.15(19204780) MS Stage: Polarity:Pos Segment1 - Event1 Precursor: Cutoff Ionization Mode:$IonizationMode$





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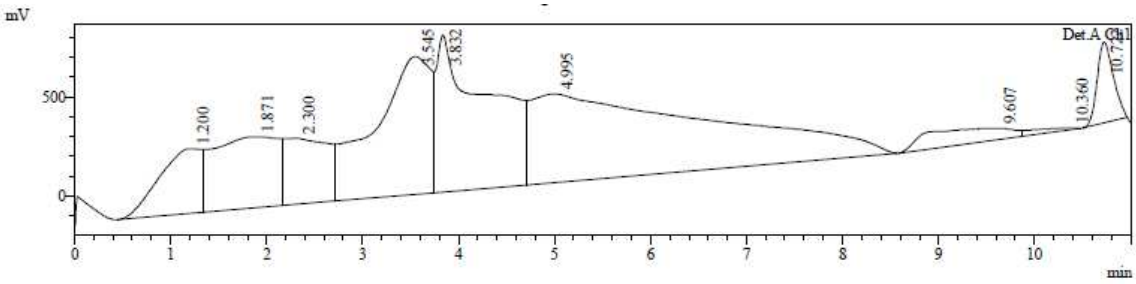
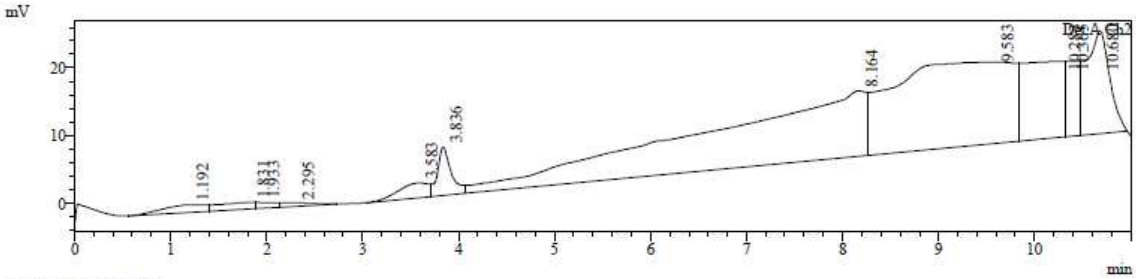
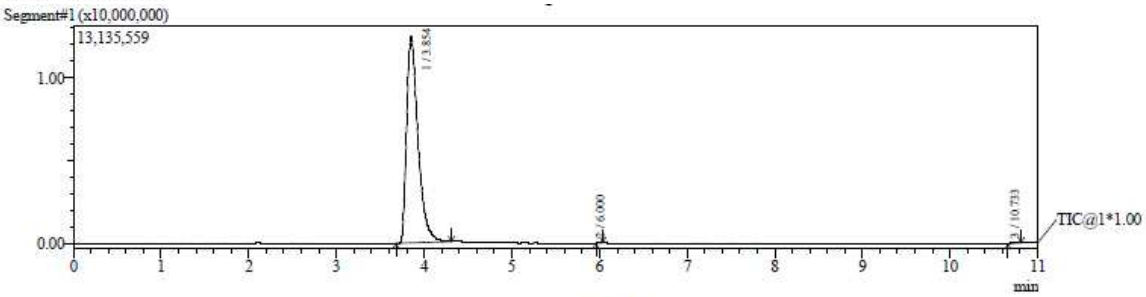


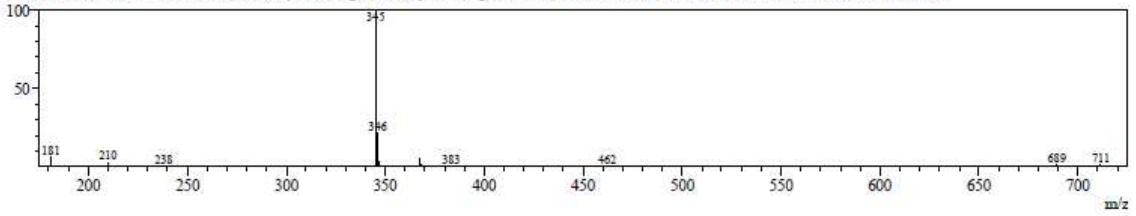


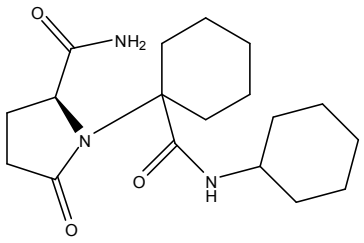
1 Det.A Ch1 / 214nm
2 Det.A Ch2 / 254nm



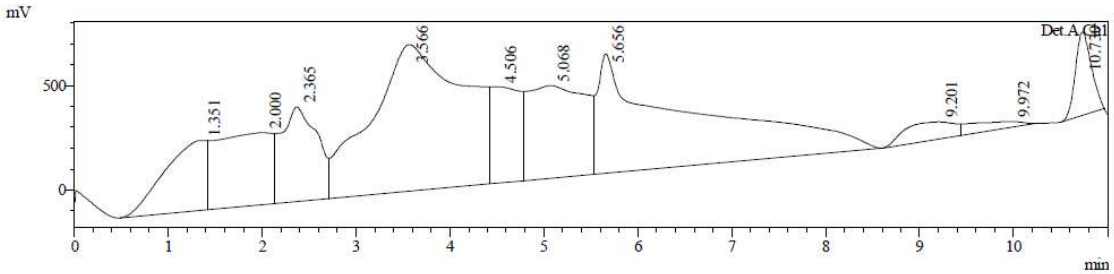
MS Spectrum Graph

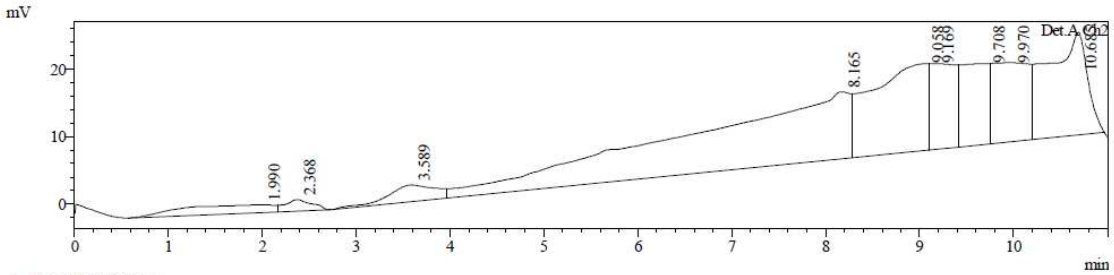
Peak#:1 Ret.Time:Averaged 3.850-3.857(Scan#:1156-1158)
BG Mode:Calc 3.680<->4.313(1105<->1295)
Mass Peaks:25 Base Peak:345.05(8993042) MS Stage: Polarity:Pos Segment1 - Event1 Precursor: Cutoff: Ionization Mode:$IonizationMode$



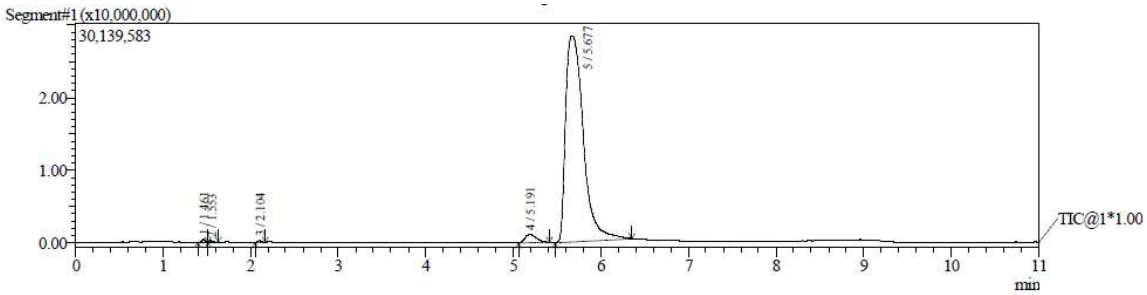


5 b



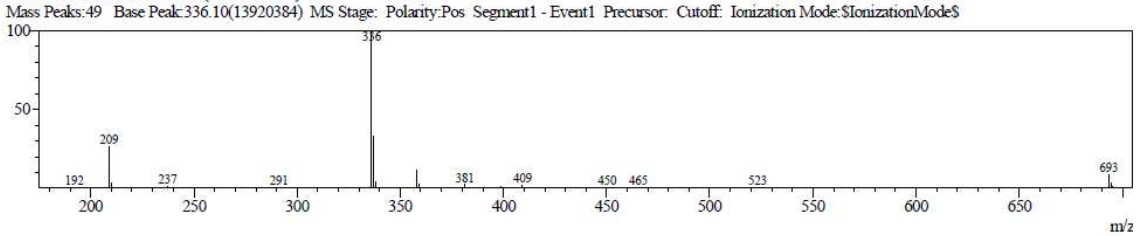


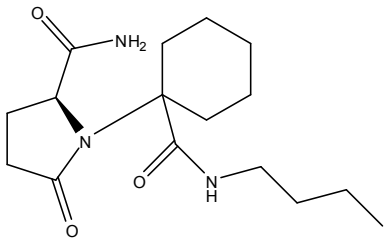
1 Det.A Ch1 / 214nm
2 Det.A Ch2 / 254nm



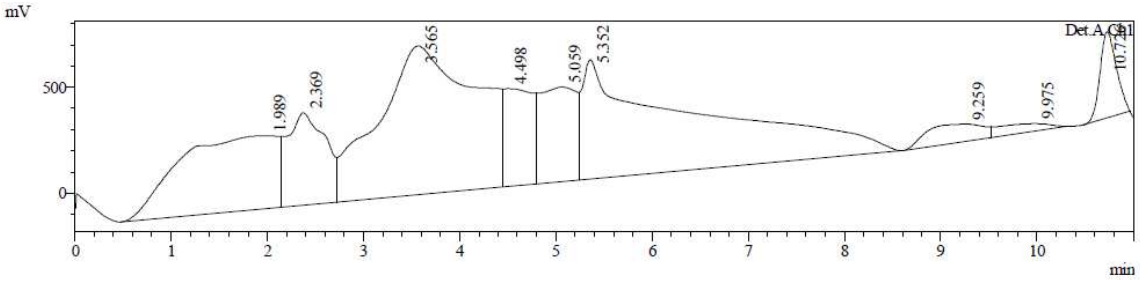
MS Spectrum Graph

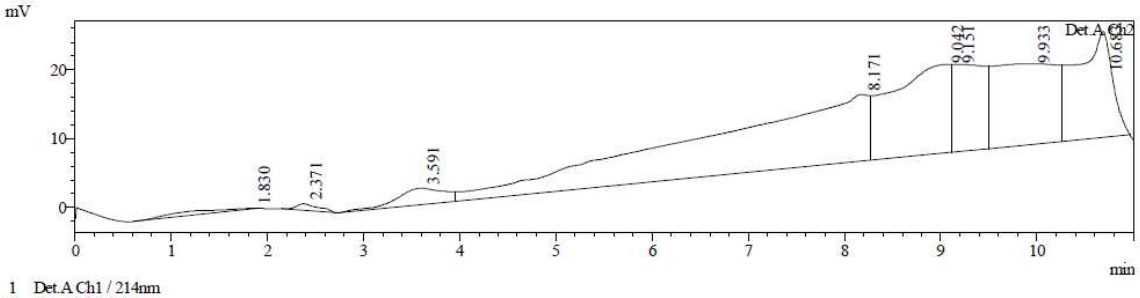
Peak#:5 Ret.Time:Averaged 5.673-5.680(Scan#:1703-1705)
BG Mode:Calc 5.480<->6.353(1645<>1907)
Mass Peaks:49 Base Peak:336.10(13920384) MS Stage: Polarity:Pos Segment1 - Event1 Precursor: Cutoff: Ionization Mode:$IonizationMode$



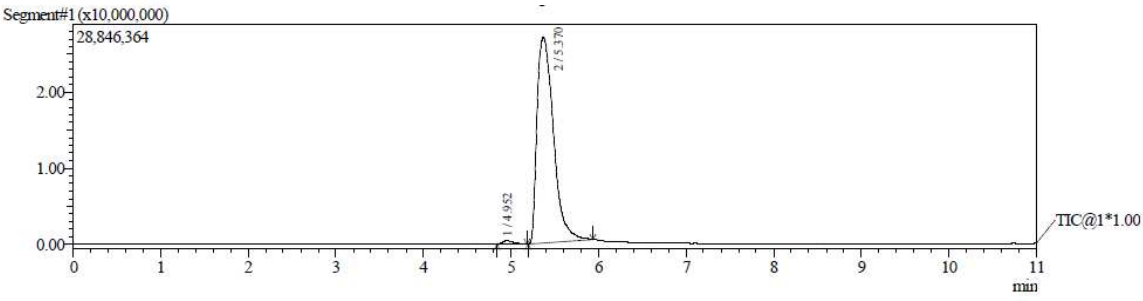


5 c



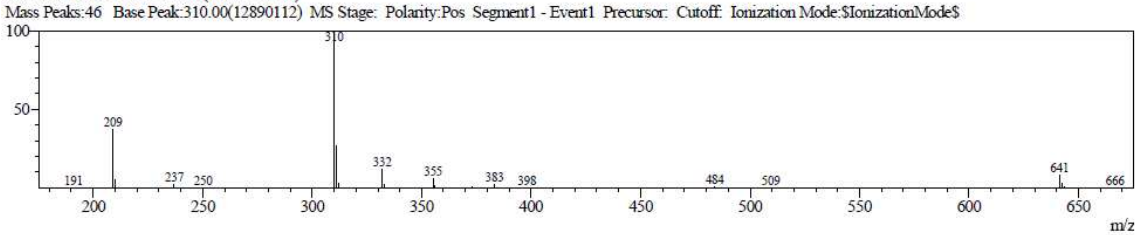


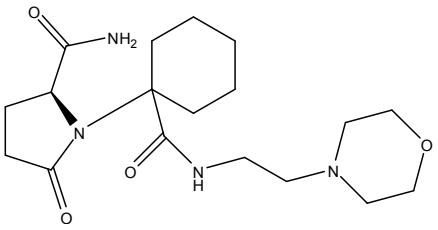
1 Det.A Ch1 / 214nm
2 Det.A Ch2 / 254nm



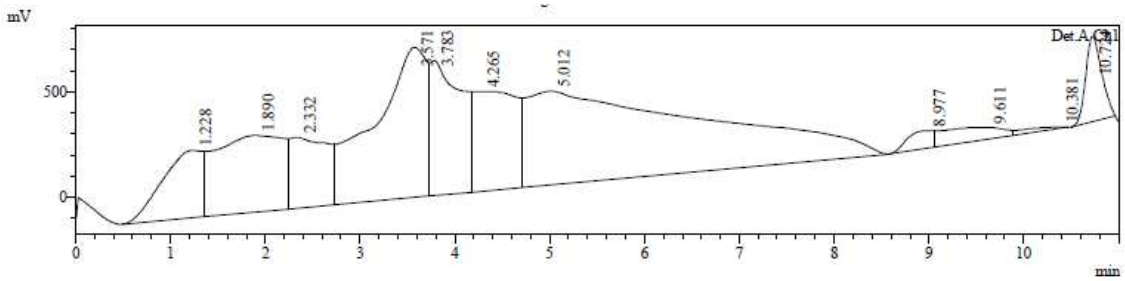
MS Spectrum Graph

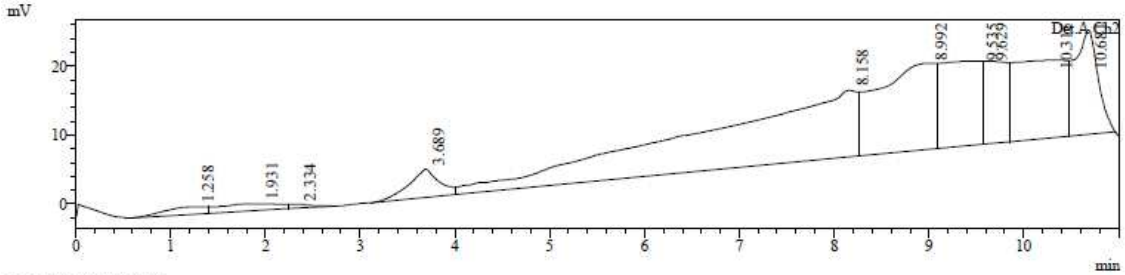
Peak#:2 Ret.Time:Averaged 5.367-5.373(Scan#:1611-1613)
BG Mode:Calc 5.193<->5.933(1559<>1781)
Mass Peaks:46 Base Peak:310.00(12890112) MS Stage: Polarity:Pos Segment1 - Event1 Precursor: Cutoff: Ionization Mode:$IonizationMode$



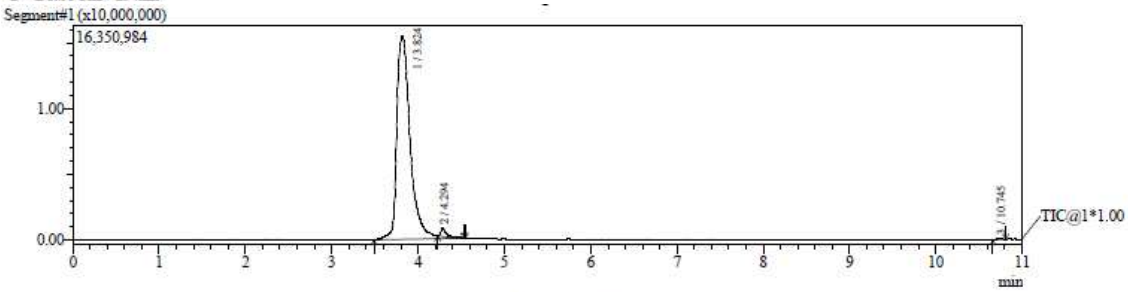


5 d



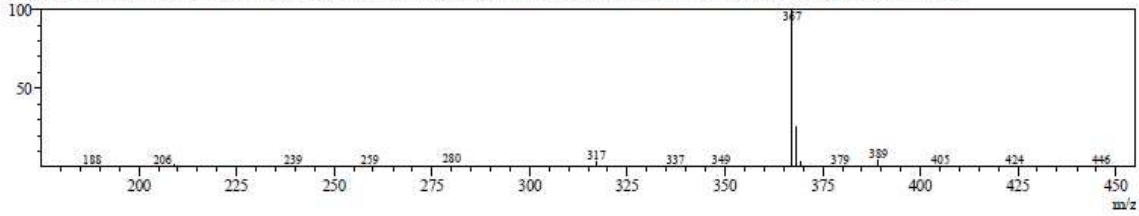


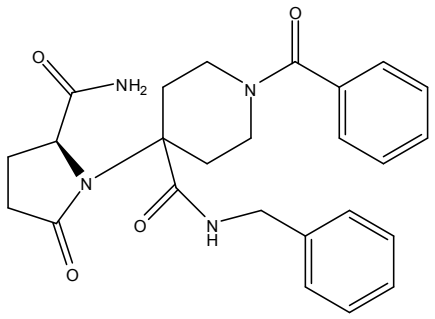
1 Det.A Ch1 / 214nm
2 Det.A Ch2 / 254nm



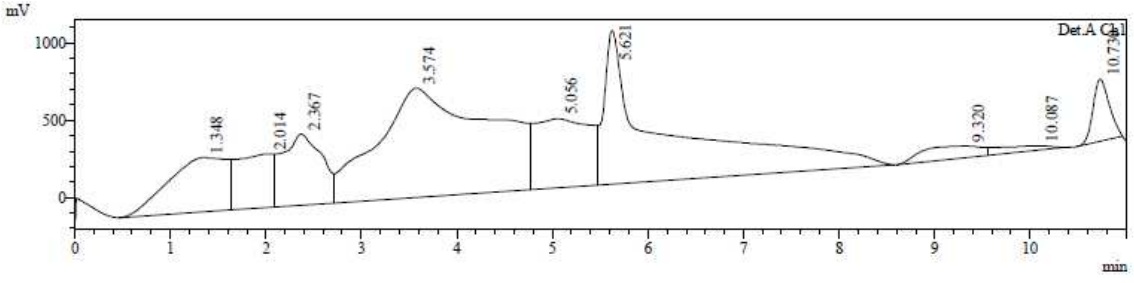
MS Spectrum Graph

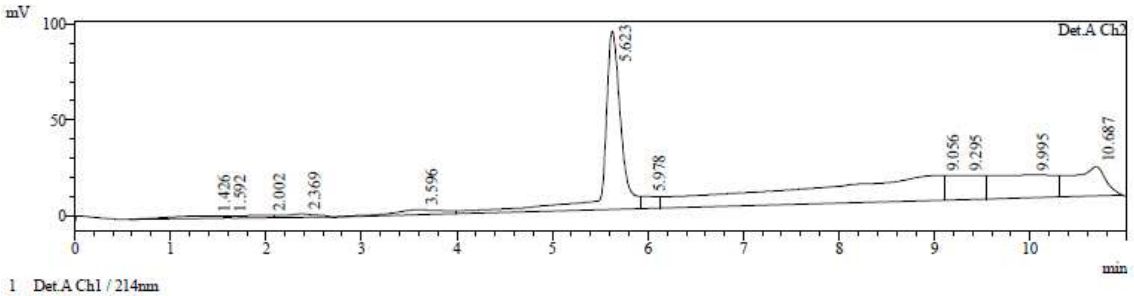
Peak#:1 Ret.Time:Averaged 3.820-3.827(Scan#:1147-1149)
BG Mode:Calc 3.487<->4.547(1047<->1365)
Mass Peaks:26 Base Peak:367.10(11167229) MS Stage: Polarity:Pos Segment1 - Event1 Precursor: Cutoff: Ionization Mode:$IonizationMode$



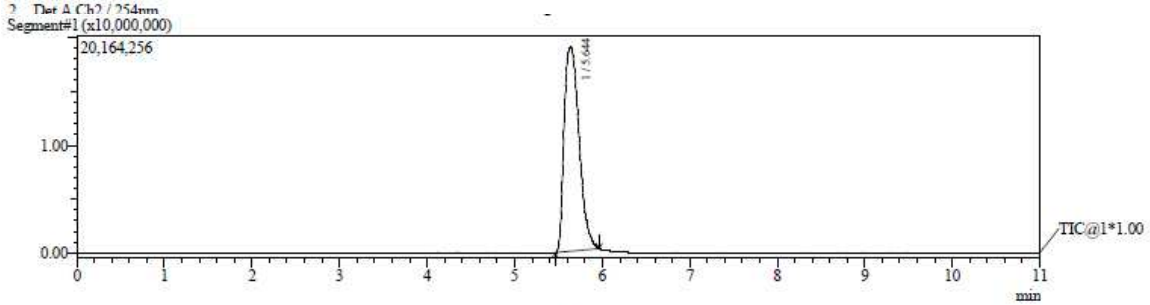


8 a



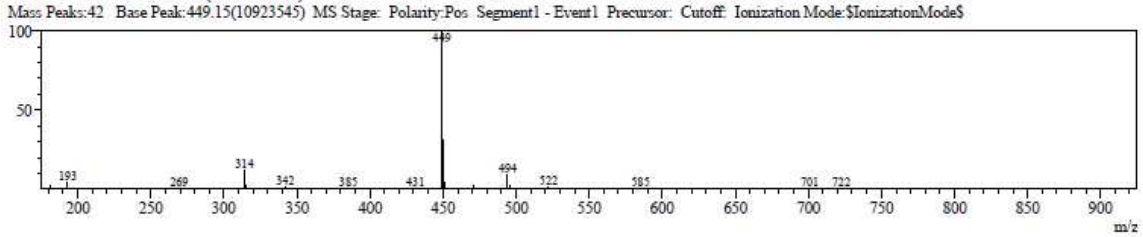


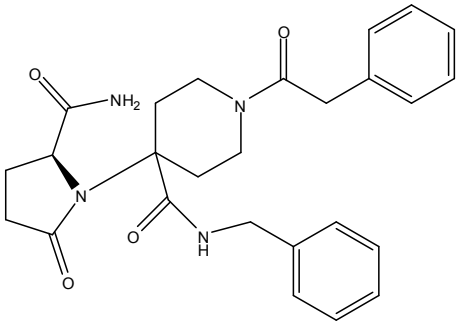
1 Det.A Ch1 / 214nm



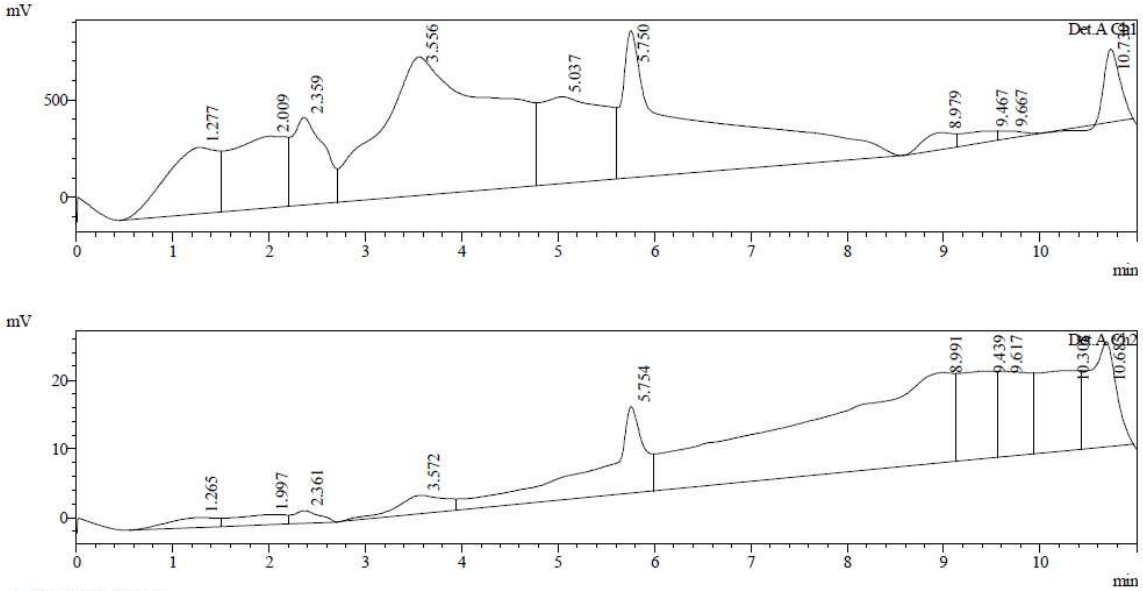
MS Spectrum Graph

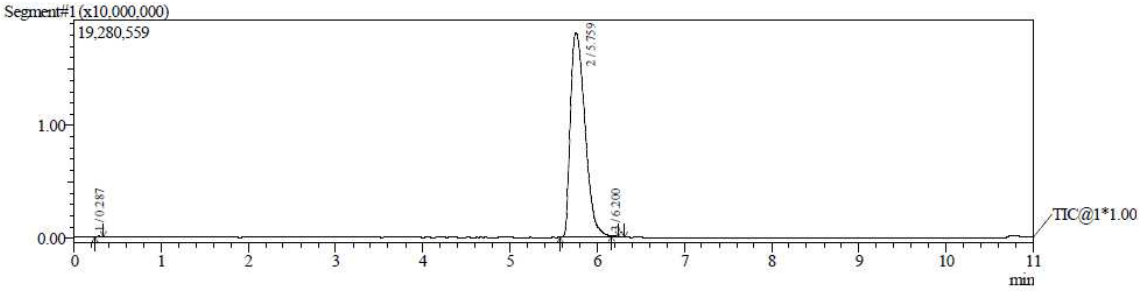
Peak#:1 Ret.Time:Averaged 5.640-5.647(Scan#:1693-1695)
BG Mode:Calc 5.467<->5.967(1641<->1791)
Mass Peaks:42 Base Peak:449.15(10923545) MS Stage: Polarity:Pos Segment1 - Event1 Precursor: Cutoff: Ionization Mode:$IonizationMode$





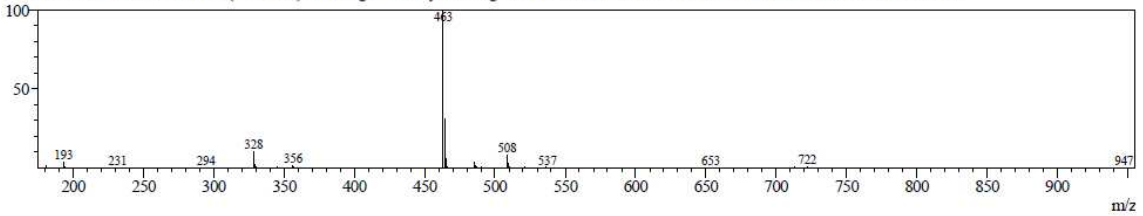
8 b

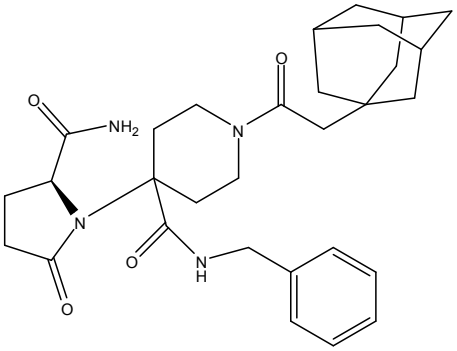




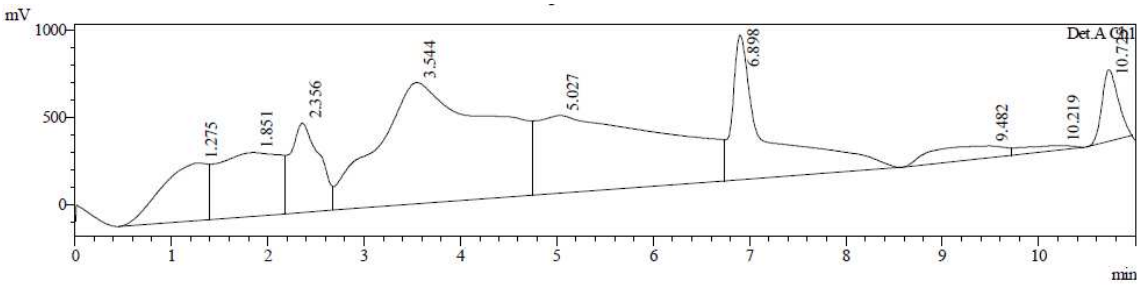
MS Spectrum Graph

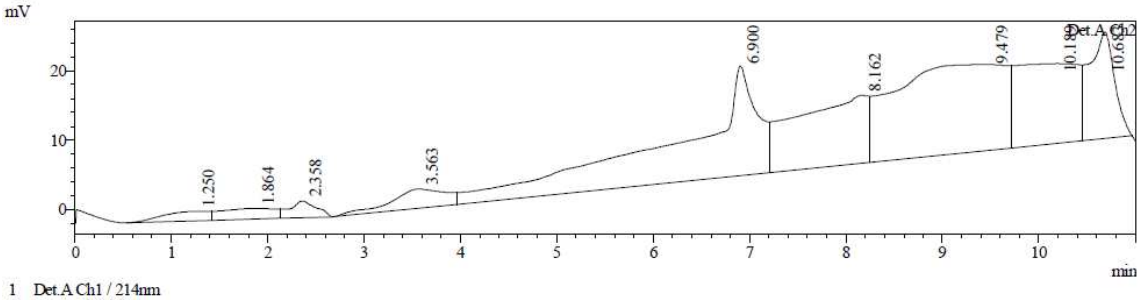
Peak#:2 Ret.Time:Averaged 5.757-5.763(Scan#:1728-1730)
BG Mode:Calc 5.573<->6.313(1673<->1895)
Mass Peaks:51 Base Peak:463.20(10202180) MS Stage: Polarity:Pos Segment1 - Event1 Precursor: Cutoff: Ionization Mode:$IonizationMode$



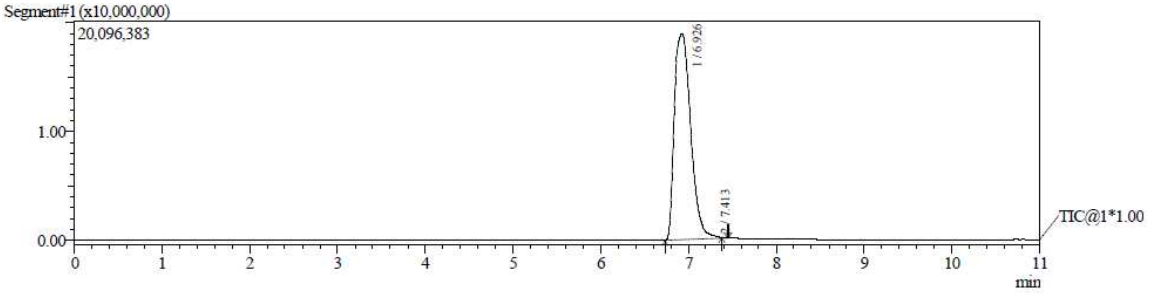


8 c



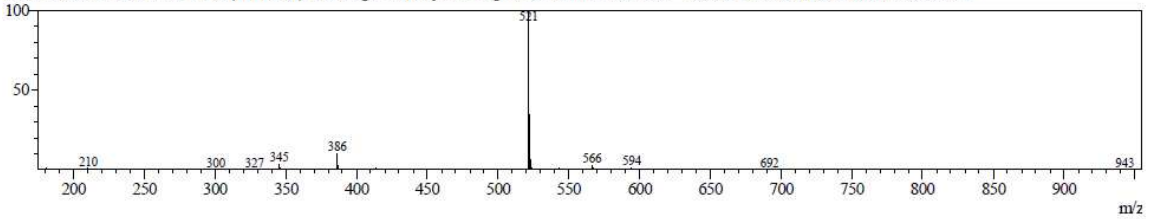


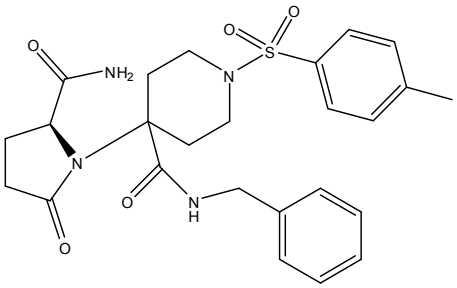
1 Det.A Ch1 / 214nm
2 Det.A Ch2 / 254nm



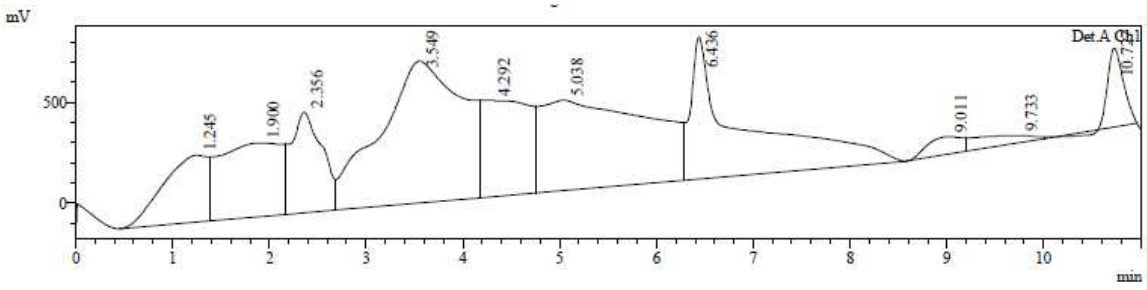
MS Spectrum Graph

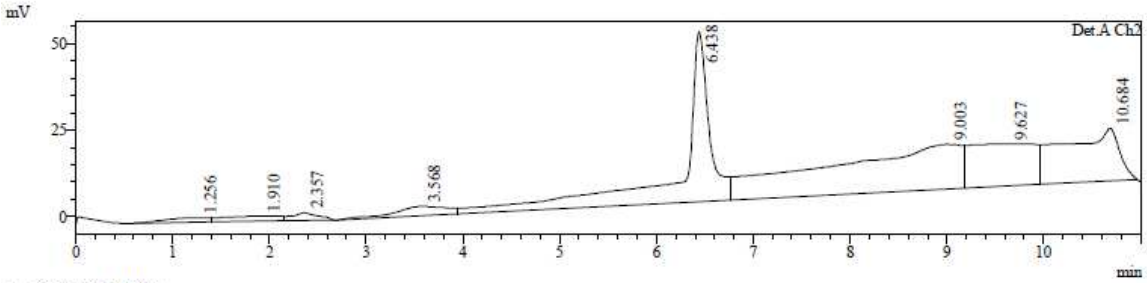
Peak#:1 Ret.Time:Averaged 6.923-6.930(Scan#:2078-2080)
BG Mode:Calc 6.733<->7.460(2021<>2239)
Mass Peaks:41 Base Peak:521.25(11140561) MS Stage: Polarity:Pos Segment1 - Event1 Precursor: Cutoff: Ionization Mode:$IonizationMode$



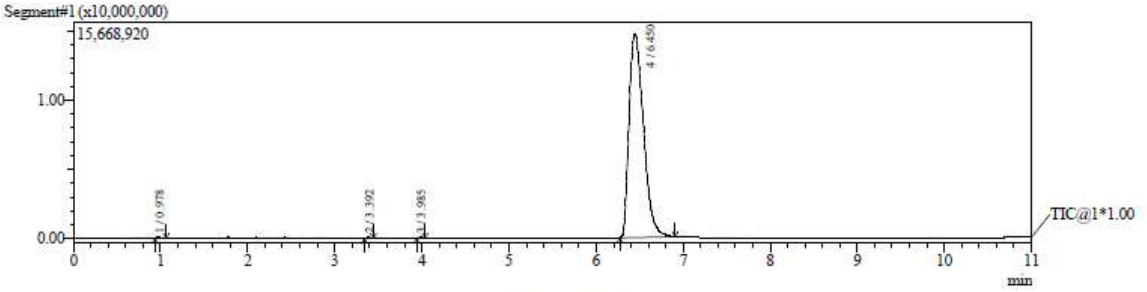


8 d



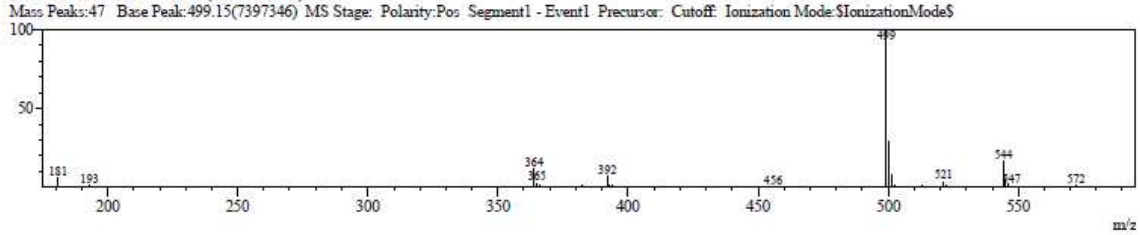


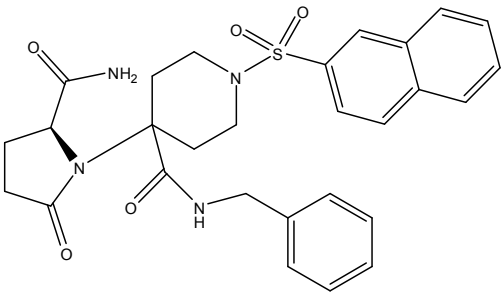
1 Det.A Ch1 / 214nm
2 Det.A Ch2 / 254nm



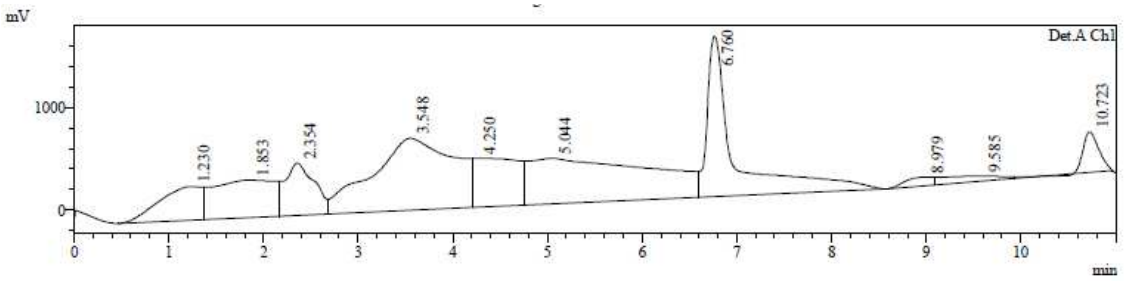
MS Spectrum Graph

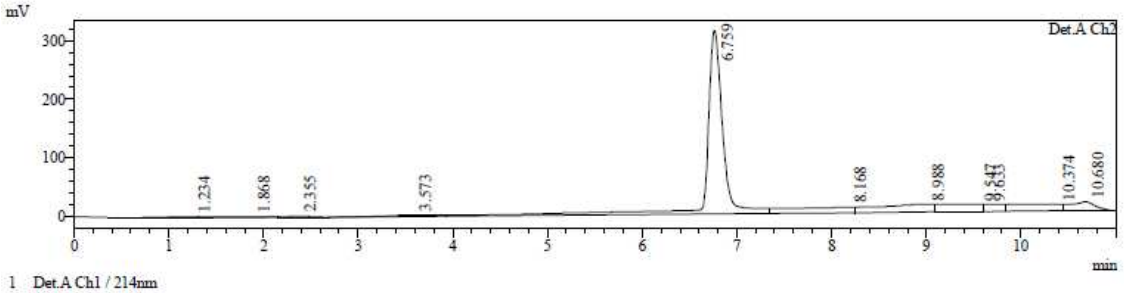
Peak#:4 Ret.Time:Averaged 6.447-6.453(Scan#:1935-1937)
BG Mode:Calc 6.273<->6.907(1883<->2073)
Mass Peaks:47 Base Peak:499.15(7397346) MS Stage: Polarity:Pos Segment1 - Event1 Precursor: Cutoff: Ionization Mode:$IonizationMode$



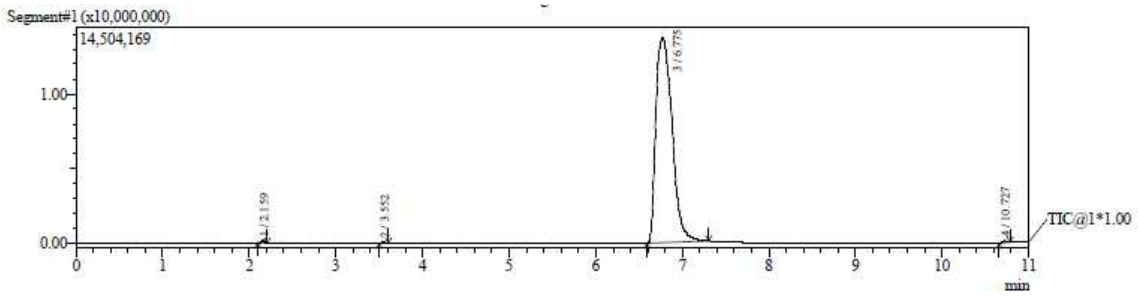


8 e



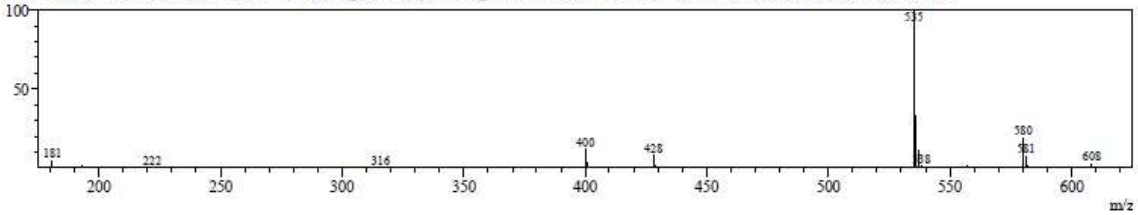


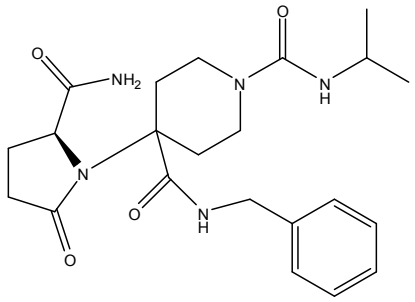
1 Det.A Ch1 / 214nm
2 Det.A Ch2 / 254nm



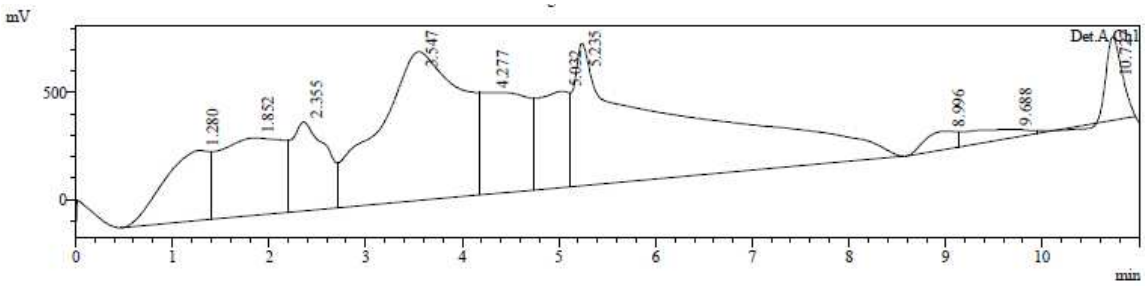
MS Spectrum Graph

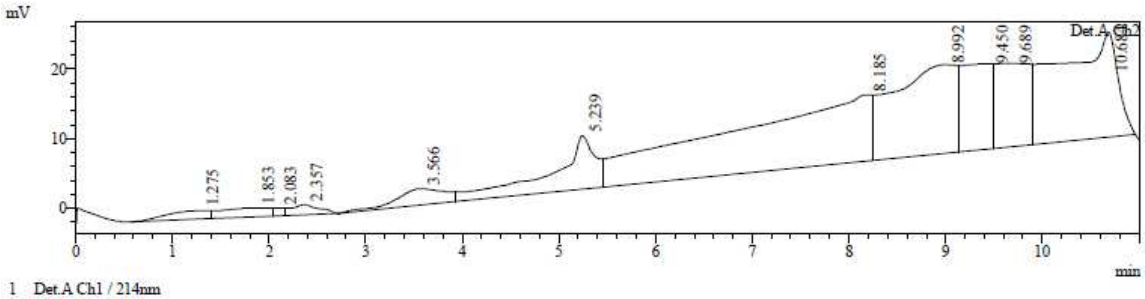
Peak#:3 Ret.Time:Averaged 6.773-6.780(Scan#:2033-2035)
BG Mode:Calc 6.593<->7.307(1979<->2193)
Mass Peaks:35 Base Peak:535.15(6419332) MS Stage: Polarity:Pos Segment1 - Event1 Precursor: Cutoff: Ionization Mode:$IonizationMode$



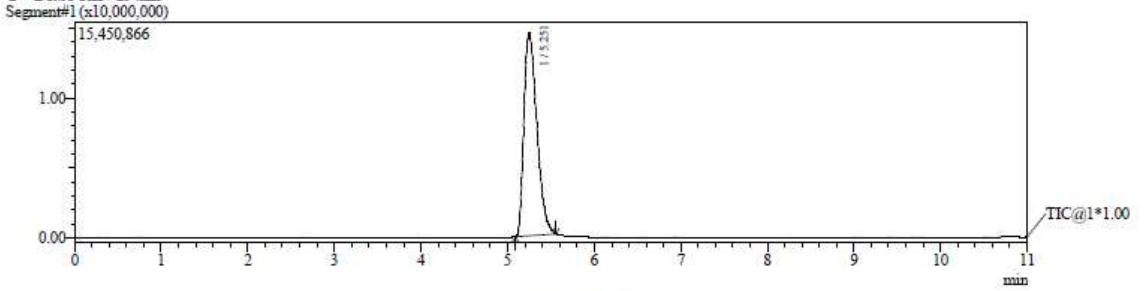


8 f



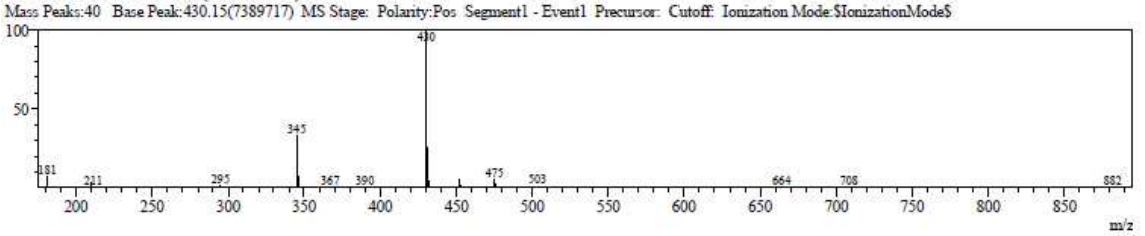


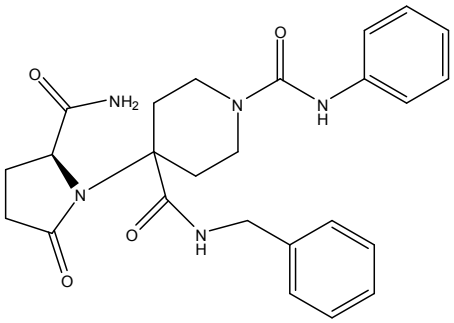
1 Det.A Ch1 / 214nm
2 Det.A Ch2 / 254nm



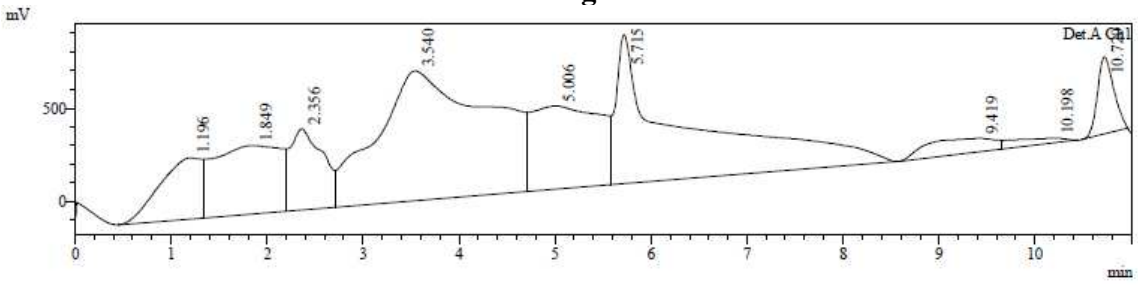
MS Spectrum Graph

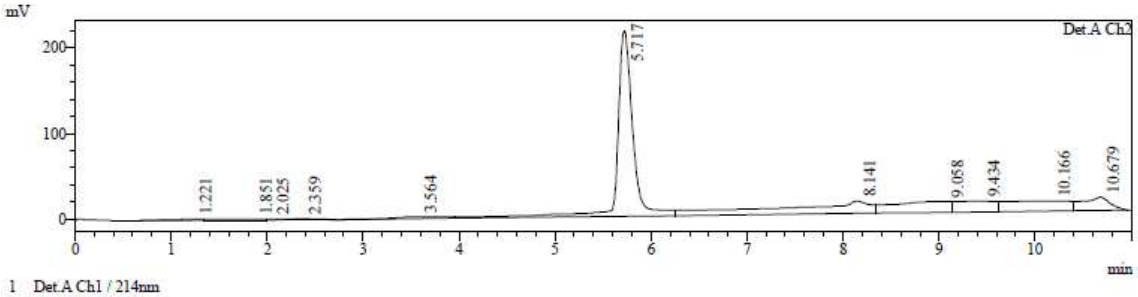
Peak#:1 Ret.Time:Averaged 5.247-5.253(Scan#:1575-1577)
BG Mode:Calc 5.093<->5.560(1529<->1669)
Mass Peaks:40 Base Peak:430.15(7389717) MS Stage: Polarity:Pos Segment1 - Event1 Precursor: Cutoff: Ionization Mode:$IonizationMode$



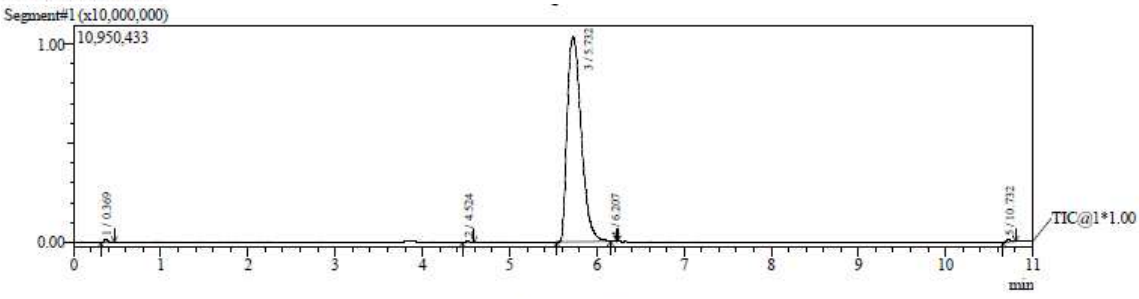


8 g



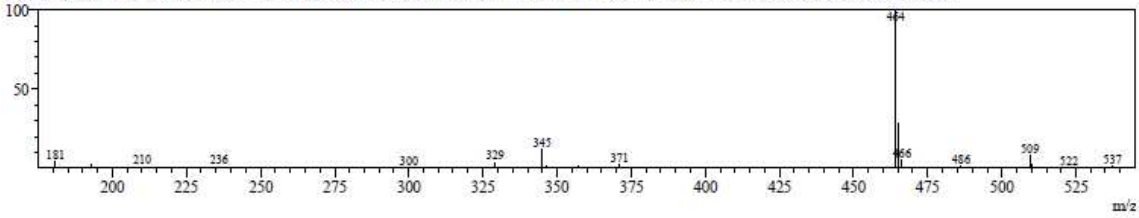


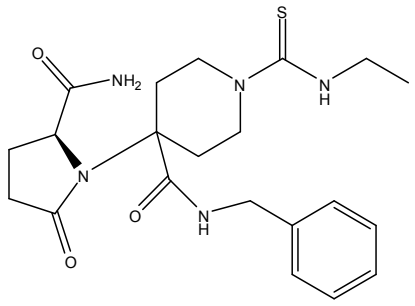
1 Det.A Ch1 / 214nm
2 Det.A Ch2 / 254nm



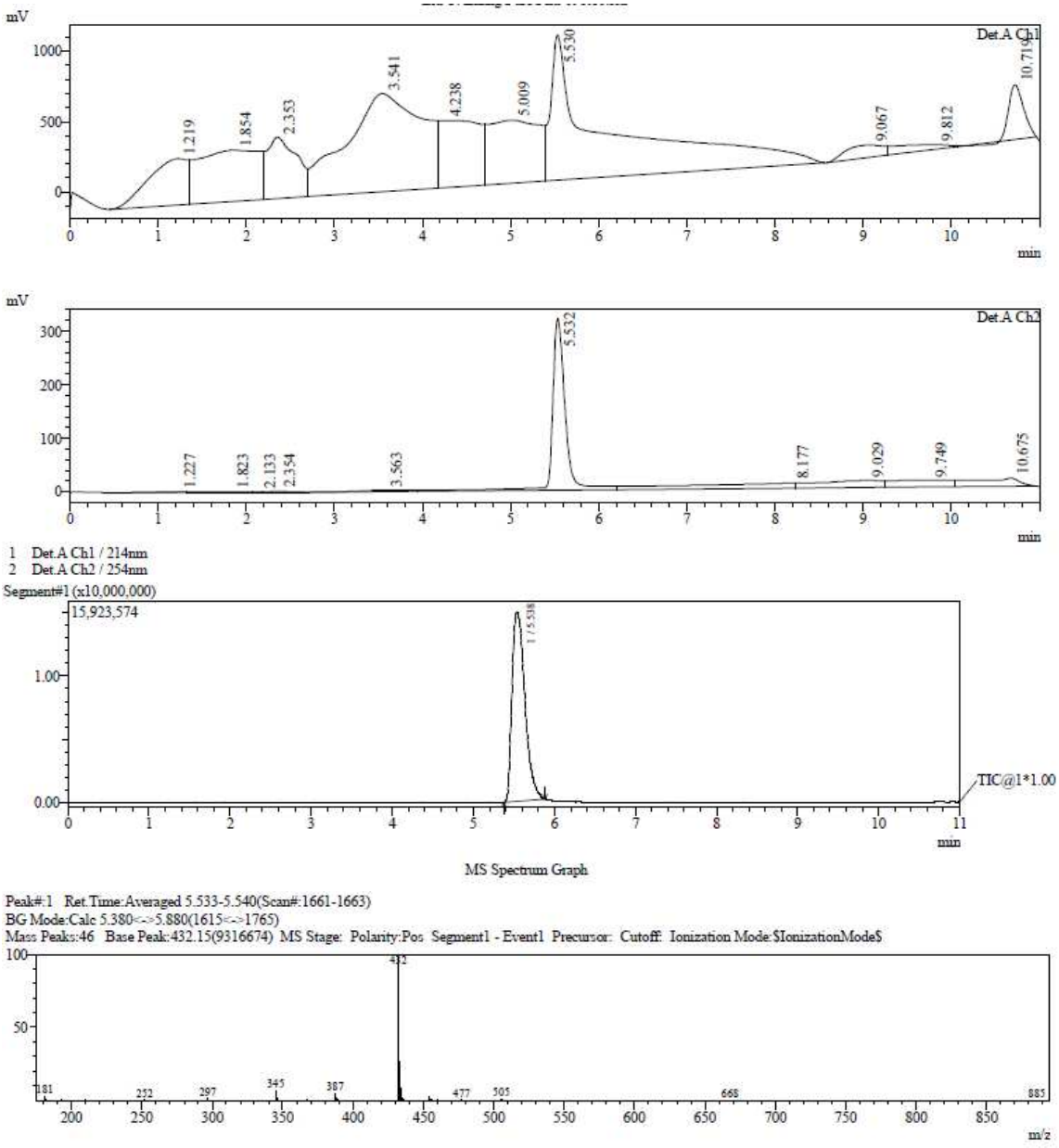
MS Spectrum Graph

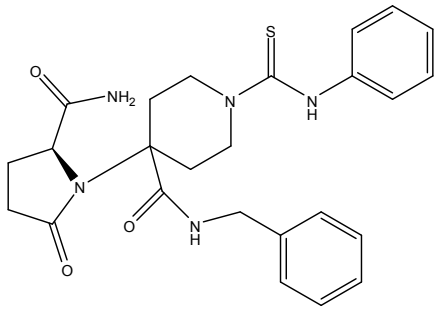
Peak#:3 Ret.Time:Averaged 5.727-5.733(Scan#:1719-1721)
BG Mode:Calc 5.540<->6.240(1663<->1873)
Mass Peaks:38 Base Peak:464.15(5725162) MS Stage: Polarity:Pos Segment1 - Event1 Precursor: Cutoff: Ionization Mode:$IonizationMode$



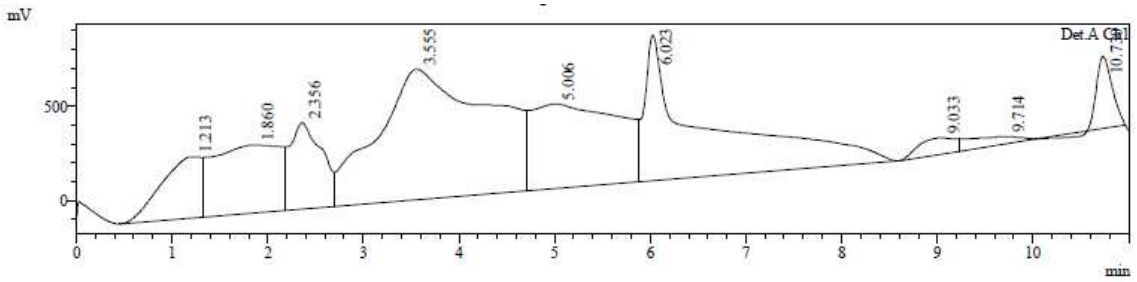


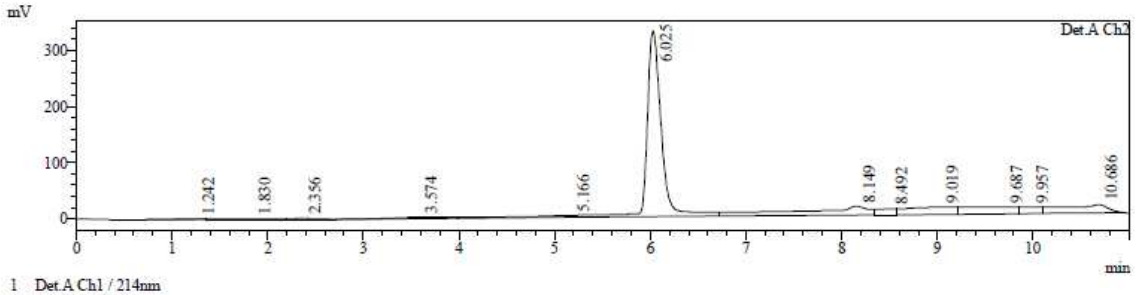
8 h


mV
Det.A Ch1
1.219
1.854
2.353
3.541
4.238
5.009
5.530
9.067
9.812
10.715
min
mV
Det.A Ch2
1.227
1.823
2.133
2.354
3.563
5.532
8.177
9.029
9.749
10.675
min
1 Det.A Ch1 / 214nm
2 Det.A Ch2 / 254nm
Segment#1 (x10,000,000)
15,923,574
TIC@1*1.00
min
MS Spectrum Graph
Peak#:1 Ret.Time:Averaged 5.533-5.540(Scan#:1661-1663)
BG Mode:Calc 5.380<->5.880(1615<->1765)
Mass Peaks:46 Base Peak:432.15(9316674) MS Stage: Polarity:Pos Segment1 - Event1 Precursor: Cutoff: Ionization Mode:$IonizationMode$
432
181
252
297
345
387
477
505
668
885
m/z

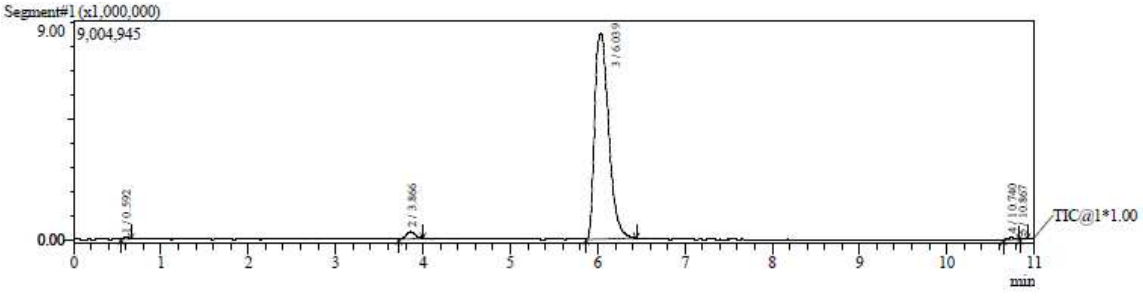


8 i





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



Peak#:3 Ret.Time:Averaged 6.037-6.043(Scan#:1812-1814)
BG Mode:Calc 5.867<->6.447(1761<->1935)
Mass Peaks:30 Base Peak:480.15(5127444) MS Stage: Polarity:Pos Segment1 - Event1 Precursor: Cutoff: Ionization Mode:$IonizationMode$