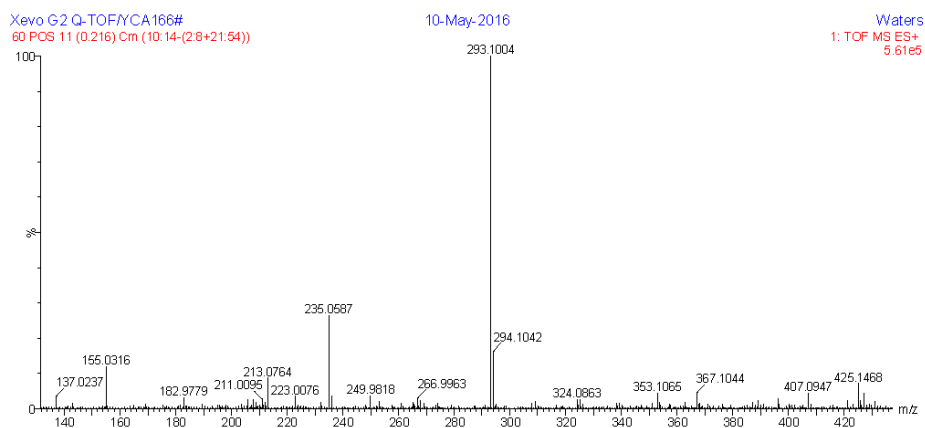
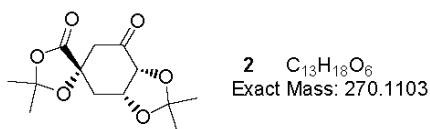


# Supplementary Materials: Synthesis, Anti-HCV, Antioxidant and Reduction of Intracellular Reactive Oxygen Species Generation of a Chlorogenic Acid Analogue with an Amide Bond Replacing the Ester Bond

Ling-Na Wang, Wei Wang, Masao Hattori, Mohsen Daneshtalab and Chao-Mei Ma

(+) HRESIMS of compound 2	S2
(+) HRESIMS of compound 3	S3
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<sup>1</sup> H-NMR spectrum of 6a	S10
<sup>13</sup> C-NMR spectrum of 6a	S10
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<sup>13</sup> C-NMR spectrum of 6b	S11
HRFABMS(-) spectrum of 6a	S12

## (+)-HRESIMS of compound 2

Elemental Composition Report of [2+Na]<sup>+</sup>

## Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

508 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

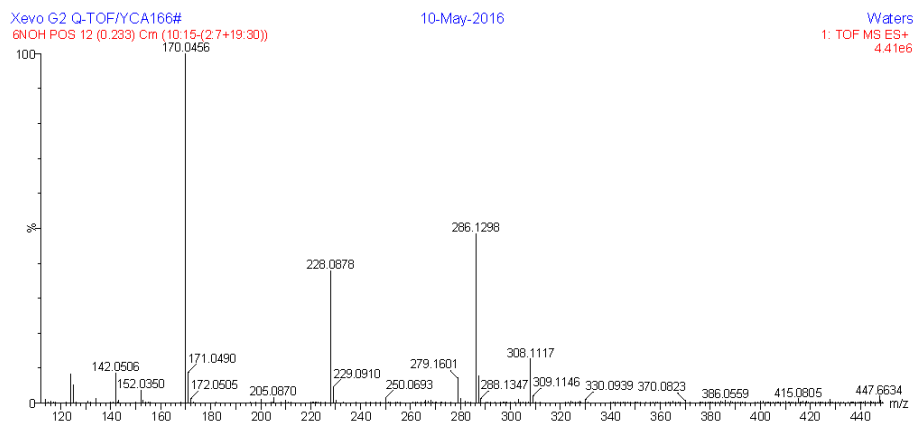
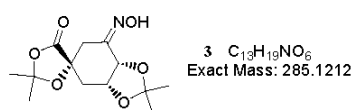
Elements Used: C: 0-100 H: 0-200 N: 0-5 O: 0-20 Na: 0-1

Minimum: -1.5

Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
293.1004	293.1001	0.3	1.0	4.5	223.4	0.386	67.95	C <sub>13</sub> H <sub>18</sub> O <sub>6</sub> Na

## (+)-HRESIMS of compound 3

Elemental Composition Report of [3+H]<sup>+</sup>

## Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

## Monoisotopic Mass, Even Electron Ions

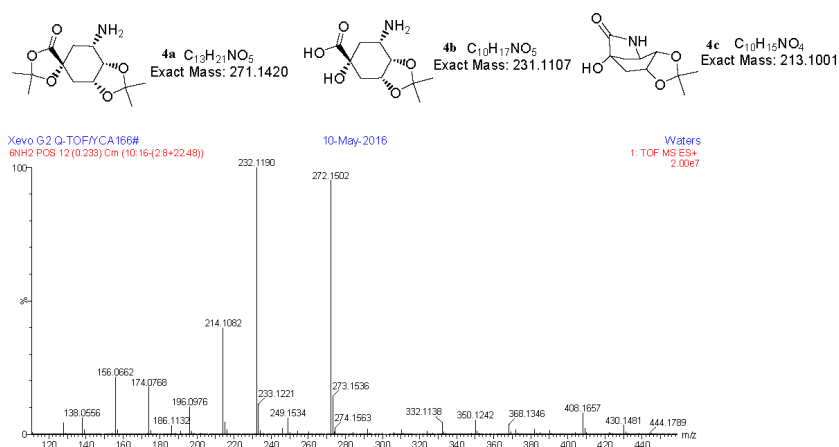
482 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

Elements Used: C: 0-100 H: 0-200 N: 0-5 O: 0-20 Na: 0-1

Minimum: -1.5

Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
286.1298	286.1291	0.7	2.4	4.5	342.1	0.008	99.19	C <sub>13</sub> H <sub>20</sub> N O <sub>6</sub>

(+)<sup>1</sup>HRESIMS of compound 4Elemental Composition Report of [4a+H]<sup>+</sup>

## Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

439 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

Elements Used: C: 0-100 H: 0-200 N: 0-5 O: 0-20 Na: 0-1

Minimum: -1.5

Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
272.1502	272.1498	0.4	1.5	3.5	659.7	0.003	99.71	C13 H22 N O5

Elemental Composition Report of [4b+H]<sup>+</sup>

## Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

332 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

Elements Used: C: 0-100 H: 0-200 N: 0-5 O: 0-20 Na: 0-1

Minimum: -1.5

Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
232.1190	232.1185	0.5	2.2	2.5	594.8	0.002	99.83	C10 H18 N O5

Elemental Composition Report of [4c+H]<sup>+</sup>

## Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

286 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

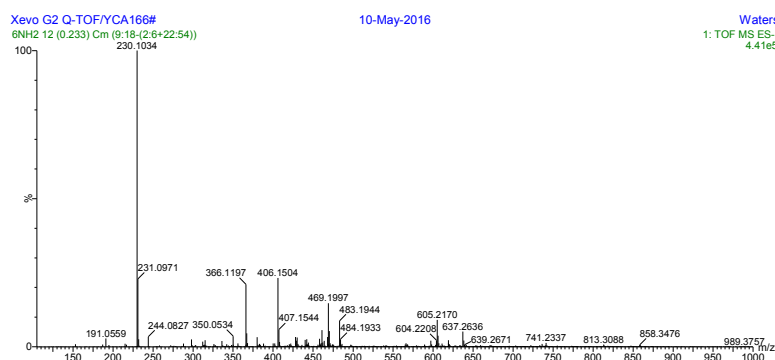
Elements Used: C: 0-100 H: 0-200 N: 0-5 O: 0-20 Na: 0-1

Minimum: -1.5

Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
214.1082	214.1079	0.3	1.4	3.5	577.3	0.322	72.47	C <sub>10</sub> H <sub>16</sub> N O <sub>4</sub>

(-) HRESIMS of 4



Elemental Composition Report of [4b-H]<sup>-</sup>

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

327 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

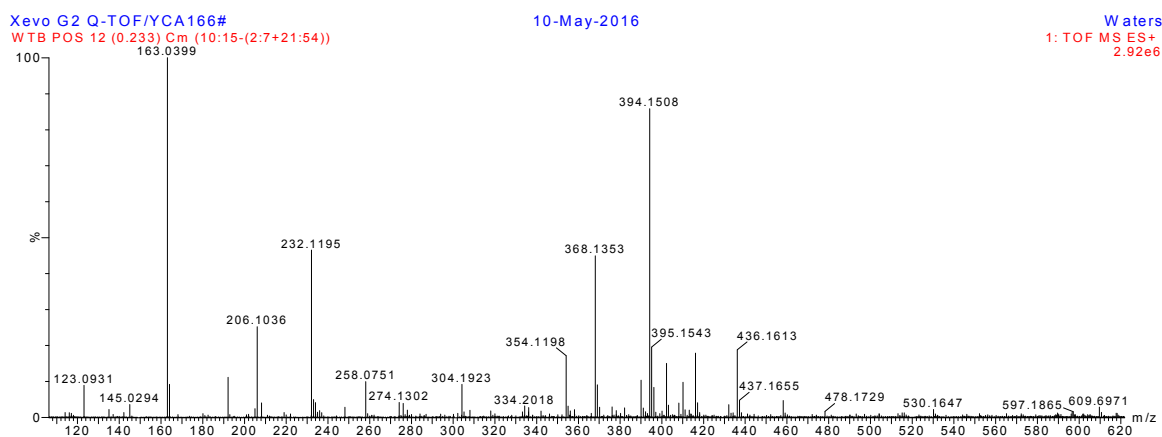
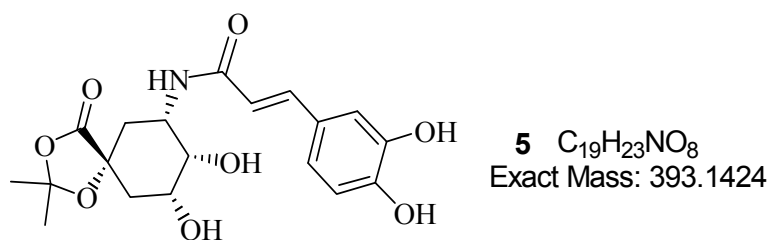
Elements Used: C: 0-100 H: 0-200 N: 0-5 O: 0-20 Na: 0-1

Minimum: -1.5

Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
230.1034	230.1028	0.6	2.6	3.5	190.3	1.160	31.36	C <sub>10</sub> H <sub>16</sub> N O <sub>5</sub>

## (+)-HRESIMS of 5

Elemental Composition Report of [5+H]<sup>+</sup>

## Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

846 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)

Elements Used: C: 0-100 H: 0-200 N: 0-5 O: 0-20 Na: 0-1

Minimum: -1.5

Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
394.1508	394.1502	0.6	1.5	8.5	379.8	0.867	42.01	C <sub>19</sub> H <sub>24</sub> N O <sub>8</sub>

Elemental Composition Report of [5+Na]<sup>+</sup>

## Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

915 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)

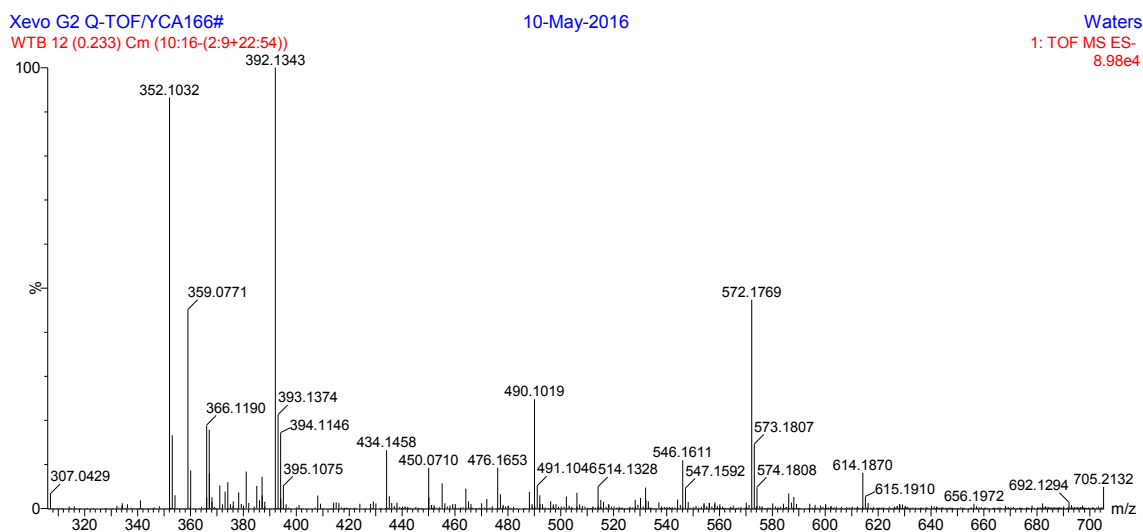
Elements Used: C: 0-100 H: 0-200 N: 0-5 O: 0-20 Na: 0-1

Minimum: -1.5

Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
416.1327	416.1321	0.6	1.4	8.5	329.3	1.330	26.46	C <sub>19</sub> H <sub>23</sub> N O <sub>8</sub> Na

## (-) HRESIMS of 5

Elemental Composition Report of [5-H]<sup>-</sup>

## Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

## Monoisotopic Mass, Even Electron Ions

840 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)

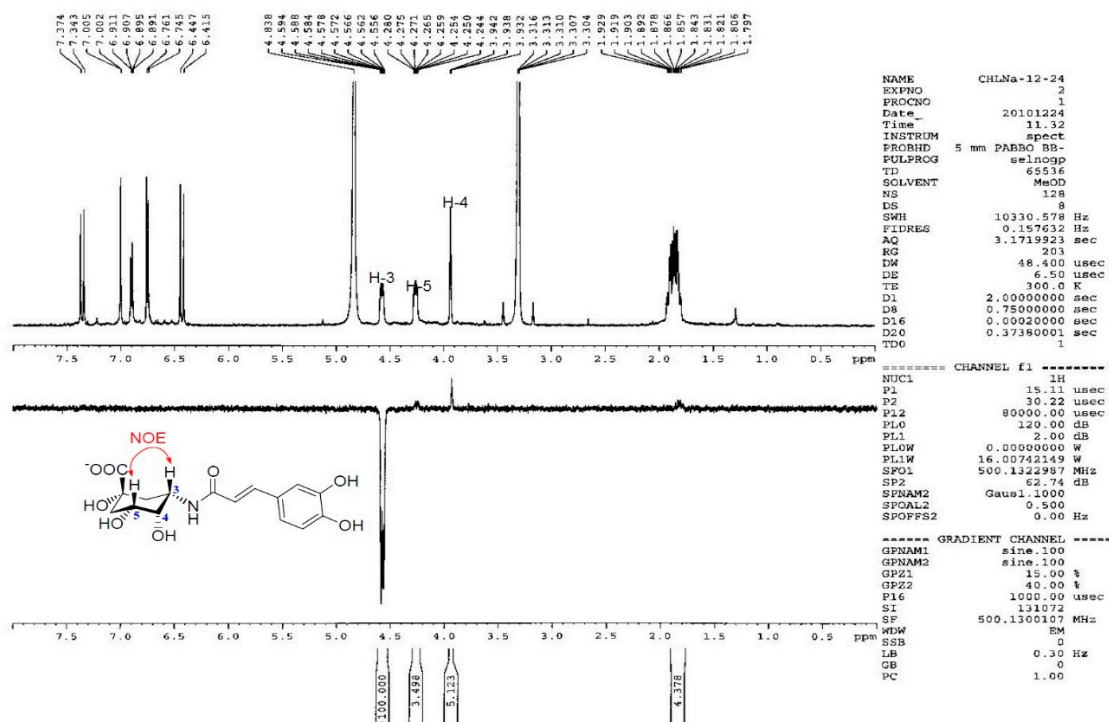
Elements Used: C: 0-100 H: 0-200 N: 0-5 O: 0-20 Na: 0-1

Minimum: -1.5

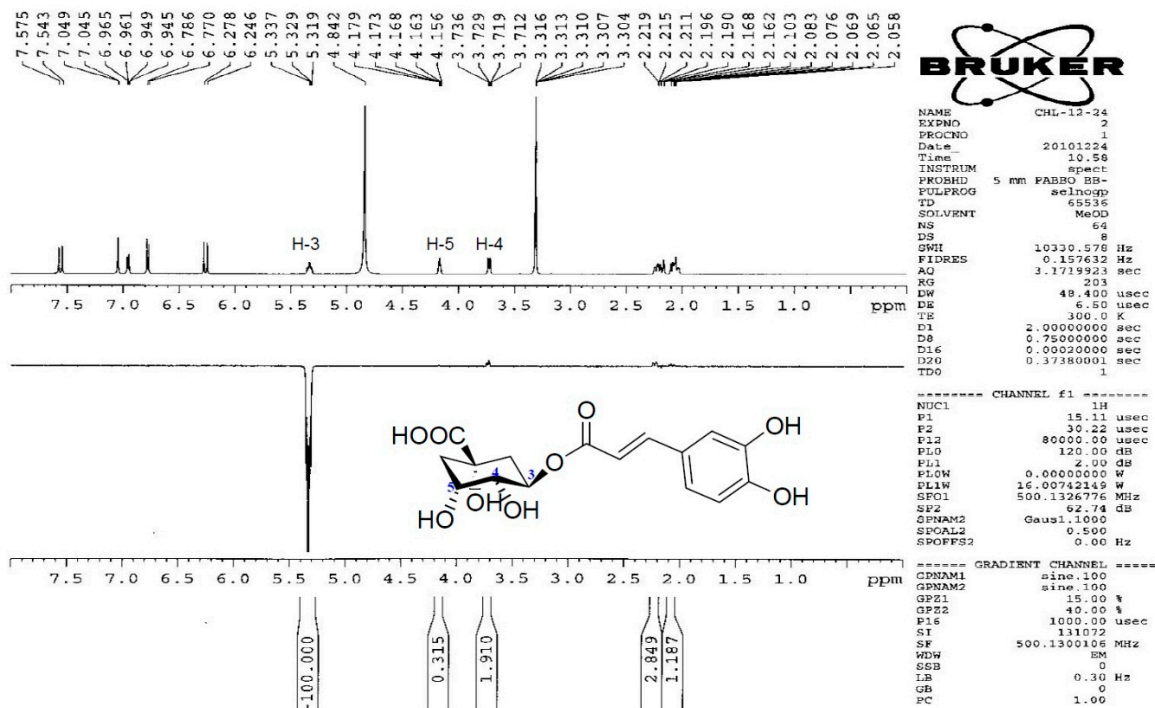
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
392.1343	392.1345	-0.2	-0.5	9.5	154.1	2.425	8.85	C <sub>19</sub> H <sub>22</sub> N <sub>1</sub> O <sub>8</sub>

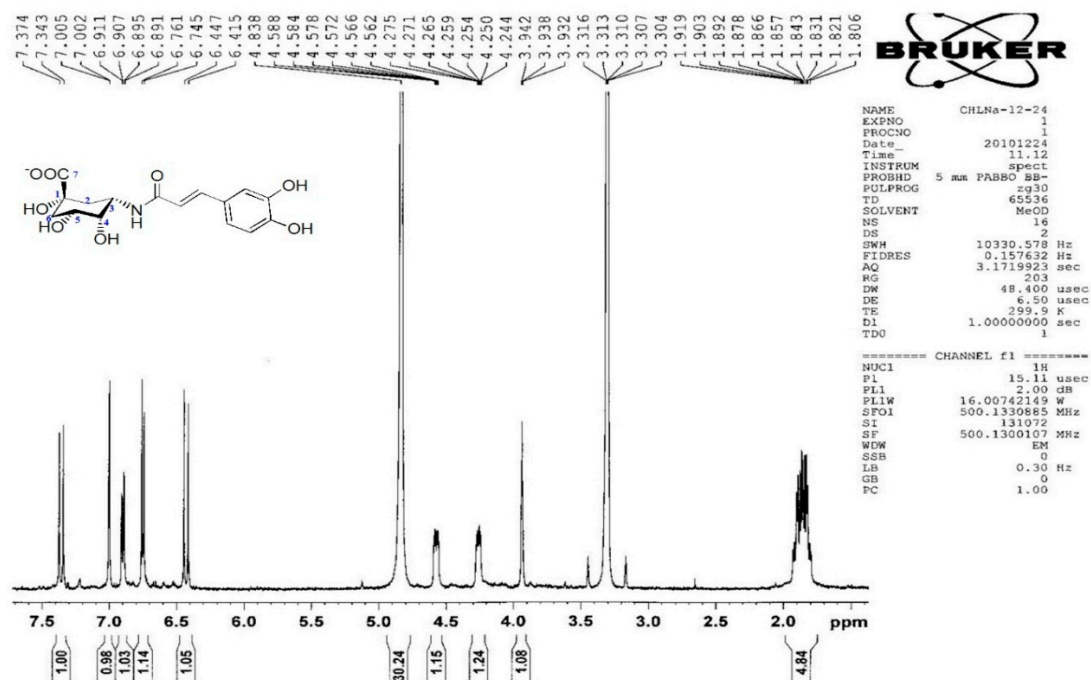
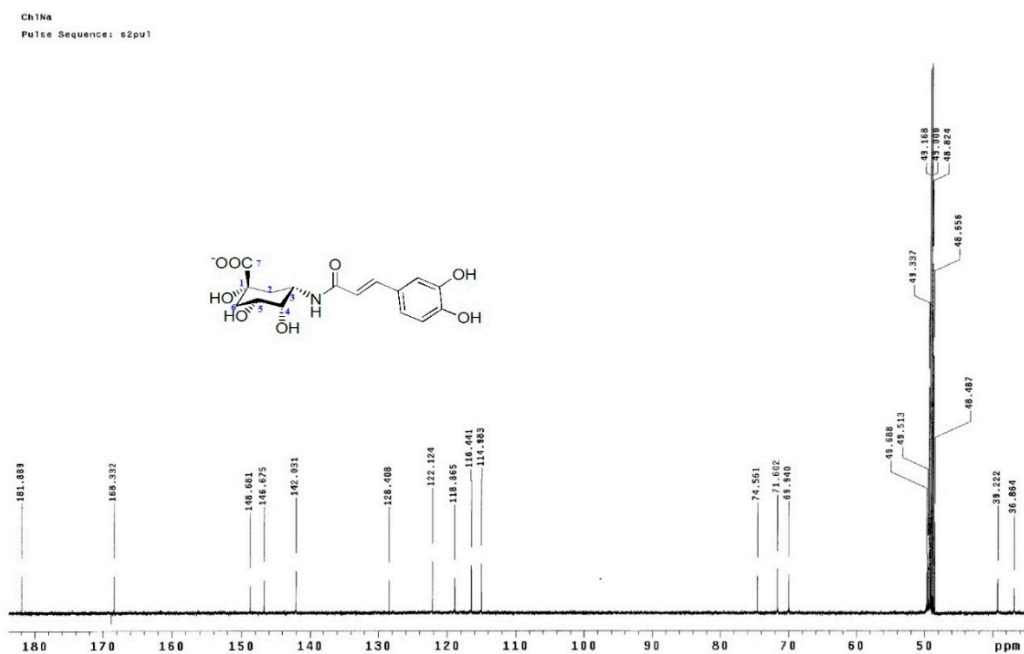
NOE spectrum of 6a

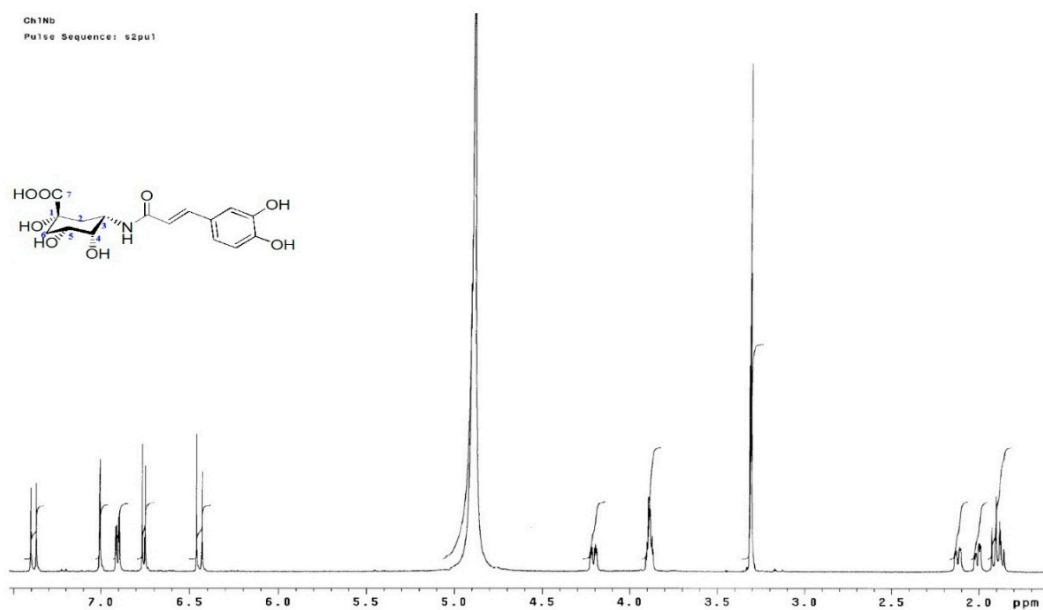
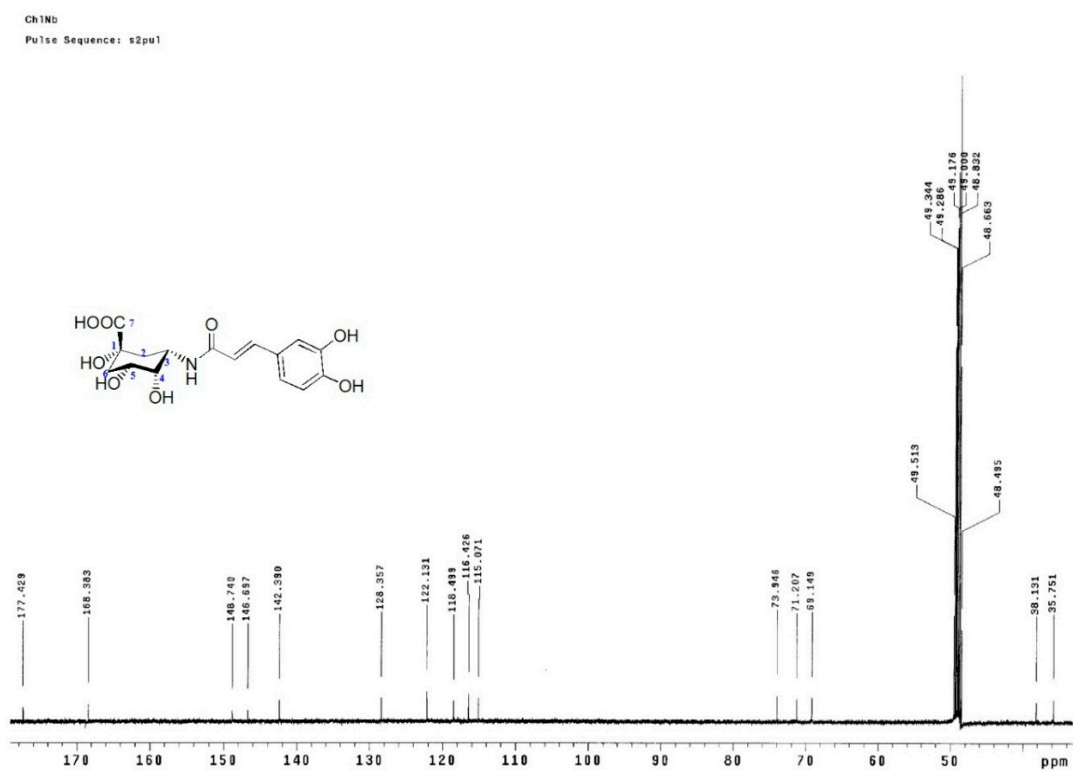


NOE spectrum of chlorogenic acid





<sup>1</sup>H-NMR spectrum of 6a<sup>13</sup>C-NMR spectrum of 6a

<sup>1</sup>H-NMR spectrum of **6b**<sup>13</sup>C-NMR spectrum of **6b**

## (-) HRFABMS of 6a

File: ChIN007  
Sample: - -  
Instrument: AX505W  
Inlet: Direct

Date Run: 7-16-2009 (Time Run: 13:16:24)

Ionization mode: FAB-

Scan: 3  
Base: m/z 352; 38.8%FS TIC: 3626674

R.T.: .18

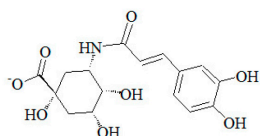
#Ions: 65

Selected Isotopes : H C<sub>0-16</sub> O<sub>0-8</sub> N<sub>0-1</sub>

Error Limit : 20 mmu

Unsaturation Limits : 0 to 50

<u>Measured Mass</u>	<u>% Base</u>	<u>Formula</u>	<u>Calculated Mass</u>	<u>Error</u>	<u>Unsaturation</u>
352.10167	100.0%	C <sub>16</sub> H <sub>18</sub> O <sub>8</sub> N	352.10322	-1.6	8.5



**6a** C<sub>16</sub>H<sub>18</sub>NO<sub>8</sub><sup>-</sup>  
Exact Mass: 352.1032