

Isoakuranetin

5,7-Dihydroxy-4'-methoxyflavanone

CAS-Number: 480-43-3

Formula: C₁₆H₁₄O₅ Exact mass: 286.08412

Molecular mass: 286.28

Column: Zorbax LiChrosphere Kinetex

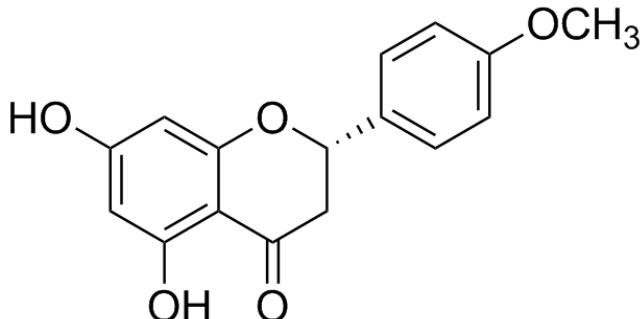
Abs.RetentionTime [min]: 27.68 24.35 12.16

Rel. RetentionTime (k') : 22.46 22.41 21.94

k' rel. to Rutin : 1.70 1.81 1.84

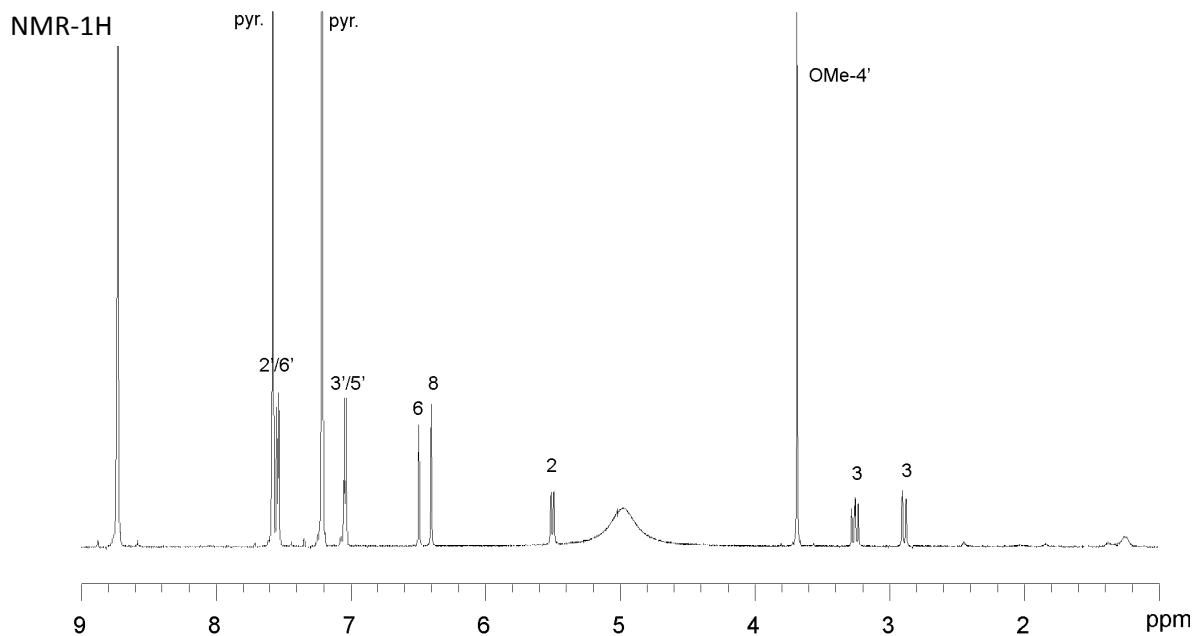
MS1: 285.3 MS2: 270.1 MS3: 164.1

UV/Vis: 290–330(sh)

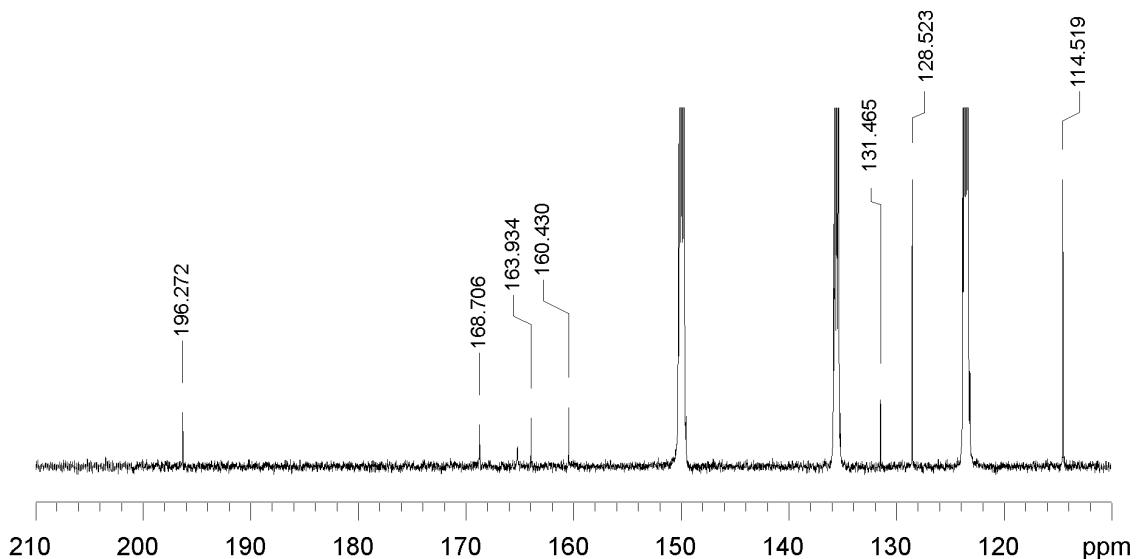


NMR - Resonance Assignments:

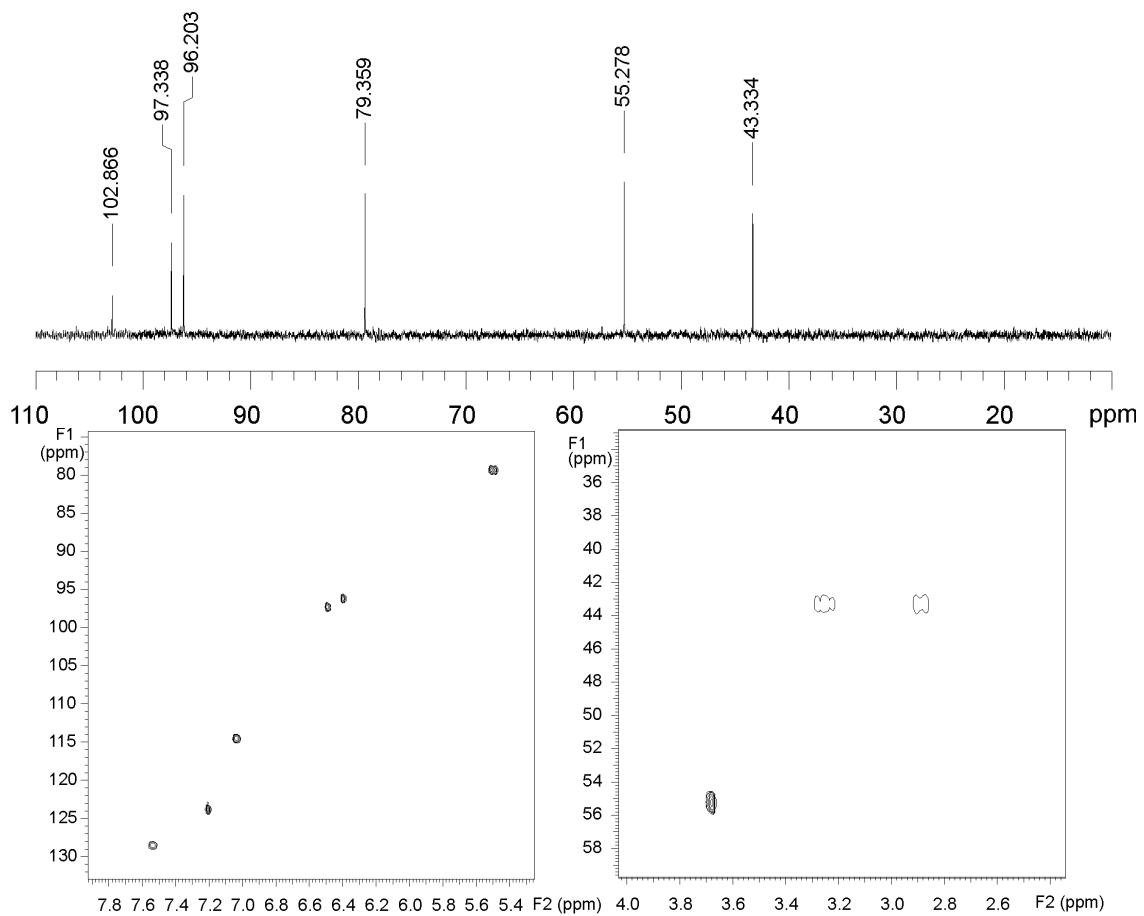
| | δ_C | δ_H |
|--------|------------|------------|
| 2 | 79.4d | 5.5 |
| 3 | 43.3t | 2.89/3.25 |
| 4 | 196.3s | |
| 4a | 102.9s | |
| 5 | 165.2s | |
| 6 | 97.3d | 6.49 |
| 7 | 168.7s | |
| 8 | 96.2d | 6.4 |
| 8a | 163.9s | |
| 1' | 131.5s | |
| 2' | 128.5d | 7.54 |
| 3' | 114.5d | 7.04 |
| 4' | 160.4s | |
| 5' | 114.5d | 7.04 |
| 6' | 128.5d | 7.54 |
| OMe-4' | 55.3q | 3.69 |



NMR-13C:



NMR-HSQC:



Names

Isoakuranetin; 2,3-dihydro-5,7-dihydroxy-2-(4-methoxyphenyl)-(2S)- 4H-1-benzopyran-4-one; 2,3-dihydro-5,7-dihydroxy-2-(4-methoxyphenyl)-(S)- 4H-1-benzopyran-4-one; 5,7-dihydroxy-4'-methoxy-flavanone; Isosakuranetin; (S)-Isosakuranetin; 4'-Methylnaringenin; 5,7-Dihydroxy-4'-methoxyflavanone; Citrifoliol; Naringenin-4'-methyl ether; Ponciretin

Eriodictyol

5,7,3',4'-Tetrahydroxyflavanone

CAS-Number: 552-58-9

Formula: C₁₅H₁₂O₆ Exact mass: 288.06339

Molecular mass: 288.25

Column: Zorbax LiChrosphere Kinetex

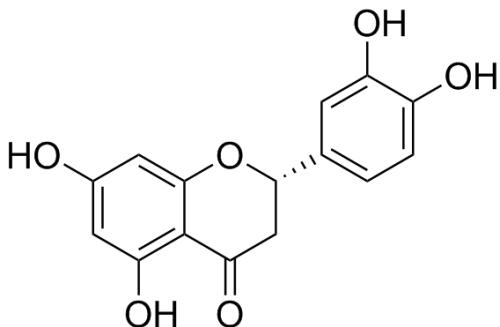
Abs.RetentionTime [min]: 20.4 17.04 8.41

Rel. RetentionTime (k') : 16.29 15.38 14.87

k' rel. to Rutin : 1.23 1.24 1.24

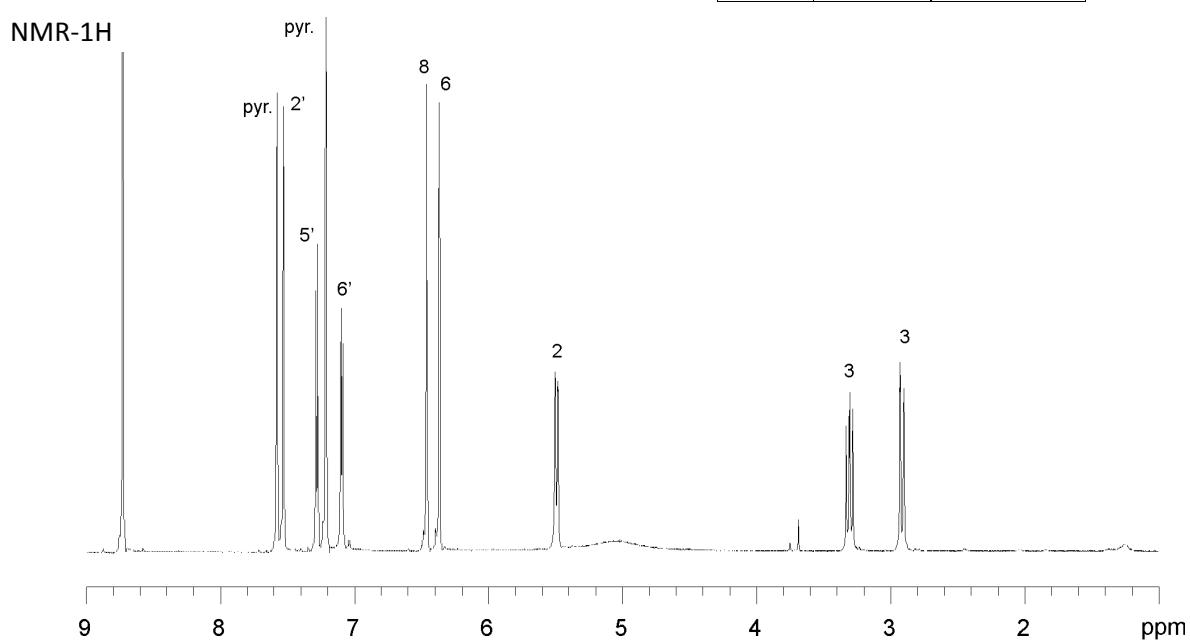
MS1: 287.1 MS2: 151.1 MS3: 107.1

UV/Vis: 285, 330(sh)

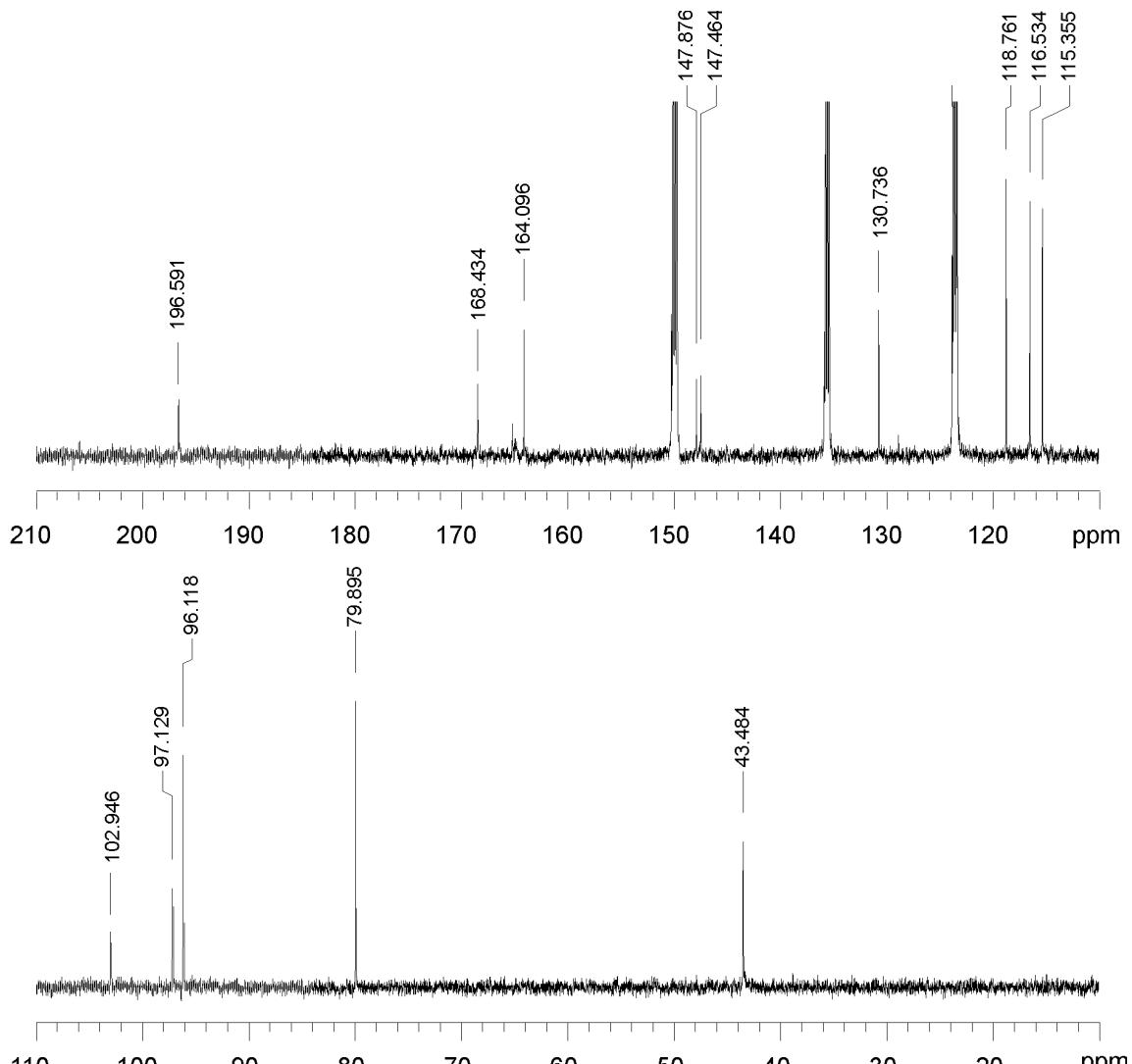


NMR - Resonance Assignments:

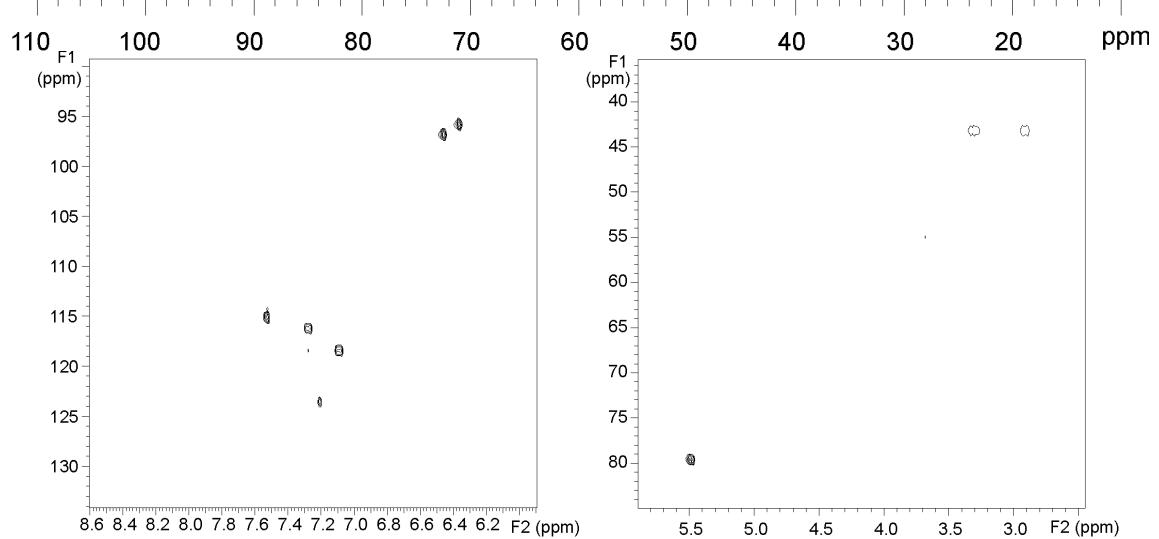
| | δ_C | δ_H |
|----|------------|------------|
| 2 | 79.9d | 5.48 |
| 3 | 43.5t | 2.91/3.3 |
| 4 | 196.6s | |
| 4a | 102.9s | |
| 5 | 165.2s | |
| 6 | 97.1d | 6.47 |
| 7 | 168.4s | |
| 8 | 96.1d | 6.36 |
| 8a | 164.1s | |
| 1' | 130.7s | |
| 2' | 115.4d | 7.53 |
| 3' | 147.5s | |
| 4' | 147.9s | |
| 5' | 116.5d | 7.28 |
| 6' | 118.8d | 7.09 |



NMR-13C:



NMR-HSQC:



Names

2-(3,4-dihydroxyphenyl)-2,3-dihydro-5,7-dihydroxy-(2S)-4H-1-benzopyran-4-one; 2-(3,4-dihydroxyphenyl)-2,3-dihydro-5,7-dihydroxy- (S)-4H-1-benzopyran-4-one; Eriodictyol; 5,7,3',4'-tetrahydroxy- flavanone; (+)-Eriodictyol; (2S)-Eriodictyol; (S)-5,7,3',4'-Tetrahydroxyflavanone; 5,7,3',4'-Tetrahydroxyflavanone; Huazhongilexone

Naringenin

5,7,4'-Trihydroxyflavanone

CAS-Number: 480-41-1

Formula: C₁₅H₁₂O₅ Exact mass: 272.06847

Molecular mass: 272.25

Column: Zorbax LiChrosphere Kinetex

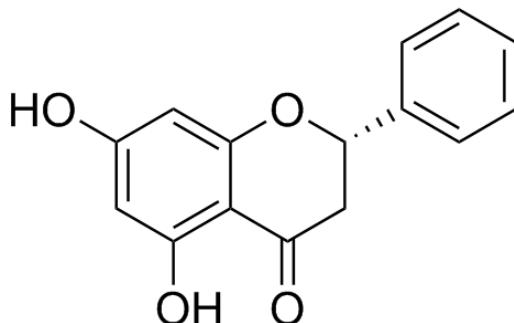
Abs.RetentionTime [min]: 22.43 19.33 9.57

Rel. RetentionTime (k') : 18.01 17.59 17.06

k' rel. to Rutin : 1.36 1.42 1.43

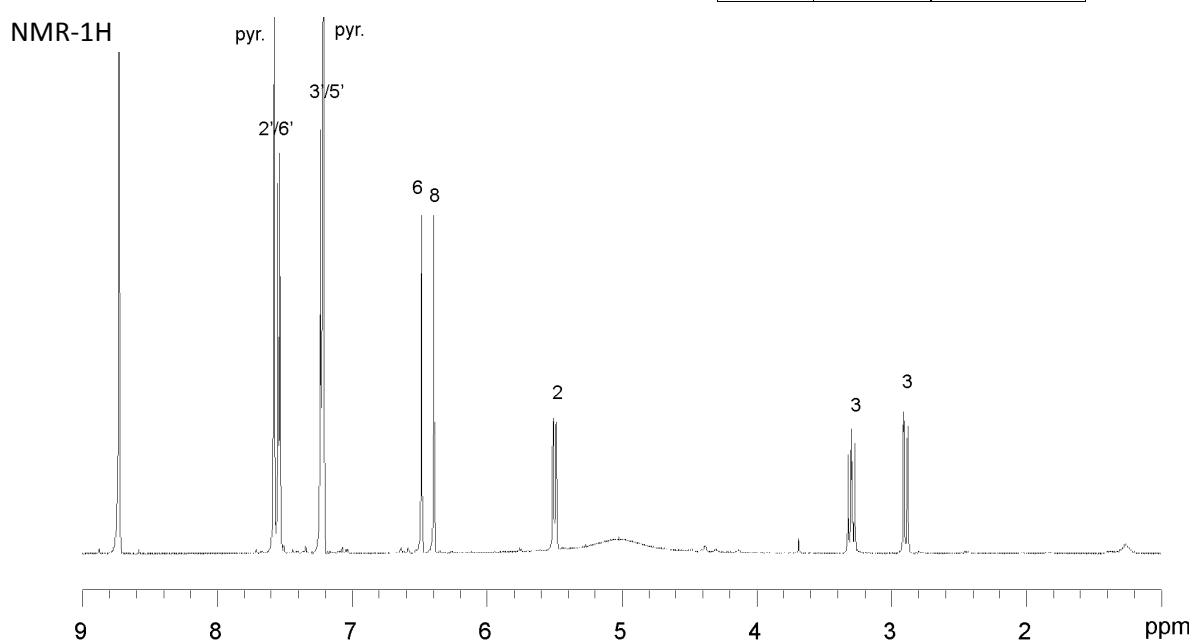
MS1: 271.3 MS2: 151.1 MS3: 107.1

UV/Vis: 290–330(sh)

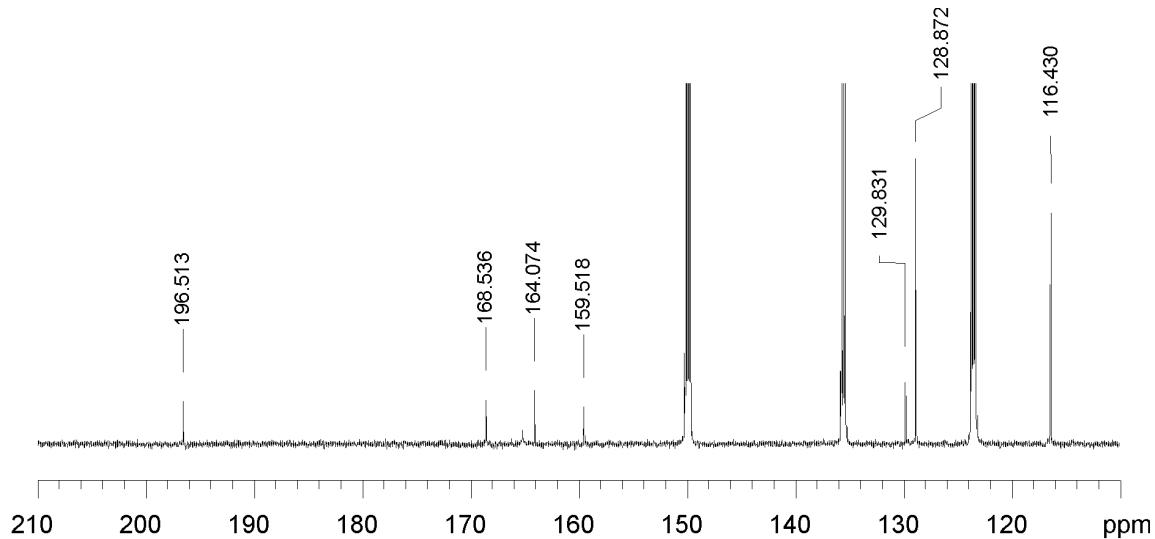


NMR - Resonance Assignments:

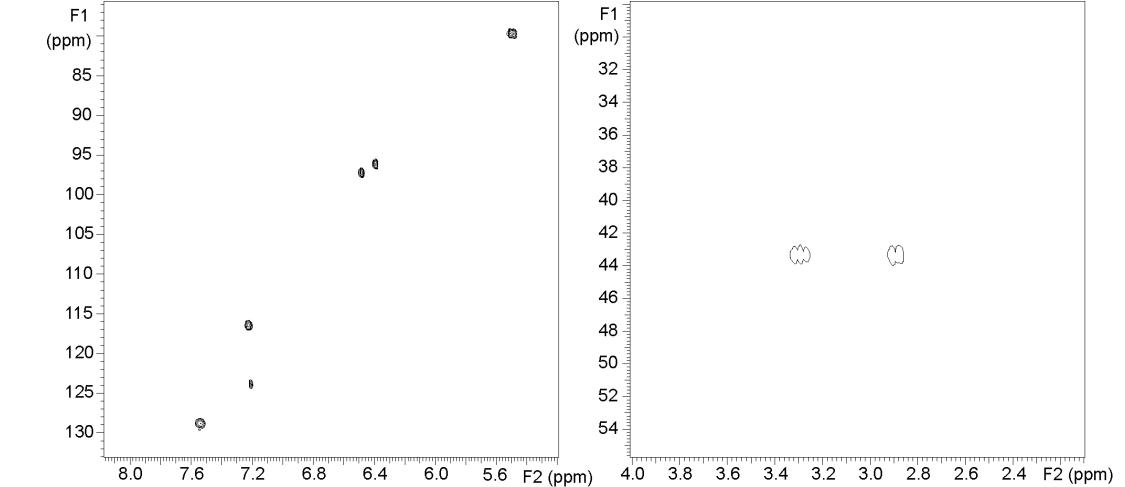
| | δ_C | δ_H |
|----|------------|------------|
| 2 | 79.7d | 5.49 |
| 3 | 43.4t | 2.89/3.29 |
| 4 | 196.5s | |
| 4a | 102.9s | |
| 5 | 165.2s | |
| 6 | 97.2d | 6.49 |
| 7 | 168.5s | |
| 8 | 96.1d | 6.39 |
| 8a | 164.1s | |
| 1' | 129.8s | |
| 2' | 128.9d | 7.54 |
| 3' | 116.4d | 7.23 |
| 4' | 159.5s | |
| 5' | 116.4d | 7.23 |
| 6' | 128.9d | 7.54 |



NMR-13C:



NMR-HSQC:



Names

2,3-dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-, (2S)-4H-1-benzopyran-4-one; 2,3-dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-, (S)-4H-1-benzopyran-4-one; 5,7,4'-trihydroxy-flavanone; Naringenin; (-)-(2S)-Naringenin; (-)-Naringenin; (2S)-5,7,4'-Trihydroxy-flavanone; (2S)-Naringenin; (S)-Naringenin; NSC 11855; NSC 34875; Naringenine; Naringetol; S-Dihydrogenistein; Salipurol; Salipurpo

Hesperidin

Hesperetin-7-O- β -D-rutinosid

CAS-Number: 520-26-3

Formula: C₂₈H₃₄O₁₅ Exact mass: 610.18977

Molecular mass: 610.56

Column: Zorbax LiChrosphere Kinetex

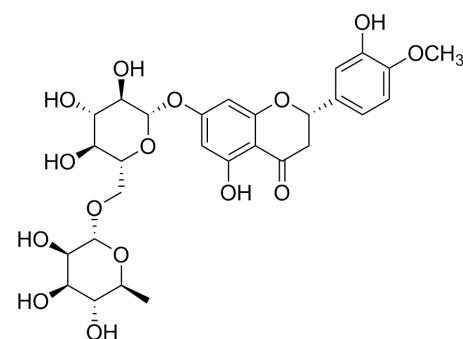
Abs.RetentionTime [min]: 18.32 14.99 7.43

Rel. RetentionTime (k'): 14.53 13.41 13.02

k' rel. to Rutin : 1.10 1.08 1.09

MS1: 609.3 MS2: 301.2 MS3: 286.1

UV/Vis: 285, 330(sh)

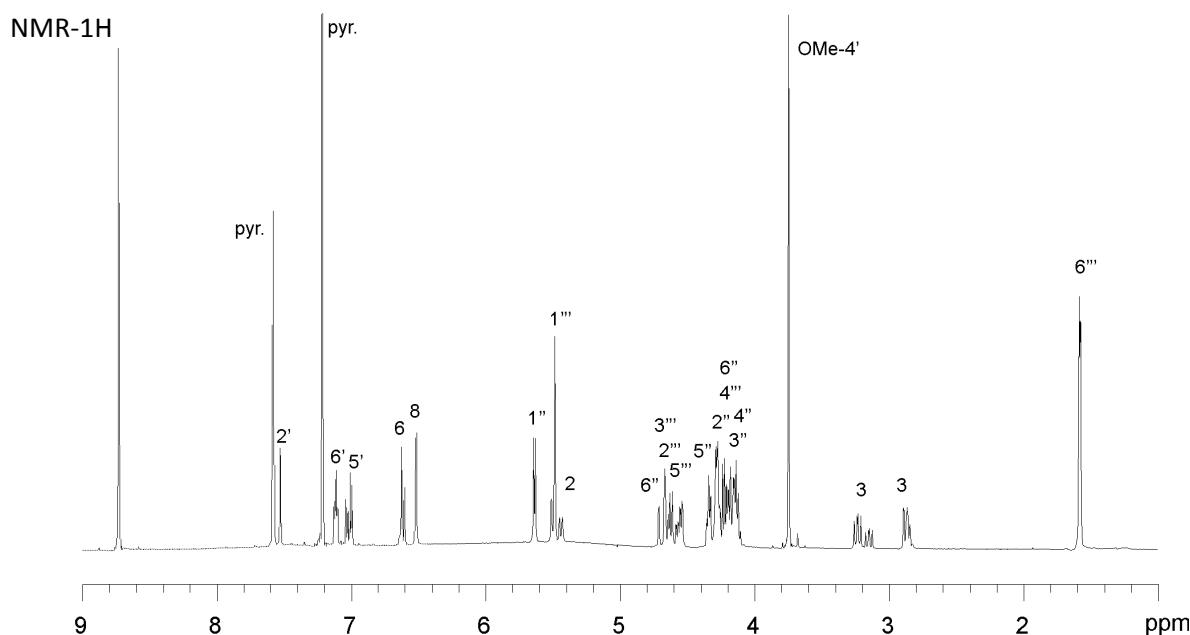


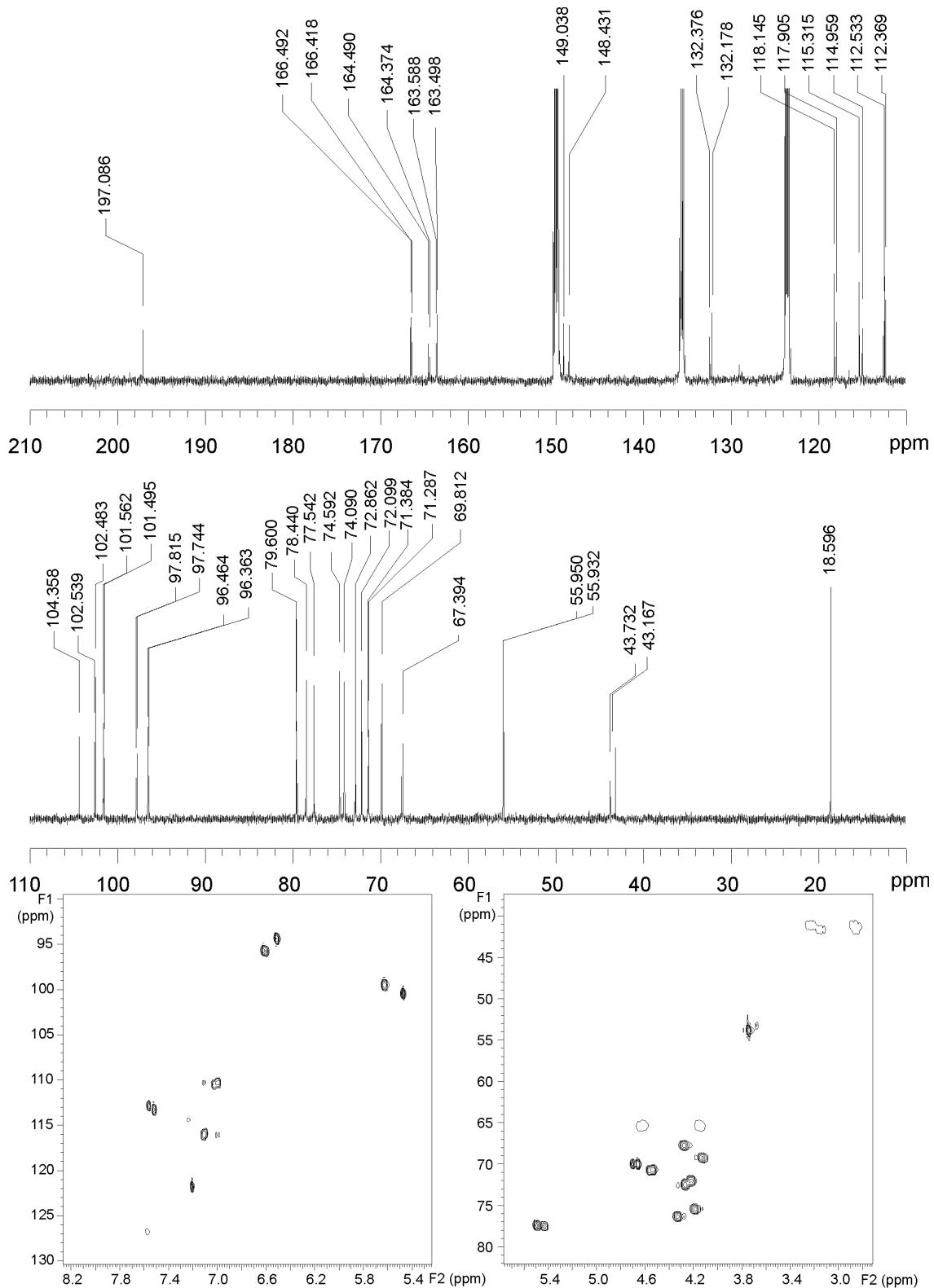
NMR - Resonance Assignments:

Flavone Core

Sugar

| | δ_{C} | δ_{H} | | δ_{C} | δ_{H} |
|----|---------------------|---------------------|--------|---------------------|---------------------|
| 2 | 79.6d | 5.5 | 1" | 101.5d | 5.65 |
| 3 | 43.2t | 3.24/2.88 | 2" | 74.6d | 4.28 |
| 4 | 196.9s | | 3" | 77.6d | 4.2 |
| 4a | 104.5s | | 4" | 71.4d | 4.13 |
| 5 | 164.8s | | 5" | 78.5d | 4.33 |
| 6 | 98d | 6.64 | 6" | 67.5t | 4.63/4.17 |
| 7 | 166.4s | | 1''' | 102.5d | 5.49 |
| 8 | 96.3d | 6.51 | 2''' | 72.1d | 4.69 |
| 8a | 163.5s | | 3''' | 72.7d | 4.55 |
| 1' | 132.1s | | 4''' | 74.1d | 4.22 |
| 2' | 115.3d | 7.52 | 5''' | 69.9d | 4.29 |
| 3' | 148.5s | | 6''' | 18.6q | 1.58 |
| 4' | 149s | | OMe-4' | 55.9q | 3.75 |
| 5' | 112.4d | 7 | | | |
| 6' | 118.1d | 7.11 | | | |



NMR-¹³C:

Names

7-[[6-O-(6-deoxy- α -L-mannopyranosyl)- β -D-glucopyranosyl]oxy]-2,3-dihydro-5-hydroxy-2-(3-hydroxy-4-methoxyphenyl)-(2S)-4H-1-benzopyran-4-one; 7-[[6-O-(6-deoxy- α -L-mannopyranosyl)- β -D-glucopyranosyl]oxy]-2,3-dihydro-5-hydroxy-2-(3-hydroxy-4-methoxyphenyl)-(S)-4H-1-benzopyran-4-one; 5,7,3'-trihydroxy-4'-methoxy-7-(6-O- α -L-rhamnosyl-D-glucoside)-flavanone; Hesperidin; (2S)-Hesperidin; Atripliside B; Cirantin; Hesperetin 7-rhamnoglucoside; Hesperetin 7-rutinoside; Hesperidine; Hesperidoside; NSC 44184

Naringin

Naringenin-7-O- β -D-neohesperidoside

CAS-Number: 10236-47-2

Formula: C₂₇H₃₂O₁₄ Exact mass: 580.17921

Molecular mass: 580.53

Column: Zorbax LiChrosphere Kinetex

Abs.RetentionTime [min]: 17.97 14.53 7.21

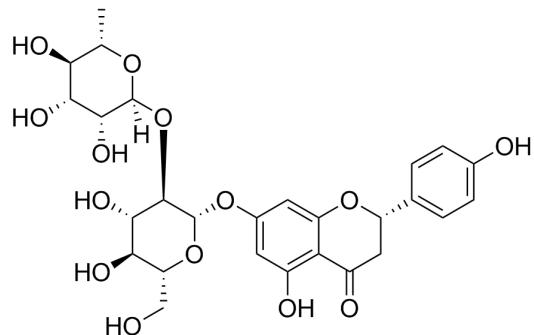
Rel. RetentionTime (k'): 14.23 12.97 12.60

k' rel. to Rutin : 1.08 1.05 1.06

MS1: 579.3 MS2: 459.2 MS3: 357.2

UV/Vis: 285, 330(sh)

Naringin

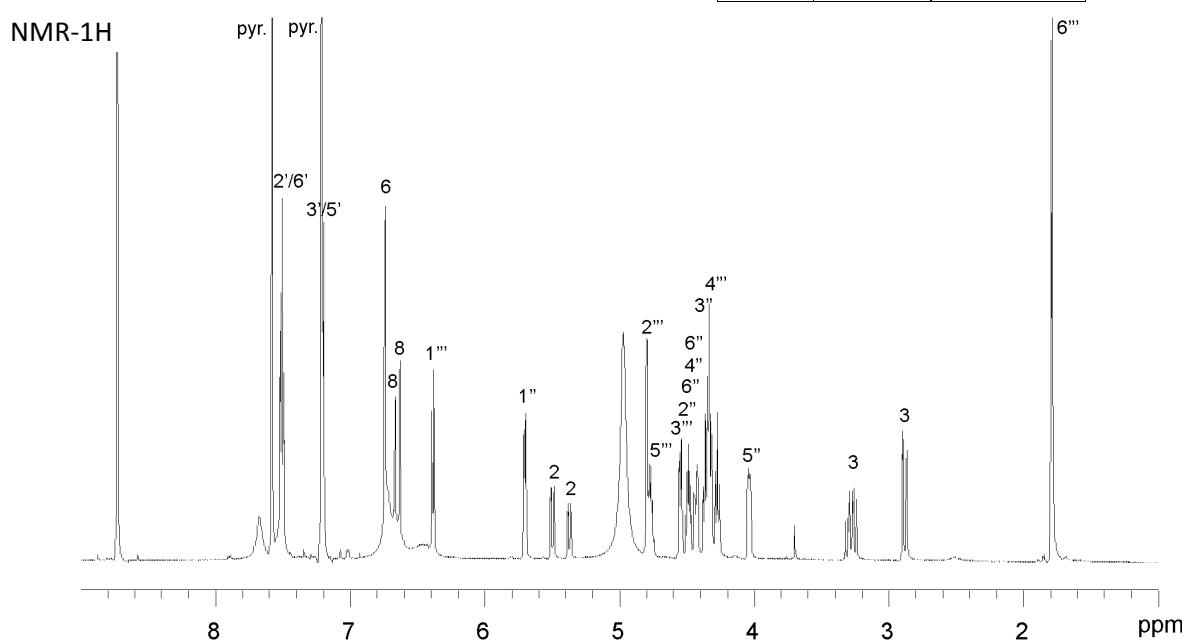


NMR - Resonance Assignments:

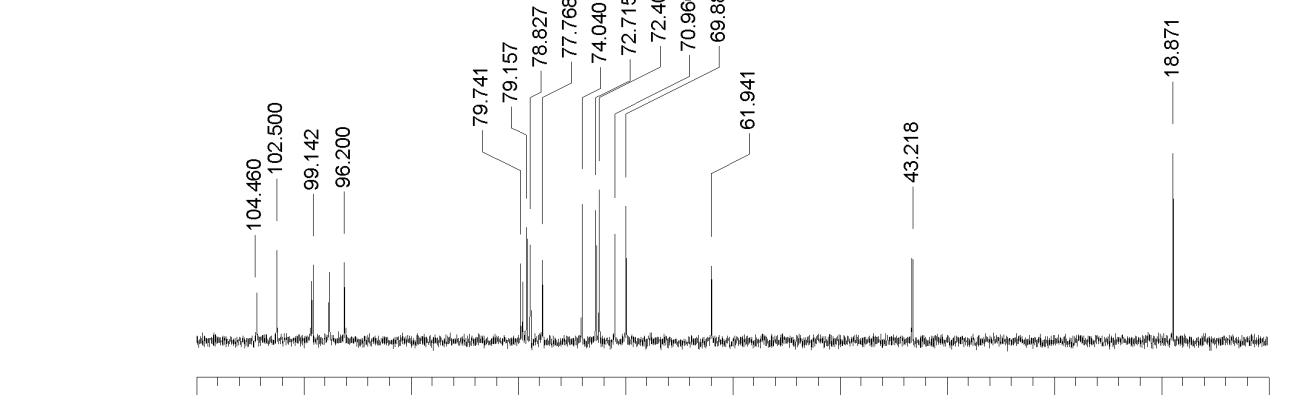
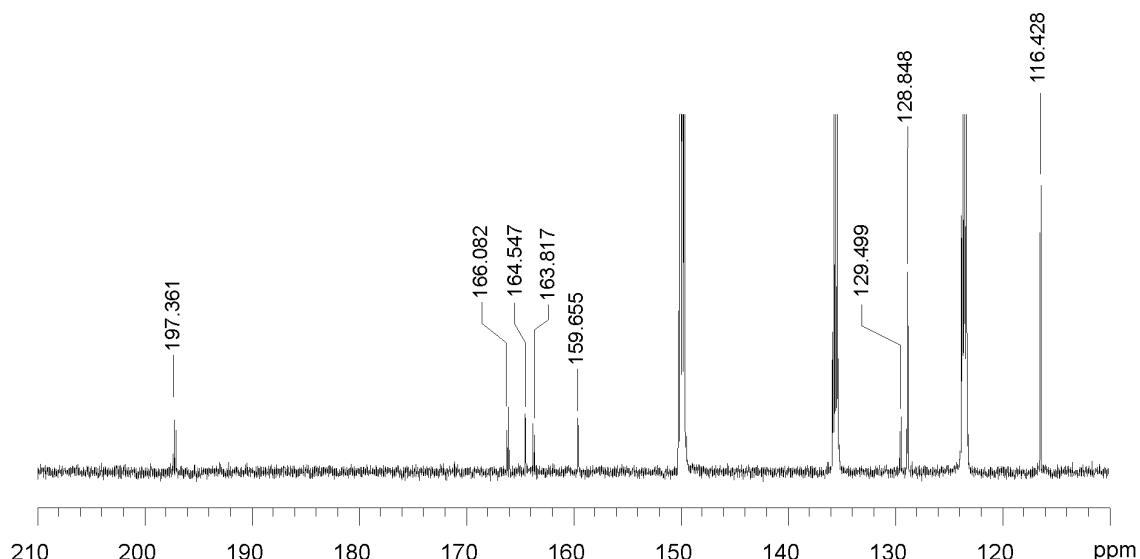
Flavone Core

Sugar

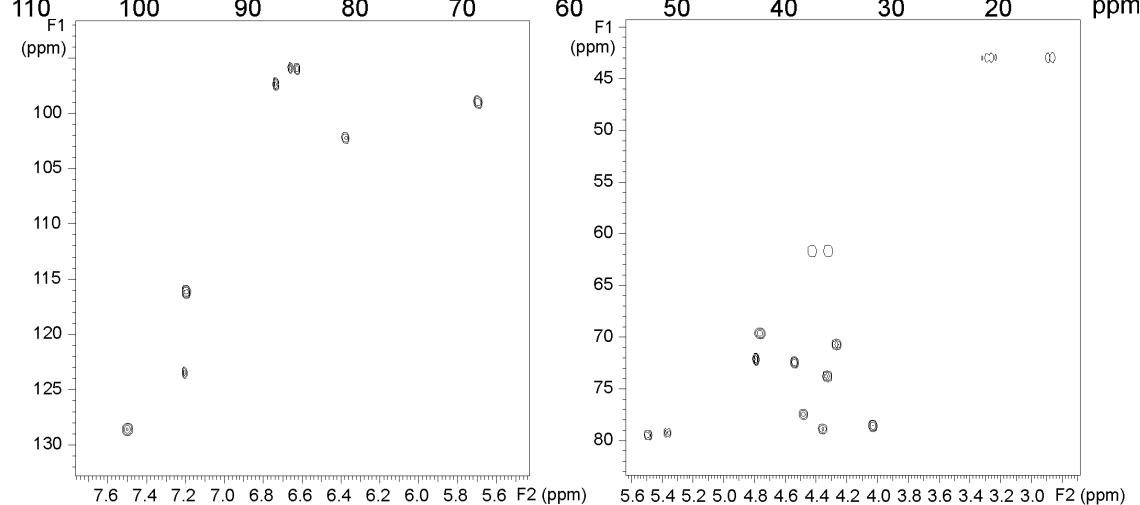
| | δ_C | δ_H | | δ_C | δ_H |
|----|------------|------------|------|------------|------------|
| 2 | 79.6d | 5.37/5.5 | 1" | 99.3d | 5.7 |
| 3 | 43.3t | 2.88/3.28 | 2" | 77.8d | 4.49 |
| 4 | 197.3s | | 3" | 79.2d | 4.36 |
| 4a | 104.4s | | 4" | 71.1d | 4.27 |
| 5 | 164.5s | | 5" | 78.9d | 4.04 |
| 6 | 97.7d | 6.75 | 6" | 62t | 4.33/4.44 |
| 7 | 166.2s | | 1''' | 102.5d | 6.38 |
| 8 | 96.2d | 6.67 | 2''' | 72.5d | 4.8 |
| 8a | 163.7s | | 3''' | 72.8d | 4.55 |
| 1' | 129.5s | | 4''' | 74.1d | 4.33 |
| 2' | 128.9d | 7.51 | 5''' | 70d | 4.77 |
| 3' | 116.5d | 7.2 | 6''' | 19q | 1.79 |
| 4' | 159.6s | | | | |
| 5' | 116.5d | 7.2 | | | |
| 6' | 128.9d | 7.51 | | | |



NMR-13C:



NMR-HSQC:



Names

7-[[2-O-(6-deoxy- α -L-mannopyranosyl)- β -D-glucopyranosyl]oxy]-2,3-dihydro-5-hydroxy-2-(4-hydroxyphenyl)-(2S)-4H-1-benzopyran-4-one; 7-[[2-O-(6-deoxy- α -L-mannopyranosyl)- β -D-glucopyranosyl]oxy]-2,3-dihydro-5-hydroxy-2-(4-hydroxyphenyl)-(S)-4H-1-benzopyran-4-one; Naringin; (2S)-Naringin; 7-[2-O-(6-Deoxy- α -L-mannopyranosyl)- β -D-glucopyranosyloxy]-2,3-dihydro-5,7,4'-trihydroxyflavone; Aurantiin; Naringenin 7-O-neohesperidoside; Naringenin 7-O- β -D-neohesperidoside; Naringenin 7-neohesperidoside; Naringenin 7-rhamnoglucoside; Naringenin 7 β -neohesperidoside; Naringoside

Naringenin-7-O-glucosidNaringenin-7-O- β -D-glucopyranoside

CAS-Number: 529-55-5

Formula: C₂₁H₂₂O₁₀ Exact mass: 434.12130

Molecular mass: 434.39

Column: Zorbax LiChrosphere Kinetex

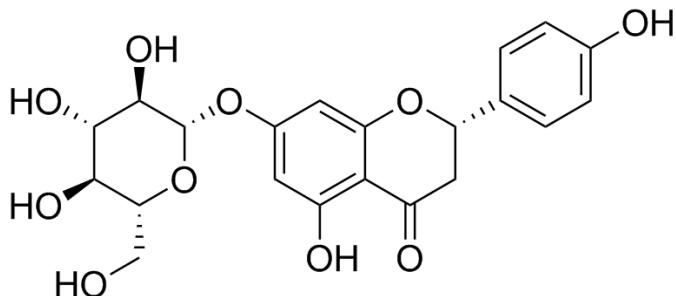
Abs.RetentionTime [min]: 17.81 14.45 7.07

Rel. RetentionTime (k'): 14.09 12.89 12.34

k' rel. to Rutin : 1.07 1.04 1.03

MS1: 433.2 MS2: 271.2 MS3: 151.1

UV/Vis: 285, 330(sh)

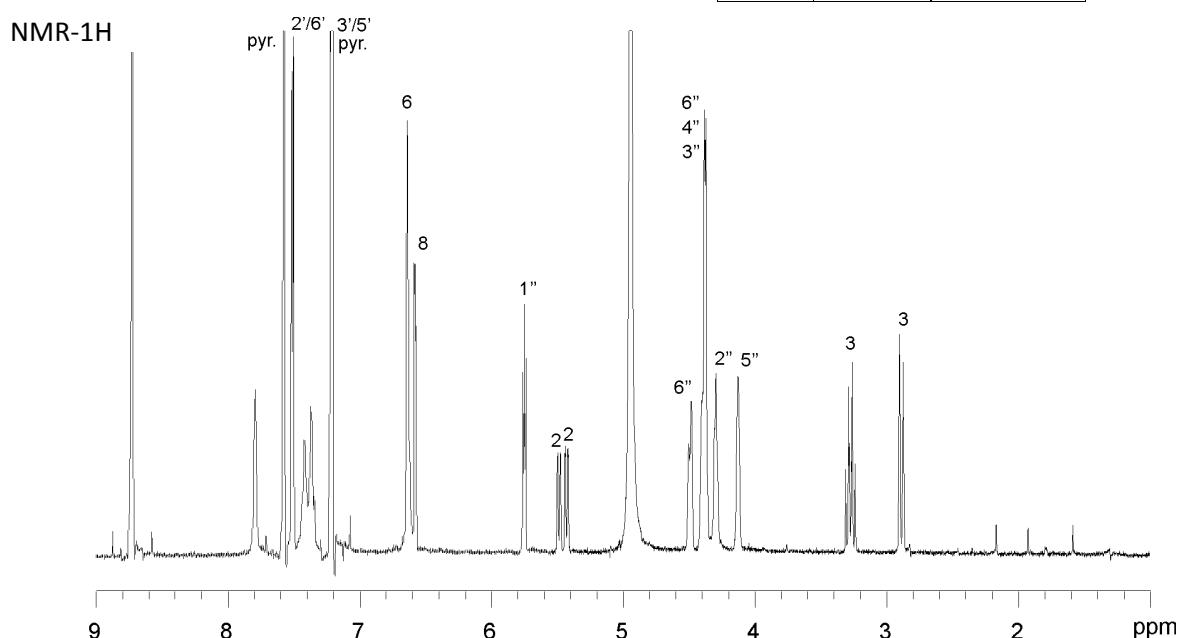


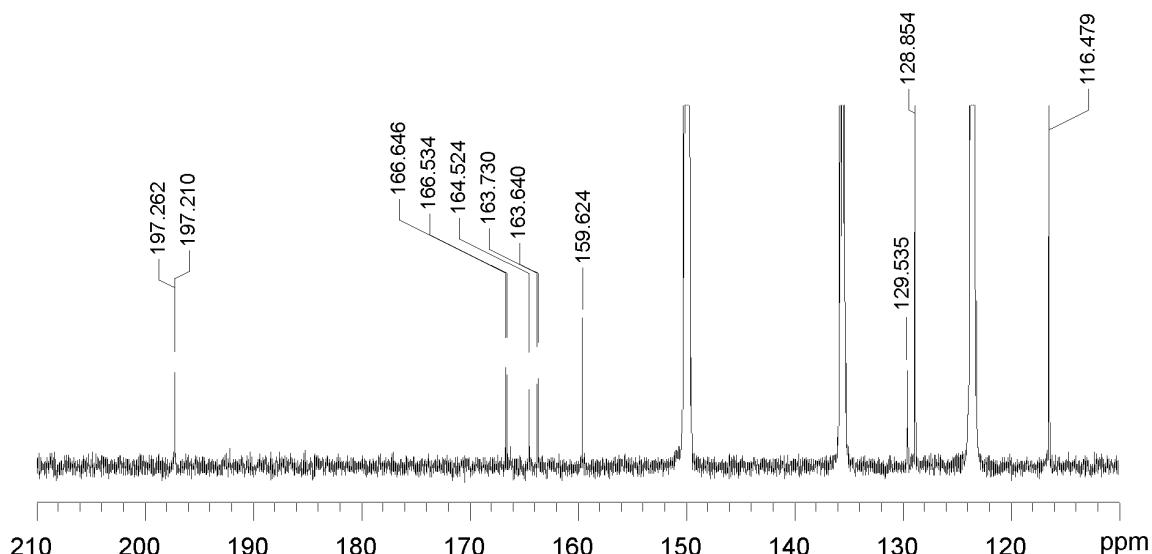
NMR - Resonance Assignments:

Flavone Core

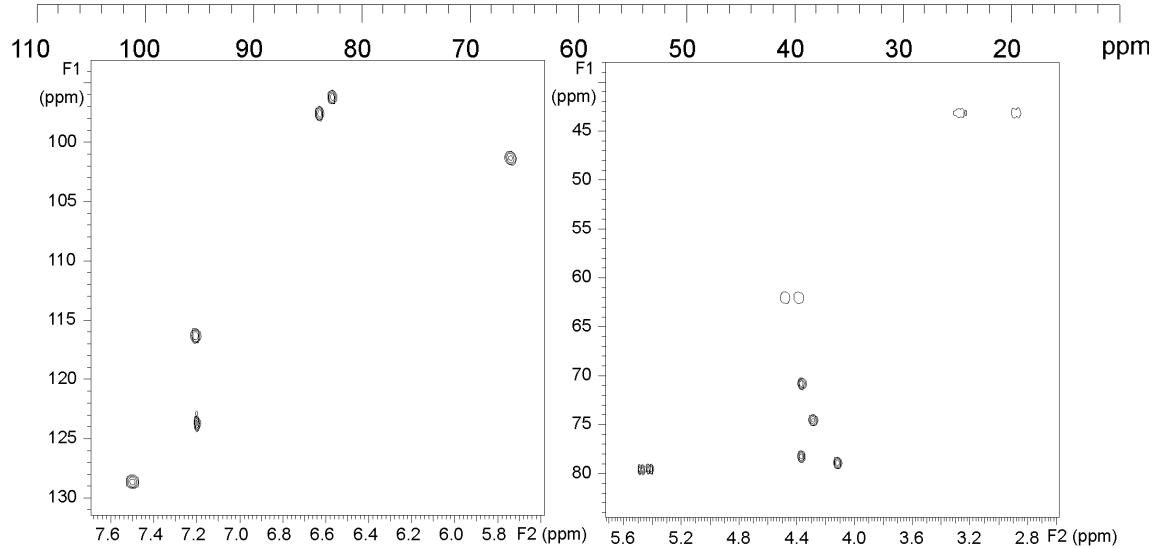
Sugar

| | δ_C | δ_H | | δ_C | δ_H |
|----|------------|------------|----|------------|------------|
| 2 | 79.8d | 5.49/5.43 | 5" | 79.1d | 4.12 |
| 3 | 43.3t | 3.29/2.89 | 6" | 62.2t | 4.45/4.39 |
| 4 | 197.3s | | 1" | 101.4d | 5.75 |
| 4a | 104.3s | | 2" | 74.7d | 4.29 |
| 5 | 169.5s | | 3" | 78.4d | 4.38 |
| 6 | 97.6d | 6.64 | 4" | 71d | 4.38 |
| 7 | 166.6s | | | | |
| 8 | 96.3d | 6.58 | | | |
| 8a | 163.6s | | | | |
| 1' | 129.5s | | | | |
| 2' | 128.9d | 7.51 | | | |
| 3' | 116.6d | 7.22 | | | |
| 4' | 159.6s | | | | |
| 5' | 116.5d | 7.22 | | | |
| 6' | 128.9d | 7.51 | | | |



NMR-¹³C:

NMR-HSQC:



Names

7-(β -D-glucopyranosyloxy)-2,3-dihydro-5-hydroxy-2-(4-hydroxyphenyl)-, (2S)-4H-1-benzopyran-4-one; 7-(β -D-glucopyranosyloxy)-2,3-dihydro-5-hydroxy-2-(4-hydroxyphenyl)-(S)-4H-1-benzopyran-4-one; Prunin; (-)-Naringenin 7- β -D-glucoside; 5,7,4'-trihydroxyflavanone 7-O- β -D-glucopyranoside; NSC 135064; Naringenin 7-O-glucoside; Naringenin 7-O- β -D-glucopyranoside; Naringenin 7-O- β -D-glucoside; Naringenin 7-glucoside

Hesperetin

5,7,3'-Trihydroxy-4'-methoxyflavanone

CAS-Number: 520-33-2

Formula: C₁₆H₁₄O₆ Exact mass: 302.07904

Molecular mass: 302.28

Column: Zorbax LiChrosphere Kinetex

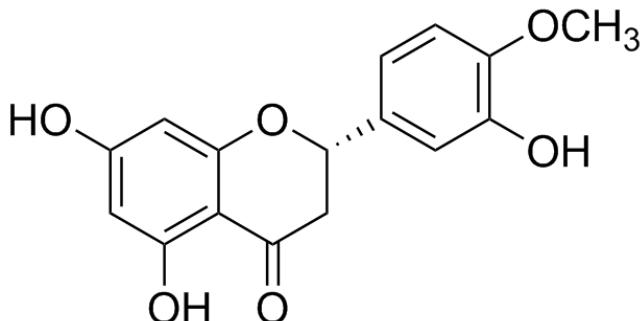
Abs.RetentionTime [min]: 23.33 20.19 10.04

Rel. RetentionTime (k') : 18.77 18.41 17.94

k' rel. to Rutin : 1.42 1.48 1.50

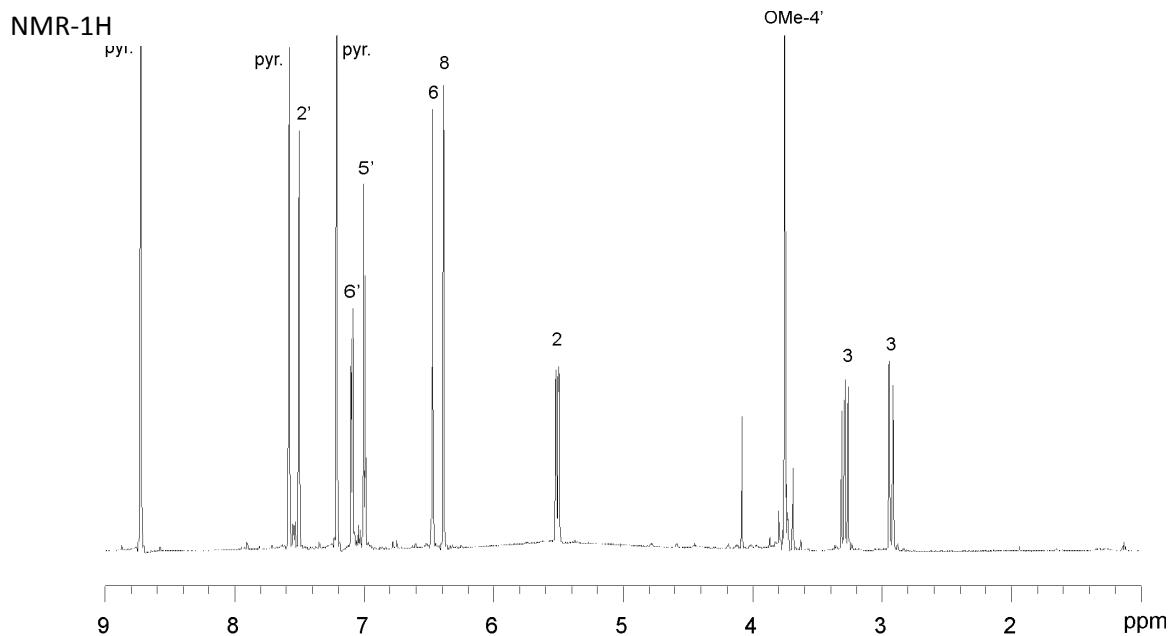
MS1: 301.2 MS2: 286.1 MS3: 258.1

UV/Vis: 285, 330(sh)

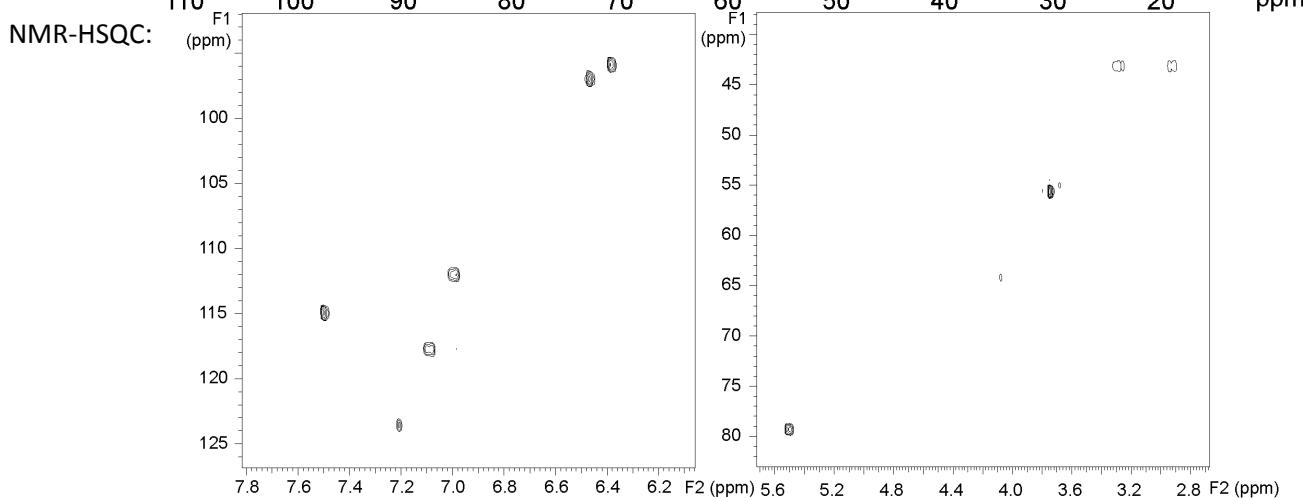
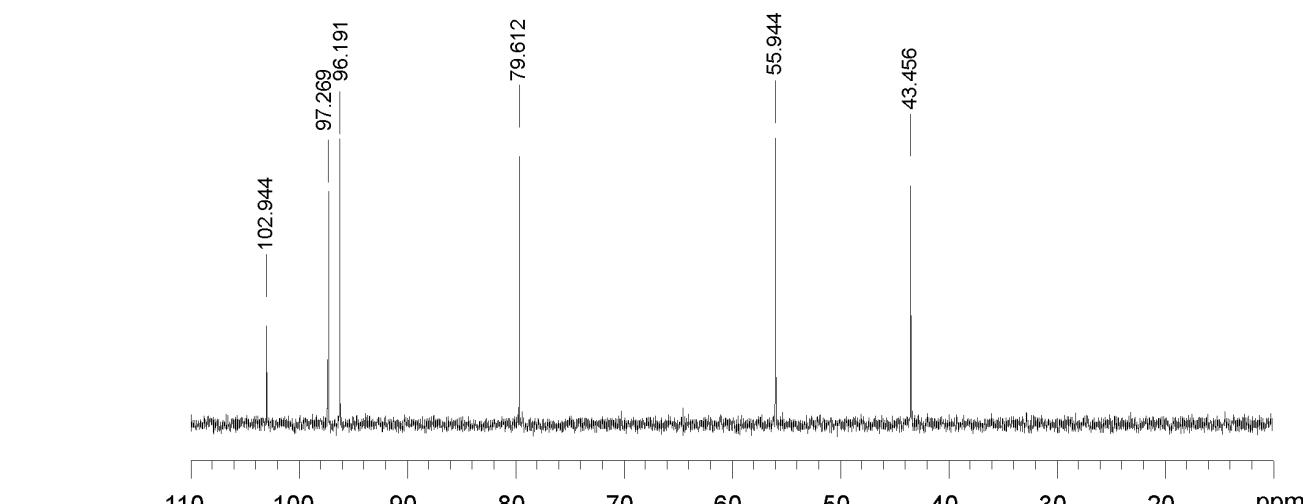
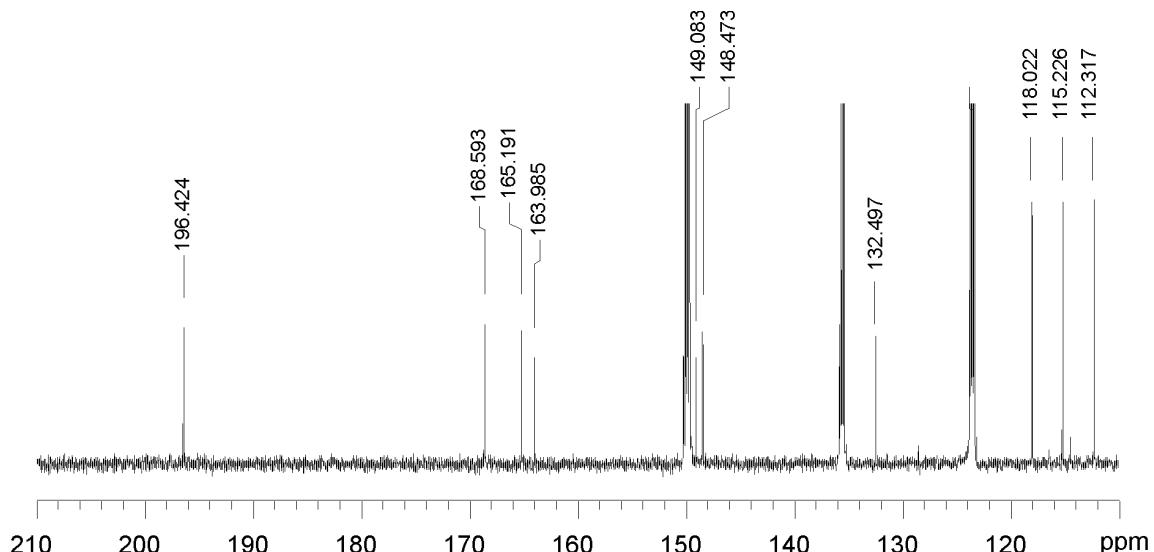


NMR - Resonance Assignments:

| | δ_C | δ_H |
|--------|------------|------------|
| 2 | 79.6d | 5.51 |
| 3 | 43.4t | 3.29/2.93 |
| 4 | 196.4s | |
| 4a | 102.9s | |
| 5 | 165.2s | |
| 6 | 97.3d | 6.47 |
| 7 | 168.6s | |
| 8 | 96.2d | 6.39 |
| 8a | 164s | |
| 1' | 132.5s | |
| 2' | 115.2d | 7.5 |
| 3' | 148.5s | |
| 4' | 149.1s | |
| 5' | 112.3d | 6.99 |
| 6' | 118d | 7.09 |
| OMe-4' | 55.9q | 3.75 |



NMR-13C:



Names

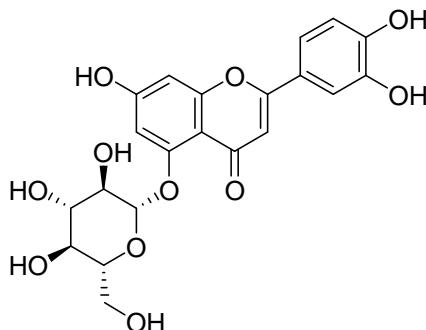
2,3-dihydro-5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-(2S)-4H-1-benzopyran-4-one; 2,3-dihydro-5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-(S)-4H-1-benzopyran-4-one; 5,7,3'-trihydroxy-4'-methoxy-flavanone; Hesperetin; (-)-Hesperetin; 2,3-Dihydro-5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-4H-1-benzopyran-4-one; 5,7,3'-Trihydroxy-4'-methoxyflavanone; 5,7,3'-Trihydroxy-4'-methoxyflavanone; Eriodictyol 4'-monomethyl ether; Hesperitin; NSC 57654

Luteolin-5-O-glucosidLuteolin-5-O- β -D-glucopyranoside

CAS-Number: 20344-46-1

Formula: C₂₁H₂₀O₁₁ Exact mass: 448.10056

Molecular mass: 448.38



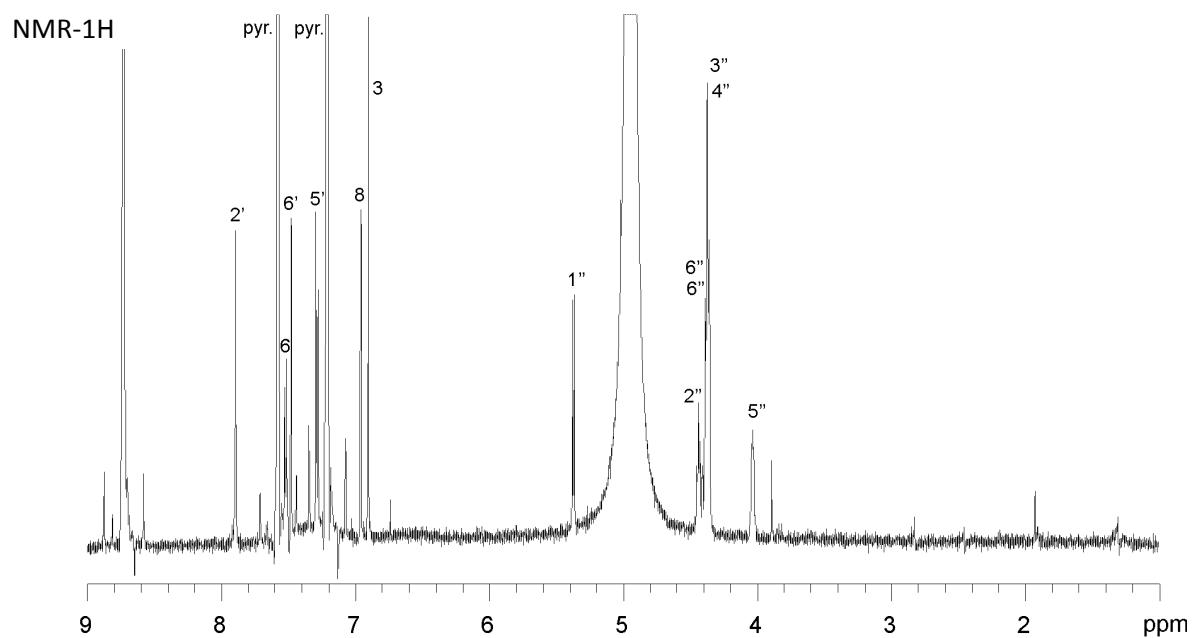
| Column: | Zorbax | LiChrosphere | Kinetex |
|---------------------------|--------|--------------|---------|
| Abs.RetentionTime [min]: | 15.84 | 13.20 | 6.33 |
| Rel. RetentionTime (k') : | 12.42 | 11.69 | 10.94 |
| k' rel. to Rutin : | 0.94 | 0.94 | 0.92 |

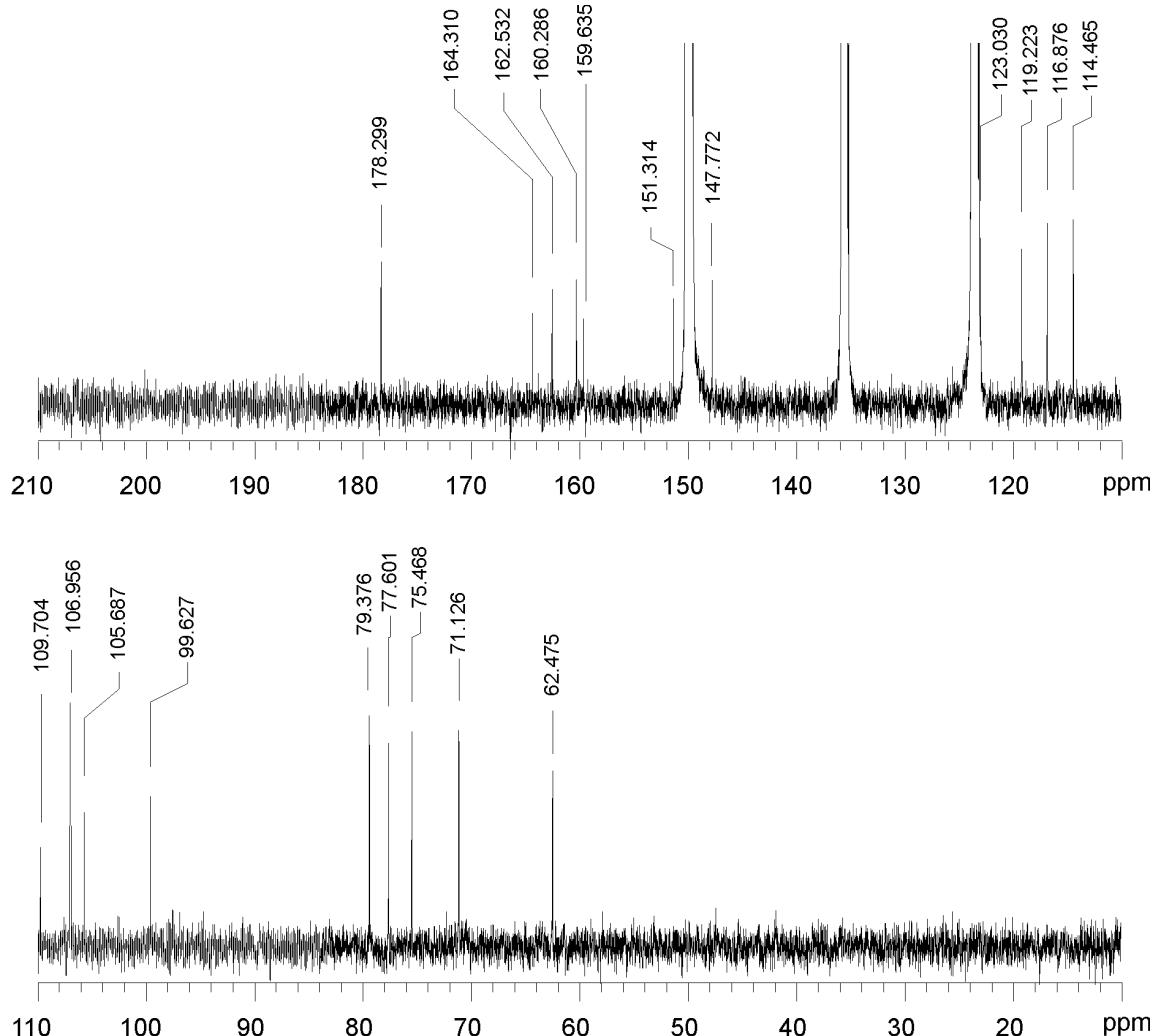
MS1: 447.3 MS2: 285.2 MS3: 241.2

UV/Vis: 255, 305(sh), 3

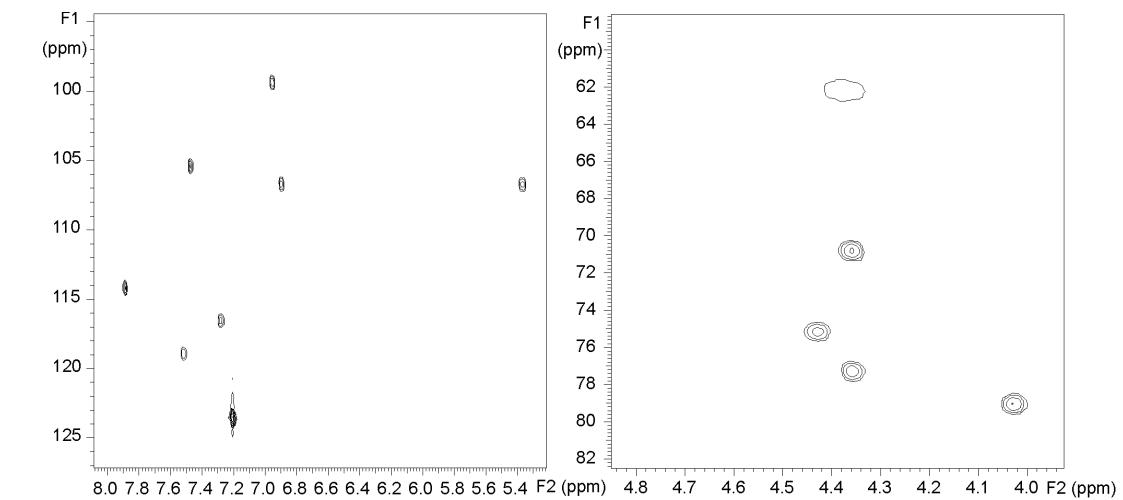
NMR - Resonance Assignments:
Flavone Core Sugar

| | δ_C | δ_H | | δ_C | δ_H |
|----|------------|------------|----|------------|------------|
| 2 | 162.5s | | 1" | 106.9d | 5.37 |
| 3 | 106.9d | 6.9 | 2" | 75.5d | 4.43 |
| 4 | 178.3s | | 3" | 77.6d | 4.35 |
| 4a | 109.7s | | 4" | 71.1d | 4.35 |
| 5 | 160.3s | | 5" | 79.4d | 4.03 |
| 6 | 105.7d | 7.48 | 6" | 62.5t | 4.37 |
| 7 | 164.3s | | | | |
| 8 | 99.6d | 6.96 | | | |
| 8a | 159.6s | | | | |
| 1' | 123s | | | | |
| 2' | 114.5d | 7.89 | | | |
| 3' | 147.8s | | | | |
| 4' | 151.3s | | | | |
| 5' | 116.9d | 7.28 | | | |
| 6' | 119.2d | 7.52 | | | |



NMR-¹³C:

NMR-HSQC:



Names

2-(3,4-dihydroxyphenyl)-5-(β -D-glucopyranosyloxy)-7-hydroxy-flavone-5,7,3',4'-tetrahydroxy- 5- β -D-glucopyranoside-4H-1-benzopyran-4-one; Galuteolin; Luteolin 5-O- β -D-glucopyranoside; Luteolin 5-glucoside; Luteolin 5- β -D-glucopyranoside; Luteolin-5-O-glucoside; Luteolin-5-O- β -D-glucoside

Galangin-3-rutinosidGalangin-3-O- β -D-rutinoside

CAS-Number: 16268-50-1

Formula: C₂₇H₃₀O₁₄ Exact mass: 578.16356

Molecular mass: 578.52

Column: Zorbax LiChrosphere Kinetex

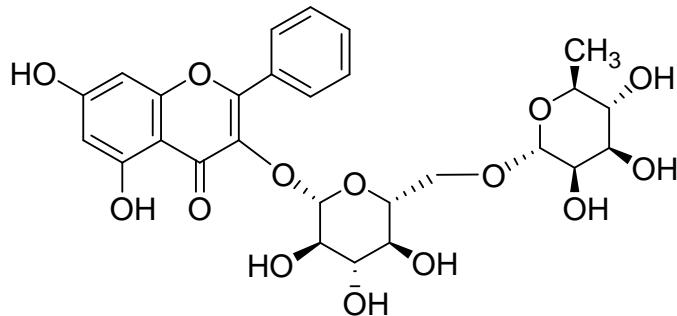
Abs.RetentionTime [min]: 19.81 16.96 8.42

Rel. RetentionTime (k'): 15.79 15.31 14.89

k' rel. to Rutin : 1.20 1.23 1.25

MS1: 577.3 MS2: 269.2 MS3: 241.2

UV/Vis: 265, 310(sh)



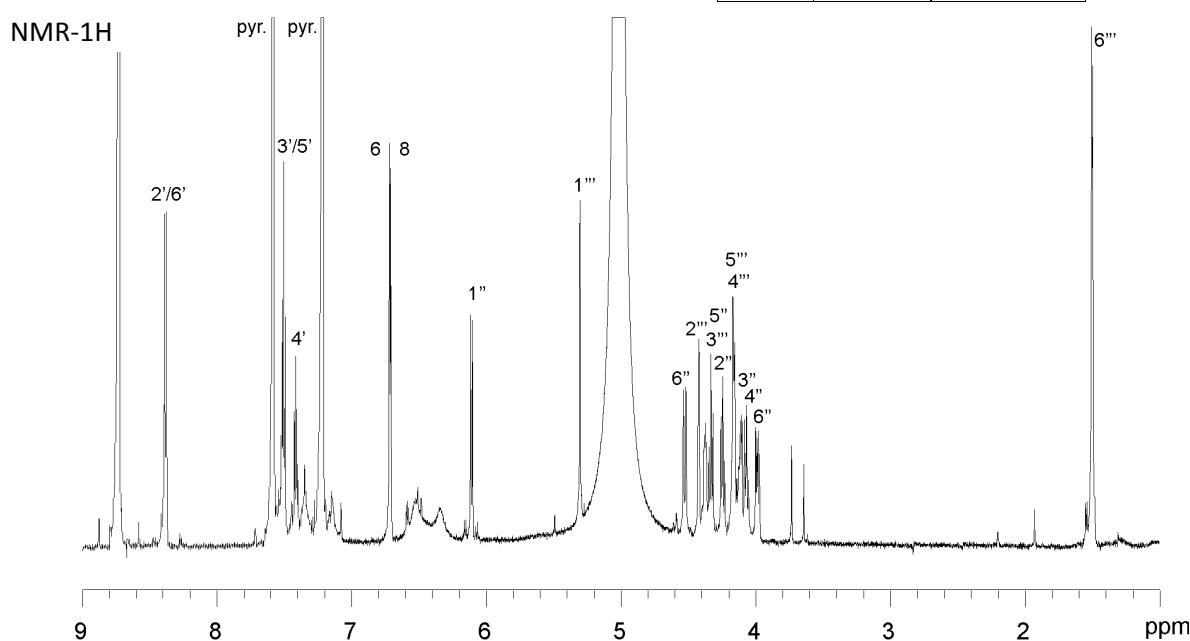
NMR - Resonance Assignments:

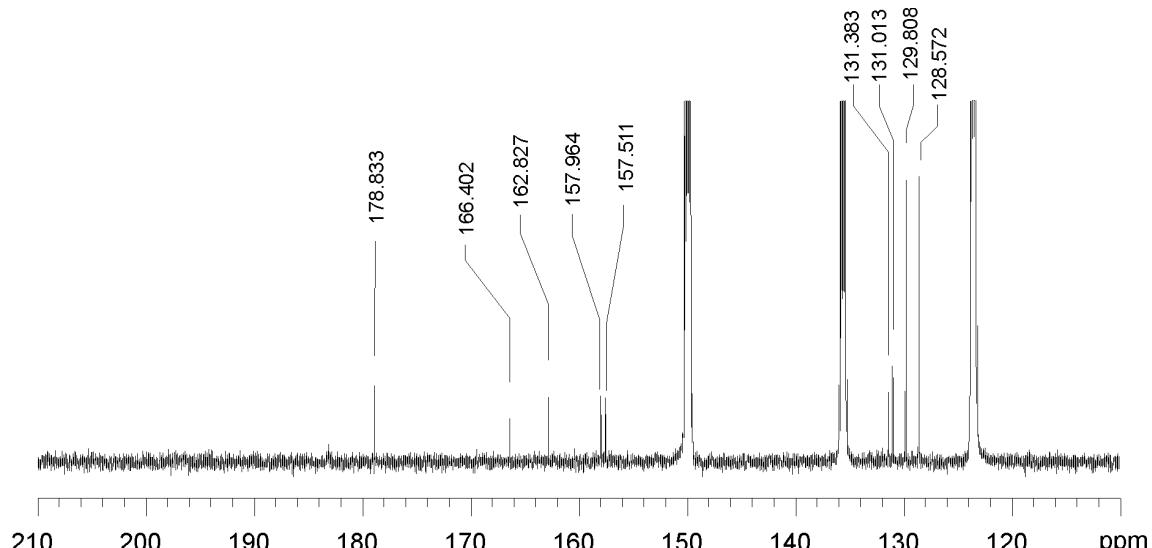
Flavone Core

Sugar

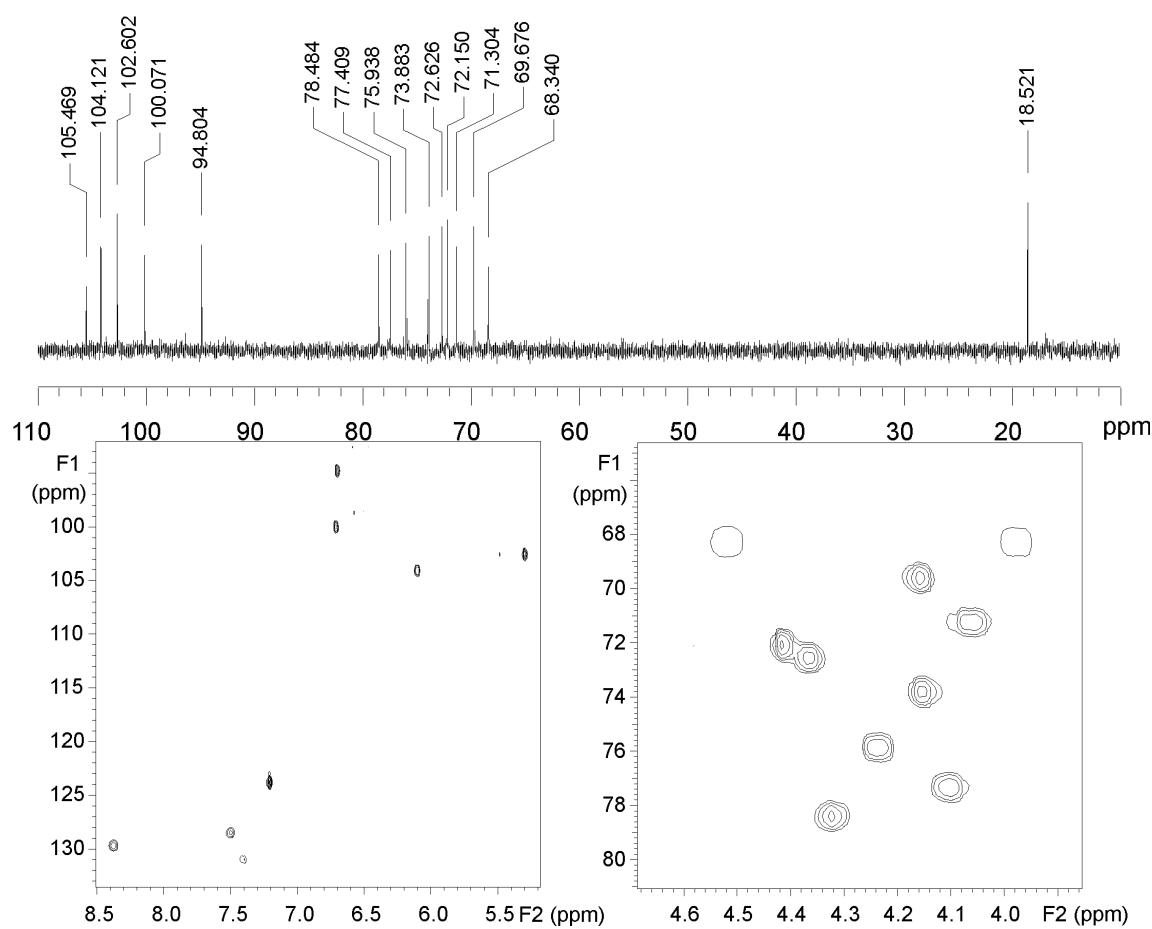
| | δ_C | δ_H |
|----|------------|------------|
| 2 | 157.5s | |
| 3 | 136s | |
| 4 | 178.8s | |
| 4a | 105.5s | |
| 5 | 162.8s | |
| 6 | 100.1d | 6.72 |
| 7 | 166.4s | |
| 8 | 94.8d | 6.71 |
| 8a | 158s | |
| 1' | 131.4s | |
| 2' | 129.8d | 8.38 |
| 3' | 128.6d | 7.5 |
| 4' | 131d | 7.41 |
| 5' | 128.6d | 7.5 |
| 6' | 129.8d | 8.38 |

| | δ_C | δ_H |
|------|------------|------------|
| 1'' | 104.1d | 6.11 |
| 2'' | 75.9d | 4.24 |
| 3'' | 77.5d | 4.1 |
| 4'' | 71.3d | 4.06 |
| 5'' | 78.5d | 4.32 |
| 6'' | 68.3t | 4.52/3.98 |
| 1''' | 102.6d | 5.3 |
| 2''' | 72.1d | 4.42 |
| 3''' | 72.6d | 4.37 |
| 4''' | 73.9d | 4.16 |
| 5''' | 69.7d | 4.16 |
| 6''' | 18.5q | 1.5 |



NMR-¹³C:

NMR-HSQC:



Names

3-[[6-O-(6-deoxy- α -L-mannopyranosyl)- β -D-glucopyranosyl]oxy]-5,7-dihydroxy-2-phenyl-4H-1-benzopyran-4-one;
3,5,7-trihydroxy-flavone, 3-[6-O-(6-deoxy- α -L-mannopyranosyl)- β -D-glucopyranoside]; Galangin 3-rutinoside;
Galanginoside

Hyperosid

Quercetin-3-O- β -D-galactopyranoside

CAS-Number: 482-36-0

Formula: C₂₁H₂₀O₁₂ Exact mass: 464.09548

Molecular mass: 464.38

Column: Zorbax LiChrosphere Kinetex

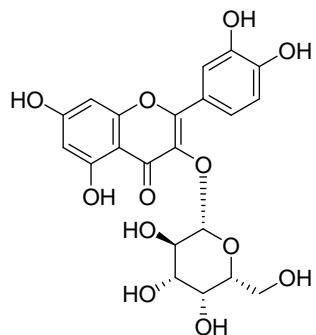
Abs.RetentionTime [min]: 16.67 14.05 6.83

Rel. RetentionTime (k'): 13.13 12.51 11.89

k' rel. to Rutin : 0.99 1.01 1.00

MS1: 463.2 MS2: 301.2 MS3: 178.9

UV/Vis: 255, 300(sh), 3

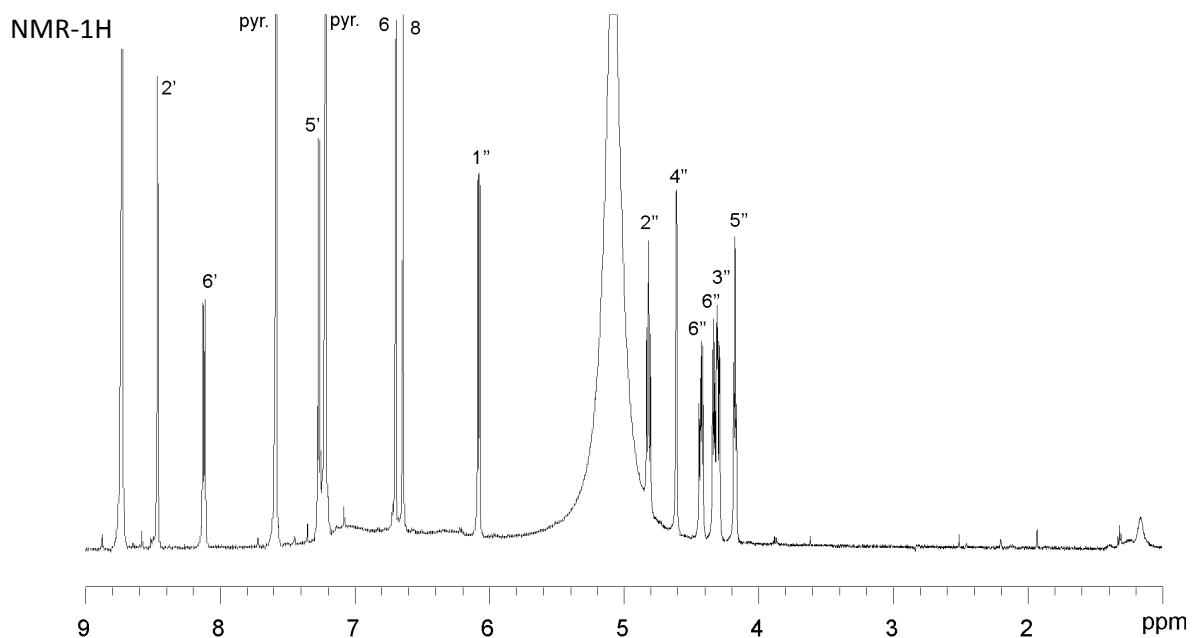


NMR - Resonance Assignments:

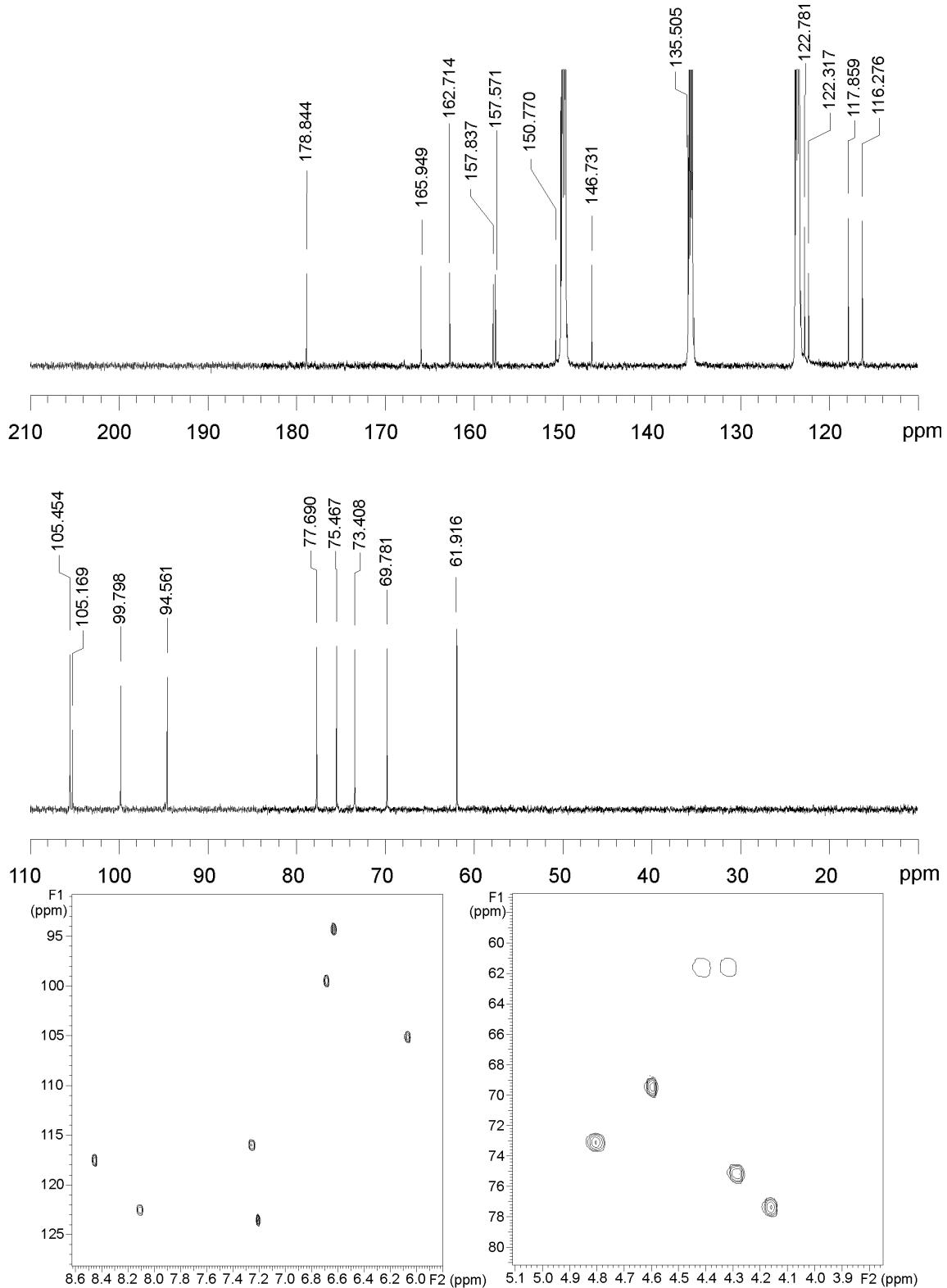
Flavone Core

Sugar

| | δ_C | δ_H | | δ_C | δ_H |
|----|------------|------------|----|------------|------------|
| 2 | 157.8s | | 1" | 105.5d | 6.07 |
| 3 | 135.5s | | 2" | 73.4d | 4.8 |
| 4 | 178.8s | | 3" | 75.5d | 4.29 |
| 4a | 105.2s | | 4" | 69.8d | 4.6 |
| 5 | 162.7s | | 5" | 77.7d | 4.17 |
| 6 | 99.8d | 6.68 | 6" | 61.9t | 4.42/4.31 |
| 7 | 165.9s | | | | |
| 8 | 94.6d | 6.63 | | | |
| 8a | 157.6s | | | | |
| 1' | 122.3s | | | | |
| 2' | 117.9d | 8.41 | | | |
| 3' | 146.7s | | | | |
| 4' | 150.8s | | | | |
| 5' | 116.3d | 7.26 | | | |
| 6' | 122.8d | 8.12 | | | |



NMR-13C:



Names

2-(3,4-dihydroxyphenyl)-3-(β -D-galactopyranosyloxy)-5,7-dihydroxy-4H-1-benzopyran-4-one; Hyperin; 3,5,7,3',4'-pentahydroxyflavone 3-O- β -D-galactopyranoside; 3-O- β -D-Galactopyranosyl quercetin; 3-O- β -D-galactopyranosylquercetin; Hyperosid; Hyperoside; NSC 407304; Quercetin 3-O-galactopyranoside; Quercetin 3-O- β -D-galactopyranoside; Quercetin 3-O- β -D-galactoside; Quercetin 3-O- β -galactopyranoside; Quercetin 3-O- β -galactoside; Quercetin 3-galactoside; Quercetin 3- β -D-galactoside; Quercetin 3- β -galactoside

Isoquercitrin

Quercetin-3-O-β-D-glucopyranoside

CAS-Number: 482-35-9

Formula: C₂₁H₂₀O₁₂ Exact mass: 464.09548

Molecular mass: 464.38

Column: Zorbax LiChrosphere Kinetex

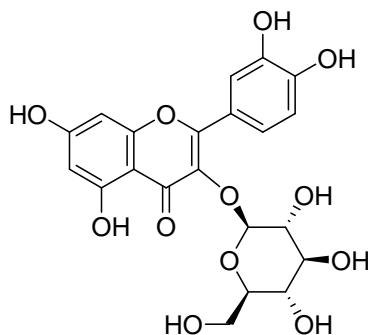
Abs.RetentionTime [min]: 16.88 14.24 6.96

Rel. RetentionTime (k') : 13.31 12.69 12.13

k' rel. to Rutin : 1.01 1.02 1.02

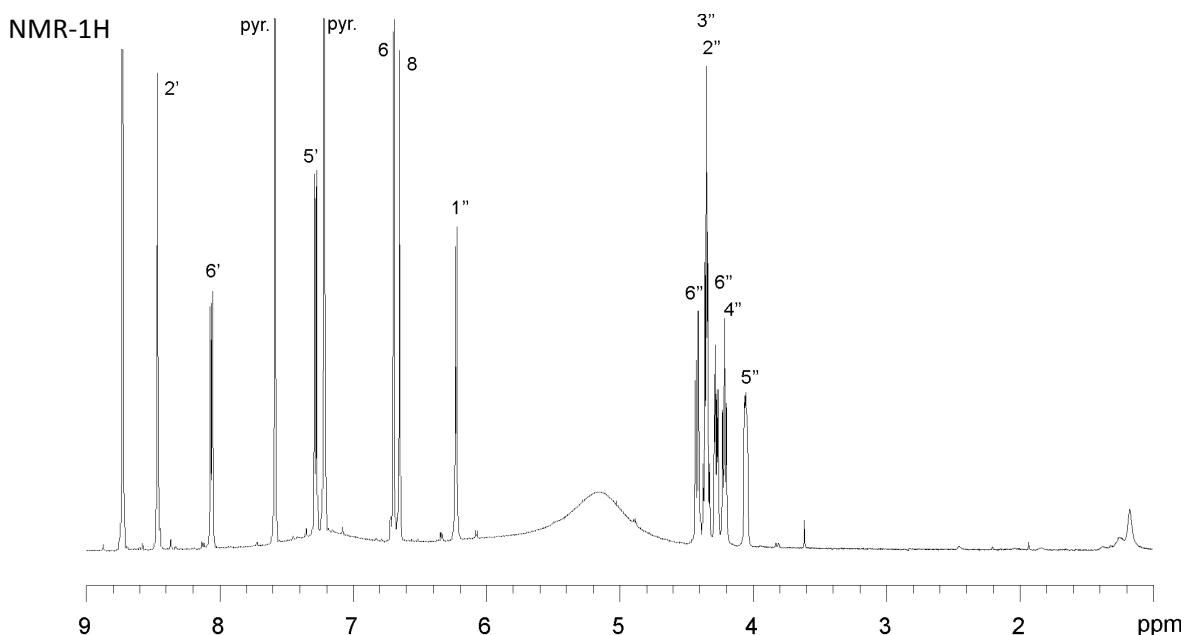
MS1: 463 2 MS2: 301 2 MS3: 178 9

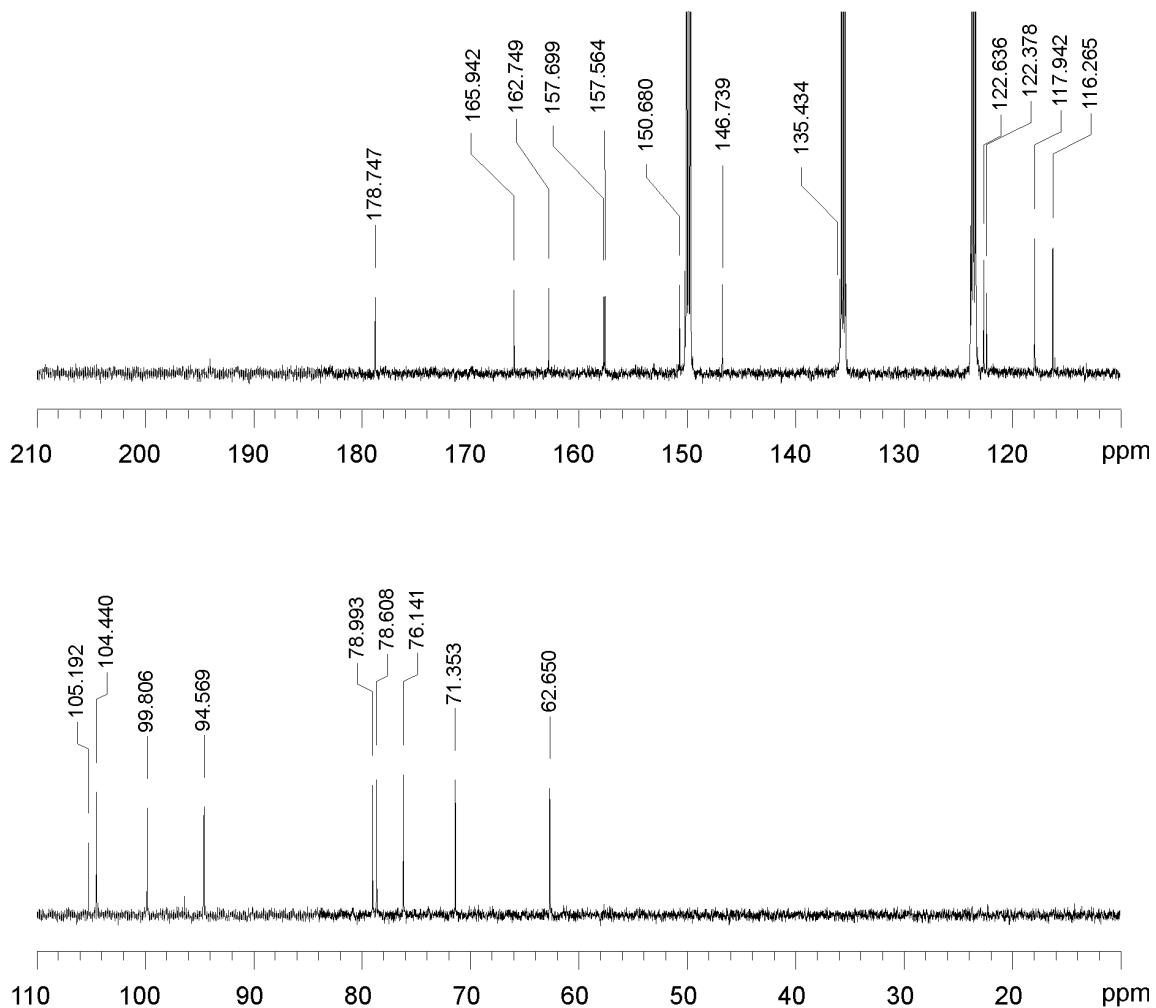
UV/Vis: 255, 305 (sh), 3



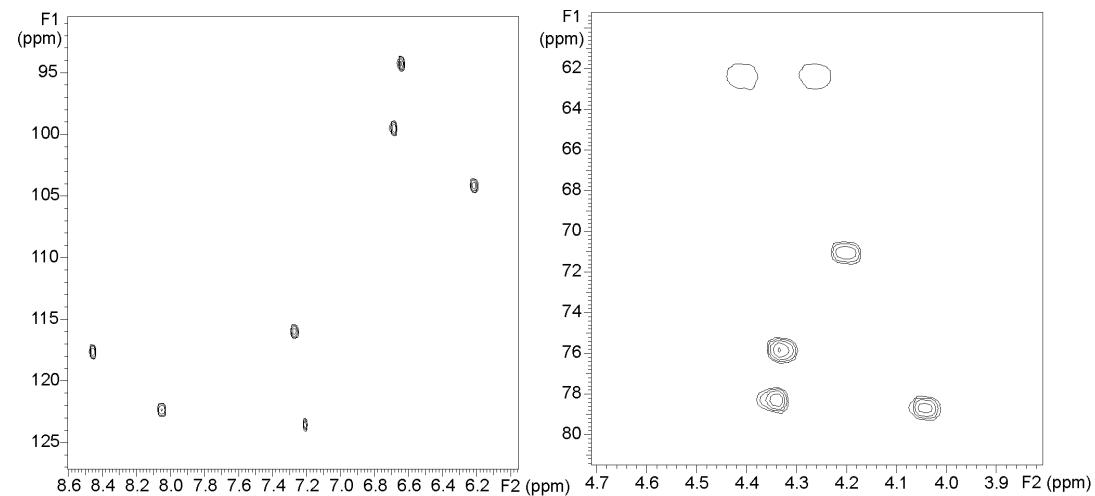
NMR - Resonance Assignments:

| | δ_C | δ_H | | δ_C | δ_H |
|----|------------|------------|----|------------|------------|
| 2 | 157.7s | | 1" | 104.4d | 6.22 |
| 3 | 135.4s | | 2" | 76.1d | 4.33 |
| 4 | 178.7s | | 3" | 78.6d | 4.34 |
| 4a | 105.2s | | 4" | 71.3d | 4.2 |
| 5 | 162.7s | | 5" | 79d | 4.04 |
| 6 | 99.8d | 6.69 | 6" | 62.6t | 4.41/4.27 |
| 7 | 165.9s | | | | |
| 8 | 94.6d | 6.64 | | | |
| 8a | 157.6s | | | | |
| 1' | 122.4s | | | | |
| 2' | 117.9d | 8.46 | | | |
| 3' | 146.7s | | | | |
| 4' | 150.6s | | | | |
| 5' | 116.3d | 7.28 | | | |
| 6' | 122.6d | 8.05 | | | |



NMR-¹³C:

NMR-HSQC:



Names

2-(3,4-dihydroxyphenyl)-3-(β -D-glucopyranosyloxy)-5,7-dihydroxy-4H-1-benzopyran-4-one; Hirsutrin; 3-Glucosylquercetin; 3-O- β -D-glucopyranosylquercetin; 5,7,3',4'-tetrahydroxyflavone-3- β -D-glucopyranoside; Contigoside B; Glucosyl-3-quercetin; Isoquercetin; Isoquercetrin; Isoquercitrin; NSC 115918; Q 5; Quercetin 3-D-glucoside; Quercetin 3-O-glucopyranoside; Quercetin 3-O-glucoside; Quercetin 3-O- β -D-glucopyranoside; Quercetin 3-O- β -D-glucoside; Quercetin 3-O- β -glucoside; Quercetin 3-glucoside; Quercetin 3-mono-D-glucoside; Quercetin 3-monoglucoside; Quercetin 3- β -D-glucopyranoside; Quercetin 3- β -D-glucoside; Quercetin 3 β -O-glucoside; Quercetin 3 β -glucoside; Quercetin glucoside; Quercetin-3-glucose; Quercetin-3- β -glucopyranoside; Quercetol 3-glucoside; Quercetol 3-monoglucoside

Kaempferol-7-neohesperosidKaempferol-7-O- β -D-neohesperidoside

CAS-Number: 17353-03-6

Formula: C₂₇H₃₀O₁₅ Exact mass: 594.15847

Molecular mass: 594.52

Column: Zorbax LiChrosphere Kinetex

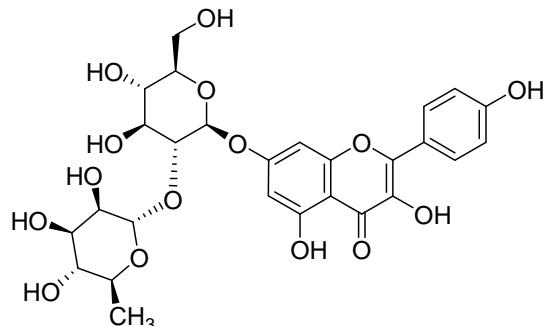
Abs.RetentionTime [min]: 18 15.20 7.53

Rel. RetentionTime (k'): 14.25 13.62 13.21

k' rel. to Rutin : 1.08 1.10 1.11

MS1: 593.2 MS2: 285.3 MS3: 285.2

UV/Vis: 250, 265(sh), 3

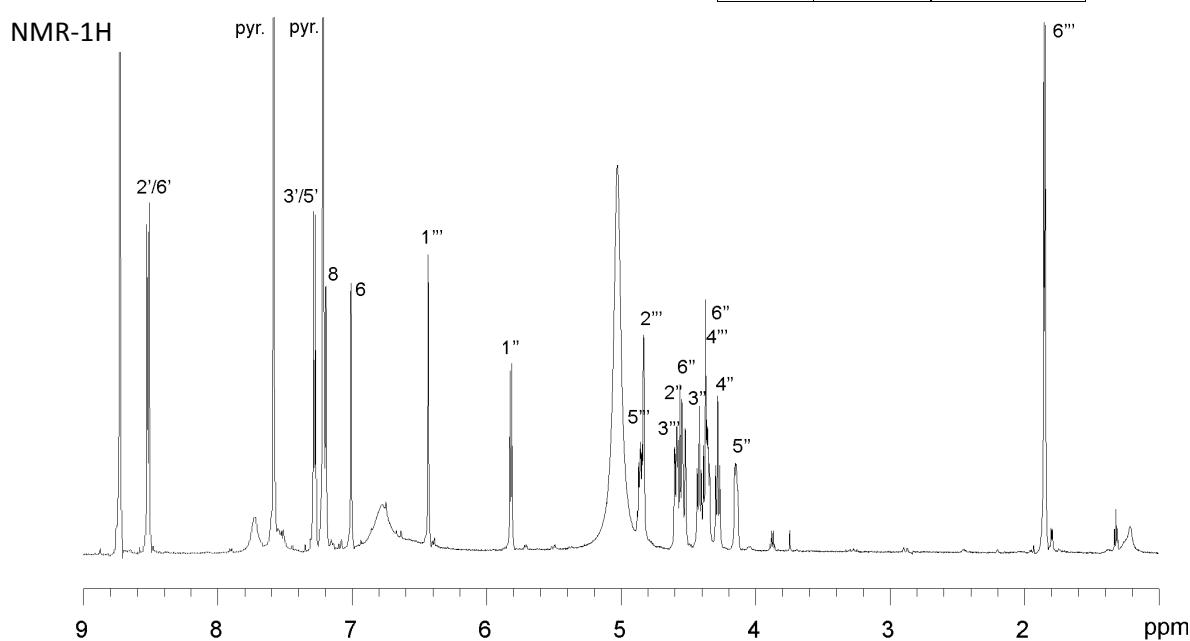


NMR - Resonance Assignments:

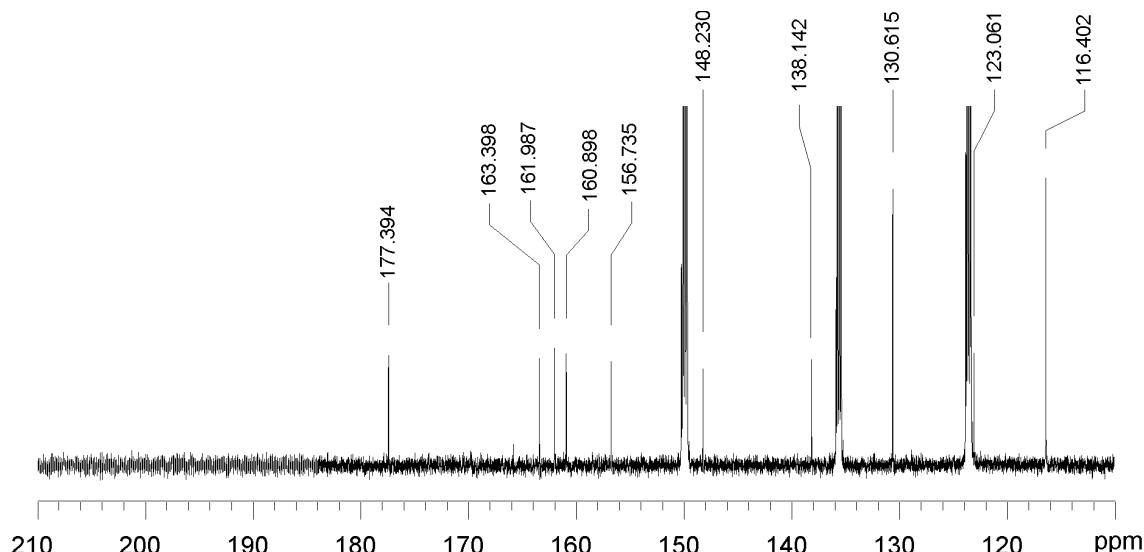
Flavone Core

Sugar

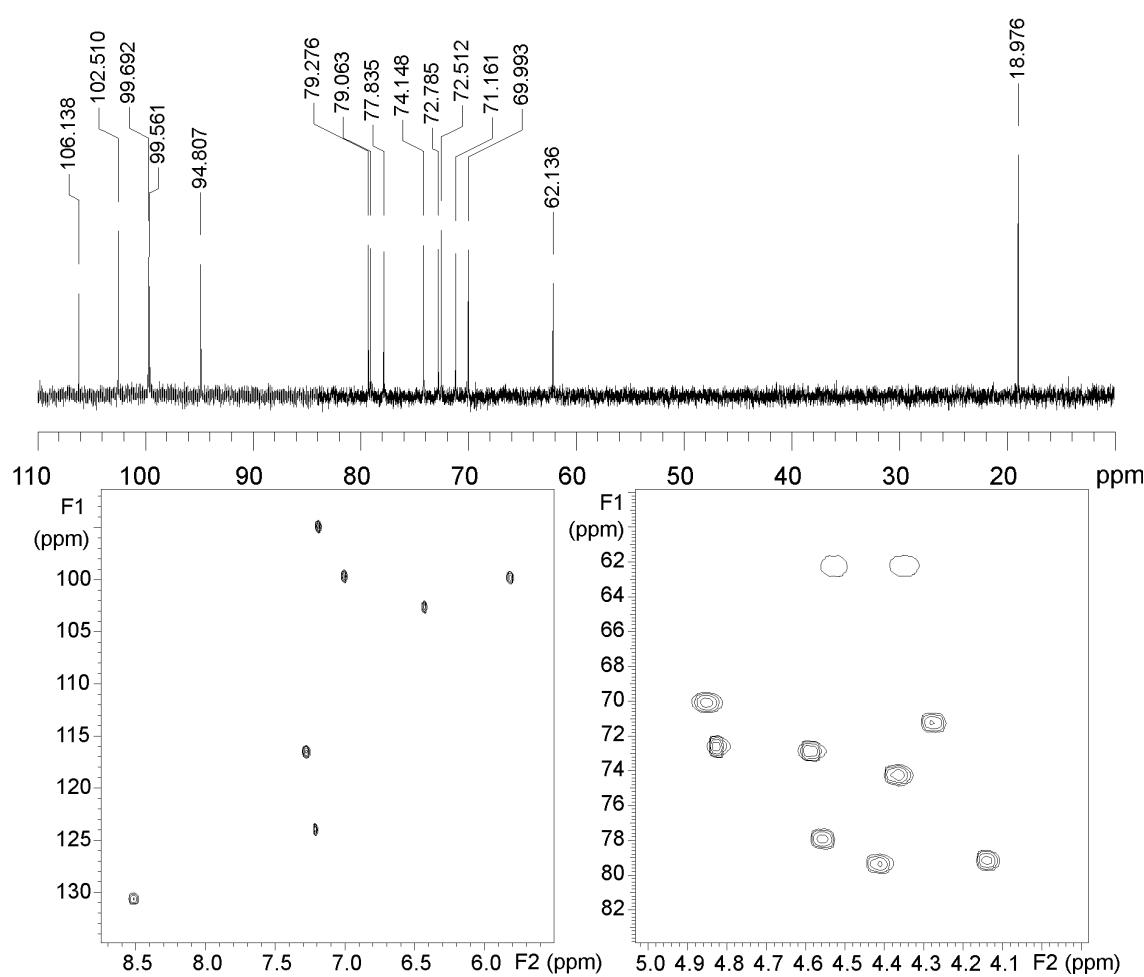
| | δ_C | δ_H | | δ_C | δ_H |
|----|------------|------------|------|------------|------------|
| 2 | 148.2s | | 1'' | 99.7d | 5.82 |
| 3 | 138.1s | | 2'' | 77.8d | 4.56 |
| 4 | 177.4s | | 3'' | 79.3d | 4.42 |
| 4a | 106.1s | | 4'' | 71.2d | 4.28 |
| 5 | 162s | | 5'' | 79.1d | 4.14 |
| 6 | 99.6d | 7.01 | 6'' | 62.1t | 4.53/4.36 |
| 7 | 163.4s | | 1''' | 102.5d | 6.43 |
| 8 | 94.8d | 7.2 | 2''' | 72.5d | 4.83 |
| 8a | 156.7s | | 3''' | 72.8d | 4.6 |
| 1' | 123.1s | | 4''' | 74.1d | 4.37 |
| 2' | 130.6d | 8.52 | 5''' | 70d | 4.86 |
| 3' | 116.4d | 7.28 | 6''' | 19q | 1.85 |
| 4' | 160.9s | | | | |
| 5' | 116.4d | 7.28 | | | |
| 6' | 130.6d | 8.52 | | | |



NMR-13C:



NMR-HSQC:



Names

7-[[2-O-(6-deoxy- α -L-mannopyranosyl)- β -D-glucopyranosyl]oxy]-3,5-dihydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one; 3,5,7,4'-tetrahydroxy-7-neohesperidoside-flavone; 3,5,7,4-Tetrahydroxyflavone 7-[2-O-(6-deoxy- α -L-mannopyranosyl)- β -D-glucopyranoside]; Kaempferol 7-O-neohesperidoside; Kaempferol 7-neohesperidoside

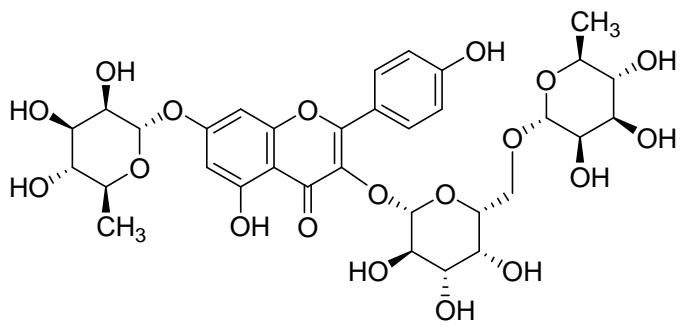
Robinin

Kaempferol 3-O- α -L-rhamnopyranosyl-(1 \rightarrow 6)- β -D-galactopyranosyl 7-O- α -L-rhamnopyranoside

CAS-Number: 301-19-9

Formula: C₃₃H₄₀O₁₉ Exact mass: 740.21638

Molecular mass: 740.66



Column: Zorbax LiChrosphere Kinetex

Abs.RetentionTime [min]: 15.95 13.23 6.42

Rel. RetentionTime (k'): 12.52 11.72 11.11

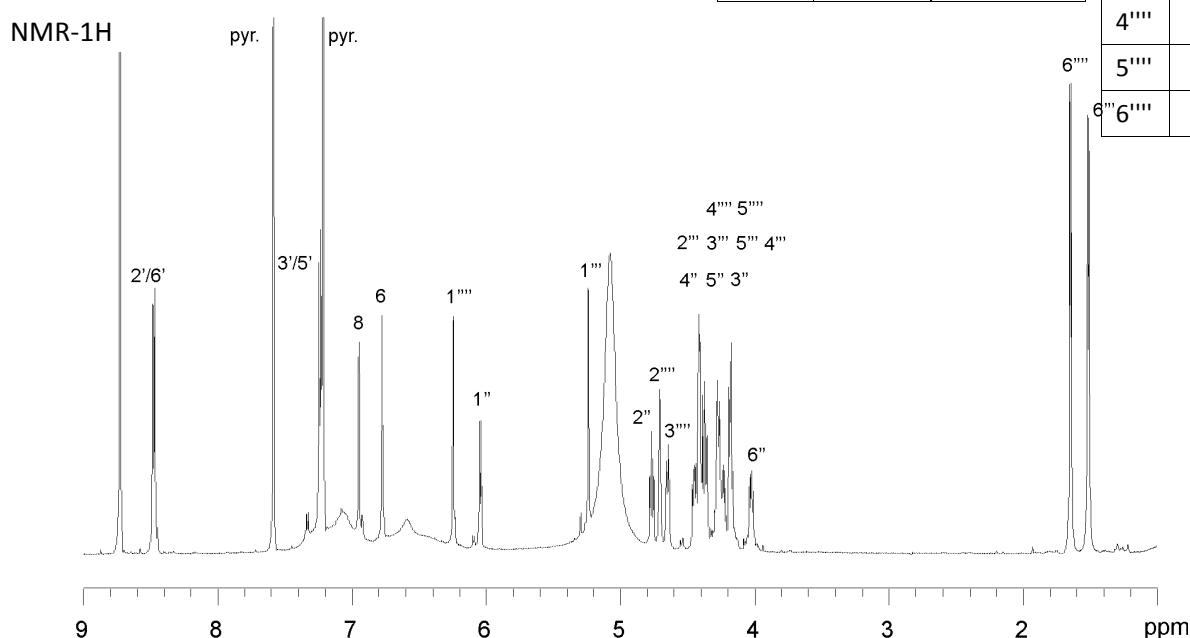
k' rel. to Rutin : 0.95 0.94 0.93

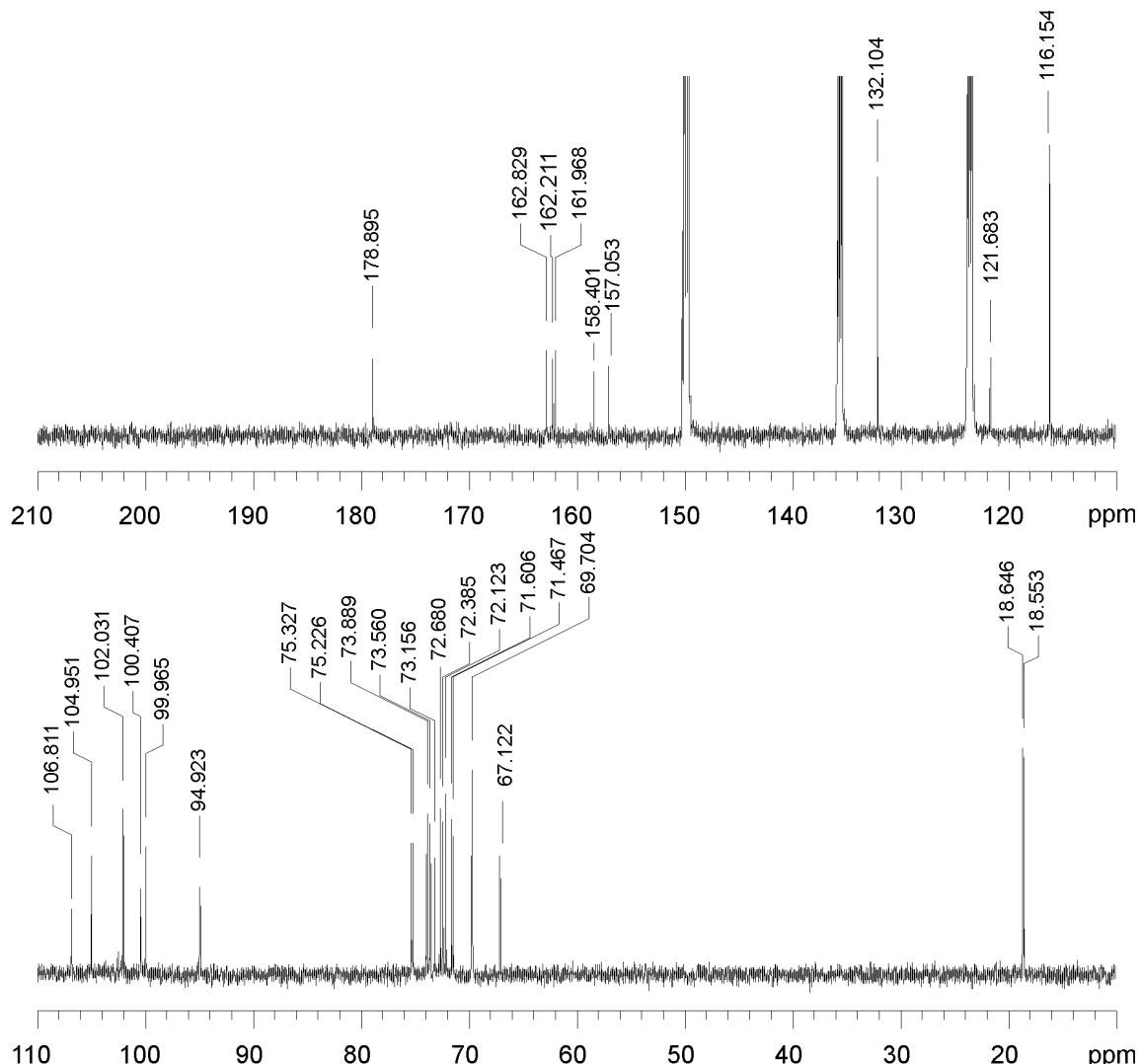
MS1: 739.2 MS2: 593.1 MS3: 285.2

UV/Vis: 265, 320(sh), 3

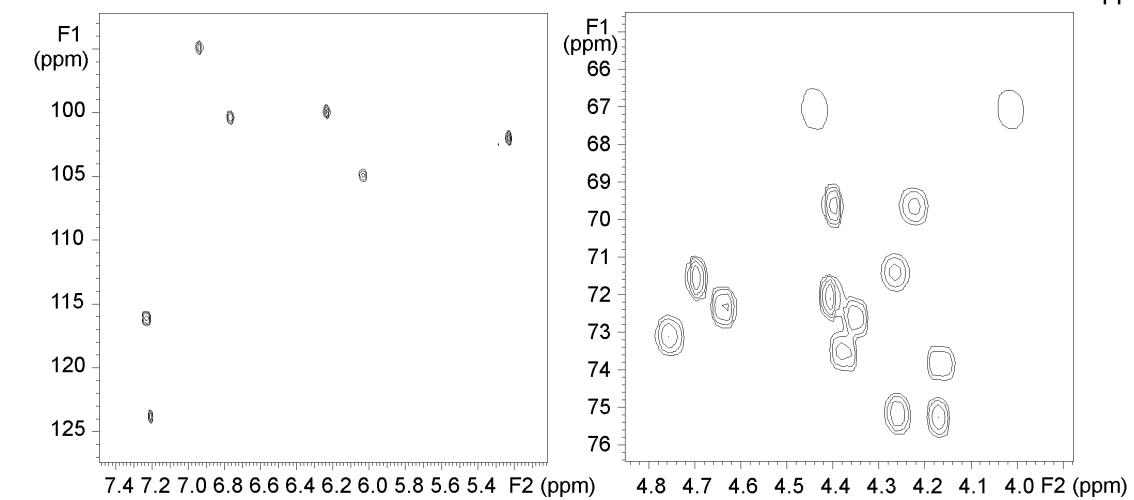
NMR - Resonance Assignments:
Flavone Core Sugar

| | δ_C | δ_H | | δ_C | δ_H |
|----|------------|------------|-------|------------|------------|
| 2 | 158.4s | | 1'' | 105 | 6.05 |
| 3 | 135.4s | | 2'' | 73.2d | 4.77 |
| 4 | 178.9s | | 3'' | 75.2d | 4.27 |
| 4a | 106.8s | | 4'' | 69.7d | 4.41 |
| 5 | 162.2s | | 5'' | 75.3d | 4.19 |
| 6 | 100.4d | 6.78 | 6'' | 67.1t | 4.45/4.03 |
| 7 | 162.8s | | 1''' | 102 | 5.24 |
| 8 | 94.9d | 6.95 | 2''' | 72.1 | 4.42 |
| 8a | 157.1s | | 3''' | 72.7 | 4.36 |
| 1' | 121.7s | | 4''' | 73.9 | 4.18 |
| 2' | 132.1d | 8.48 | 5''' | 69.7 | 4.24 |
| 3' | 116.2d | 7.24 | 6''' | 18.6 | 1.52 |
| 4' | 162s | | 1'''' | 100d | 6.25 |
| 5' | 116.2d | 7.24 | 2'''' | 71.6d | 4.72 |
| 6' | 132.1d | 8.48 | 3'''' | 74d | 4.65 |



NMR-¹³C:

NMR-HSQC:



Names

3-[[6-O-(6-deoxy- α -L-mannopyranosyl)- β -D-galactopyranosyl]oxy]-7-[(6-deoxy- α -L-mannopyranosyl)oxy]-5-hydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one; Robinin; 3-[[6-O-(6-deoxy- α -L-mannopyranosyl)- β -D-galactopyranosyl]oxy]-7-[(6-deoxy- α -L-mannopyranosyl)oxy]-5-hydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one; Kaempferol 3-O- α -L-rhamnopyranosyl-(1 \rightarrow 6)- β -D-galactopyranosyl 7-O- α -L-rhamnopyranoside

Apiin

Apigenin-7-[O- β -D-apiofuranosyl(1 \rightarrow 2)- β -D-glucopyranoside]

CAS-Number: 26544-34-3

Formula: C₂₆H₂₈O₁₄ Exact mass: 564.14791

Molecular mass: 564.49

Column: Zorbax LiChrosphere Kinetex

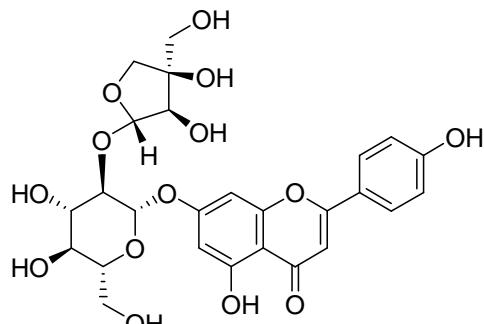
Abs.RetentionTime [min]: 18.03 15.25 7.56

Rel. RetentionTime (k'): 14.28 13.66 13.26

k' rel. to Rutin : 1.08 1.10 1.11

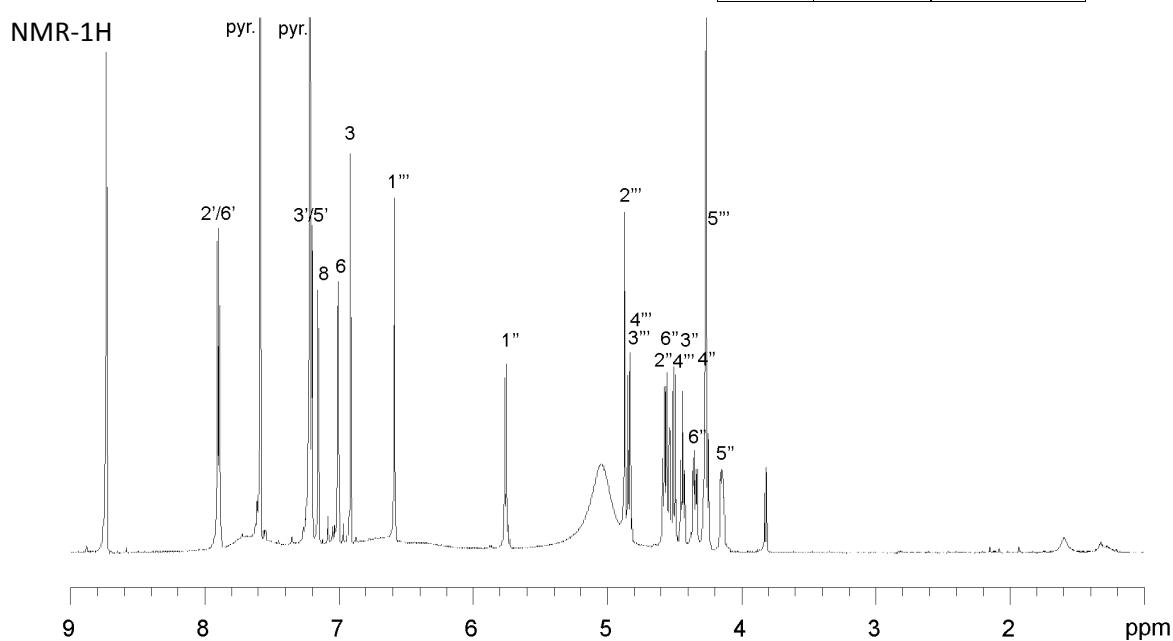
MS1: 563.3 MS2: 269.3 MS3: 225.1

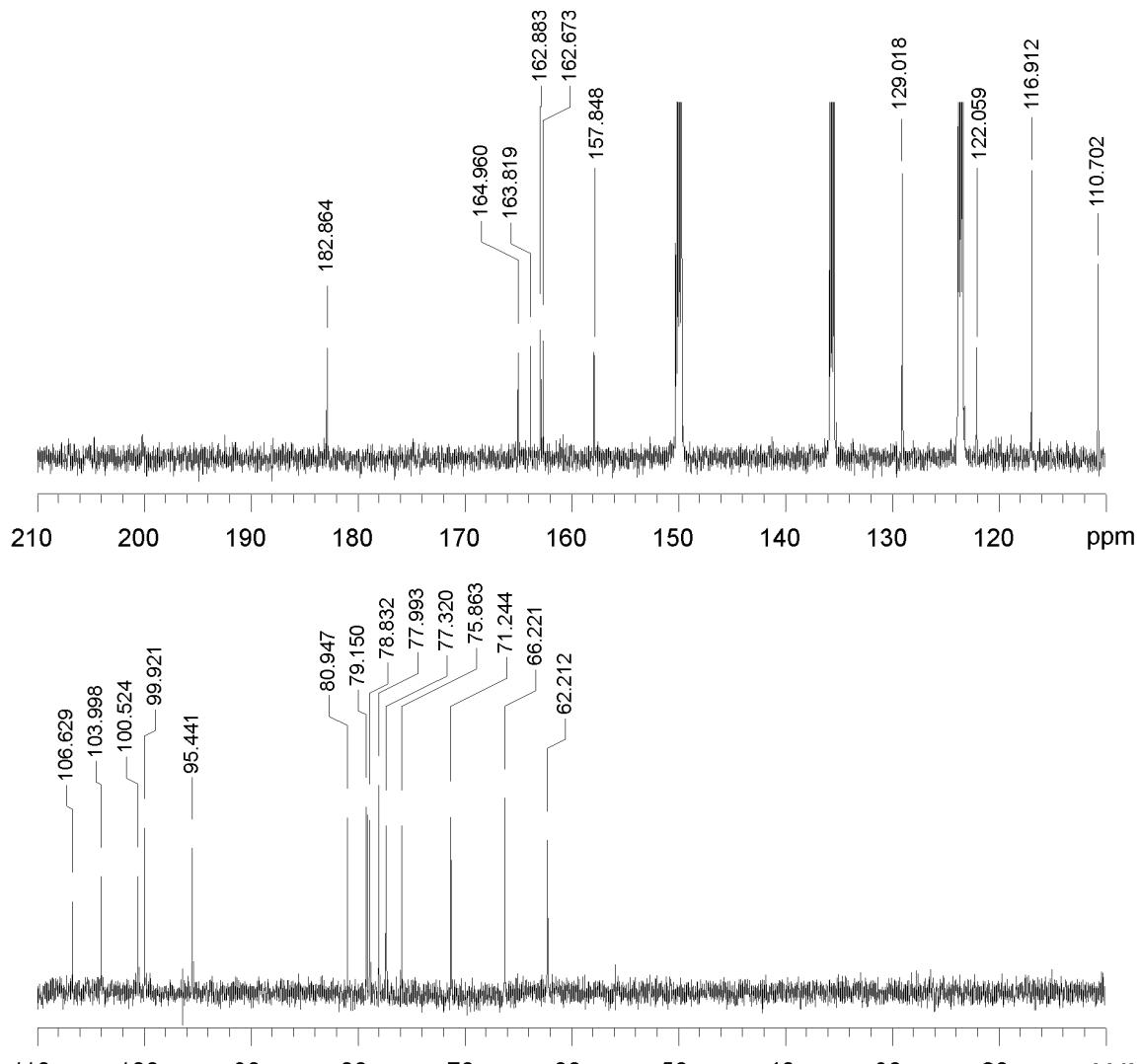
UV/Vis: 265, 335



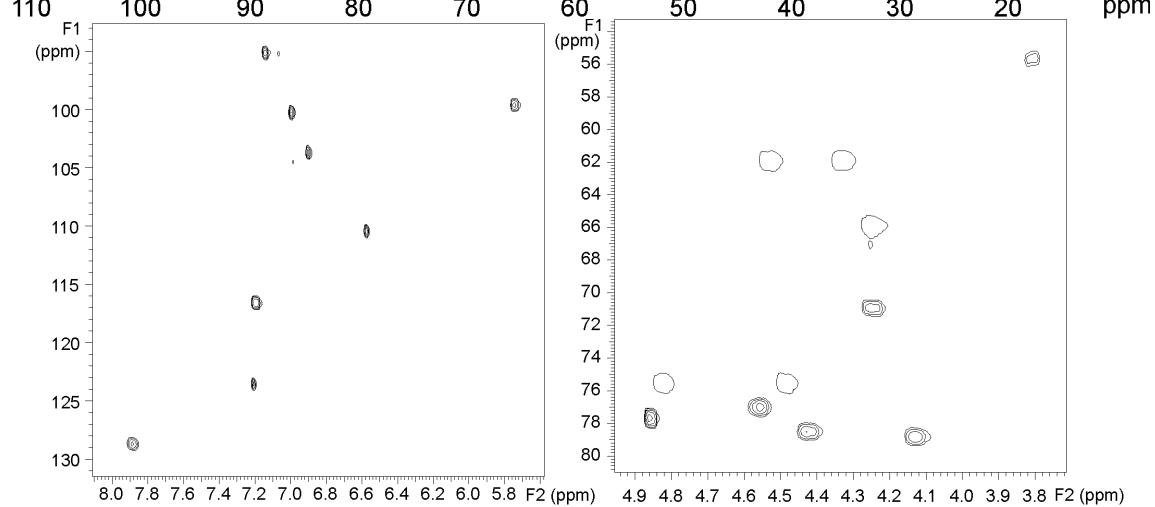
NMR - Resonance Assignments:
Flavone Core Sugar

| | δ_C | δ_H | | δ_C | δ_H |
|----|------------|------------|------|------------|------------|
| 2 | 165s | | 1" | 99.9d | 5.75 |
| 3 | 104d | 6.91 | 2" | 77.3d | 4.56 |
| 4 | 182.7s | | 3" | 78.8d | 4.42 |
| 4a | 106.6s | | 4" | 71.2d | 4.23 |
| 5 | 162.7s | | 5" | 79.2d | 4.13 |
| 6 | 100.5d | 7 | 6" | 62.2t | 4.53/4.33 |
| 7 | 163.8s | | 1''' | 110.7d | 6.59 |
| 8 | 95.4d | 7.15 | 2''' | 78d | 4.86 |
| 8a | 157.8s | | 3''' | 81.1s | |
| 1' | 122s | | 4''' | 75.9t | 4.83/4.49 |
| 2' | 129d | 7.9 | 5''' | 66.2t | 4.25/4.25 |
| 3' | 116.9d | 7.2 | | | |
| 4' | 162.9s | | | | |
| 5' | 116.9d | 7.2 | | | |
| 6' | 129d | 7.9 | | | |



NMR-¹³C:

NMR-HSQC:



Names

7-[(2-O-D-apio-β-D-furanosyl-β-D-glucopyranosyl)oxy]-5-hydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one; Apiin;
Apigenin-7-O-β-D-apiofuranosyl(1→2)-β-D-glucopyranoside

Apigenin

5,7,4'-Trihydroxyflavone

CAS-Number: 520-36-5

Formula: C₁₅H₁₀O₅ Exact mass: 270.05282

Molecular mass: 270.24

Column: Zorbax LiChrosphere Kinetex

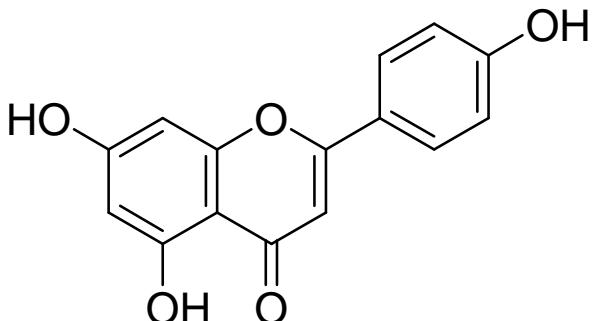
Abs.RetentionTime [min]: 23.57 21.25 10.48

Rel. RetentionTime (k') : 18.97 19.43 18.77

k' rel. to Butin : 1.44 1.57 1.57

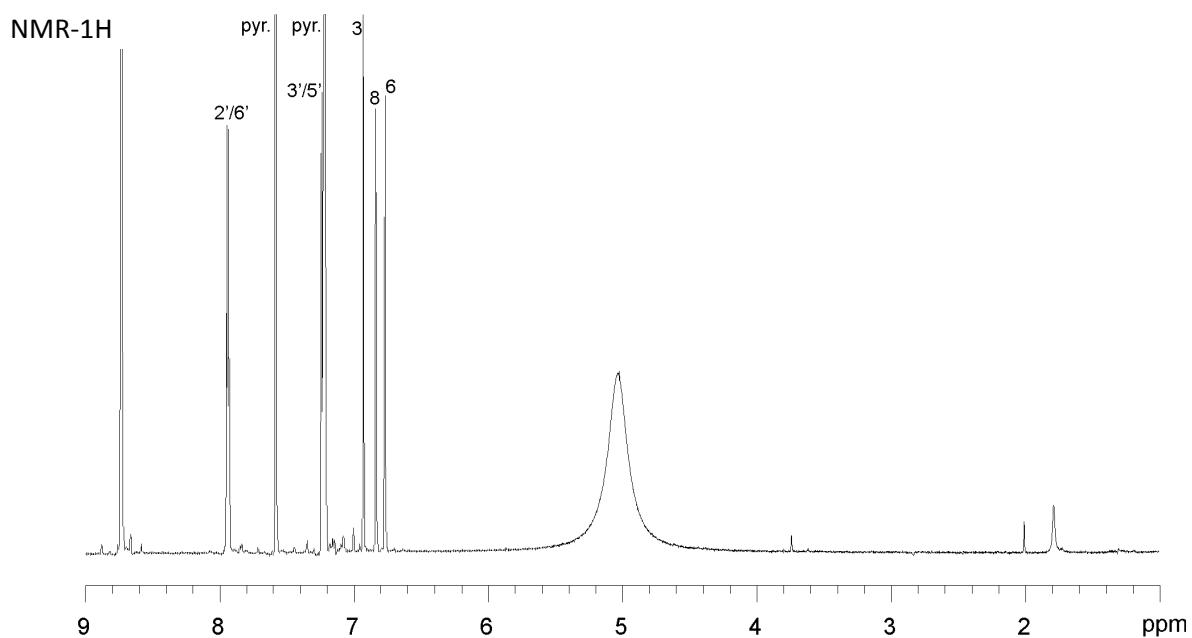
MS1: 269 3 MS2: 225 2 MS3: 181 1

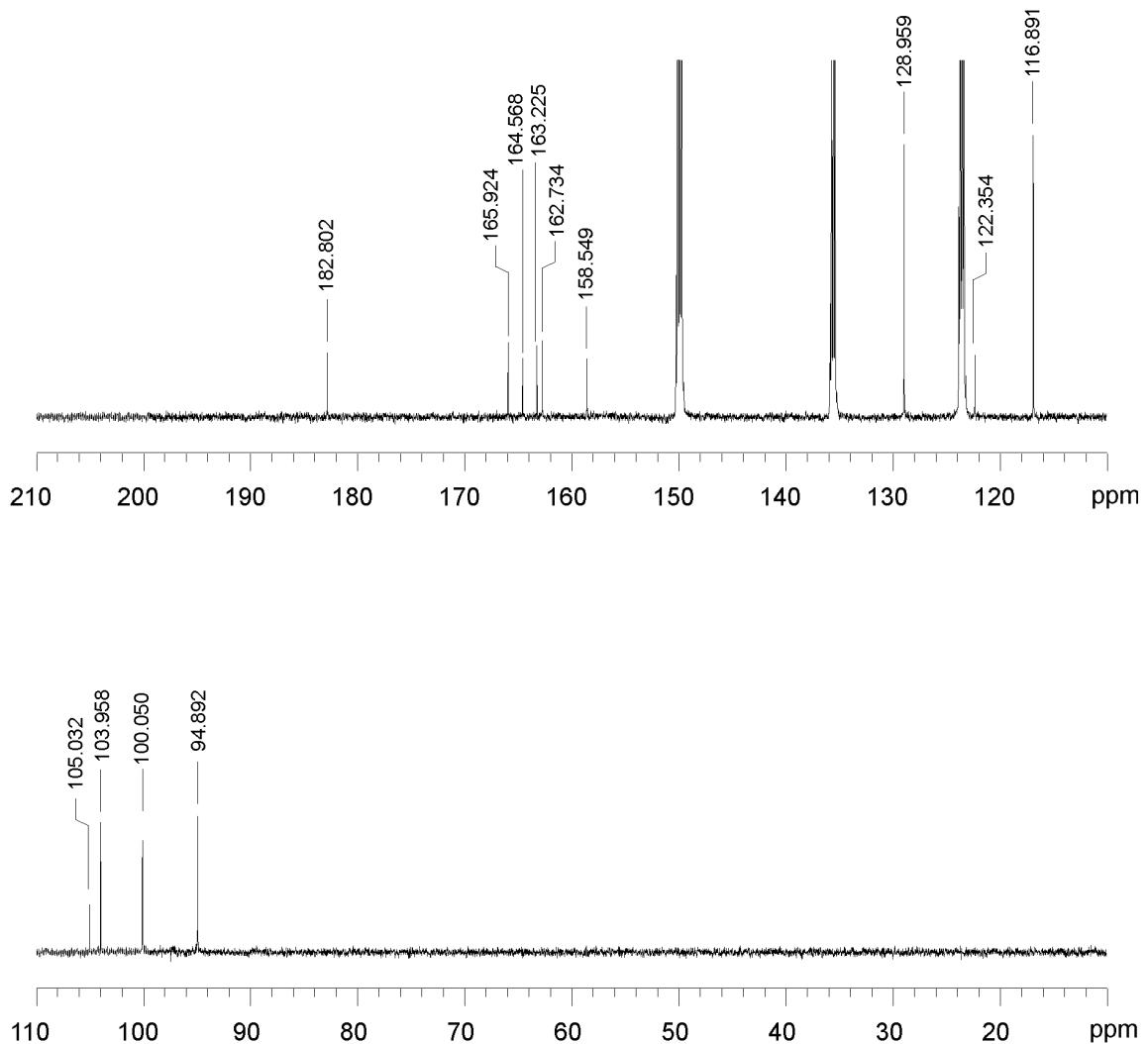
UV/Vis: 265, 335



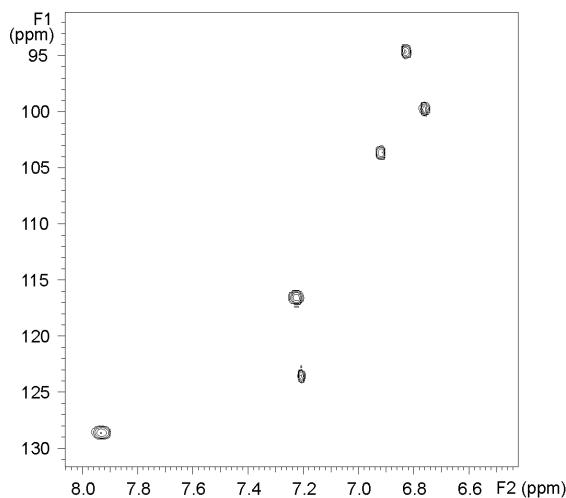
NMR - Resonance Assignments:

| | δ_C | δ_H |
|----|------------|------------|
| 2 | 164.6s | |
| 3 | 104d | 6.94 |
| 4 | 182.8s | |
| 4a | 105s | |
| 5 | 163.2s | |
| 6 | 100.1s | 6.76 |
| 7 | 165.9s | |
| 8 | 95d | 6.84 |
| 8a | 158.5s | |
| 1' | 122.3s | |
| 2' | 129d | 7.94 |
| 3' | 116.9d | 7.23 |
| 4' | 162.7s | |
| 5' | 116.9d | 7.23 |
| 6' | 129d | 7.94 |



NMR-¹³C:

NMR-HSQC:



Names

5,7-dihydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one; 5,7,4'-trihydroxy-flavone; 5,7,4'-trihydroxyflavone; 5,7,4'-Trihydroxyflavone; 5,7-Dihydroxy-2-(4-hydroxyphenyl)chromen-4-one; 5,7-Dihydroxy-2-p-hydroxyphenyl-4-chromenone; Apegenin; Apigenin; Apigenine; Apigenol; C.I. Natural Yellow 1; Chamomile; LY 080400; NSC 83244; Pelargidene 1449; UCCF 031; Versulin

Acacetin

5,7-Dihydroxy-4'-methoxyflavone

CAS-Number: 480-44-4

Formula: C₁₆H₁₂O₅ Exact mass: 284.06847

Molecular mass: 284.26

Column: Zorbax LiChrosphere Kinetex

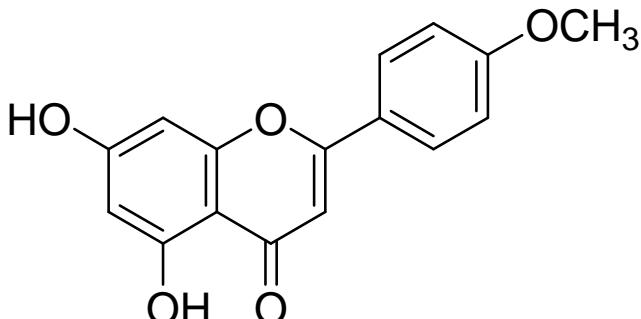
Abs.RetentionTime [min]: 28.35 26.08 12.88

Rel. RetentionTime (k') : 23.03 24.08 23.30

k' rel. to Rutin : 1.75 1.94 1.95

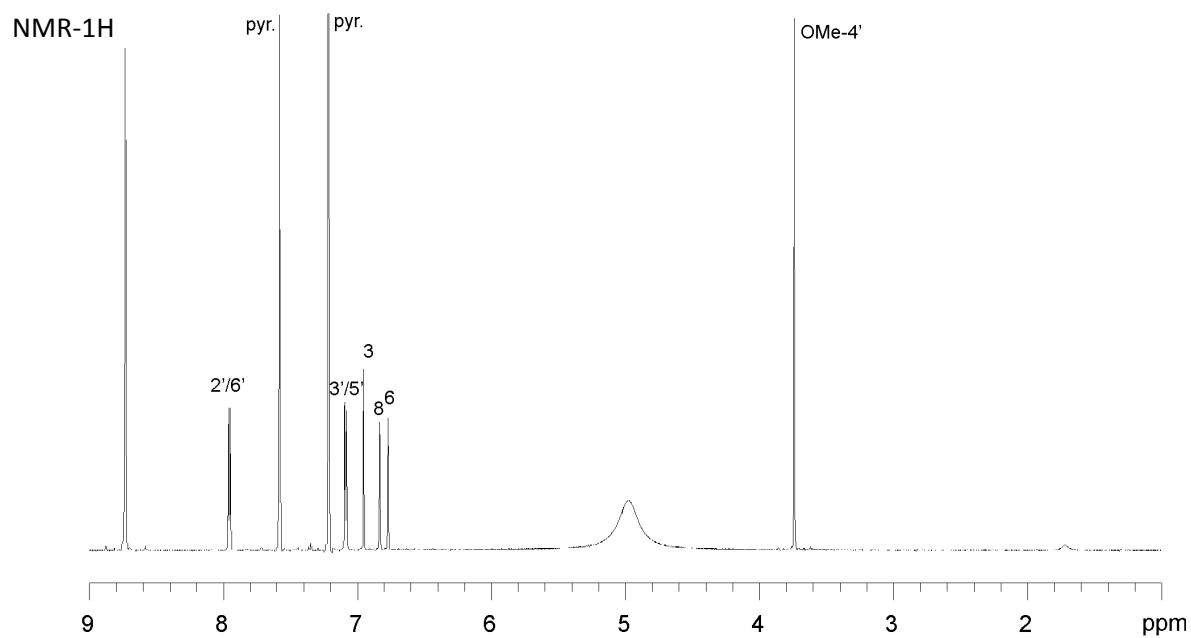
MS1: 283.2 MS2: 268.1 MS3: 268.1

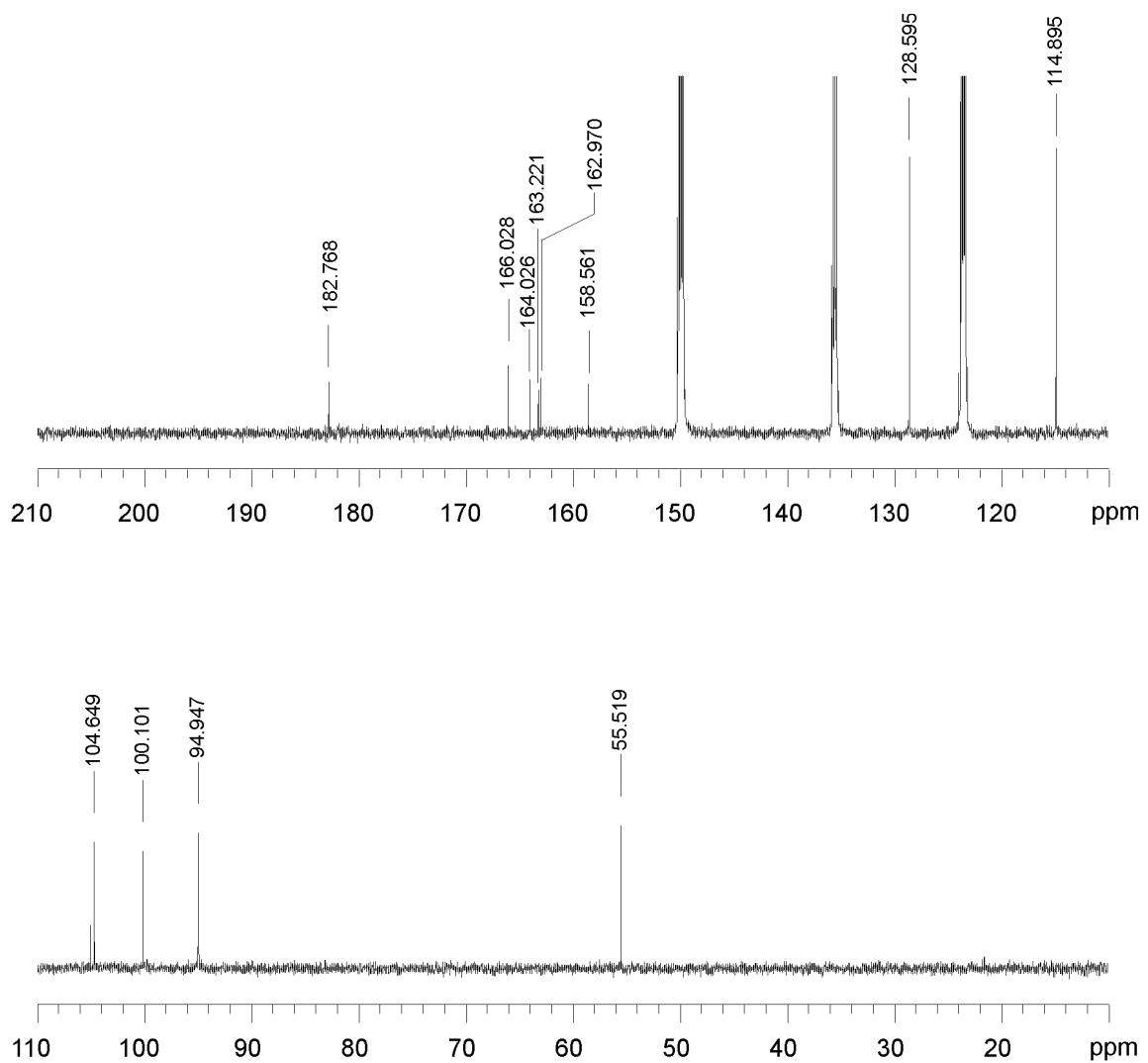
UV/Vis 265–335



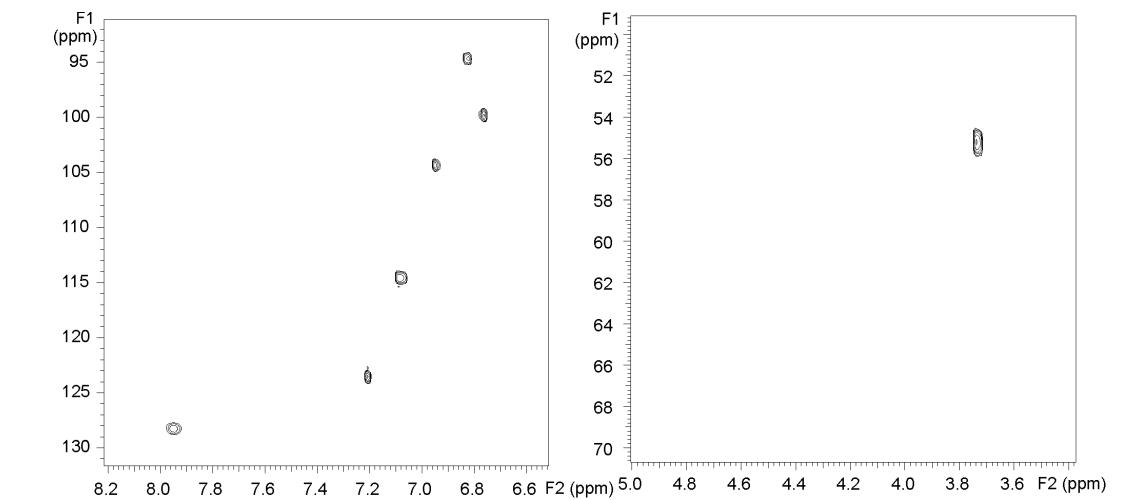
NMR - Resonance Assignments:

| | δ_C | δ_H |
|--------|------------|------------|
| 2 | 164.6s | |
| 3 | 104.7d | 6.95 |
| 4 | 182.8s | |
| 4a | 105.1s | |
| 5 | 163.2s | |
| 6 | 100.1d | 6.77 |
| 7 | 166s | |
| 8 | 95d | 6.84 |
| 8a | 158.6s | |
| 1' | 123.8s | |
| 2' | 128.6d | 7.95 |
| 3' | 114.9d | 7.08 |
| 4' | 163s | |
| 5' | 114.9d | 7.08 |
| 6' | 128.6d | 7.95 |
| OMe-4' | 55.3q | 3.74 |



NMR-¹³C:

NMR-HSQC:



Names

5,7-dihydroxy-2-(4-methoxyphenyl)-4H-1-benzopyran-4-one; Acacetin; 5,7-dihydroxy-4'-methoxy-flavone; 2-(4-methoxyphenyl)-5,7-dihydroxy-4H-1-benzopyran-4-one; 4'-methylapigenin; 4'-O-methylapigenin; 5,7-dihydroxy-4'-methoxyflavone; Apigenin 4'-methyl ether; Buddleoflavonol; LY 064233; Linarigenin; NSC 76061

RhoifolinApigenin-7-O- β -D-neohesperidoside

CAS-Number: 17306-46-6

Formula: C₂₇H₃₀O₁₄ Exact mass: 578.16356

Molecular mass: 578.52

Column: Zorbax LiChrosphere Kinetex

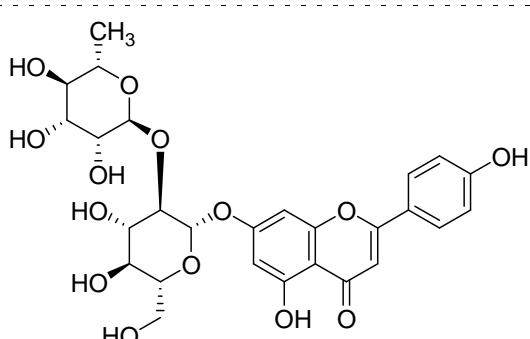
Abs.RetentionTime [min]: 18.35 15.49 7.70

Rel. RetentionTime (k'): 14.55 13.89 13.53

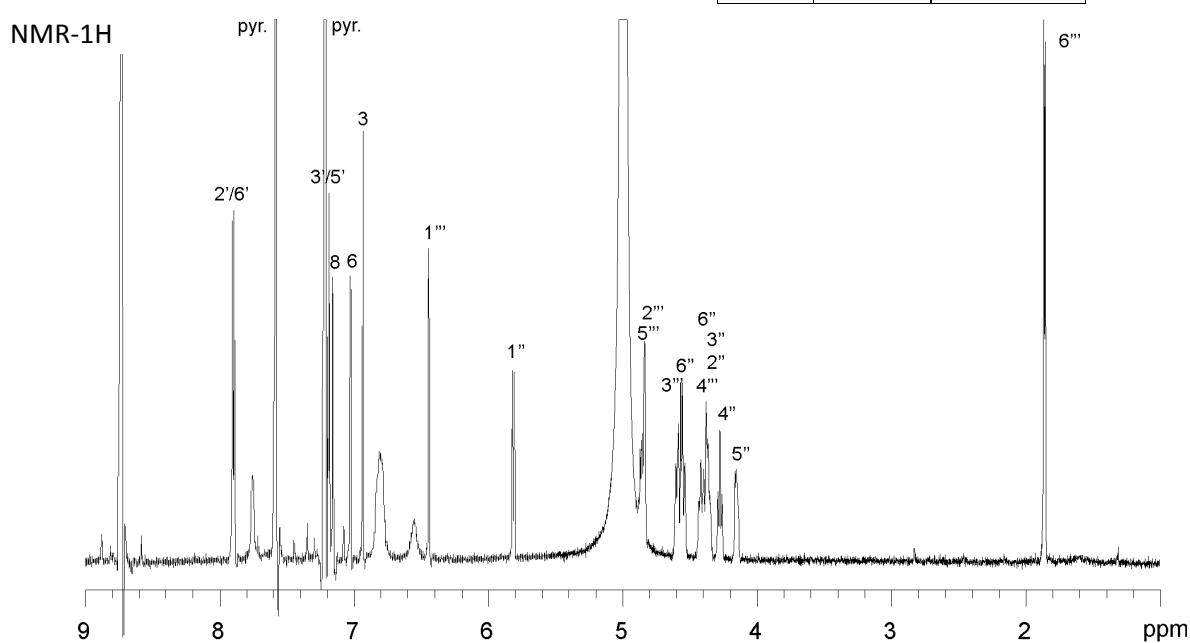
k' rel. to Rutin : 1.10 1.12 1.13

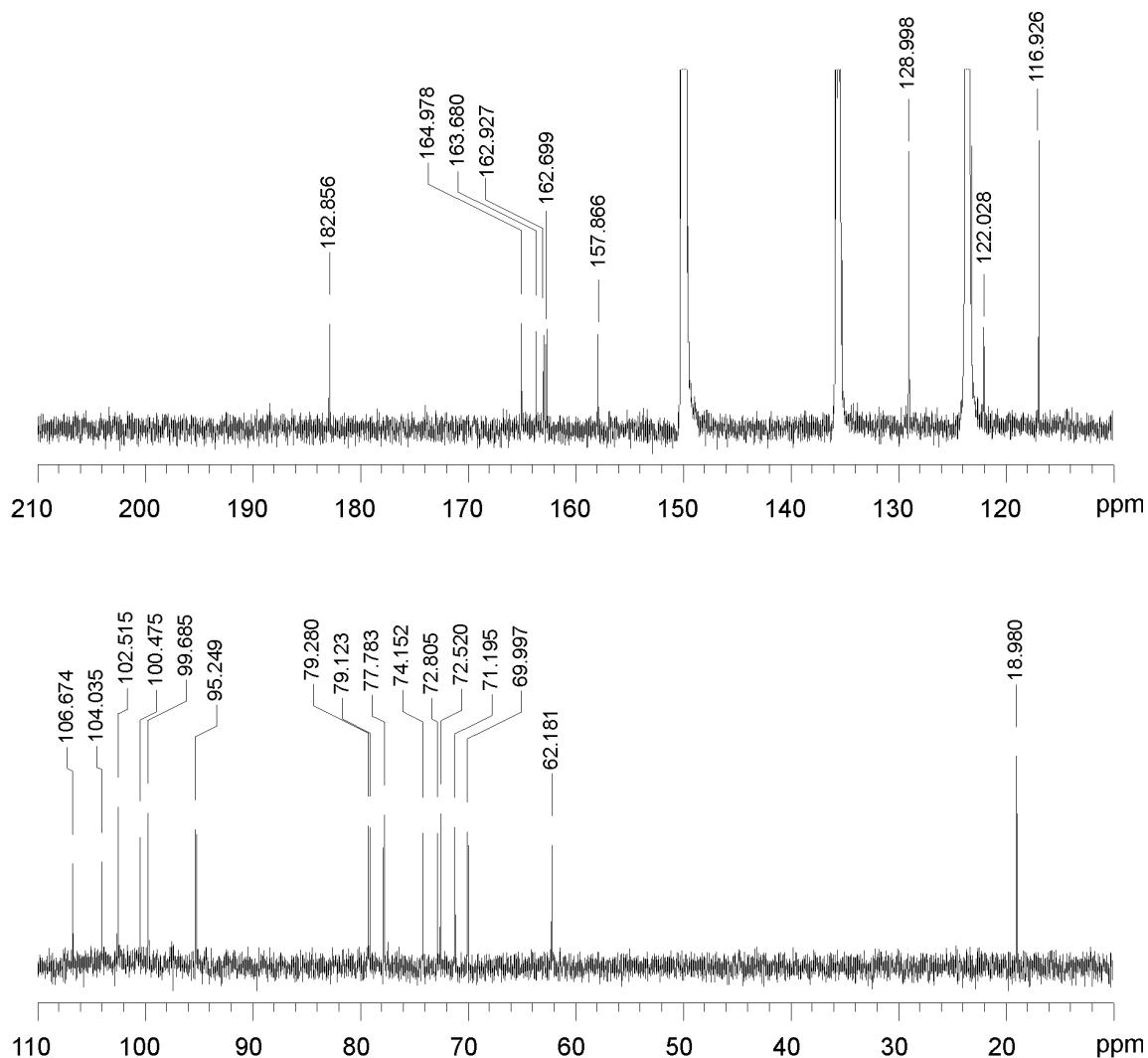
MS1: 577.4 MS2: 269.3 MS3: 225.1

UV/Vis: 265, 335

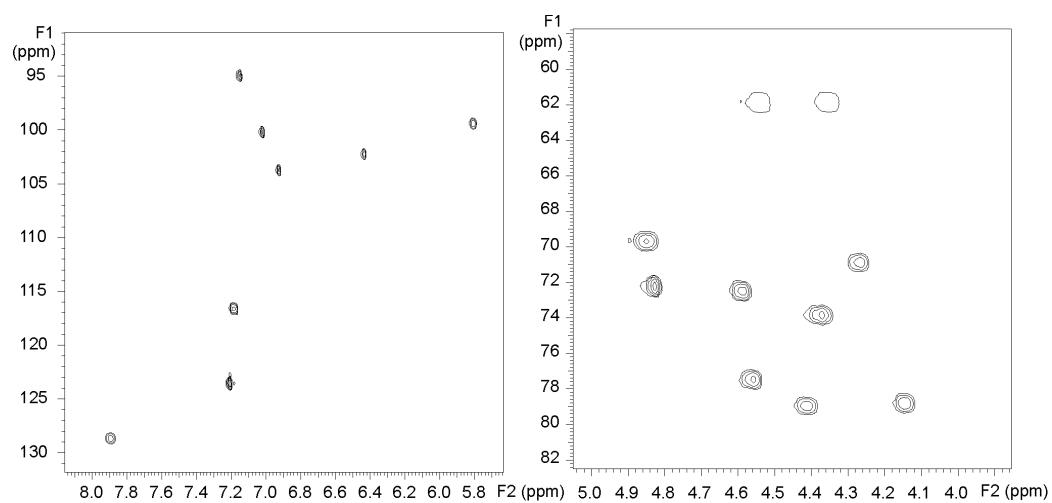
NMR - Resonance Assignments:
Flavone Core Sugar

| | δ_C | δ_H | | δ_C | δ_H |
|----|------------|------------|------|------------|------------|
| 2 | 165s | | 1" | 99.7d | 5.81 |
| 3 | 104d | 6.93 | 2" | 77.8d | 4.56 |
| 4 | 182.9s | | 3" | 79.3d | 4.41 |
| 4a | 106.7s | | 4" | 71.2d | 4.27 |
| 5 | 162.7s | | 5" | 79.1d | 4.15 |
| 6 | 100.5d | 7.02 | 6" | 62.2t | 4.54/4.36 |
| 7 | 163.7s | | 1''' | 102.5d | 6.44 |
| 8 | 95.2d | 7.16 | 2''' | 72.5d | 4.83 |
| 8a | 157.9s | | 3''' | 72.8d | 4.6 |
| 1' | 122s | | 4''' | 74.2d | 4.38 |
| 2' | 129d | 7.91 | 5''' | 70d | 4.86 |
| 3' | 116.9d | 7.18 | 6''' | 19q | 1.85 |
| 4' | 162.9s | | | | |
| 5' | 116.9d | 7.18 | | | |
| 6' | 129d | 7.91 | | | |



NMR-¹³C:

NMR-HSQC:



Names

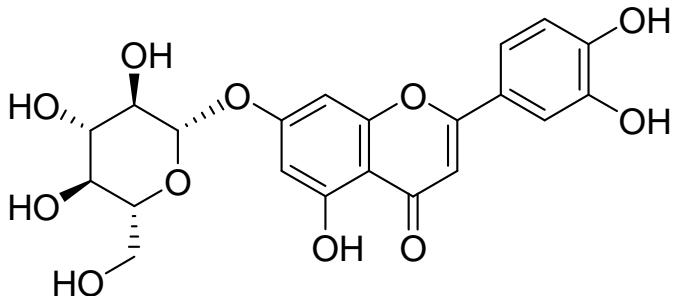
7-[[2-O-(6-deoxy- α -L-mannopyranosyl)- β -D-glucopyranosyl]oxy]-5-hydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one; Rhoifolin; Apigenin-7- β -neohesperidoside; Apigenin 7-O-neohesperidoside; Apigenin 7-O- β -D-neohesperidoside; Apigenin 7-O- β -neohesperidoside; Apigenin 7-neohesperidoside; Rhoifoloside

Luteolin-7-O-glucosidLuteolin-7-O- β -D-glucopyranoside

CAS-Number: 5373-11-5

Formula: C₂₁H₂₀O₁₁ Exact mass: 432.10565

Molecular mass: 448.38



Column: Zorbax LiChrosphere Kinetex

Abs.RetentionTime [min]: 16.75 13.92 6.81

Rel. RetentionTime (k'): 13.19 12.38 11.85

k' rel. to Rutin : 1.00 1.00 0.99

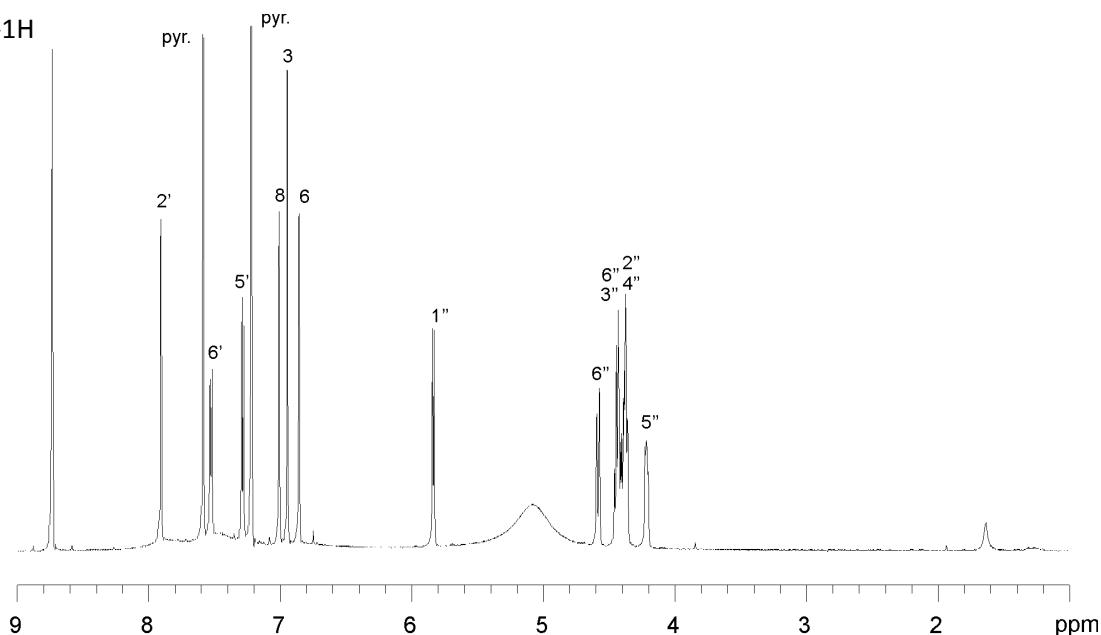
MS1: 447.3 MS2: 285.2 MS3: 241.2

UV/Vis: 255, 265(sh), 3

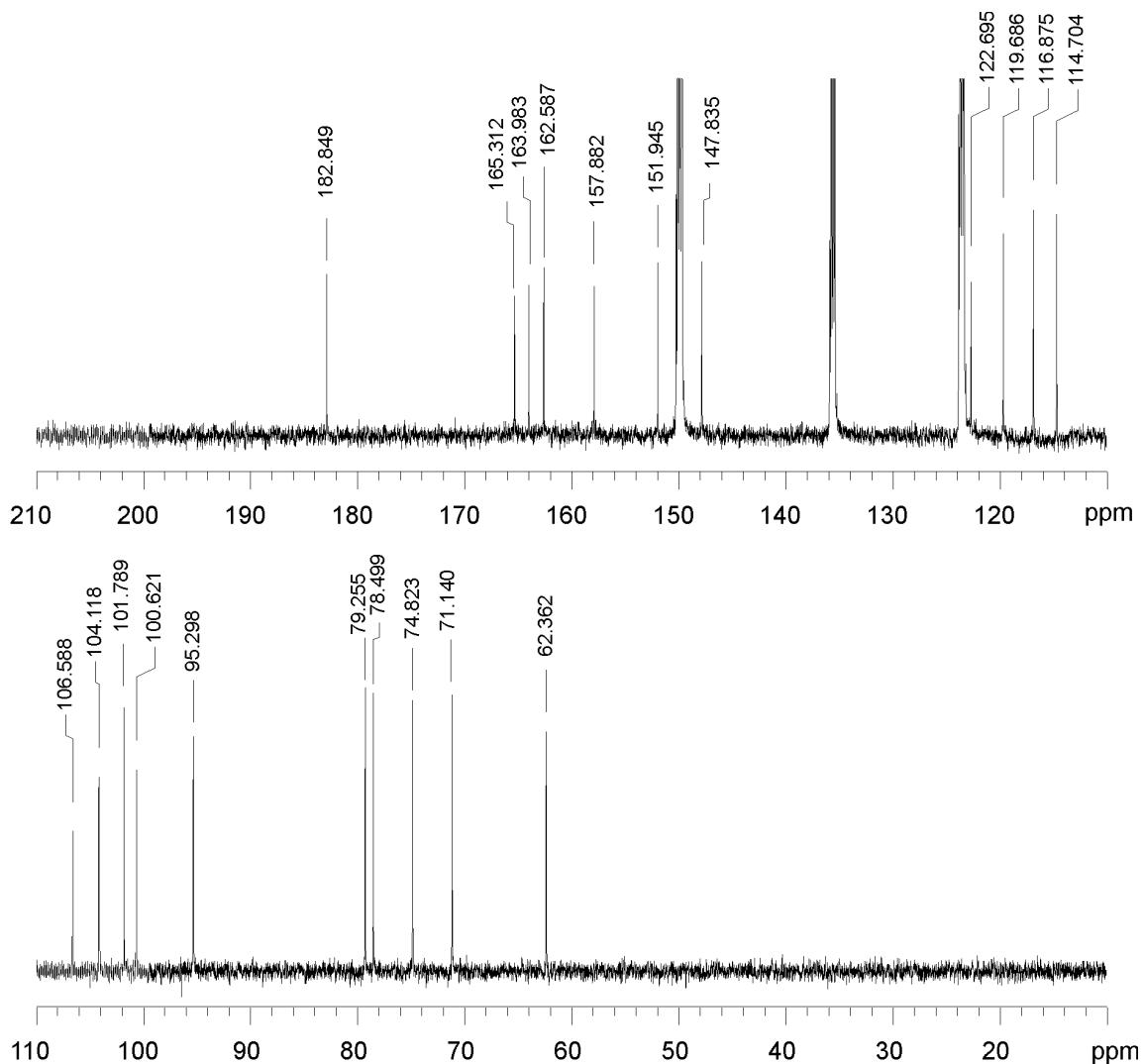
NMR - Resonance Assignments:
Flavone Core Sugar

| | δ_C | δ_H | | δ_C | δ_H |
|----|------------|------------|----|------------|------------|
| 2 | 165.3s | | 1" | 101.8d | 5.83 |
| 3 | 104.1d | 6.95 | 2" | 74.8d | 4.36 |
| 4 | 182.8s | | 3" | 78.5d | 4.43 |
| 4a | 106.6s | | 4" | 71.1d | 4.36 |
| 5 | 162.6s | | 5" | 79.2d | 4.2 |
| 6 | 100.6d | 6.85 | 6" | 62.4t | 4.57/4.41 |
| 7 | 164s | | | | |
| 8 | 95.3d | 7 | | | |
| 8a | 157.9s | | | | |
| 1' | 122.7s | | | | |
| 2' | 114.7d | 7.91 | | | |
| 3' | 147.8s | | | | |
| 4' | 152s | | | | |
| 5' | 116.9d | 7.29 | | | |
| 6' | 119.7d | 7.52 | | | |

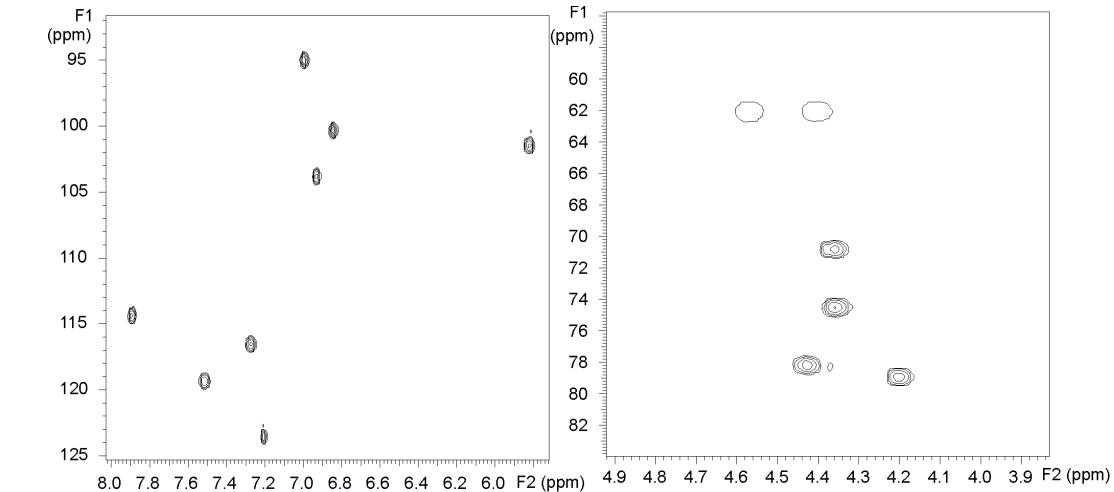
NMR-1H



NMR-13C:



NMR-HSQC:



Names

2-(3,4-dihydroxyphenyl)-7-(β -D-glucopyranosyloxy)-5-hydroxy-4H-1-benzopyran-4-one; Cynaroside; Luteolin, 7- β -D-glucopyranoside; 7-Glucoluteolin; 7- β -D-Glucosylluteolin; 7- β -Glucosylluteolin; Cinaroside; Glucoluteolin; Luteolin 7-O-glucopyranoside; Luteolin 7-O-glucoside; Luteolin 7-O-monoglucoside; Luteolin 7-O- β -D-glucopyranoside; Luteolin 7-O- β -D-glucoside; Luteolin 7-O- β -glucopyranoside; Luteolin 7-O- β -glucoside; Luteolin 7-glucoside; Luteolin 7-monoglucoside; Luteolin 7- β -D-glucoside; Luteolin 7- β -glucoside; Luteolin 7- β -monoglucoside; Luteolin-7-D-glucopyranoside; Luteoloside; Nephrocizin; Nephrocizine

Luteolin

5,7,3',4'-Tetrahydroxyflavone

CAS-Number: 491-70-3

Formula: C₁₅H₁₀O₆ Exact mass: 286.04774

Molecular mass: 286.24

Column: Zorbax LiChrosphere Kinetex

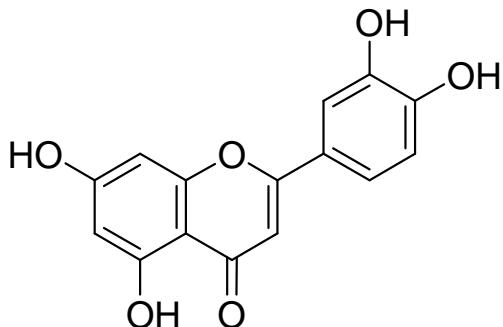
Abs.RetentionTime [min]: 21.63 18.99 9.42

Rel. RetentionTime (k') : 17.33 17.26 16.77

k' rel. to Rutin : 1.31 1.39 1.40

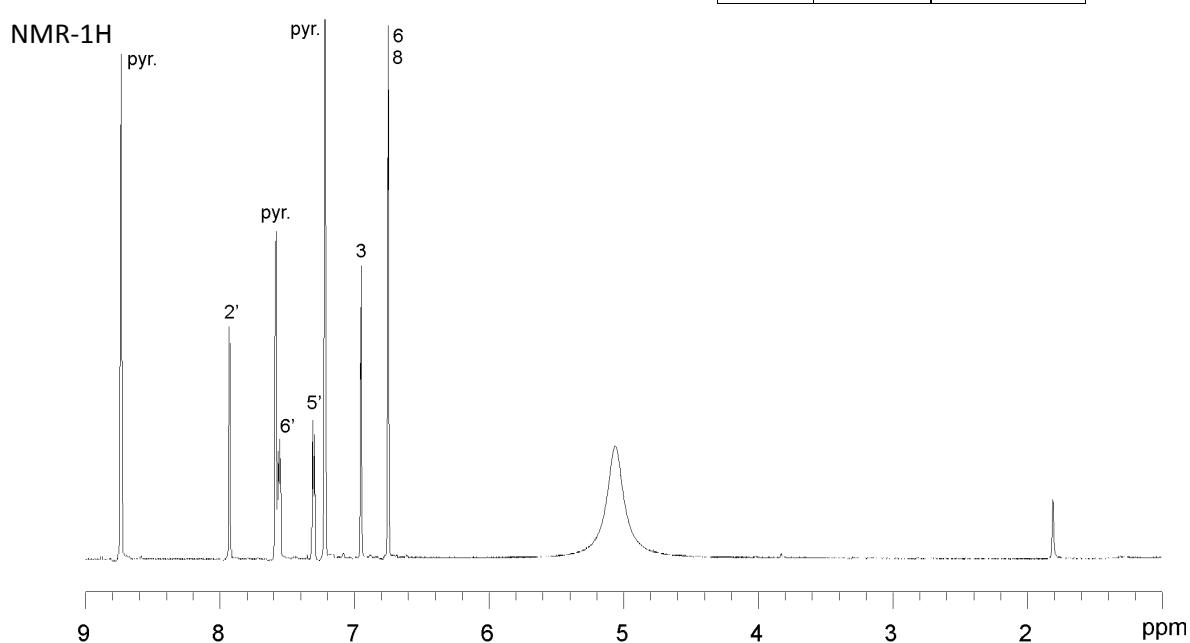
MS1: 285.4 MS2: 241.3 MS3: 198

UV/Vis: 255, 265(sh), 3

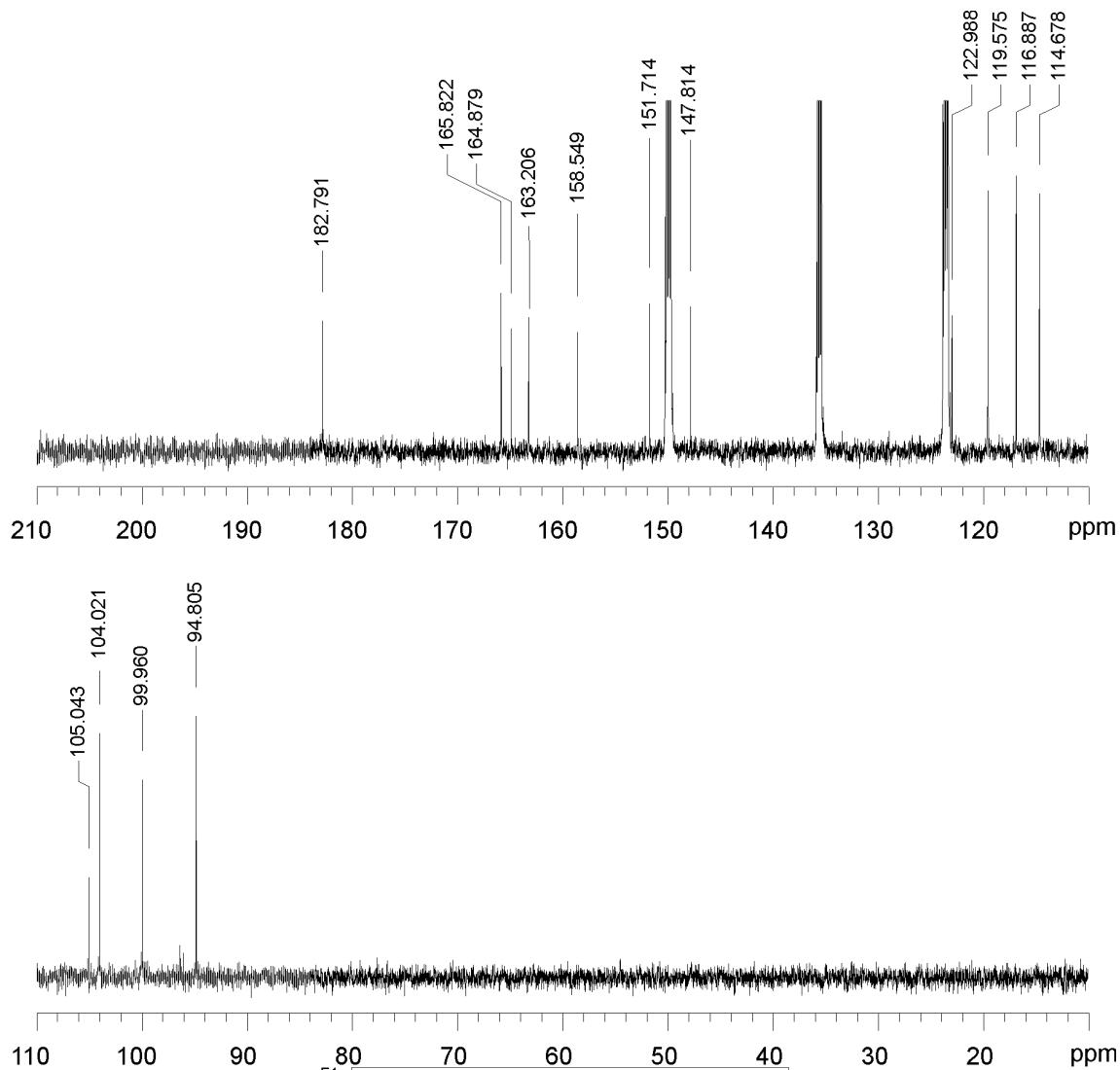


NMR - Resonance Assignments:

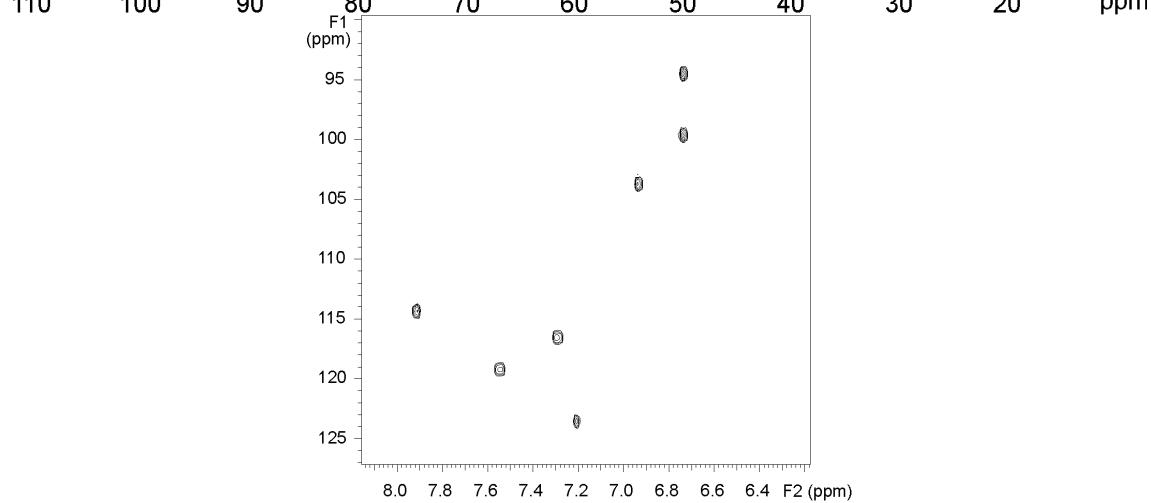
| | δ_C | δ_H |
|----|------------|------------|
| 2 | 164.9s | |
| 3 | 104d | 6.95 |
| 4 | 182.8s | |
| 4a | 105s | |
| 5 | 163.2s | |
| 6 | 100d | 6.75 |
| 7 | 165.8s | |
| 8 | 94.8d | 6.75 |
| 8a | 158.5s | |
| 1' | 123s | |
| 2' | 114.7d | 7.93 |
| 3' | 147.8s | |
| 4' | 151.7s | |
| 5' | 116.9d | 7.31 |
| 6' | 119.6d | 7.56 |



NMR-13C:



NMR-HSQC:



Names

2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4H-1-benzopyran-4-one; 5,7,3',4'-tetrahydroxy-flavone; Luteolin; 2-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-4H-1-benzopyran-4-one; 2-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-4H-benzopyran-4-one; 5,7,3',4'-tetrahydroxyflavone; 5,7,3',4'-Tetrahydroxyflavone; Cyanidenon; Cyanidenon 1470; Digitoflavone; Flacitran; Luteoline; Luteolol; Salifazide; Weld lake; Yama Kariyasu

Chrysoeriol

5,7,4'-Trihydroxy-3'-methoxyflavone

CAS-Number: 491-71-4

Formula: C₁₆H₁₂O₆ Exact mass: 300.06339

Molecular mass: 300.26

Column: Zorbax LiChrosphere Kinetex

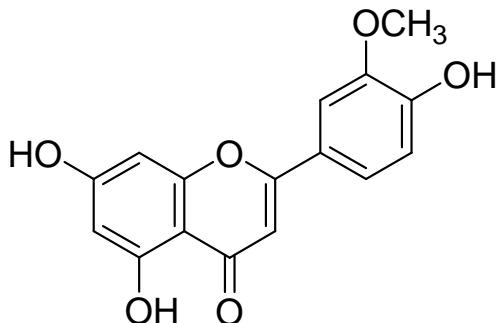
Abs.RetentionTime [min]: 24.03 21.60 10.69

Rel. RetentionTime (k') : 19.36 19.77 19.17

k' rel. to Rutin : 1.47 1.59 1.61

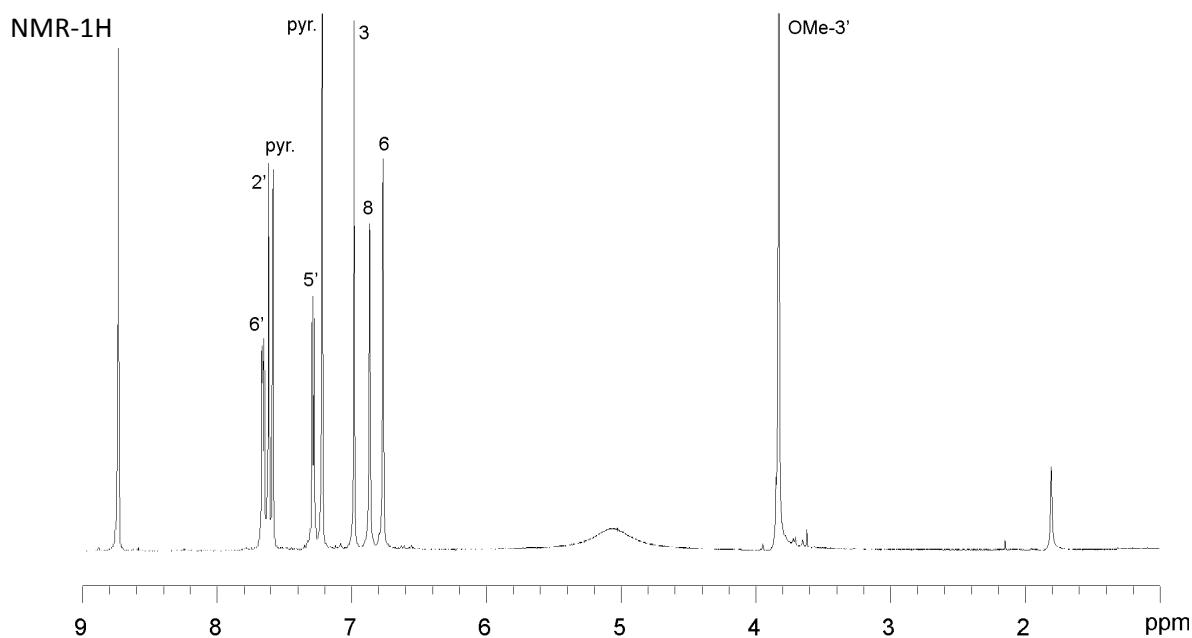
MS1: 299.3 MS2: 284.2 MS3: 256.2

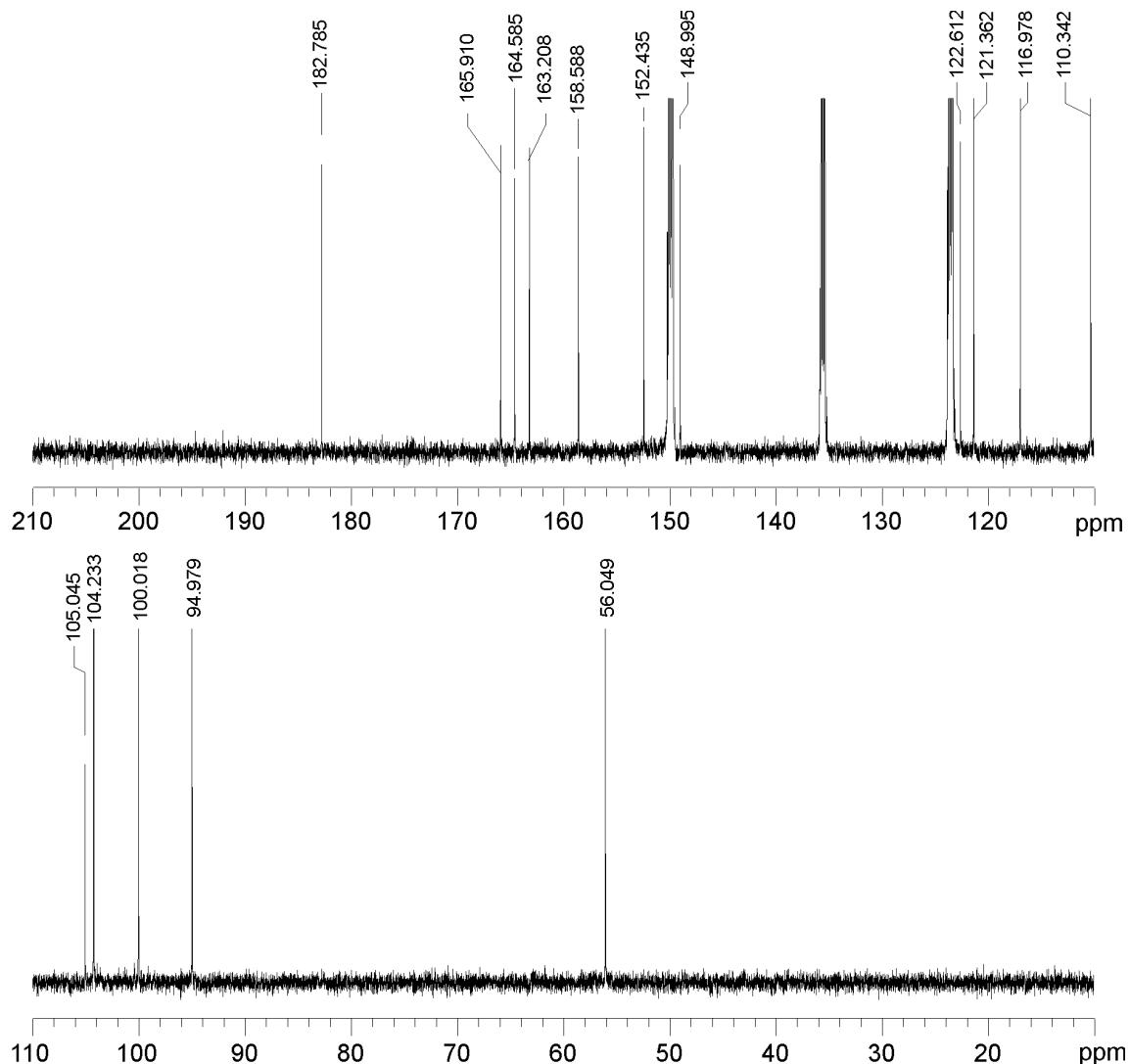
UV/Vis: 255, 265(sh), 3



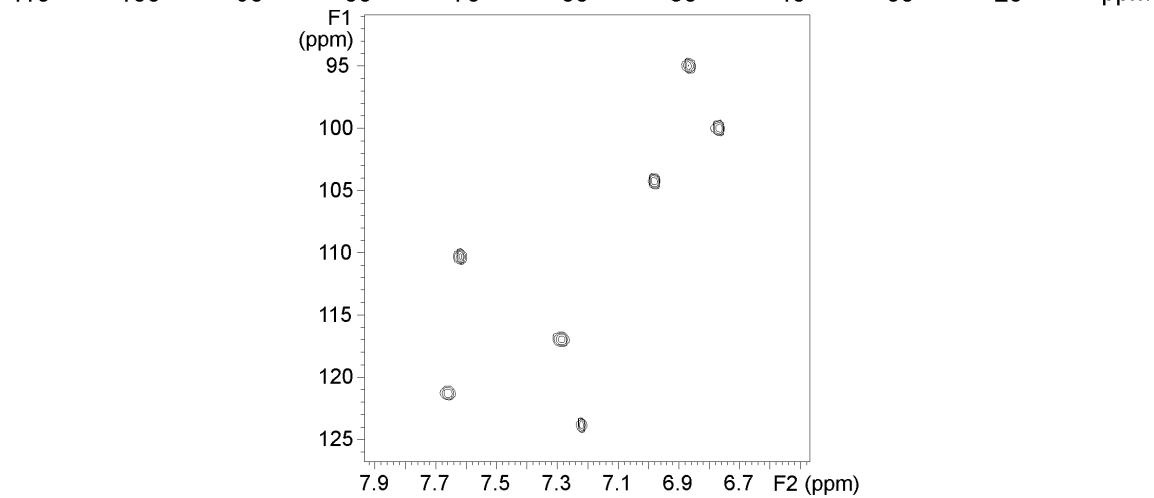
NMR - Resonance Assignments:

| | δ_C | δ_H |
|--------|------------|------------|
| 2 | 164.6s | |
| 3 | 104.2d | 6.98 |
| 4 | 182.8s | |
| 4a | 105s | |
| 5 | 163.2s | |
| 6 | 100d | 6.77 |
| 7 | 165.9s | |
| 8 | 95d | 6.87 |
| 8a | 158.6s | |
| 1' | 122.6s | |
| 2' | 110.3d | 7.62 |
| 3' | 149s | |
| 4' | 152.4s | |
| 5' | 117d | 7.28 |
| 6' | 121.4d | 7.66 |
| OMe-3' | 56q | 3.83 |



NMR-¹³C:

NMR-HSQC:



Names

5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-4H-1-benzopyran-4-one; 5,7,4'-trihydroxy-3'-methoxy-flavone; 3'-methoxy-5,7,4'-trihydroxyflavone; 3'-methoxyapigenin; 3'-O-Methyluteolin; 5,7,4'-trihydroxy-3'-methoxyflavone; Chrysoeriol; Chrysoriol; Luteolin 3'-methyl ether

RutinQuercetin-3-O- β -D-rutinoside

CAS-Number: 153-18-4

Formula: C₂₇H₃₀O₁₆ Exact mass: 610.15338

Molecular mass: 610.52

Column: Zorbax LiChrosphere Kinetex

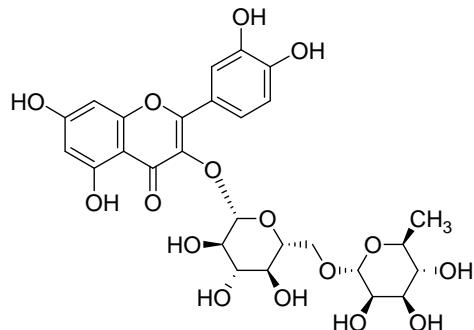
Abs.RetentionTime [min]: 16.75 13.95 6.86

Rel. RetentionTime (k'): 13.19 12.41 11.94

k' rel. to Rutin : 1.00 1.00 1.00

MS1: 609.3 MS2: 301.1 MS3: 178.9

UV/Vis: 255, 265(sh), 3

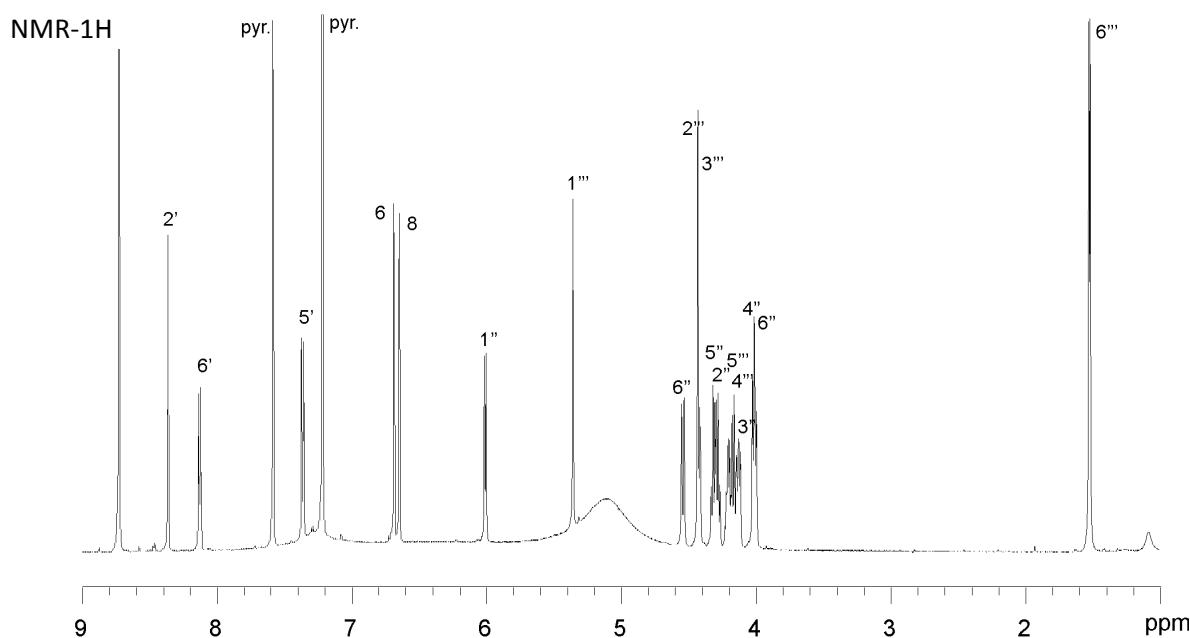


NMR - Resonance Assignments:

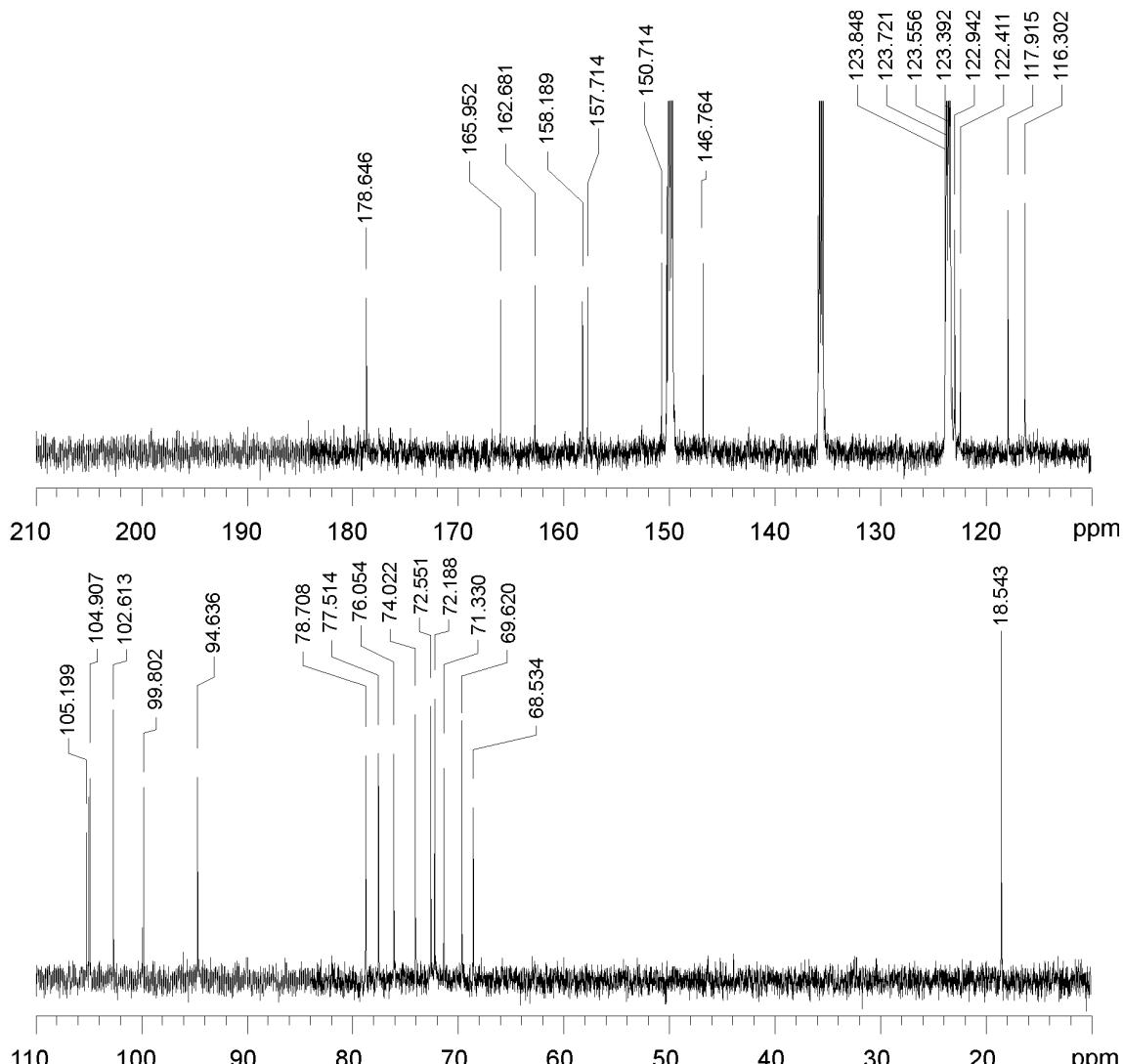
Flavone Core

Sugar

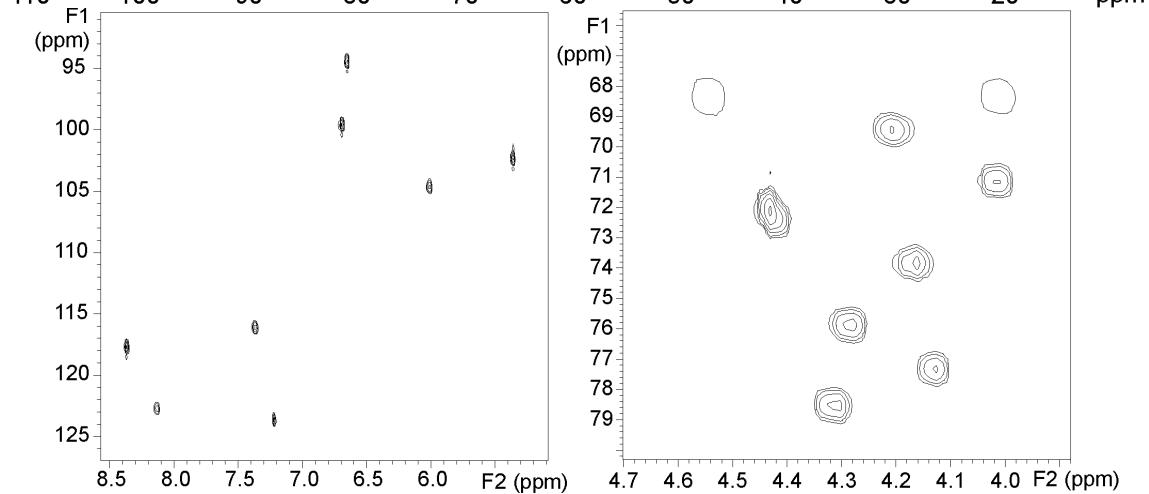
| | δ_{C} | δ_{H} | | δ_{C} | δ_{H} |
|----|---------------------|---------------------|------|---------------------|---------------------|
| 2 | 158.2s | | 1" | 104.9d | 6/4 |
| 3 | 135.6s | | 2" | 76.1d | 4.27 |
| 4 | 178.6s | | 3" | 77.5d | 4.12 |
| 4a | 105.2s | | 4" | 71.3d | 4.01 |
| 5 | 162.7s | | 5" | 78.7d | 4.32 |
| 6 | 99.8d | 6.69 | 6" | 68.5t | 4.53 |
| 7 | 166s | | 1''' | 102.6d | 5.35 |
| 8 | 94.6d | 6.64 | 2''' | 72.2d | 4.42 |
| 8a | 157.7s | | 3''' | 72.6d | 4.41 |
| 1' | 122.4s | | 4''' | 74d | 4.15 |
| 2' | 117.9d | 8.36 | 5''' | 69.6d | 4.2 |
| 3' | 146.7s | | 6''' | 18.5t | 1.53 |
| 4' | 150.7s | | | | |
| 5' | 116.3d | 7.37 | | | |
| 6' | 122.9d | 8.12 | | | |



NMR-13C:



NMR-HSQC:



Names

3-[[6-O-(6-deoxy- α -L-mannopyranosyl)- β -D-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4H-1-benzopyran-4-one; Flavone 3,5,7,3',4',5'-hexahydroxy-(6-O- α -L-rhamnosyl- β -D-glucoside); Ilixanthin; Rutin; 3,5,7,3',4'-Pentahydroxyflavone 3-O-rutinoside; 3,5,7,3',4'-Pentahydroxyflavone 3-rutinoside; 3-O-Rutinosyl-quercetin; 3-Rutinosylquercetin; 5,7,3',4'-tetrahydroxyflavonol-3-O-rutinoside; Birutan; C.I. 75730; Eldrin; Globulariacitrin; Globularicitrin; Ilixathin; Melin; Myrticalorin; Myrticolorin; Myticolorin; NSC 9220; Novarrutina; Oxyritin; Osyririn; Oxyritin; Paliurosides; Phytomelin; Quercetin 3-O-rutinoside; Quercetin 3-O- α -L-rhamnopyranosyl-(1 \rightarrow 6)- β -D-glucopyranoside; Quercetin 3-O- α -rhamnopyranosyl(1 \rightarrow 6)- β -glucopyranoside; Quercetin 3-O- β -D-rutinoside; Quercetin 3-O- β -rutinoside; Quercetin 3-rhamnoglucoside; Quercetin 3-rutinoside; Quercetin 3- β -rutinoside; Rutabion; Rutine; Rutinic acid; Rutosid; Rutoside; Rutozid; Sophorin; Tanrutin; Violaquerçetin; Violaquerçitrin; Yunxianggan

Diosmetin

5,7,3'-Trihydroxy-4'-methoxyflavone

CAS-Number: 520-34-3

Formula: C₁₆H₁₂O₆ Exact mass: 300.06339

Molecular mass: 300.26

Column: Zorbax LiChrosphere Kinetex

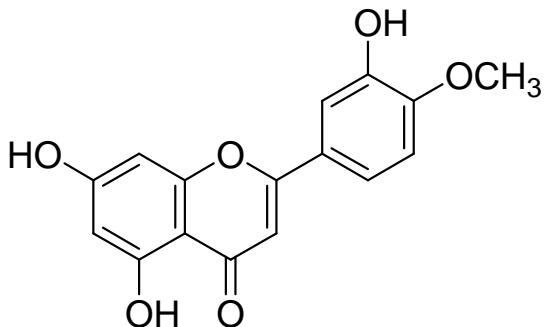
Abs.RetentionTime [min]: 24.21 21.81 10.79

Rel. RetentionTime (k') : 19.52 19.97 19.36

k' rel. to Rutin : 1.48 1.61 1.62

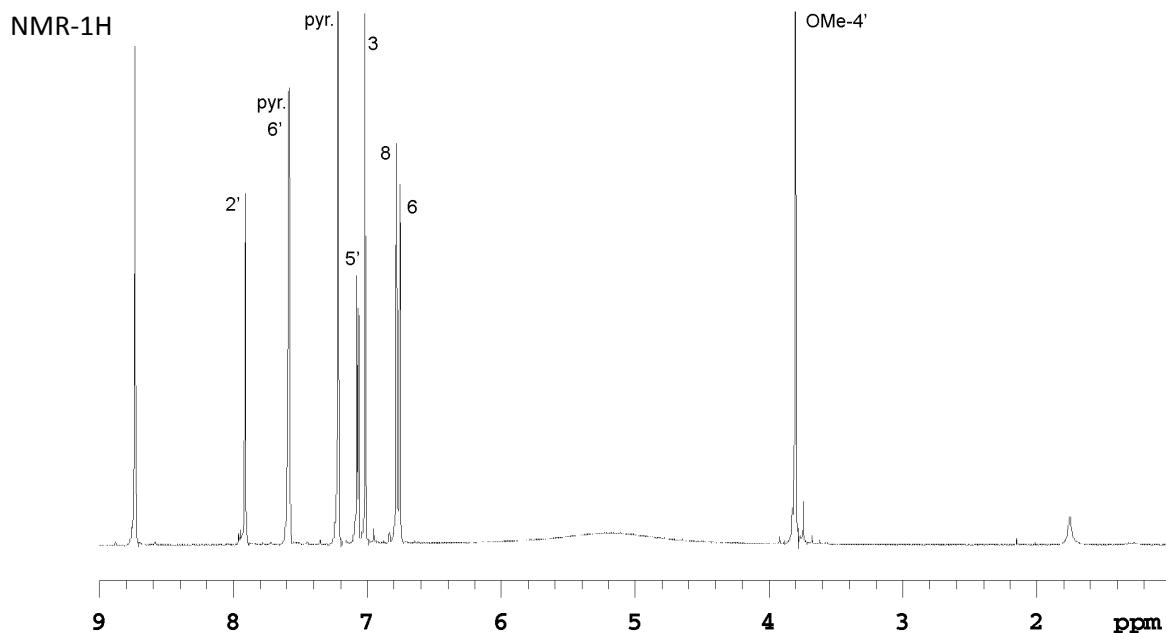
MS1: 299.2 MS2: 284.2 MS3: 256.1

UV/Vis: 255, 265(sh), 3

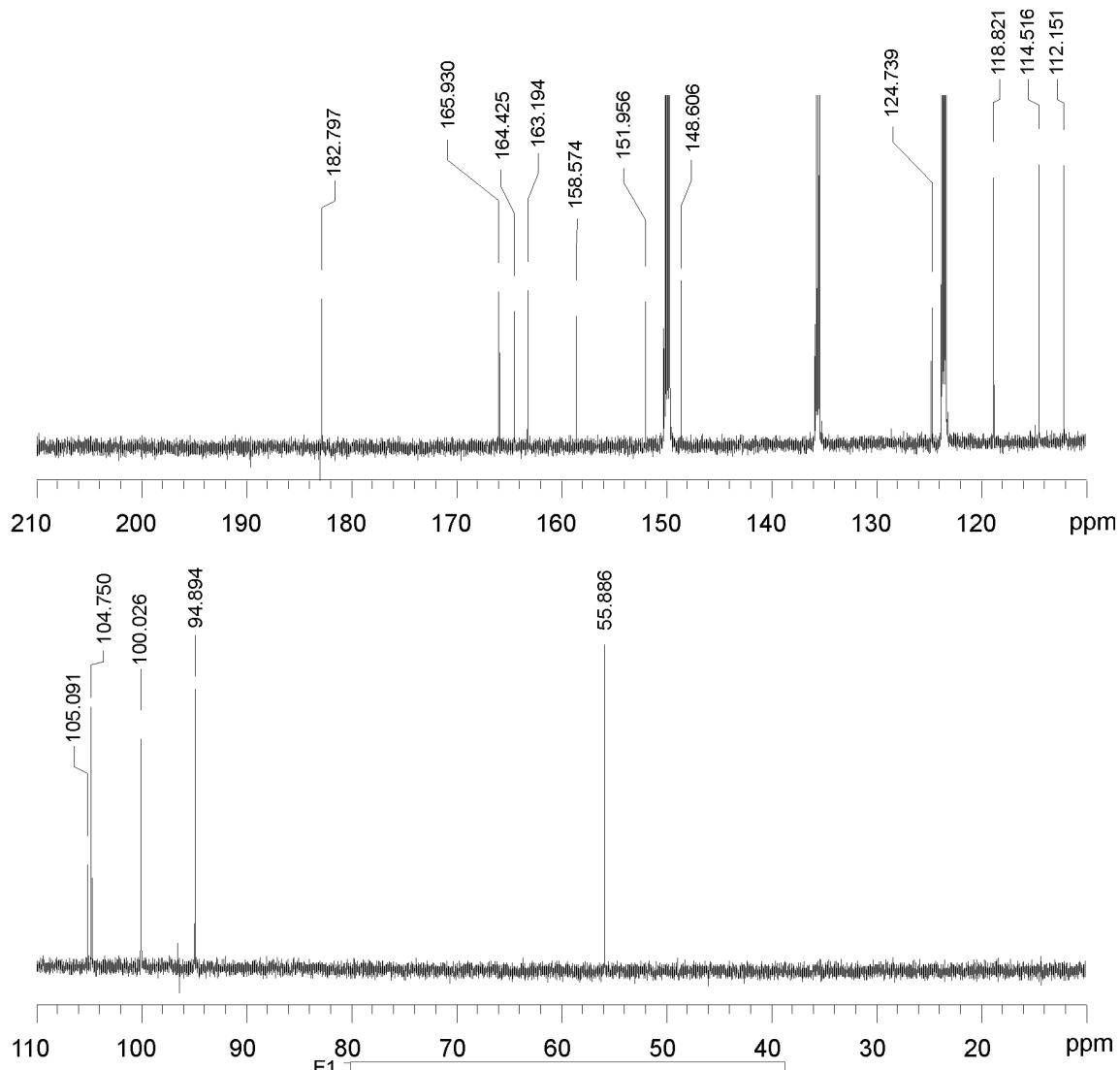


NMR - Resonance Assignments:

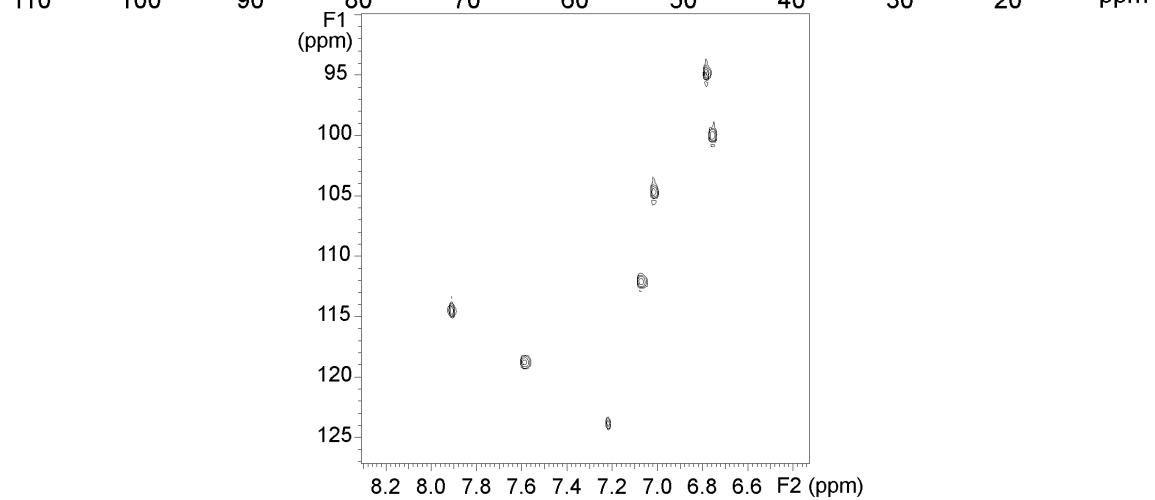
| | δ_C | δ_H |
|--------|------------|------------|
| 2 | 164.4s | |
| 3 | 104.8d | 7.01 |
| 4 | 182.8s | |
| 4a | 105.1s | |
| 5 | 163.2s | |
| 6 | 100d | 6.75 |
| 7 | 165.9s | |
| 8 | 94.9d | 6.78 |
| 8a | 158.6s | |
| 1' | 124.7s | |
| 2' | 114.5d | 7.91 |
| 3' | 148.6s | |
| 4' | 152s | |
| 5' | 112.2d | 7.07 |
| 6' | 118.8d | 7.58 |
| OMe-4' | 55.9q | 3.8 |



NMR-13C:



NMR-HSQC:



Names

5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-4H-1-benzopyran-4-one; Diosmetin; 5,7,3'-trihydroxy-4'-methoxyflavone; 5,7,3'-trihydroxy-4'-methoxyflavone; 4'-methyluteolin; 5,7,3'-trihydroxy-4'-methoxyflavone; Diosmetine; Diosmetol; Luteolin 4'-methyl ether; Pillon

Centaurein

5,7,3'-Trihydroxy-3,6,4'-trimethoxy-flavone-7-O- β -D-glucoside

CAS-Number: 35595-03-0

Formula: C₂₄H₂₆O₁₃ Exact mass: 522.13734

Molecular mass: 522.46

Column: Zorbax LiChrosphere Kinetex

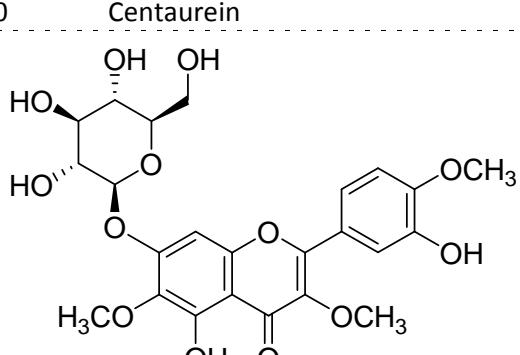
Abs.RetentionTime [min]: 20.53 17.33 8.76

Rel. RetentionTime (k'): 16.4 15.66 15.53

k' rel. to Rutin : 1.24 1.26 1.30

MS1: 521.2 MS2: 359.3 MS3: 153.1

UV/Vis: 255, 265(sh), 3



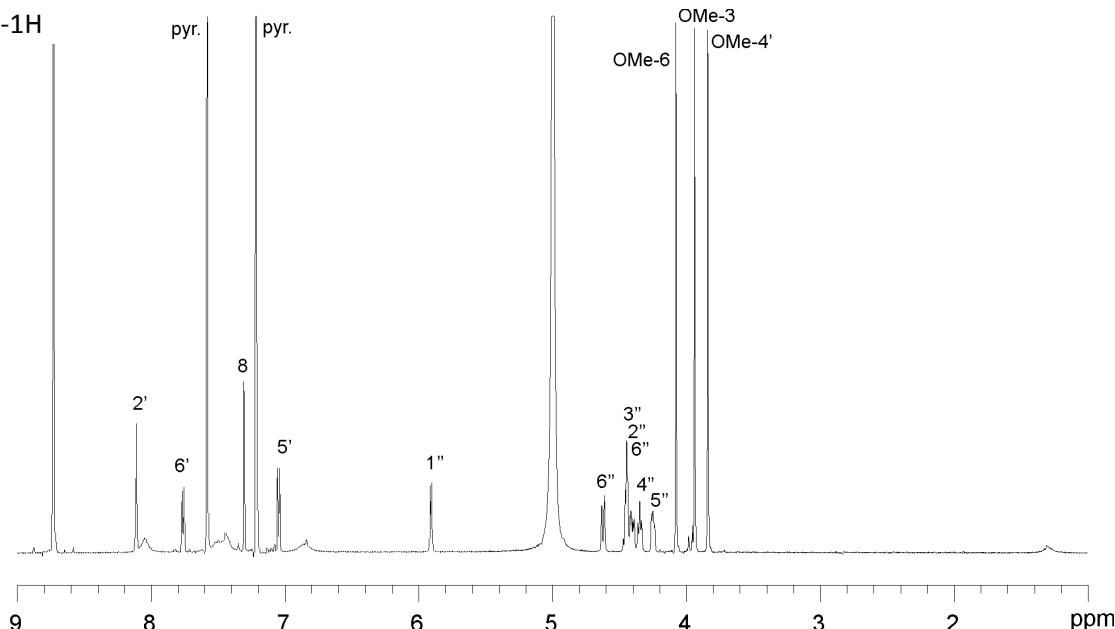
NMR - Resonance Assignments:

Flavone Core

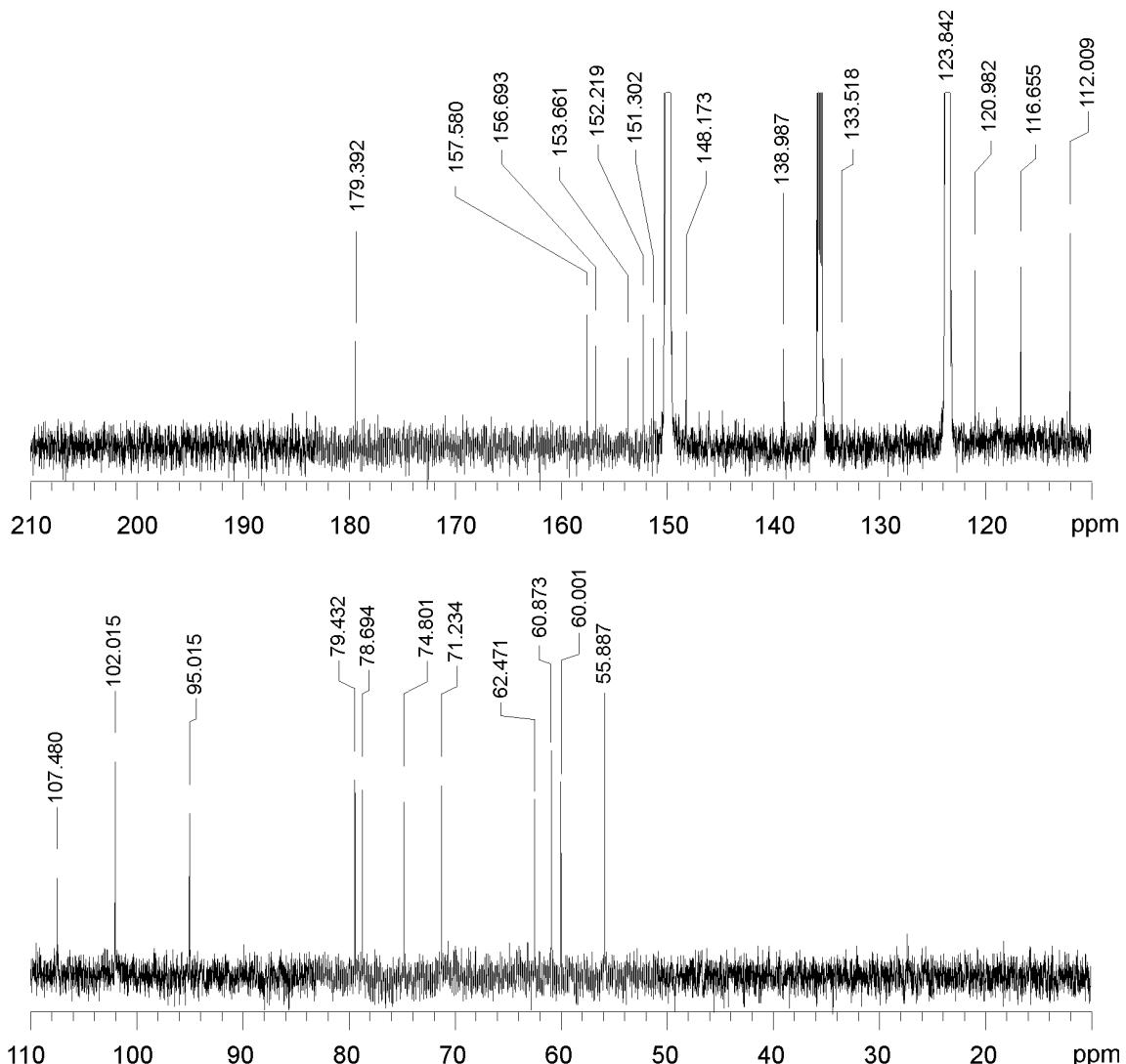
Sugar

| | δ_C | δ_H | | δ_C | δ_H |
|--------|------------|------------|----|------------|------------|
| 2 | 156.7s | | 1" | 102d | 5.91 |
| 3 | 139s | | 2" | 74.8d | 44.4 |
| 4 | 179.4s | | 3" | 78.4d | 4.45 |
| 4a | 107.5s | | 4" | 71.2d | 4.35 |
| 5 | 153.6s | | 5" | 79.4d | 4.25 |
| 6 | 133.5s | | 6" | 62.5t | 4.63/4.4 |
| 7 | 157.6s | | | | |
| 8 | 95d | 7.31 | | | |
| 8a | 152.2s | | | | |
| 1' | 123.9s | | | | |
| 2' | 116.7d | 8.12 | | | |
| 3' | 148.2s | | | | |
| 4' | 151.3s | | | | |
| 5' | 112d | 7.05 | | | |
| 6' | 121d | 7.76 | | | |
| OMe-3' | 60q | 3.94 | | | |
| OMe-6 | 60.9q | 4.08 | | | |
| OMe-4' | 55.9q | 3.84 | | | |

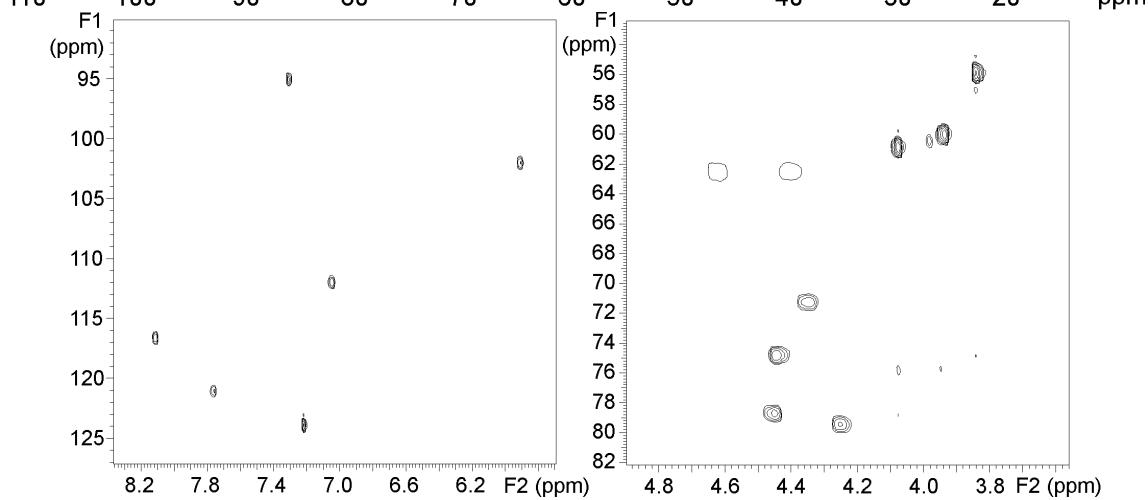
NMR-1H



NMR-13C:



NMR-HSQC:



Names

7-(β -D-glucopyranosyloxy)-5-hydroxy-2-(3-hydroxy-4-methoxyphenyl)-3,6-dimethoxy-4H-1-benzopyran-4-one;
Centaurein; 5,7,3'-Trihydroxy-3,6,4'-trimethoxy-flavone-7-O- β -D-glucoside

Galangin

3,5,7-Trihydroxyflavone

CAS-Number: 548-83-4

Formula: C₁₅H₁₀O₅ Exact mass: 270.05282

Molecular mass: 270.24

Column: Zorbax LiChrosphere Kinetex

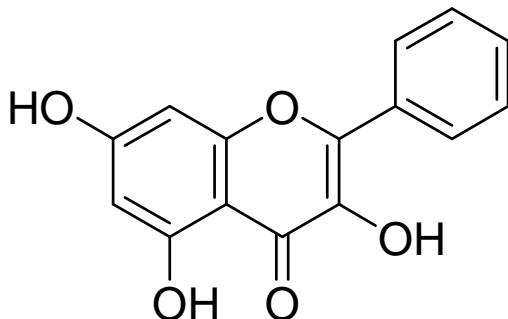
Abs.RetentionTime [min]: 28.32 25.73 12.82

Rel. RetentionTime (k'): 23 23.74 23.19

k' rel. to Rutin : 1.74 1.91 1.94

MS1: 269.3 MS2: 227.1 MS3: 153.1

UV/Vis: 265, 310(sh), 3



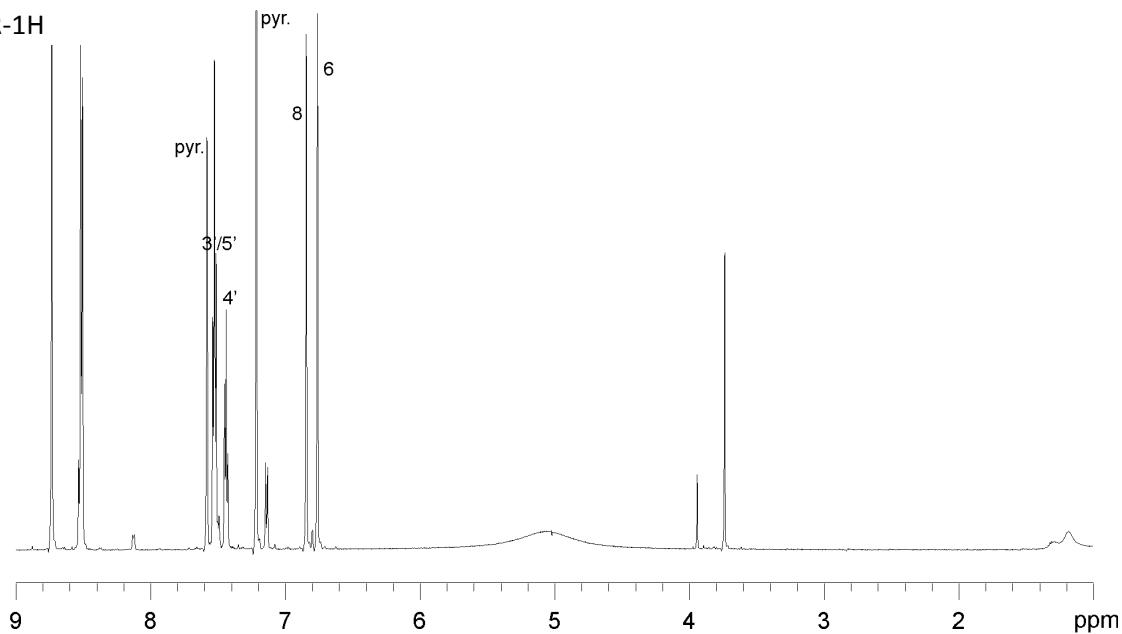
NMR - Resonance Assignments:

Flavone Core

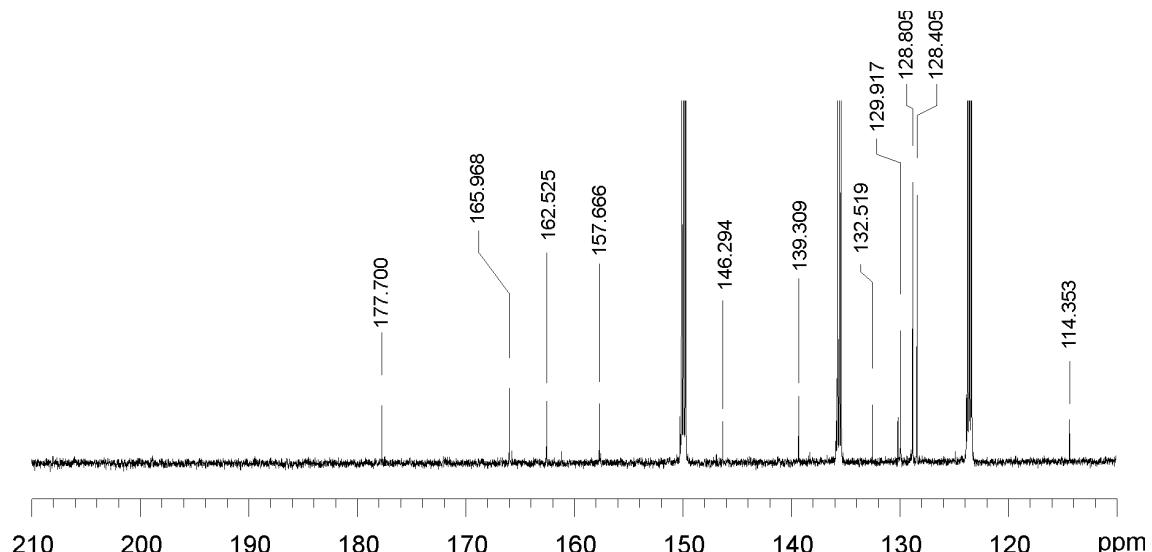
Sugar

| | δ_{C} | δ_{H} |
|----|---------------------|---------------------|
| 2 | 146.3s | |
| 3 | 139.3s | |
| 4 | 177.7s | |
| 4a | 104.6s | |
| 5 | 162.5s | |
| 6 | 99.4d | 6.76 |
| 7 | 166s | |
| 8 | 94.4d | 6.84 |
| 8a | 157.7s | |
| 1' | 132.5s | |
| 2' | 128.4d | 8.51 |
| 3' | 128.8d | 7.53 |
| 4' | 129.9d | 7.44 |
| 5' | 128.8d | 7.53 |
| 6' | 128.4d | 8.51 |

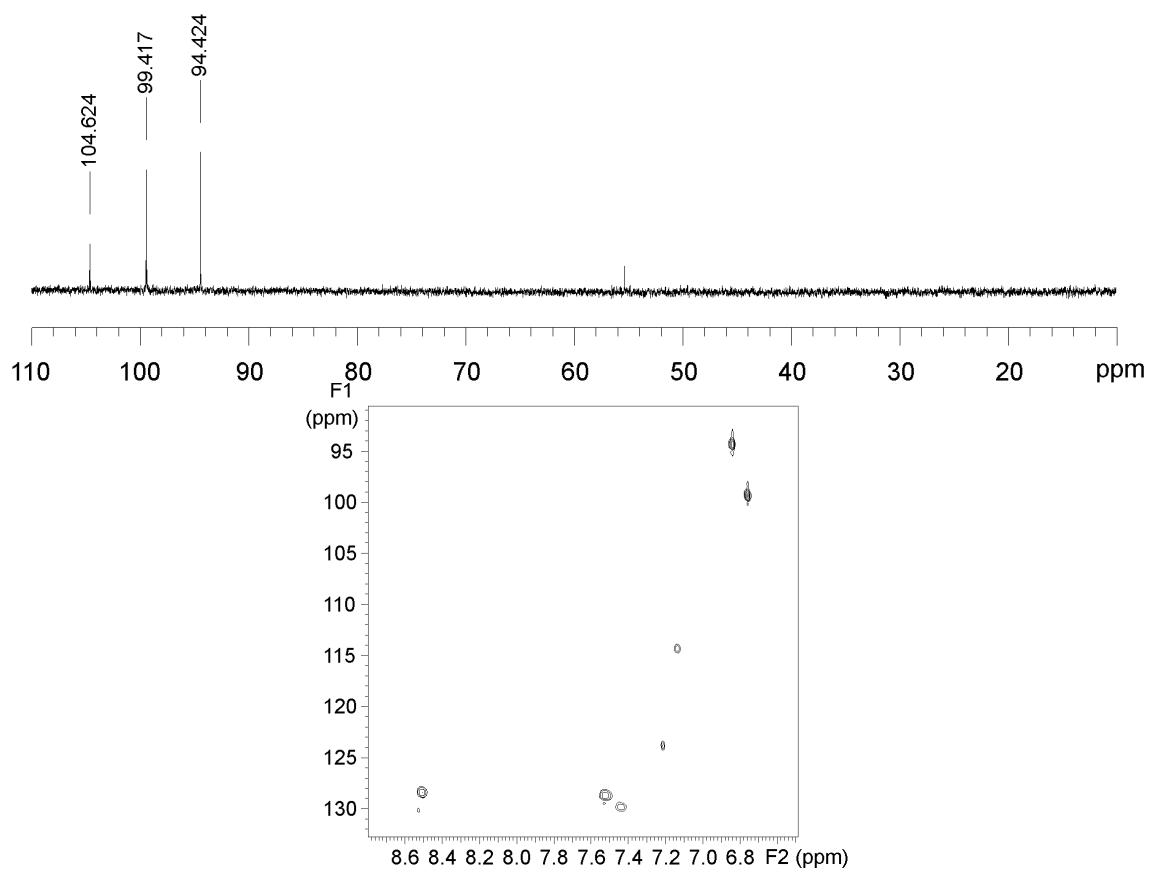
NMR-1H



NMR-13C:



NMR-HSQC:



Names

3,5,7-trihydroxy-2-phenyl-4H-1-benzopyran-4-one; 3,5,7-trihydroxy-flavone; Galangin; 3,5,7-trihydroxyflavone; NSC 407229; Norizalpinin

Kaempferol

3,5,7,4'-Tetrahydroxyflavone

CAS-Number: 520-18-3

Formula: C₁₅H₁₀O₆ Exact mass: 286.04774

Molecular mass: 286.24

Column: Zorbax LiChrosphere Kinetex

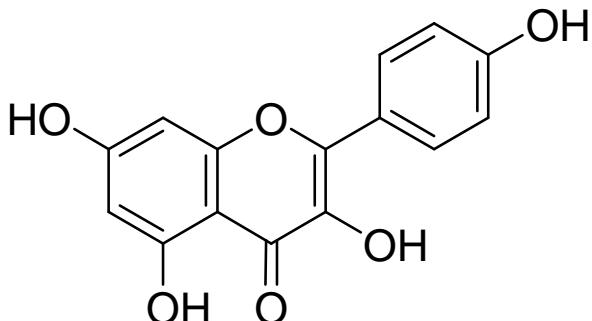
Abs.RetentionTime [min]: 23.52 21.09 10.43

Rel. RetentionTime (k') : 18.93 19.28 18.68

k' rel. to Butin : 1.43 1.55 1.56

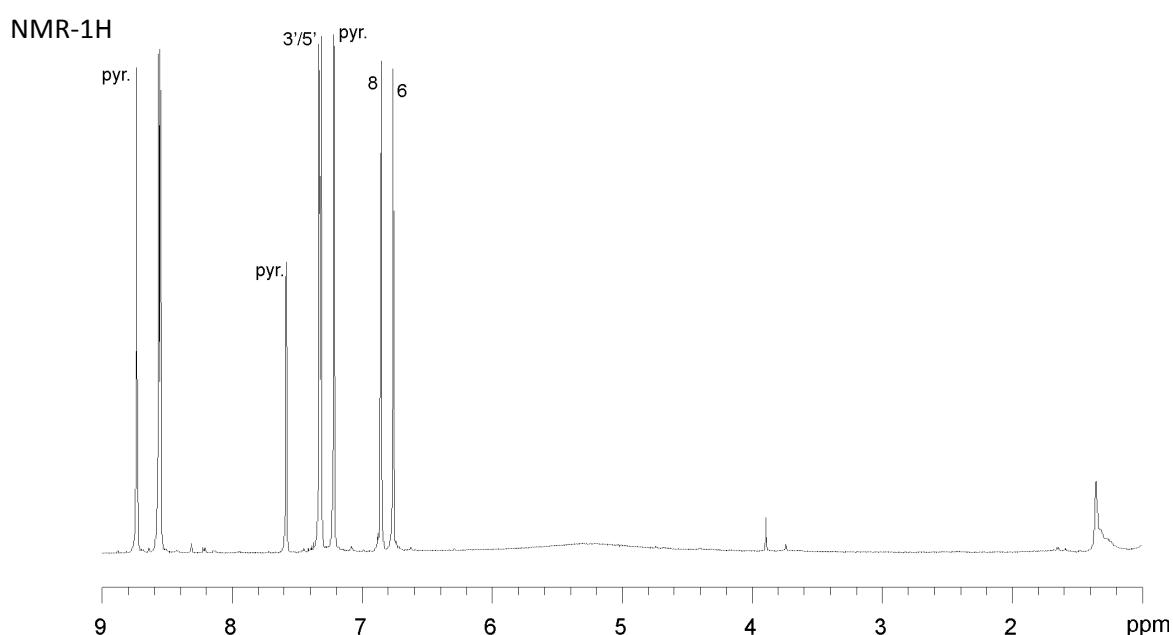
MS1: 285.3 MS2: 258 MS3: 151.1

UV/Vis: 265, 320(sh), 3

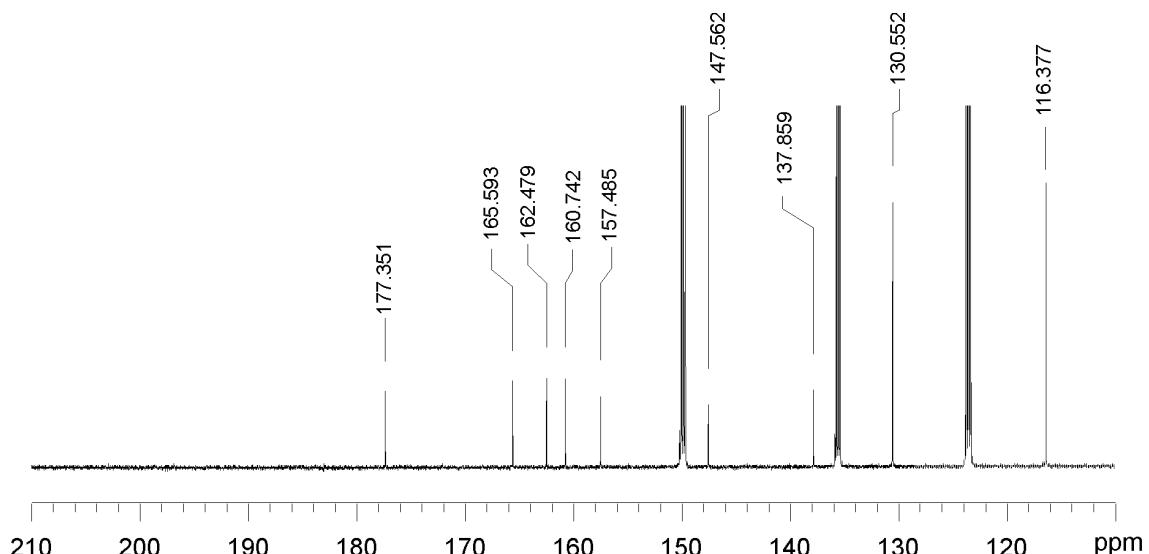


NMR - Resonance Assignments:

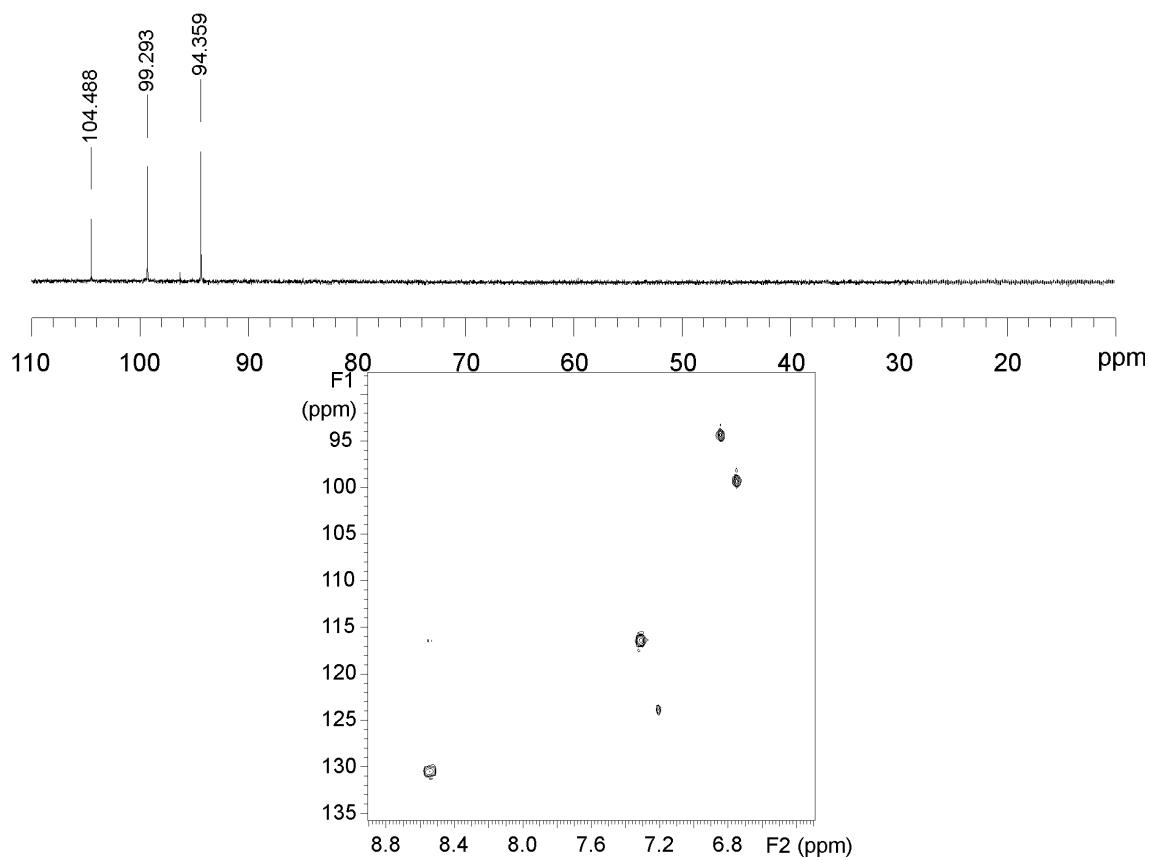
| | δ_C | δ_H |
|----|------------|------------|
| 2 | 147.6s | |
| 3 | 147.9s | |
| 4 | 177.4s | |
| 4a | 104.5s | |
| 5 | 162.5s | |
| 6 | 99.3d | 6.76 |
| 7 | 165.6s | |
| 8 | 94.4d | 6.85 |
| 8a | 157.5s | |
| 1' | 123.3s | |
| 2' | 130.6d | 8.55 |
| 3' | 116.4d | 7.32 |
| 4' | 160.7s | |
| 5' | 116.4d | 7.32 |
| 6' | 130.6d | 8.55 |



NMR-13C:



NMR-HSQC:



Names

3,5,7-trihydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one; 3,5,7,4'-tetrahydroxy-flavone; 3,5,7,4'-tetrahydroxyflavone; 3,5,7,4'-tetrahydroxyflavone; 3'-Deoxyquercetin; 5,7,4'-trihydroxyflavonol; C.I. 75640; Indigo Yellow; Kaempferol; Kaempferol; Kampcetin; Kempferol; NSC 407289; NSC 656277; Nimbecetin; Pelargidenolon; Pelargidenon; Populinetin; Rhamnolutein; Rhamnolutin; Robigenin; Swartziolin; Trifolitin

Isorhamnetin

3,5,7,4'-Tetrahydroxy-3'-methoxyflavone

CAS-Number: 480-19-3

Formula: C₁₆H₁₂O₇ Exact mass: 316.05830

Molecular mass: 316.26

Column: Zorbax LiChrosphere Kinetex

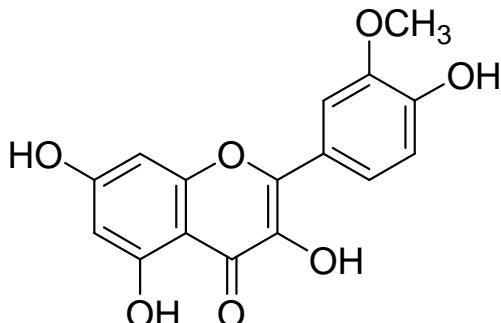
Abs.RetentionTime [min]: 24.03 21.60 10.67

Rel. RetentionTime (k') : 19.36 19.77 19.13

k' rel. to Rutin : 1.47 1.59 1.60

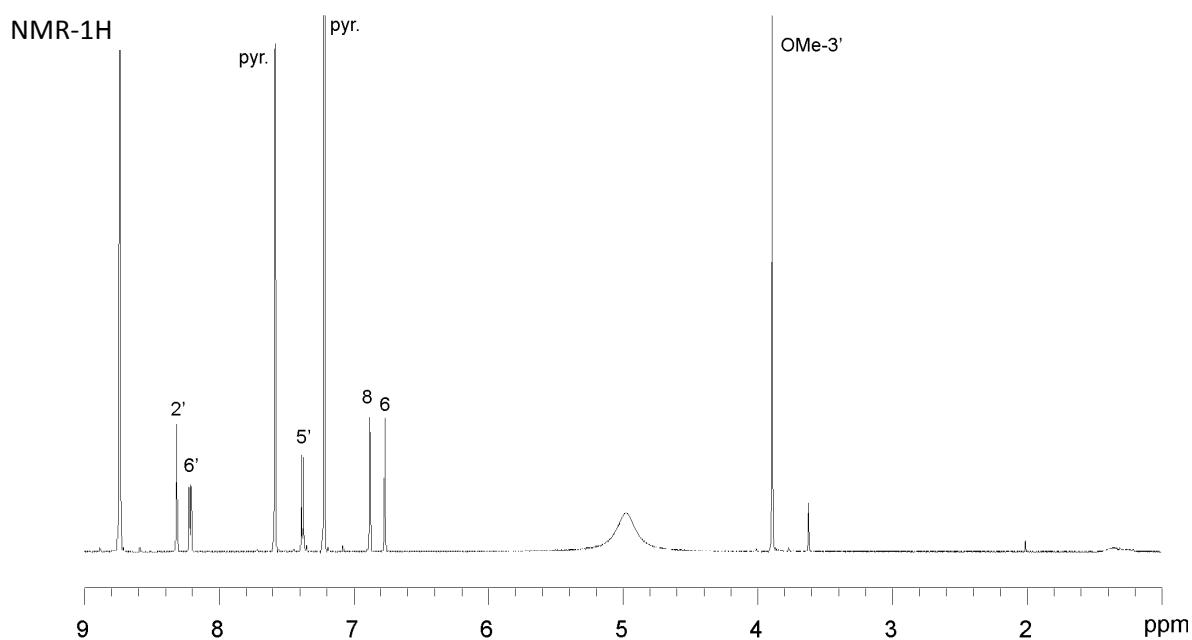
MS1: 315.2 MS2: 300.2 MS3: 271.3

UV/Vis: 255, 265(sh), 3

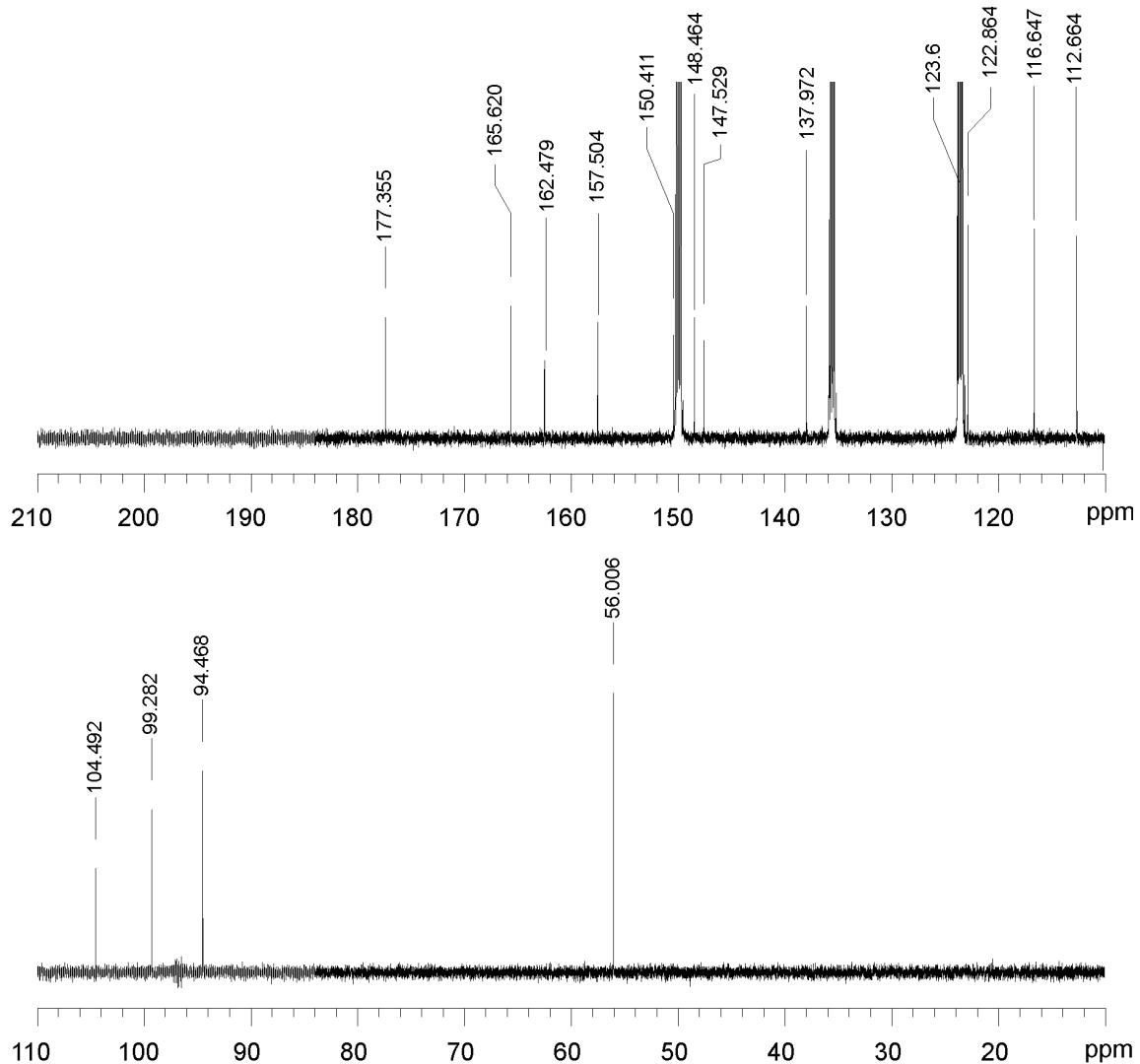


NMR - Resonance Assignments:

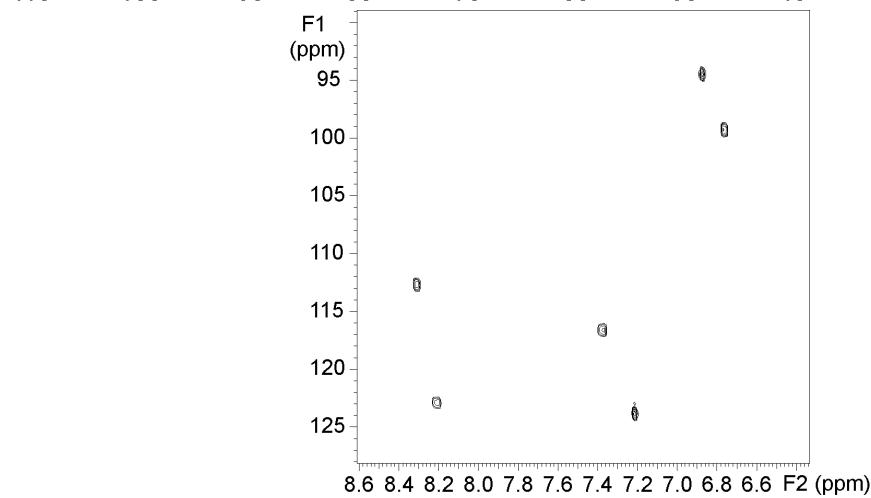
| | δ_C | δ_H |
|--------|------------|------------|
| 2 | 147.5s | |
| 3 | 138s | |
| 4 | 177.4s | |
| 4a | 104.5s | |
| 5 | 162.5s | |
| 6 | 99.3d | 6.77 |
| 7 | 165.6s | |
| 8 | 94.5d | 6.88 |
| 8a | 157.5s | |
| 1' | 123.6s | |
| 2' | 112.7d | 8.31 |
| 3' | 148.5s | |
| 4' | 150.4s | |
| 5' | 116.6d | 7.38 |
| 6' | 122.9d | 8.21 |
| OMe-3' | 56q | 3.89 |



NMR-13C:



NMR-HSQC:



Names

3,5,7-trihydroxy-2-(4-hydroxy-3-methoxyphenyl)-4H-1-benzopyran-4-one; 3,5,7,4'-tetrahydroxy-3'-methoxy-flavone; Isorhamnetin; 3,5,7,4'-tetrahydroxy-3'-methoxyflavone; 3,5,7,4'-Tetrahydroxy-3'-methoxyflavone; 3'-Methoxyquercetin; 3'-Methylquercetin; 3'-O-Methylquercetin; C.I. 75680; Isorhamnetol; Quercetin 3'-methyl ether

Robinetin

3,7,3',4',5'-Pentahydroxyflavone

CAS-Number: 490-31-3

Formula: C₁₅H₁₀O₇ Exact mass: 302.04265

Molecular mass: 302.24

Column: Zorbax LiChrosphere Kinetex

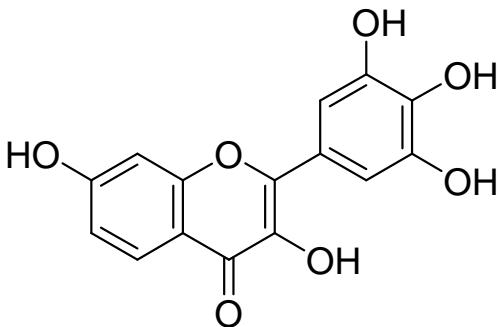
Abs.RetentionTime [min]: 16.4 13.71 6.60

Rel. RetentionTime (k') : 12.9 12.18 11.45

k' rel. to Rutin : 0.98 0.98 0.96

MS1: 301.2 MS2: 162.9 MS3: 135

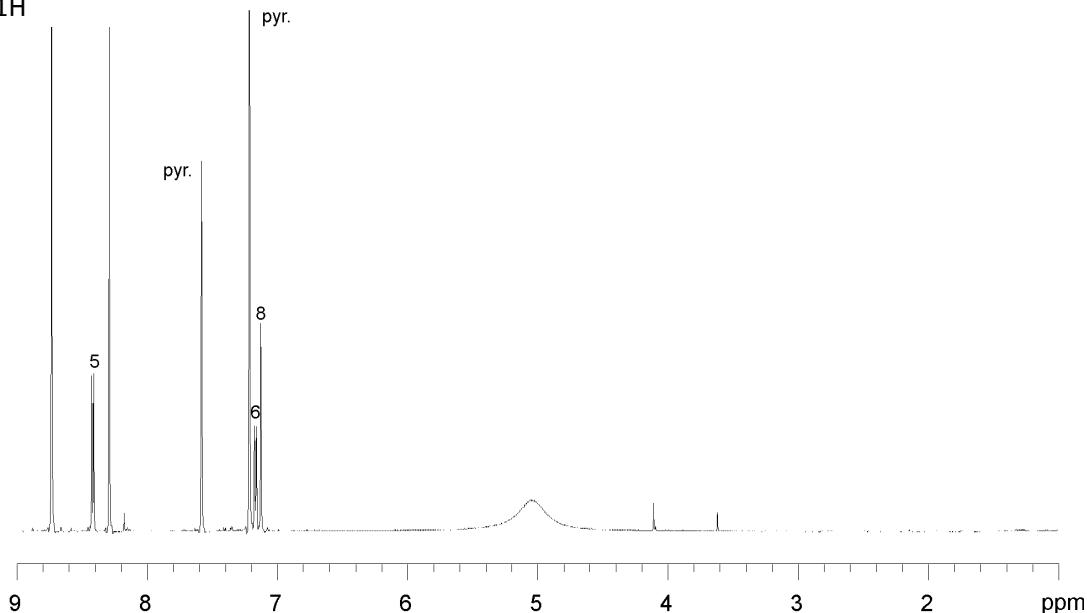
UV/Vis: 255, 320(sh), 3



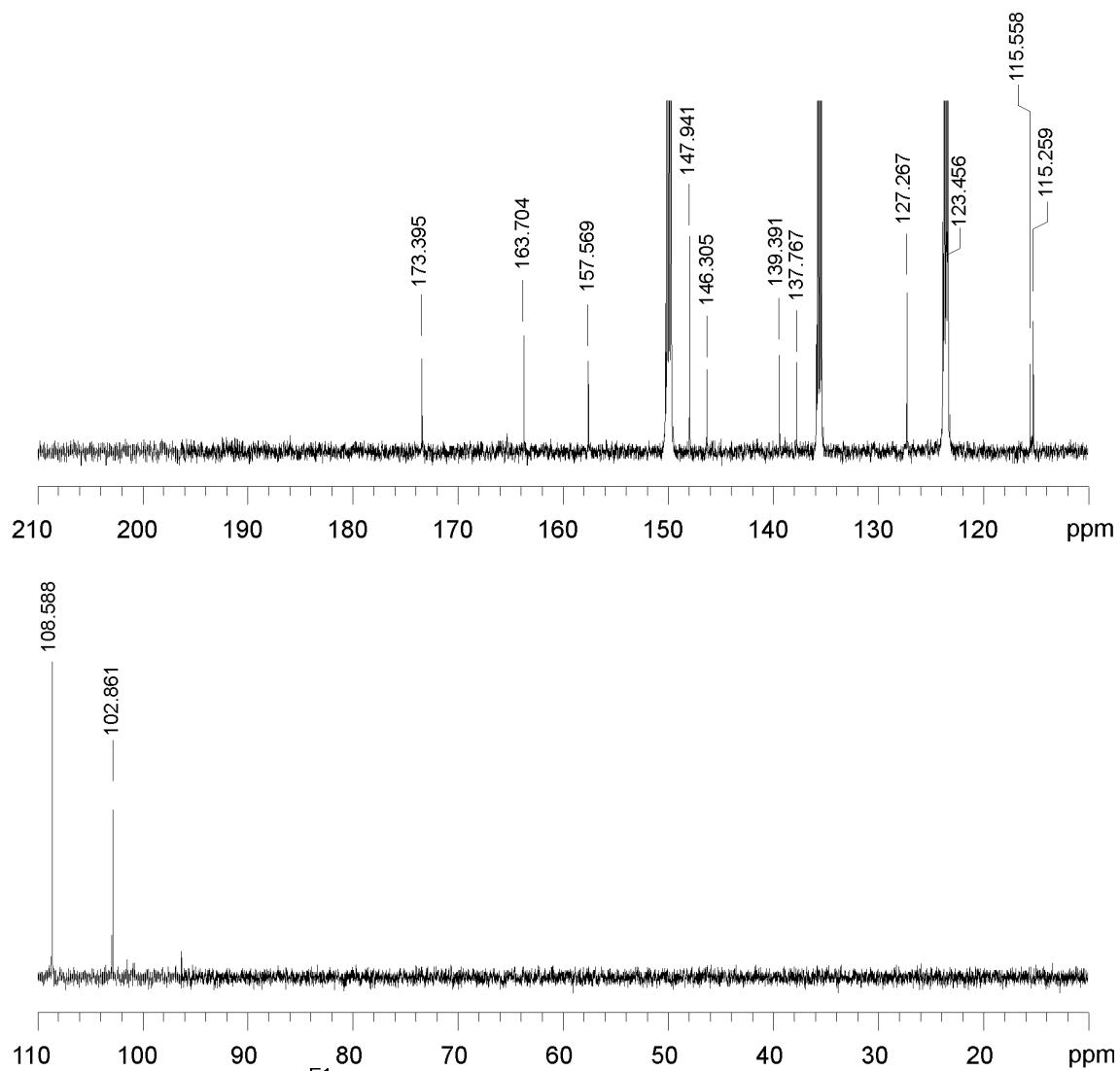
NMR - Resonance Assignments:

| | δ_C | δ_H |
|----|------------|------------|
| 2 | 147.9s | |
| 3 | 139.4s | |
| 4 | 173.4s | |
| 4a | 115.5s | |
| 5 | 127.3d | 8.42 |
| 6 | 115.3d | 7.17 |
| 7 | 163.7s | |
| 8 | 102.8d | 7.13 |
| 8a | 157.6s | |
| 1' | 123.5s | |
| 2' | 108.6d | 8.29 |
| 3' | 146.3s | |
| 4' | 137.8s | |
| 5' | 146.3s | |
| 6' | 108.6d | 8.29 |

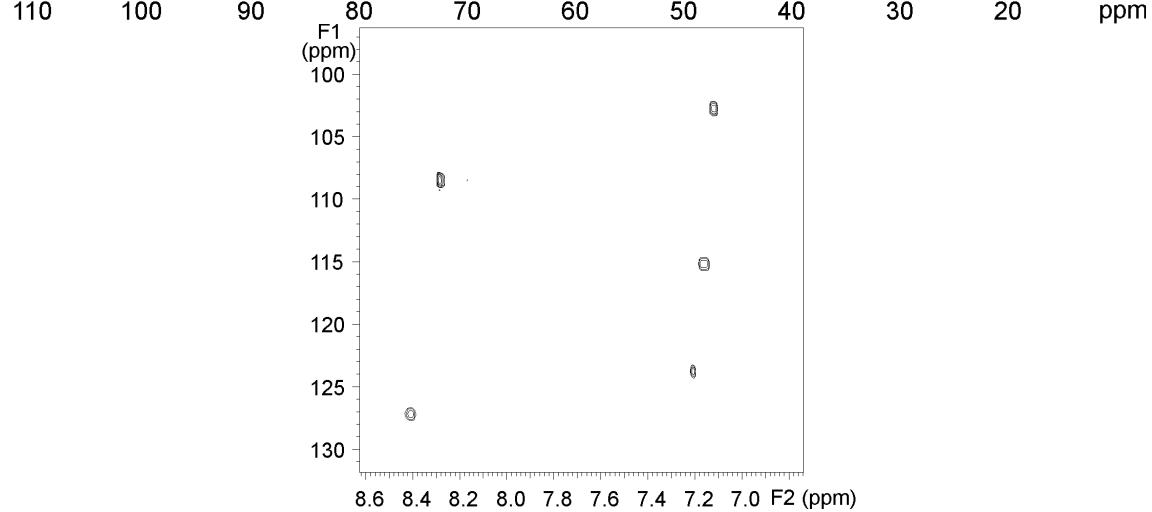
NMR-¹H



NMR-13C:



NMR-HSQC:



Names

3,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-4H-1-benzopyran-4-one; 3,7,3',4',5'-pentahydroxy-flavone; Robinetin; 3,7,3',4',5'-pentahydroxyflavone; 3,7,3',4',5'-pentahydroxyflavone; NSC 407331; NSC 656274; Norkanugin

Vitexin

Apigenin-8-C- β -D-glucoside

CAS-Number: 3681-93-4

Formula: C₂₁H₂₀O₁₀ Exact mass: 432.10565

Molecular mass: 432.1

Column: Zorbax LiChrosphere Kinetex

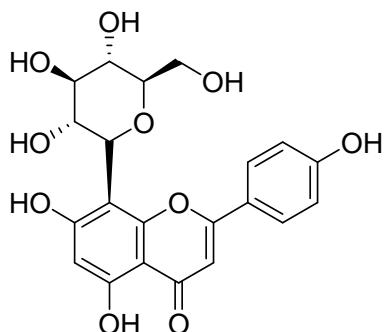
Abs.RetentionTime [min]: 16.05 12.96 6.34

Rel. RetentionTime (k') : 12.6 11.46 10.96

k' rel. to Rutin : 0.96 0.92 0.92

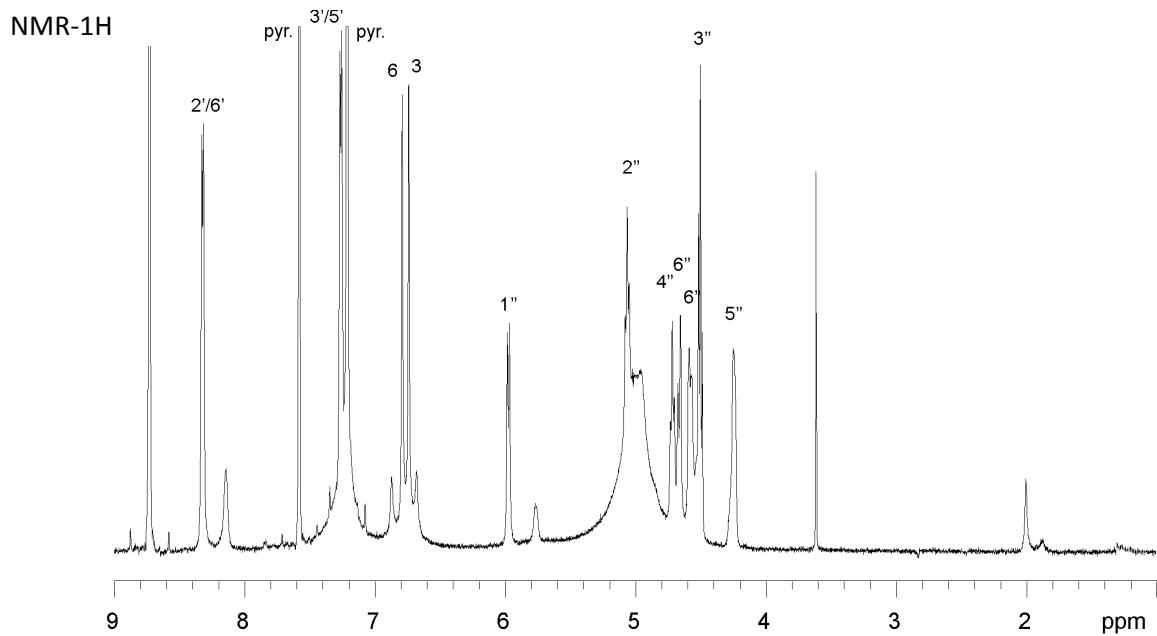
MS1: 431 2 MS2: 311 2 MS3: 283 3

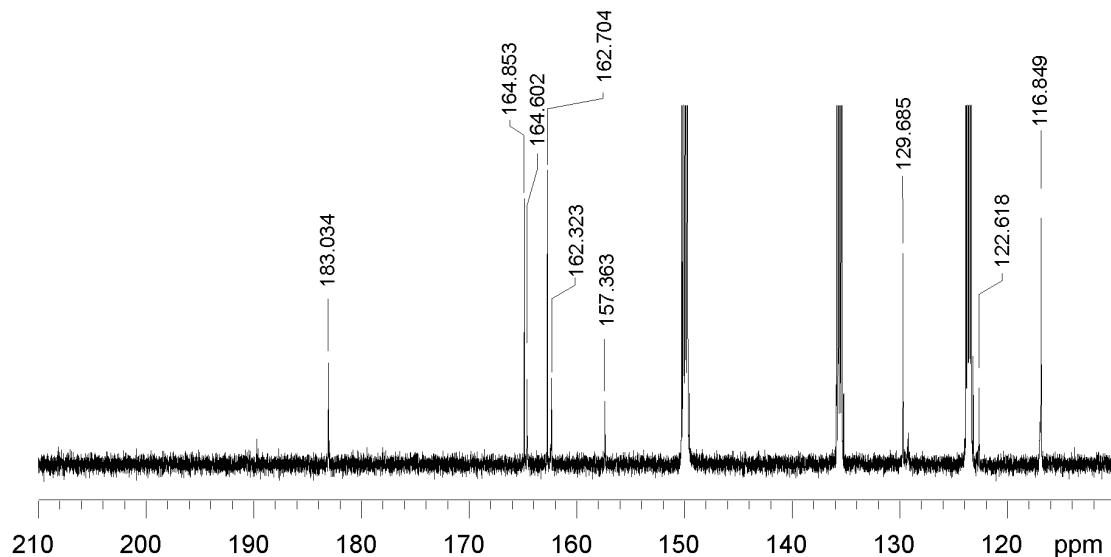
UV/Vis: 265, 335



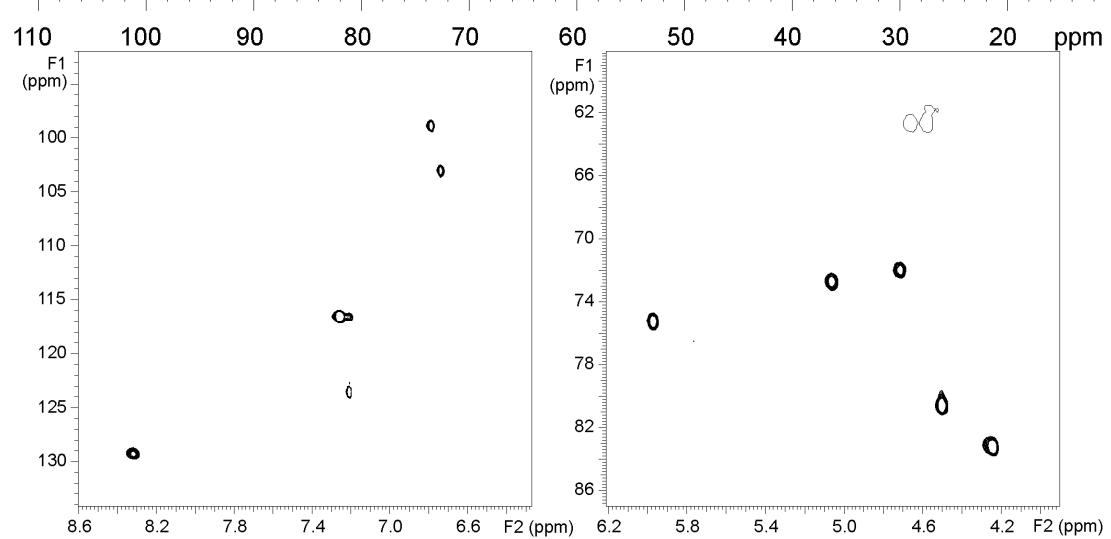
NMR - Resonance Assignments:

| | δ_C | δ_H | | δ_C | δ_H |
|----|------------|------------|----|------------|------------|
| 2 | 165.8s | | 1" | 75.6d | 5.97 |
| 3 | 103.3d | 6.74 | 2" | 73d | 5.06 |
| 4 | 183s | | 3" | 80.9d | 4.5 |
| 4a | 105.4s | | 4" | 72.3d | 4.72 |
| 5 | 162.3s | | 5" | 83.6d | 4.24 |
| 6 | 99.2d | 6.79 | 6" | 63t | 4.66/4.58 |
| 7 | 164.6s | | | | |
| 8 | 106.2s | | | | |
| 1' | 122.6s | | | | |
| 2' | 129.7d | 8.32 | | | |
| 3' | 116.8d | 7.26 | | | |
| 4' | 162.7s | | | | |
| 5' | 116.8d | 7.26 | | | |
| 6' | 129.7d | 8.32 | | | |



NMR-¹³C:

NMR-HSQC:



Names

8- β -D-glucopyranosyl-5,7-dihydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one; 8-D-glucosyl-5,7,4'-trihydroxy-flavone; Vitexin; 8-C- β -D-Glucopyranosylapigenin; Apigenin 8-C- β -D-glucoside; Orientoside; Vitexina

Vitexin-2"-O-rhamnosid

Apigenin-8-[C- α -L-rhamnopyranosyl-(1 \rightarrow 2)- β -D-glucopyranoside]

CAS-Number: 64820-99-1

Formula: C₂₇H₃₀O₁₄ Exact mass: 578.16356

Molecular mass: 578.16

Column: Zorbax LiChrosphere Kinetex

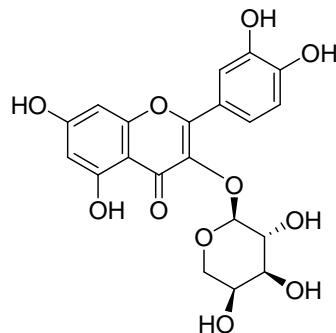
Abs.RetentionTime [min]: 16.11 12.96 6.37

Rel. RetentionTime (k'): 12.65 11.46 11.02

k' rel. to Rutin : 0.96 0.92 0.92

MS1: 577.3 MS2: 413.2 MS3: 293.3

UV/Vis: 265, 335

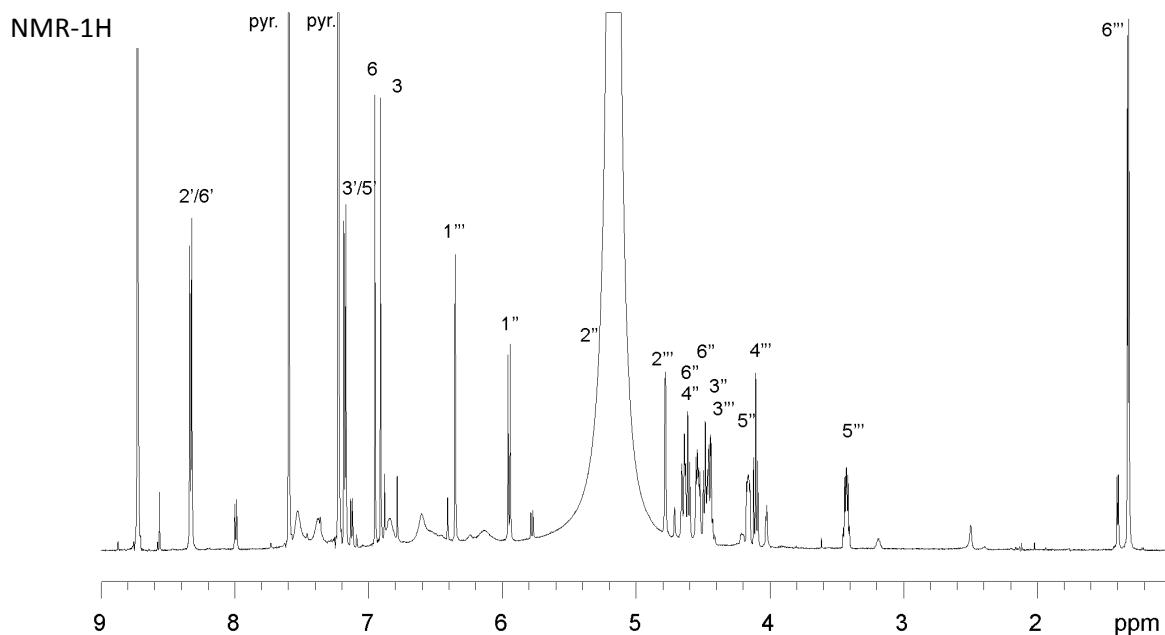


NMR - Resonance Assignments:

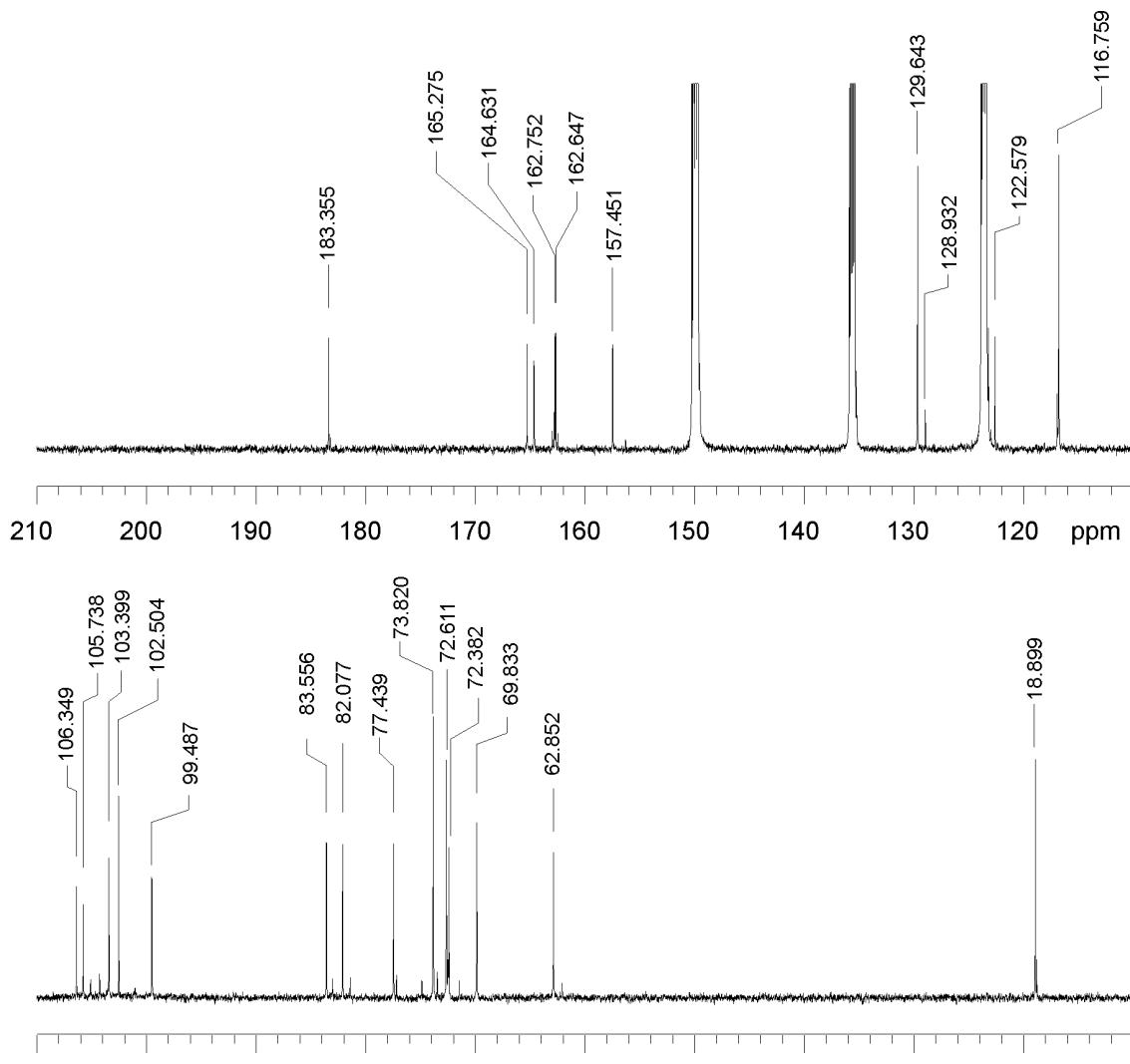
Flavone Core

Sugar

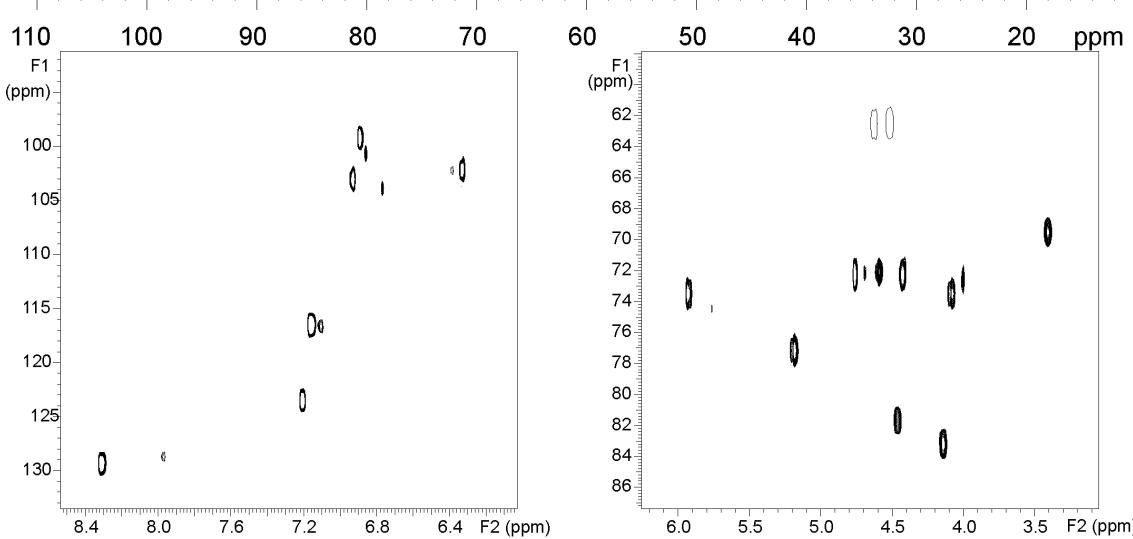
| | δ_C | δ_H | | δ_C | δ_H |
|----|------------|------------|------|------------|------------|
| 2 | 165.3s | | 1" | 73.8d | 5.95 |
| 3 | 103.4d | 6.95 | 2" | 77.4d | 5.21 |
| 4 | 183.4s | | 3" | 82.1d | 4.49 |
| 4a | 105.7s | | 4" | 72.4d | 4.62 |
| 5 | 162.8s | | 5" | 83.6d | 4.16 |
| 6 | 99.5d | 6.92 | 6" | 62.9t | 4.65/4.54 |
| 7 | 164.6s | | 1''' | 102.5d | 6.36 |
| 8 | 106.4s | | 2''' | 72.6d | 4.79 |
| 1' | 122.6s | | 3''' | 72.6d | 4.45 |
| 2' | 129.6d | 8.33 | 4''' | 73.8d | 4.12 |
| 3' | 116.8d | 7.18 | 5''' | 69.8d | 3.44 |
| 4' | 162.7s | | 6''' | 18.9q | 1.33 |
| 5' | 116.8d | 7.18 | | | |
| 6' | 129.6d | 8.33 | | | |



NMR-13C:



NMR-HSQC:



Names

8-[2-O-(6-deoxy- α -L-mannopyranosyl)- β -D-glucopyranosyl]-5,7-dihydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one; 2"-O-rhamnosylvitexin; 2"-O- α -L-rhamnopyranosylvitexin; 2"-rhamnosylvitexin; Apigenin 8-[C- α -L-rhamnopyranosyl-(1 \rightarrow 2)- β -D-glucopyranoside]; Vitexin 2"-O-rhamnoside; Vitexin 2"-rhamnoside

GuaijaverinQuercetin-3-O- α -L-arabinopyranoside

CAS-Number: 22255-13-6

Formula: C₂₀H₁₈O₁₁ Exact mass: 434.08491

Molecular mass: 434.08

Column: Zorbax LiChrosphere Kinetex

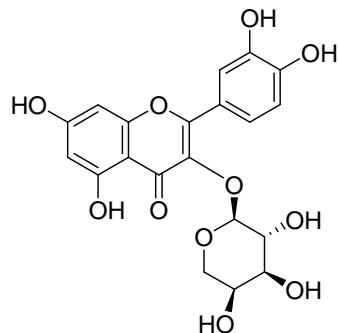
Abs.RetentionTime [min]: 17.63 14.93 7.40

Rel. RetentionTime (k'): 13.94 13.36 12.96

k' rel. to Rutin : 1.06 1.08 1.09

MS1: 433.3 MS2: 301.1 MS3: 178.9

UV/Vis: 230, 265(sh), 3



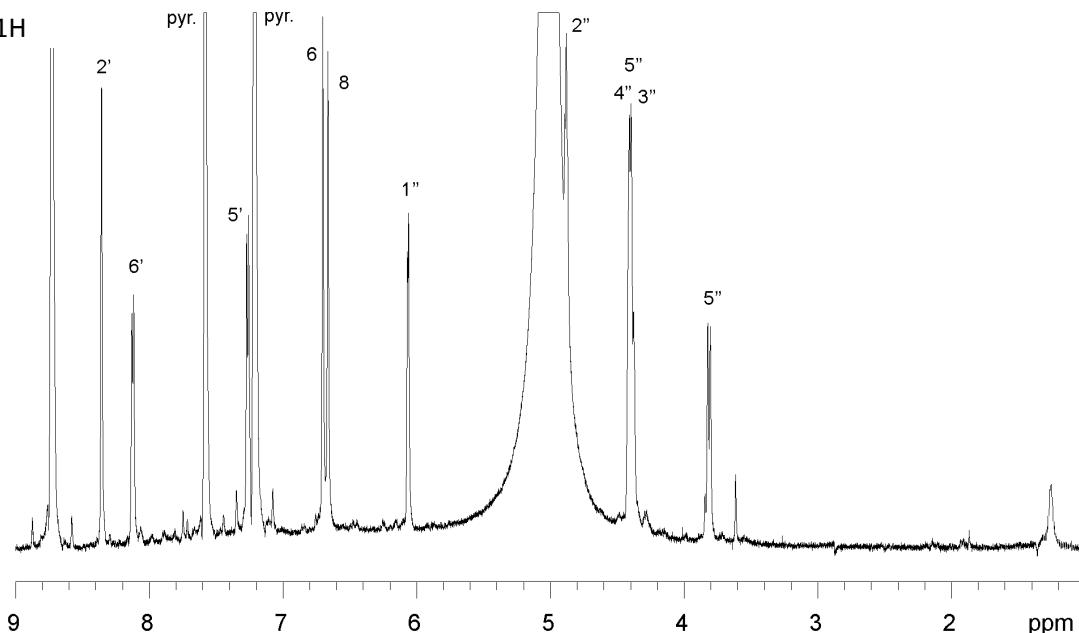
NMR - Resonance Assignments:

Flavone Core

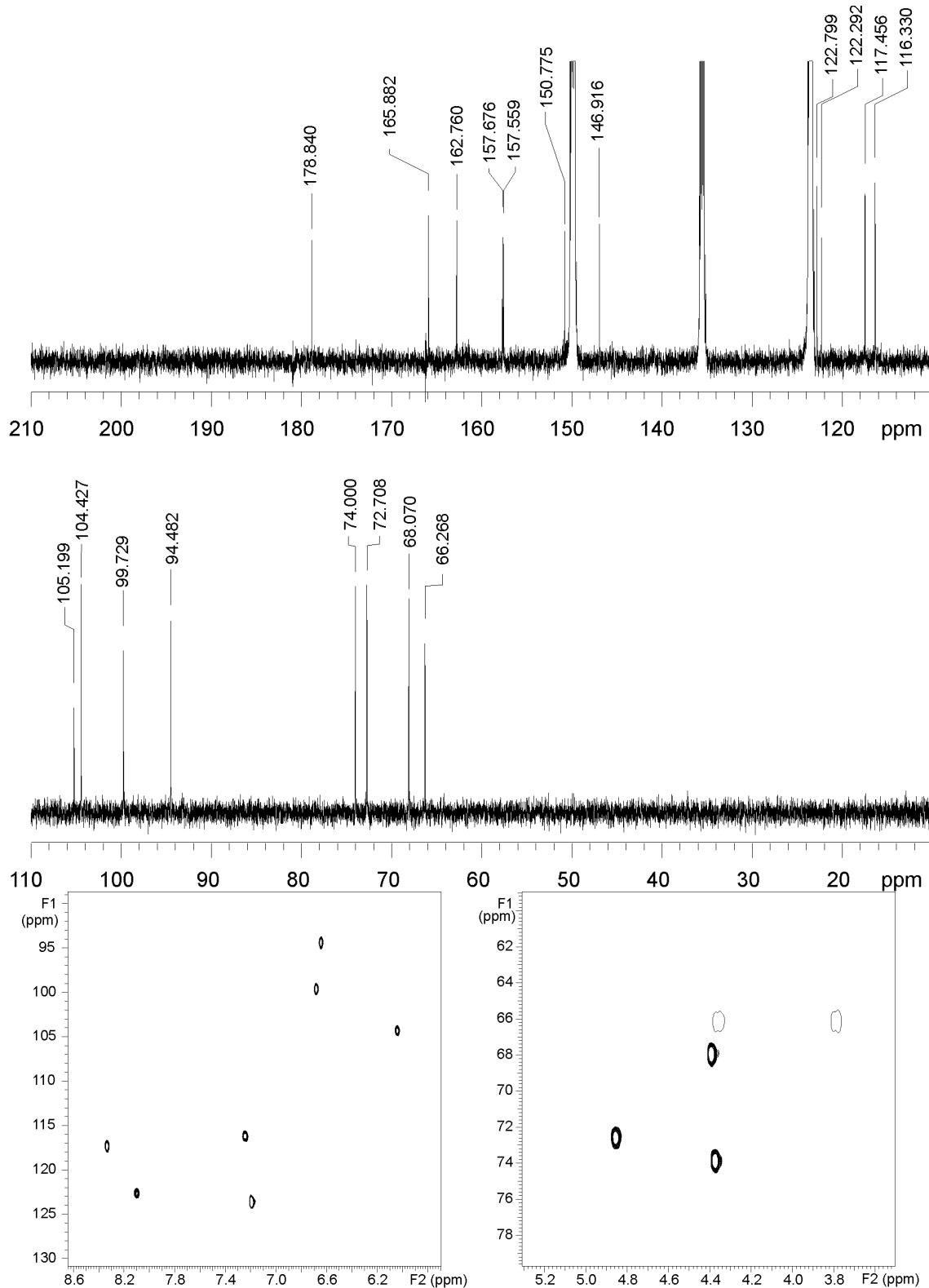
Sugar

| | δ_C | δ_H | | δ_C | δ_H |
|----|------------|------------|----|------------|------------|
| 2 | 157.7s | | 1" | 104.4d | 6.06 |
| 3 | 135.3s | | 2" | 72.7d | 4.87 |
| 4 | 178.8s | | 3" | 74d | 4.39 |
| 4a | 105.2s | | 4" | 68.1d | 4.41 |
| 5 | 162.8s | | 5" | 66.3t | 4.38/3.81 |
| 6 | 99.7d | 6.7 | | | |
| 7 | 165.9s | | | | |
| 8 | 94.5d | 6.66 | | | |
| 1' | 122.3s | | | | |
| 2' | 117.4d | 8.36 | | | |
| 3' | 146.9s | | | | |
| 4' | 150.8s | | | | |
| 5' | 116.3d | 7.26 | | | |
| 6' | 122.8d | 8.12 | | | |

NMR-1H



NMR-13C:



Names

3-(α -L-arabinopyranosyloxy)-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4H-1-benzopyran-4-one; Guaijaverin; quercetin-3, α -L-arabinopyranoside; 5,7,3',4'-tetrahydroxyflavone 3-O- α -L-arabinoside; Feniculin; Feniculine; Foeniculin; Foeniculin (glycoside); Guaiaverin; Guajavarin; Guajaverin; Quercetin 3-O- α -L-arabinopyranoside; Quercetin 3- α -L-arabinopyranoside; Quercetin-3-O- α -L-arabinoside

Quercetin-3-arabino-glucosid

Quercetin-3-O-[β -arabinopyranosyl-(1" \rightarrow 6")- β -glucopyranoside]

CAS-Number: 391639-37-5

Formula: C₂₆H₁₈O₁₆ Exact mass: 596.13773

Molecular mass: 596.49

Column: Zorbax LiChrosphere Kinetex

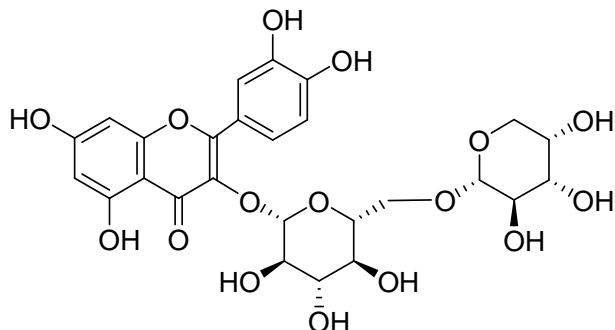
Abs.RetentionTime [min]: 15.95 13.12 6.41

Rel. RetentionTime (k'): 12.52 11.62 11.09

k' rel. to Rutin : 0.95 0.94 0.93

MS1: 595.4 MS2: 301.2 MS3: 178.9

UV/Vis: 255, 265(sh)



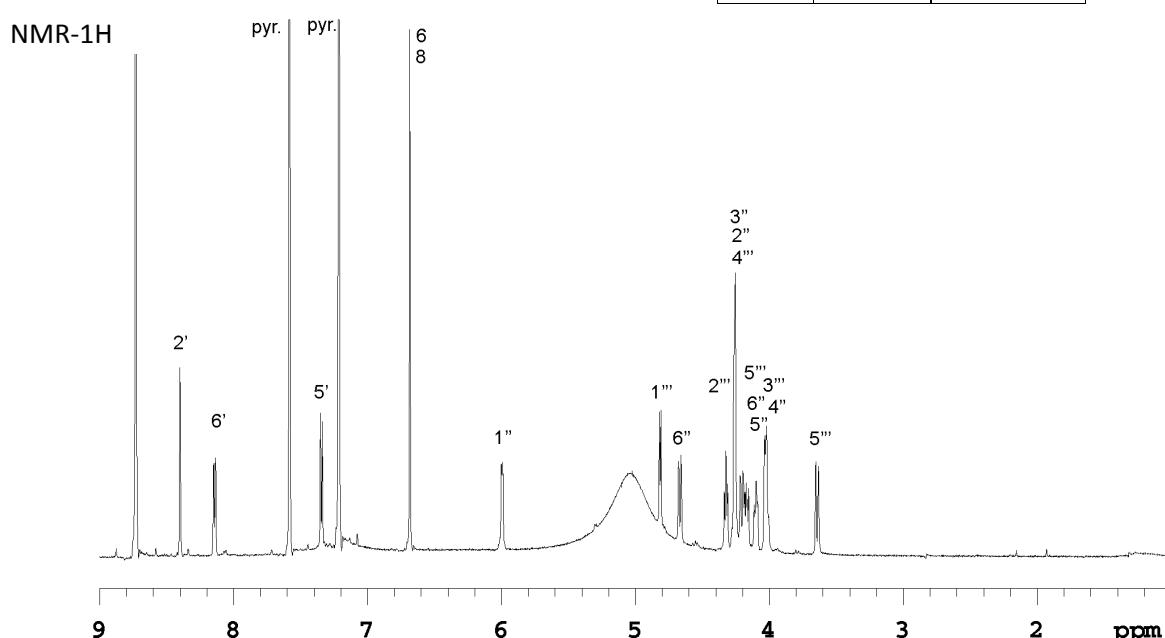
NMR - Resonance Assignments:

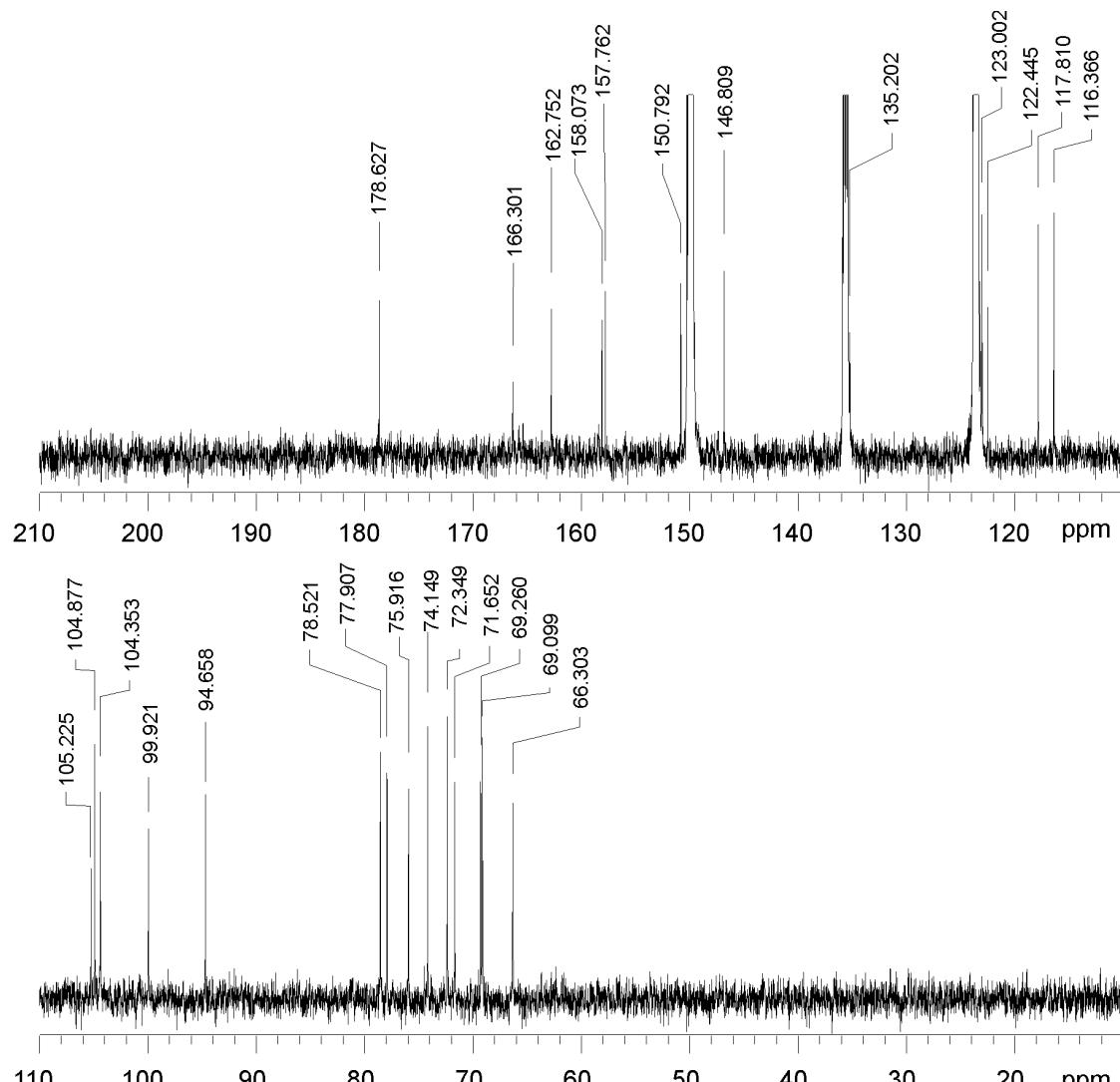
Flavone Core

Sugar

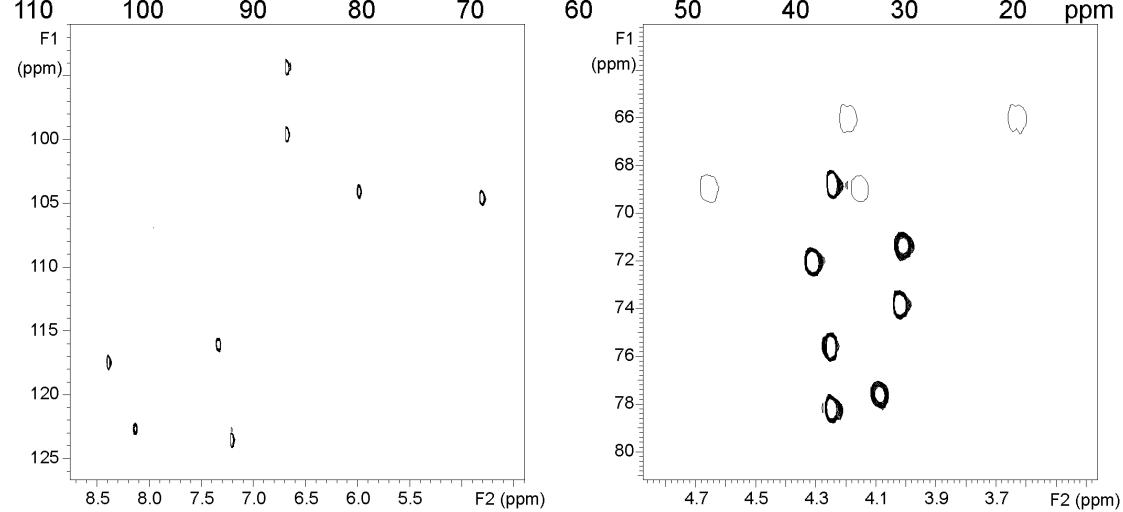
| | δ_C | δ_H |
|----|------------|------------|
| 2 | 158.1s | |
| 3 | 135.2s | |
| 4 | 178.6s | |
| 4a | 105.2s | |
| 5 | 162.7s | |
| 6 | 99.9d | 6.68 |
| 7 | 166.3s | |
| 8 | 94.6d | 6.68 |
| 8a | 157.7s | |
| 1' | 122.4s | |
| 2' | 117.8d | 8.4 |
| 3' | 146.8s | |
| 4' | 150.8s | |
| 5' | 116.4d | 7.34 |
| 6' | 123d | 8.14 |

| | δ_C | δ_H |
|------|------------|------------|
| 1" | 104.4d | 5.99 |
| 2" | 75.9d | 4.25 |
| 3" | 78.5d | 4.25 |
| 4" | 71.1d | 4.01 |
| 5" | 77.9d | 4.09 |
| 6" | 69.3t | 4.65/4.15 |
| 1''' | 104.9d | 4.81 |
| 2''' | 72.3d | 4.31 |
| 3''' | 74.1d | 4.02 |
| 4''' | 69.1d | 4.24 |
| 5''' | 66.3t | 4.19/3.63 |



NMR-¹³C:

NMR-HSQC:



Names

3-[(6-O- β -L-arabinopyranosyl- β -D-glucopyranosyl)oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4H-1-benzopyran-4-one;
Quercetin-3-O-[β -arabinopyranosyl-(1 \rightarrow 6)- β -glucopyranoside]

Tiliroside

Kaempferol-3-O- β -D-(6"-O-(E)-p-coumaroyl)glucopyranoside
CAS-Number: 20316-62-5

Formula: C₃₀H₂₆O₁₃ Exact mass: 594.13734

Molecular mass: 594.53

Column: Zorbax LiChrosphere Kinetex

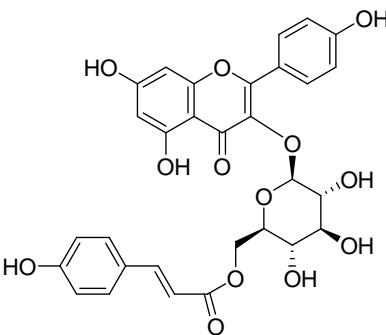
Abs.RetentionTime [min]: 22.21 19.65 9.98

Rel. RetentionTime (k'): 17.82 17.89 17.83

k' rel. to Rutin : 1.35 1.44 1.49

MS1: 593.3 MS2: 285.3 MS3: 257.1

UV/Vis: 265, 315



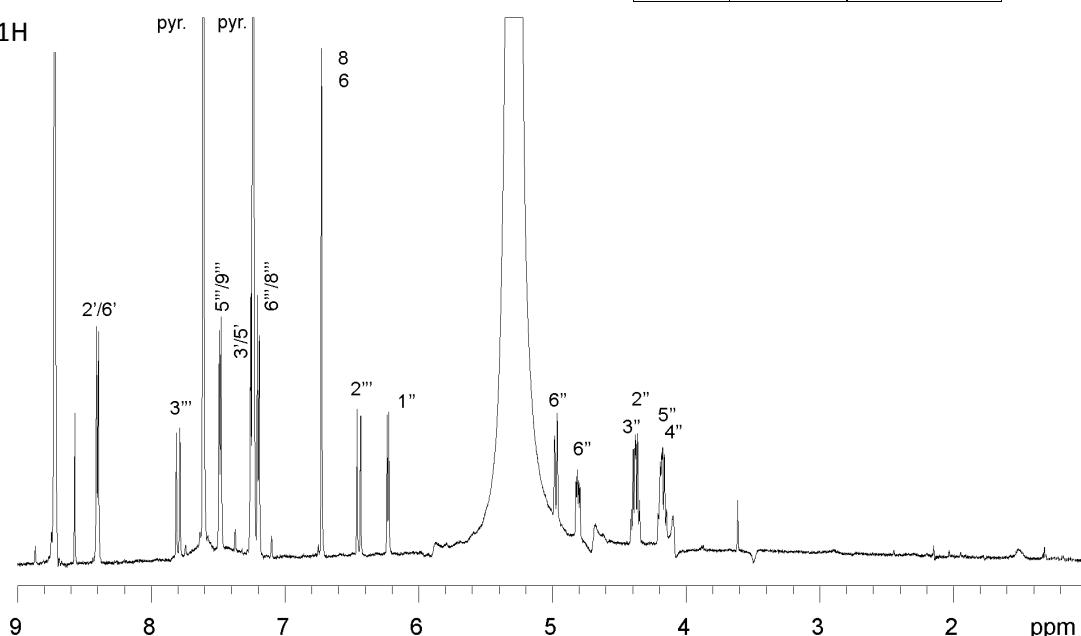
NMR - Resonance Assignments:

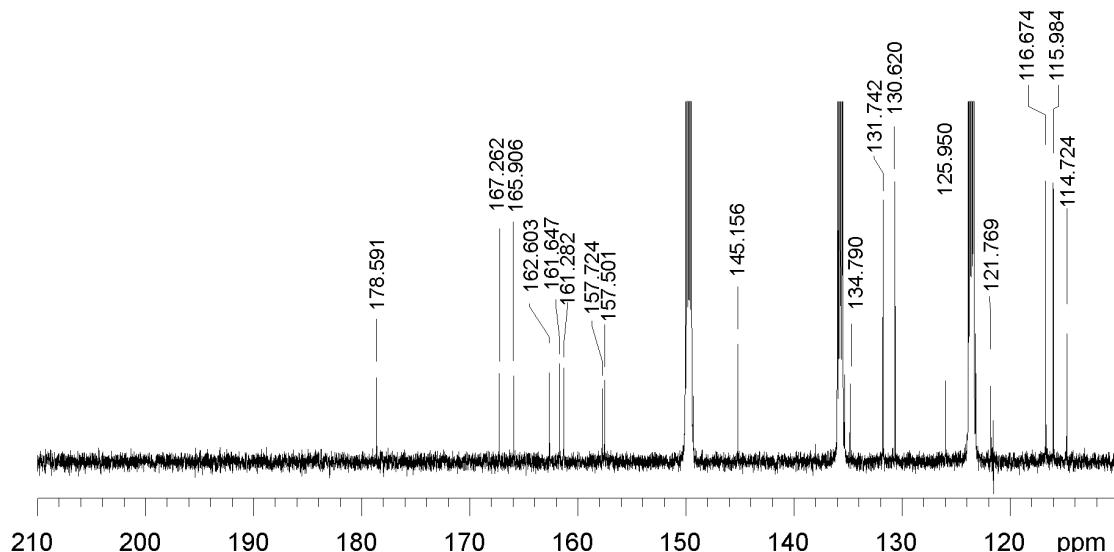
Flavone Core

Sugar

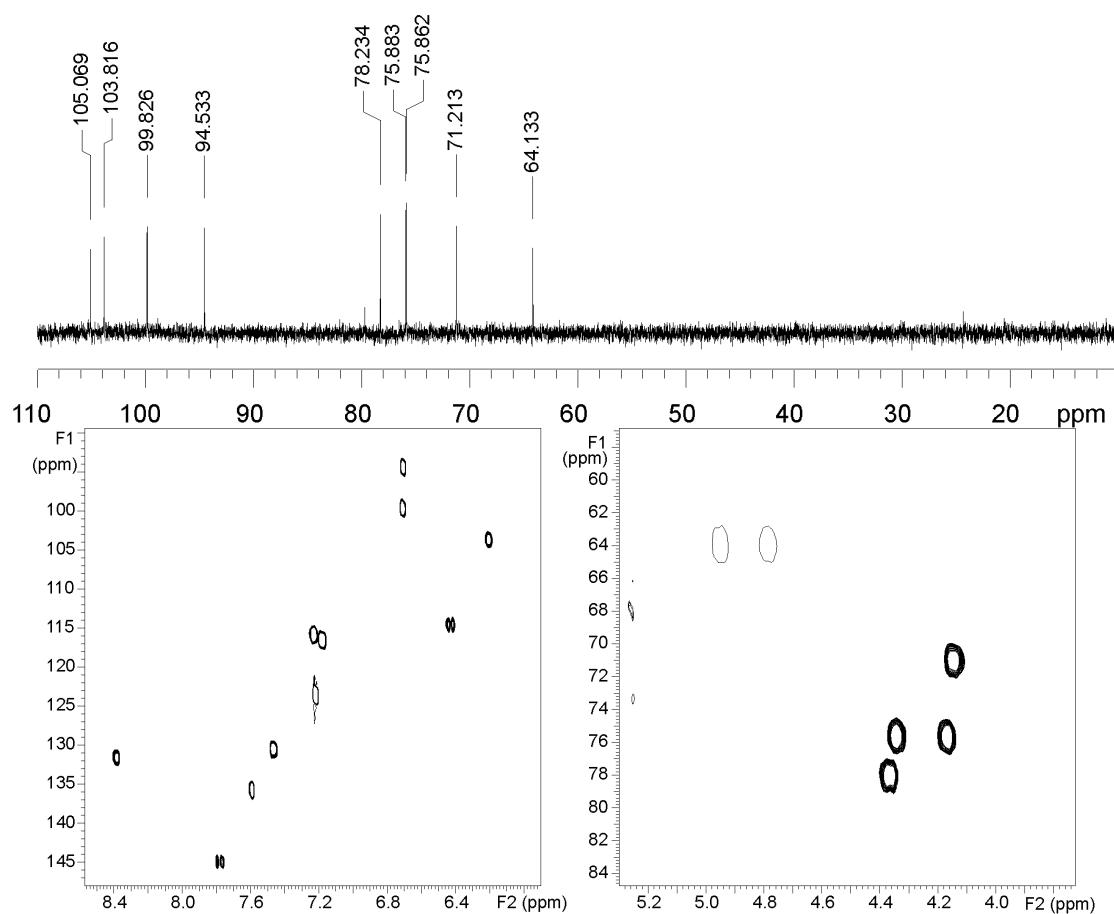
| | δ_{C} | δ_{H} | | δ_{C} | δ_{H} |
|----|---------------------|---------------------|------|---------------------|---------------------|
| 2 | 157.7s | | 1" | 103.8d | 6.22 |
| 3 | 134.8s | | 2" | 75.9d | 4.35 |
| 4 | 178.6s | | 3" | 78.2d | 4.38 |
| 4a | 105.1s | | 4" | 71.2d | 4.16 |
| 5 | 162.6s | | 5" | 75.9d | 4.18 |
| 6 | 99.8d | 6.72 | 6" | 64.1t | 4.96/4.8 |
| 7 | 165.9s | | 1''' | 167.3s | |
| 8 | 94.5d | 6.72 | 2''' | 144.7d | 6.44 |
| 8a | 157.5s | | 3''' | 145.2d | 7.8 |
| 1' | 121.8s | | 4''' | 126s | |
| 2' | 131.8d | 8.4 | 5''' | 130.6d | 7.48 |
| 3' | 116d | 7.24 | 6''' | 116.7d | 7.2 |
| 4' | 161.7s | | 7''' | 161.3s | |
| 5' | 116d | 7.24 | 8''' | 116.7d | 7.2 |
| 6' | 131.8d | 8.4 | 9''' | 130.6d | 7.48 |

NMR-1H



NMR-¹³C:

NMR-HSQC:



Names

5,7-dihydroxy-2-(4-hydroxyphenyl)-3-[[6-O-[(2E)-3-(4-hydroxyphenyl)-1-oxo-2-propen-1-yl]-β-D-glucopyranosyl]oxy]-4H-1-benzopyran-4-one; 3-(4-hydroxyphenyl)-6'-ester with 3-(β-D-glucopyranosyloxy)-5,7-dihydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one-(E)-2-propenoic acid; 5,7-dihydroxy-2-(4-hydroxyphenyl)-3-[[6-O-[(2E)-3-(4-hydroxyphenyl)-1-oxo-2-propenyl]-β-D-glucopyranosyl]oxy]-4H-1-benzopyran-4-one; Tiliroside; 3-O-Kaempferol 6-O-(trans-p-coumaroyl)-β-D-glucopyranoside; 5,7-dihydroxy-2-(4-hydroxyphenyl)-3-[[6-O-[3-(4-hydroxyphenyl)-1-oxo-2-propenyl]-β-D-glucopyranosyl]oxy]-(E)-4H-1-benzopyran-4-one; Astragalin-6"-trans-p-coumarate; Kaempferol 3-O-(6"-O-p-coumaroyl)glucoside; Kaempferol 3-O-(6"-trans-p-coumaroyl)-β-D-glucopyranoside; Kaempferol 3-O-[6"-O-(E)-p-coumaroyl]-β-D-glucopyranoside; Kaempferol 3-O-[6"-O-(trans-p-coumaroyl)]-β-D-glucopyranoside; Kaempferol 3-O-β-D-(6-O-trans-p-coumaroyl)glucopyranoside; Kaempferol 3-O-β-D-(6"-E-p-coumaroyl)glucopyranoside; Kaempferol 3-O-β-D-(6"-O-p-coumaryl)glycoside; Kaempferol 3-β-D-(6-O-trans-p-coumaryl)glucopyranoside; Kaempferol-3-O-β-D-(6"-O-(E)-p-coumaroyl)glucopyranoside; Kaempferol-3-O-β-D-(6"-trans-p-coumaroyl) glucopyranoside; Potengriffioside A; RonaCareTiliroside; trans-Tiliroside

MyricitrinMyricetin 3-O- α -L-rhamnopyranoside

CAS-Number: 17912-87-7

Formula: C₂₁H₂₀O₁₂ Exact mass: 464.09548

Molecular mass: 464.38

Column: Zorbax LiChrosphere Kinetex

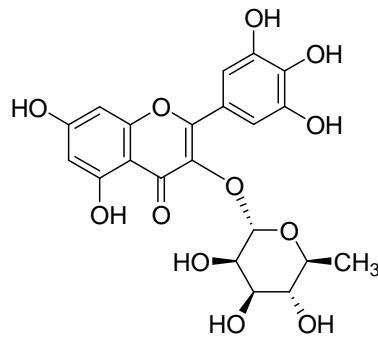
Abs.RetentionTime [min]: 16.4 13.52 6.65

Rel. RetentionTime (k'): 12.9 12.00 11.55

k' rel. to Rutin : 0.98 0.97 0.97

MS1: 463.2 MS2: 316.2 MS3: 271.2

UV/Vis: 255, 265(sh), 3

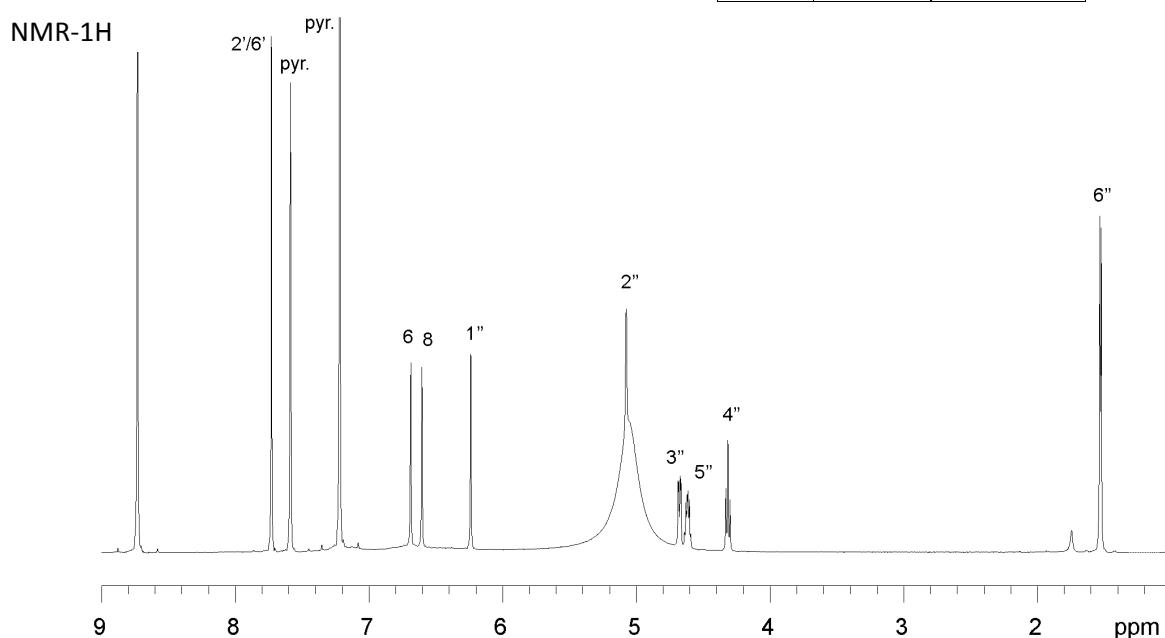


NMR - Resonance Assignments:

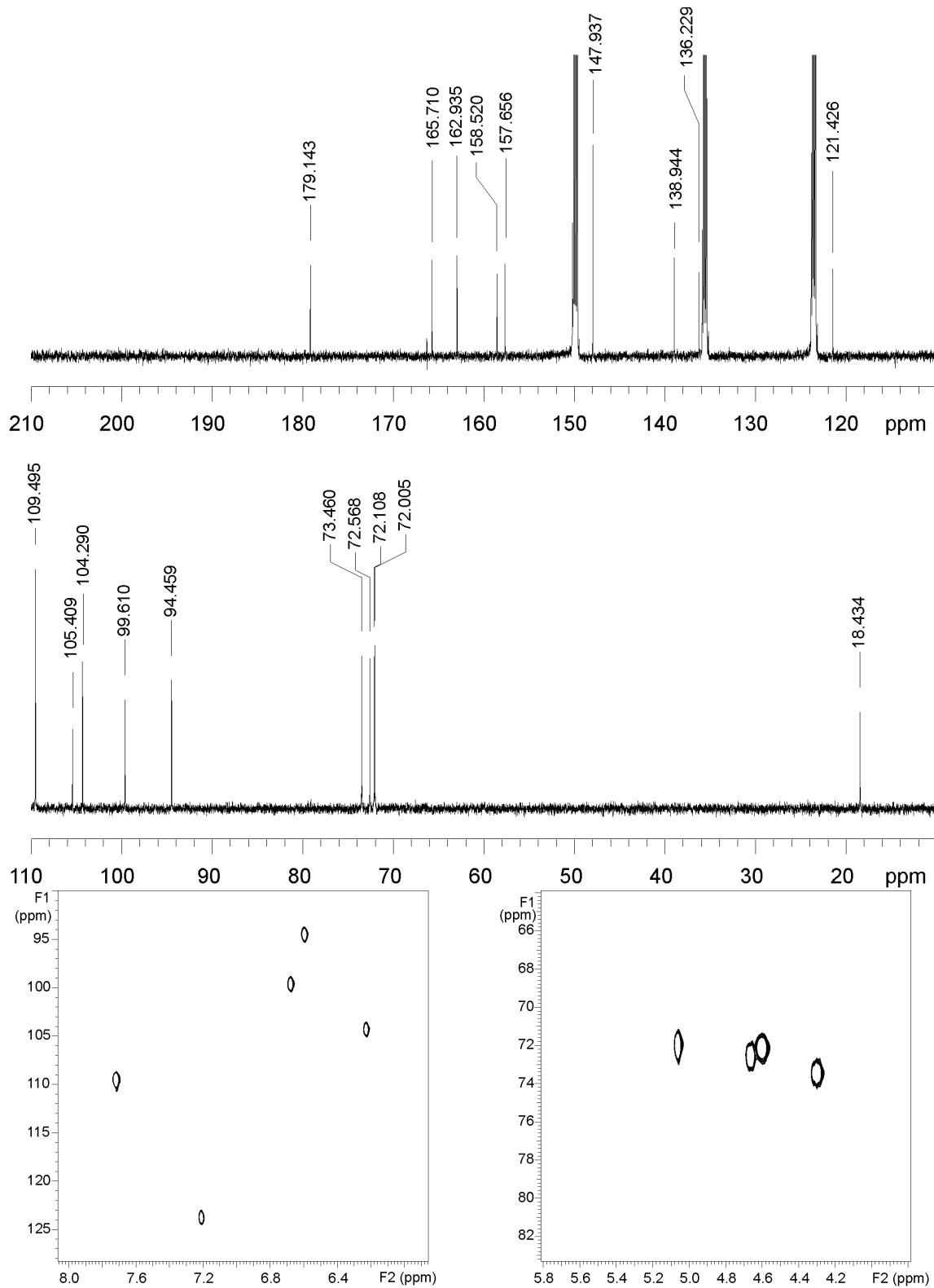
Flavone Core

Sugar

| | δ_{C} | δ_{H} | | δ_{C} | δ_{H} |
|----|---------------------|---------------------|----|---------------------|---------------------|
| 2 | 158.6s | | 1" | 104.3d | 6.24 |
| 3 | 136.2s | | 2" | 72d | 5.08 |
| 4 | 179.1s | | 3" | 72.6d | 4.68 |
| 4a | 105.4s | | 4" | 73.5d | 4.32 |
| 5 | 162.9s | | 5" | 72.1d | 4.62 |
| 6 | 99.6d | 6.69 | 6" | 18.4q | 1.53 |
| 7 | 165.7s | | | | |
| 8 | 94.5d | 6.61 | | | |
| 8a | 157.7s | | | | |
| 1' | 121.4s | | | | |
| 2' | 109.5d | 7.74 | | | |
| 3' | 147.9s | | | | |
| 4' | 138.9s | | | | |
| 5' | 147.9s | | | | |
| 6' | 109.5d | 7.74 | | | |



NMR-13C:



Names

3-[(6-deoxy- α -L-mannopyranosyl)oxy]-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-4H-1-benzopyran-4-one; Myricitrin; 3,5,7,3',4',5'-hexahydroxyflavone-3-rhamnoside; Myricetin 3-O-rhamnoside; Myricetin 3-O- α -L-rhamnopyranoside; Myricetin 3-O- α -L-rhamnoside; Myricetin 3-O- α -L-rhamnopyranoside; Myricetin 3-O- α -rhamnopyranoside; Myricetin 3-rhamnoside; Myricetin-3-O- α -rhamnoside; Myricitrine; Myricitroside; NSC 19803

Jacein

5,7,4'-Trihydroxy-3,6,3'-trimethoxy-flavone-7-O- β -D-glucoside

CAS-Number: 35305-11-4

Formula: C₂₄H₂₆O₁₃ Exact mass: 522.13734

Molecular mass: 522.46

Column: Zorbax LiChrosphere Kinetex

Abs.RetentionTime [min]: 20.24 17.07 8.63

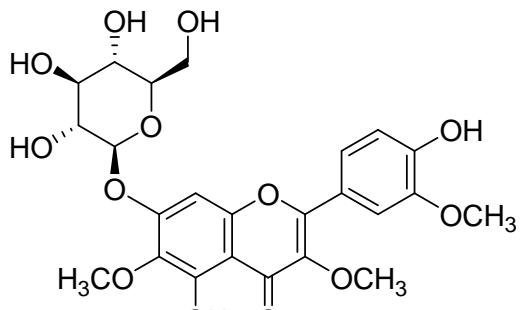
Rel. RetentionTime (k'): 16.15 15.41 15.28

k' rel. to Rutin : 1.22 1.24 1.28

MS1: 521.3 MS2: 506.1 MS3: 343.1

UV/Vis: 255, 265(sh), 3

Jacein



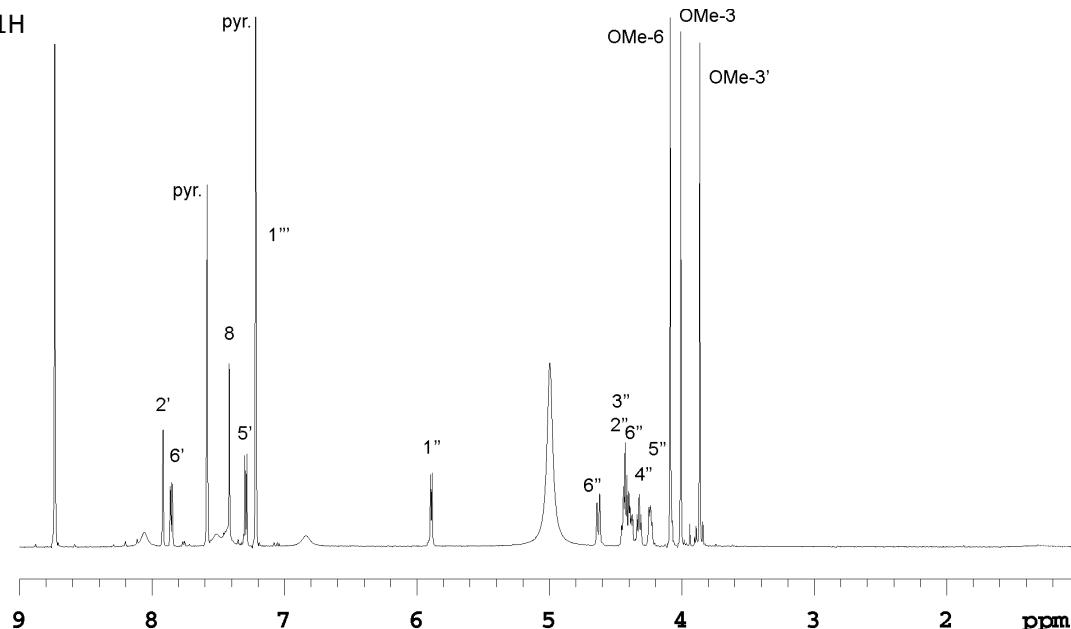
NMR - Resonance Assignments:

Flavone Core

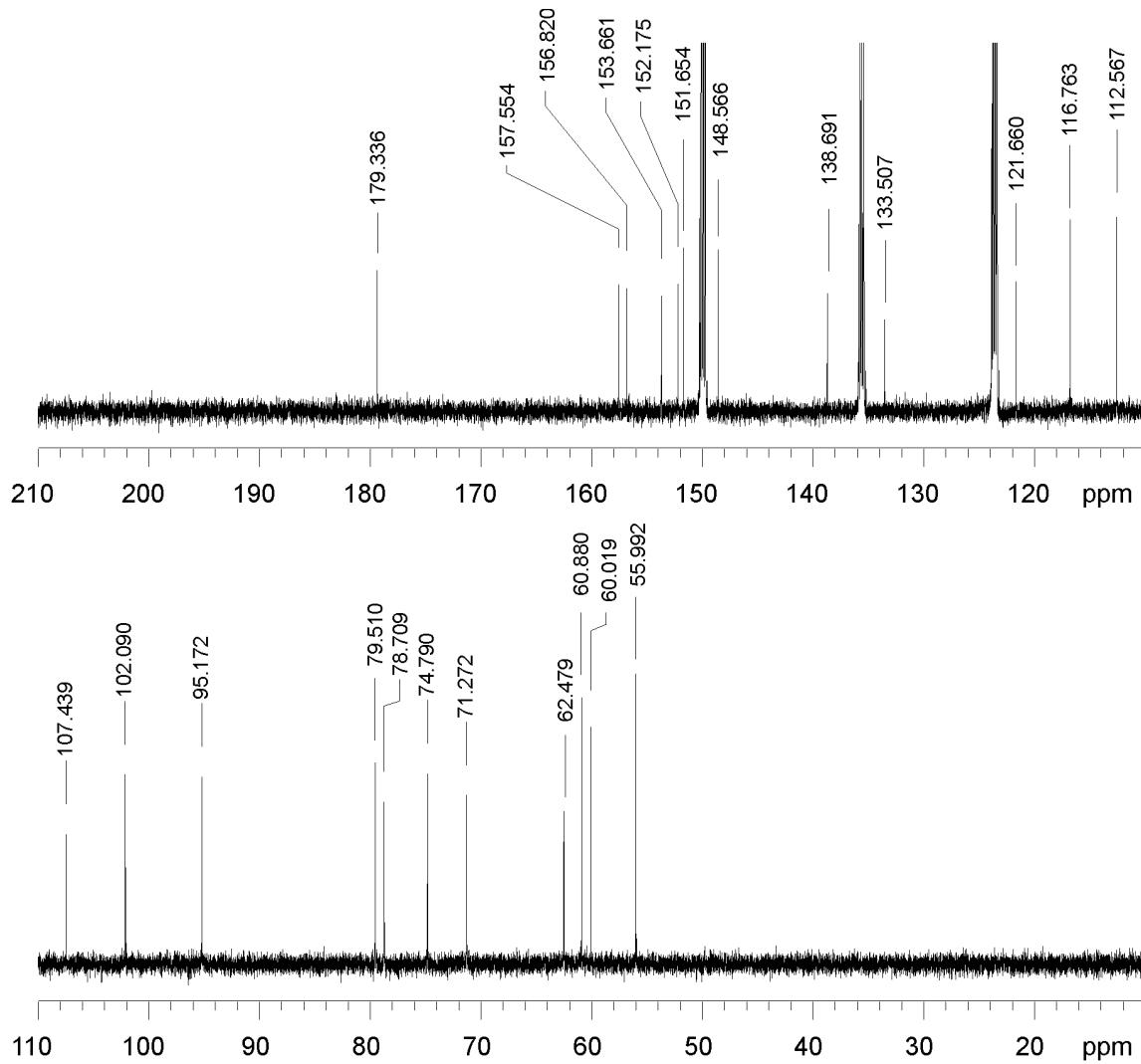
Sugar

| | δ_C | δ_H | | δ_C | δ_H |
|--------|------------|------------|-----|------------|------------|
| 2 | 156.8s | | 1'' | 102.1d | 5.89 |
| 3 | 138.7s | | 2'' | 74.8d | 4.43 |
| 4 | 179.3s | | 3'' | 78.7d | 4.41 |
| 4a | 107.4s | | 4'' | 71.3d | 4.31 |
| 5 | 153.7s | | 5'' | 79.5d | 4.23 |
| 6 | 135.6s | | 6'' | 62.5t | 4.62/4.37 |
| 7 | 157.6s | | | | |
| 8 | 95.2d | 7.41 | | | |
| 8a | 152.2s | | | | |
| 1' | 121.7s | | | | |
| 2' | 112.6d | 7.91 | | | |
| 3' | 148.6s | | | | |
| 4' | 151.7s | | | | |
| 5' | 116.8d | 7.29 | | | |
| 6' | 123.4d | 7.85 | | | |
| OMe-3 | 60q | 4 | | | |
| OMe-6 | 60.9q | 4.08 | | | |
| OMe-3' | 55.9q | 3.86 | | | |

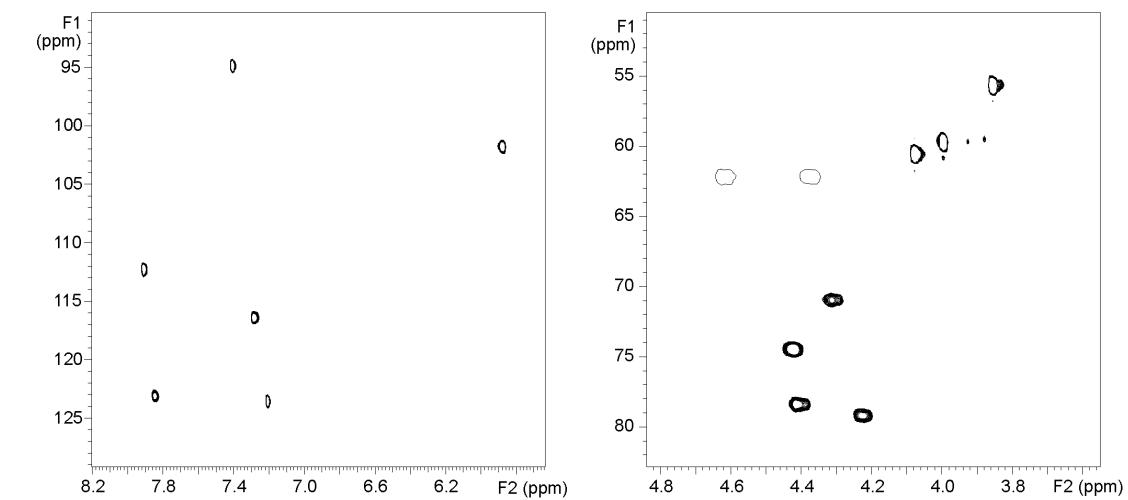
NMR-1H



NMR-13C:



NMR-HSQC:



Names

7-(β -D-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxy-3-methoxyphenyl)-3,6-dimethoxy-4H-1-benzopyran-4-one; Flavone 5,7,4'-trihydroxy-3,6,3'-trimethoxy-7- β -D-glucoside; 5,7,4'-trihydroxy-3,3',6-trimethoxy-flavone-7-O- β -D-glucoside; 5,7,4'-Trihydroxy-3,6,3'-trimethoxy-flavone-7-O- β -D-glucoside; Jacein; Jaceine

Quercetin

3,5,7,3',4'-Pentahydroxyflavone

CAS-Number: 117-39-5

Formula: C₁₅H₁₀O₇ Exact mass: 302.04265

Molecular mass: 302.24

Column: Zorbax LiChrosphere Kinetex

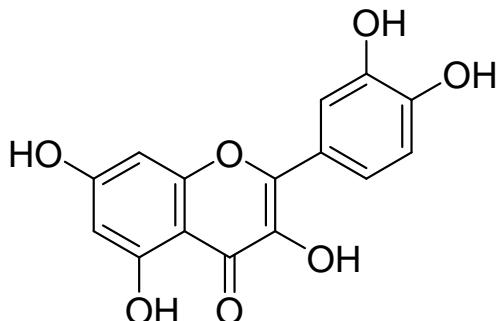
Abs.RetentionTime [min]: 21.25 18.56 9.16

Rel. RetentionTime (k') : 17.01 16.85 16.28

k' rel. to Rutin : 1.29 1.36 1.36

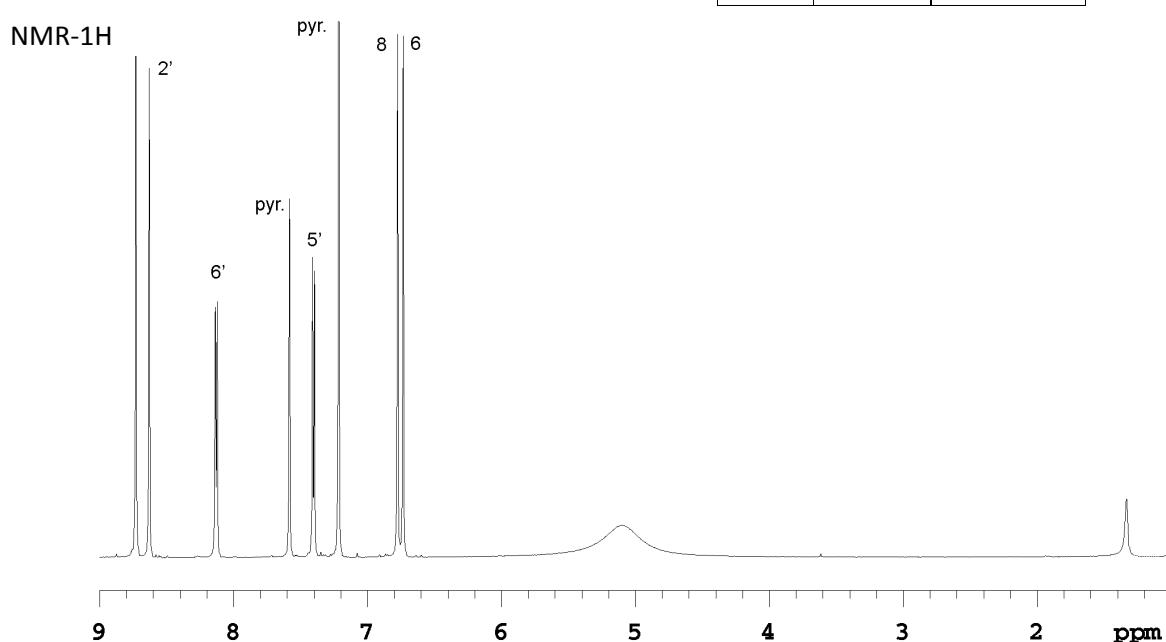
MS1: 301 2 MS2: 271 3 MS3: 227

UV/Vis: 255, 265(sh), 3

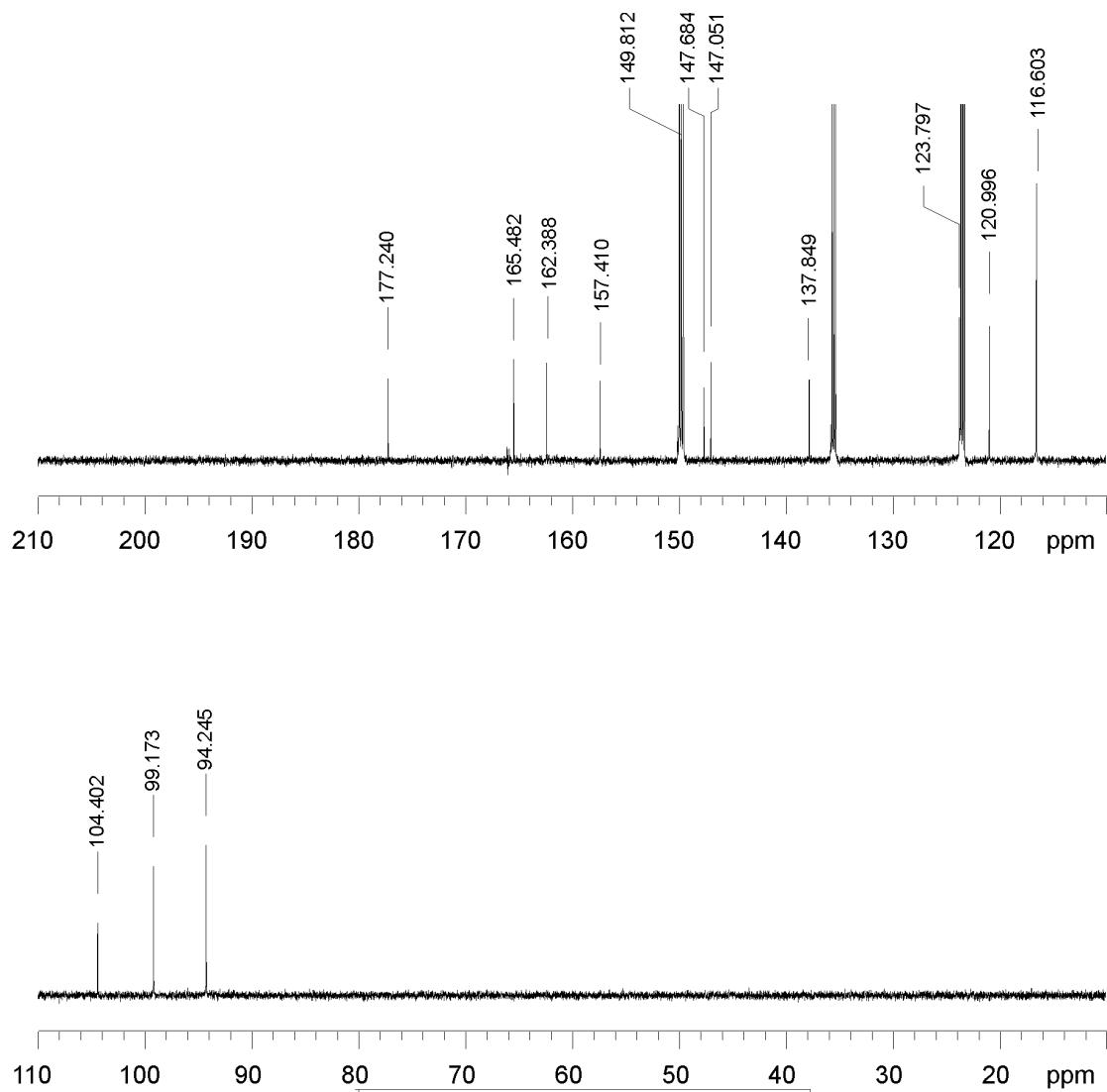


NMR - Resonance Assignments:

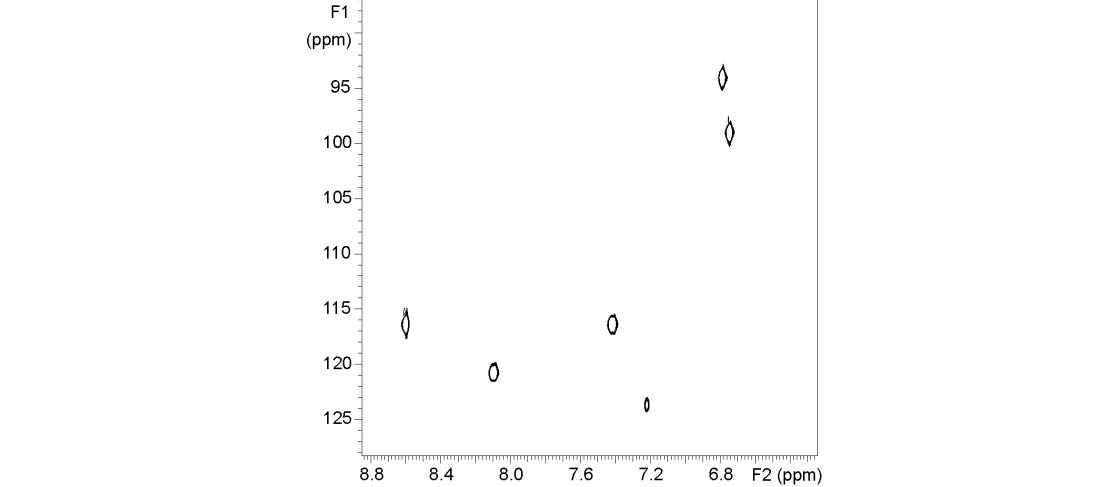
| | δ_C | δ_H |
|----|------------|------------|
| 2 | 147.7s | |
| 3 | 137.9s | |
| 4 | 177.3s | |
| 4a | 104.4s | |
| 5 | 162.4s | |
| 6 | 99.2d | 6.74 |
| 7 | 165.5s | |
| 8 | 94.3d | 6.78 |
| 8a | 157.4s | |
| 1' | 128.8s | |
| 2' | 116.6d | 8.63 |
| 3' | 147.1s | |
| 4' | 149.6s | |
| 5' | 116.6d | 7.41 |
| 6' | 121d | 8.13 |



NMR-13C:



NMR-HSQC:



Names

2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-4H-1-benzopyran-4-one; 3,5,7,3',4'-pentahydroxy-flavone; 3,5,7,4',5'-pentahydroxy-flavone; 2-(3,4-Dihydroxyphenyl)-3,5,7-trihydroxy-4H-benzopyran-4-one; 3,5,7,3',4'-pentahydroxyflavone; 3,5,7,3',4'-pentahydroxyflavone; 3'-hydroxykaempferol; C.I. 75670; Corvitin; Cyanidelonon 1522; Korvitin; Meletin; NSC 57655; NSC 9219; Quercetin; Quercetine; Quercetol; Quertin; Quertine; Sophoretin; Xanthaurine

Myricetin

3,5,7,3',4',5'-Hexahydroxyflavone

CAS-Number: 529-44-2

Formula: C₁₅H₁₀O₈ Exact mass: 318.03757

Molecular mass: 318.04

Column: Zorbax LiChrosphere Kinetex

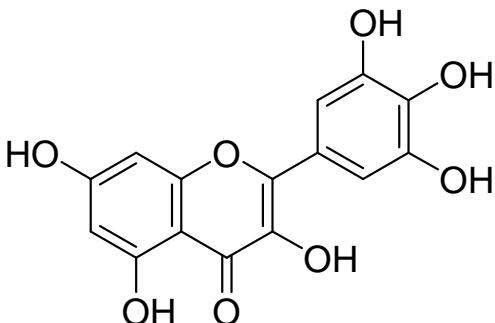
Abs.RetentionTime [min]: 18.64 15.87 7.74

Rel. RetentionTime (k') : 14.8 14.26 13.60

k' rel. to Rutin : 1.12 1.15 1.14

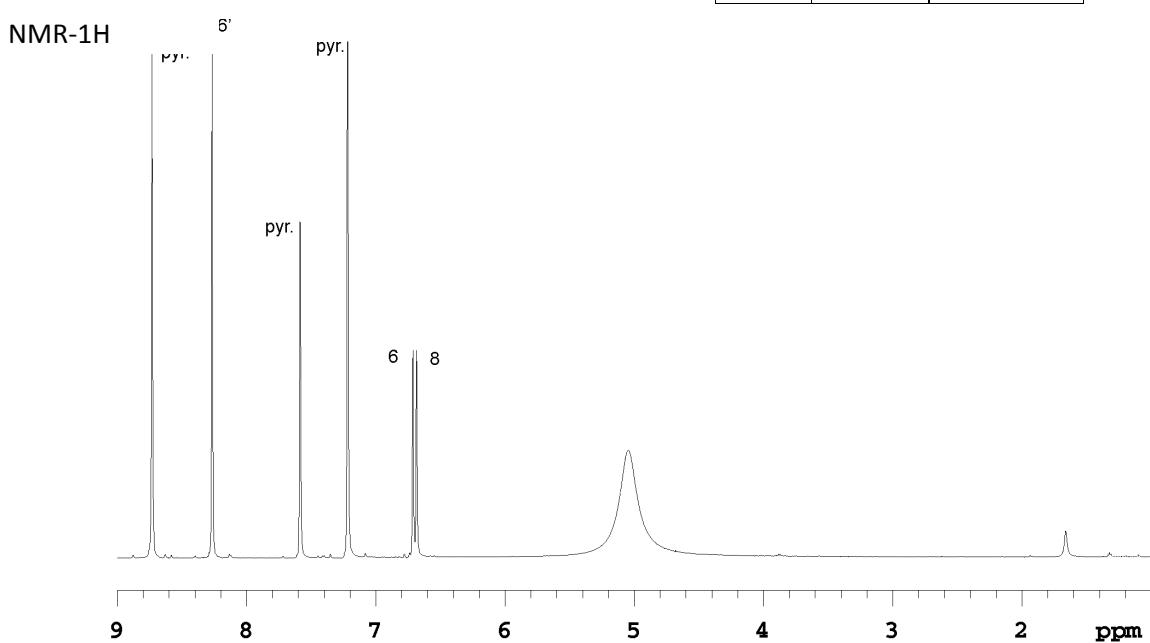
MS1: 317.2 MS2: 179.1 MS3: 151.1

UV/Vis: 250, 265(sh), 3

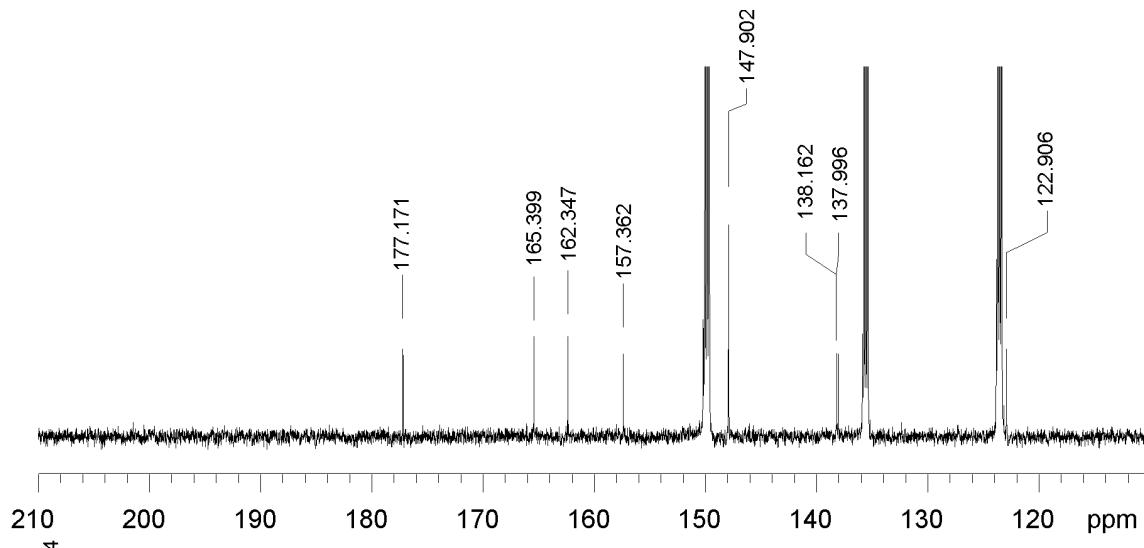


NMR - Resonance Assignments:

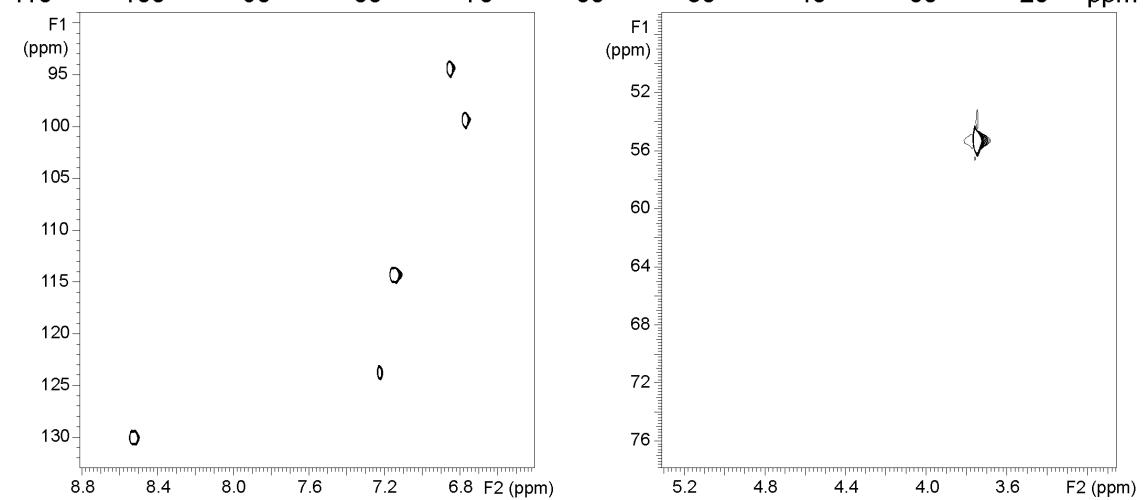
| | δ_C | δ_H |
|----|------------|------------|
| 2 | 147.9s | |
| 3 | 138s | |
| 4 | 177.2s | |
| 4a | 104.4s | |
| 5 | 162.3s | |
| 6 | 99.1d | 6.71 |
| 7 | 165.4s | |
| 8 | 94.2d | 6.68 |
| 8a | 157.4s | |
| 1' | 122.9s | |
| 2' | 108.7d | 8.26 |
| 3' | 147.9s | |
| 4' | 138.2s | |
| 5' | 147.9s | |
| 6' | 108.7d | 8.26 |



NMR-13C:



NMR-HSQC:



Names

3,5,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)-4H-1-benzopyran-4-one; 3,5,7,3',4',5'-hexahydroxy-flavone; 3,5,7,3',4',5'-hexahydroxyflavone; 3,5,7,3',4',5'-Hexahydroxyflavone; Cannabiscetin; Myricetin; Myricetol; NSC 407290

Chrysin

5,7-Dihydroxyflavone

CAS-Number: 480-40-0

Formula: C₁₅H₁₀O₄ Exact mass: 254.05791

Molecular mass: 254.06

Column: Zorbax LiChrosphere Kinetex

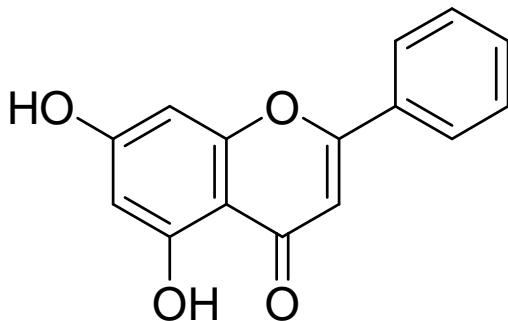
Abs.RetentionTime [min]: 27.81 25.23 12.52

Rel. RetentionTime (k') : 22.57 23.26 22.62

k' rel. to Rutin : 1.71 1.87 1.89

MS1: 253.3 MS2: 209.2 MS3: 181.1

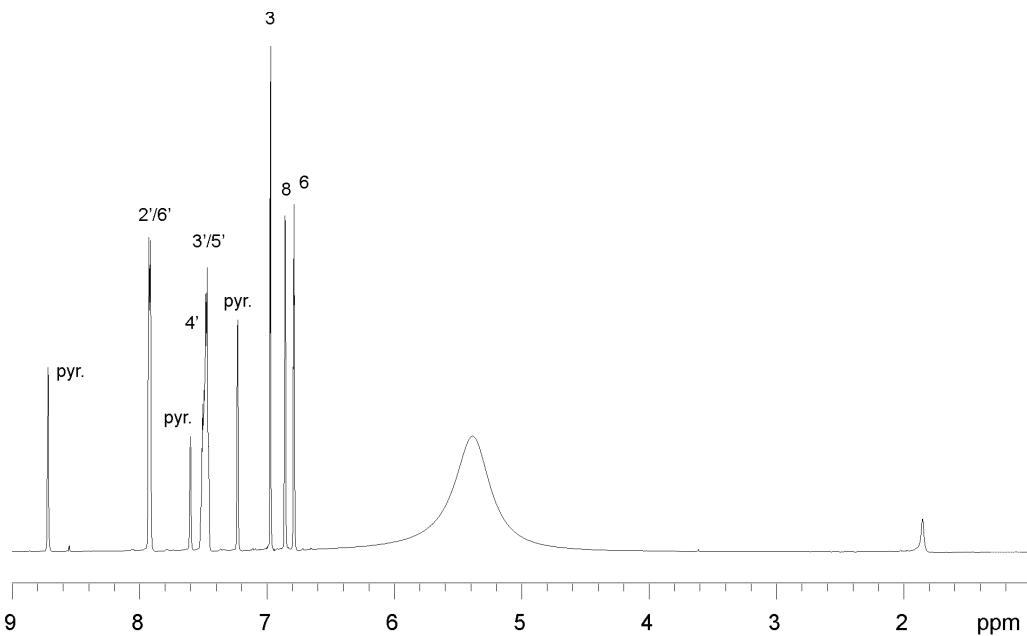
UV/Vis: 265, 315

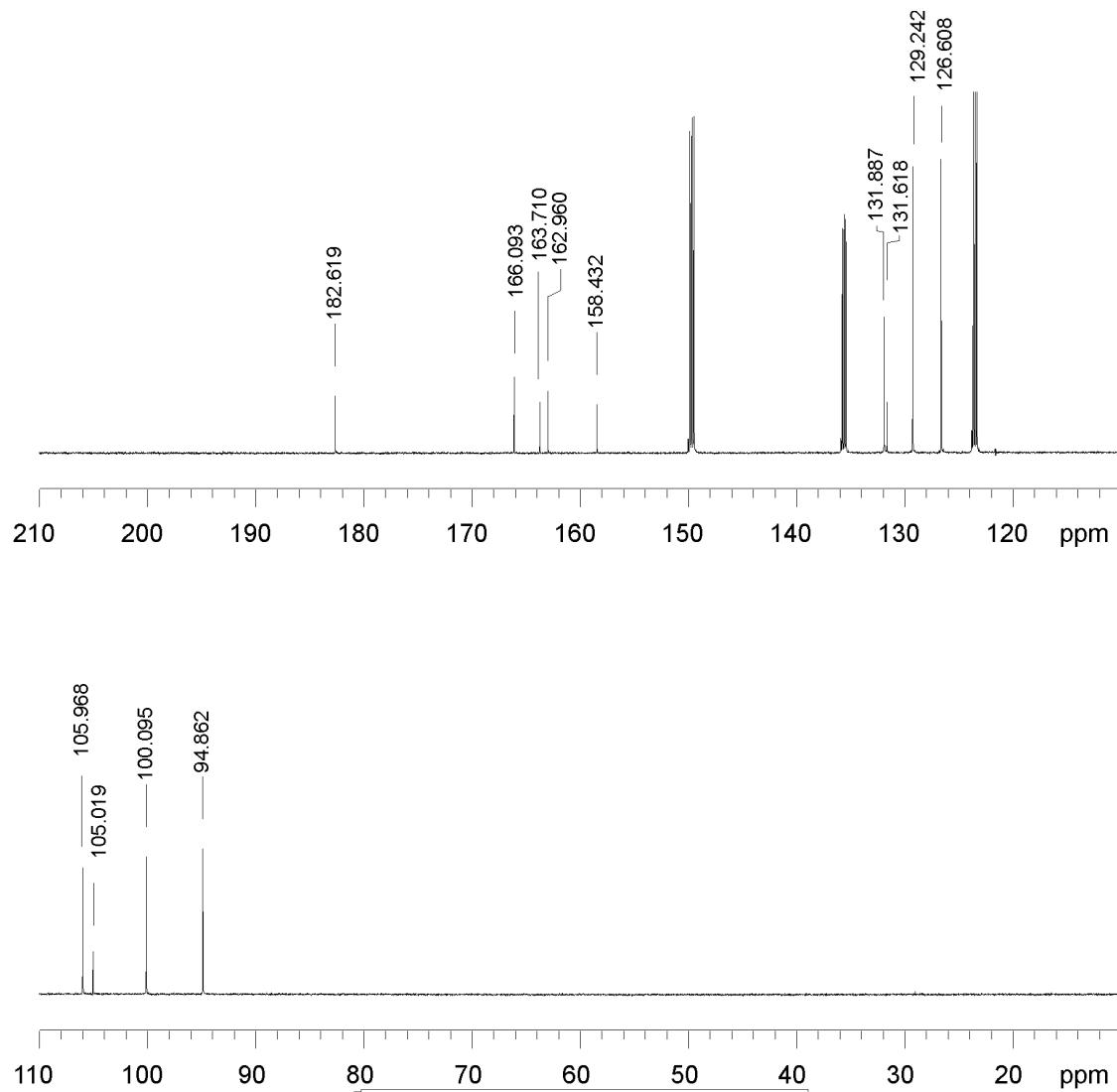


NMR - Resonance Assignments:

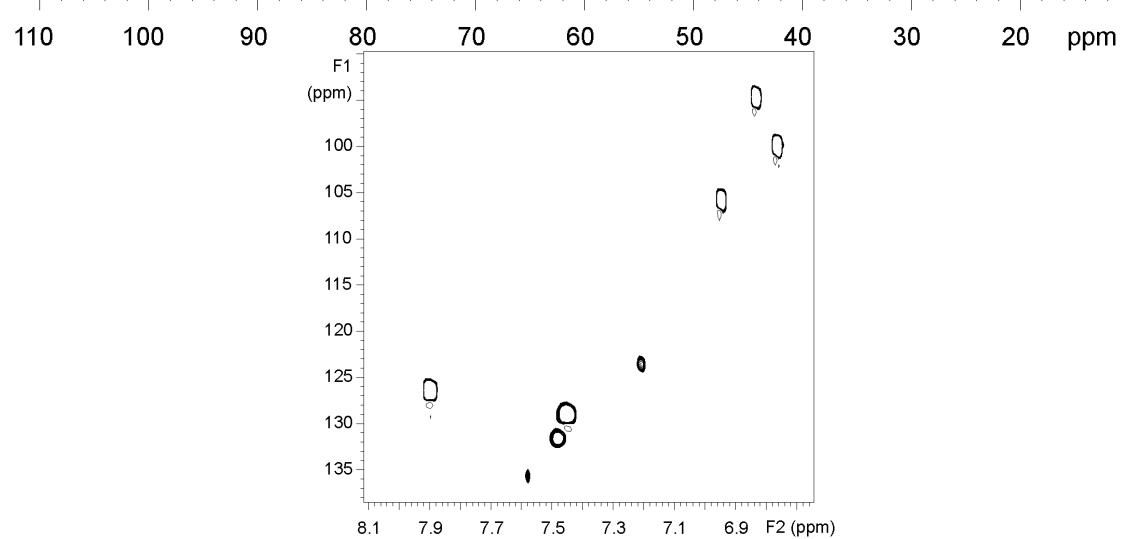
| | δ_C | δ_H |
|----|------------|------------|
| 2 | 163.7s | |
| 3 | 106d | 6.98 |
| 4 | 182.6d | |
| 4a | 105s | |
| 5 | 163.9s | |
| 6 | 100.1d | 6.78 |
| 7 | 166.1s | |
| 8 | 94.9d | 6.86 |
| 8a | 158.4s | |
| 1' | 131.6s | |
| 2' | 126.6d | 7.93 |
| 3' | 129.3d | 7.48 |
| 4' | 131.9d | 7.5 |
| 5' | 129.3d | 7.48 |
| 6' | 126.6d | 7.93 |

NMR-1H



NMR-¹³C:

NMR-HSQC:



Names

5,7-dihydroxy-2-phenyl-4H-1-benzopyran-4-one; Chrysin; 5,7-dihydroxy-flavone; 5,7-Dihydroxy-2-phenylchromen-4-one; 5,7-Dihydroxyflavone; Crysin; NSC 407436

Avicularin

Quercetin-3-O- α -L-arabinofuranoside

CAS-Number: 572-30-5

Formula: C₂₀H₁₈O₁₁ Exact mass: 434.08491

Molecular mass: 434.08

Column: Zorbax LiChrosphere Kinetex

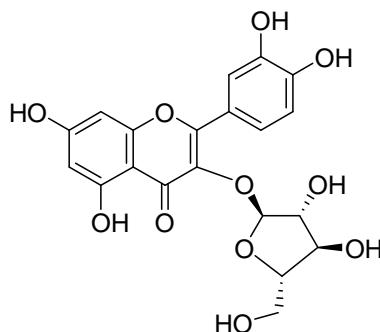
Abs.RetentionTime [min]: 18 15.25 7.54

Rel. RetentionTime (k'): 14.25 13.66 13.23

k' rel. to Rutin : 1.08 1.10 1.11

MS1: 433.4 MS2: 301.2 MS3: 178.9

UV/Vis: 255, 265(sh), 3



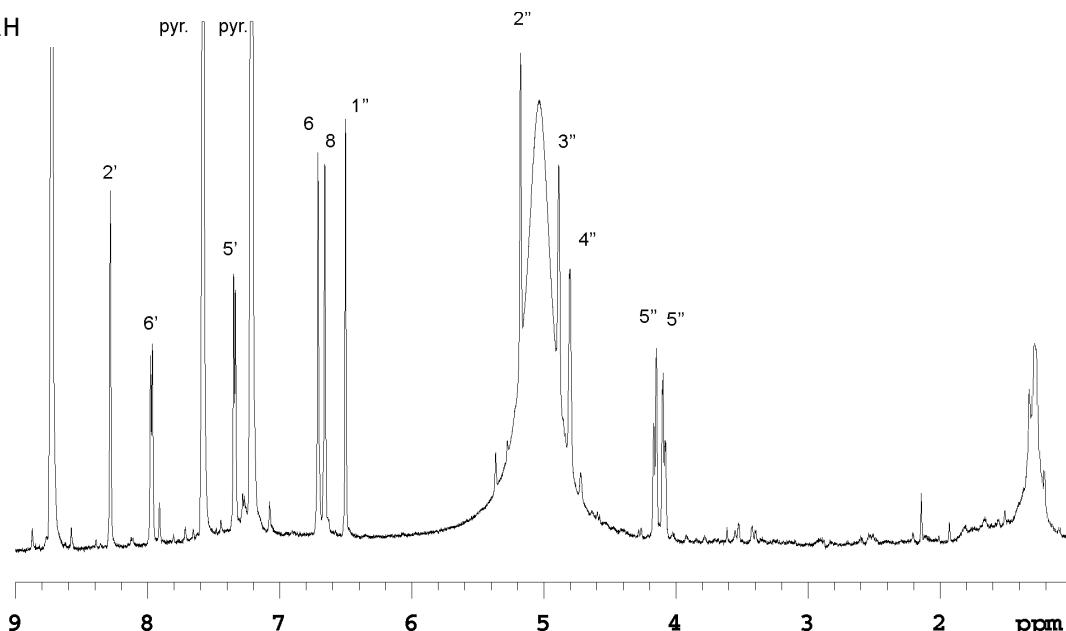
NMR - Resonance Assignments:

Flavone Core

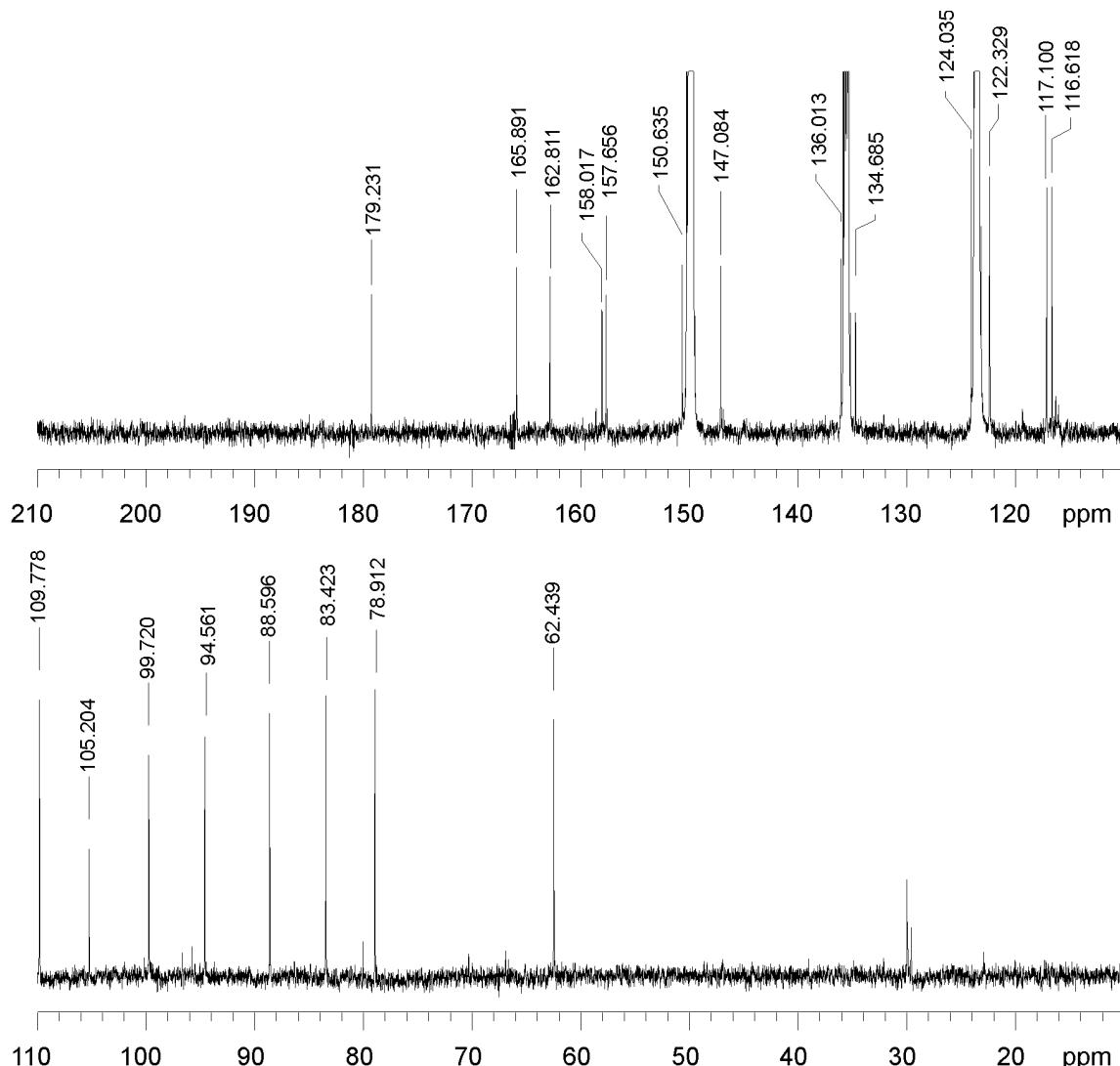
Sugar

| | δ_C | δ_H | | δ_C | δ_H |
|----|------------|------------|----|------------|------------|
| 2 | 158s | | 1" | 109.8d | 6.5 |
| 3 | 134.7s | | 2" | 83.4d | 5.17 |
| 4 | 179.2s | | 3" | 78.9d | 4.88 |
| 4a | 105.2s | | 4" | 88.6d | 4.8 |
| 5 | 162.8s | | 5" | 62.4t | 4.15/4.1 |
| 6 | 99.7d | 6.7 | | | |
| 7 | 165.9s | | | | |
| 8 | 94.6d | 6.65 | | | |
| 8a | 157.7s | | | | |
| 1' | 122.4s | | | | |
| 2' | 117.1d | 8.28 | | | |
| 3' | 147.1s | | | | |
| 4' | 150.6s | | | | |
| 5' | 116.6d | 7.34 | | | |
| 6' | 123.3d | 7.97 | | | |

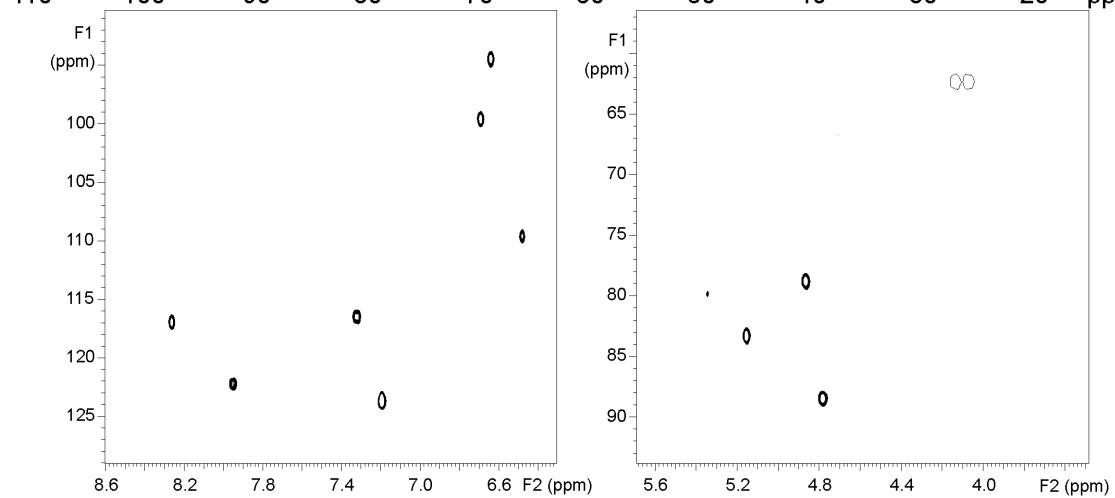
NMR-1H



NMR-13C:



NMR-HSQC:



Names

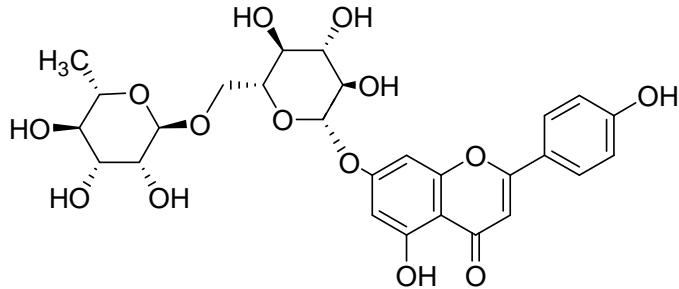
3-(α -L-arabinofuranosyloxy)-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4H-1-benzopyran-4-one; Avicularin; Avicularine; Avicularoside; Quercetin 3-O- α -L-arabinofuranoside; Quercetin 3- α -L-arabinofuranoside

IsorhoifolinApigenin-7-O- β -D-rutinoside

CAS-Number: 552-57-8

Formula: C₂₇H₃₀O₁₄ Exact mass: 578.16356

Molecular mass: 578.53



Column: Zorbax LiChrosphere Kinetex

Abs.RetentionTime [min]: 17.84 15.04 7.51

Rel. RetentionTime (k'): 14.12 13.46 13.17

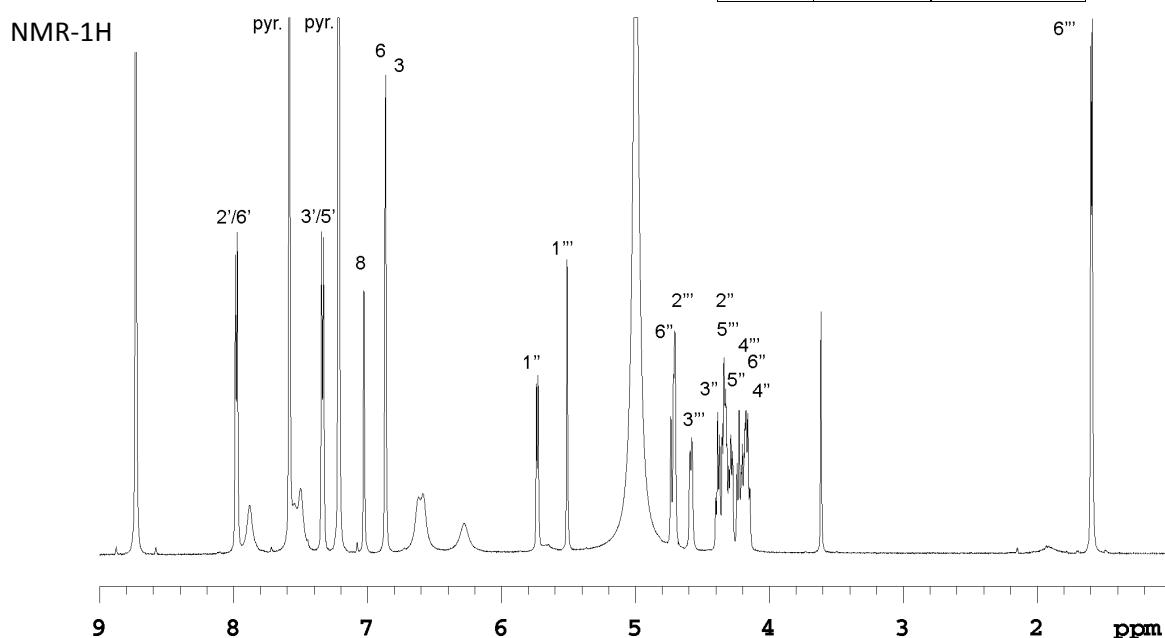
k' rel. to Rutin : 1.07 1.08 1.10

MS1: 577.3 MS2: 269.3 MS3: 225

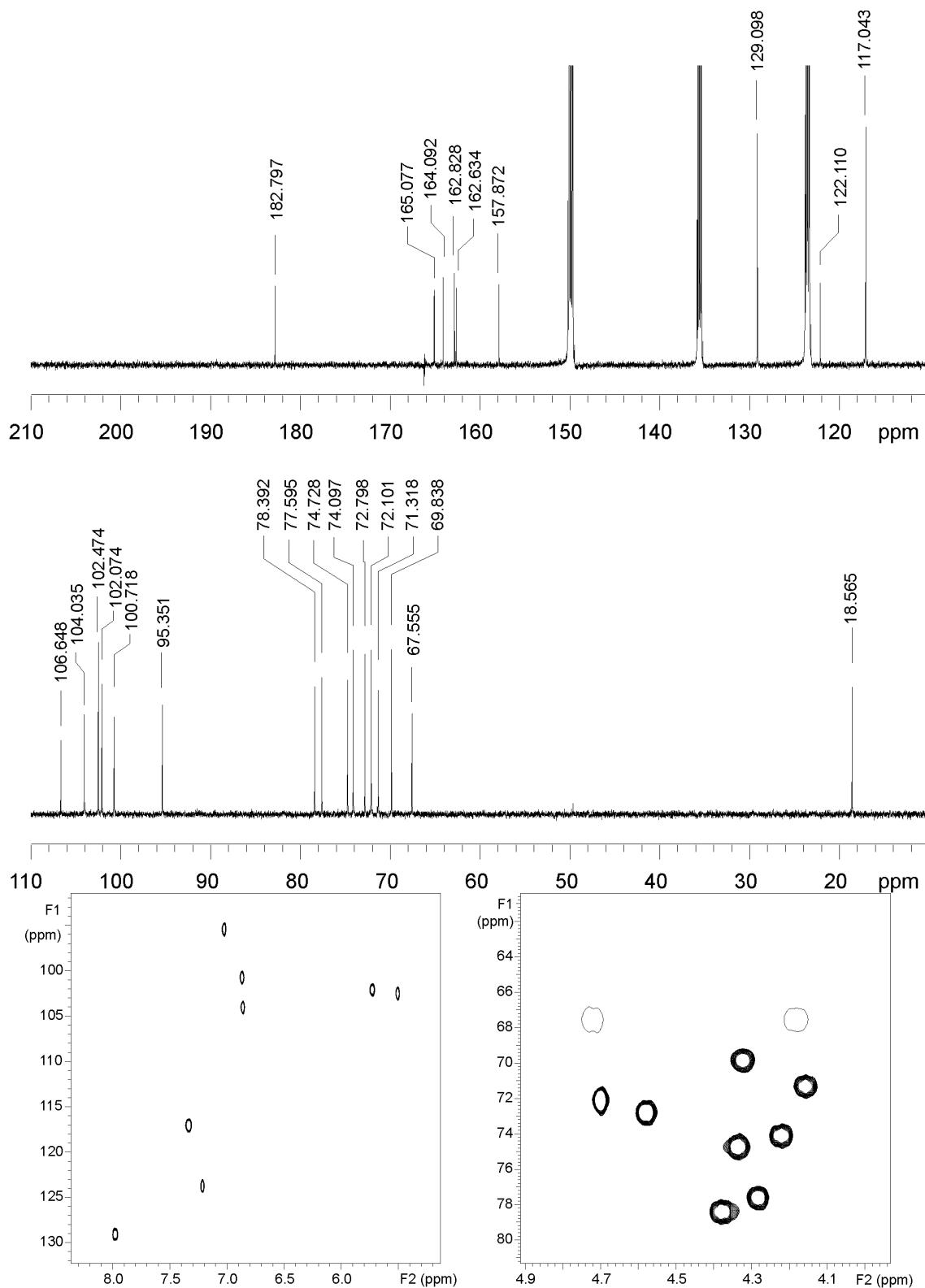
UV/Vis: 265, 340

NMR - Resonance Assignments:
Flavone Core Sugar

| | δ_C | δ_H | | δ_C | δ_H |
|----|------------|------------|------|------------|------------|
| 2 | 165.1s | | 1'' | 102.1d | 5.73 |
| 3 | 104d | 6.86 | 2'' | 74.7d | 4.33 |
| 4 | 182.8s | | 3'' | 78.4d | 4.38 |
| 4a | 106.6s | | 4'' | 71.3d | 4.16 |
| 5 | 162.6s | | 5'' | 77.6d | 4.28 |
| 6 | 100.7d | 6.87 | 6'' | 67.6t | 4.72/4.18 |
| 7 | 164.1s | | 1''' | 102.5d | 5.51 |
| 8 | 95.4d | 7.03 | 2''' | 72.1d | 4.7 |
| 8a | 157.9s | | 3''' | 72.8d | 4.58 |
| 1' | 122.1s | | 4''' | 74.1d | 4.22 |
| 2' | 129.1d | 7.98 | 5''' | 69.8d | 4.32 |
| 3' | 117d | 7.33 | 6''' | 18.6q | 1.59 |
| 4' | 162.8s | | | | |
| 5' | 117d | 7.33 | | | |
| 6' | 129.1d | 7.98 | | | |



NMR-13C:



Names

7-[[6-O-(6-deoxy- α -L-mannopyranosyl)- β -D-glucopyranosyl]oxy]-5-hydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one; 5,7,4'-trihydroxy-7- β -rutinoside-flavone; Isorhoifolin; 5,7,4'-trihydroxyflavone 7-O-rutinoside; Apigenin 7-O-rutinoside; Apigenin 7-O- α -L-rhamnopyranosyl-(1 \rightarrow 6)- β -D-glucopyranoside; Apigenin 7-O- α -L-rhamnosyl-(1 \rightarrow 6)- β -D-glucopyranoside; Apigenin 7-O- β -D-glucopyranosyl-(6 \rightarrow 1)- α -L-rhamnopyranoside; Apigenin 7-rutinoside; Apigenin 7- β -rutinoside; Apigenin-7-O-gluco(6'-1'') rhamnoside; Apigenin-7-O- β -D-rutinoside

7-Methylpinocembrin

5-Hydroxy-7-methoxyflavanone

CAS-Number: 480-37-5

Formula: C₁₆H₁₄O₄ Exact mass: 270.08921

Molecular mass: 270.09

Column: Zorbax LiChrosphere Kinetex

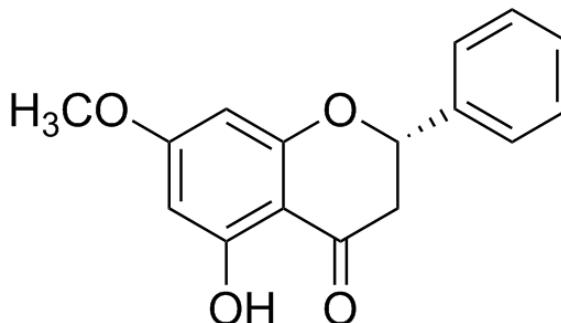
Abs.RetentionTime [min]: 31.97 28.72 14.43

Rel. RetentionTime (k') : 26.09 26.62 26.23

k' rel. to Butin : 1.98 2.14 2.20

MS1: 269.3 MS2: 254.1 MS3: 226.1

UV/Vis: 290–330(sh)



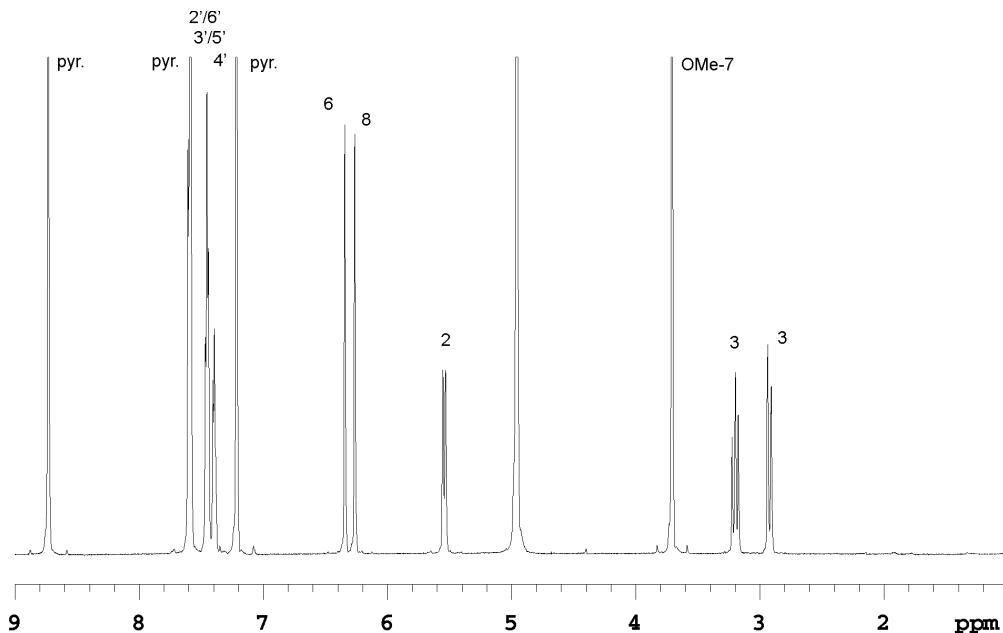
NMR - Resonance Assignments:

Flavone Core

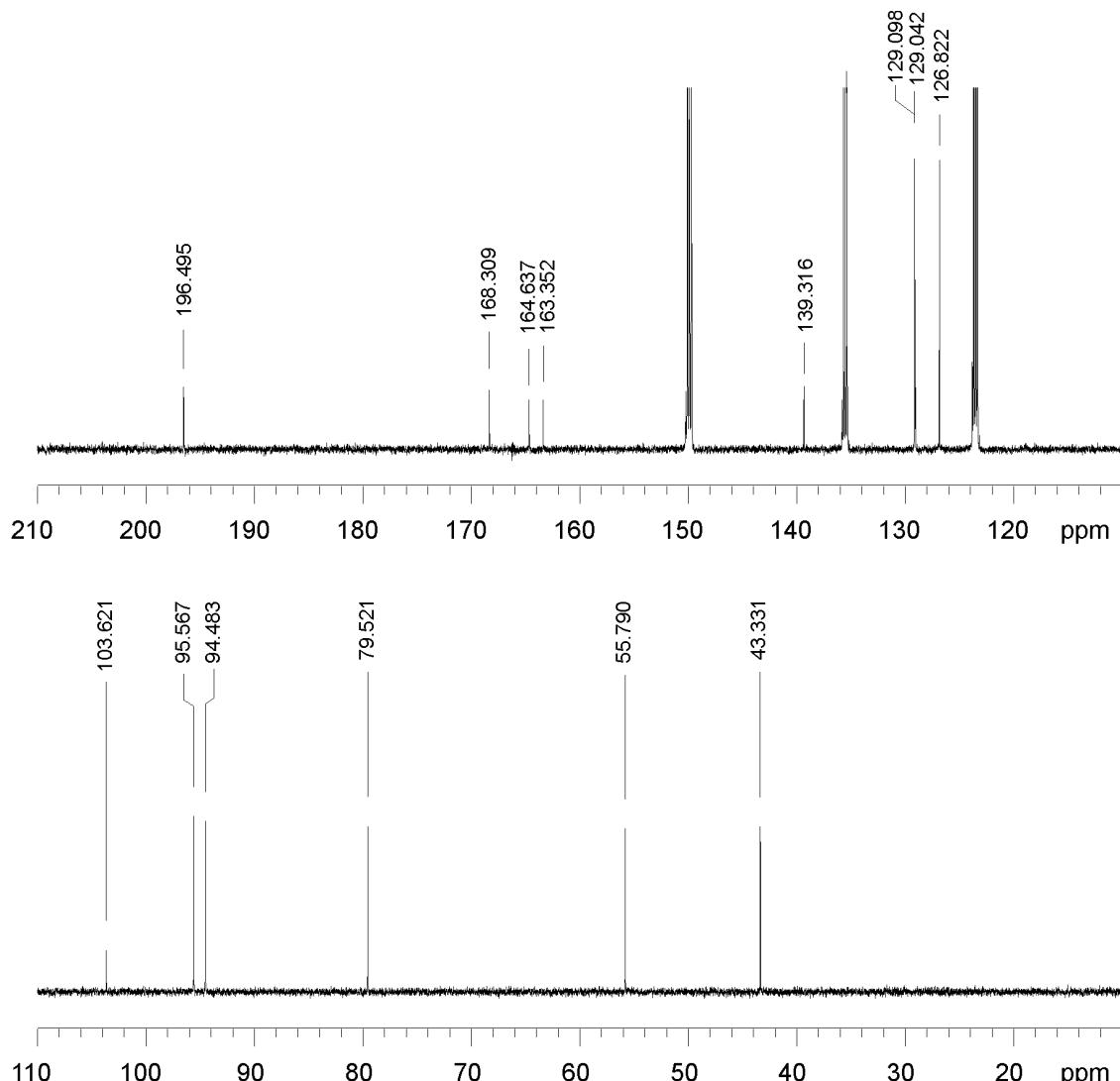
Sugar

| | δ_C | δ_H |
|-------|------------|------------|
| 2 | 79.5d | 5.54 |
| 3 | 43.3t | 3.19/2.92 |
| 4 | 196.5s | |
| 4a | 103.6s | |
| 5 | 164.6s | |
| 6 | 95.6d | 6.34 |
| 7 | 168.3s | |
| 8 | 94.5d | 6.26 |
| 8a | 163.4s | |
| 1' | 139.3s | |
| 2' | 126.8d | 7.59 |
| 3' | 129.1d | 7.45 |
| 4' | 129d | 7.38 |
| 5' | 129.1d | 7.45 |
| 6' | 126.8d | 7.59 |
| OMe-7 | 55.8q | 3.7 |

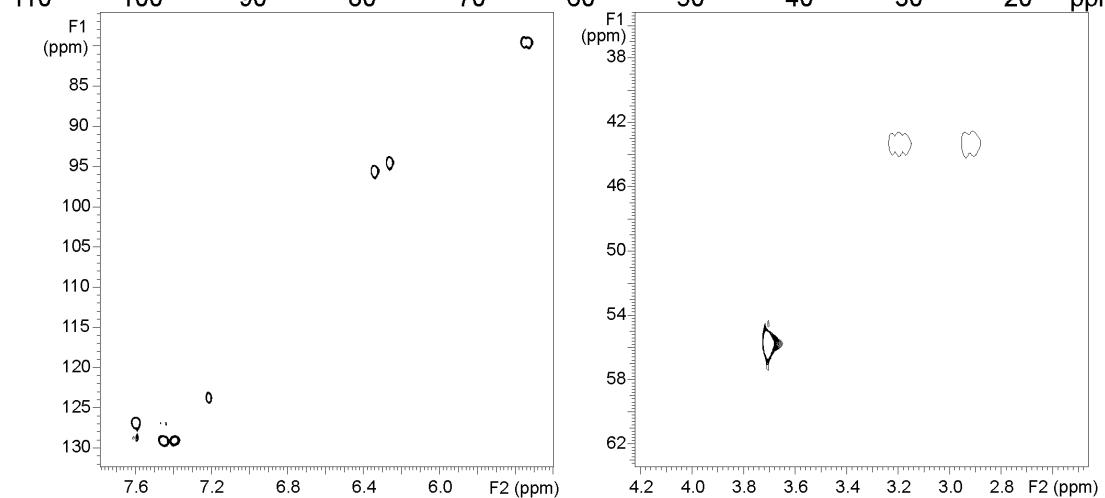
NMR-1H



NMR-13C:



NMR-HSQC:



Names

2,3-dihydro-5-hydroxy-7-methoxy-2-phenyl-(2S)-4H-1-benzopyran-4-one; 2,3-dihydro-5-hydroxy-7-methoxy-2-phenyl-(S)-4H-1-benzopyran-4-one; 5-hydroxy-7-methoxy-flavanone; Pinostrobin; (-)-2S-Pinocembrin; (-)-Pinostrobin; (2S)-Pinostrobin; 5-hydroxy-7-methoxyflavanone; 7-methylpinocembrin; Dihydrotectochrysin; Pinocembrin 7-methyl ether; Pinostrombin

DidyminIsosakuranetin-7-O- β -D-rutinosid

CAS-Number: 14259-47-3

Formula: C₂₈H₃₄O₁₄ Exact mass: 594.19486

Molecular mass: 594.56

Column: Zorbax LiChrosphere Kinetex

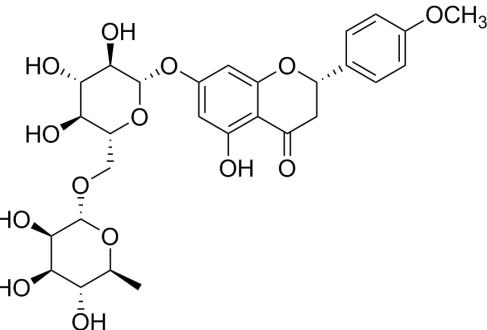
Abs.RetentionTime [min]: 21.33 18.24 9.08

Rel. RetentionTime (k'): 17.08 16.54 16.13

k' rel. to Rutin : 1.31 1.33 1.35

MS1: 593.2 MS2: 285 MS3: 270.1

UV/Vis: 280, 330(sh)

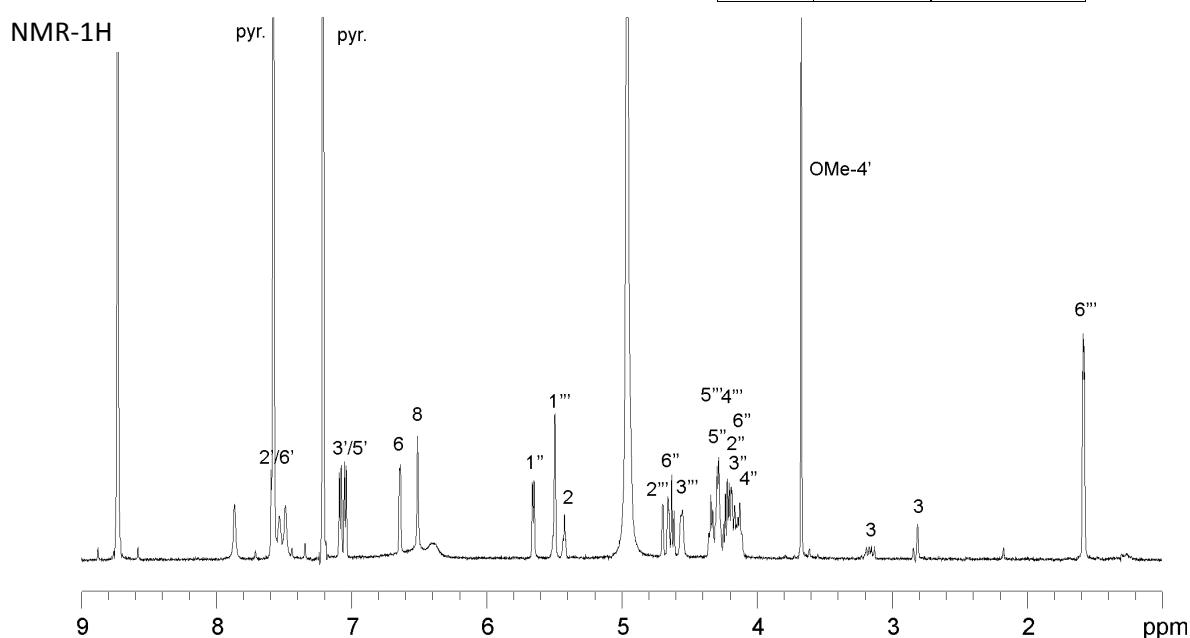


NMR - Resonance Assignments:

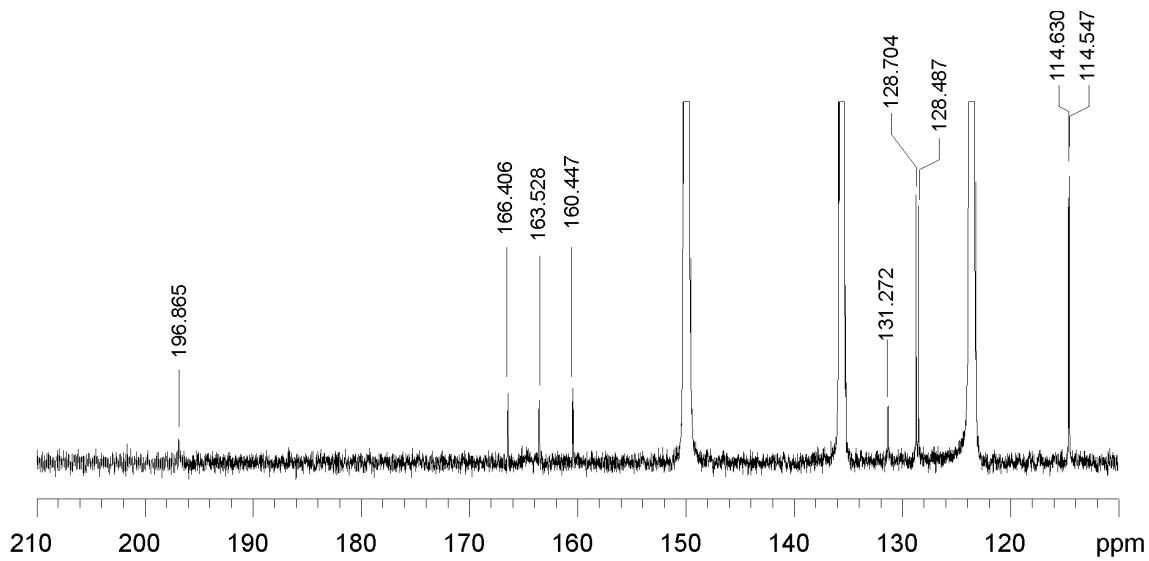
Flavone Core

Sugar

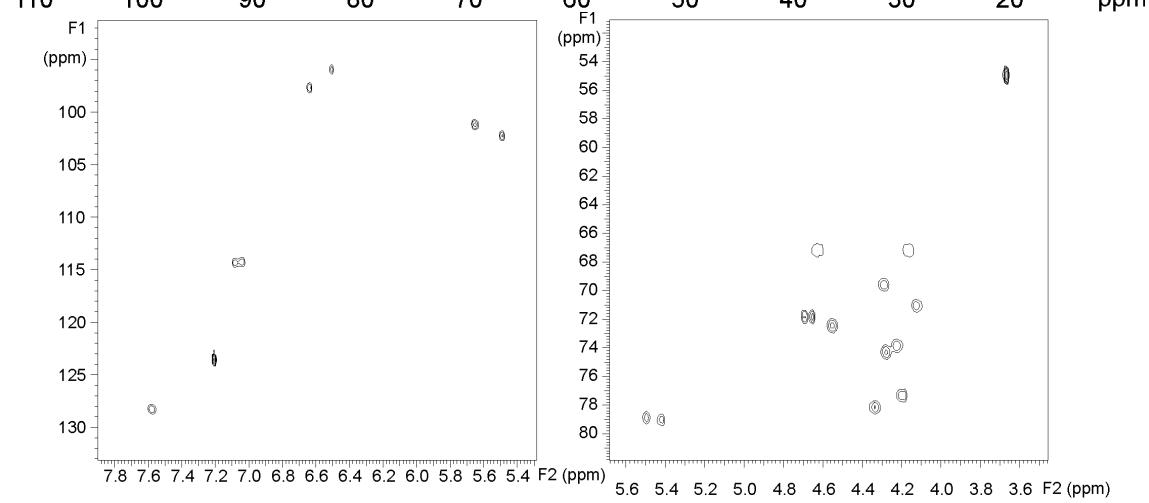
| | δ_C | δ_H | | δ_C | δ_H |
|----|------------|------------|------|------------|------------|
| 2 | 79.3s | 5.5 | 1" | 105d | 5.65 |
| 3 | 43.2t | 3.17/2.82 | 2" | 74.6d | 4.28 |
| 4 | 196.9s | | 3" | 77.6d | 4.2 |
| 4a | 104.5s | | 4" | 71.4d | 4.13 |
| 5 | 164.8s | | 5" | 78.5d | 4.33 |
| 6 | 98d | 6.64 | 6" | 67.5t | 4.63/4.17 |
| 7 | 166.4s | | 1''' | 102.5d | 5.49 |
| 8 | 96.3d | 6.51 | 2''' | 72.1d | 4.67 |
| 8a | 163.5s | | 3''' | 72.7d | 4.55 |
| 1' | 131.3s | | 4''' | 74.1d | 4.22 |
| 2' | 128.5d | 7.58 | 5''' | 69.9d | 4.29 |
| 3' | 114.5d | 7.04 | 6''' | 18.6q | 1.58 |
| 4' | 160.4s | | | | |
| 5' | 114.5d | 7.04 | | | |
| 6' | 128.5d | 7.58 | | | |



NMR-13C:



NMR-HSQC:



Names

Neponcirin; Isokuranetin-7-O-rutinoside; (2S)-5-hydroxy-2-(4-methoxyphenyl)-4-oxo-3,4-dihydro-2H-chromen-7-yl 6-O-(6-deoxy- α -L-mannopyranosyl)- β -D-glucopyranoside; (S)-5,7-Dihydroxy-4'-methoxyflavanone-7- β -rutinoside; (S)-5,7-Dihydroxy-4'-methoxyflavanone-7-6-O-(α -L-rhamnopyranosyl)- β -D-glucopyranoside

Eriodictyol-7-glucosideEriodictyol-7-O- β -D-glucopyranoside

CAS-Number: 38965-51-4

Formula: C₂₁H₂₂O₁₁ Exact mass: 450.11621

Molecular mass: 450.39

Column: Zorbax LiChrosphere Kinetex

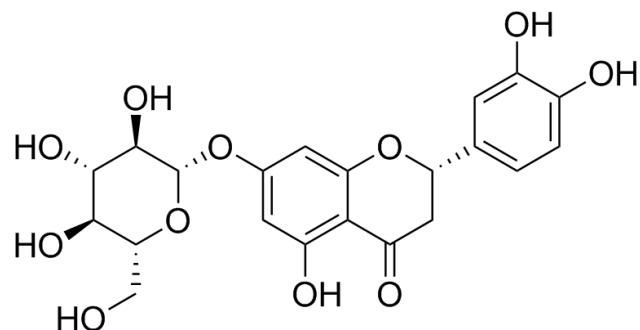
Abs.RetentionTime [min]: 16.05 12.59 6.09

Rel. RetentionTime (k'): 12.6 11.11 10.49

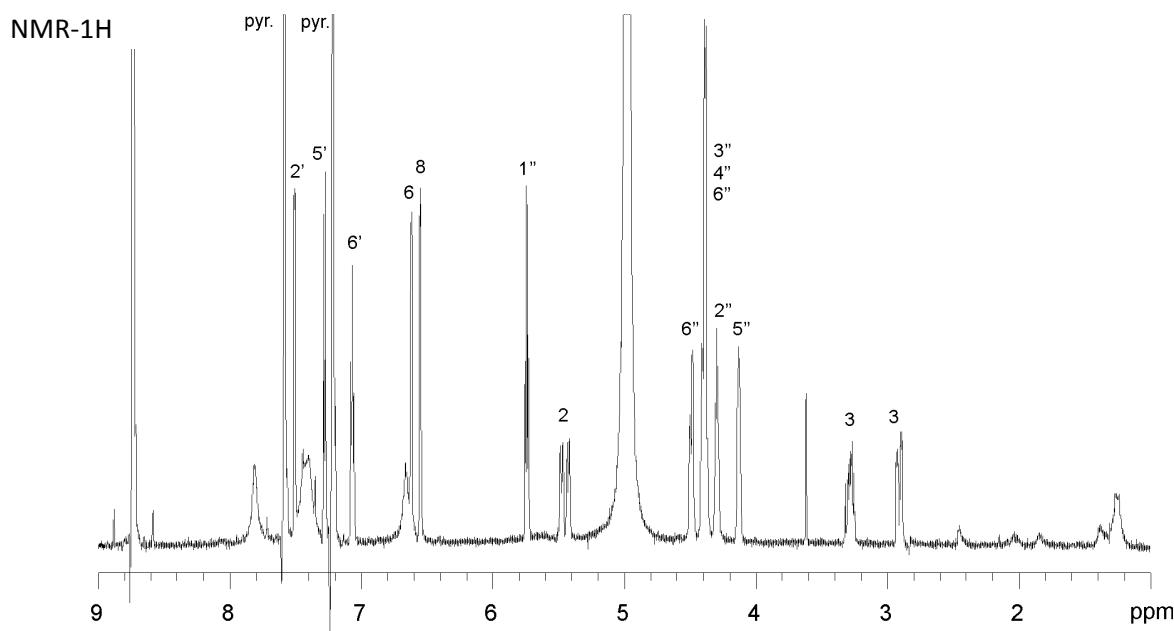
k' rel. to Rutin : 0.96 0.89 0.88

MS1: 449.3 MS2: 287.2 MS3: 151

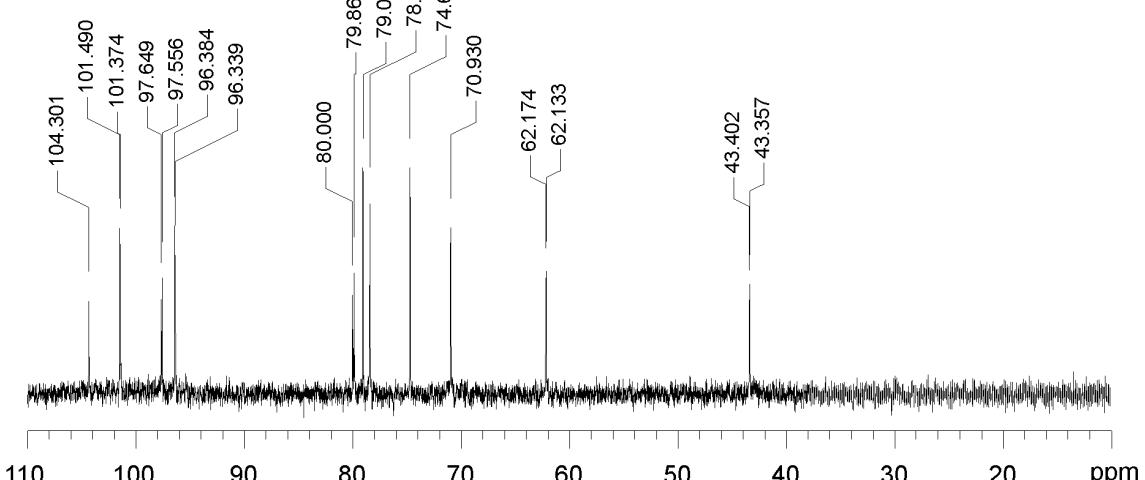
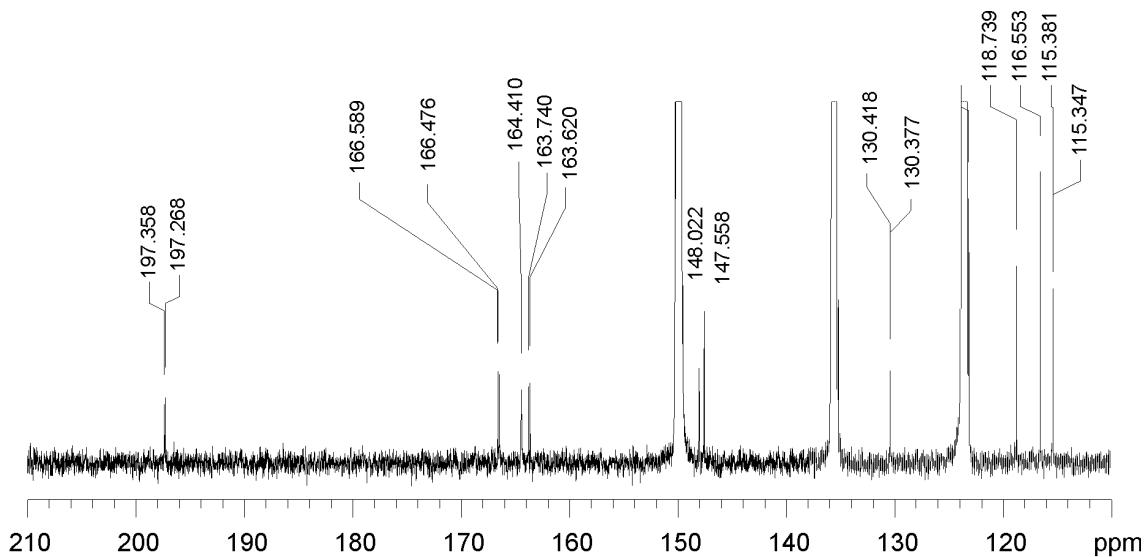
UV/Vis: 285, 330(sh)

NMR - Resonance Assignments:
Flavone Core Sugar

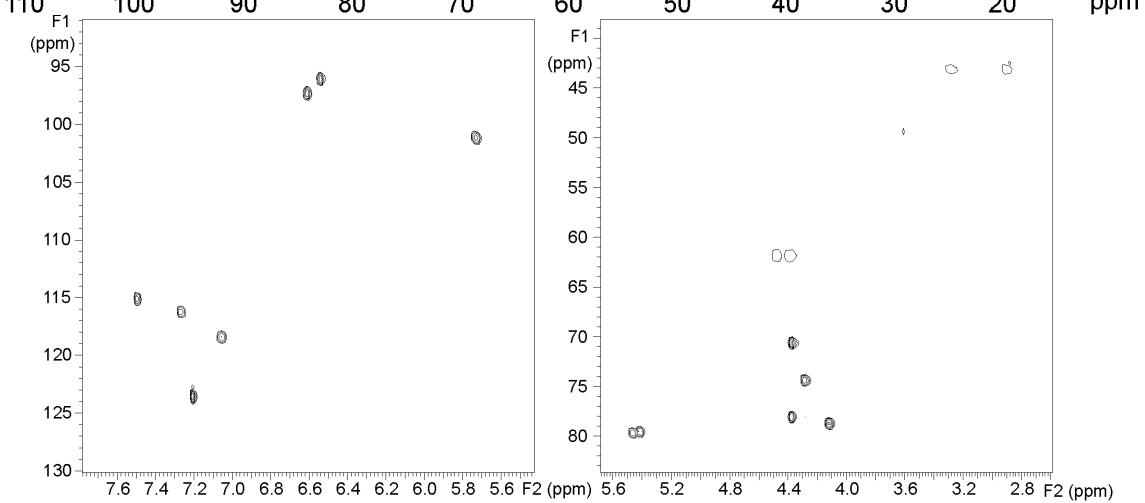
| | δ_C | δ_H | | δ_C | δ_H |
|----|------------|------------|----|------------|------------|
| 2 | 79.9d | 5.41 | 1" | 101.5d | 5.73 |
| 3 | 43.4t | 3.28/2.9 | 2" | 74.7d | 4.29 |
| 4 | 197.3s | | 3" | 78.4d | 4.38 |
| 4a | 104.3s | | 4" | 70.9d | 4.38 |
| 5 | 164.4s | | 5" | 79d | 4.12 |
| 6 | 97.6d | 6.61 | 6" | 62.1t | 4.47/4.39 |
| 7 | 166.6s | | | | |
| 8 | 96.3d | 6.54 | | | |
| 8a | 163.6s | | | | |
| 1' | 130.4s | | | | |
| 2' | 115.4d | 7.5 | | | |
| 3' | 147.6s | | | | |
| 4' | 148s | | | | |
| 5' | 116.6d | 7.27 | | | |
| 6' | 118.7d | 7.06 | | | |



NMR-13C:



NMR-HSQC:



Names

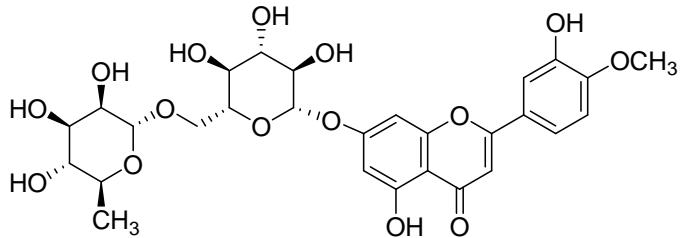
2-(3,4-dihydroxyphenyl)-7-(β -D-glucopyranosyloxy)-2,3-dihydro-5-hydroxy-(2S)-4H-1-benzopyran-4-one; 5,7,3',4'-tetrahydroxy-7- β -D-glucopyranoside-flavanone; (2S)-5,3',4'-trihydroxyflavanone-7-O-glucoside; (2S)-Eriodictyol-7-O- β -D-glucopyranoside; 5,7,3',4'-tetrahydroxyflavanone 7-glucoside; 5,7,3',4'-tetrahydroxyflavanone 7- β -D-glucopyranoside; Eriodictyol 7-O-glucoside; Eriodictyol 7-O- β -D-glucopyranoside; Eriodictyol 7-O- β -D-glucoside; Eriodictyol 7-glucoside; Eriodictyol 7- β -D-glucoside; Misanthoside

DiosminDiosmetin-7- β -D-rutinoside

CAS-Number: 520-27-4

Formula: C₂₈H₃₂O₁₅ Exact mass: 608.17412

Molecular mass: 608.54



Column: Zorbax LiChrosphere Kinetex

Abs.RetentionTime [min]: 18.27 15.93 7.43

Rel. RetentionTime (k'): 14.48 14.32 13.02

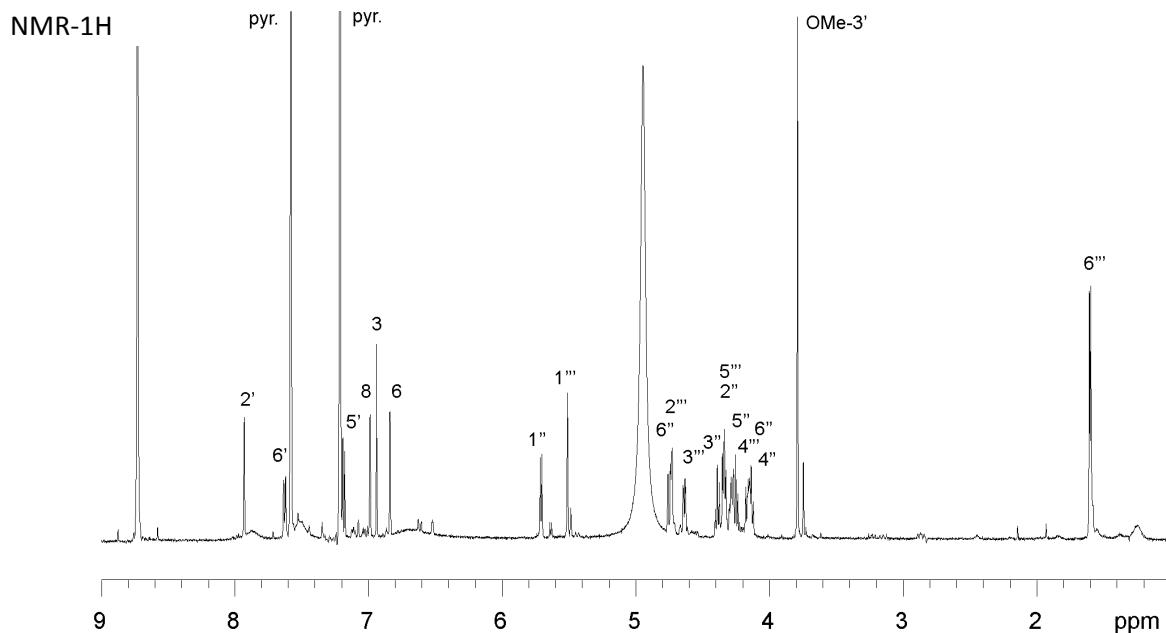
k' rel. to Rutin : 1.10 1.15 1.09

MS1: 607.1 MS2: 299.4 MS3: 284.2

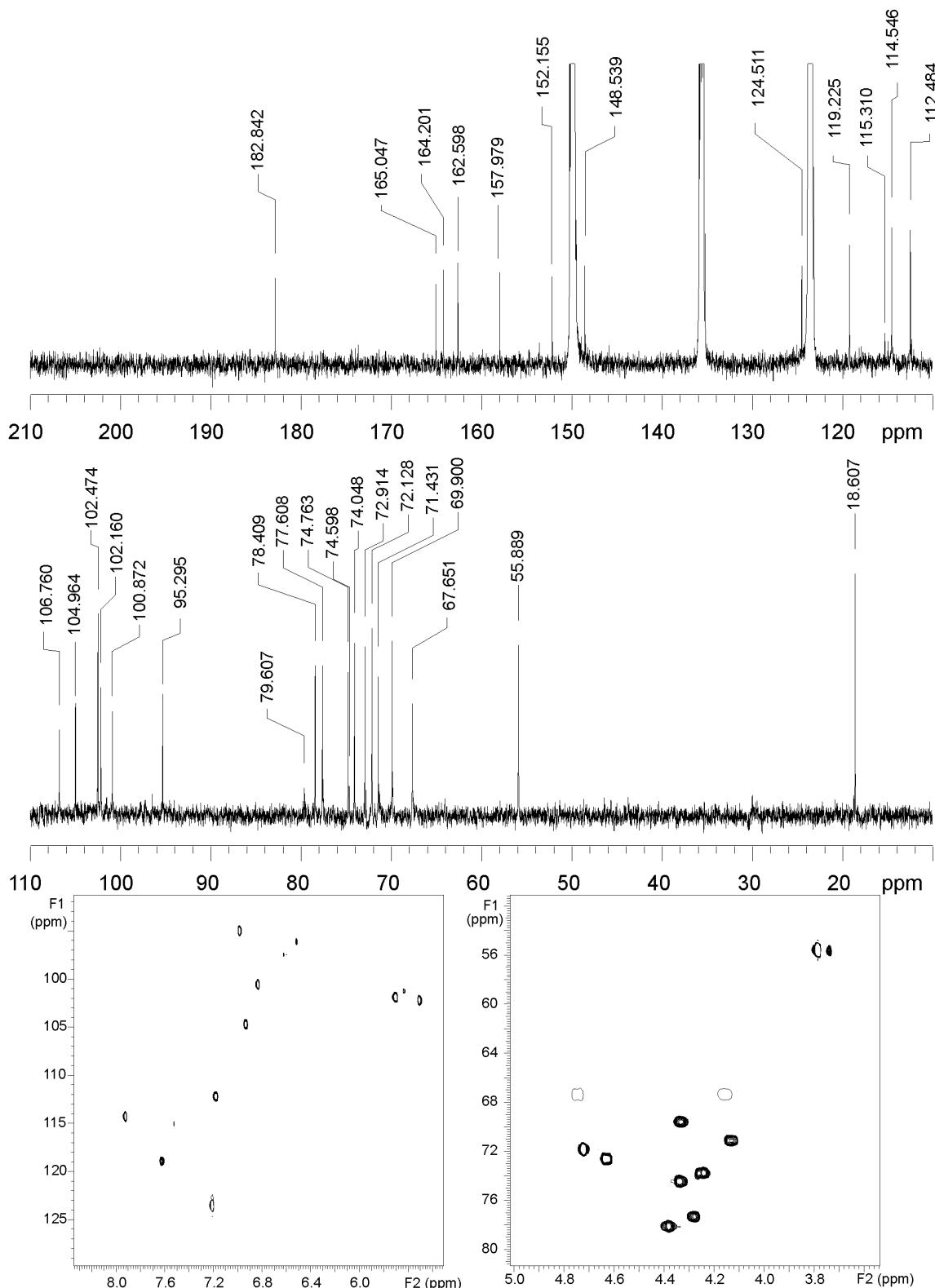
UV/Vis: 255, 265(sh), 3

NMR - Resonance Assignments:
Flavone Core Sugar

| | δ_C | δ_H | | δ_C | δ_H |
|--------|------------|------------|------|------------|------------|
| 2 | 165.1s | | 1'' | 102.5d | 5.71 |
| 3 | 105d | 6.93 | 2'' | 74.8d | 4.34 |
| 4 | 182.9s | | 3'' | 77.6d | 4.28 |
| 4a | 106.8s | | 4'' | 71.4d | 4.13 |
| 5 | 162.6s | | 5'' | 78.5d | 4.38 |
| 6 | 100.9d | 6.84 | 6'' | 67.7t | 4.75/4.16 |
| 7 | 164.2s | | 1''' | 102.2d | 5.51 |
| 8 | 95.3d | 6.98 | 2''' | 72.1d | 4.72 |
| 8a | 158s | | 3''' | 72.9d | 4.63 |
| 1' | 124.5s | | 4''' | 74.1d | 4.24 |
| 2' | 114.6d | 7.93 | 5''' | 69.9d | 4.34 |
| 3' | 148.5s | | 6''' | 18.6q | 1.6 |
| 4' | 152.2s | | | | |
| 5' | 112.5d | 7.17 | | | |
| 6' | 119.2d | 7.62 | | | |
| OMe-4' | 55.9q | 3.79 | | | |



NMR-13C:



Names

4H-1-Benzopyran-4-one, 7-[[6-O-(6-deoxy- α -L-mannopyranosyl)- β -D-glucopyranosyl]oxy]-5-hydroxy-2-(3-hydroxy-4-methoxyphenyl)-
Diosmin; 5,7,3'-Trihydroxy-4'-methoxyflavone 7-O-rutinoside;
5,3'-Dihydroxyl-4'-methoxylflavanone-7-O- α -L-rhamnosyl (1 \rightarrow 6)- β -D-glucopyranoside; Barosmin; Buchuresin;
Diosmetin 7-O-rhamnosyl(1 \rightarrow 6)-glucoside; Diosmetin 7-O- α -L-rhamnopyranosyl-(1 \rightarrow 6)- β -D-glucopyranoside;
Diosmetin 7-rutinoside; Diosmetin 7- β -rutinoside; Diosmil; Diosmine; Diosven; Dioven; Diovenor; Flebosmil; Flebosten;
Hemerven; Insuven; Litosmil; Tovene; Varinon; Ven-Detrex; Venex 500; Venosmine

Apigenin-7,4'-dimethylether

5-Hydroxy-7,4'-dimethoxyflavone

CAS-Number: 5128-44-9

Formula: C₁₇H₁₄O₅ Exact mass: 298.08412

Molecular mass: 298.29

Column: Zorbax LiChrosphere Kinetex

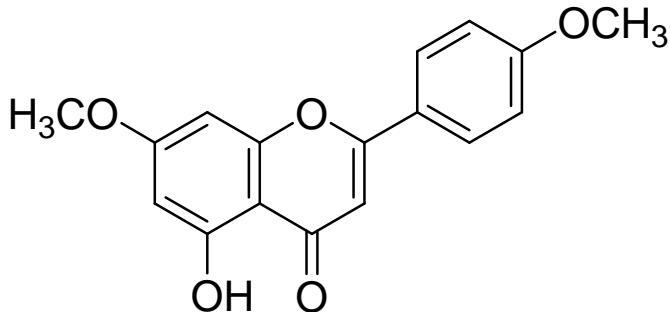
Abs.RetentionTime [min]: 33.28 31.23 15.13

Rel. RetentionTime (k') : 27.2 29.03 27.55

k' rel. to Rutin : 2.06 2.34 2.31

MS1: 297.3 MS2: MS3:

UV/Vis: 270, 330

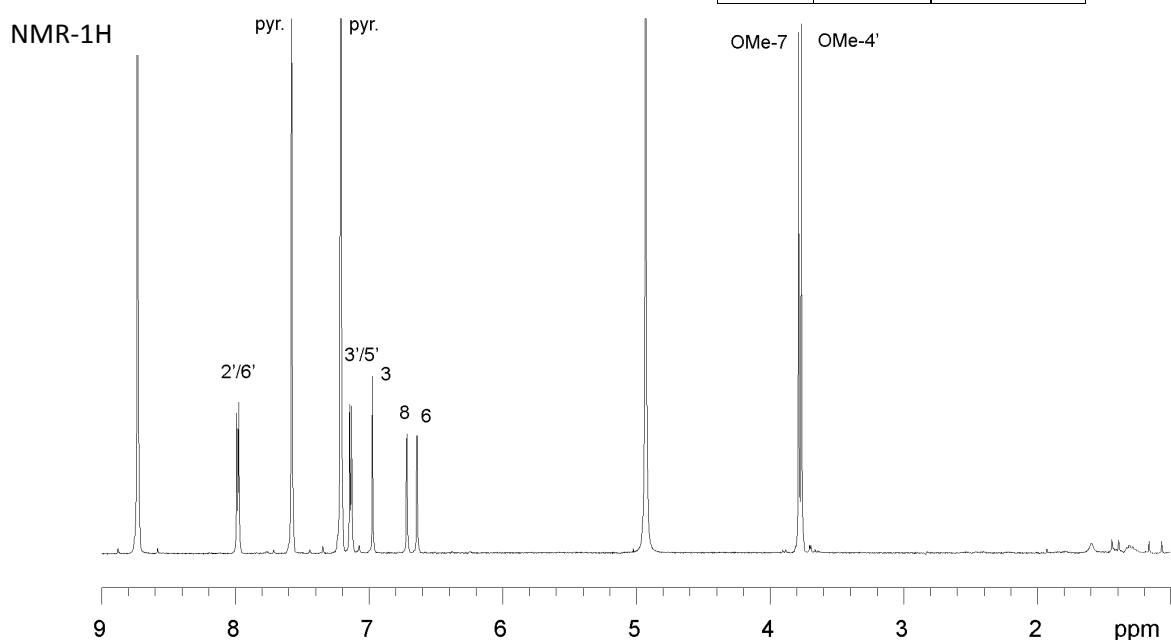


NMR - Resonance Assignments:

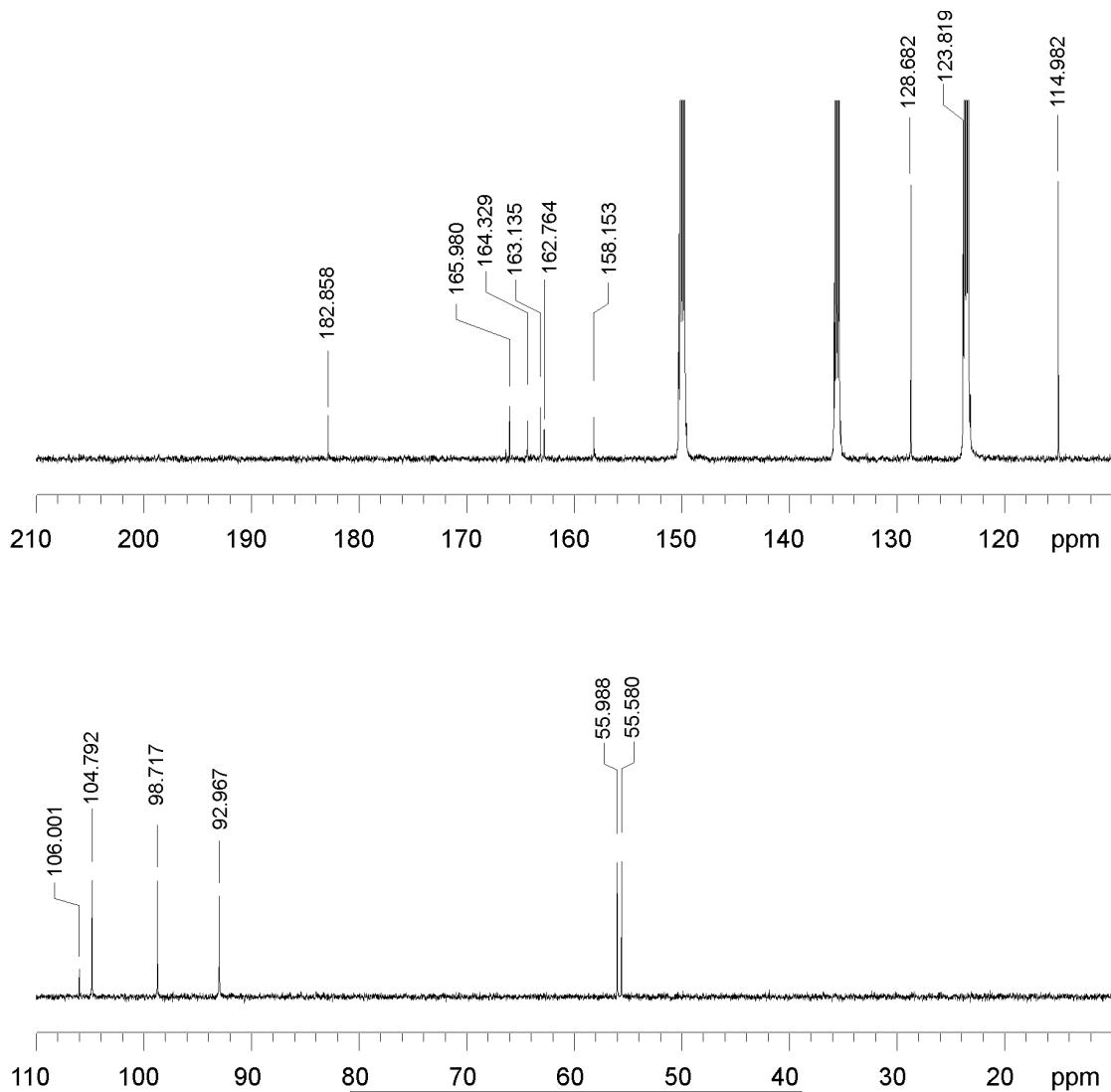
Flavone Core

Sugar

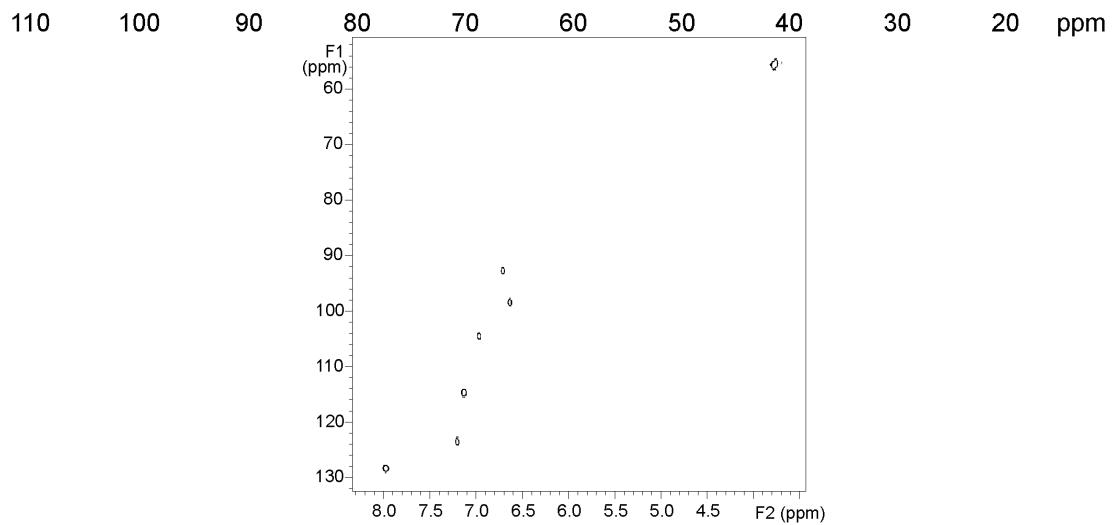
| | δ_C | δ_H |
|--------|------------|------------|
| 2 | 164.3s | |
| 3 | 104.8d | 6.97 |
| 4 | 182.9s | |
| 4a | 106s | |
| 5 | 162.8s | |
| 6 | 98.7d | 6.64 |
| 7 | 166s | |
| 8 | 93.4d | 6.72 |
| 8a | 158.2s | |
| 1' | 123.8s | |
| 2' | 128.7d | 7.98 |
| 3' | 115d | 7.13 |
| 4' | 163.1s | |
| 5' | 115d | 7.13 |
| 6' | 128.7d | 7.98 |
| OMe-7 | 56q | 3.79 |
| OMe-4' | 55.6q | 3.76 |



NMR-13C:



NMR-HSQC:



Names

5-hydroxy-7-methoxy-2-(4-methoxyphenyl)-flavone; 5-hydroxy-7, 4'-dimethoxy- 4H-1-benzopyran-4-one; 7, 4'-di-O-methylapigenin; 7, 4'-dimethylapigenin; 4'-methoxytectochrysin; 5-hydroxy-7,4'-dimethoxyflavone; 5-hydroxy-7,4'-dimethoxyflavone; 7,4'-di-O-methylapigenin; 7,4'-dimethylapigenin; 7-O-methylacetin; Acacetin 7-methyl ether; Apigenin 7,4'-dimethyl ether; Apigenin 7,4'-dimethyl ether; Apigenin dimethyl ether; Genkwanin 4'-methyl ether; NSC 94547

Kaempferide

3,5,7-Trihydroxy-4'-methoxyflavone

CAS-Number: 491-54-3

Formula: C₁₆H₁₂O₆ Exact mass: 300.06339

Molecular mass: 300.26

Column: Zorbax LiChrosphere Kinetex

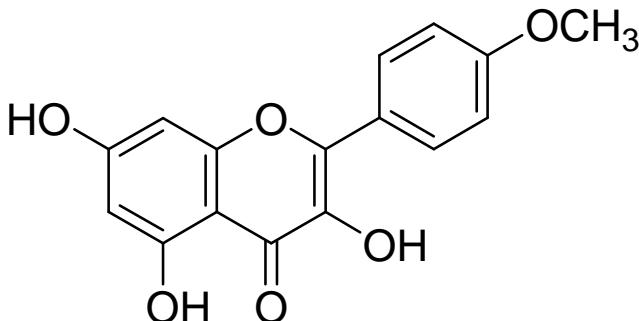
Abs.RetentionTime [min]: 28.72 26.24 13.05

Rel. RetentionTime (k') : 23.34 24.23 23.62

k' rel. to Rutin : 1.77 1.95 1.98

MS1: 299.4 MS2: 284.3 MS3: 150.9

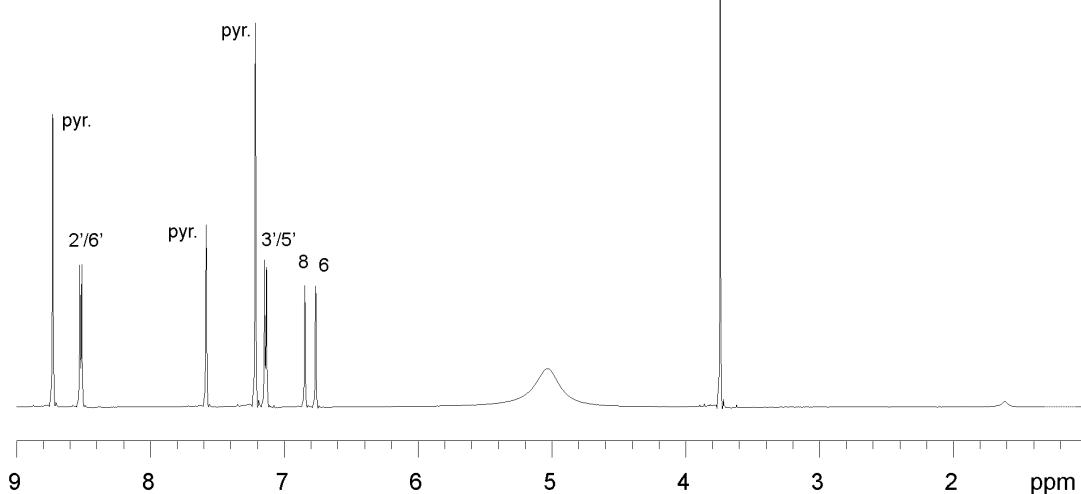
UV/Vis: 255, 265(sh)



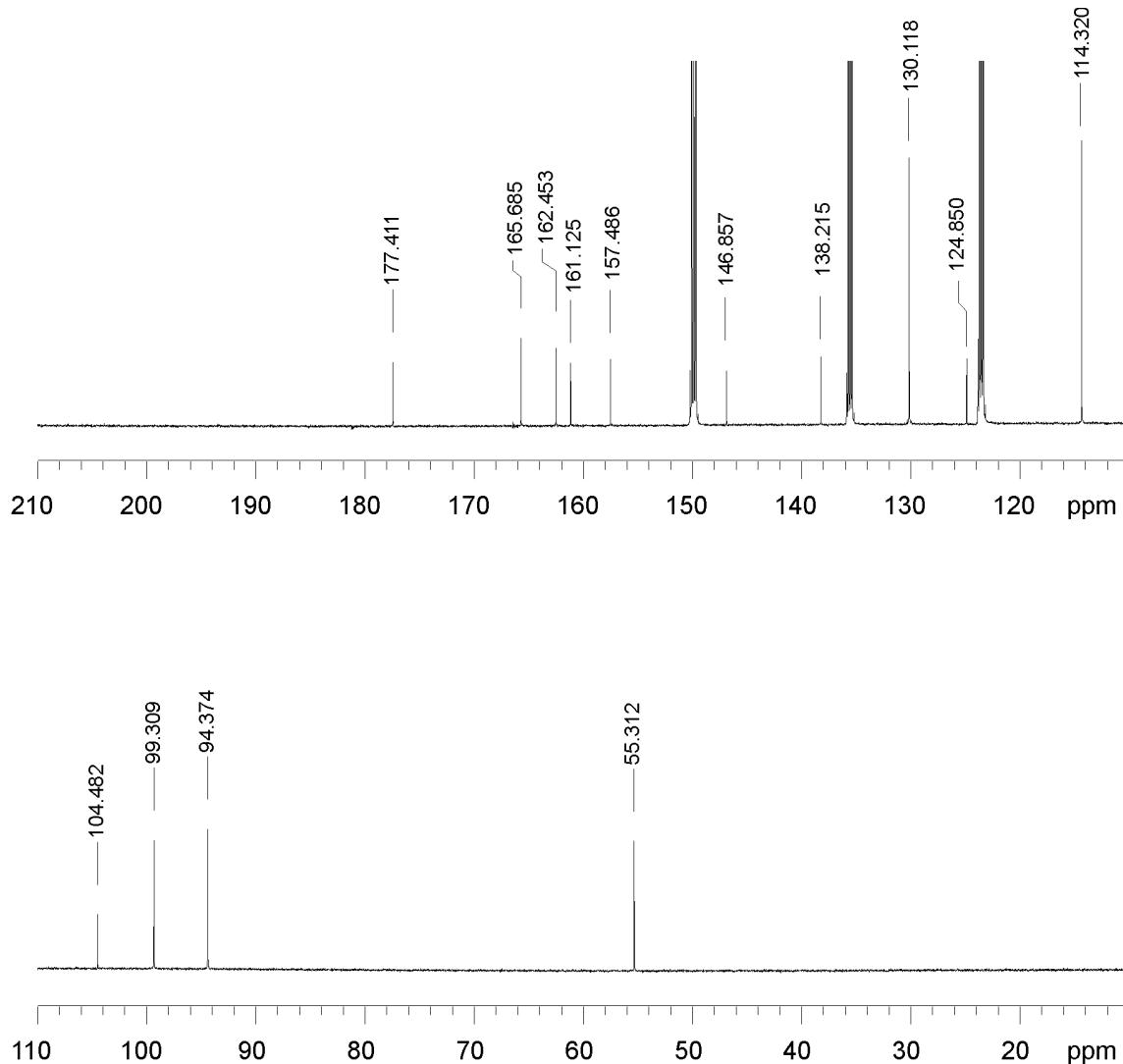
NMR - Resonance Assignments:

| | δ_C | δ_H |
|--------|------------|------------|
| 2 | 146.9s | |
| 3 | 138.2s | |
| 4 | 177.4s | |
| 4a | 104.5s | |
| 5 | 162.5s | |
| 6 | 99.3d | 6.76 |
| 7 | 165.7s | |
| 8 | 94.4d | 6.84 |
| 8a | 157.5s | |
| 1' | 124.9s | |
| 2' | 130.1d | 8.52 |
| 3' | 114.3d | 7.14 |
| 4' | 161.1s | |
| 5' | 114.3d | 7.14 |
| 6' | 130.1d | 8.52 |
| OMe-3' | 55.3q | 3.74 |

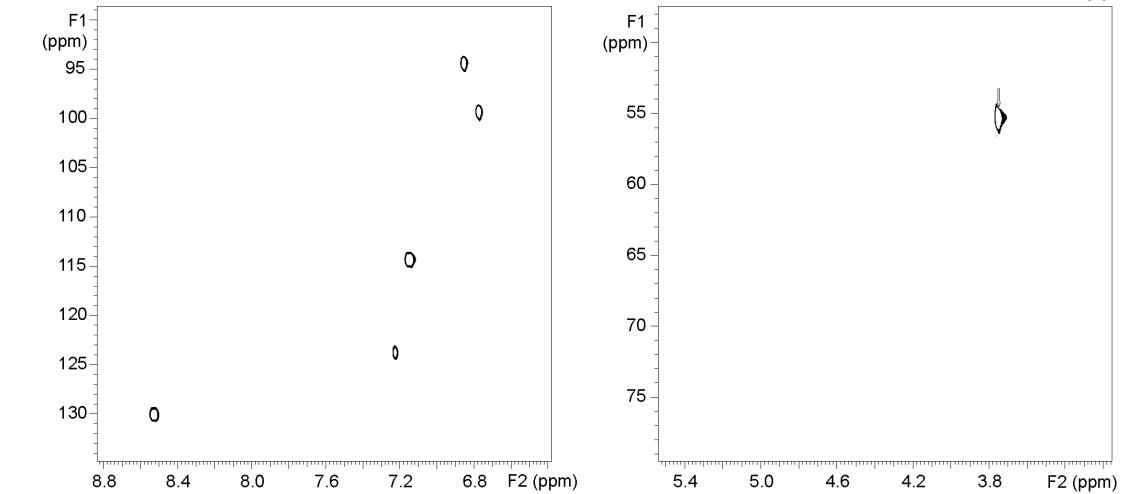
NMR-1H



NMR-13C:



NMR-HSQC:



Names

3,5,7-trihydroxy-2-(4-methoxyphenyl)-4H-1-benzopyran-4-one; 3,5,7-trihydroxy-4'-methoxy-flavone; Kaempferide; 3,5,7-trihydroxy-4'-methoxyflavone; 4'-Methoxykaempferol; 4'-Methylkaempferol; 4'-O-Methylkaempferol; 5,7-Dihydroxy-4'-methoxyflavonol; Kaempferid; Kaempferol 4'-O-methyl ether; Kaempferol 4'-methyl ether; NSC 407294

QuercitrinQuercetin-3-O- α -L-rhamnopyranoside

CAS-Number: 522-12-3

Formula: C₂₂H₂₂O₁₁ Exact mass: 462.11621

Molecular mass: 462.12

Column: Zorbax LiChrosphere Kinetex

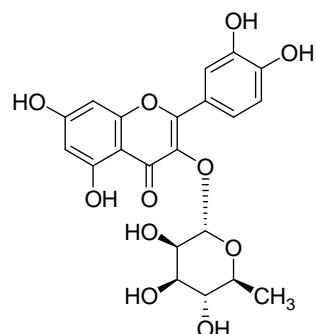
Abs.RetentionTime [min]: 18.24 15.55 7.72

Rel. RetentionTime (k'): 14.46 13.95 13.57

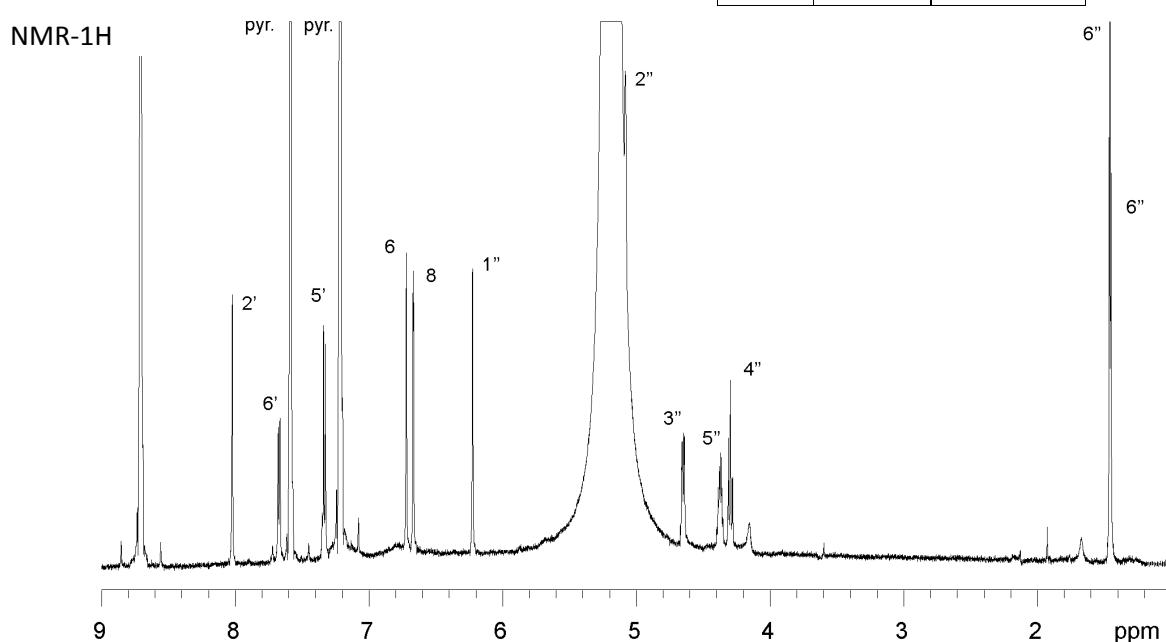
k' rel. to Rutin : 1.10 1.12 1.14

MS1: 447.4 MS2: 301.2 MS3: 178.9

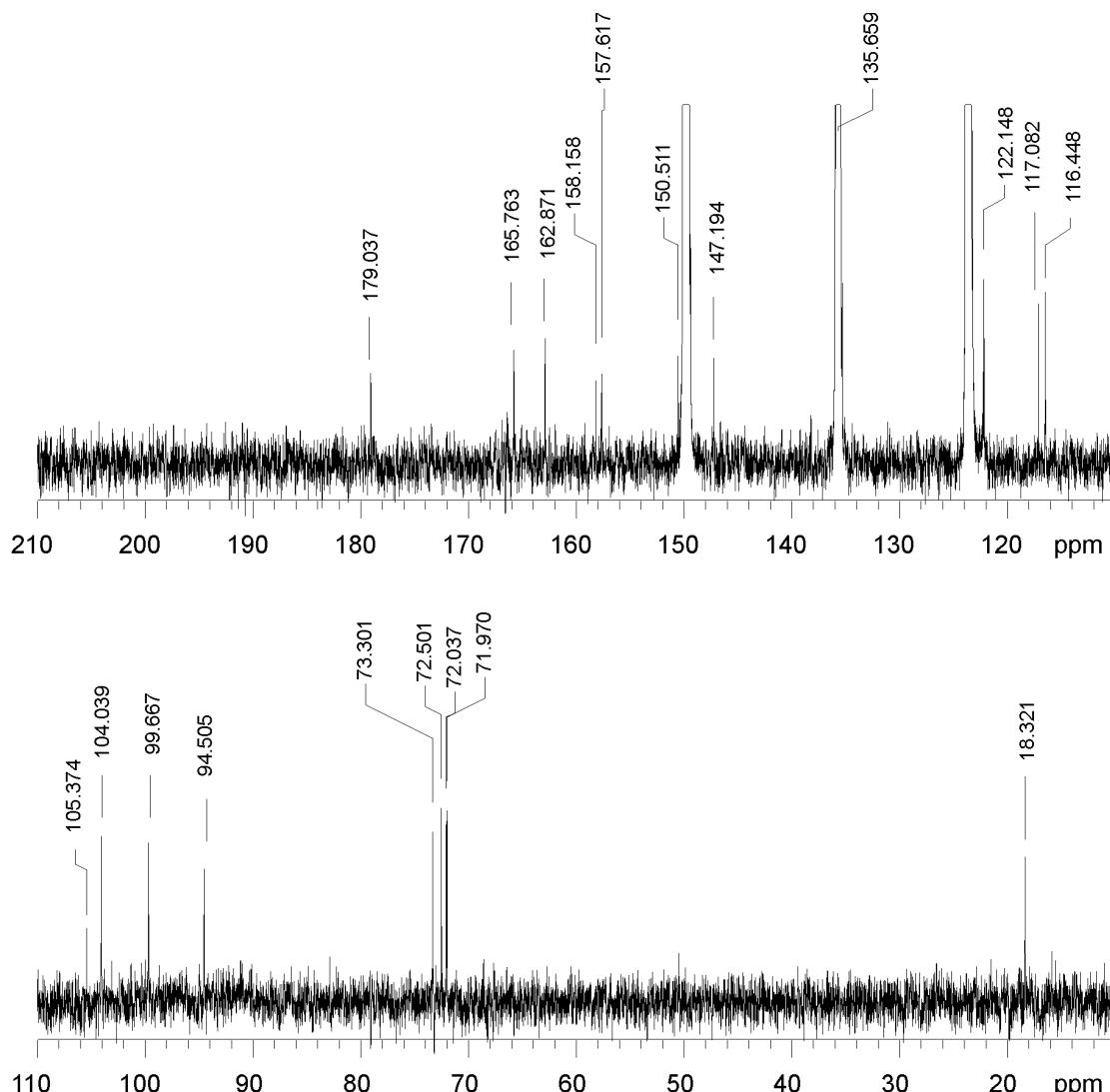
UV/Vis: 255, 265(sh), 3

NMR - Resonance Assignments:
Flavone Core Sugar

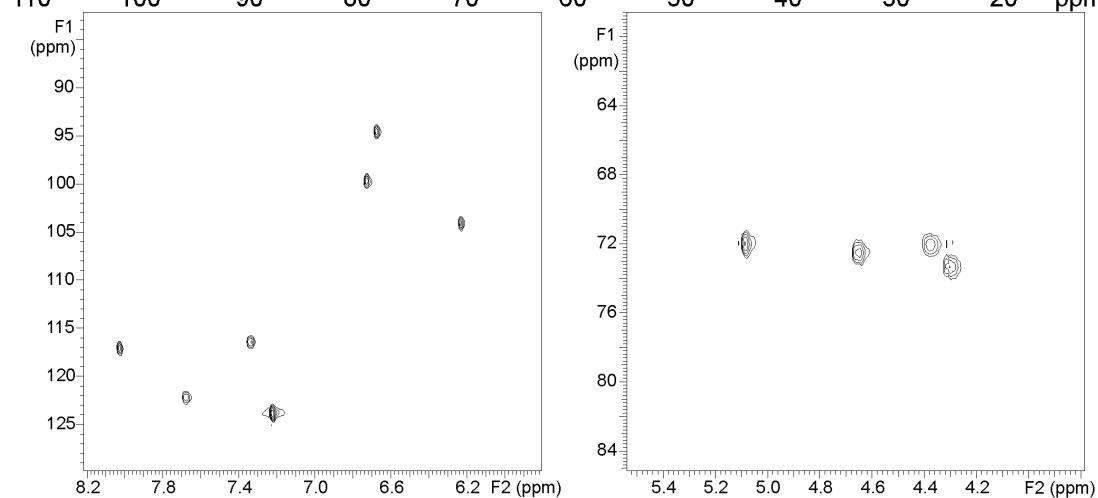
| | δ_C | δ_H | | δ_C | δ_H |
|----|------------|------------|----|------------|------------|
| 2 | 158.2s | | 1" | 104.4d | 6.23 |
| 3 | 135.8s | | 2" | 72d | 5.09 |
| 4 | 179.1s | | 3" | 72.5d | 4.66 |
| 4a | 105.4s | | 4" | 73.3d | 4.3 |
| 5 | 169.2s | | 5" | 72d | 4.37 |
| 6 | 99.7d | 6.72 | 6" | 18.3q | 1.46 |
| 7 | 165.8s | | | | |
| 8 | 94.5d | 6.66 | | | |
| 8a | 157.7s | | | | |
| 1' | 122.2s | | | | |
| 2' | 117.1d | 8.02 | | | |
| 3' | 147.2s | | | | |
| 4' | 150.5s | | | | |
| 5' | 116.5d | 7.33 | | | |
| 6' | 122.2d | 7.67 | | | |



NMR-13C:



NMR-HSQC:



Names

3-[(6-deoxy- α -L-mannopyranosyl)oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4H-1-benzopyran-4-one; Quercitrin; 3,5,7,3',4'-pentahydroxyflavone 3-L-rhamnoside; 3-O-rhamnosylquercetin; 3-O- α -L-rhamnopyranosylquercetin; 5,7,3',4'-tetrahydroxyflavonol 3-O-rhamnoside; C.I. 75720; NSC 9221; Quercetin 3-L-rhamnoside; Quercetin 3-O-L-rhamnoside; Quercetin 3-O-rhamnopyranoside; Quercetin 3-O-rhamnoside; Quercetin 3-O- α -L-rhamnopyranoside; Quercetin 3-O- α -L-rhamnoside; Quercetin 3-O-rhamnopyranoside; Quercetin 3-rhamnopyranoside; Quercetin 3-rhamnoside; Quercetin-3-O- α -rhamnoside; Quercimelin; Quercitroside; WA 17779