Supporting Information

***Rec. Nat. Prod*. 15:2 (2021) 103-110**

A New Cynaropicrin Derivative from *Cynara Scolymus* L.

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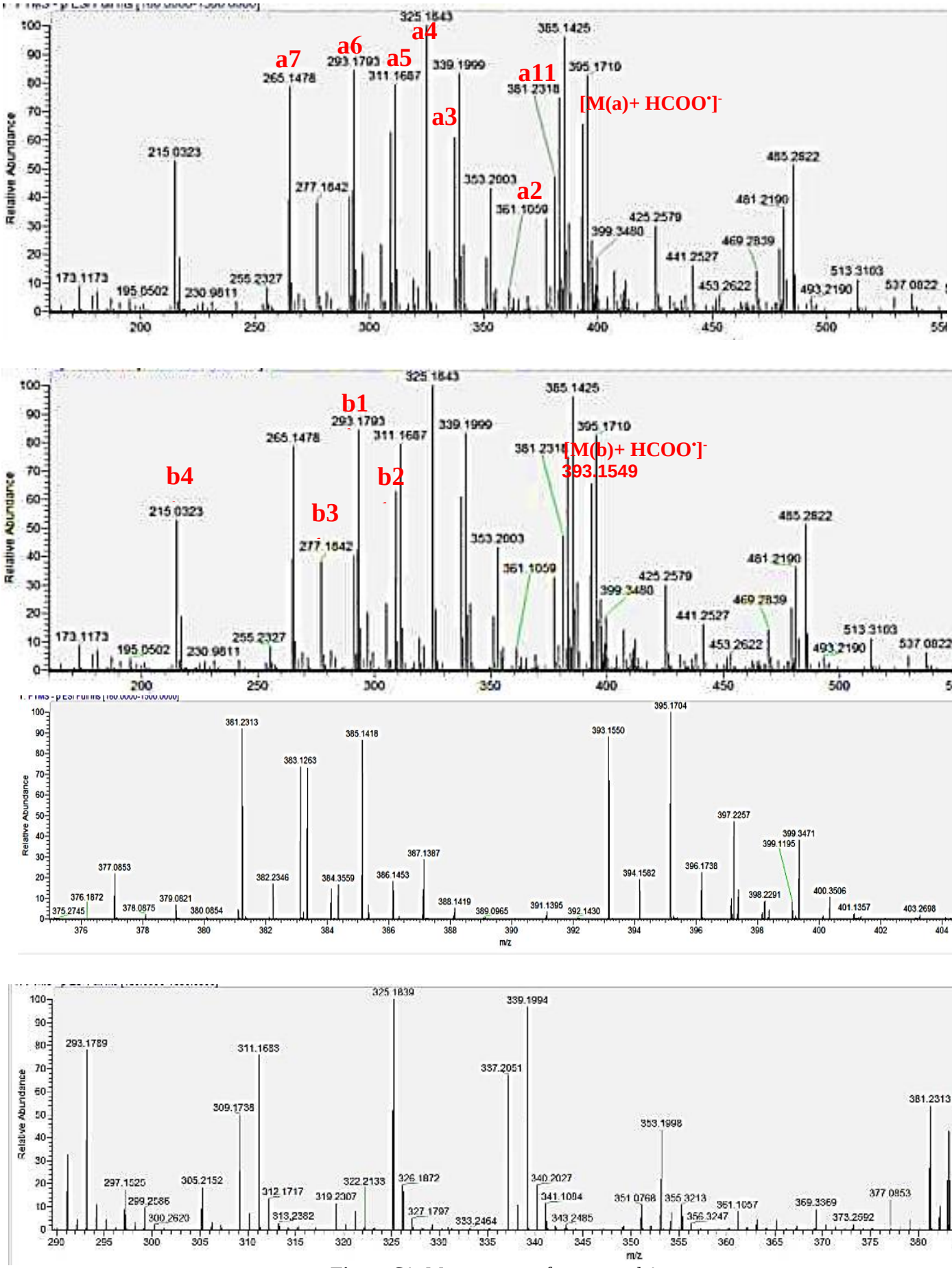


Figure S1: Mass spectra of compound **1**

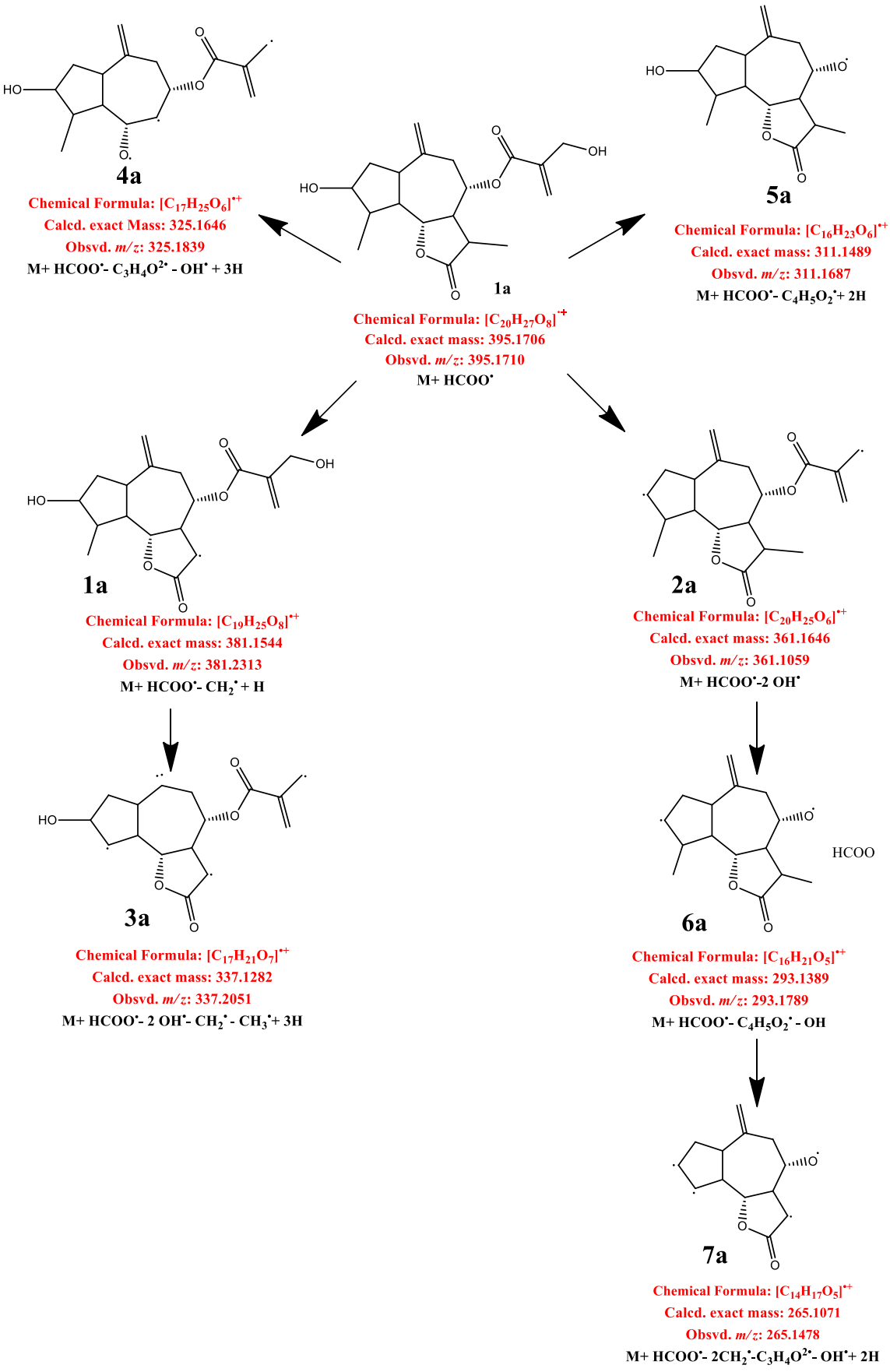


Figure S2: Mass spectrum and fragmentation pattern of **1a**

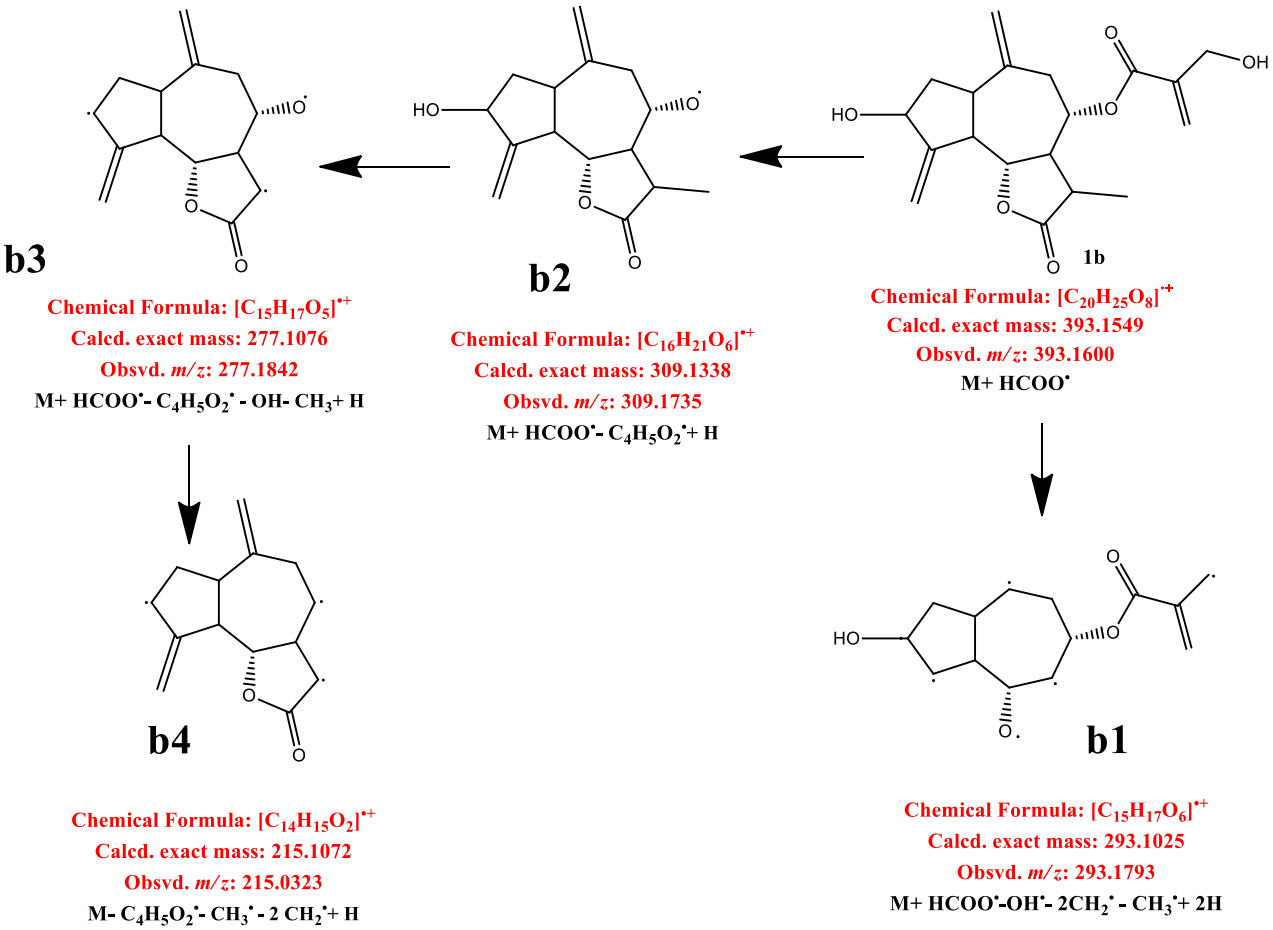


Figure S3: Mass spectrum and fragmentation pattern of **1b**

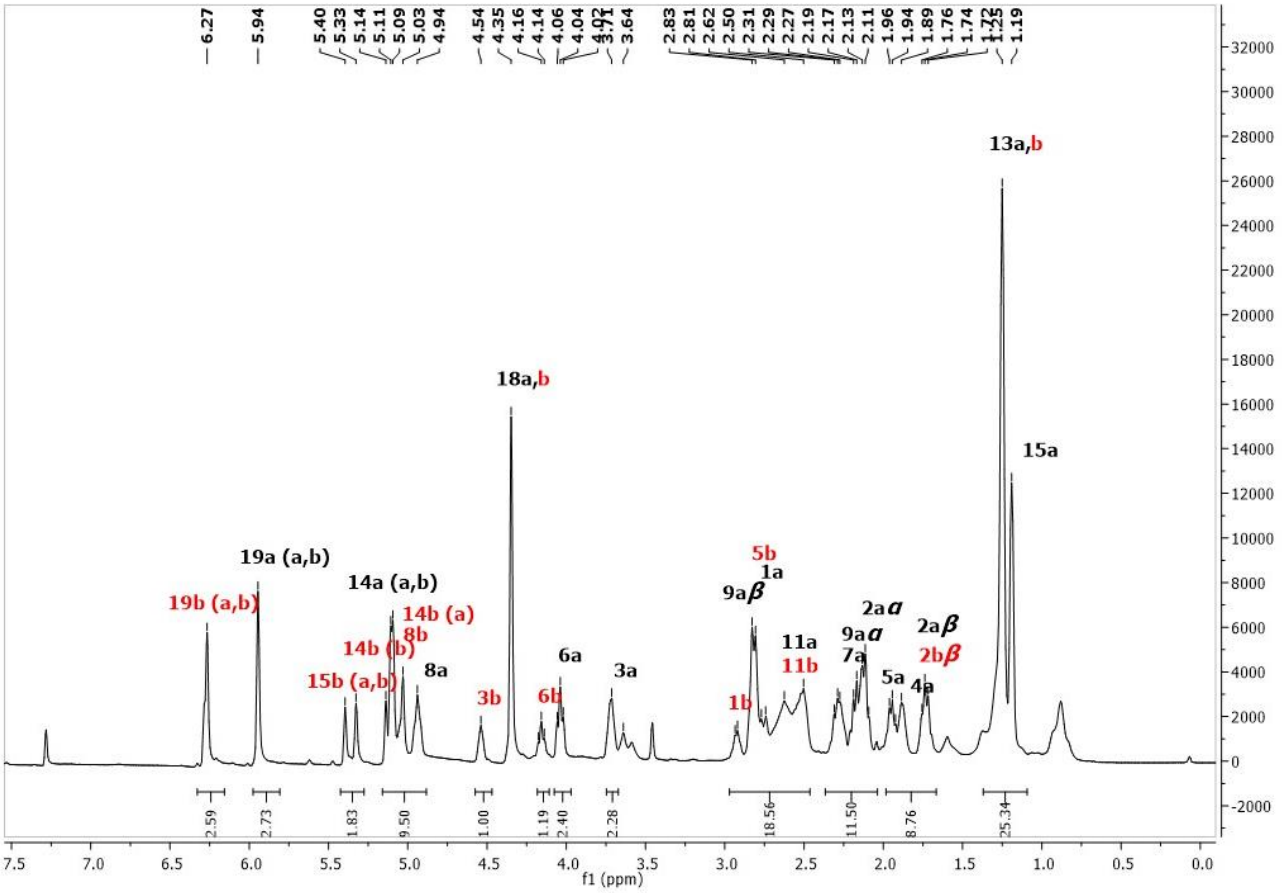


Figure S4: ^{1}H NMR spectrum of compound **1** from 1 to 7.5 ppm.

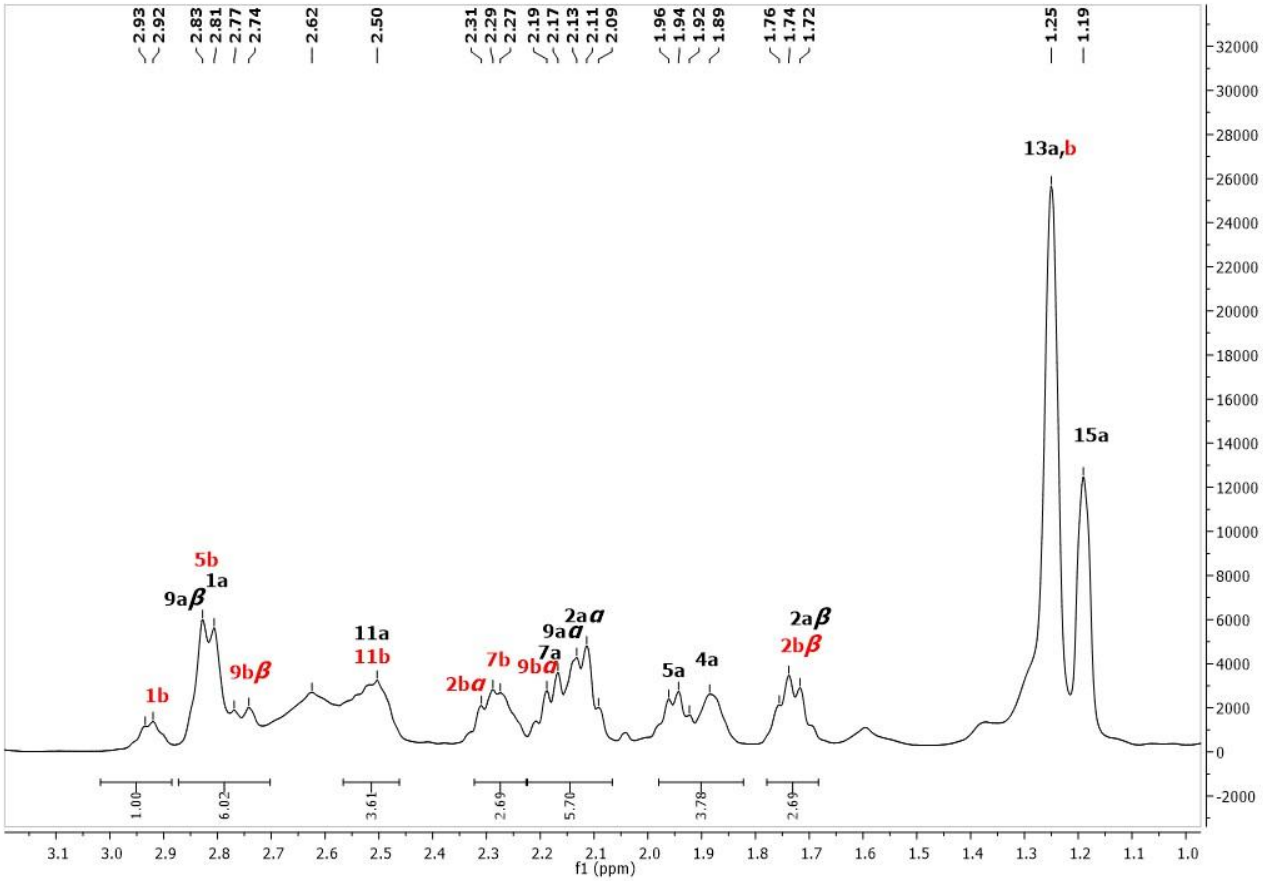


Figure S5: [1]H NMR spectrum of compound **1** from 1 to 3.1 ppm

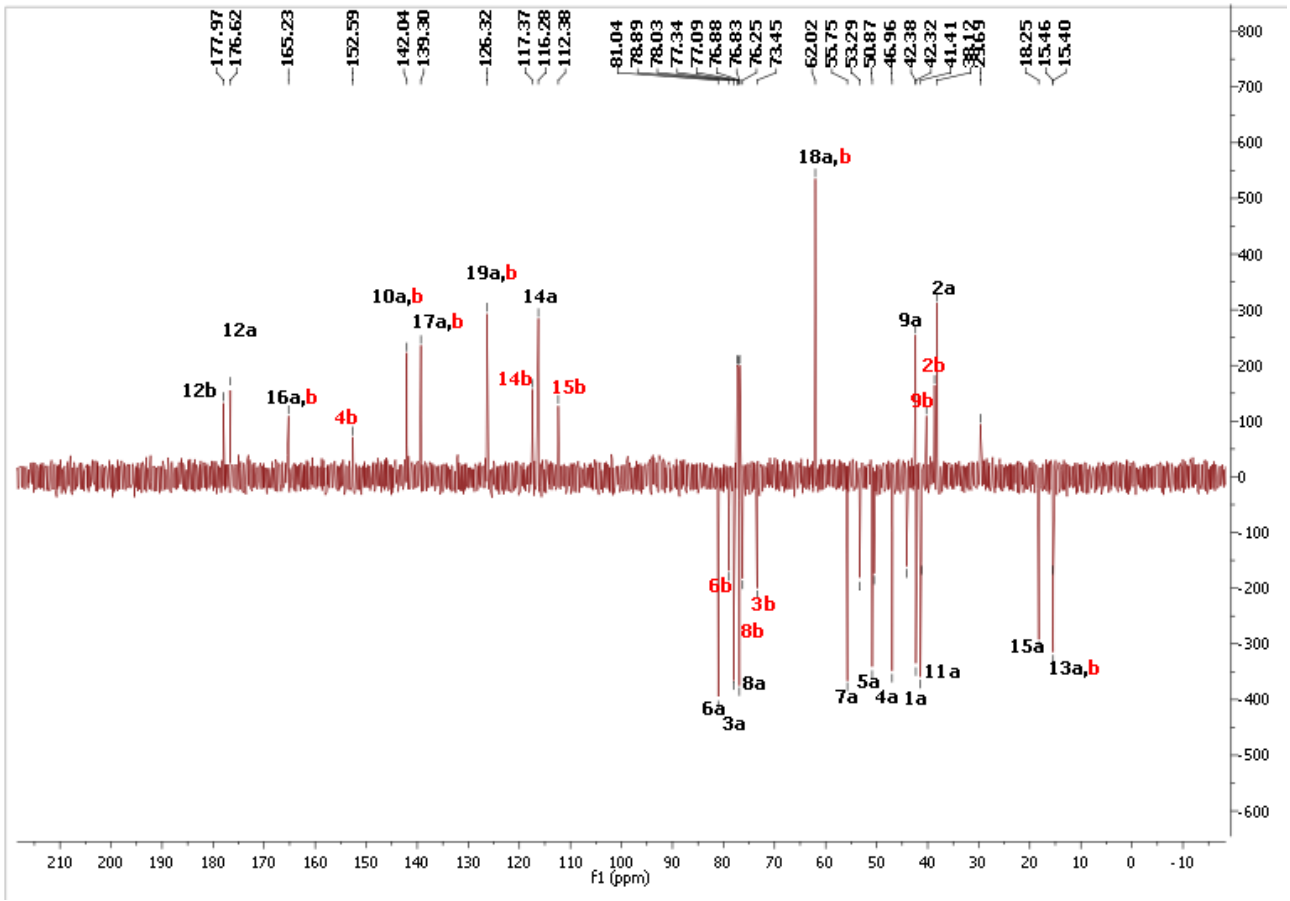


Figure S6: APT spectrum of compound **1**

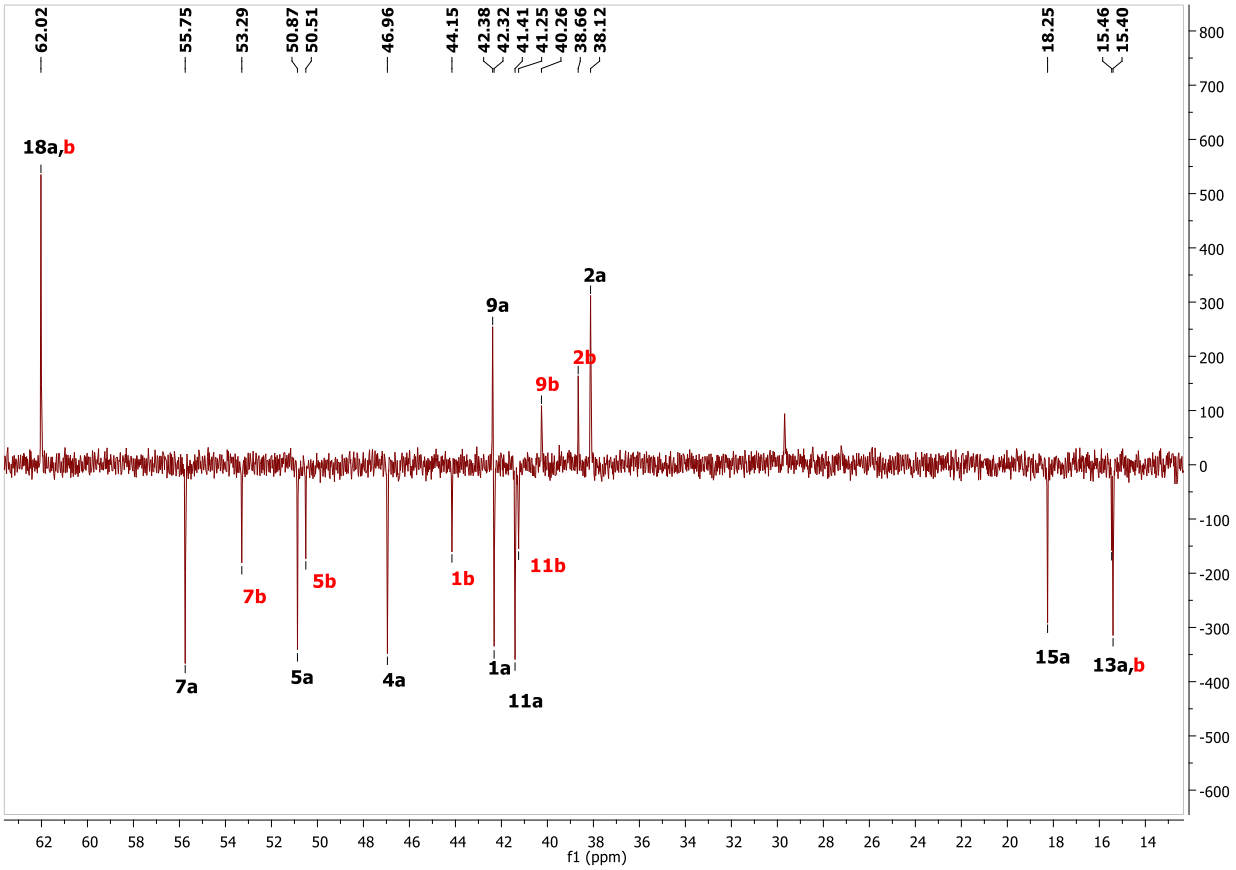


Figure S7: Expansion of APT spectrum of compound **1** from 8 to 66 ppm

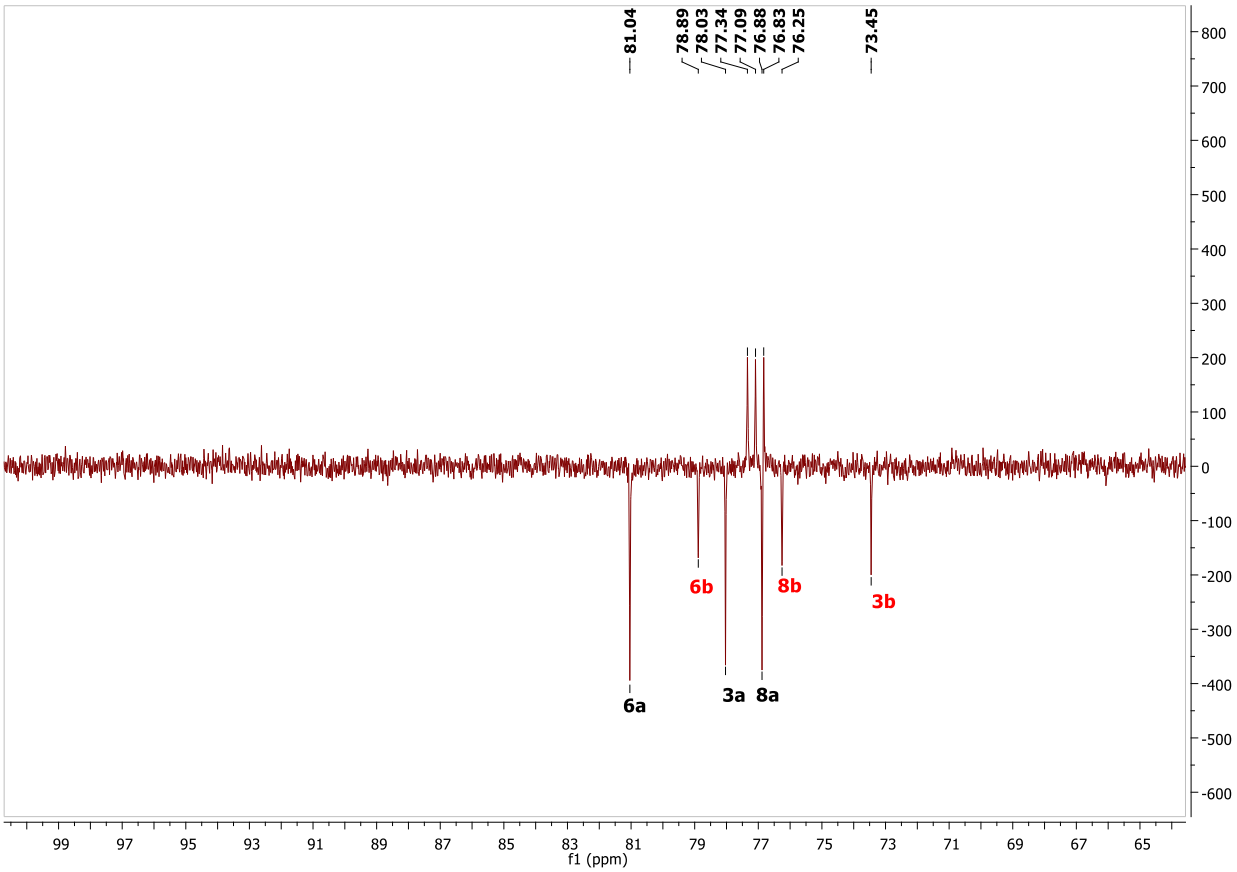


Figure S8: Expansion of APT spectrum of compound **1** from 69 to 93 ppm

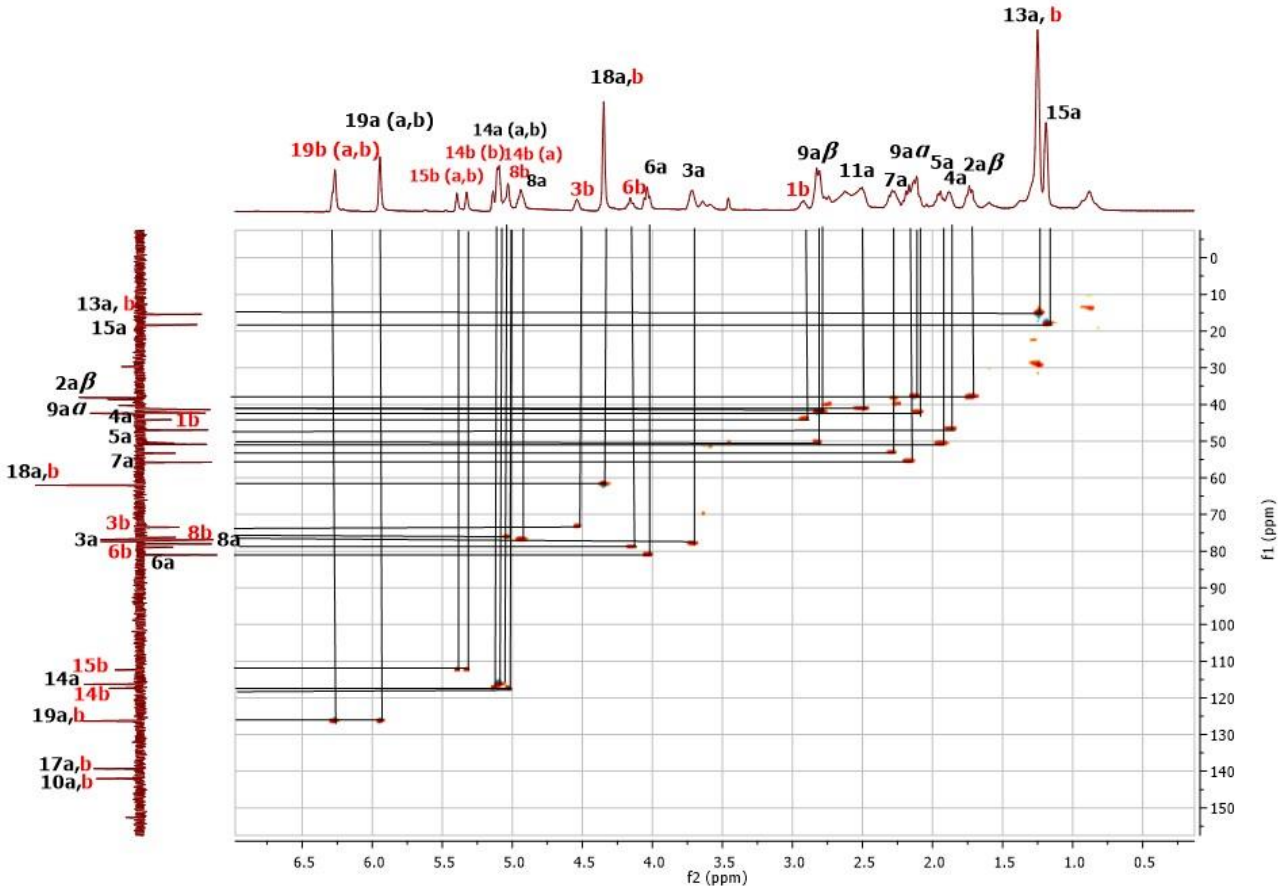


Figure S9: HSQC spectrum of compound **1**

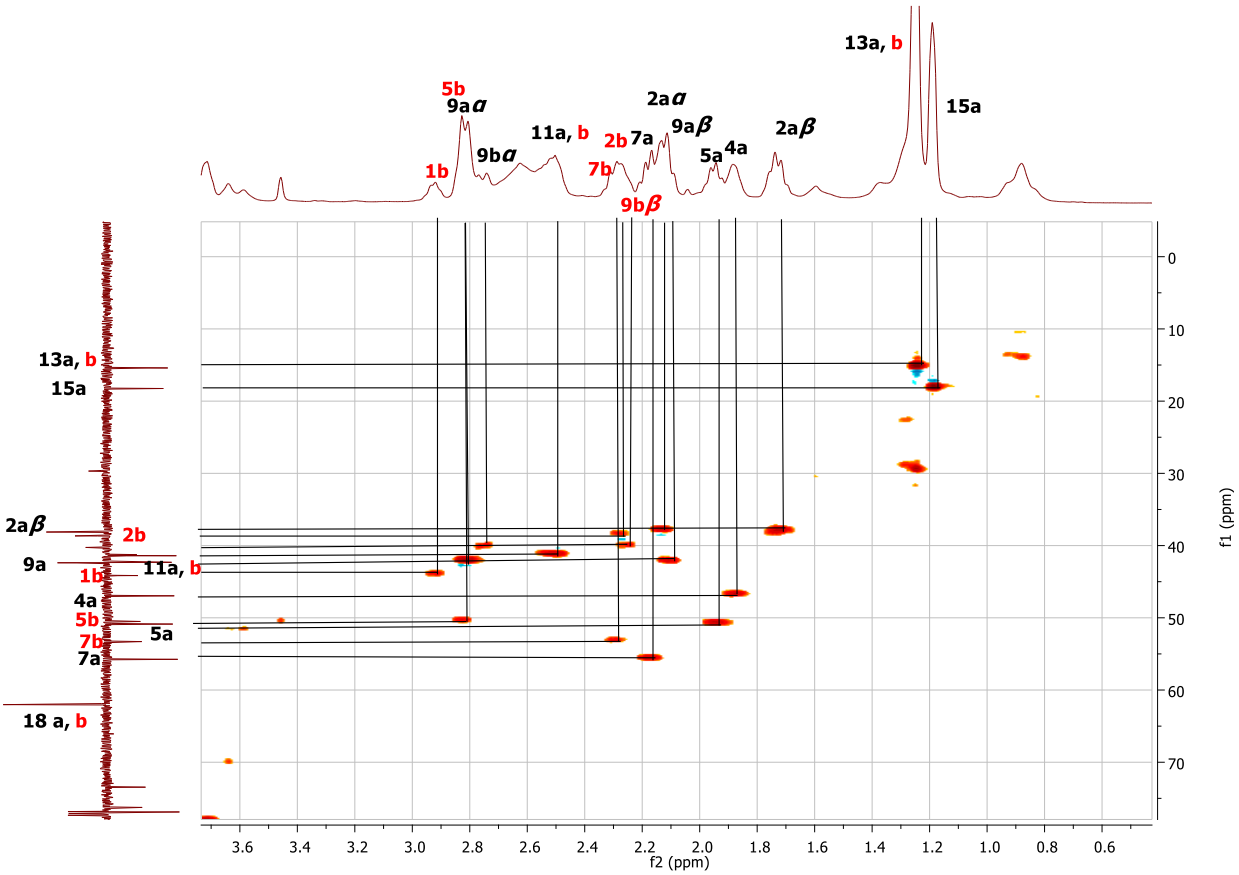


Figure S10: HSQC spectrum of compound **1**

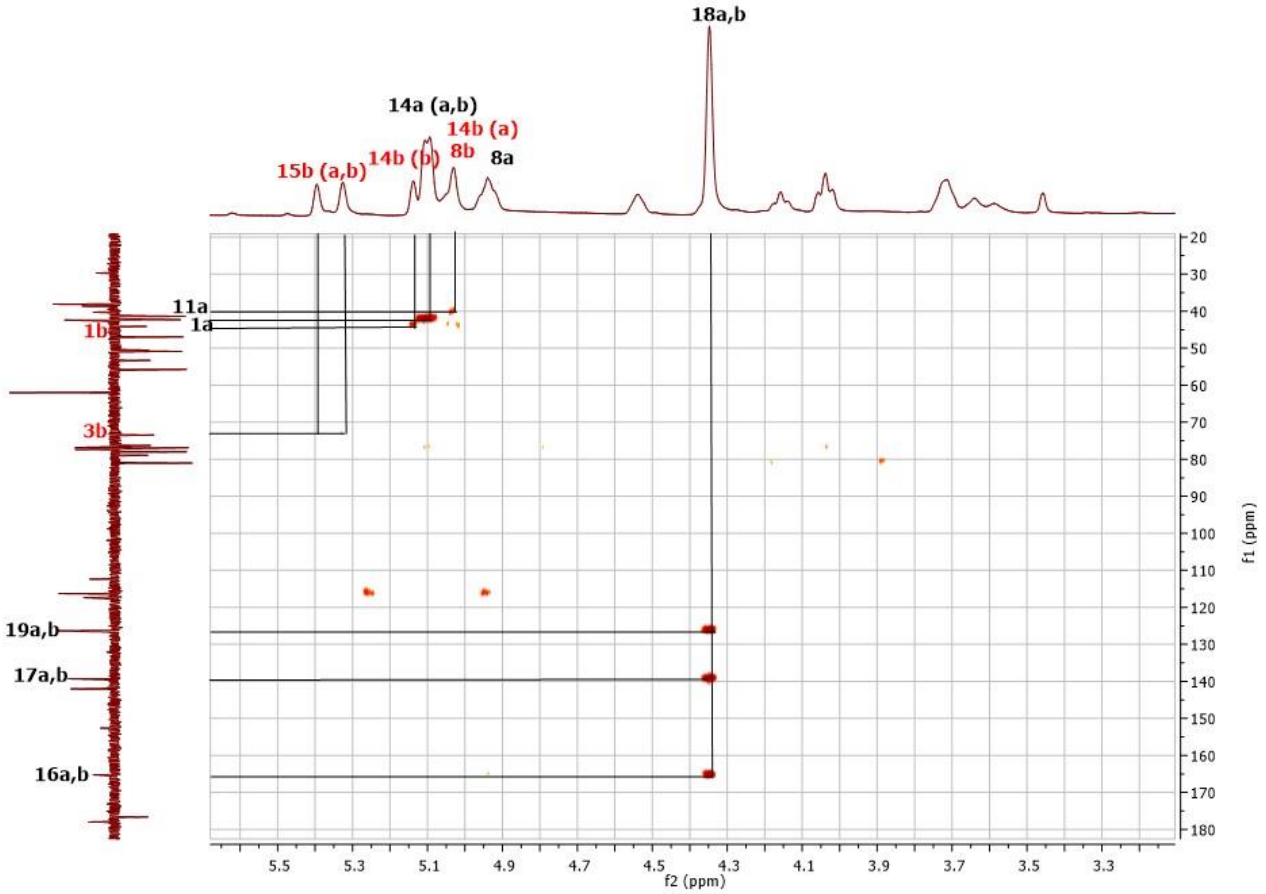


Figure S11: HMBC spectrum of compound **1** from 3.3 to 5.5 ppm

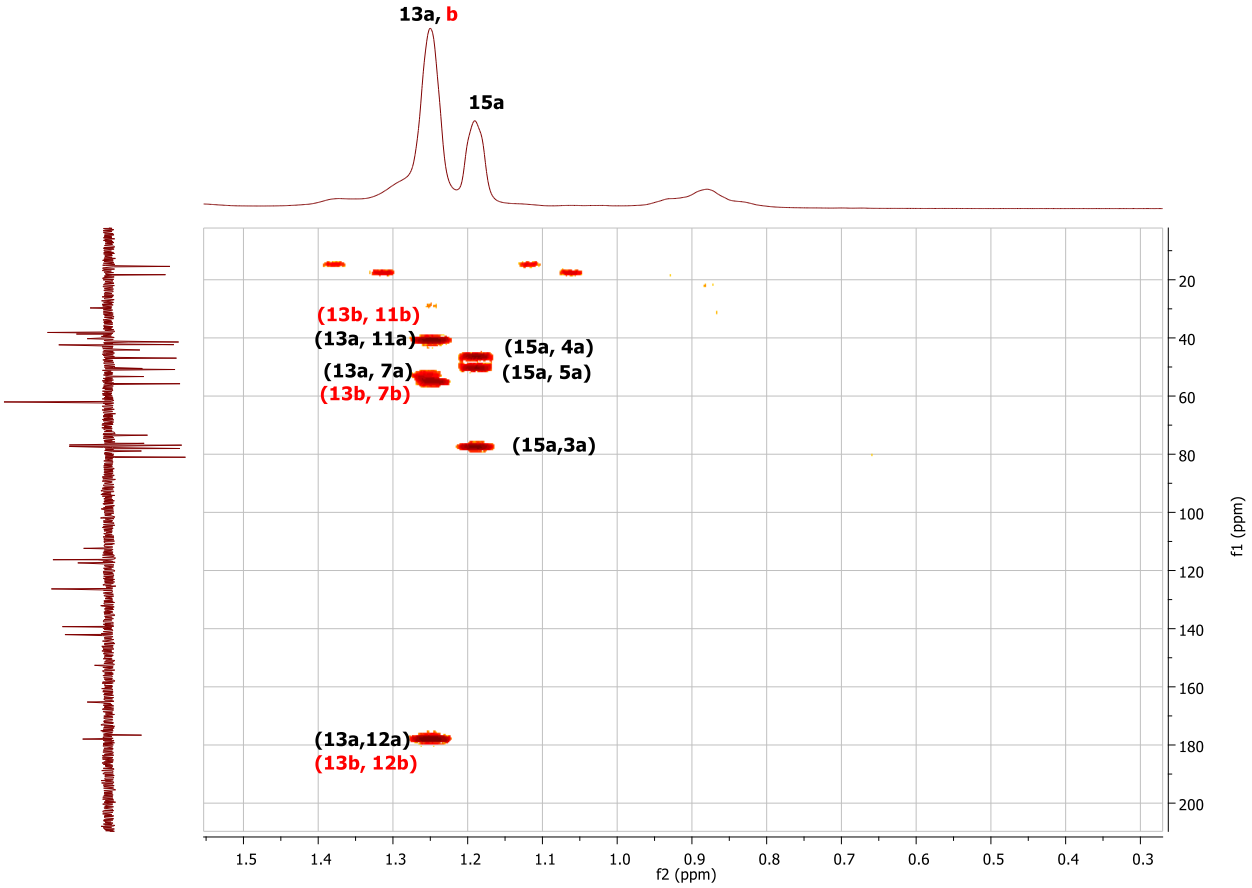


Figure S12: HMBC spectrum of compound **1** from 0.3 to 1.5 ppm

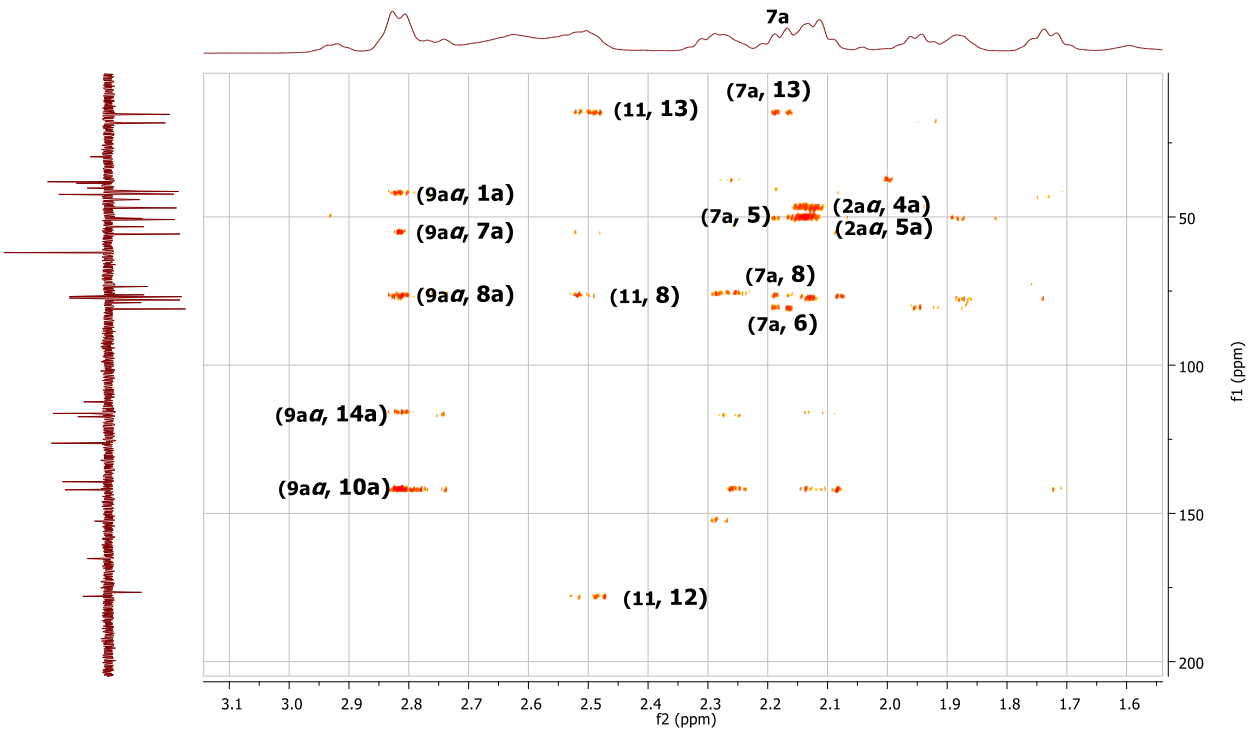


Figure S13: HMBC spectrum of compound **1** from 1.6 to 3.1 ppm

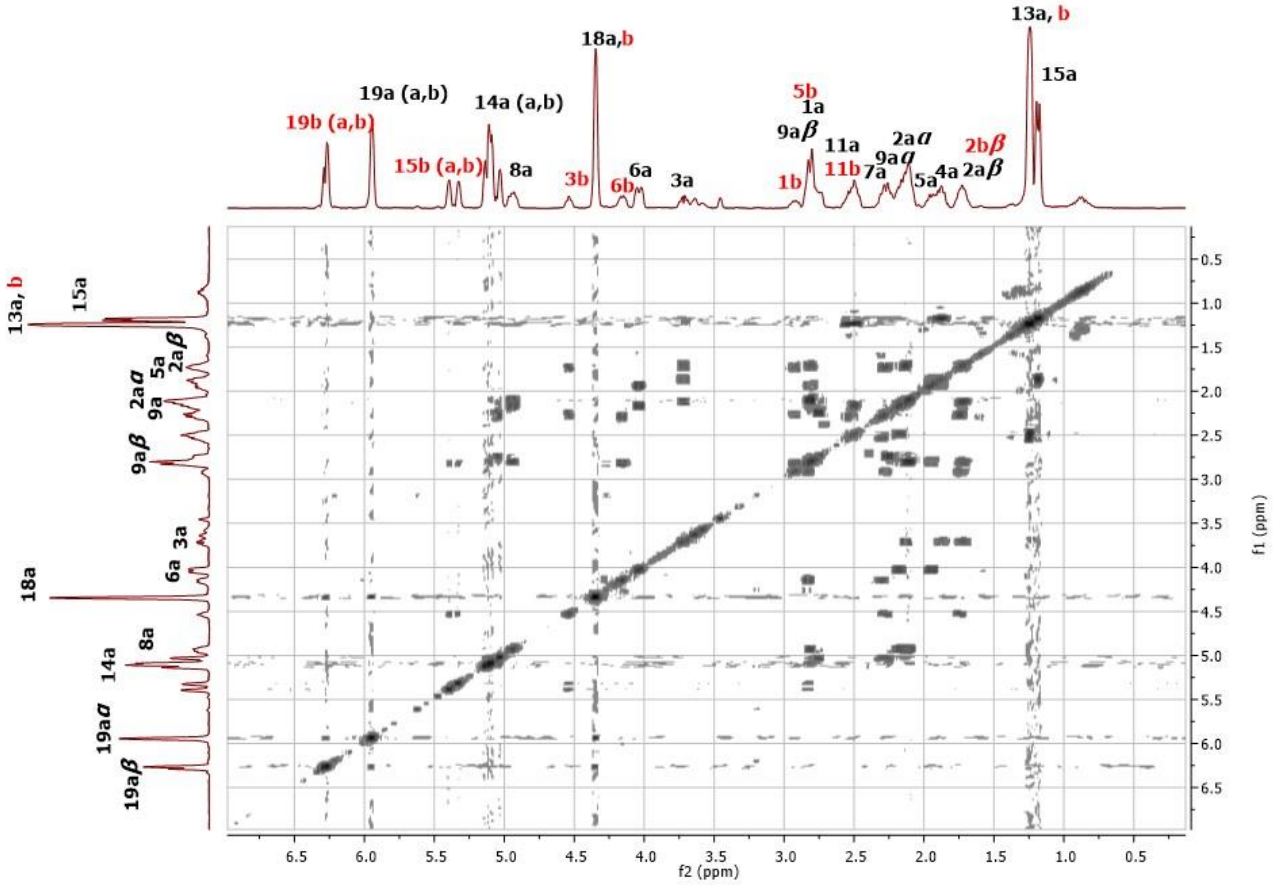


Figure S14: COSY spectrum of compound **1**

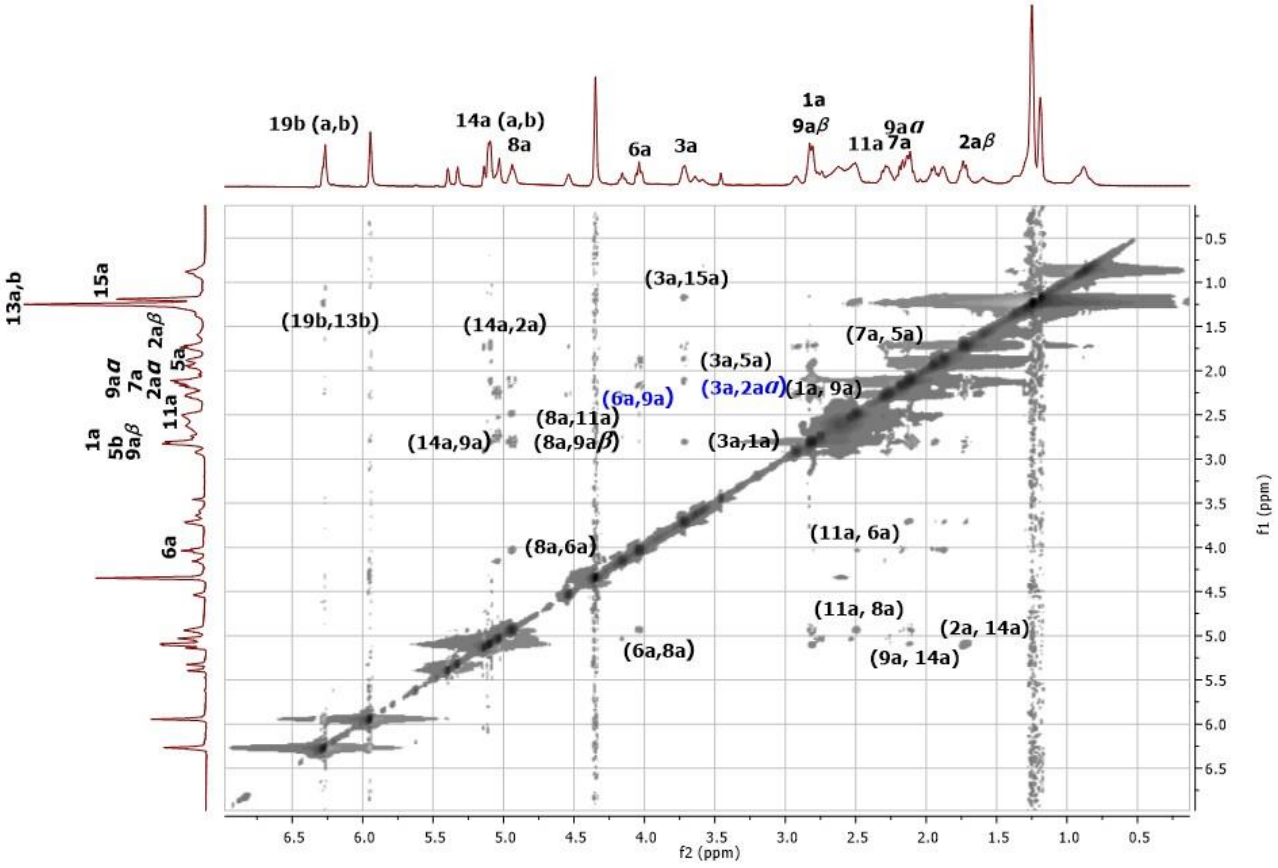


Figure S15: NOESY spectrum of compound **1**

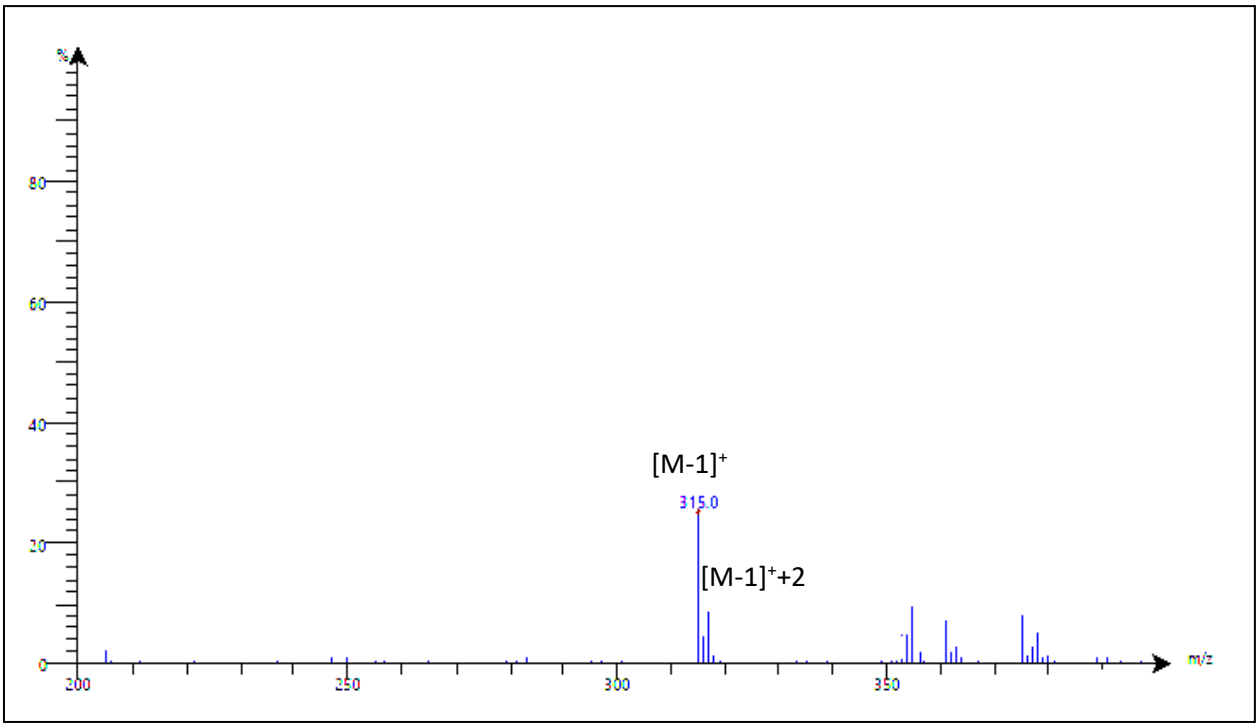


Figure S16: Mass spectrum of **2** (cynarinin B)

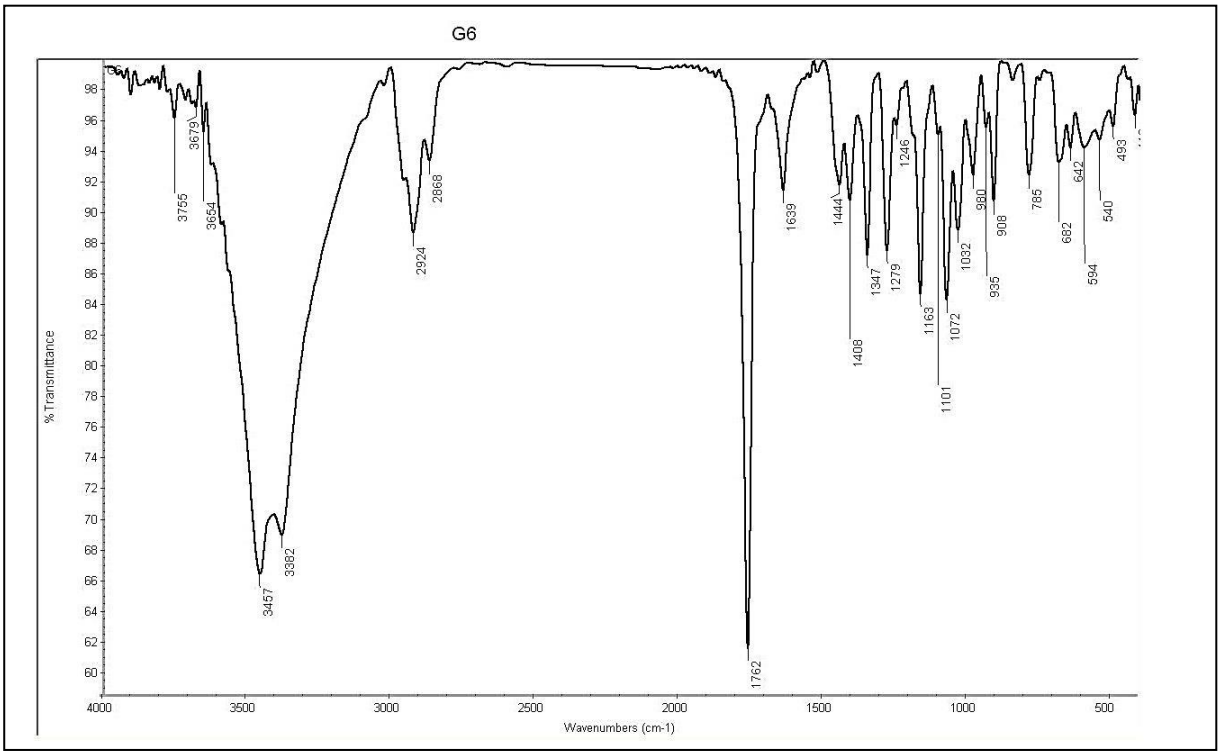


Figure S17: IR spectrum of compound **2**

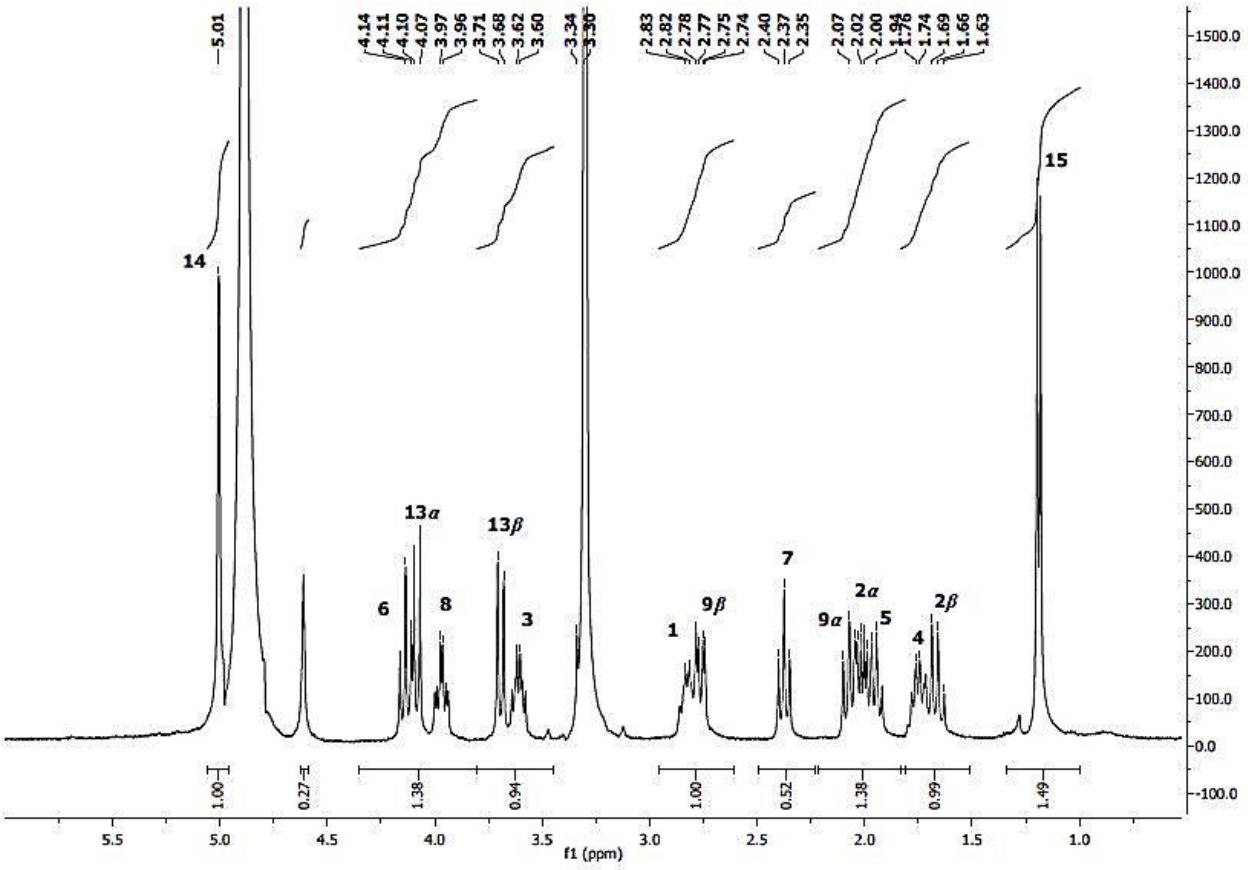


Figure S18: ^{1}H NMR spectrum of compound **2** (cynarinin B) from 1 to 5.5 ppm

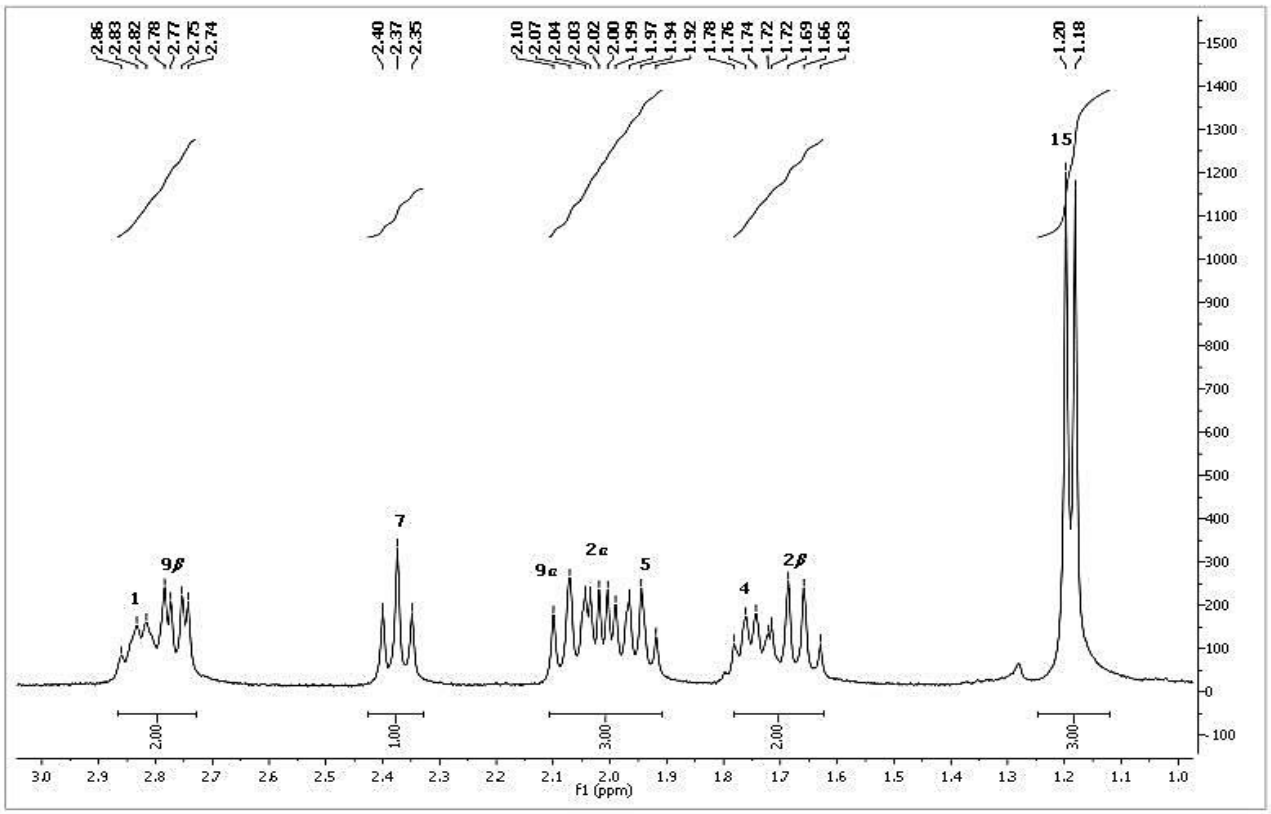


Figure S19: ^{1}H NMR spectrum of compound **2** from 1 to 3.0 ppm

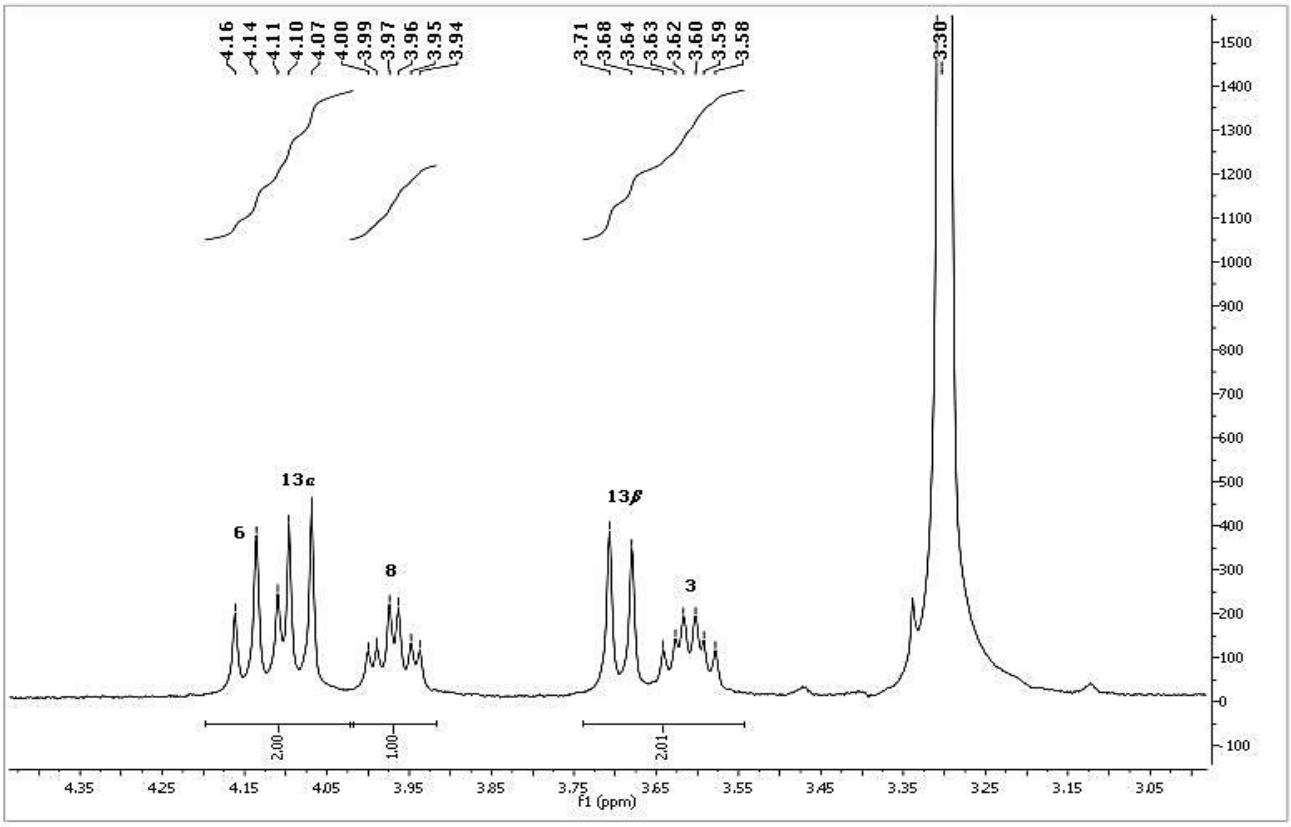


Figure S20: ^{1}H NMR spectrum of compound **2** from 3 to 4.35 ppm

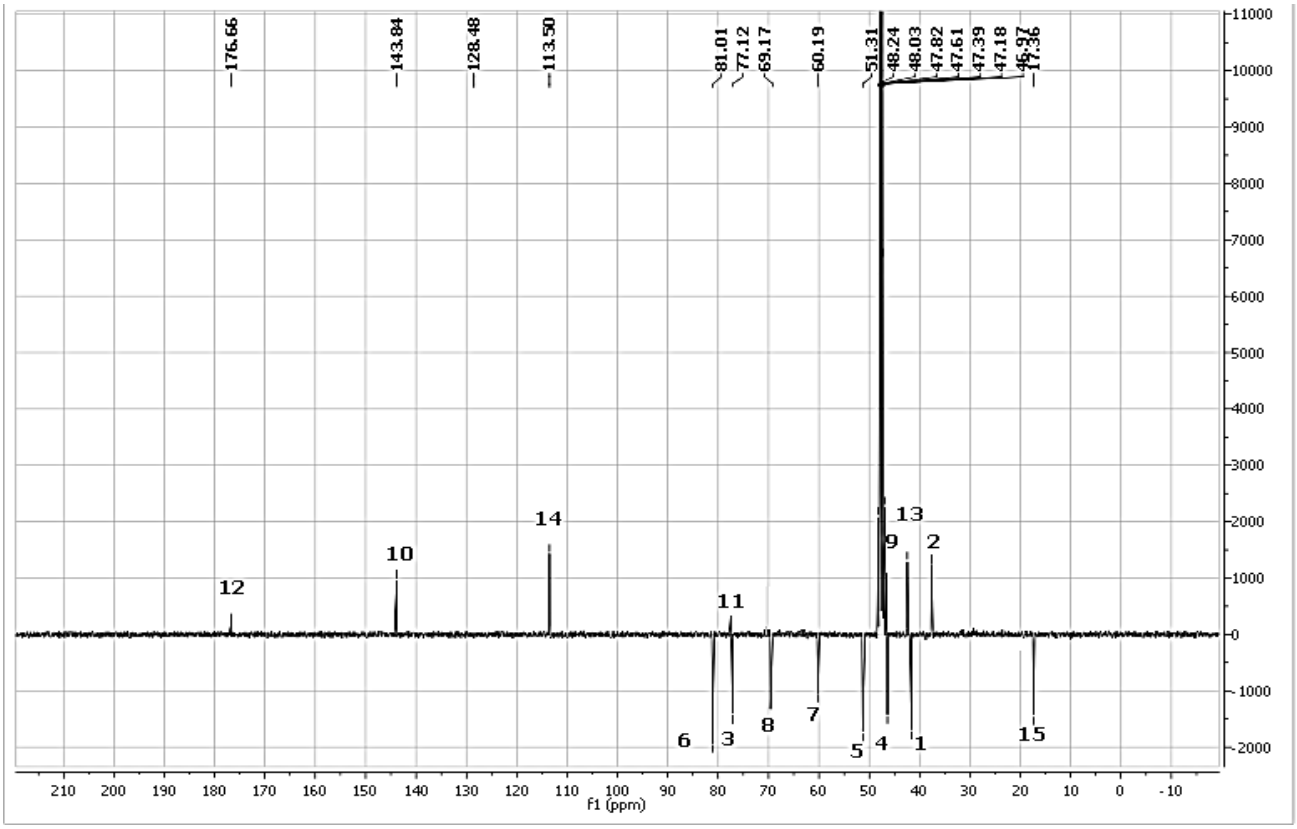


Figure S21: APT spectrum (100 MHz, CD_3OD) of compound **2** (cynarinin B)

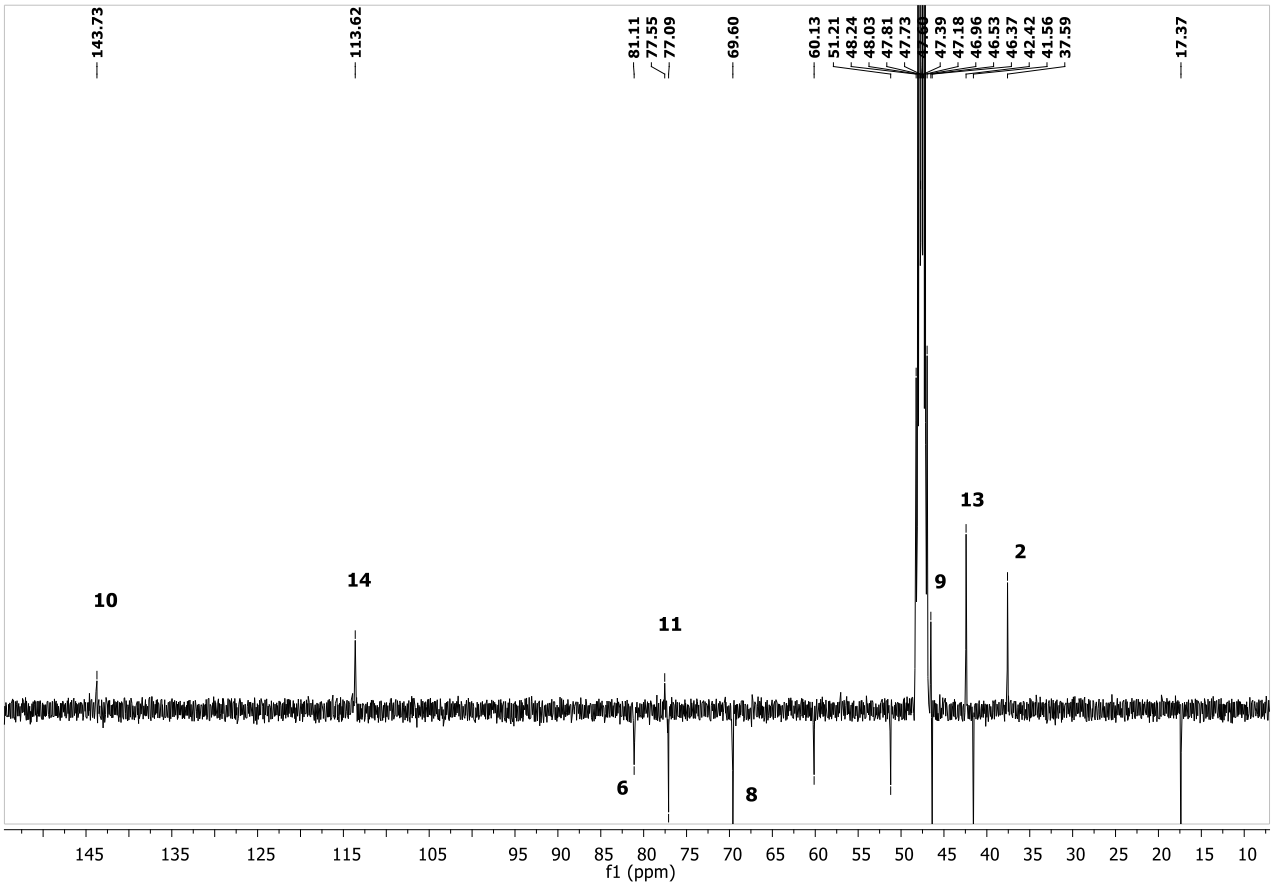


Figure S22: APT spectrum (100 MHz, CD_3OD) of compound **2** (cynarinin B) from 10 to 146.0 ppm

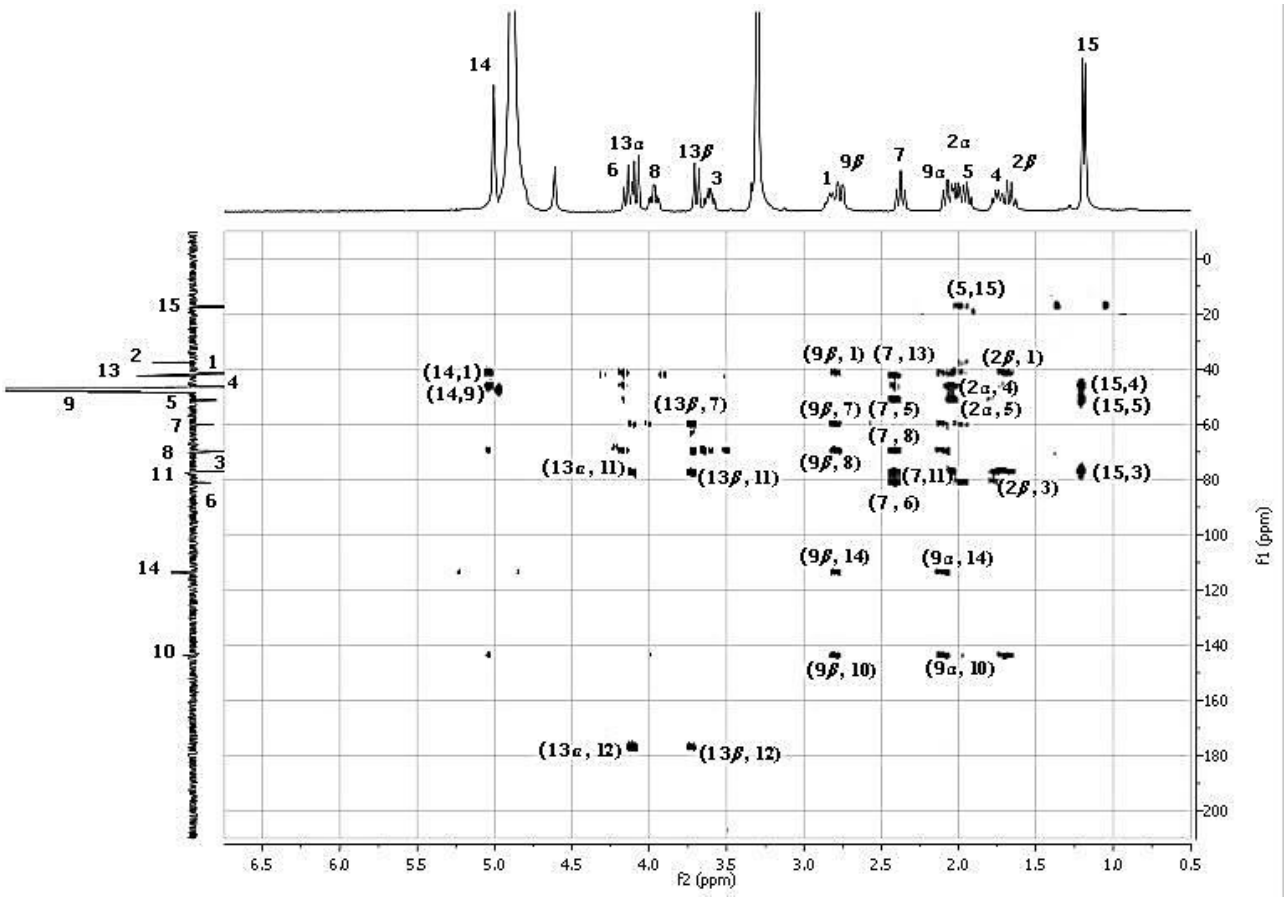


Figure S23: HSQC spectrum of compound **2**

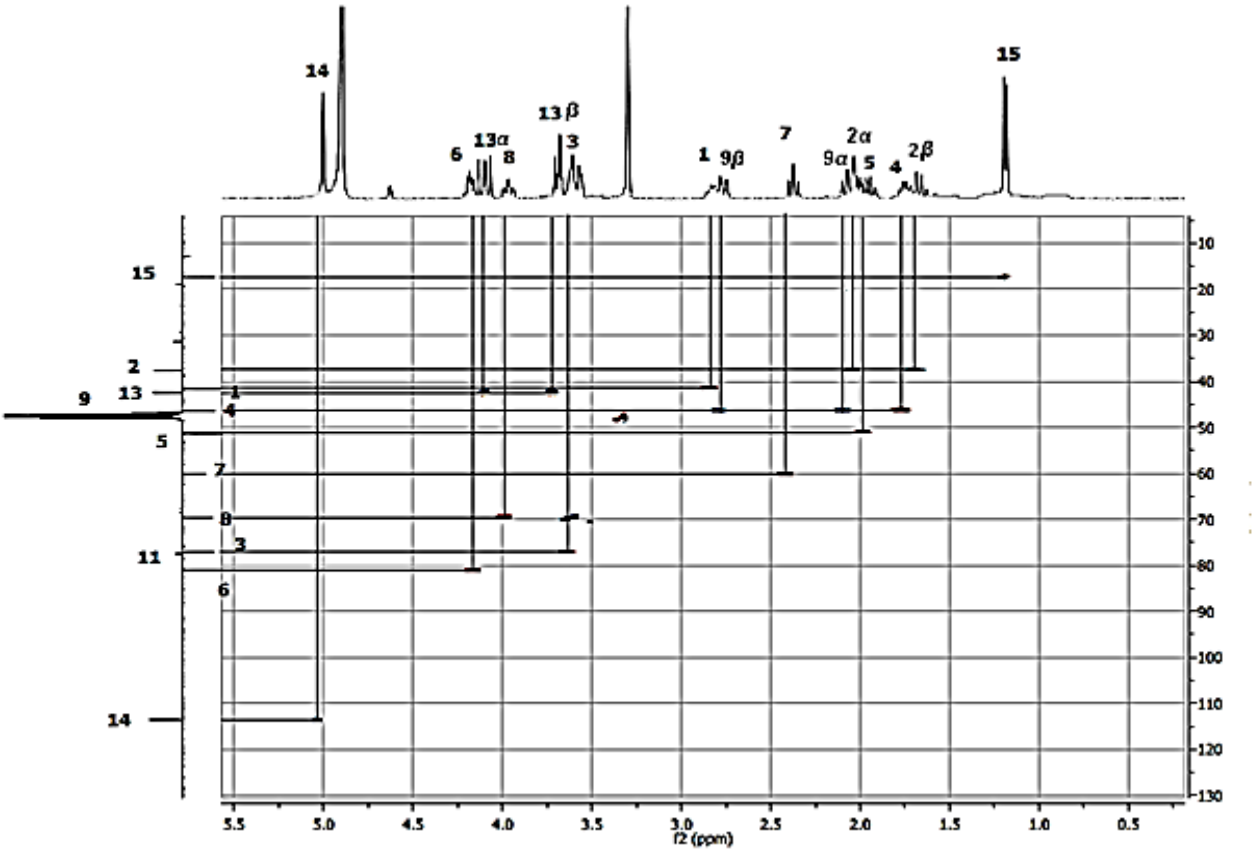


Figure S24: HMBC spectrum of compound **2**

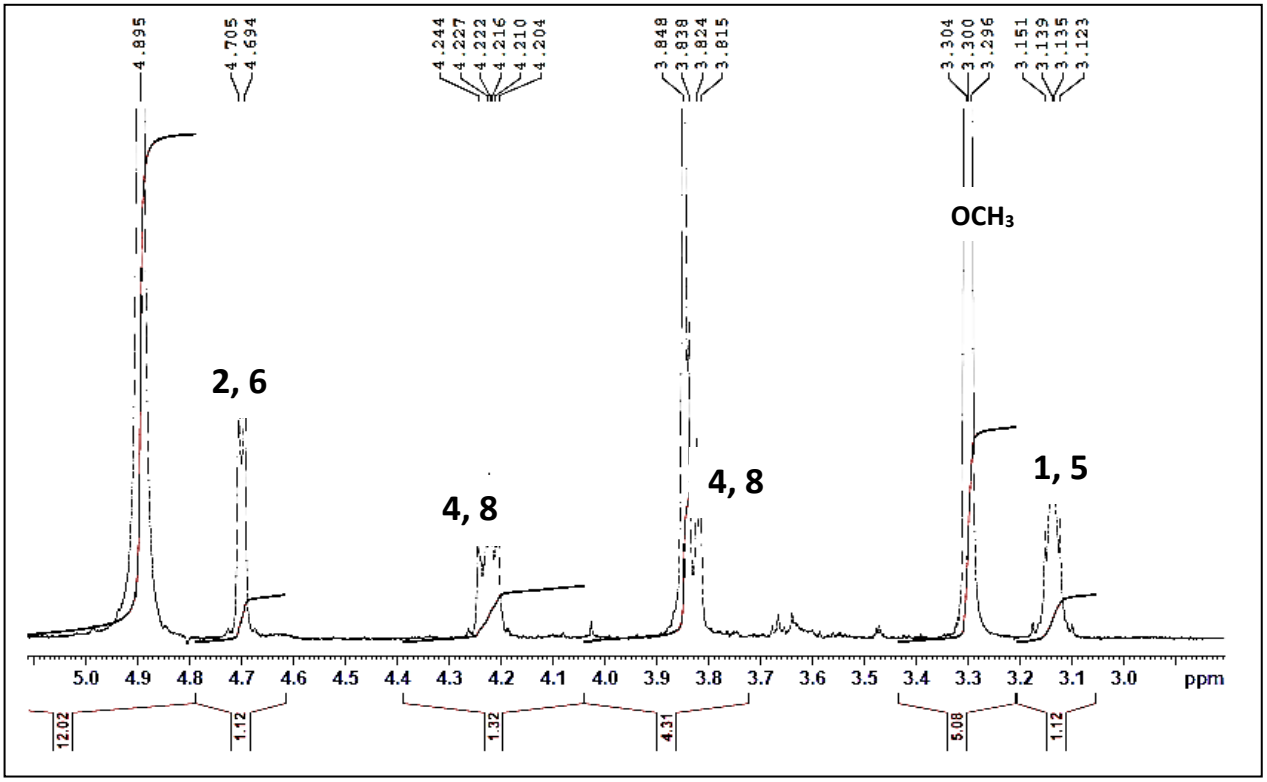


Figure S25: Expansion of ^{1}H-NMR spectrum (400 MHz, $CDCl_3$) of compound **3** (pinoresinol) from 3 to 5 ppm

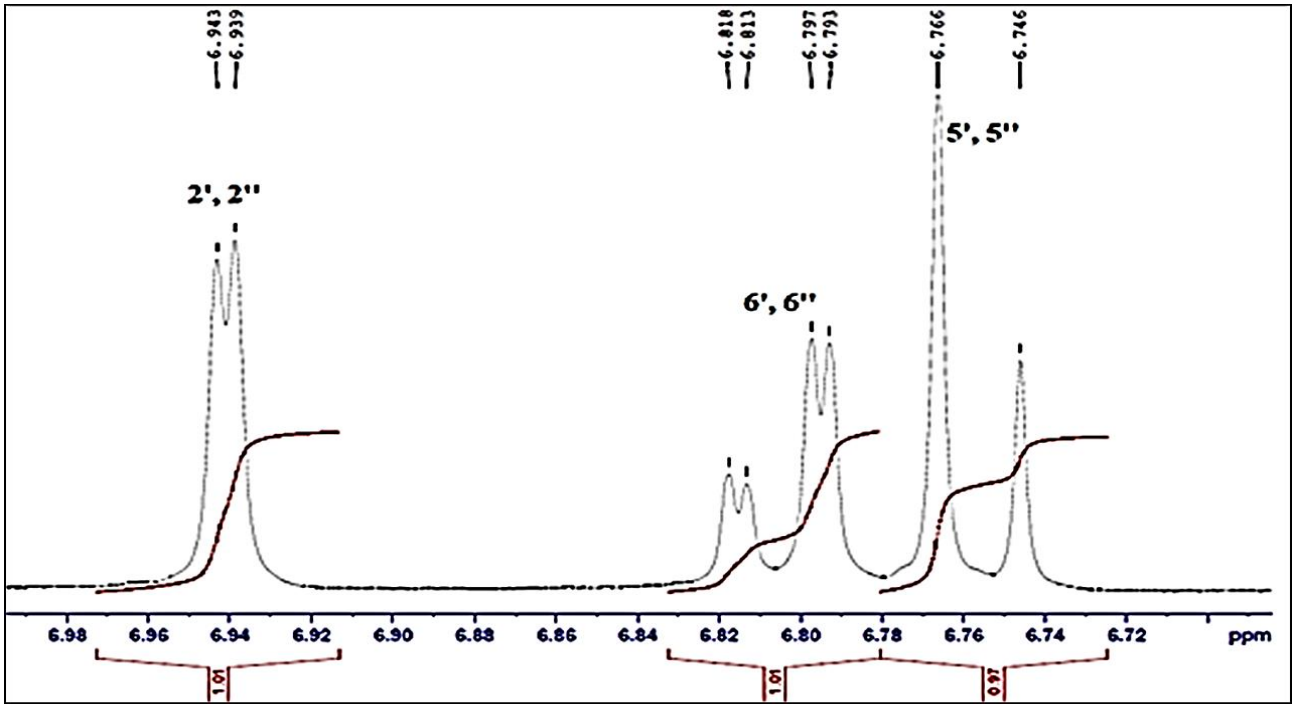


Figure S26: Expansion of ^{1}H-NMR spectrum (400 MHz, $CDCl_3$) of compound **3** from 6.72 to 6.99 ppm

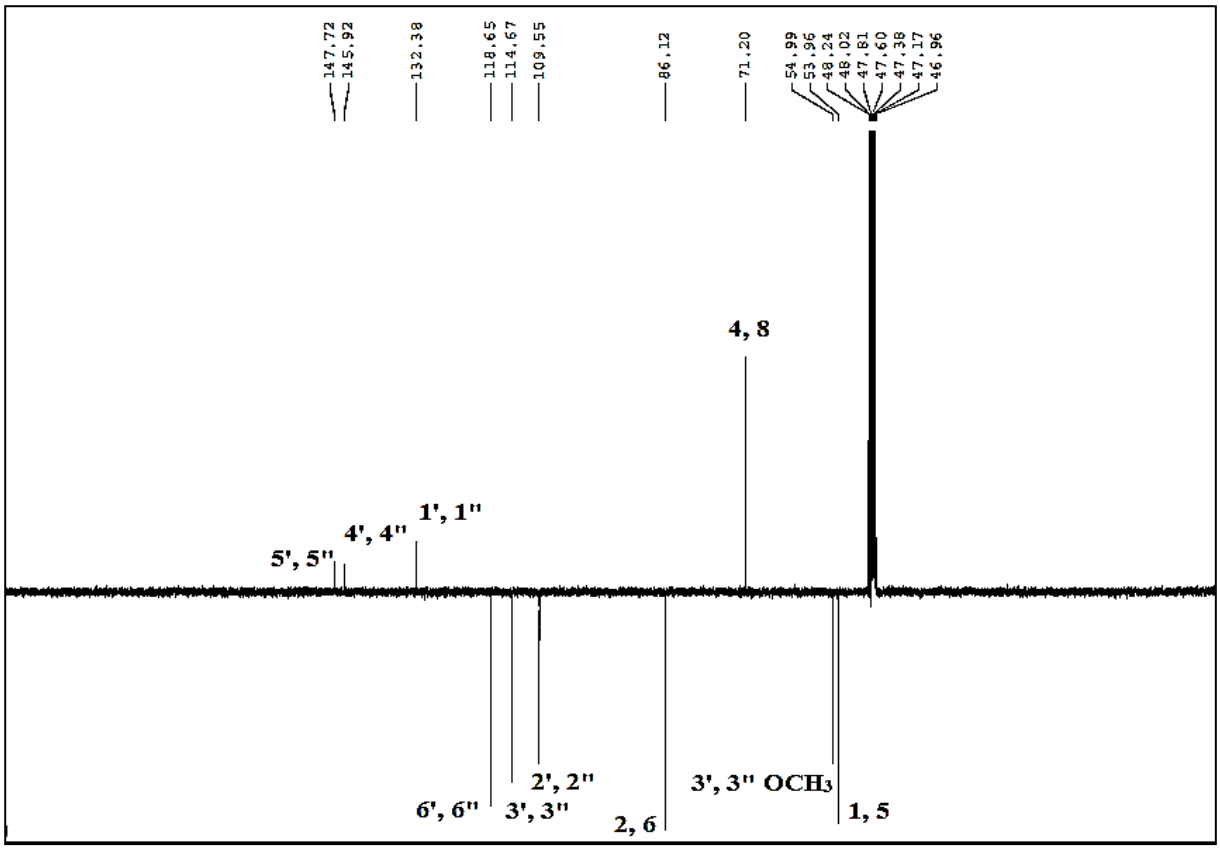


Figure S27: APT spectrum (100 MHz, CD_3OD) of compound **3** (pinoresinol)

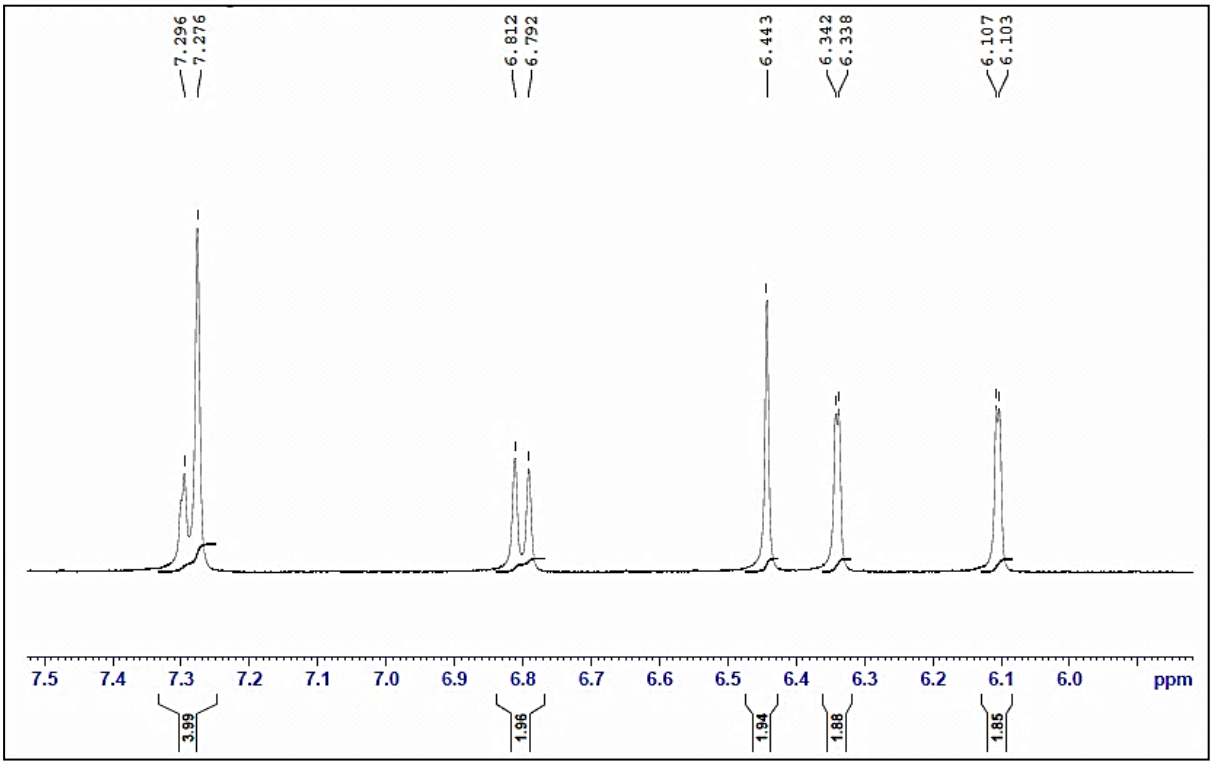


Figure S28: ^{1}H-NMR spectrum (400 MHz, CD_3OD) of compound **4** (luteolin) from 6 to 7.5 ppm

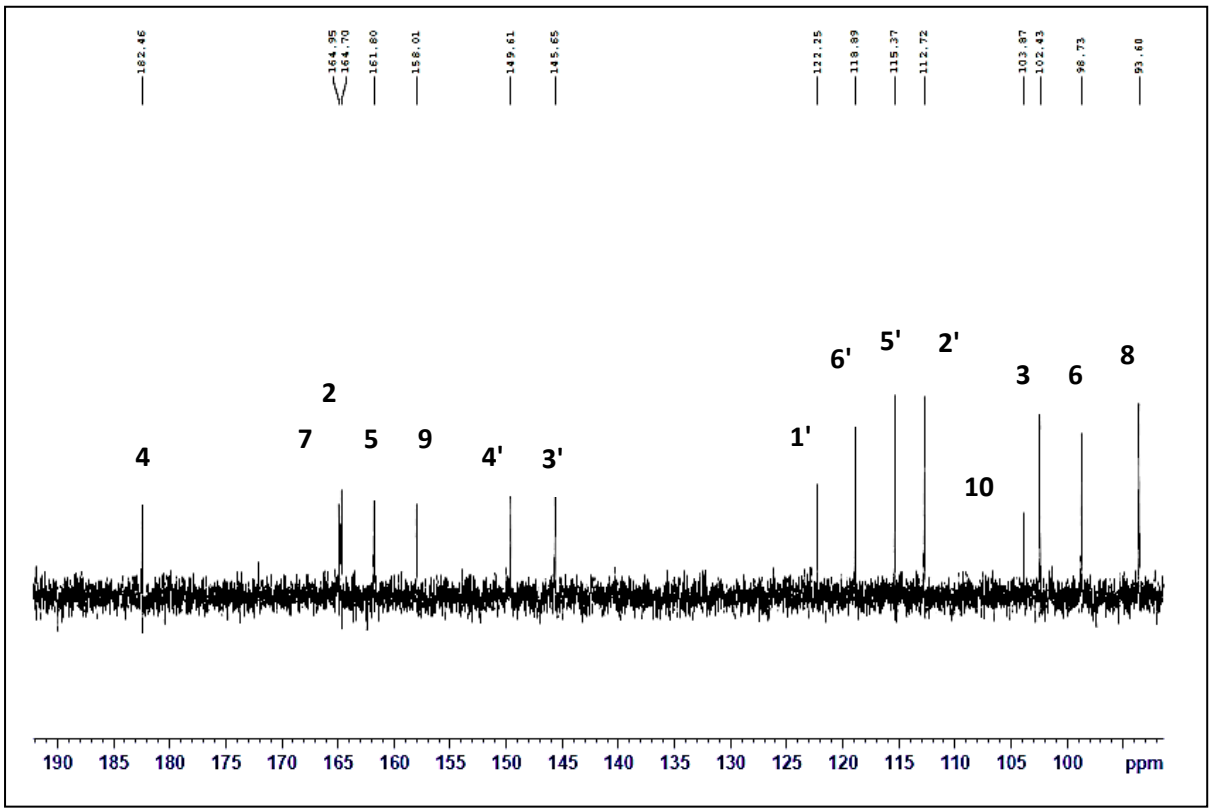
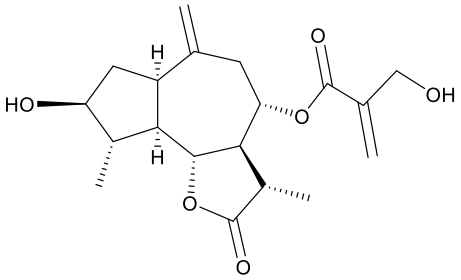
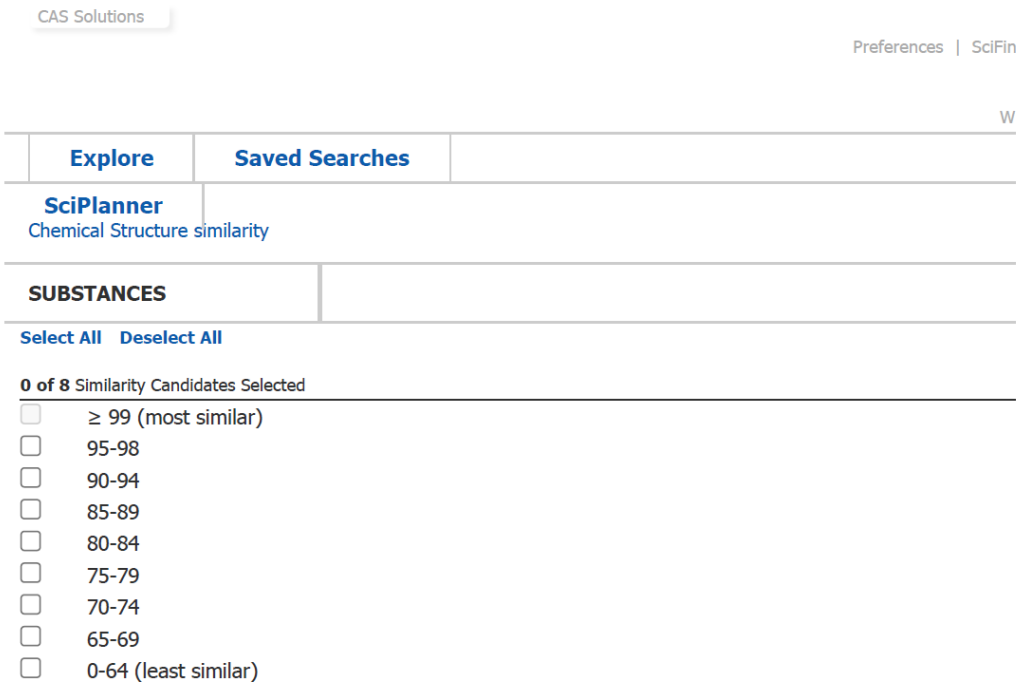


Figure S29: ^{13}C-NMR spectrum (100 MHz, CD_3OD) of compound **4** (luteolin)

Scifinder results of the new compound



No similar structure.



Results of structure similarity 95-98%

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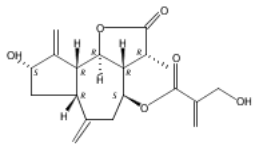

Absolute stereochemistry.
$C_{19}H_{24}O_6$
2-Propenoic acid, 2-(hydroxymethyl)-, dodecahydro-8-hydroxy-3-methyl-6,9-bis(methylene)-2-oxoazuleno[4,5-*b*]furan-4-yl ester, [3*R*-(3α,3aβ,4β,6aβ,8α,9aβ,9bα)]- (9CI)

Key Physical Properties:
Molecular Weight
348.39
Melting Point (Experimental)

Value: 131 °C
Boiling Point (Predicted)
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Density (Predicted)
Value: 1.26±0.1 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr
pKa (Predicted)
Value: 13.52±0.10 | Condition: Most Acidic Temp: 25 °C

Related Info:
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Spectra
Experimental Properties

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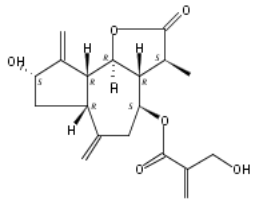

Rotation (+)., Absolute stereochemistry.
C_{19} H_{24} O_6
2-Propenoic acid, 2-(hydroxymethyl)-, dodecahydro-8-hydroxy-3-methyl-6,9-bis(methylene)-2-oxoazuleno[4,5-*b*]furan-4-yl ester, [3*S*-(3α,3aα,4α,6aα,8β,9aα,9bβ)]- (9CI)

Key Physical Properties:
Molecular Weight
348.39
Boiling Point (Predicted)
Value: 554.0±50.0 °C | Condition: Press: 760 Torr
Density (Predicted)
Value: 1.26±0.1 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr
pKa (Predicted)
Value: 13.52±0.10 | Condition: Most Acidic Temp: 25 °C

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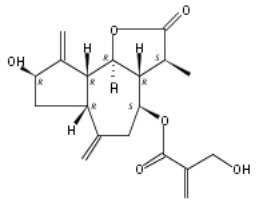

Rotation (+)., Absolute stereochemistry.
C_{19} H_{24} O_6
2-Propenoic acid, 2-(hydroxymethyl)-, (3*S*,3a*R*,4*S*,6a*R*,8*R*,9a*R*,9b*R*)-dodecahydro-8-hydroxy-3-methyl-6,9-bis(methylene)-2-oxoazuleno[4,5-*b*]furan-4-yl ester

Key Physical Properties:
Molecular Weight
348.39
Boiling Point (Predicted)
Value: 554.0±50.0 °C | Condition: Press: 760 Torr
Density (Predicted)

Value: 1.26±0.1 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr
pKa (Predicted)
Value: 13.52±0.10 | Condition: Most Acidic Temp: 25 °C

Related Info:
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~ 1 Commercial Sources
Spectra

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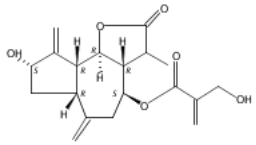

Absolute stereochemistry.
C_{19} H_{24} O_6
2-Propenoic acid, 2-(hydroxymethyl)-, (3a*R*,4*S*,6a*R*,8*S*,9a*R*,9b*R*)-dodecahydro-8-hydroxy-3-methyl-6,9-bis(methylene)-2-oxoazuleno[4,5-*b*]furan-4-yl ester

Key Physical Properties:
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Boiling Point (Predicted)
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Density (Predicted)
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pKa (Predicted)
Value: 13.52±0.10 | Condition: Most Acidic Temp: 25 °C

Related Info:
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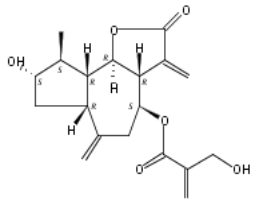

Absolute stereochemistry.
C_{19} H_{24} O_6
2-Propenoic acid, 2-(hydroxymethyl)-, (3a*R*,4*S*,6a*R*,8*S*,9*S*,9a*R*,9b*R*)-dodecahydro-8-hydroxy-9-methyl-3,6-bis(methylene)-2-oxoazuleno[4,5-*b*]furan-4-yl ester

Key Physical Properties:
Molecular Weight
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Boiling Point (Predicted)
Value: 550.1±50.0 °C | Condition: Press: 760 Torr
Density (Predicted)
Value: 1.26±0.1 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr
pKa (Predicted)
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Related Info:

~ 5 References
~ 2 Commercial Sources

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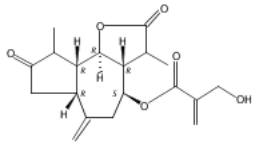

Absolute stereochemistry.
C_{19} H_{24} O_6
2-Propenoic acid, 2-(hydroxymethyl)-, (3a*R*,4*S*,6a*R*,9a*R*,9b*R*)-dodecahydro-3,9-dimethyl-6-methylene-2,8-dioxoazuleno[4,5-*b*]furan-4-yl ester

Key Physical Properties:
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pKa (Predicted)
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Related Info:
~ 2 References

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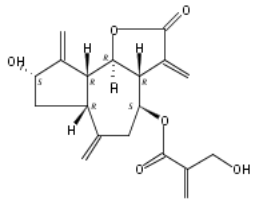

Rotation (+)., Absolute stereochemistry.
C_{19} H_{22} O_6
2-Propenoic acid, 2-(hydroxymethyl)-, (3a*R*,4*S*,6a*R*,8*S*,9a*R*,9b*R*)-dodecahydro-8-hydroxy-3,6,9-tris(methylene)-2-oxoazuleno[4,5-*b*]furan-4-yl ester

Key Physical Properties:
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Density (Predicted)
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pKa (Predicted)
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~ 259 References
Reactions
~ 39 Commercial Sources
Spectra
Experimental Properties

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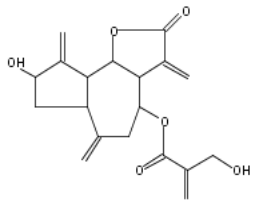
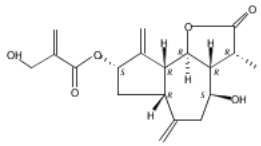


C_{19} H_{22} O_6
2-Propenoic acid, 2-(hydroxymethyl)-, dodecahydro-8-hydroxy-3,6,9-tris(methylene)-2-oxoazuleno[4,5-*b*]furan-4-yl ester
Key Physical Properties:
Molecular Weight
346.37
Boiling Point (Predicted)
Value: 566.2±50.0 °C | Condition: Press: 760 Torr
Density (Predicted)
Value: 1.28±0.1 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr
pKa (Predicted)
Value: 13.52±0.10 | Condition: Most Acidic Temp: 25 °C

Related Info:
~ 6 References
~ 8 Commercial Sources

Score: 96
9.
119403-30-4

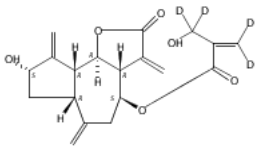


Absolute stereochemistry.
C_{19} H_{24} O_6
2-Propenoic acid, 2-(hydroxymethyl)-, dodecahydro-4-hydroxy-3-methyl-6,9-bis(methylene)-2-oxoazuleno[4,5-*b*]furan-8-yl ester, [3*R*-(3α,3aβ,4β,6aβ,8α,9aβ,9bα)]- (9CI)

Key Physical Properties:
Molecular Weight
348.39
Boiling Point (Predicted)
Value: 547.4±50.0 °C | Condition: Press: 760 Torr
Density (Predicted)
Value: 1.26±0.1 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr
pKa (Predicted)
Value: 13.54±0.10 | Condition: Most Acidic Temp: 25 °C

Related Info:
~ 1 References
Spectra
Experimental Properties

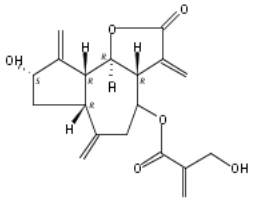
Score: 96
10.
1821519-63-4



Absolute stereochemistry.
C_{19} H_{18} D_4 O_6
INDEX NAME NOT YET ASSIGNED

Related Info:
~ 1 References
Reactions

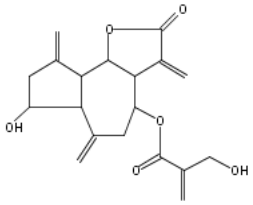
Score: 96
11.
1923795-05-4



Absolute stereochemistry.
C_{19} H_{22} O_6
2-Propenoic acid, 2-(hydroxymethyl)-, (3a*R*,6a*R*,8*S*,9a*R*,9b*R*)-dodecahydro-8-hydroxy-3,6,9-tris(methylene)-2-oxoazuleno[4,5-*b*]furan-4-yl ester

Key Physical Properties:
Molecular Weight
346.37
Boiling Point (Predicted)
Value: 566.2±50.0 °C | Condition: Press: 760 Torr
Density (Predicted)
Value: 1.28±0.1 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr
pKa (Predicted)
Value: 13.52±0.10 | Condition: Most Acidic Temp: 25 °C
Related Info:
~ 1 References

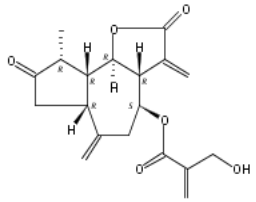
Score: 95
12.
85011-56-9



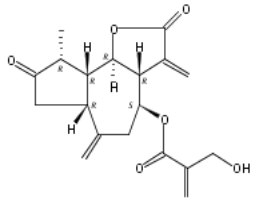
C_{19} H_{22} O_6
2-Propenoic acid, 2-(hydroxymethyl)-, dodecahydro-7-hydroxy-3,6,9-tris(methylene)-2-oxoazuleno[4,5-*b*]furan-4-yl ester (9CI)

Key Physical Properties:
Molecular Weight
346.37
Boiling Point (Predicted)
Value: 566.1±50.0 °C | Condition: Press: 760 Torr
Density (Predicted)
Value: 1.28±0.1 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr
pKa (Predicted)
Value: 13.52±0.10 | Condition: Most Acidic Temp: 25 °C

Related Info:
~ 1 References
~ 2 Commercial Sources
Score: 95
13.
1212401-38-1



Relative stereochemistry.
C_{19} H_{22} O_6
2-Propenoic acid, 2-(hydroxymethyl)-, (3a*R*,4*S*,6a*R*,9*R*,9a*R*,9b*R*)-dodecahydro-9-methyl-3,6-bis(methylene)-2,8-dioxoazuleno[4,5-*b*]furan-4-yl ester, *rel*-
Key Physical Properties:
Molecular Weight
346.37
Boiling Point (Predicted)
Value: 551.8±50.0 °C | Condition: Press: 760 Torr
Density (Predicted)
Value: 1.26±0.1 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr
pKa (Predicted)
Value: 13.52±0.10 | Condition: Most Acidic Temp: 25 °C
Related Info:
~ 1 References
~ 1 Commercial Sources
Score: 95
14.
1482499-27-3



Absolute stereochemistry.
C_{19} H_{22} O_6
2-Propenoic acid, 2-(hydroxymethyl)-, (3a*R*,4*S*,6a*R*,9*R*,9a*R*,9b*R*)-dodecahydro-9-methyl-3,6-bis(methylene)-2,8-dioxoazuleno[4,5-*b*]furan-4-yl ester
Key Physical Properties:
Molecular Weight
346.37
Boiling Point (Predicted)
Value: 551.8±50.0 °C | Condition: Press: 760 Torr
Density (Predicted)
Value: 1.26±0.1 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr
pKa (Predicted)
Value: 13.52±0.10 | Condition: Most Acidic Temp: 25 °C
Related Info:
~ 1 References