Electronic Supplementary Material (ESI) for Organic and Biomolecular Chemistry
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Asymmetric Synthesis of *α, β*-Diamino acid Derivates via Mannich-type Reaction of Chiral Ni (II) Complex of Glycine with *N*-Tolsyl Imines

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Electrionic Supplementary Information

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Supplementary Material (ESI) for Organic and Biomolecular Chemistry
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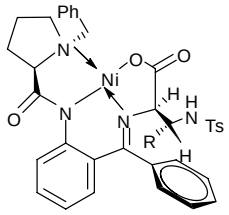
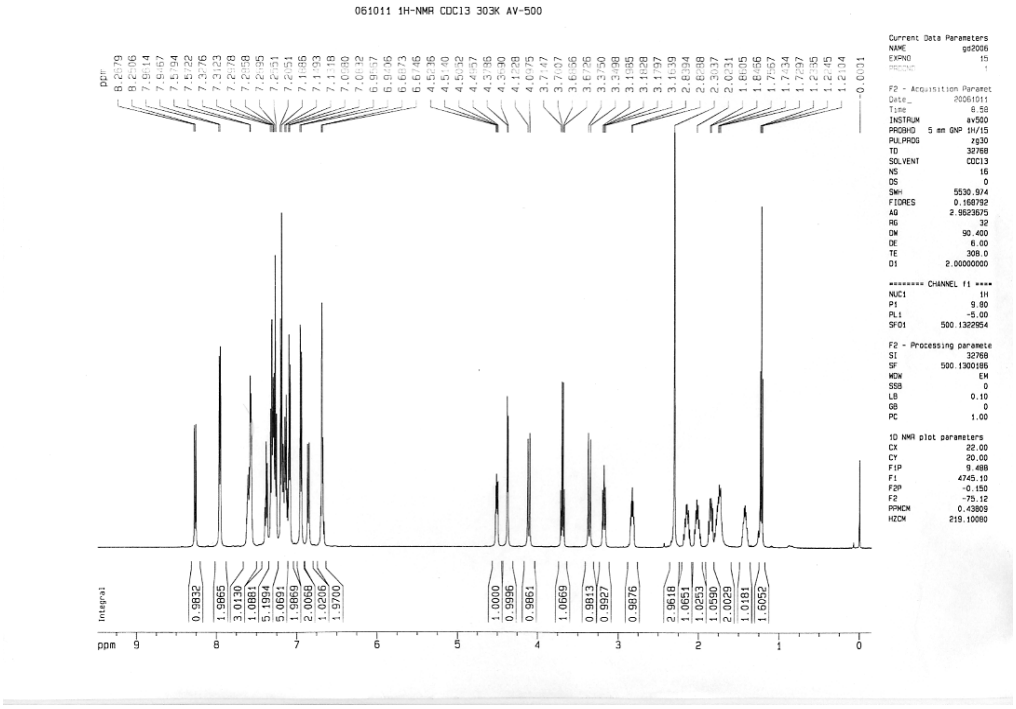
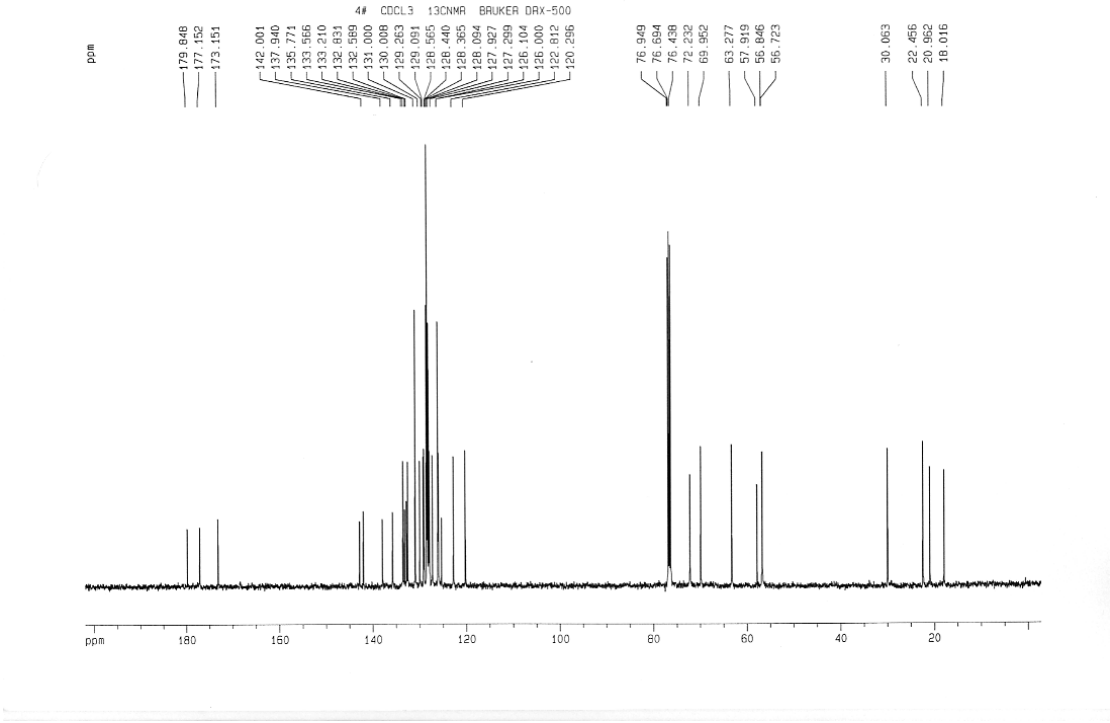
1. ^{1}H NMR, ^{13}C NMR and Mass spectras of **3a**, **3b**, **3c**, **3d**, **3e** , **3f and 3g**



R= Ph, (*R*,*R*,*S*)-3a





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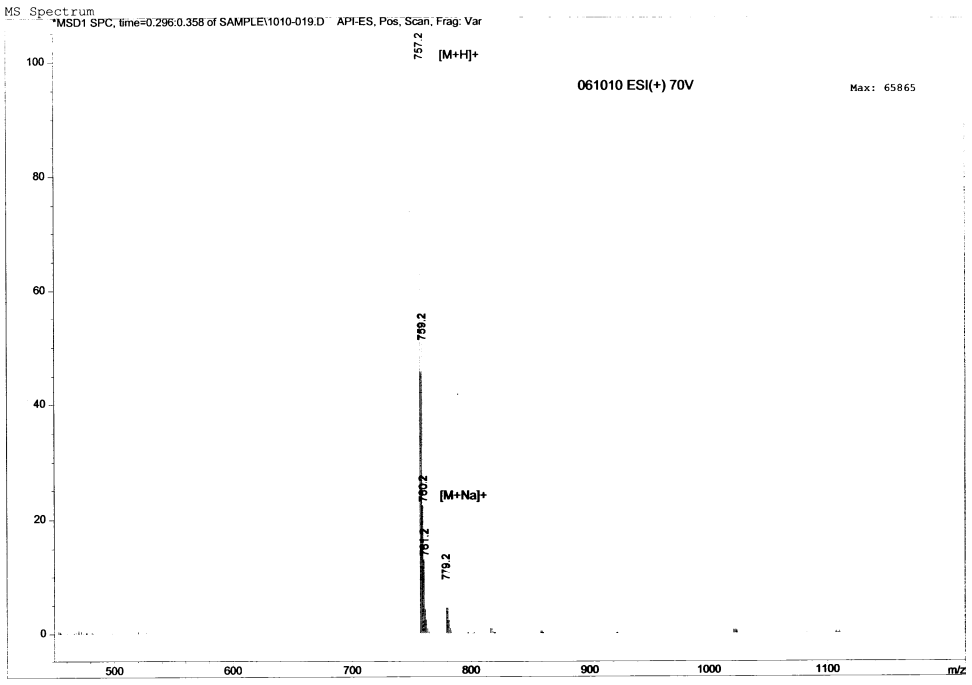

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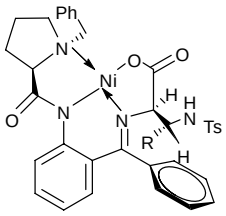

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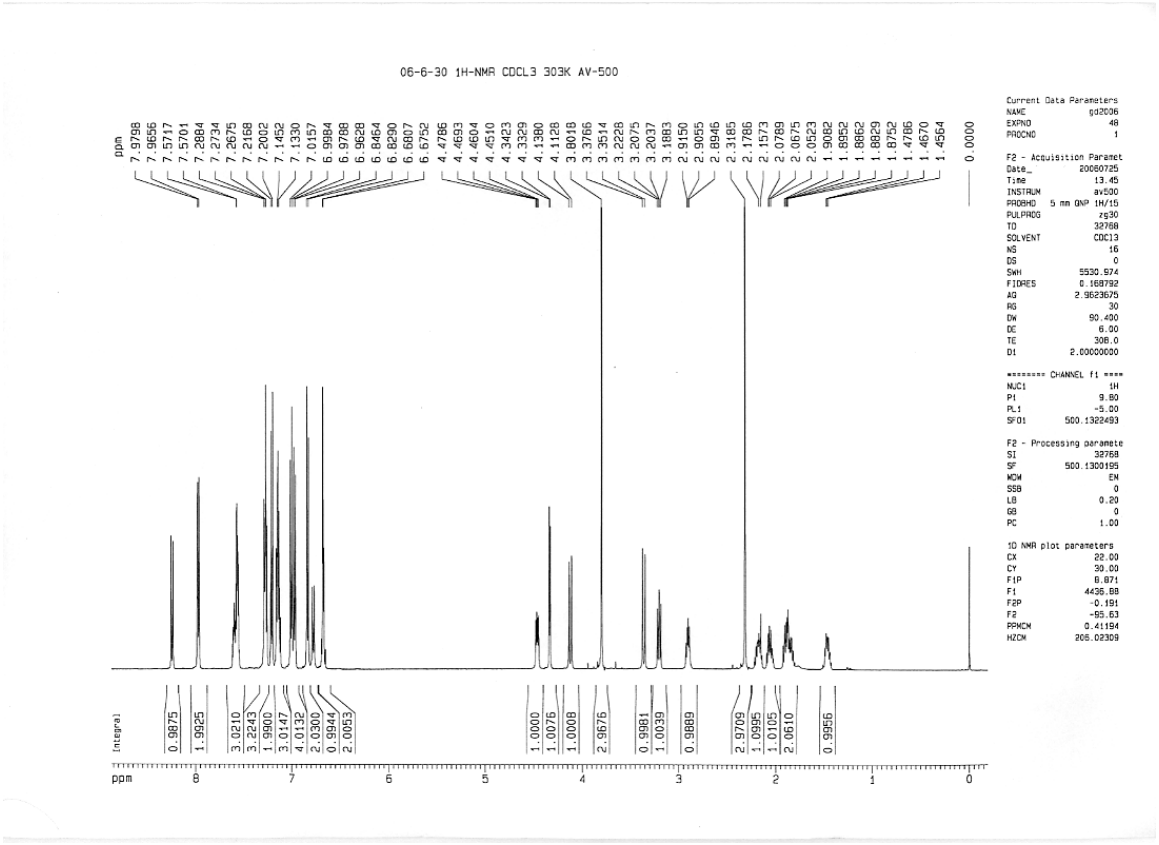

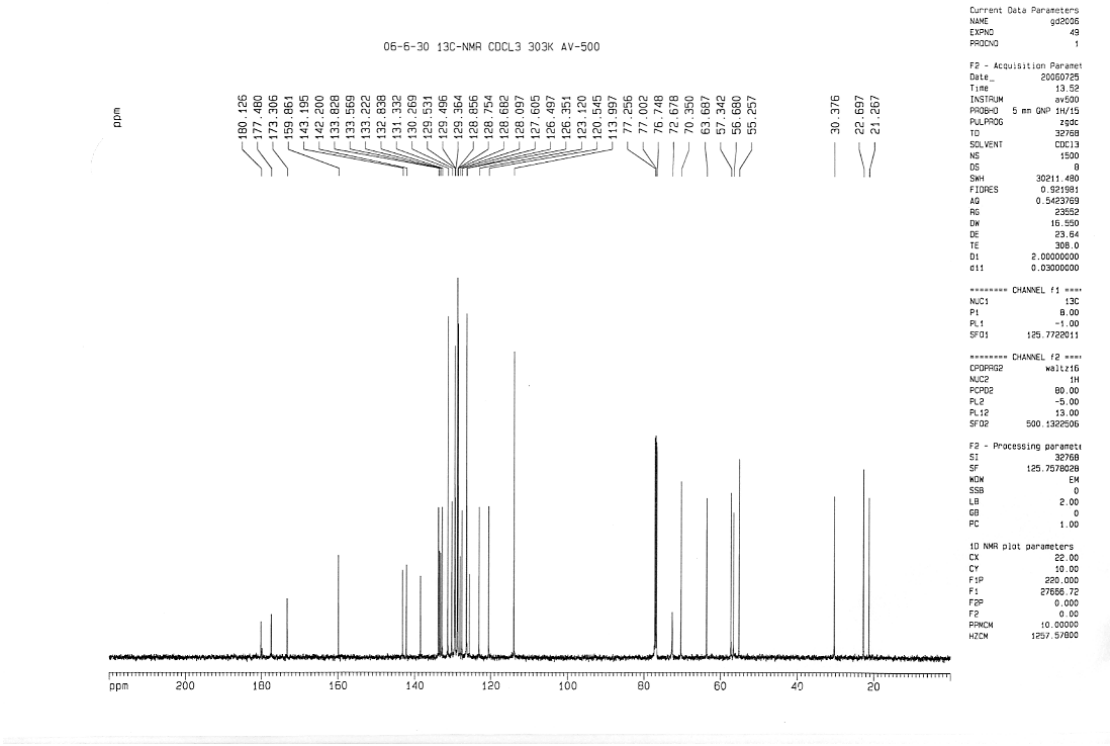

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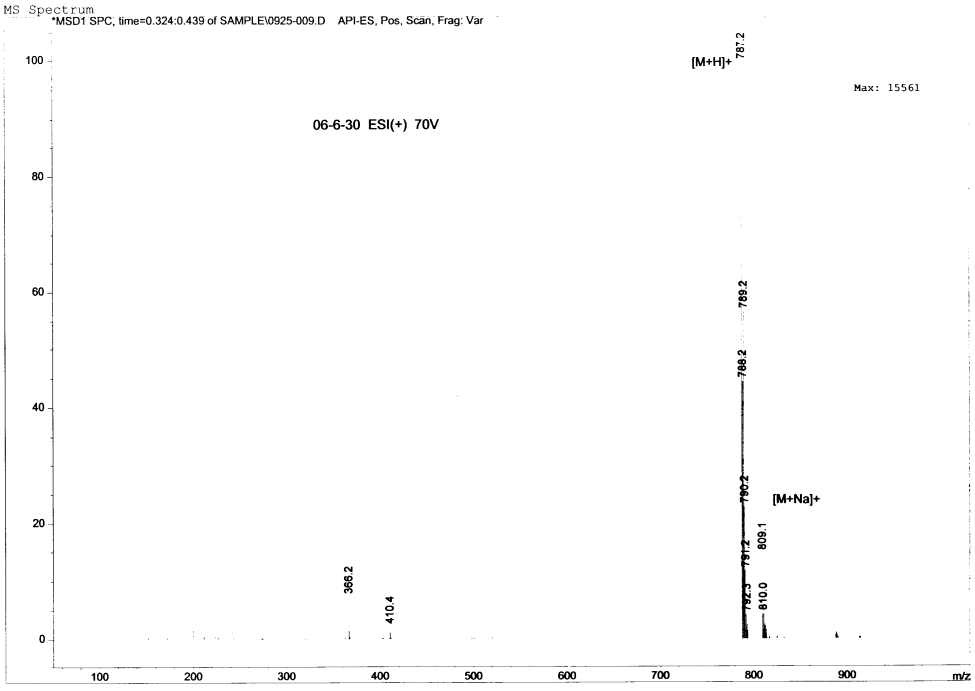

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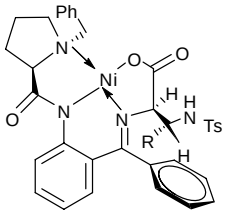

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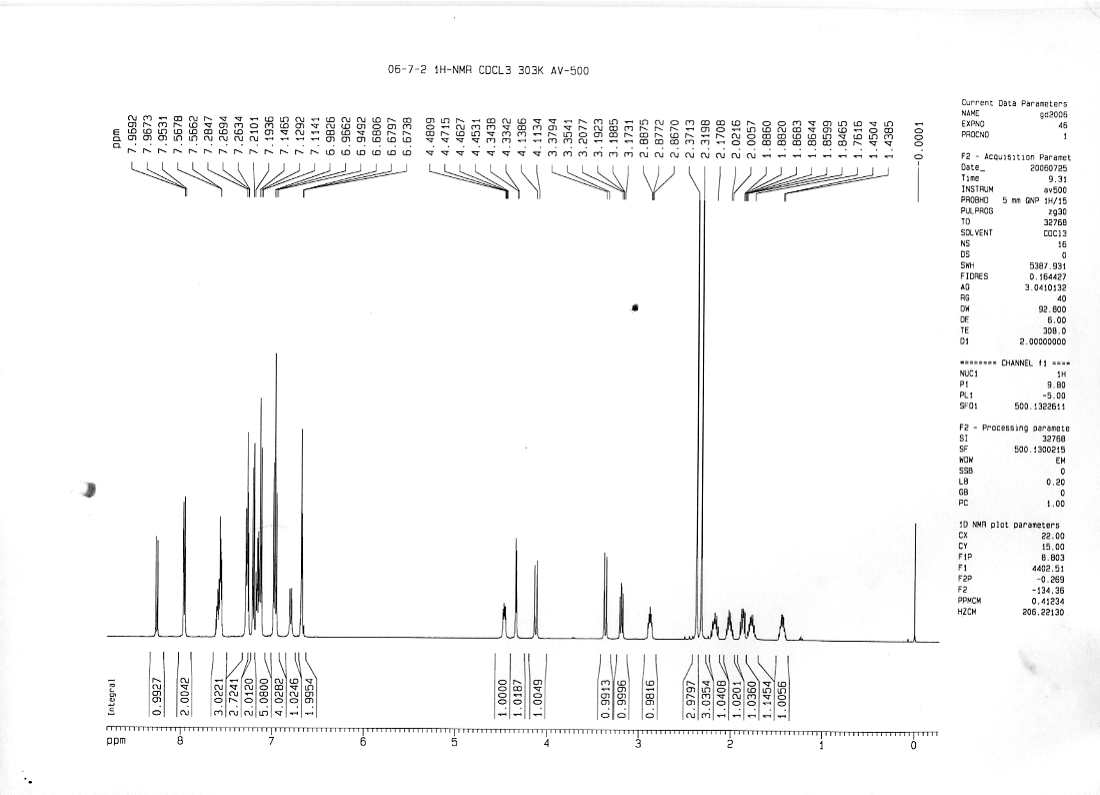

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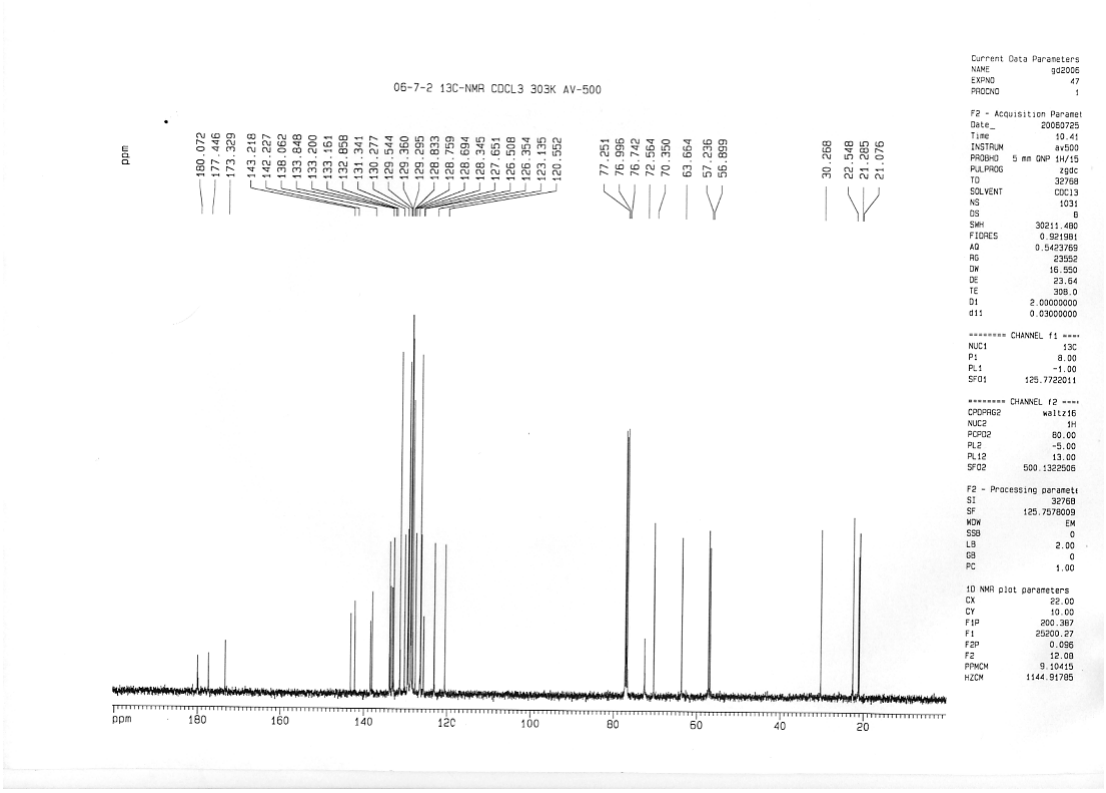

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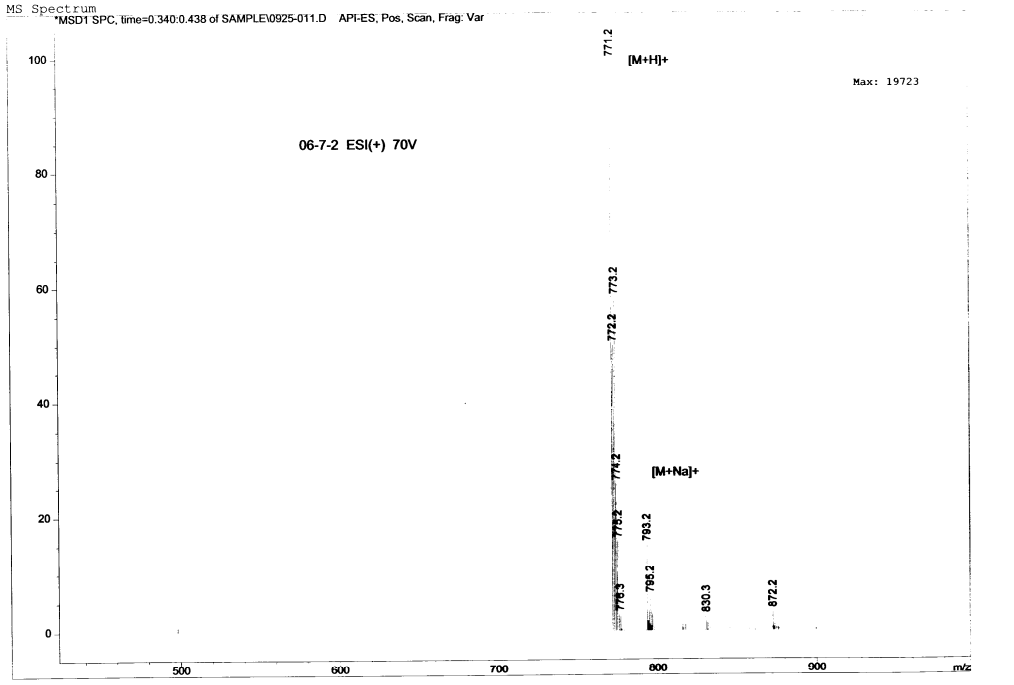

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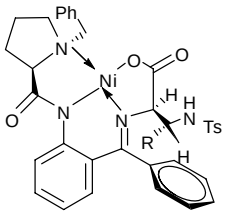

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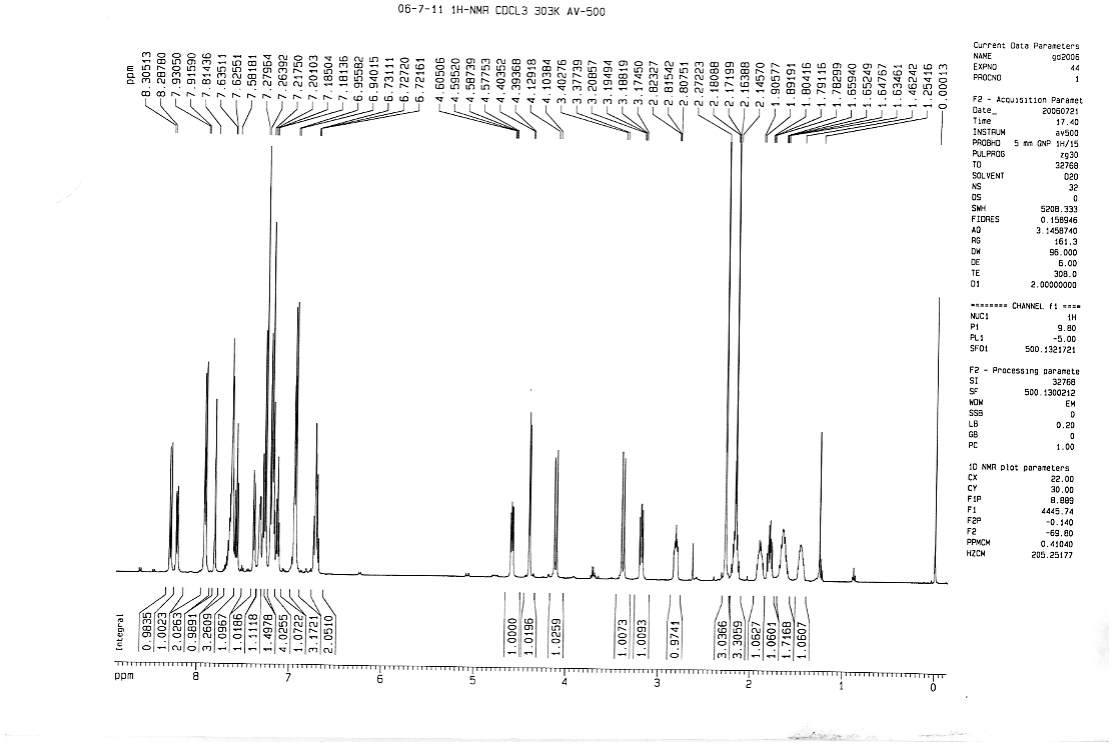

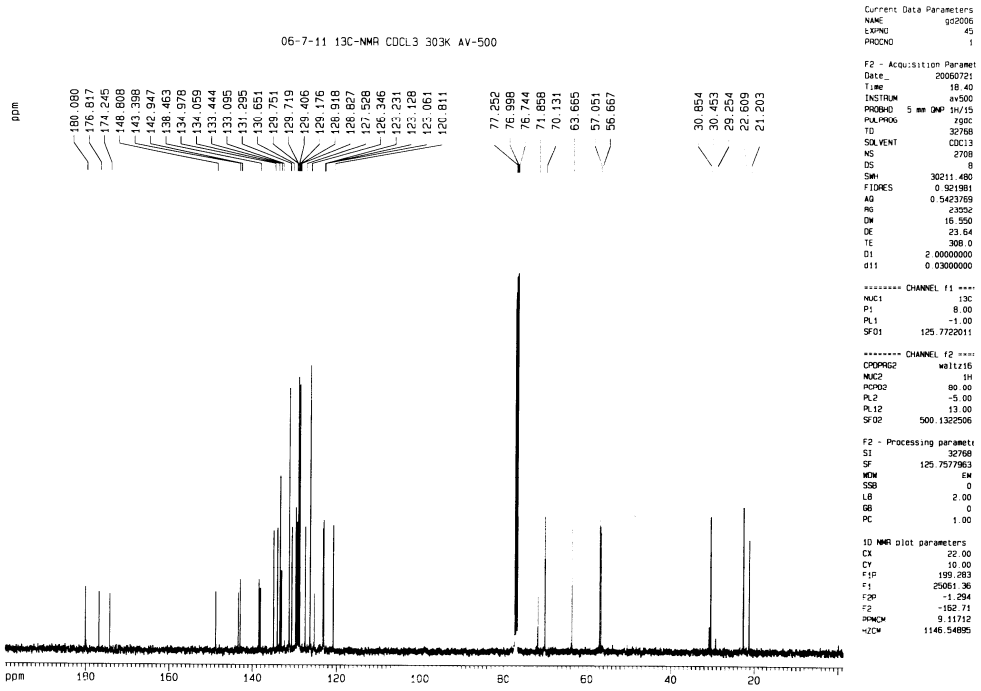

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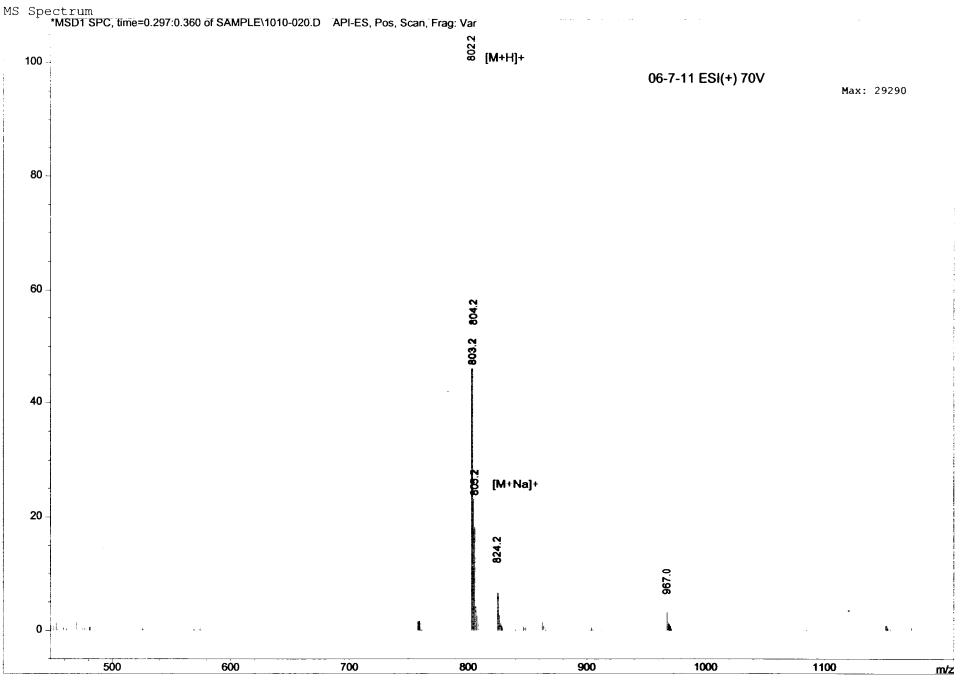

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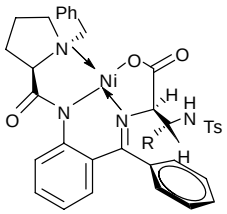

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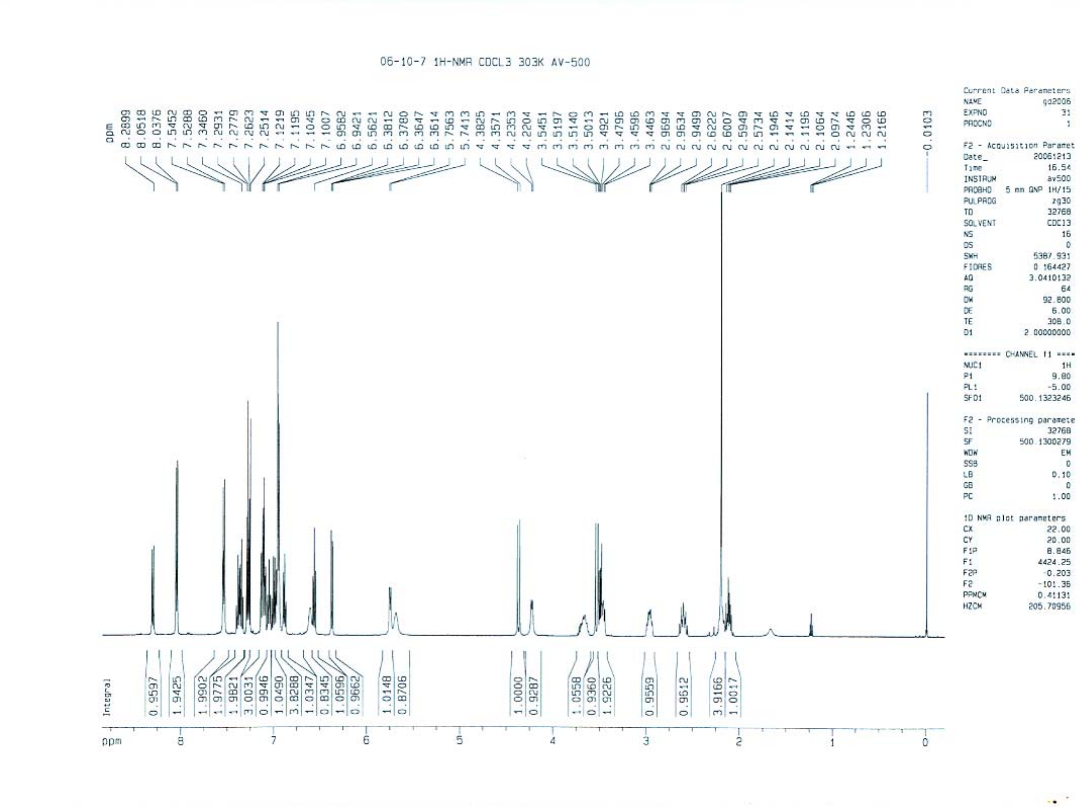
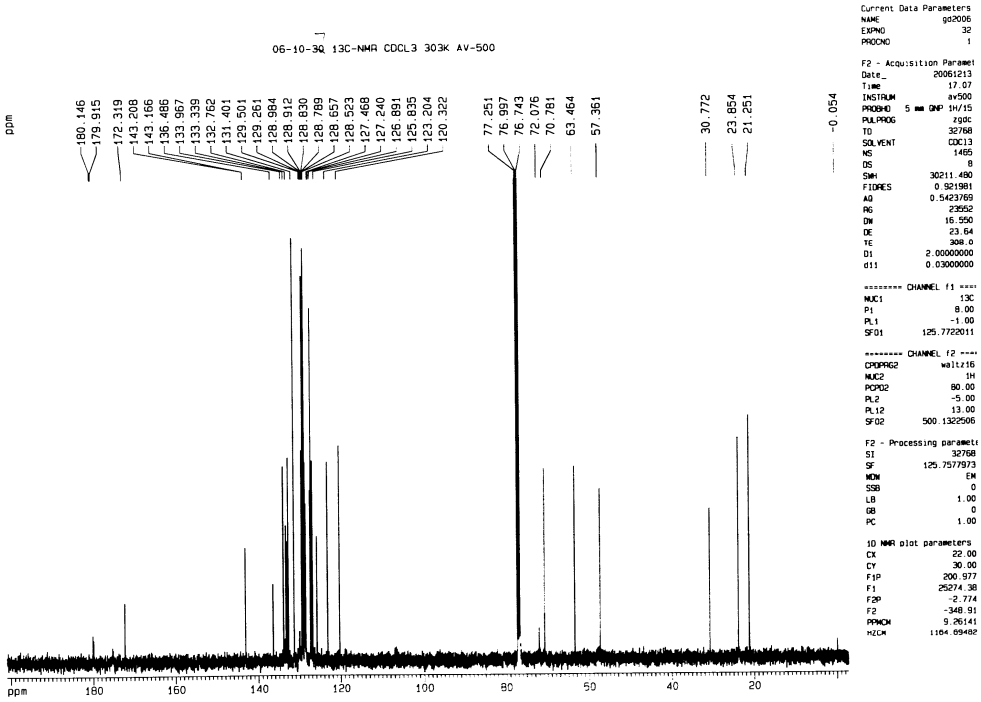
(*R*,*R*,*S*)-3e

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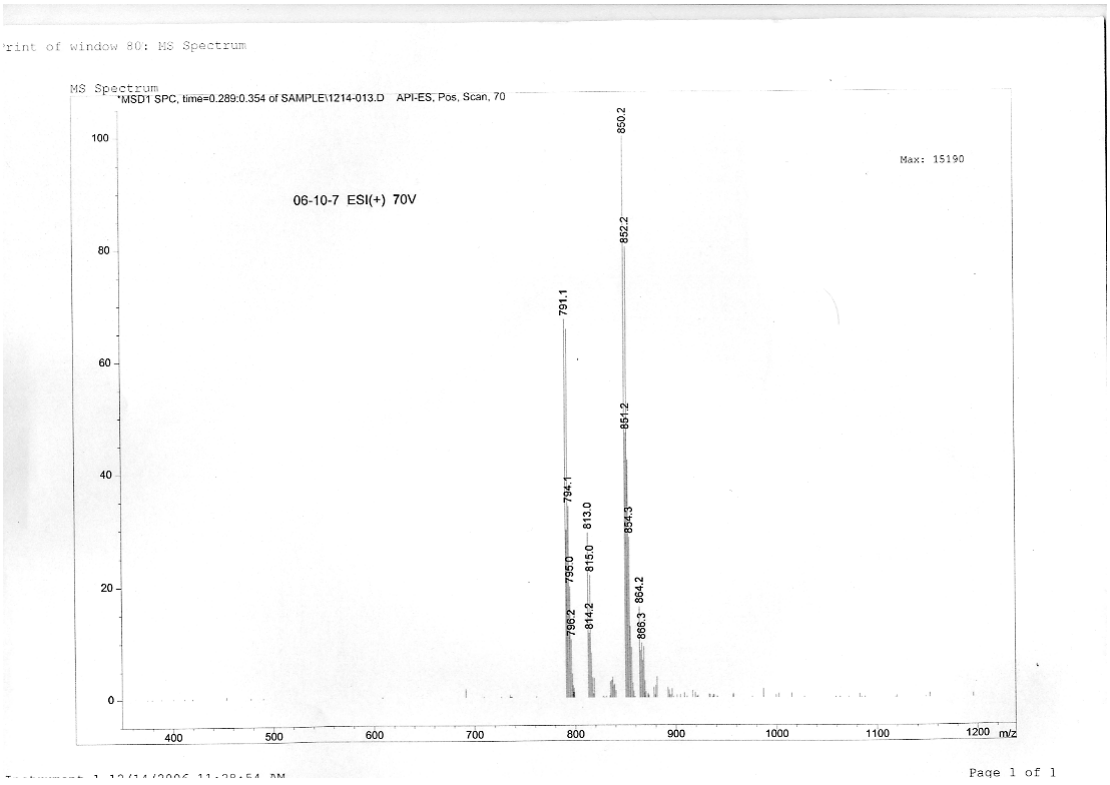
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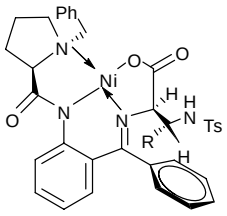
m/z
Page 1 of 1



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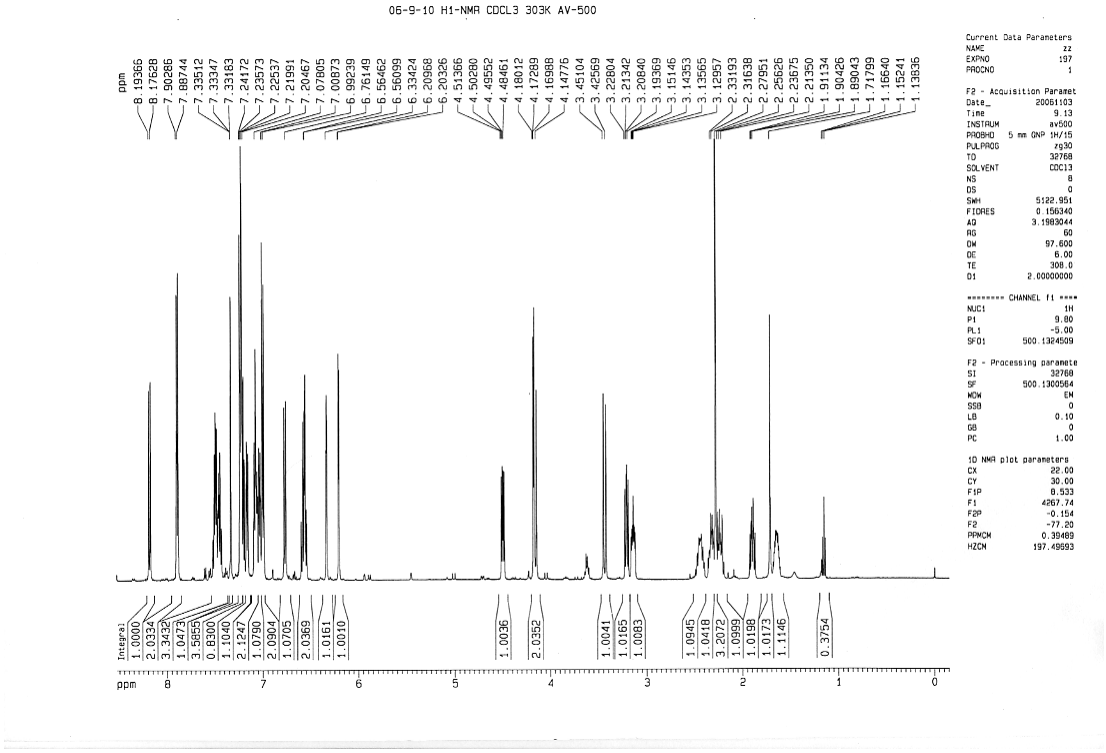

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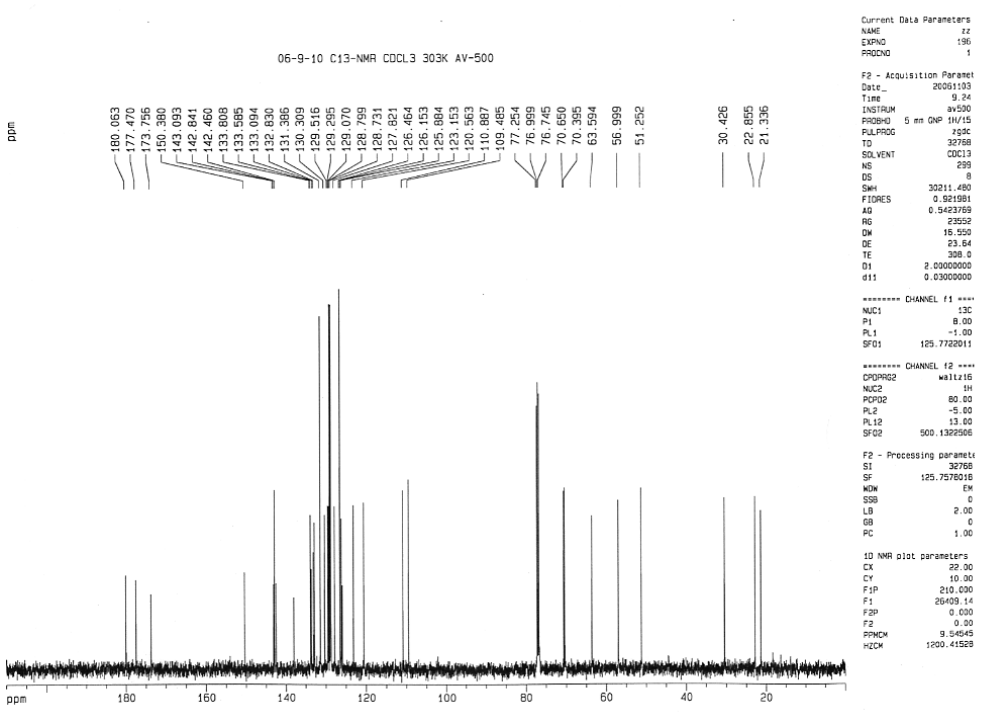

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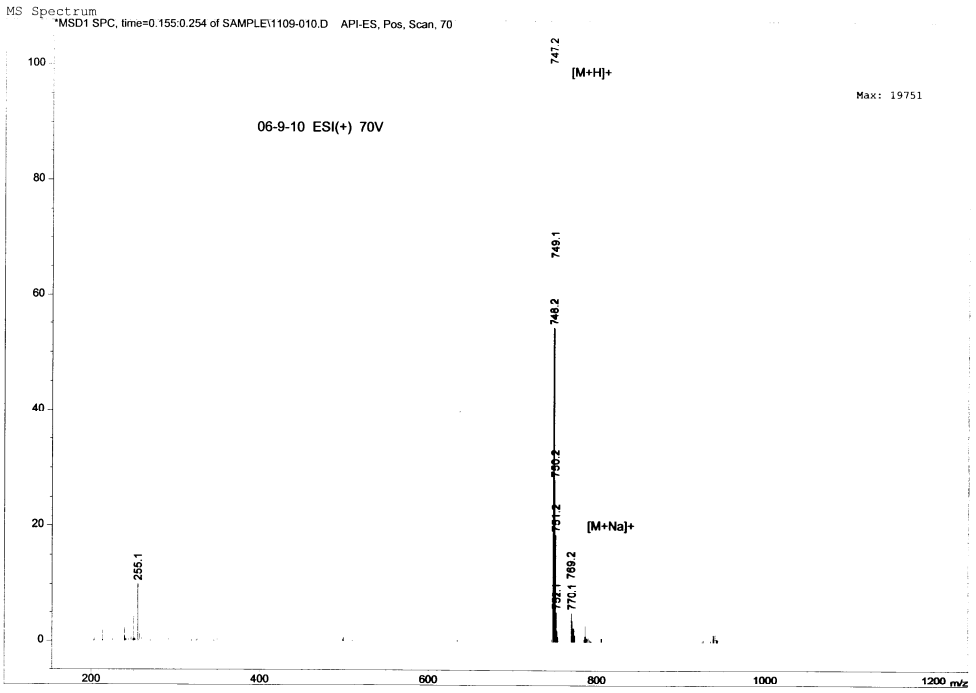

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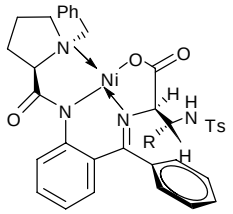
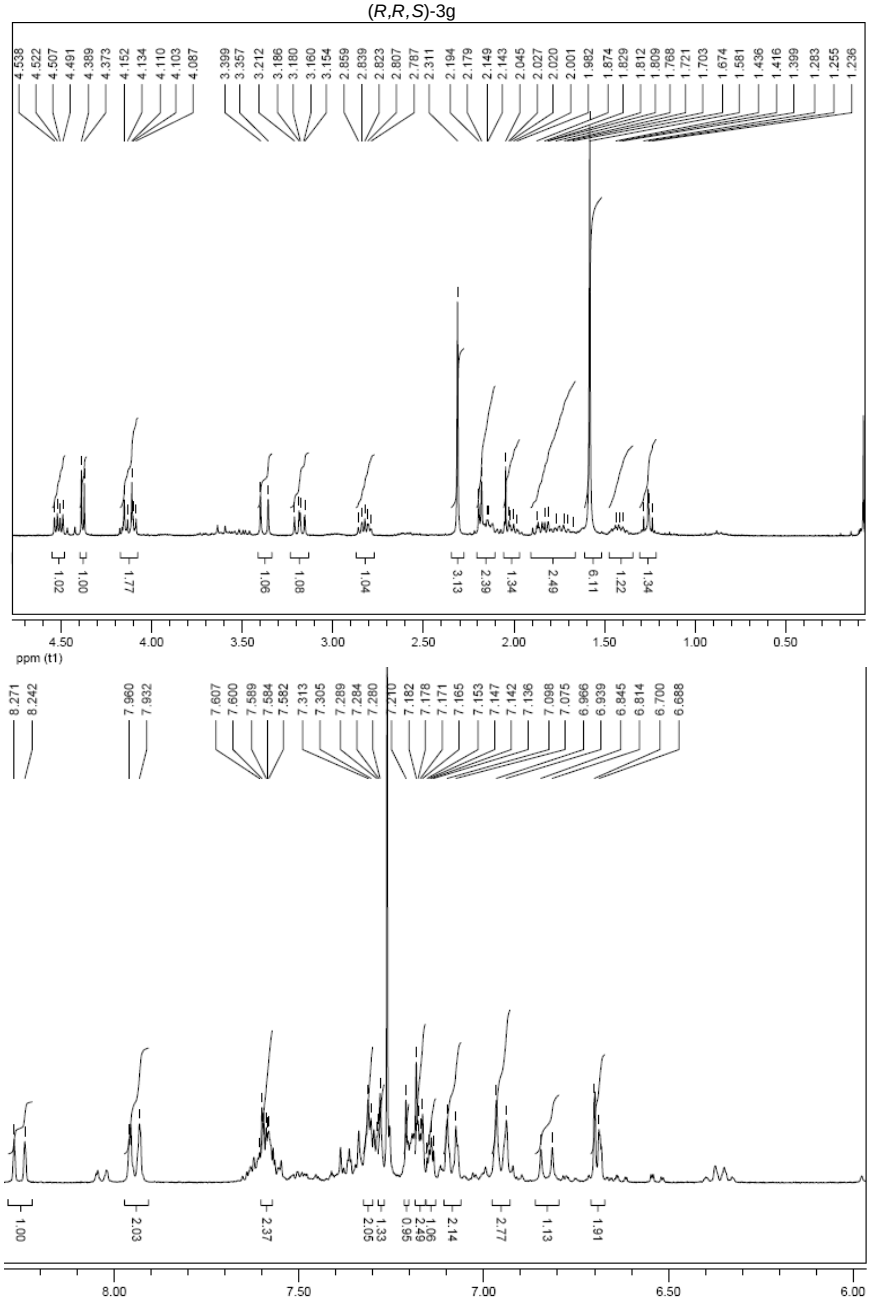


R= *I*-Bu

(*R*,*R*,*S*)-3g



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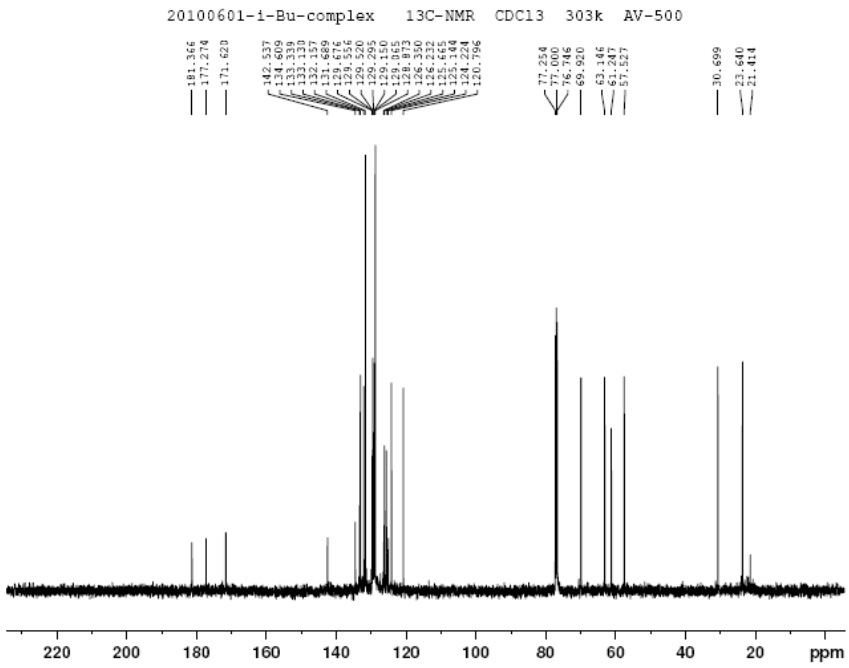

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Elemental Composition Report

Page 1

Single Mass Analysis

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Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
470 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-45 H: 0-100 N: 0-5 O: 0-5 S: 0-1 58Ni: 0-1

20100601-i-Bu-complex
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TOF MS ES+
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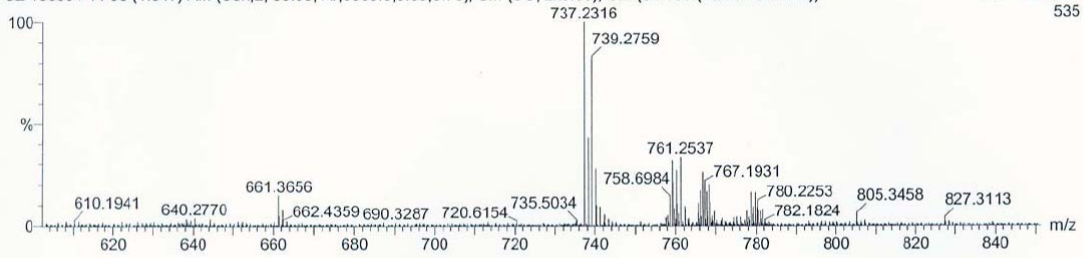

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	737.2301	1.5	2.0	30.5	41.0	C45 H37 N5 O2 58Ni
	737.2334	-1.8	-2.4	25.5	31.1	C42 H41 N5 O2 S 58Ni
	737.2348	-3.2	-4.3	25.0	31.0	C44 H43 N2 O3 S 58Ni
	737.2274	4.2	5.7	26.0	39.4	C42 H39 N4 O5 58Ni

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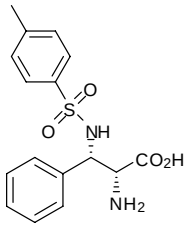
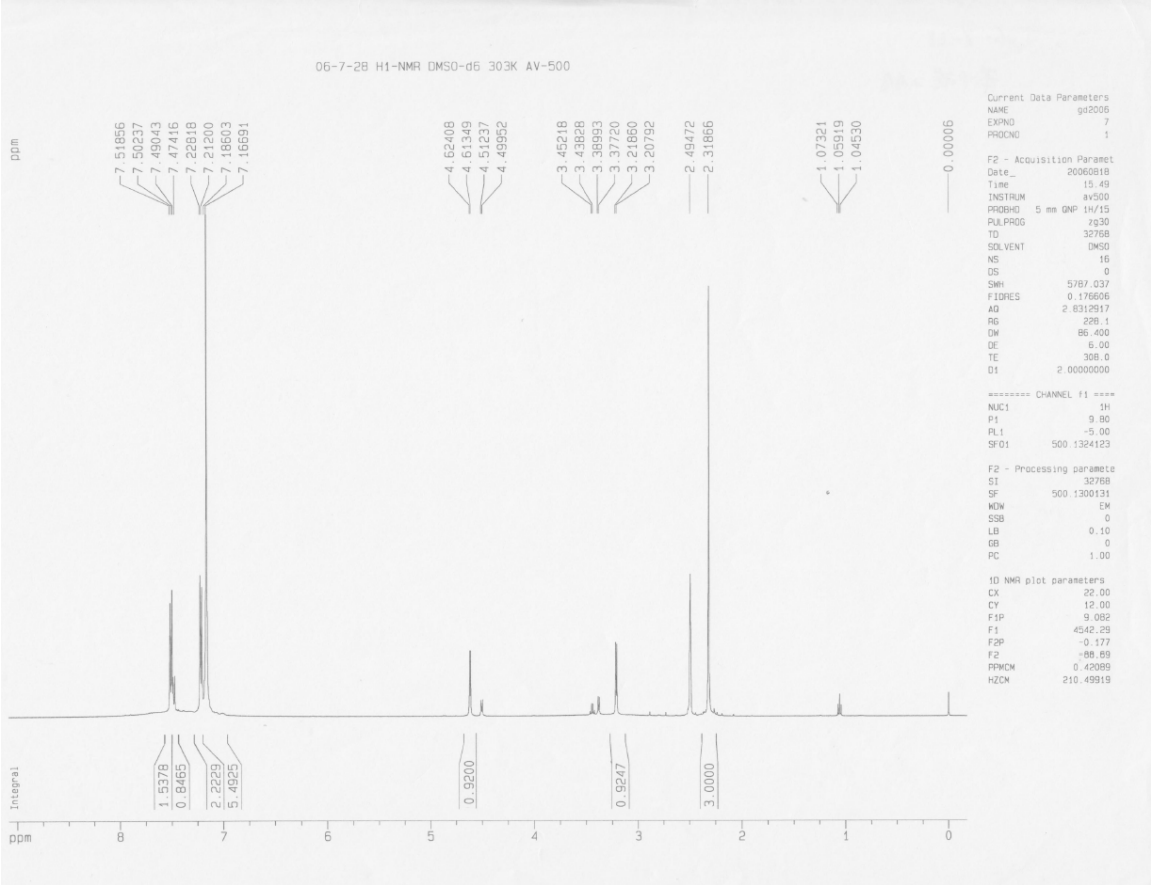
2. ^{1}H NMR, ^{13}C NMR and Mass spectra of **4a**, **4b**, **4c**, **4d**, **4e**, **4f and 4g**



(2*R*,3*S*)-4a



(2R,3S)-4a: *β*-H, δ_H 4.61-4.62
(2R,3R)-4a: *β*-H, δ_H 4.50-4.51
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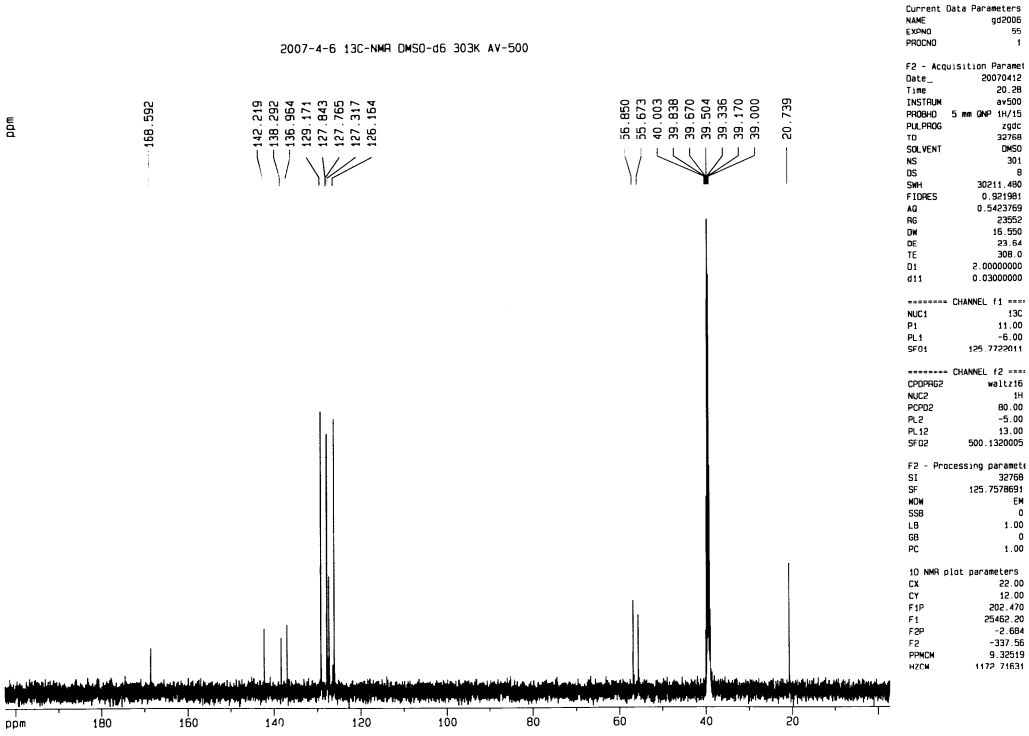

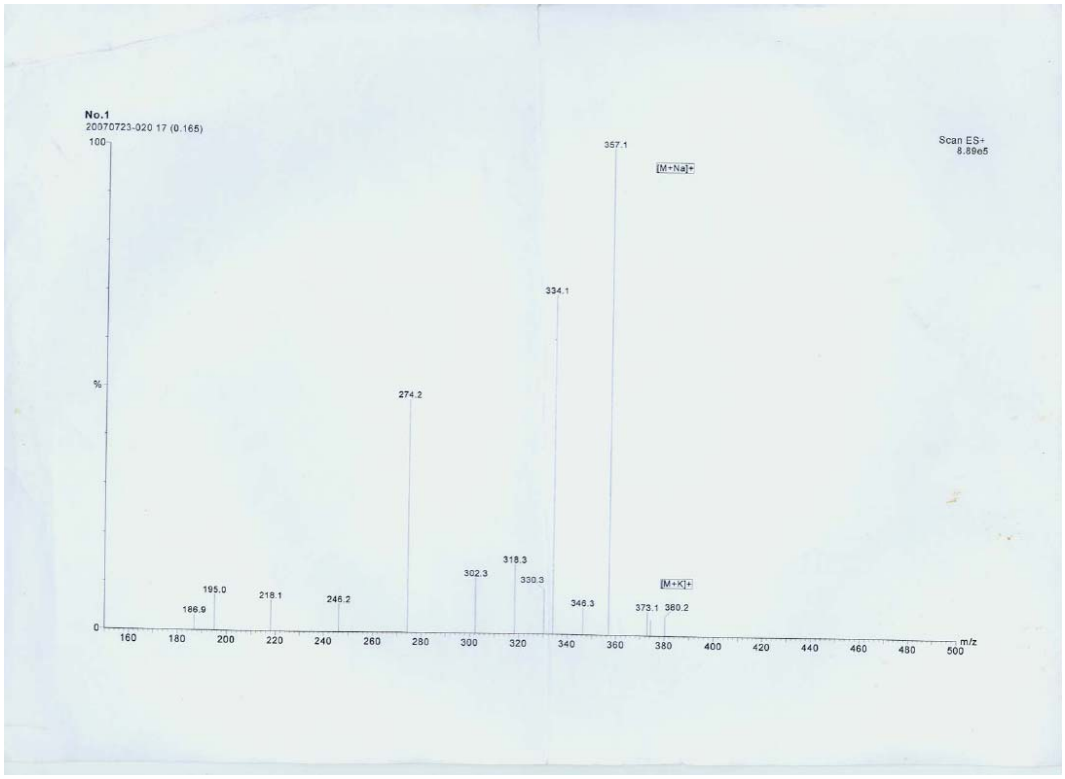

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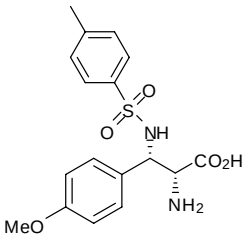

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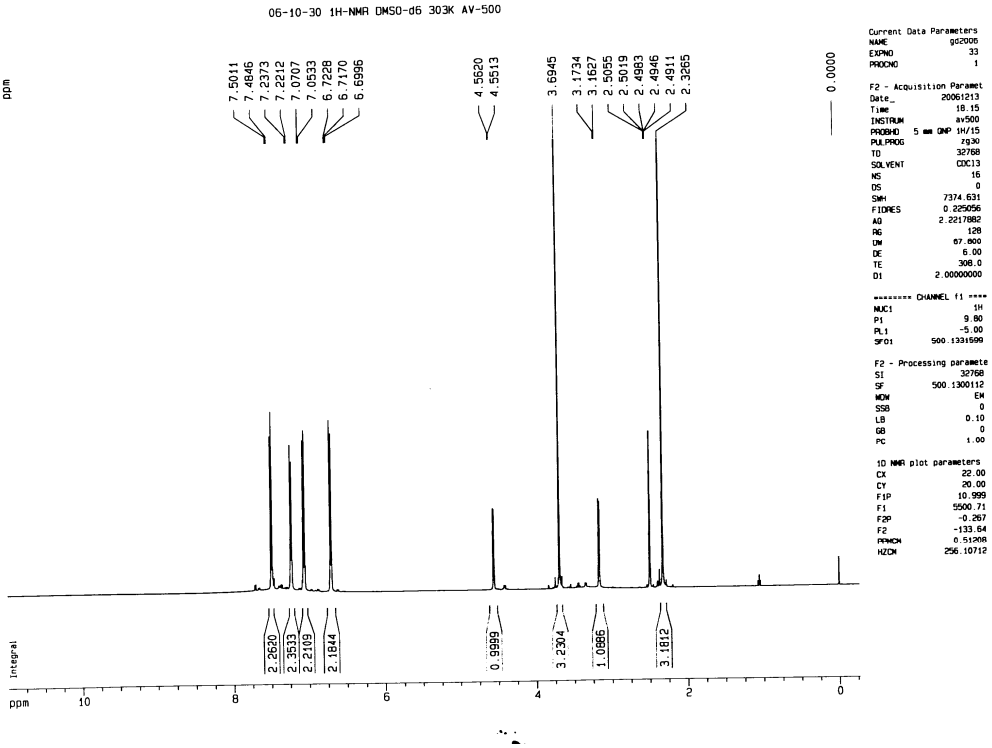

(2R,3S)-4b: *β*-H, δ_H 4.55-4.56
(2R,3R)-4b: *β*-H, δ_H 4.50-4.52
(2R,3S)-4b/(2R,3R)-4b > 99:1

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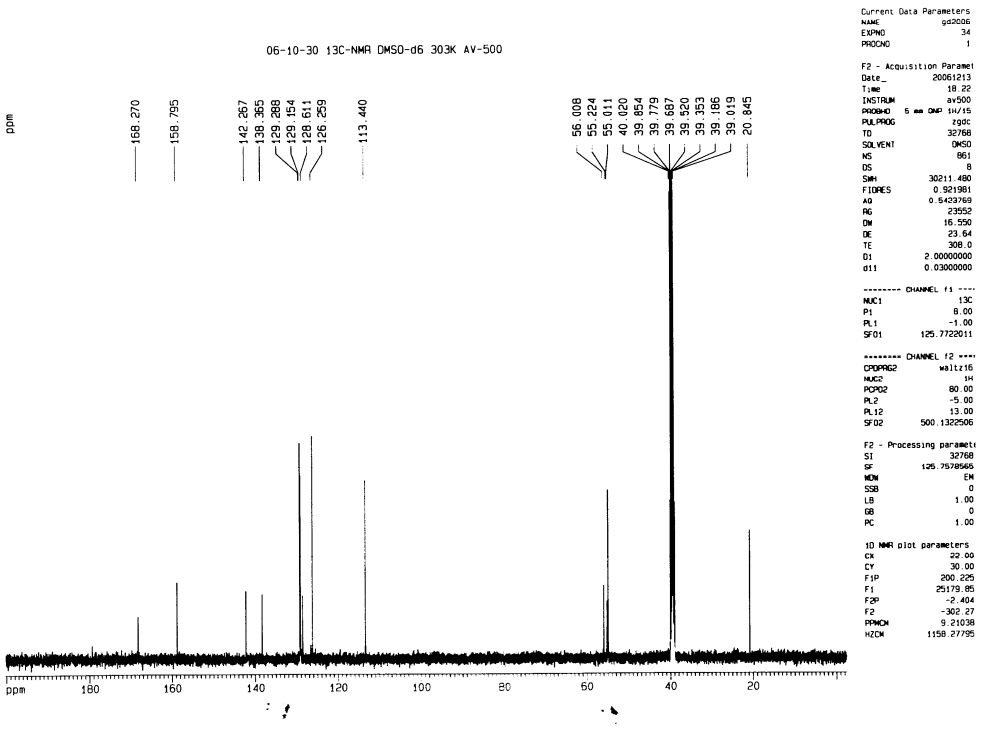

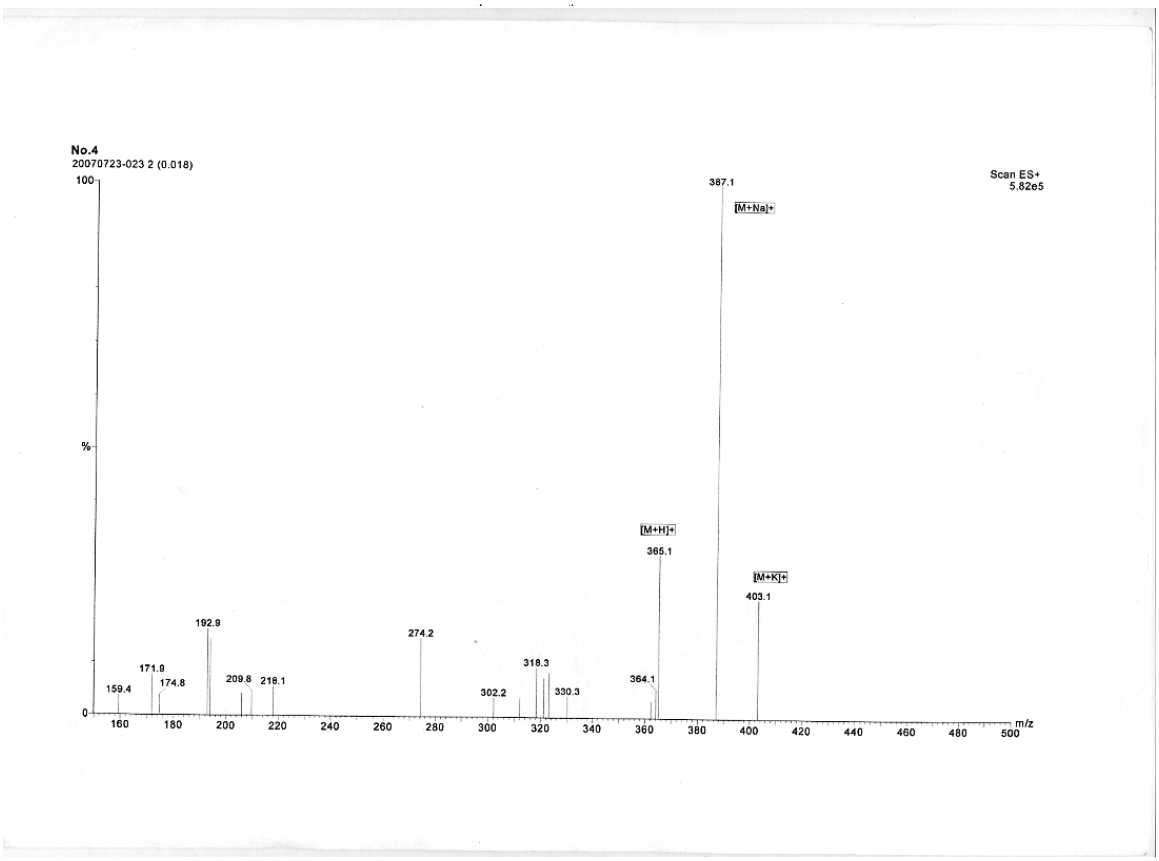

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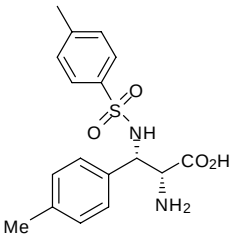

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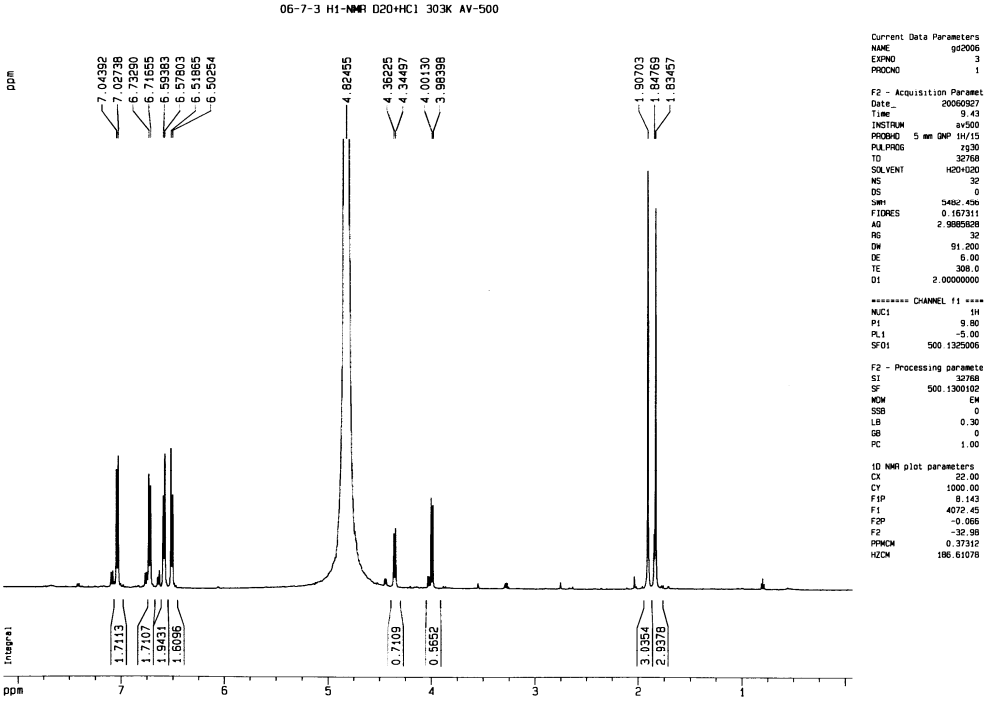

(2R,3S)-4c : β-H, δ_H 4.34-4.36
(2R,3R)-4c : β-H, δ_H 4.38-4.39
(2R,3S)-4c/(2R,3R)-4c > 99/1

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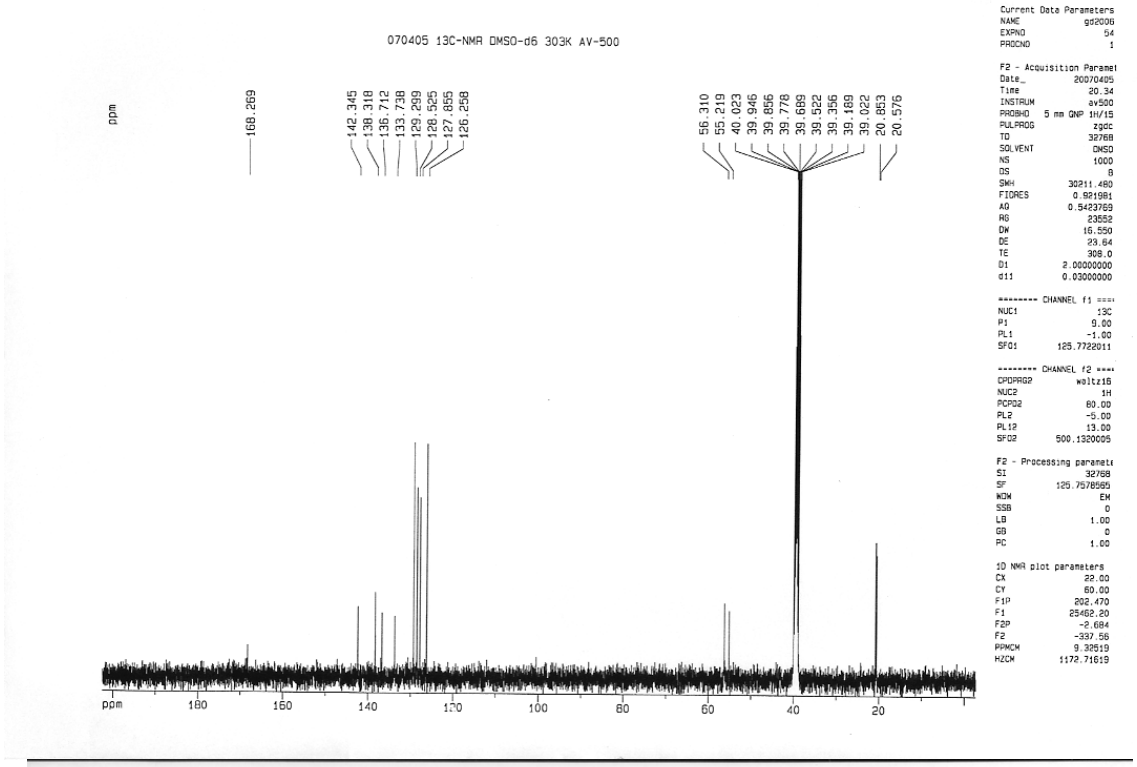

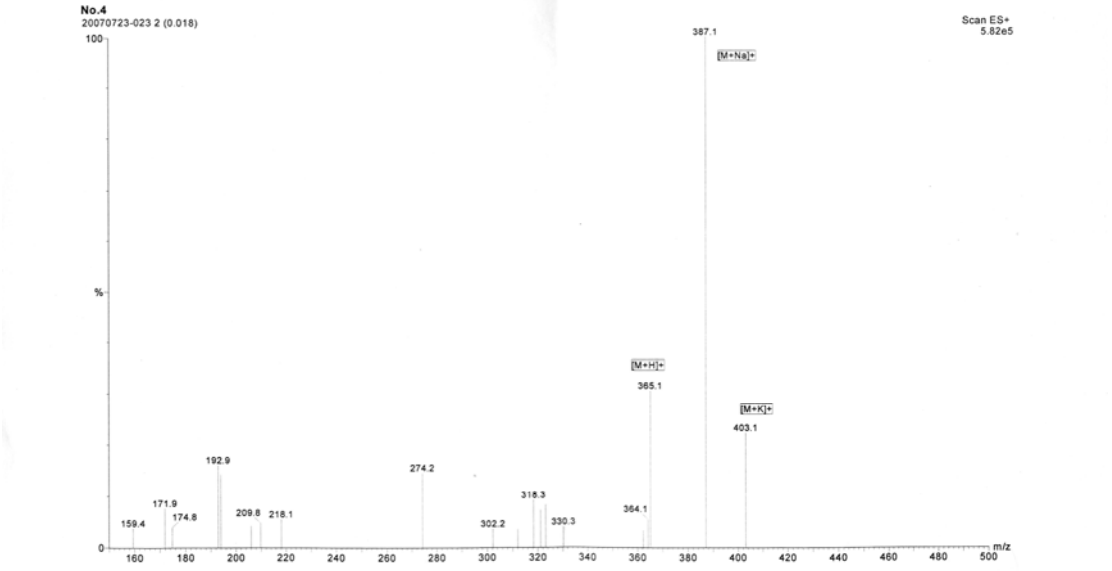

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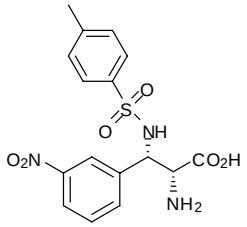
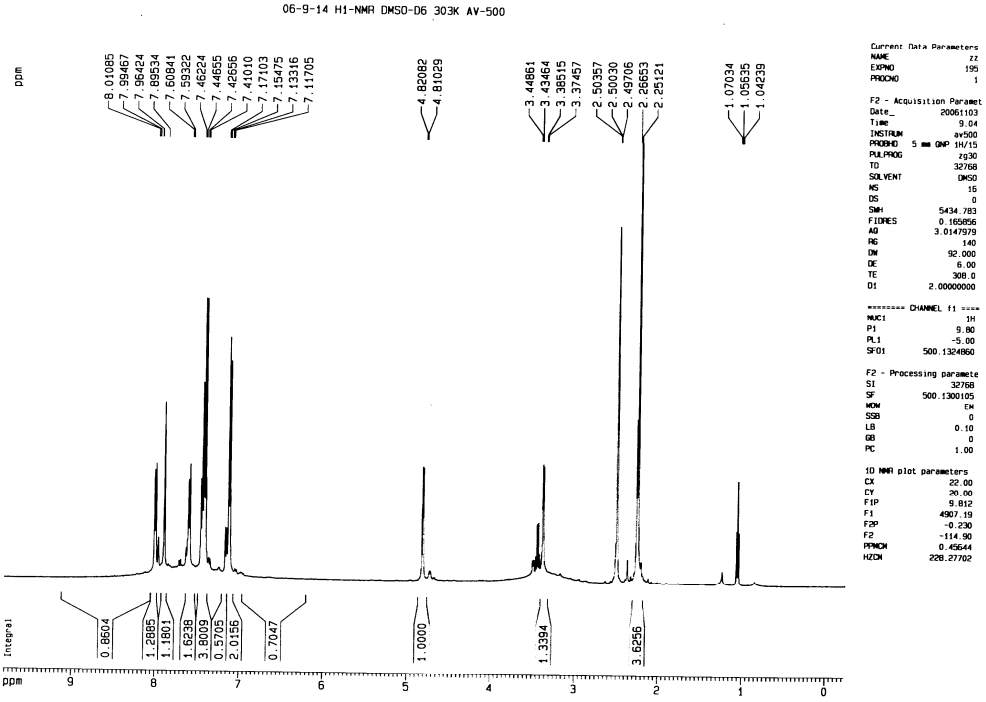


(2*R*,3*S*)-4d



(2R,3S)-4d : β-H, δ_H 4.81-4.82
(2R,3R)-4d : β-H, δ_H 4.79-4.80
(2R,3S)-4d/(2R,3R)-4d = 99/1

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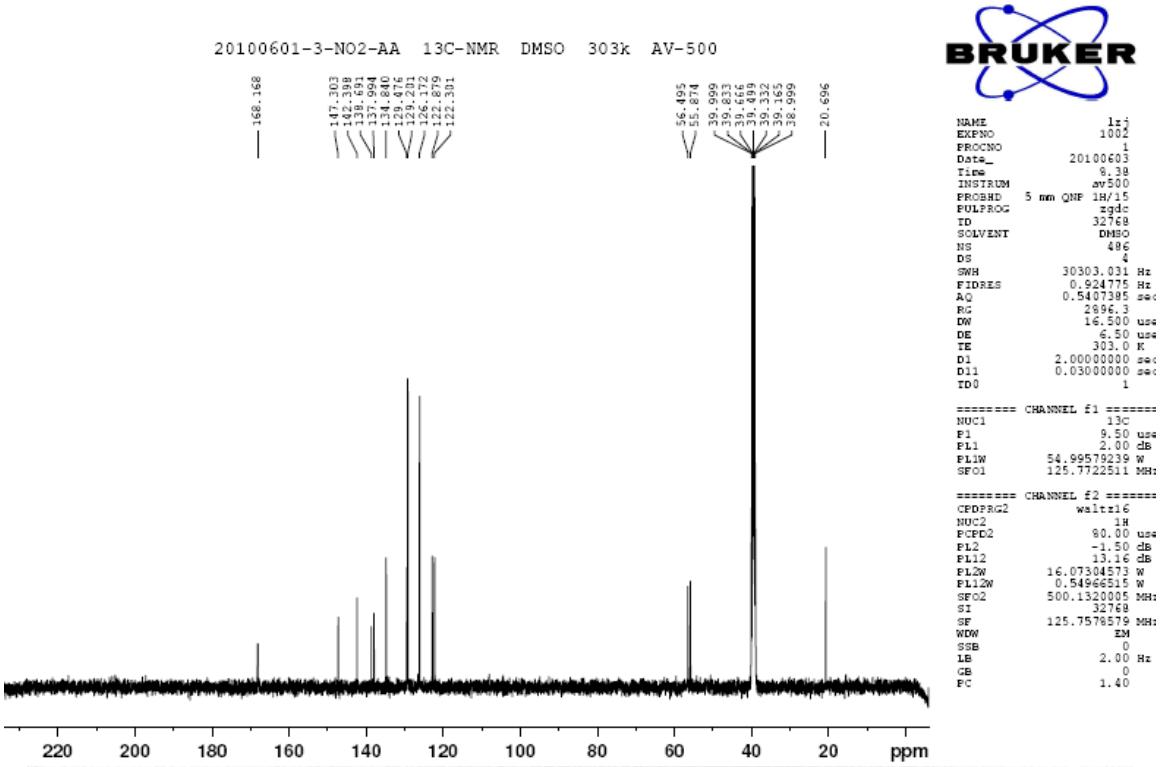

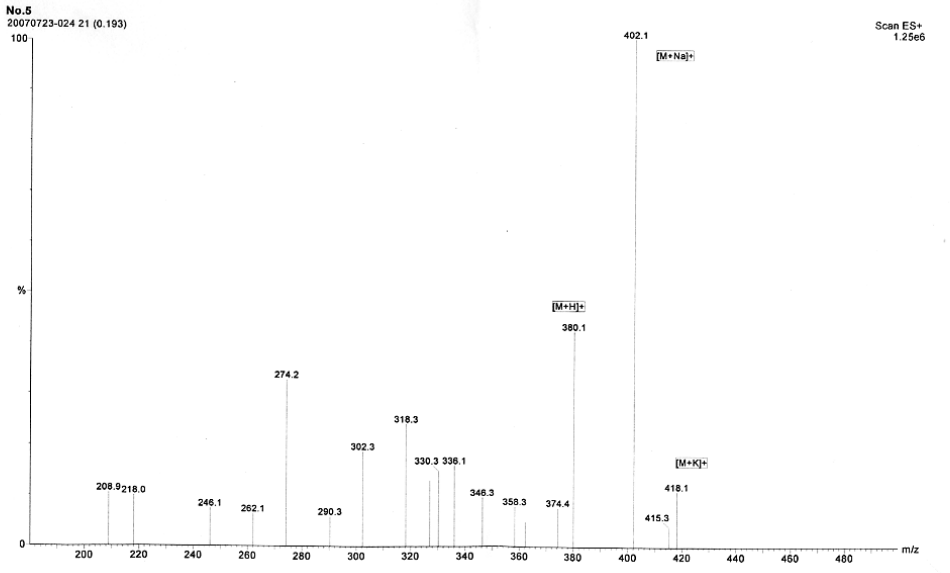

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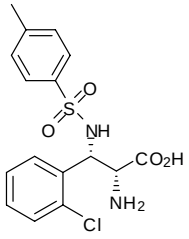
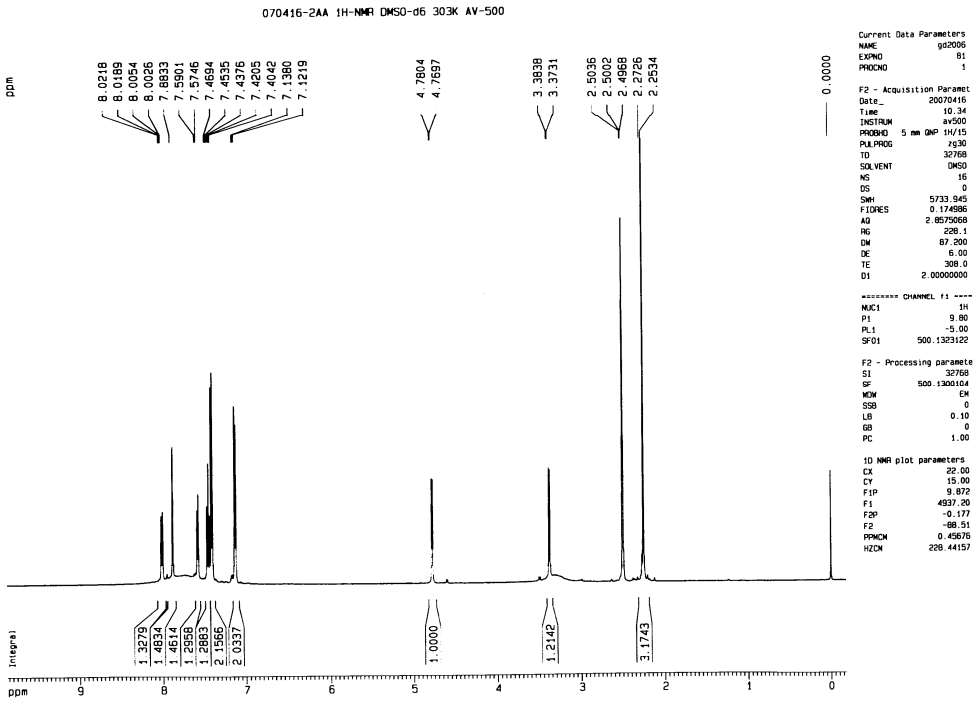


(2*R*,3*S*)-4e



(2R,3S)-4e : β-H, δ_H 4.77-4.78
(2R,3R)-4e : β-H, δ_H 4.74-4.75
(2R,3S)-4e/(2R,3R)-4e > 99/1

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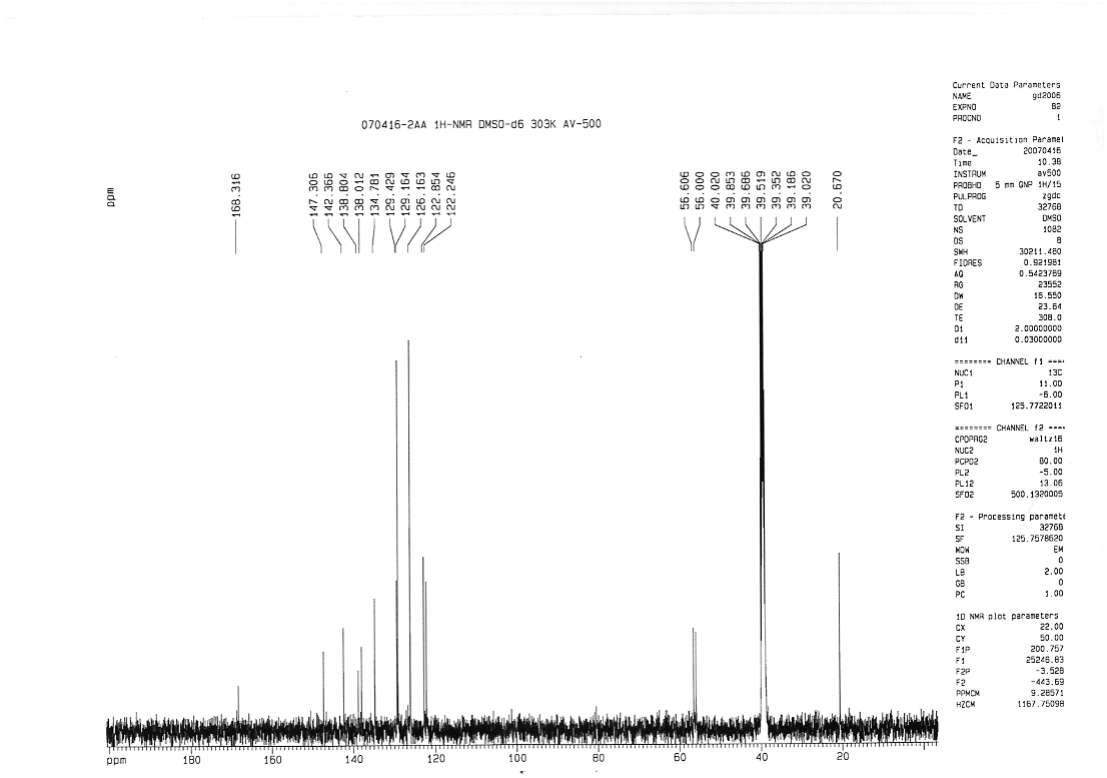

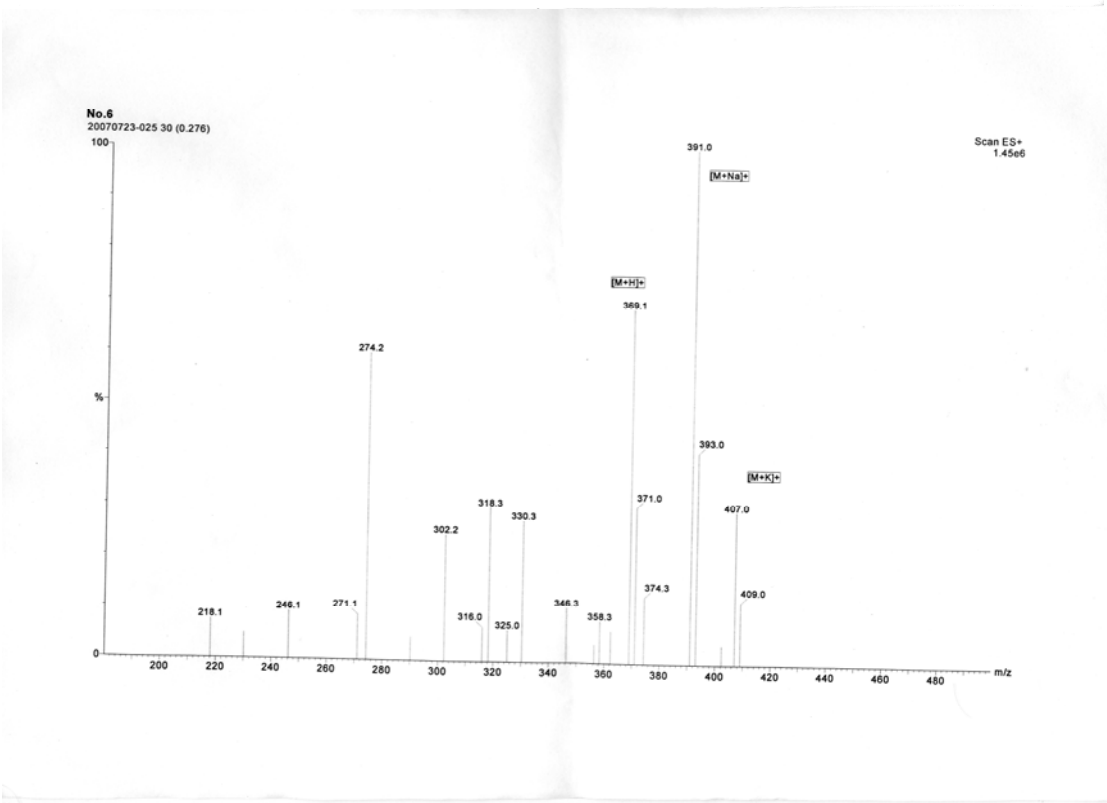

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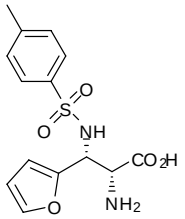
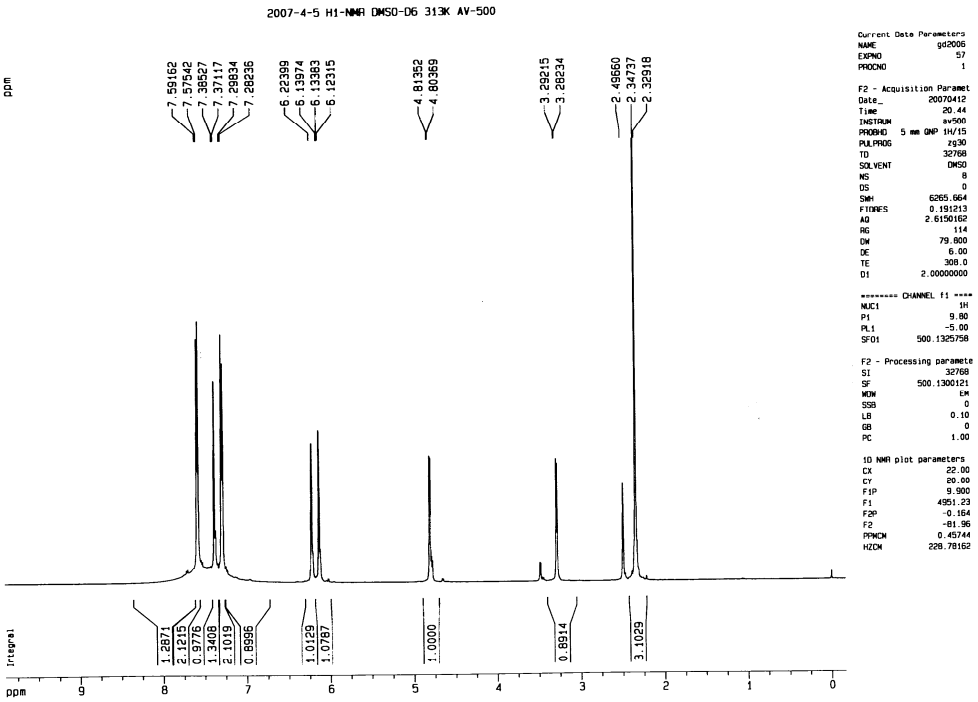


(2*R*,3*S*)-4f



(2R,3S)-4f : β-H, δ_H 4.80-4.81
(2R,3R)-4f : β-H, δ_H 4.77-4.78
(2R,3S)-4f/(2R,3R)-4f > 99/1

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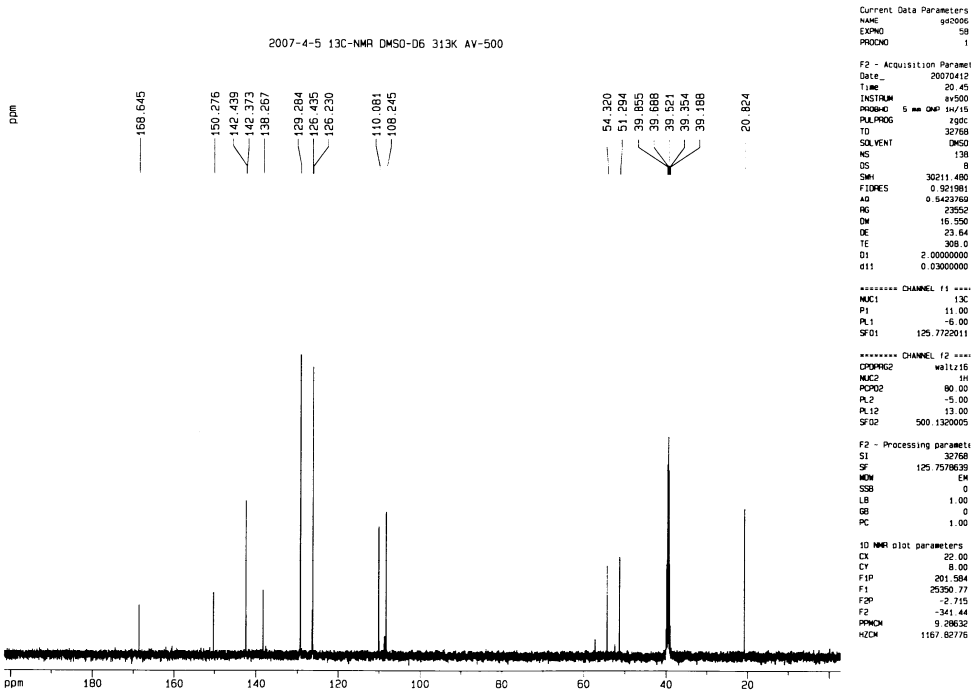

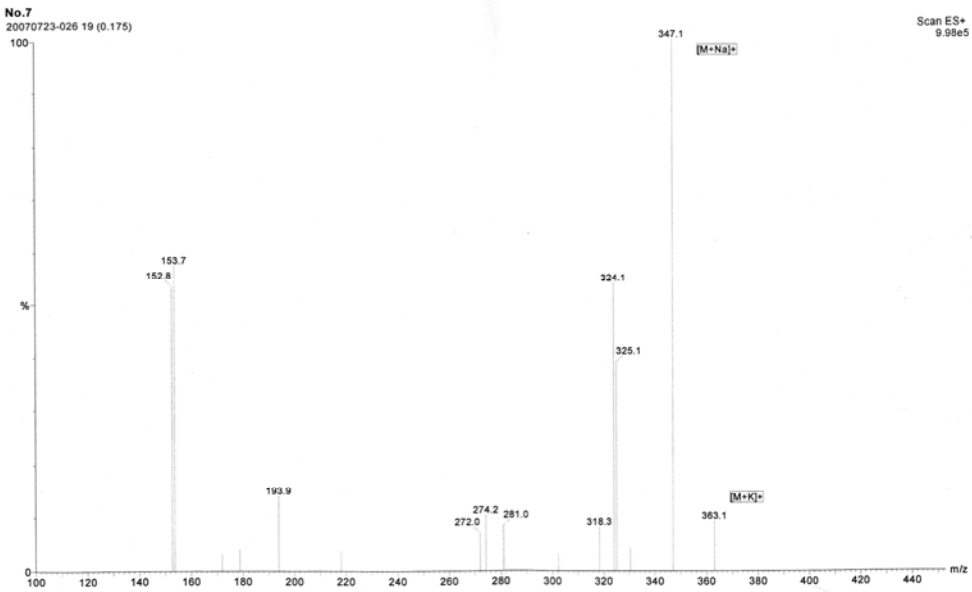

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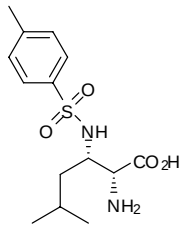
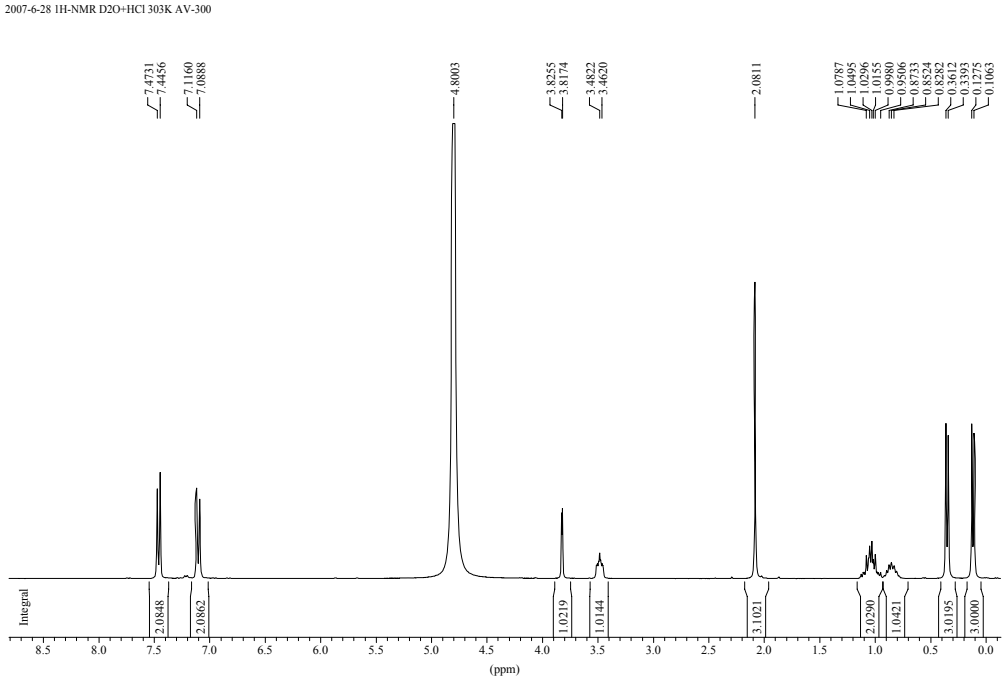


(2*R*,3*S*)-4g



(2R,3S)-4g : β-H, δ_H 4.81-4.83
(2R,3S)-4g/(2R,3R)-4g > 99/1

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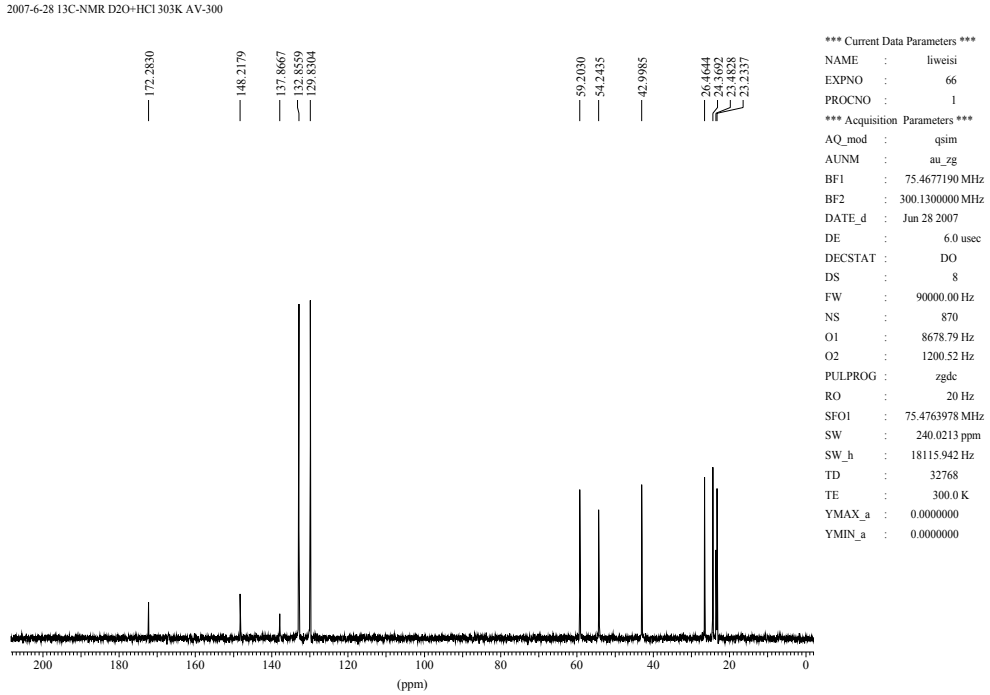

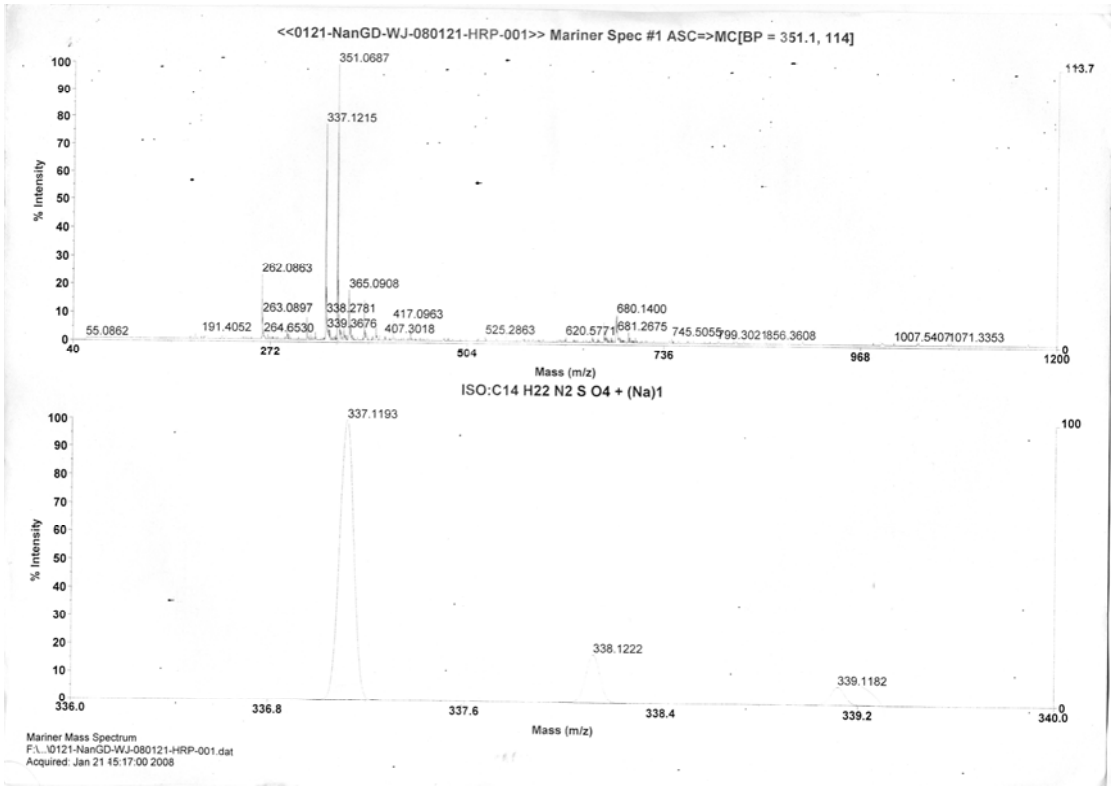

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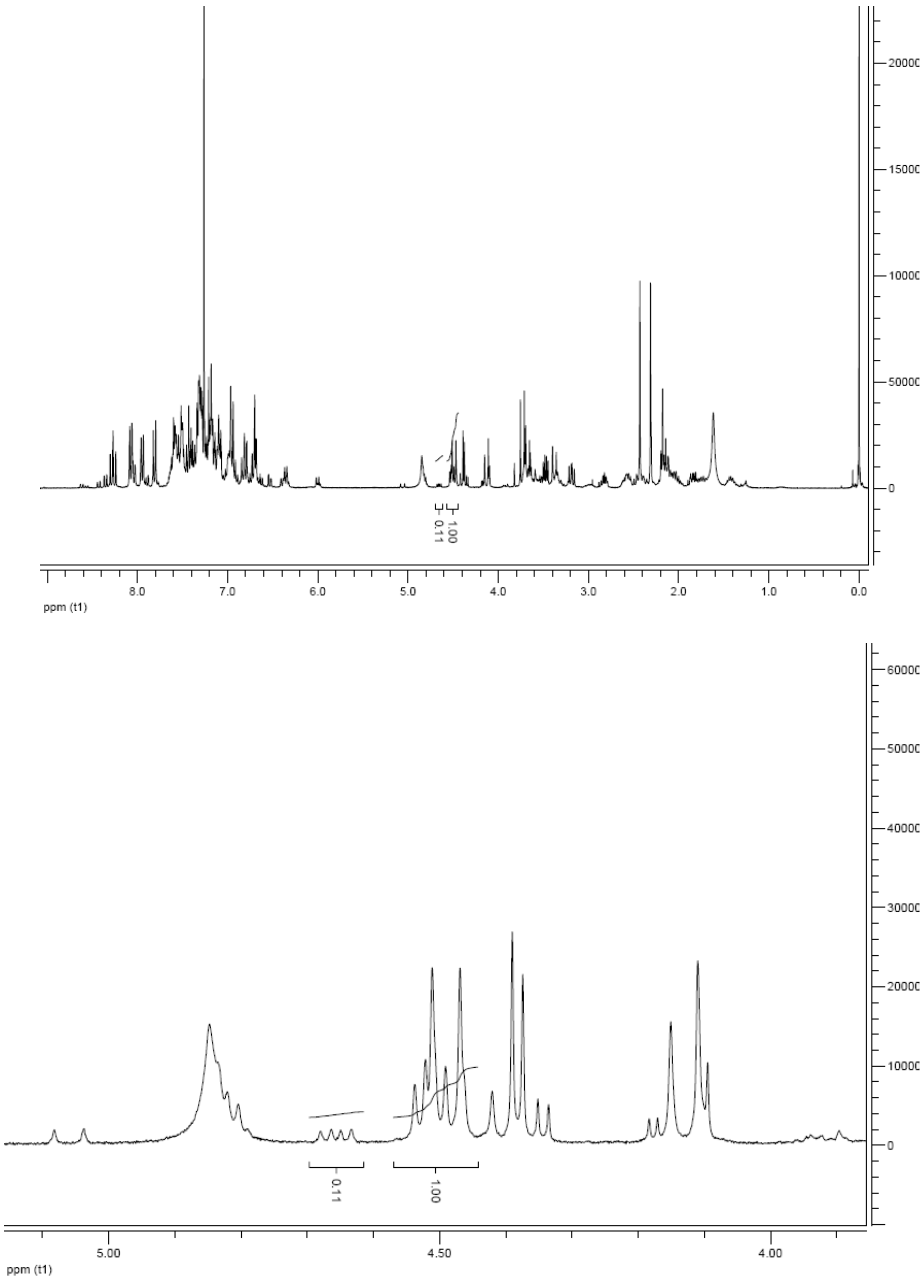
Ratio of (R,2R,3S)-3 and (R,2R,3R)-3:

The ratio was determined by ^{1}H NMR analysis of crude reaction mixtures because the chemical shifts of the protons of diastereomers (about 4.40–4.60 ppm) at β-position chiral C atoms were different.



(R,2R,3S)-3a: δ_H 4.44–4.57 (m, β-CH)
(R,2R,3R)-3a: δ_H, 4.61–4.70(m, β-CH)
(R,2R,3S)-3a/(R,2R,3R)-3a= 90:10

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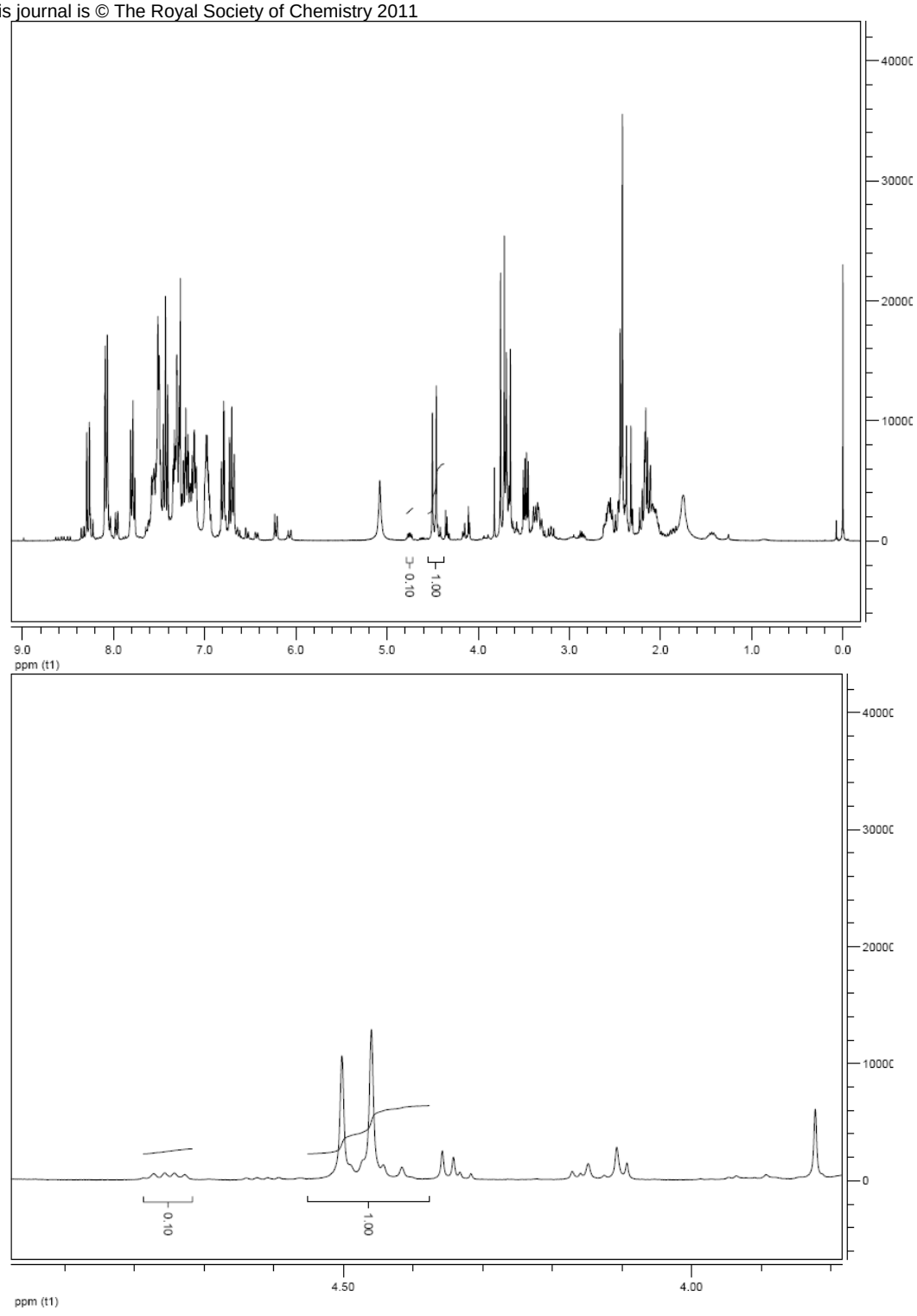

(R,2R,3S)-3b: δ_H 4.44–4.57 (m, β-CH)
(R,2R,3R)-3b: δ_H, 4.71–4.80(m, β-CH)
(R,2R,3S)-3b/(R,2R,3R)-3b = 91:9

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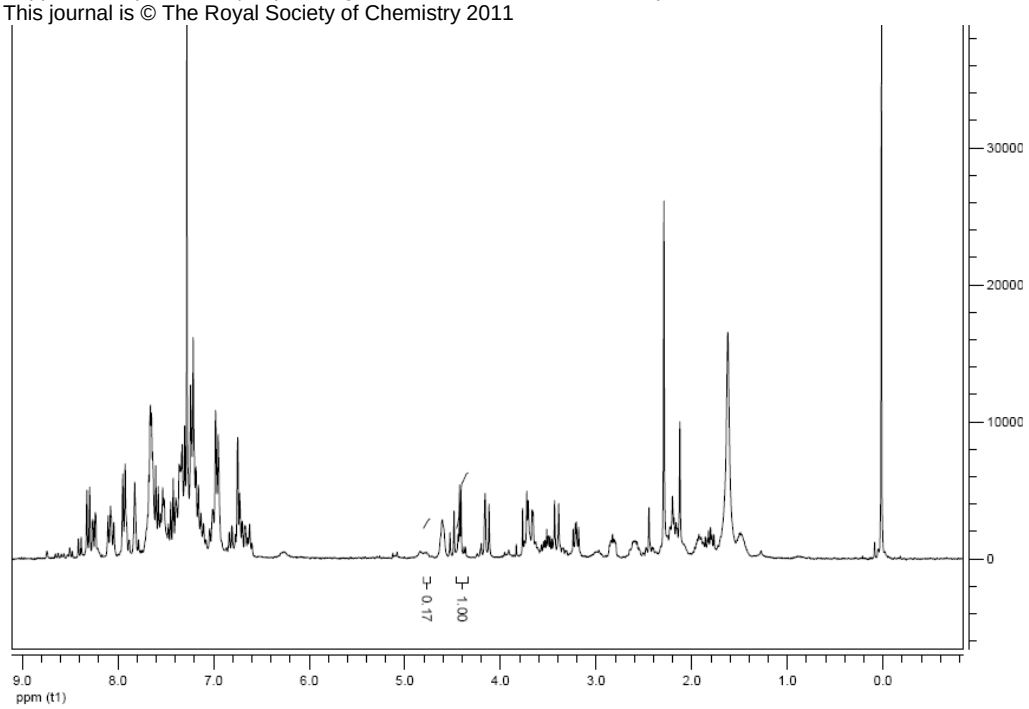

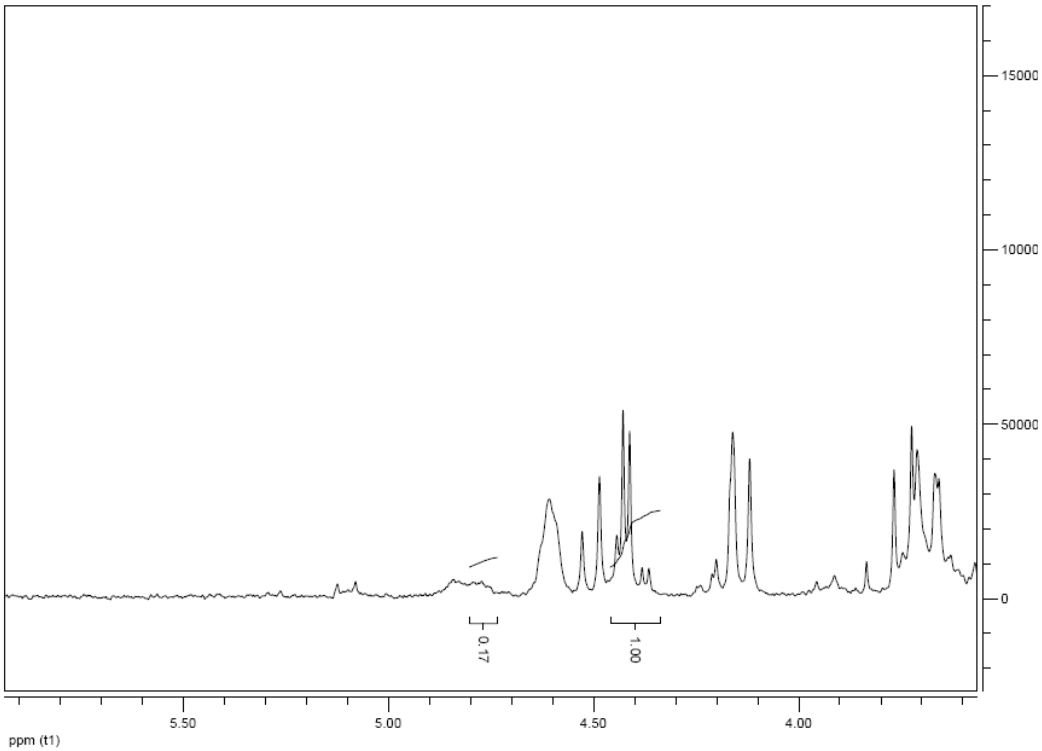

(R,2R,3S)-3d: δ_H 4.34–4.46 (m, β-CH)
(R,2R,3R)-3d: δ_H, 4.73–4.80(m, β-CH)
(R,2R,3S)-3d/(R,2R,3R)-3d =86:14

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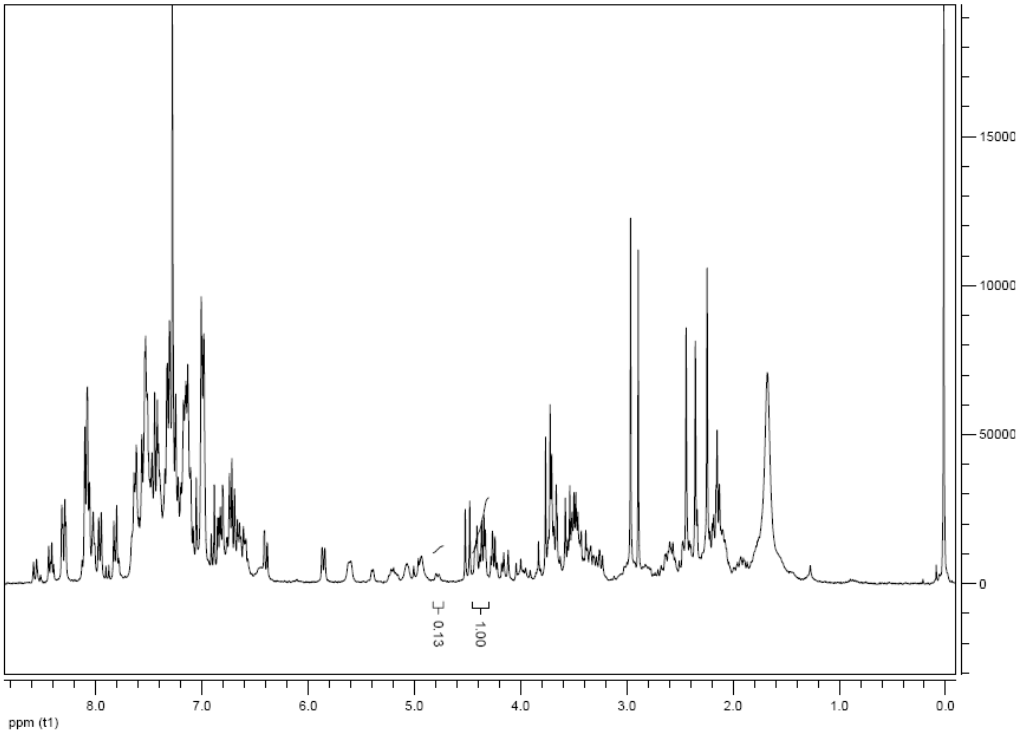

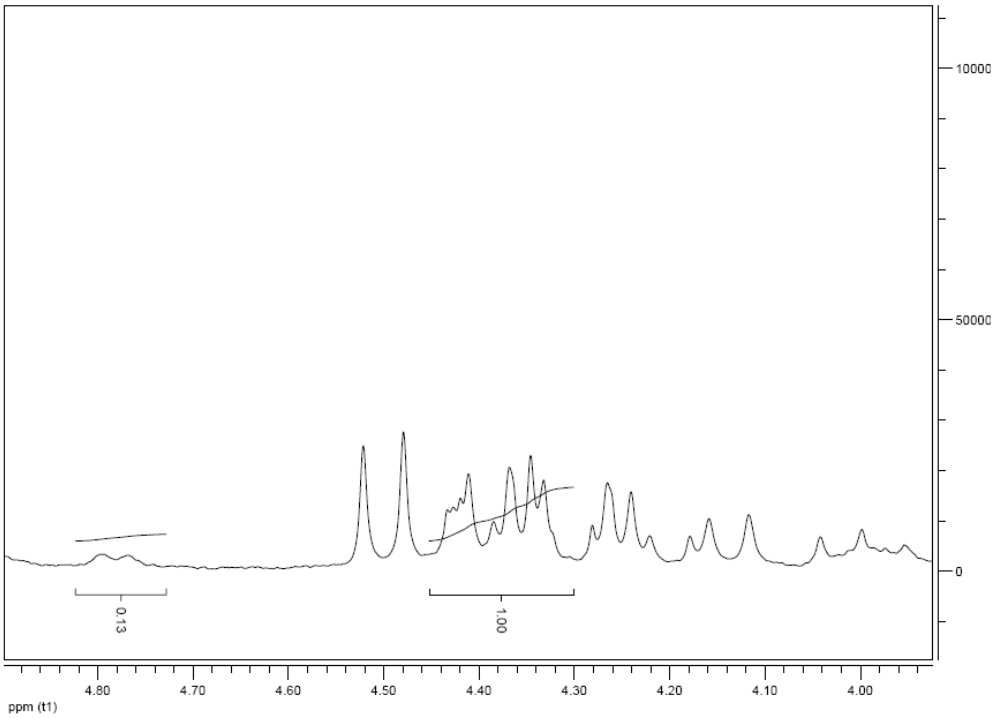

(R,2R,3S)-3e: δ_H 4.30–4.46 (m, β-CH)
(R,2R,3R)-3e: δ_H, 4.71–4.81(m, β-CH)
(R,2R,3S)-3e/(R,2R,3R)-3e =89:11

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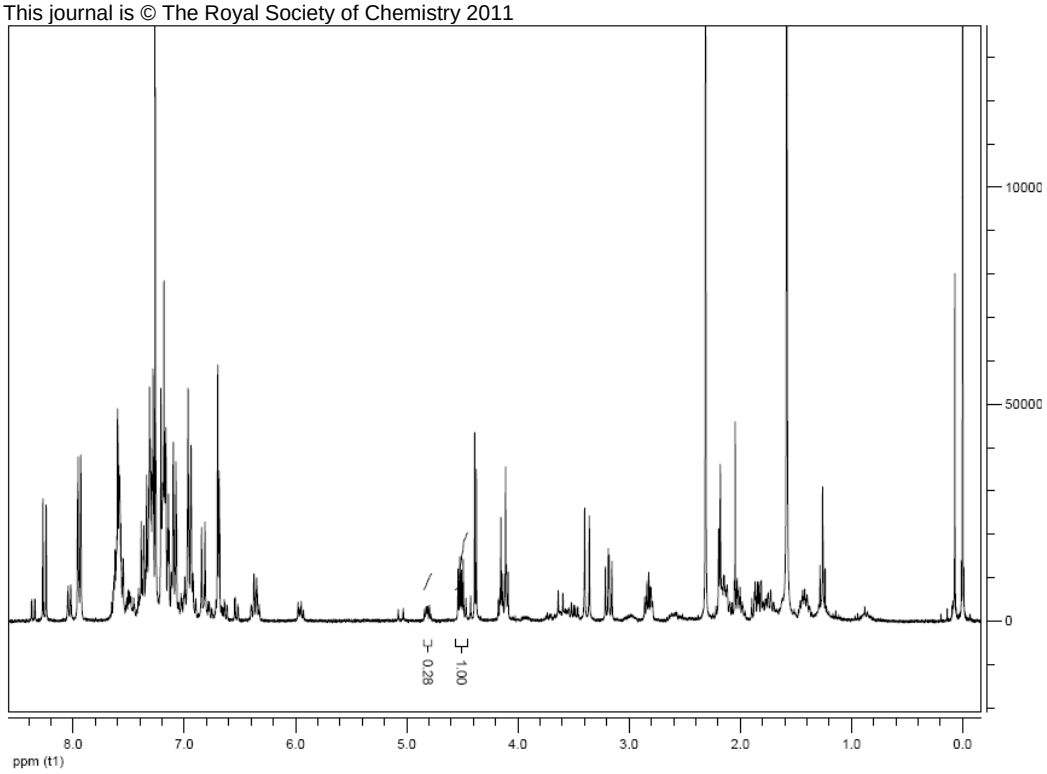

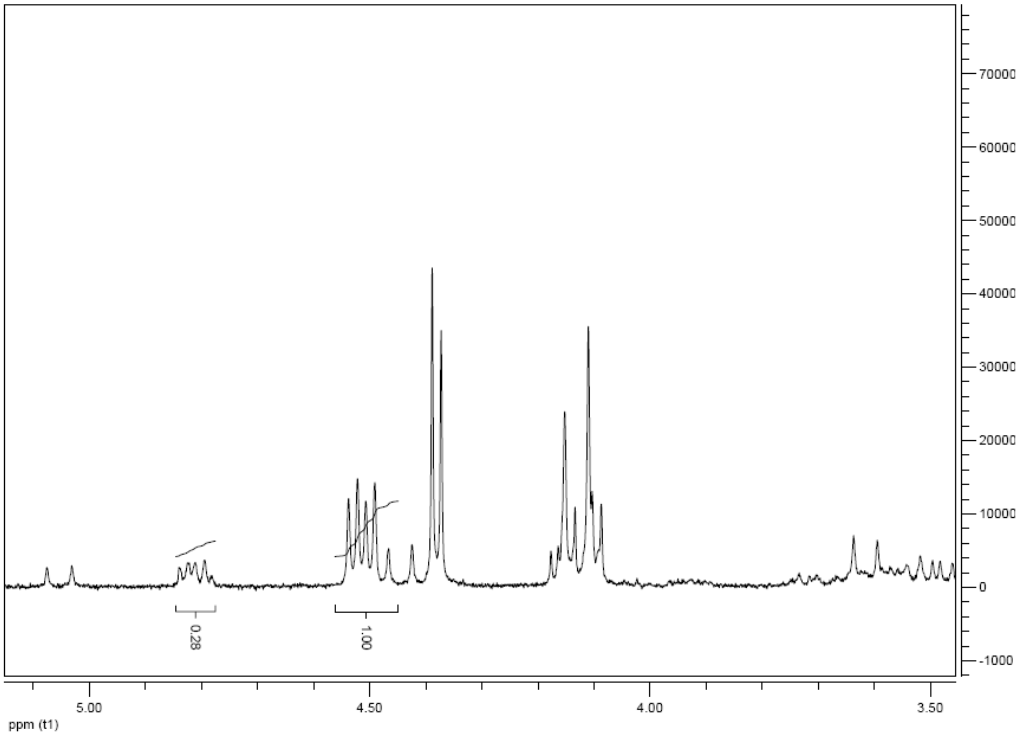

(R,2R,3S)-3g: δ_H 4.45–4.55 (m, β-CH)
(R,2R,3R)-3g: δ_H, 4.75–4.85(m, β-CH)
(R,2R,3S)-3g/(R,2R,3R)-3g =78:22