

Figure S1: ^1H NMR (600 MHz, CD_3OD) spectrum of compound 1

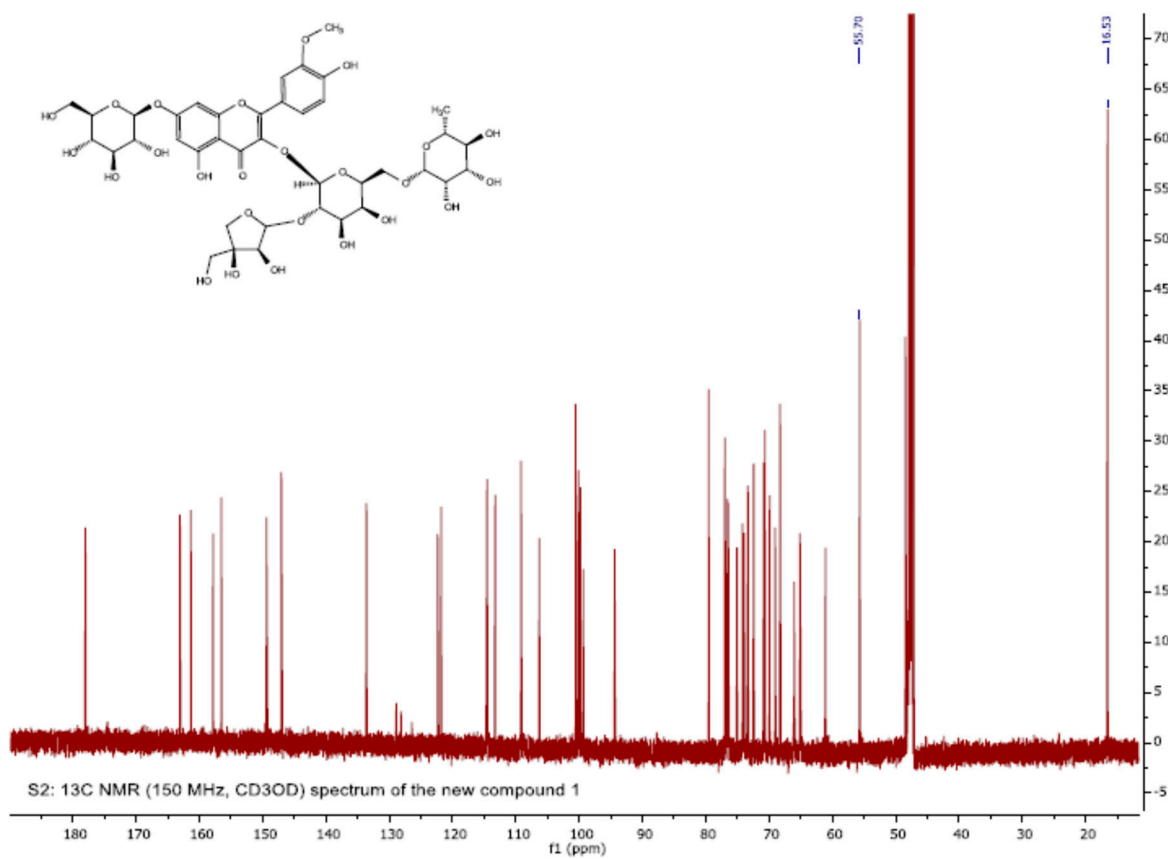


Figure S2: ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound 1

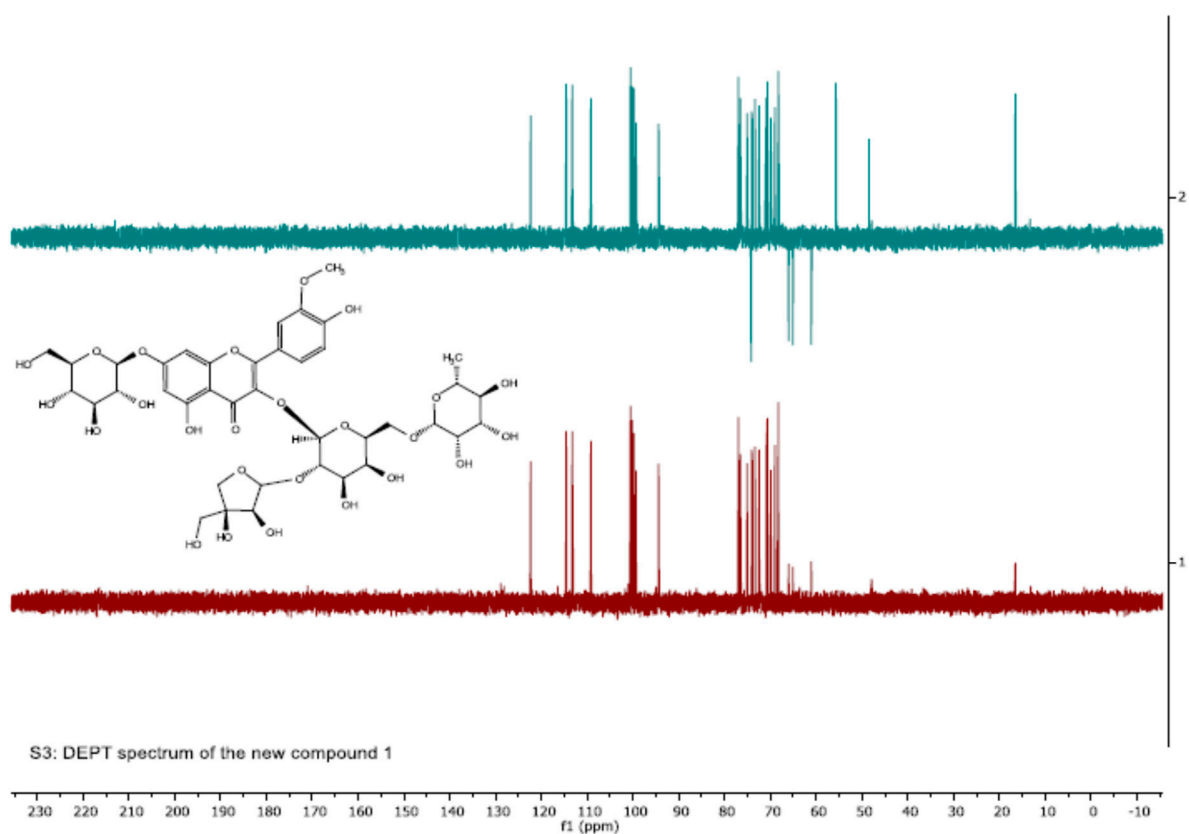


Figure S3: DEPT spectrum of compound 1

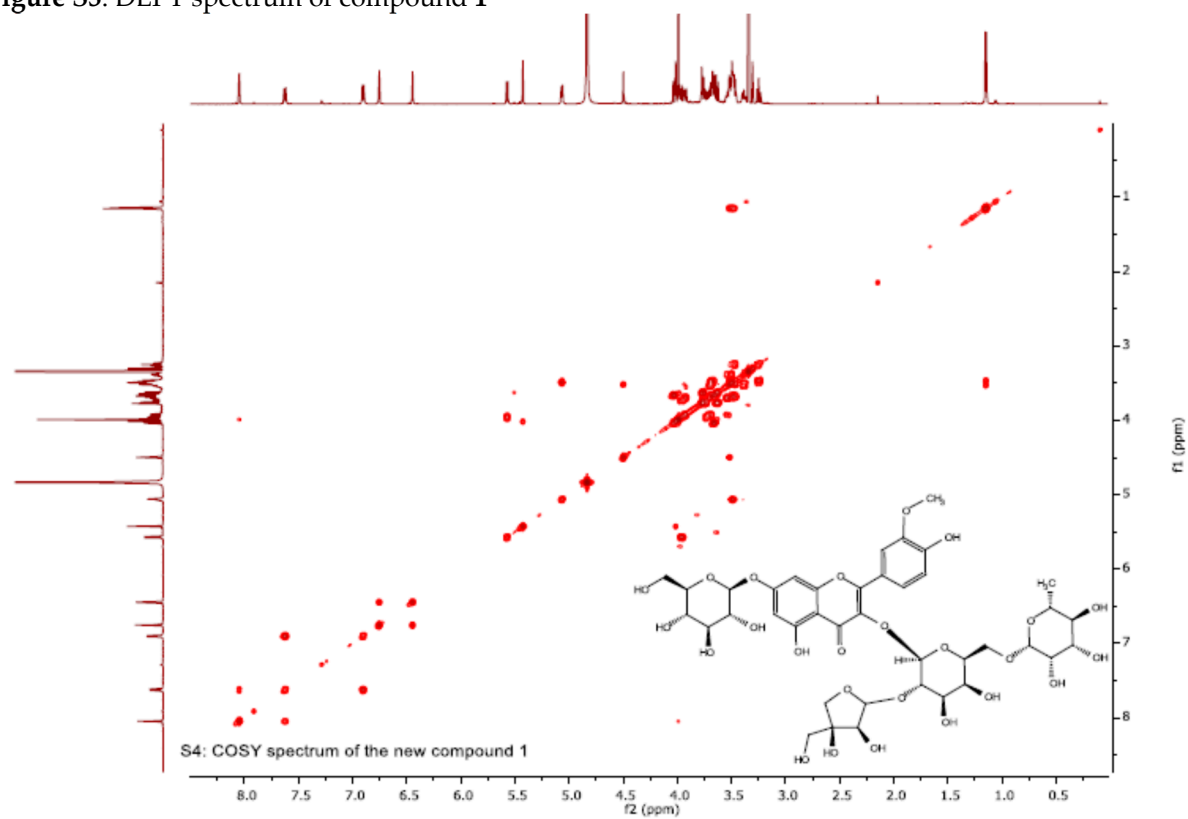


Figure S4: COSY spectrum of compound 1

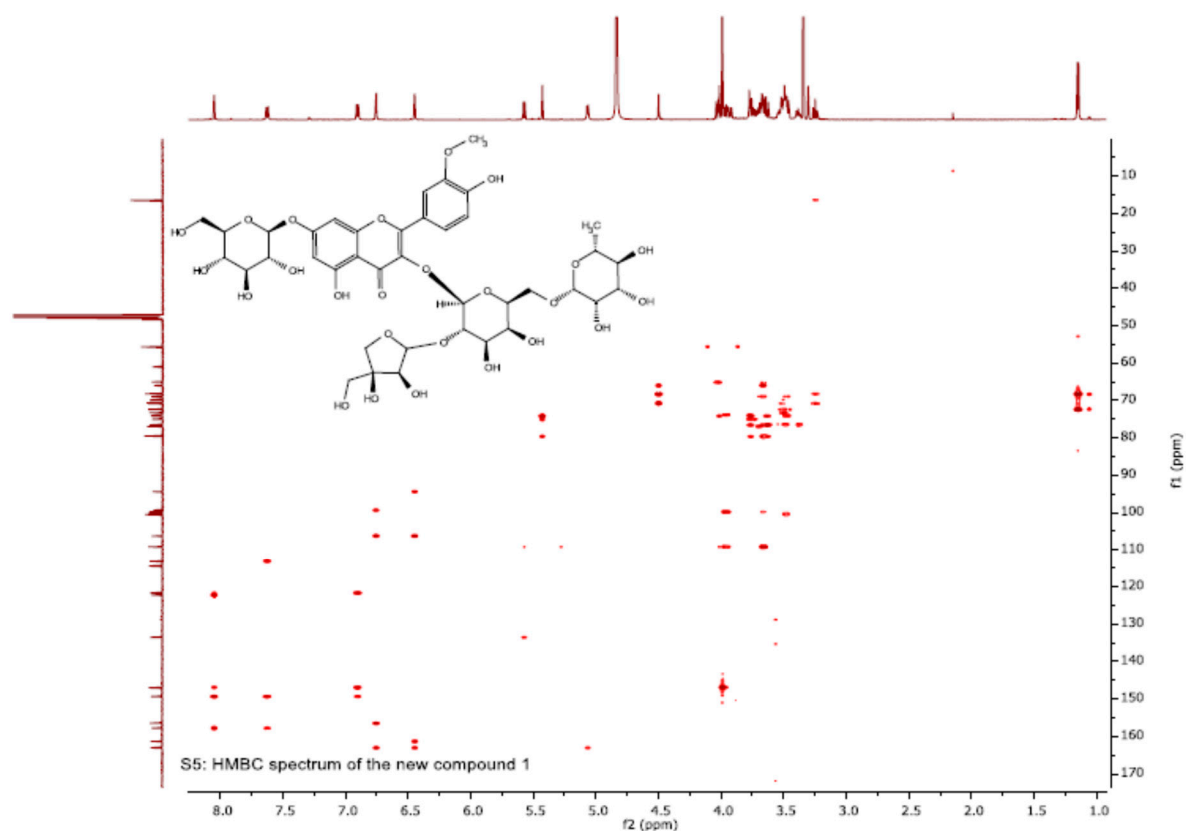


Figure S5: HMBC spectrum of compound 1

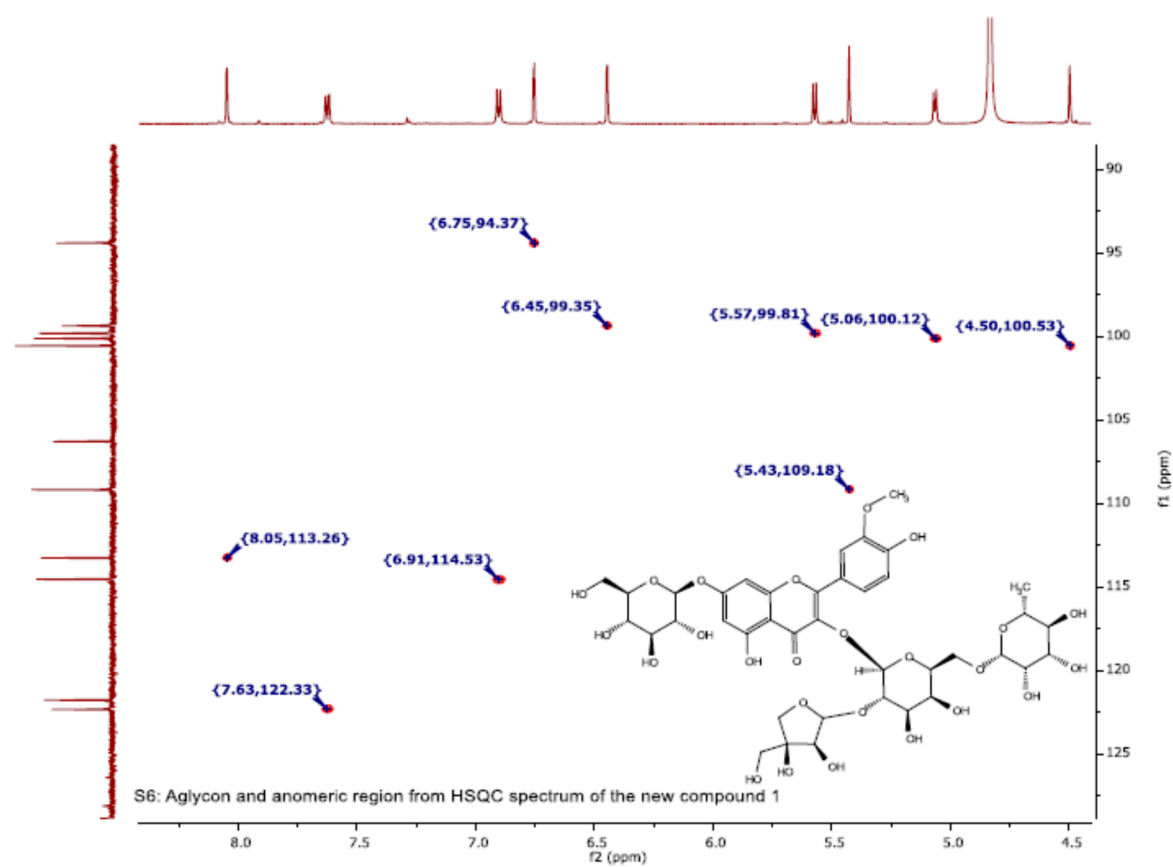


Figure S6: HSQC spectrum of compound 1 (aglycon and anomeric region)

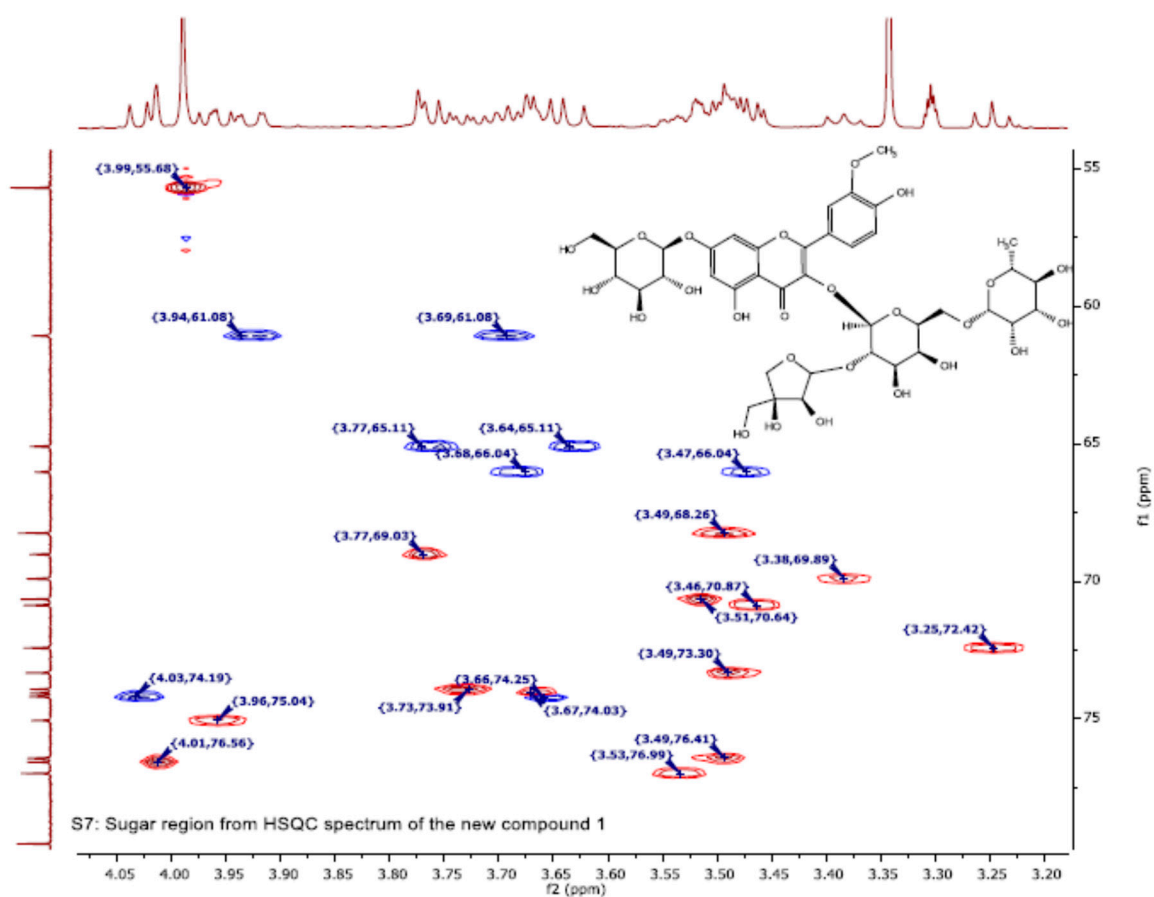


Figure S7: HSQC spectrum of compound 1 (sugar region)

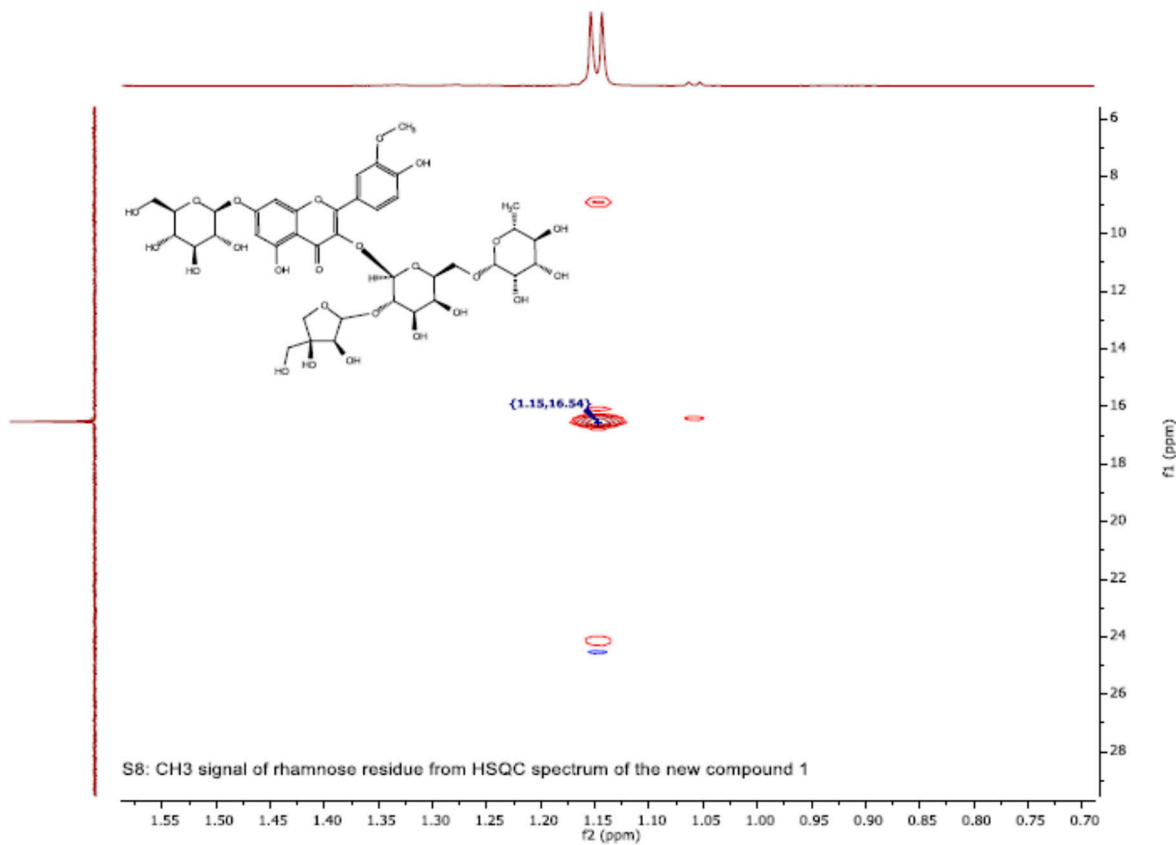
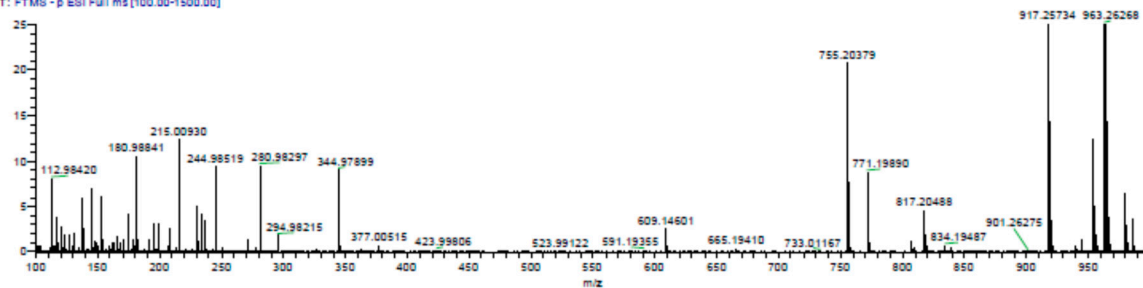
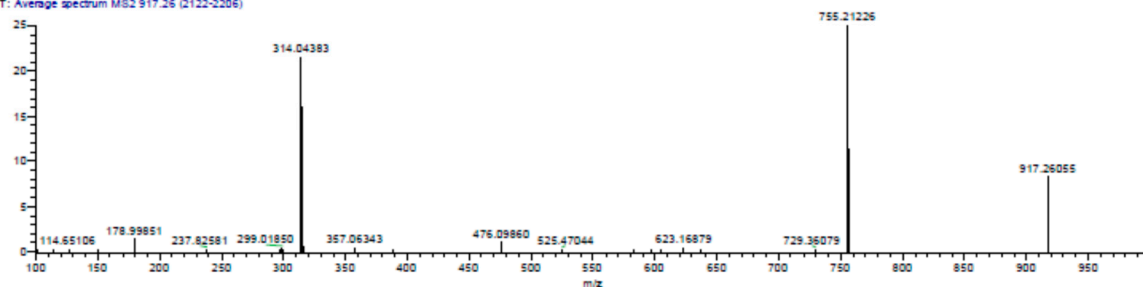


Figure S8: HSQC spectrum of compound 1 (methyl signal of rhamnose moiety)

Histo_03_161219 #2112-2173 RT: 4.90-5.0
T: FTMS - p ESI Full ms [100.00-1500.00]



Histo_03_161219 #2122-2206 RT: 4.91-5.09 AV: 2 NL: 4.15EE
T: Average spectrum MS2 917.26 (2122-2206)

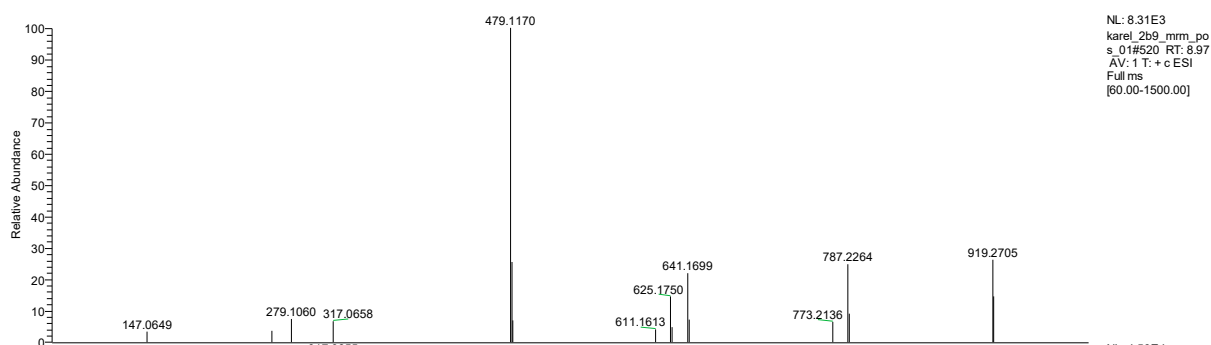


S9: HR-ESI-MS (ESI negative mode) spectrum of the new compound 1

Up: full-scan

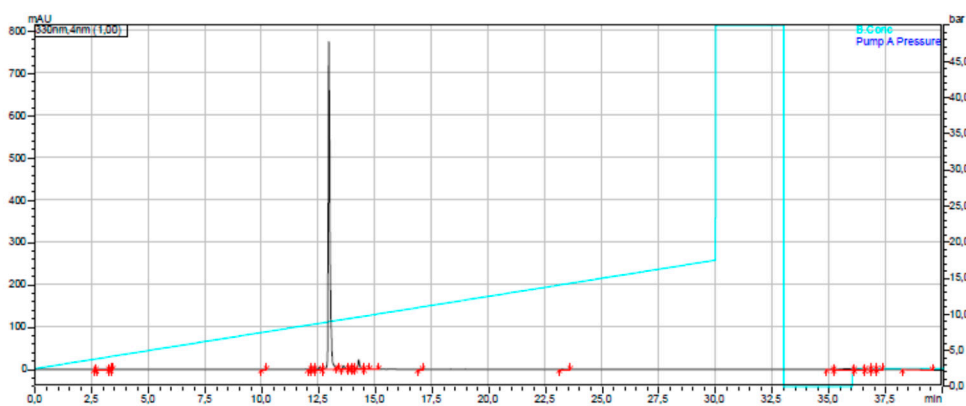
Down: MS2 of 917.25734 m/z

Figure S9: HR-ESI-MS (negative mode) of compound 1



NL: 8.31E3
karel_2b9_mm_po
s_01#520 RT: 8.97
AV: 1 T: + c ESI
Full ms
[60.00-1500.00]

Figure S10: HR-ESI-MS (positive mode) of compound 1



S10: HPLC of compound 1

Gradient 5 -> 35% Phase A (CH₃CN); Phase B (H₂O + 0.02% HCOOH) Column: Kinetex® PFP 100 A, 250 x 4.6 mm I.D., 5 µm (Phenomenex, USA).

Flow rate: 1 ml/min

Figure S11: HPLC chromatogram of compound 1

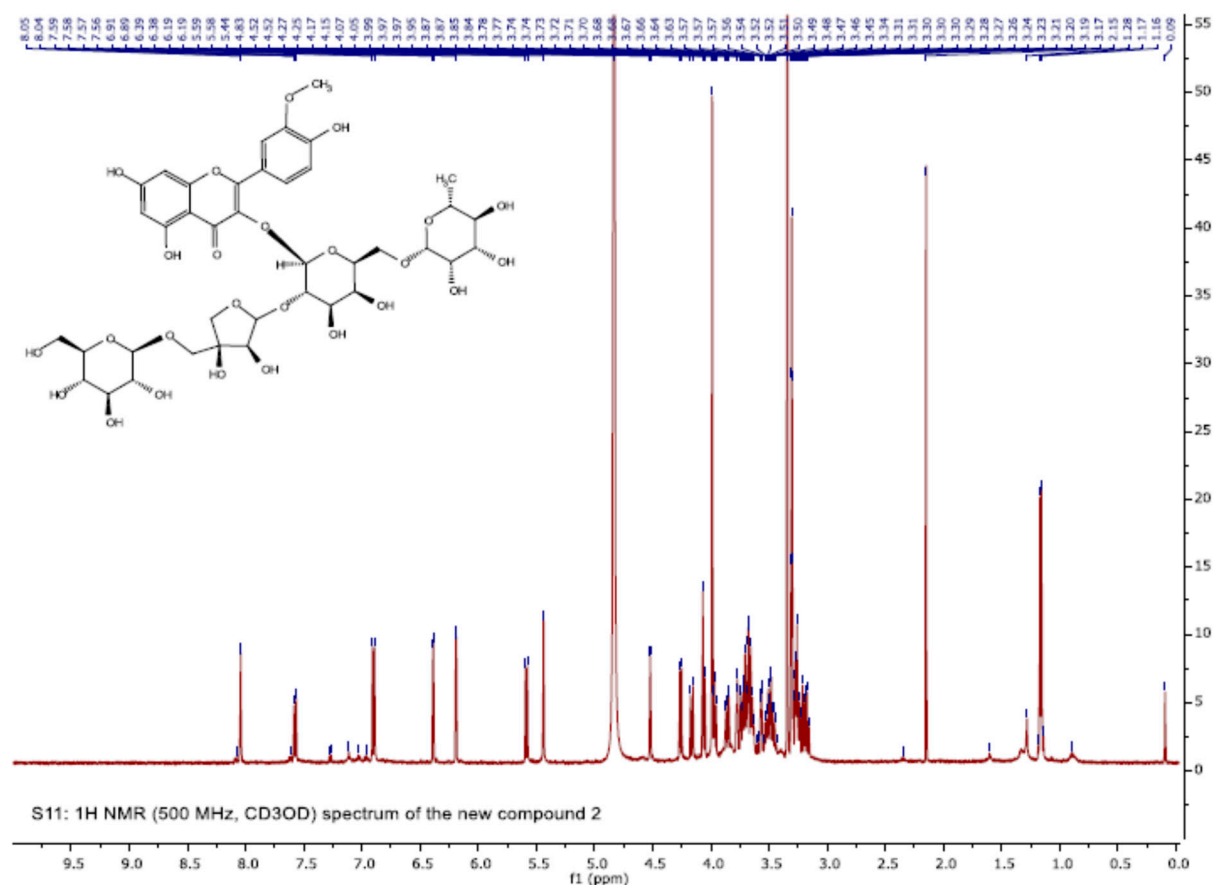


Figure S12: ¹H NMR (600 MHz, CD₃OD) spectrum of compound 2

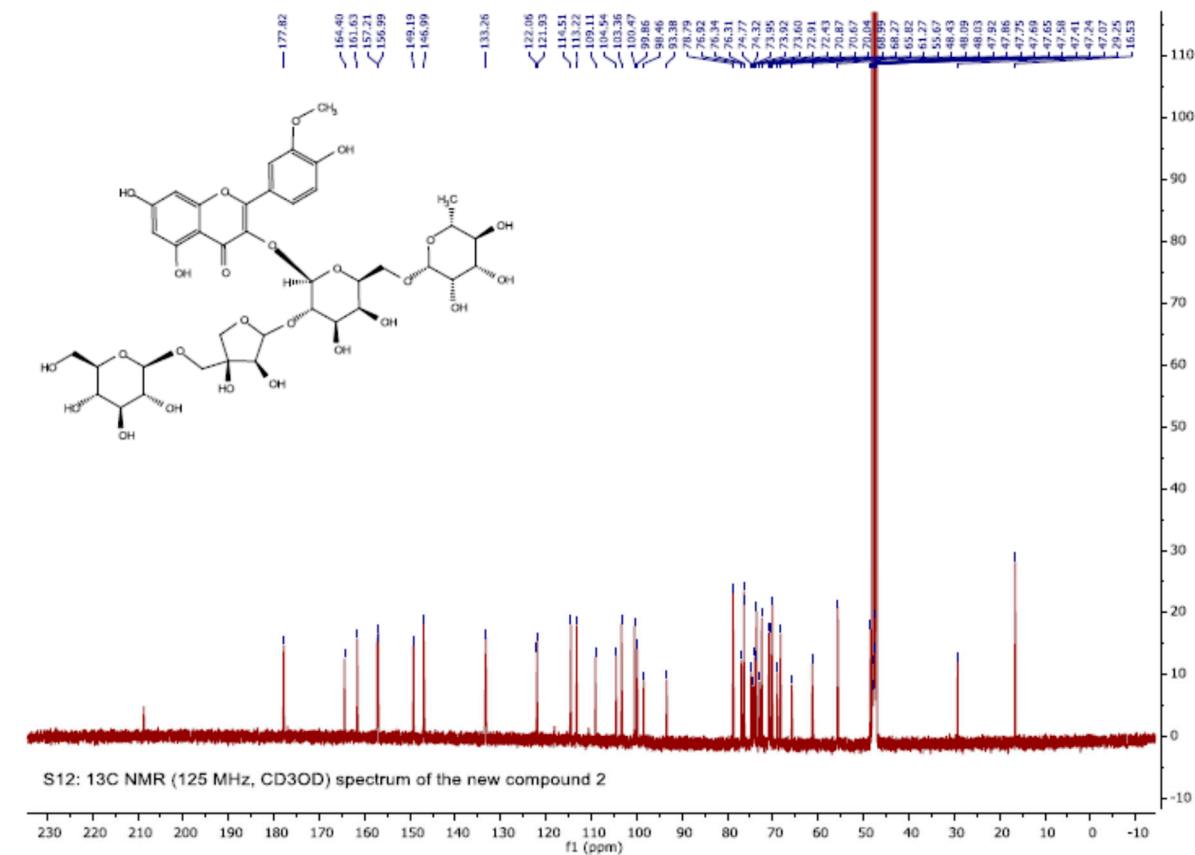


Figure S13: ¹³C NMR (125 MHz, CD₃OD) spectrum of compound 2

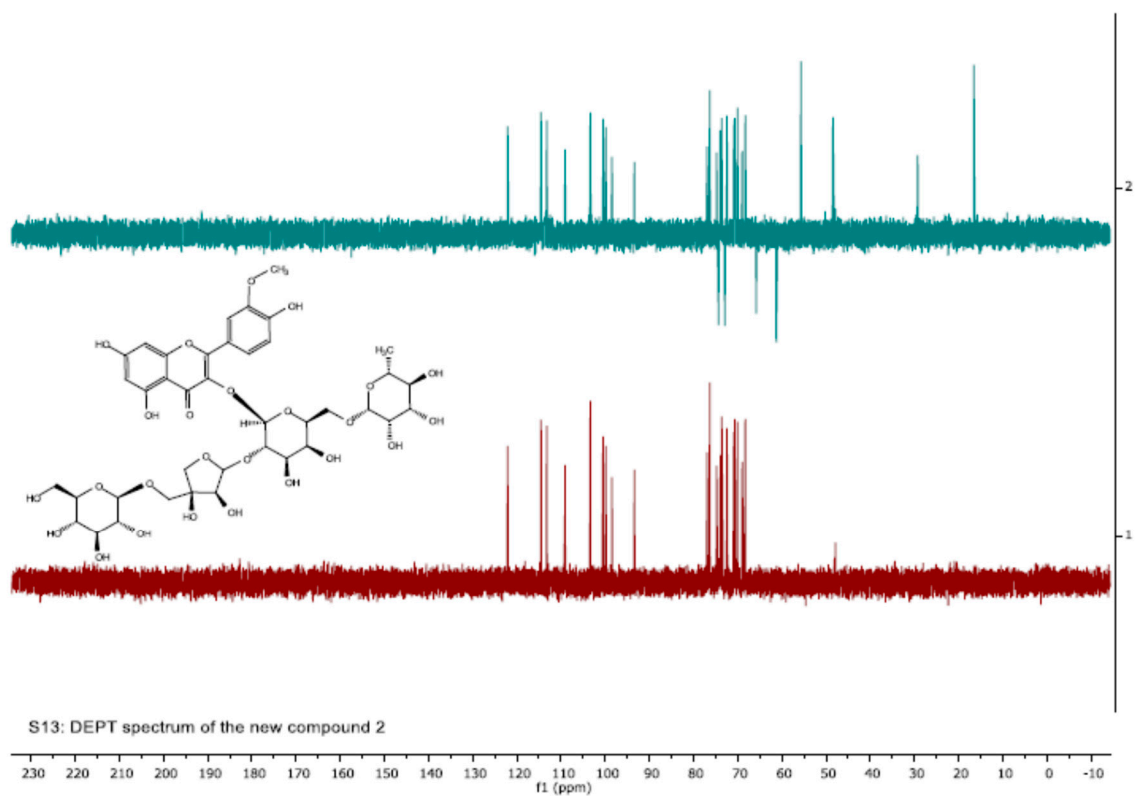


Figure S14: DEPT spectrum of compound 2

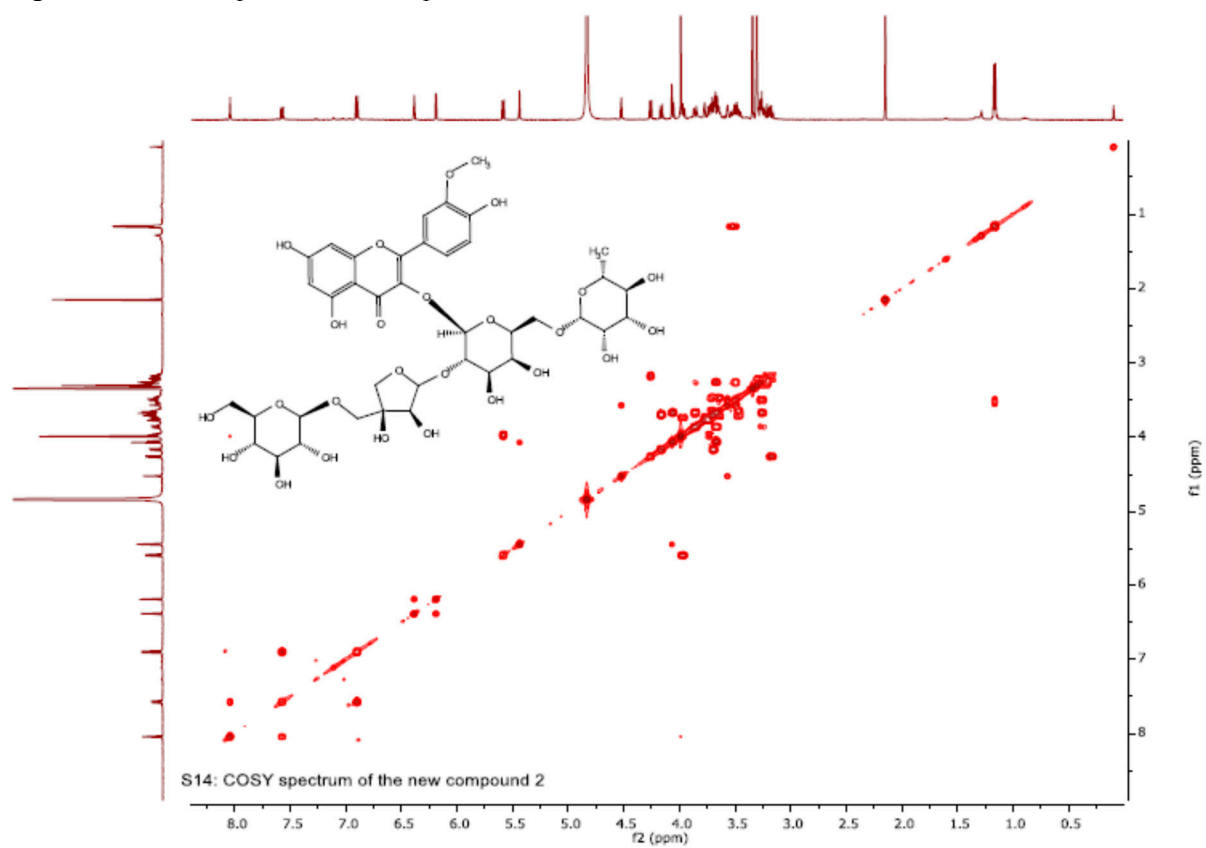


Figure S15: COSY spectrum of compound 2

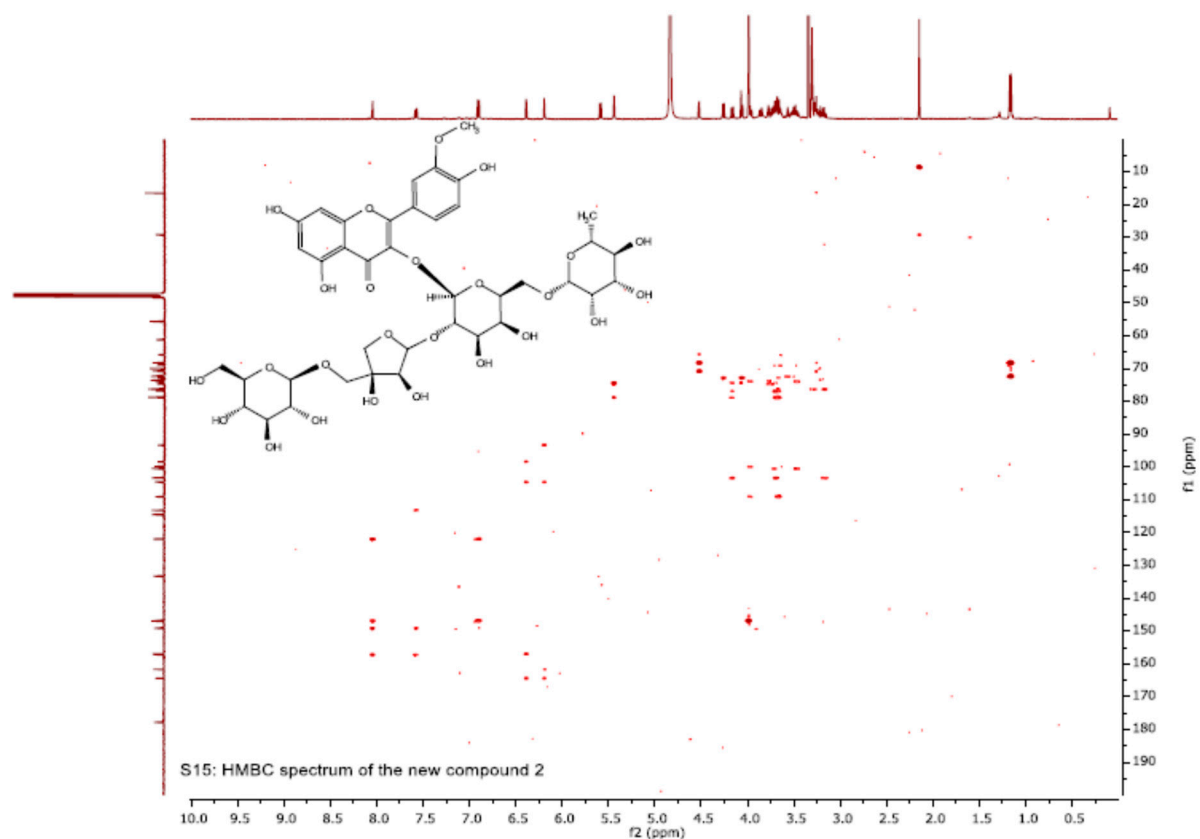


Figure S16: HMBC spectrum of compound 2

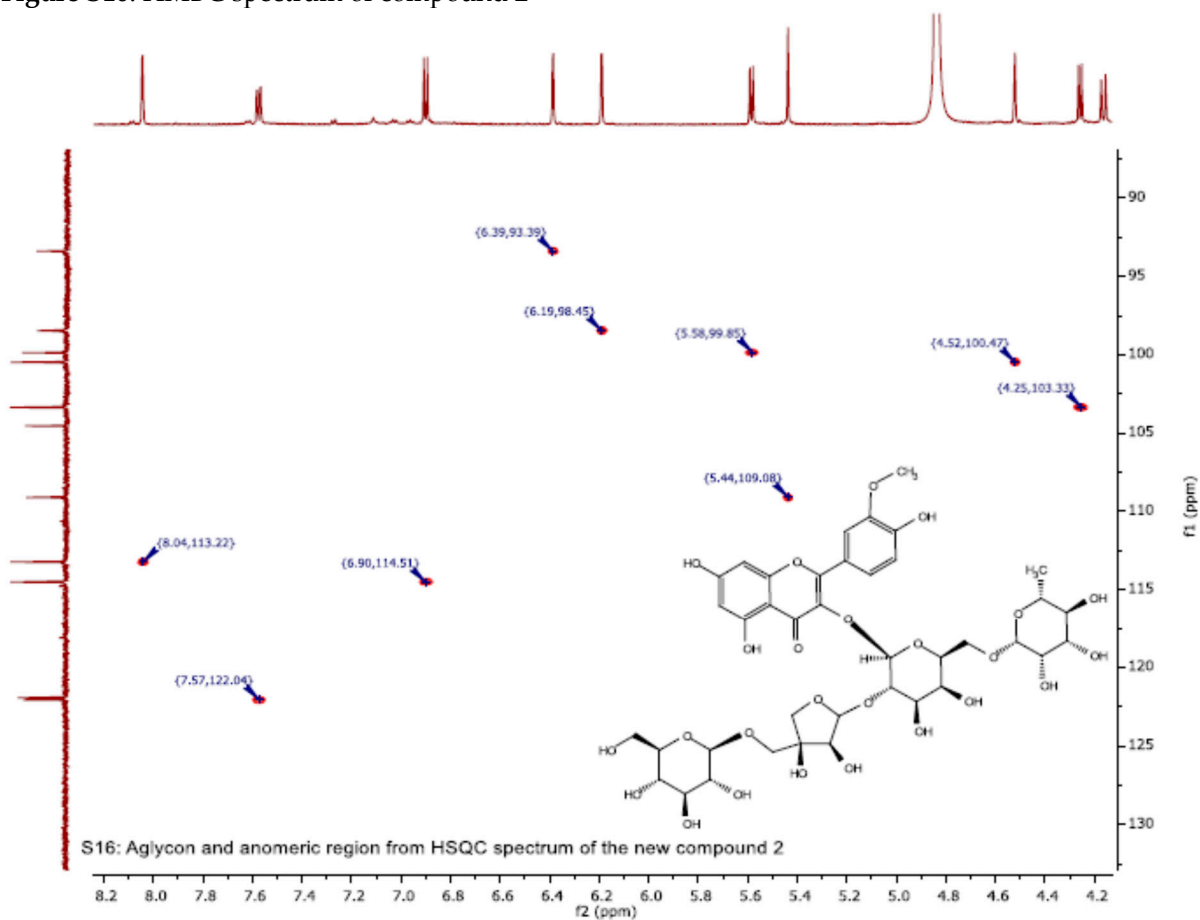


Figure S17: HSQC spectrum of compound 2 (aglycon and anomeric region)

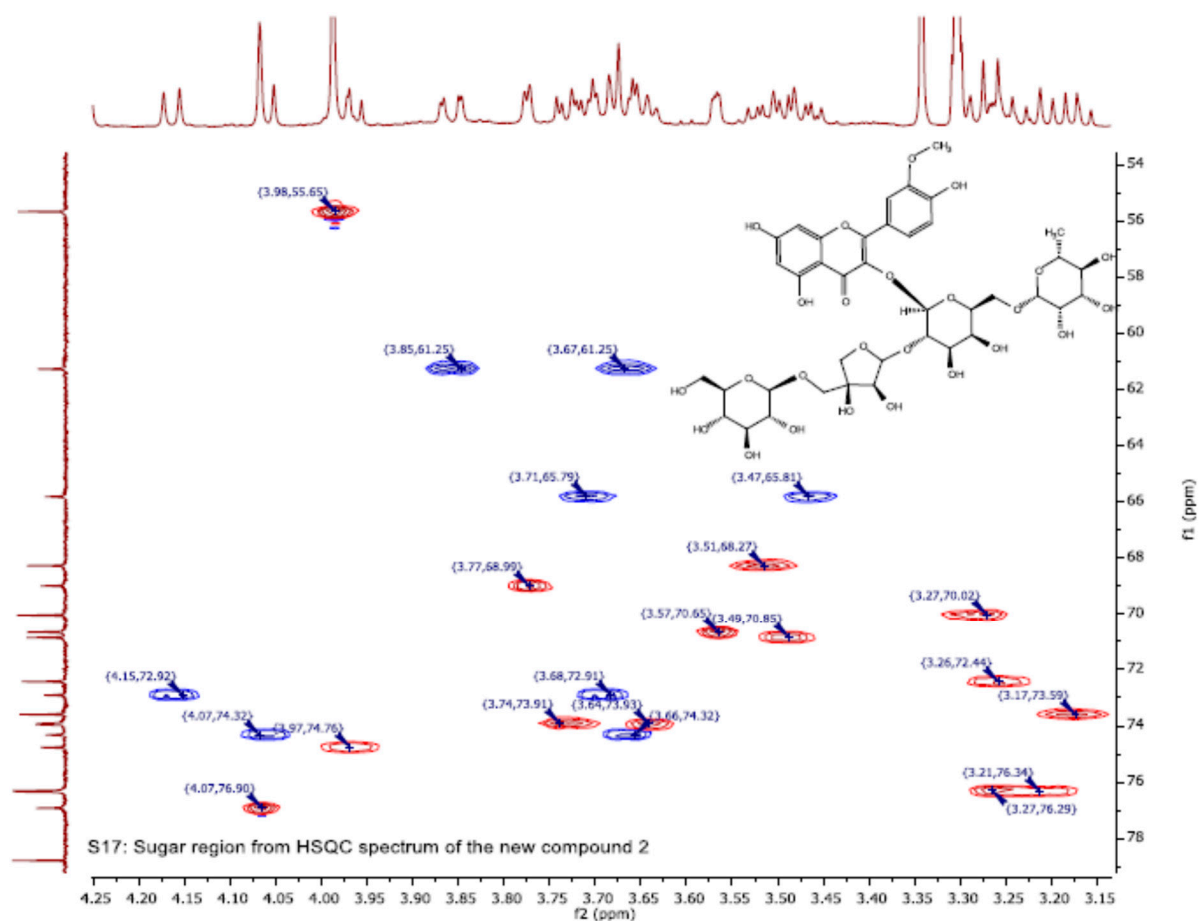


Figure S18: HSQC spectrum of compound 2 (sugar region)

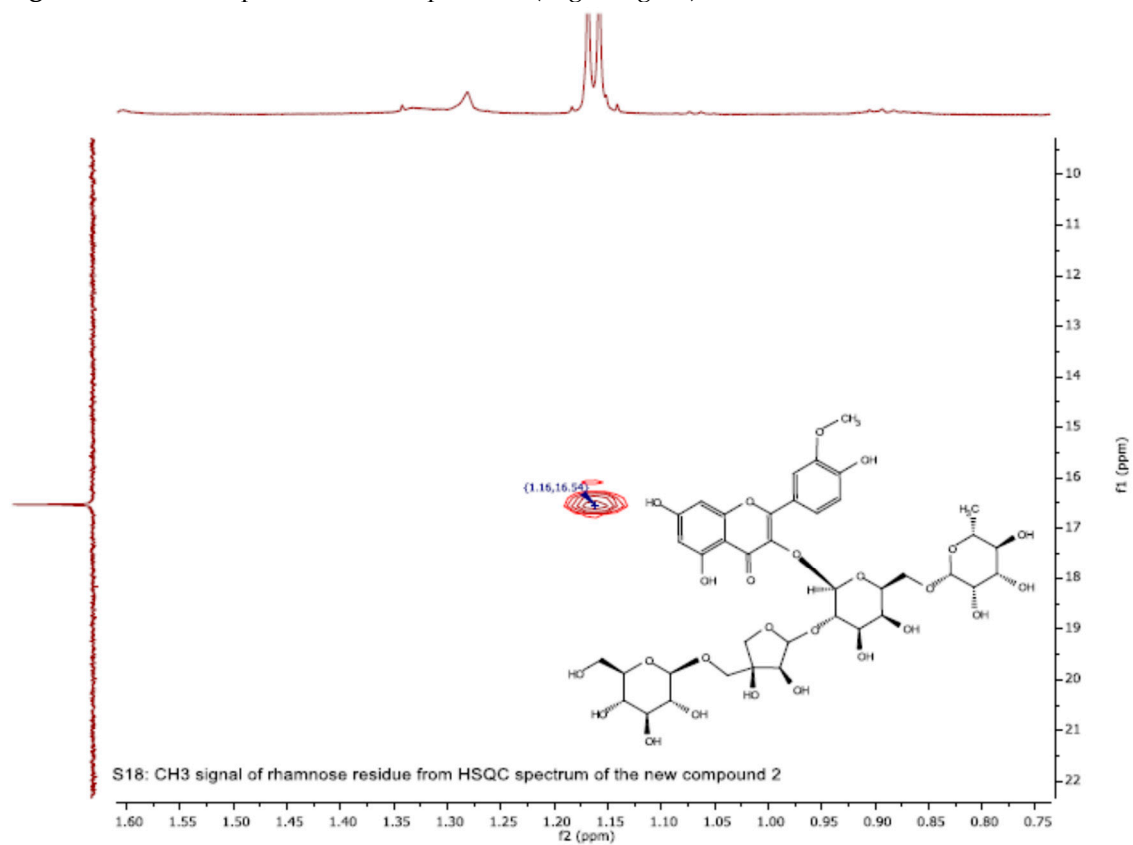


Figure S19: HSQC spectrum of compound 2 (methyl signal of rhamnose moiety)

Histo_08_161219 #2797-2849 RT: 6.40-6.5
T: FTMS - p ESI Full ms [100.00-1500.00]

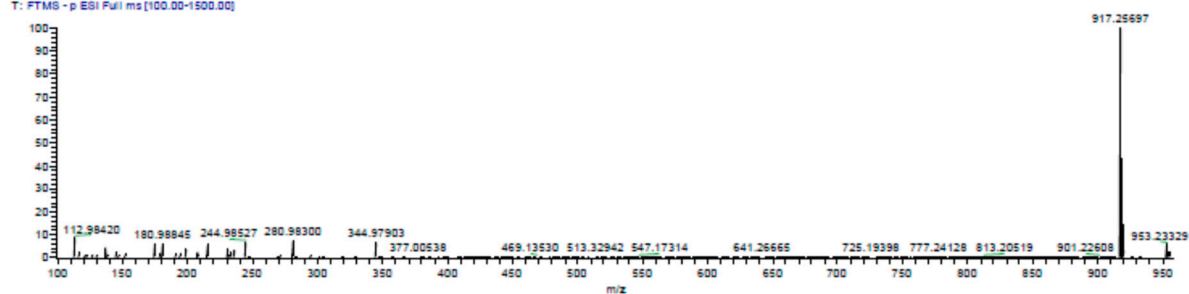


Figure S20: HR-ESI-MS (negative mode) of compound 2

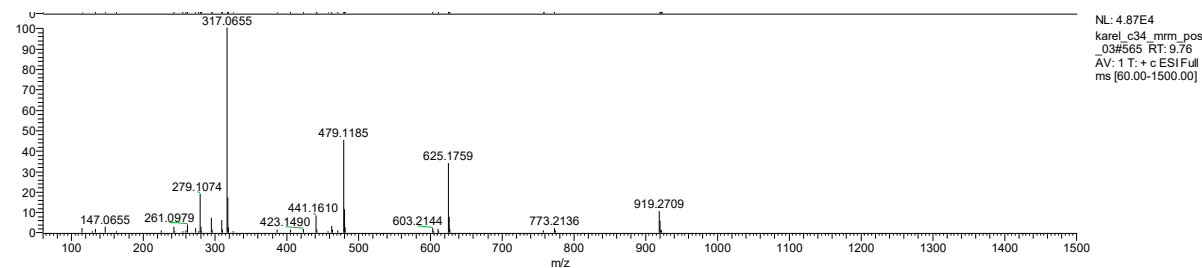


Figure S21: HR-ESI-MS (positive mode) of compound 2

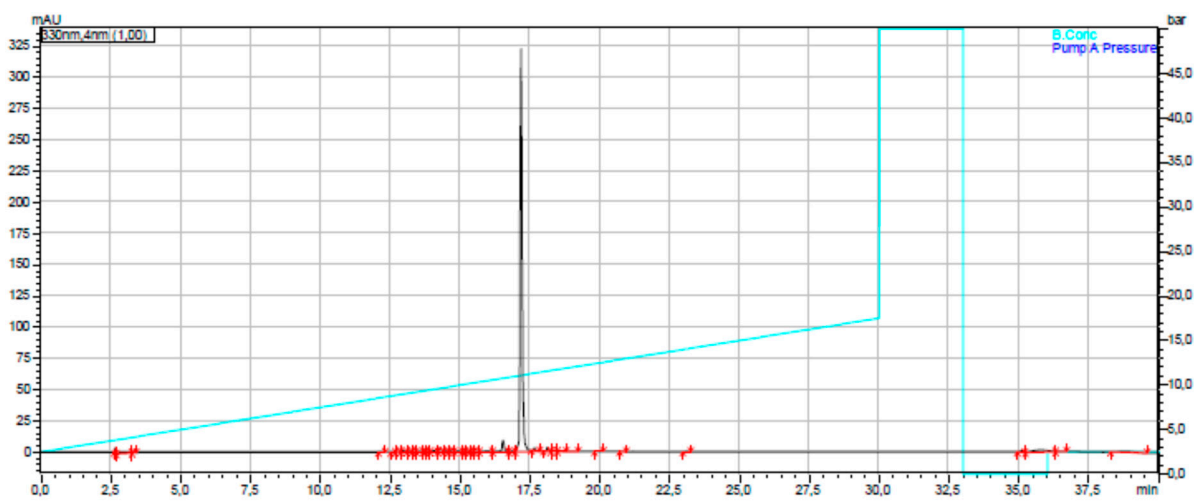


Figure S22: HPLC chromatogram of compound 2

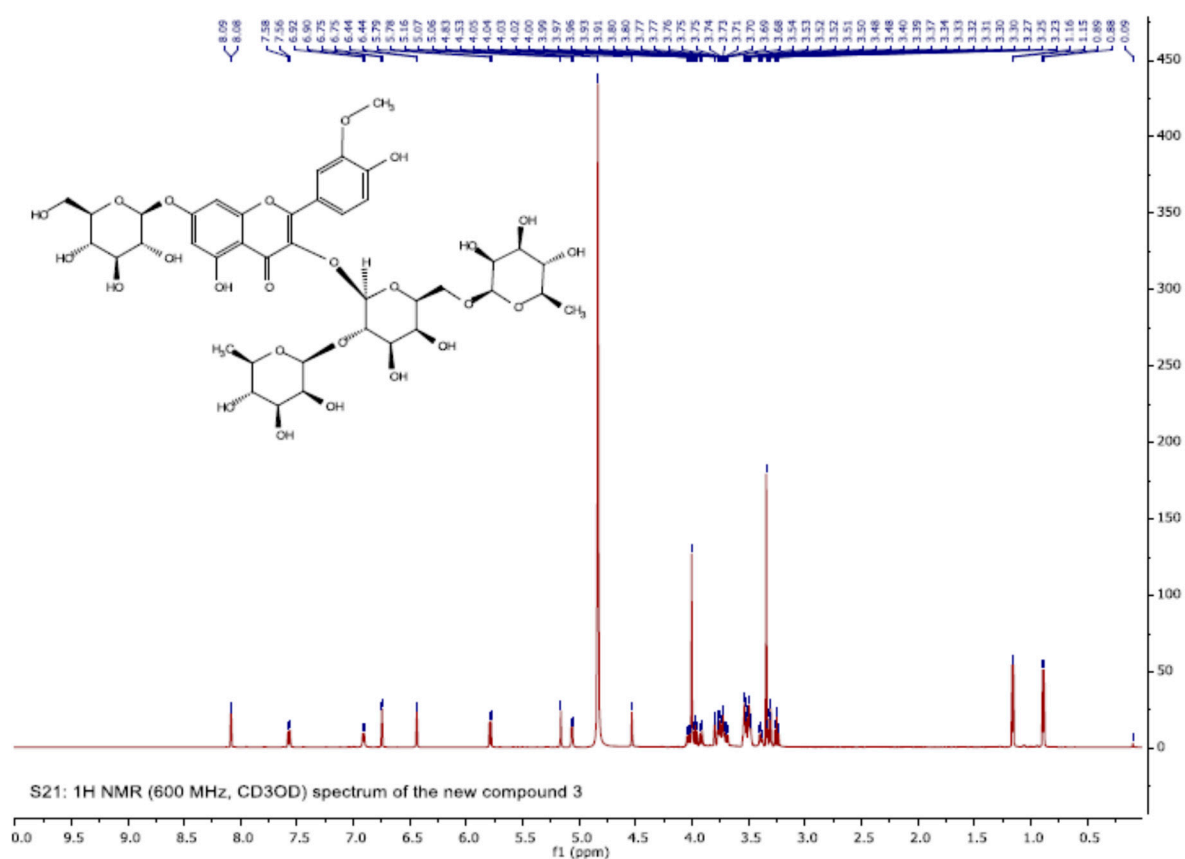


Figure S23: ¹H NMR (600 MHz, CD₃OD) spectrum of compound 3

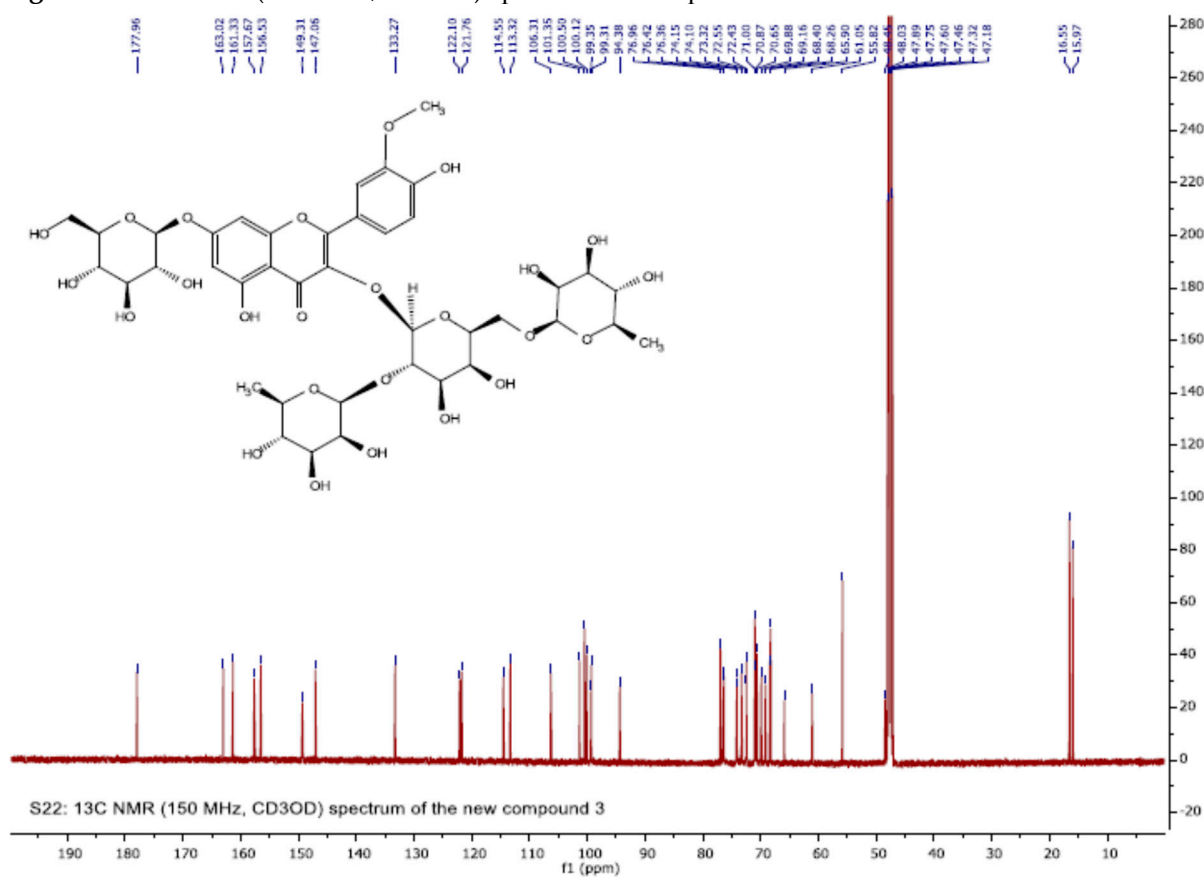


Figure S24: ¹³C NMR (600 MHz, CD₃OD) spectrum of compound 3

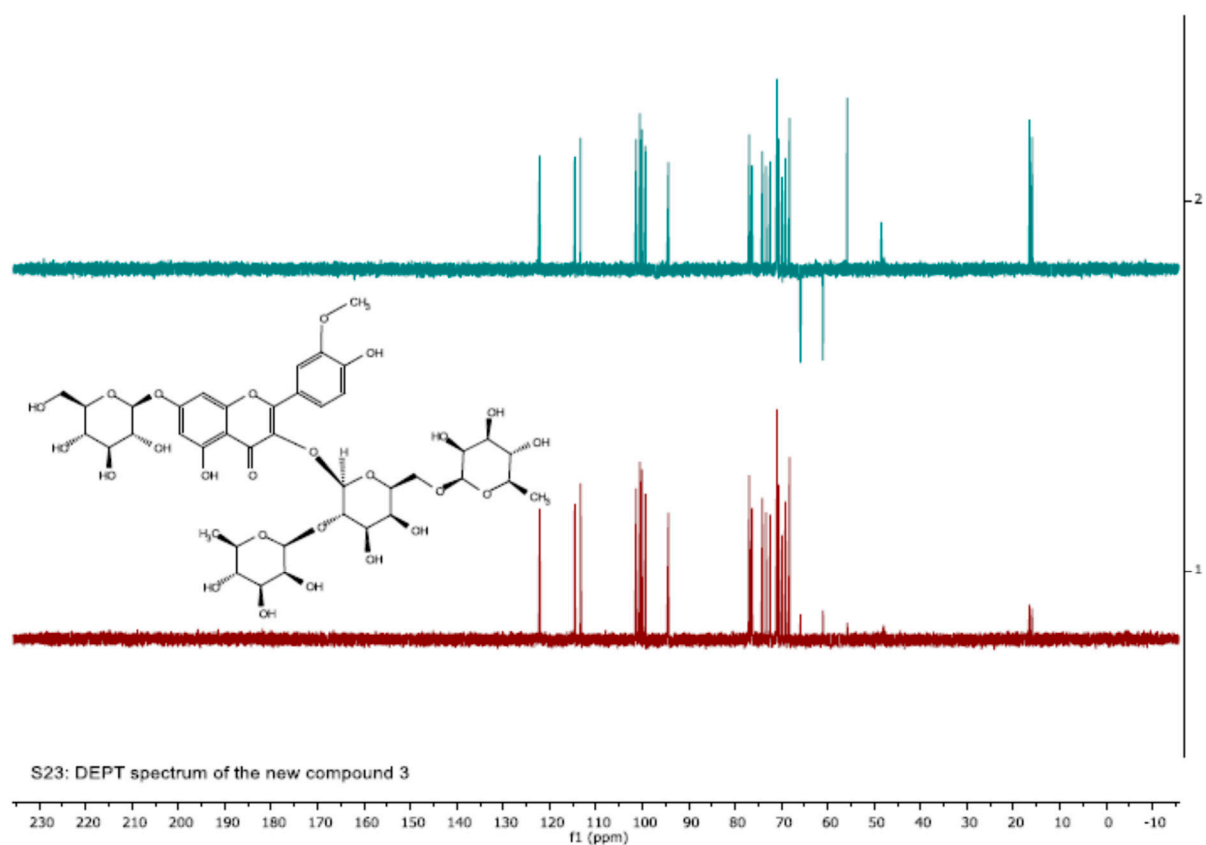


Figure S25: DEPT spectrum of compound 3

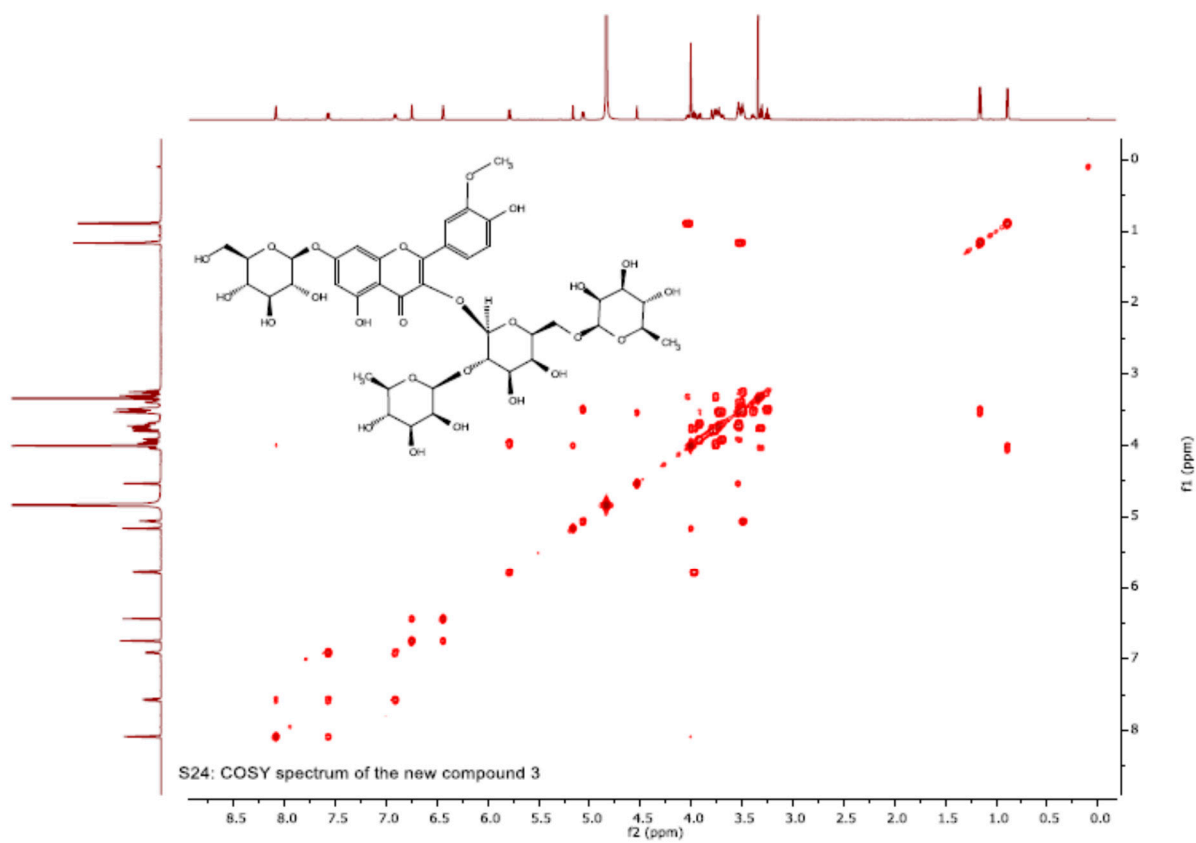


Figure S26: COSY spectrum of compound 3

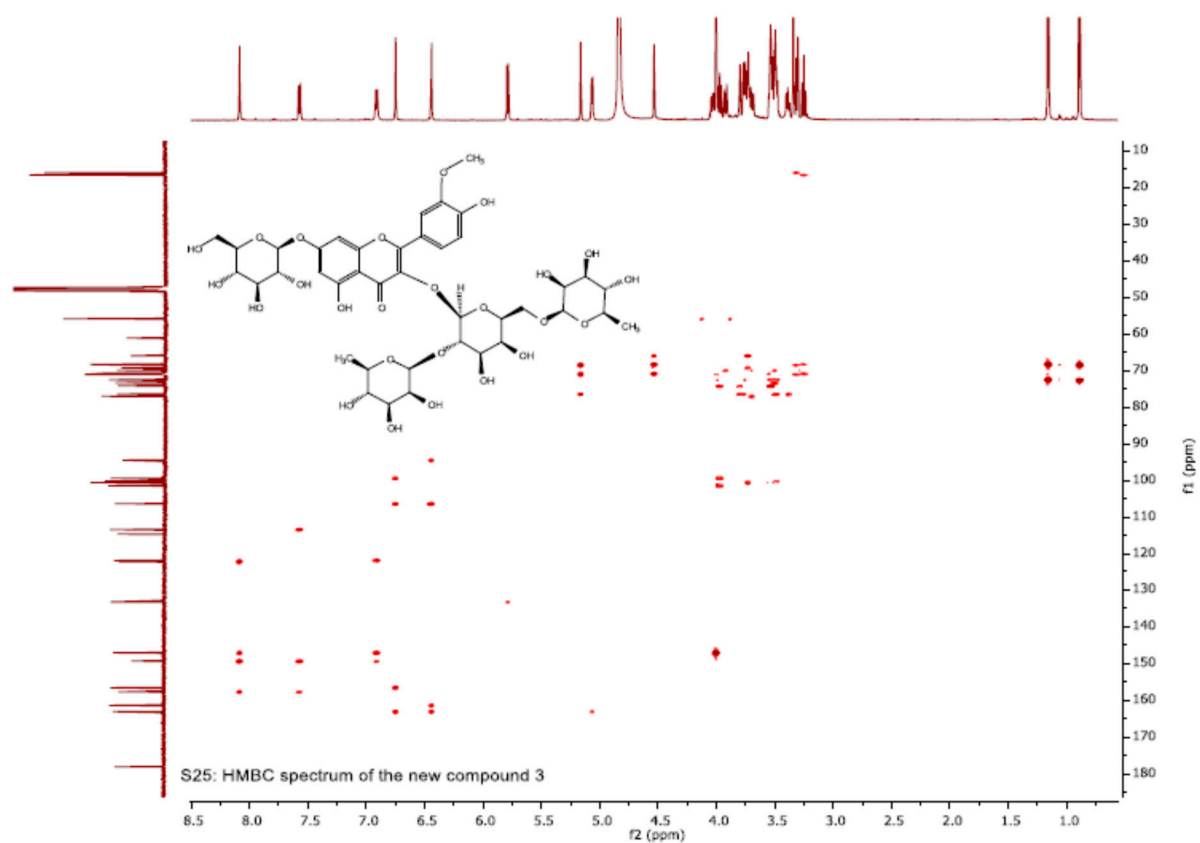


Figure S27: HMBC spectrum of compound 3

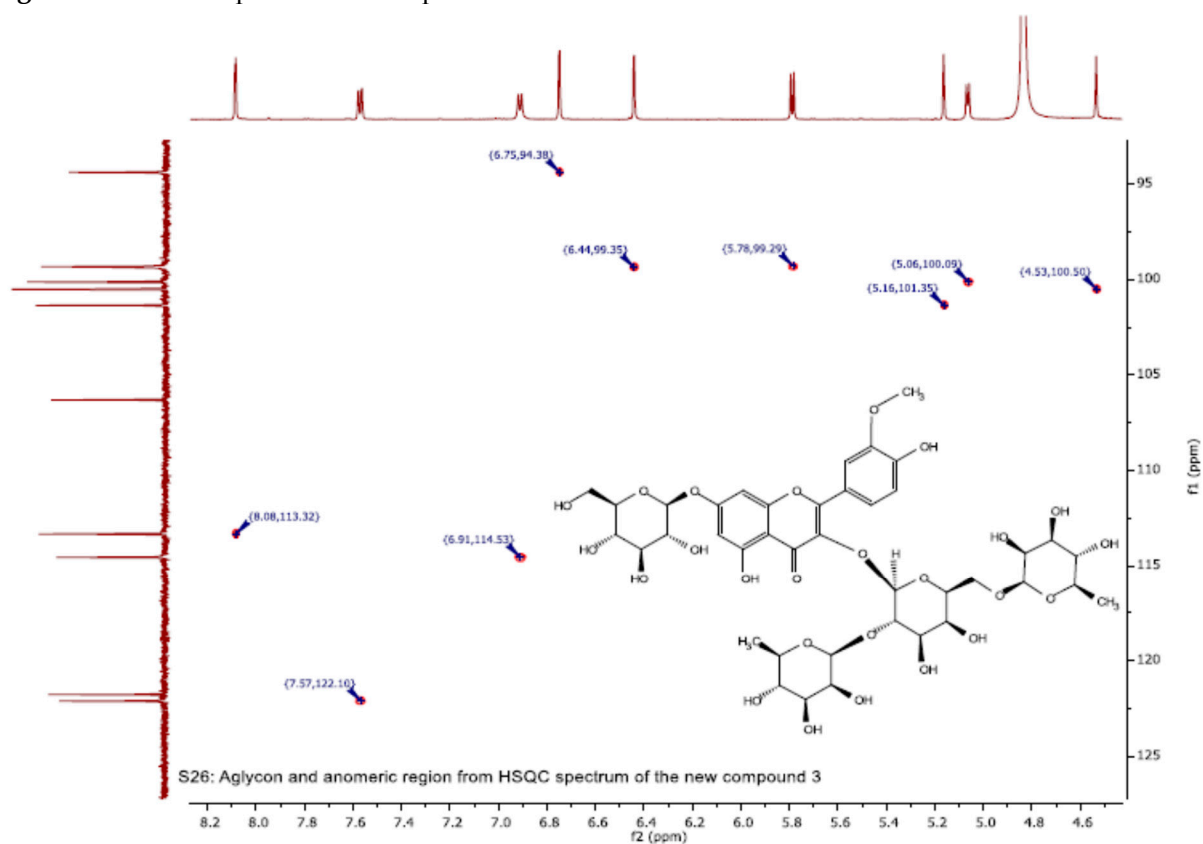


Figure S28: HSQC spectrum of compound 3 (aglycon and anomeric region)

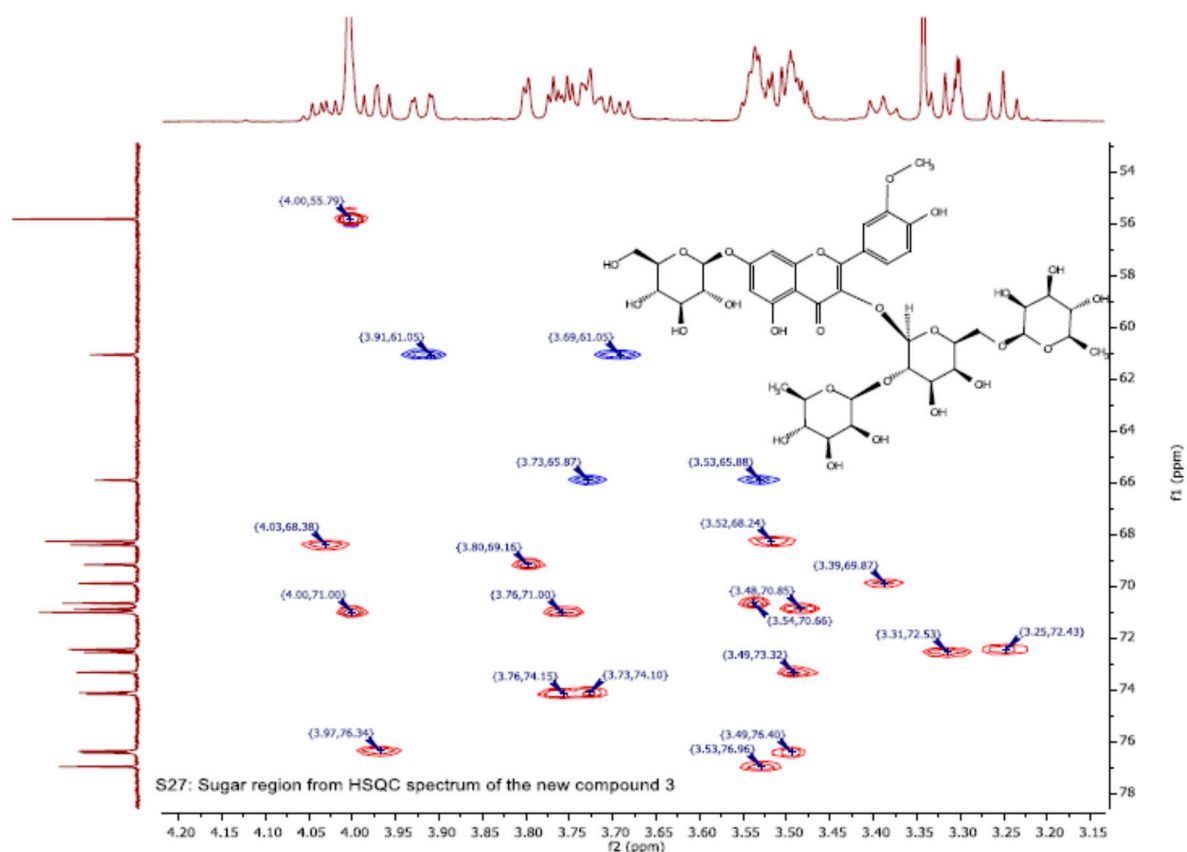


Figure S29: HSQC spectrum of compound 3 (sugar region)

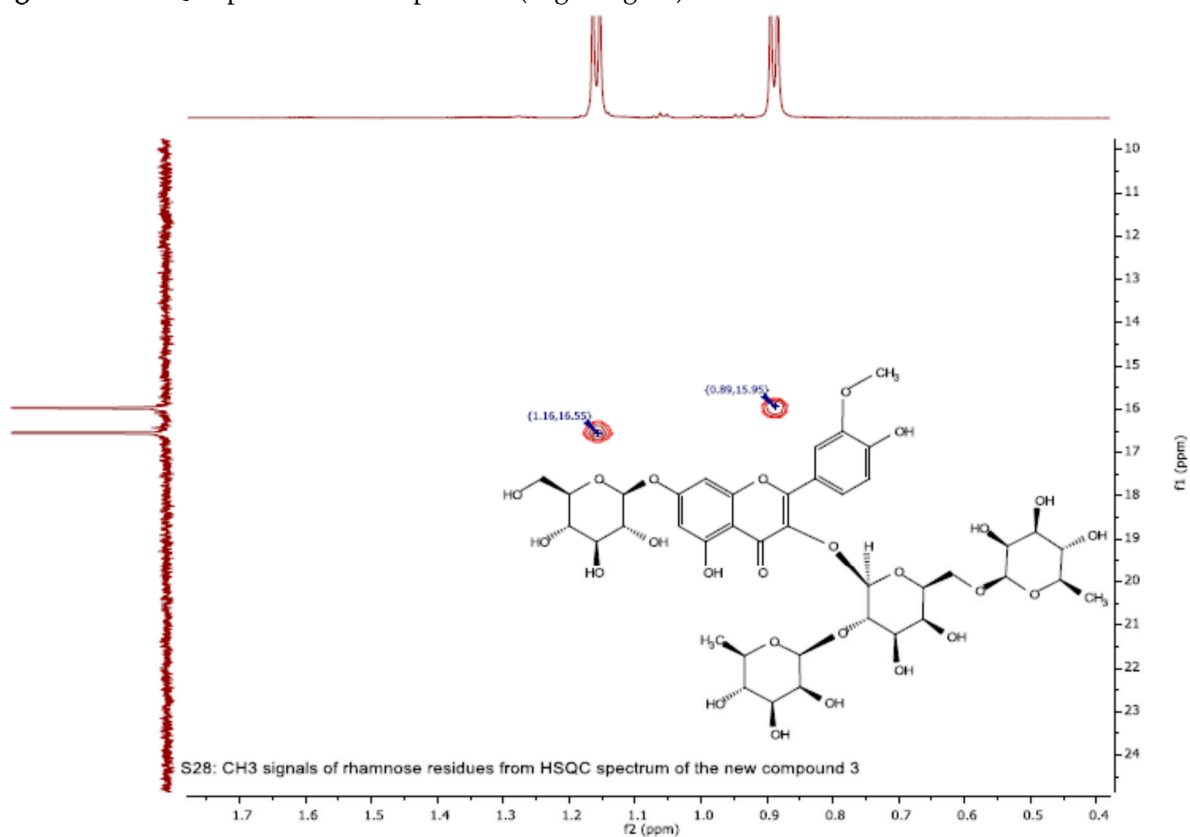
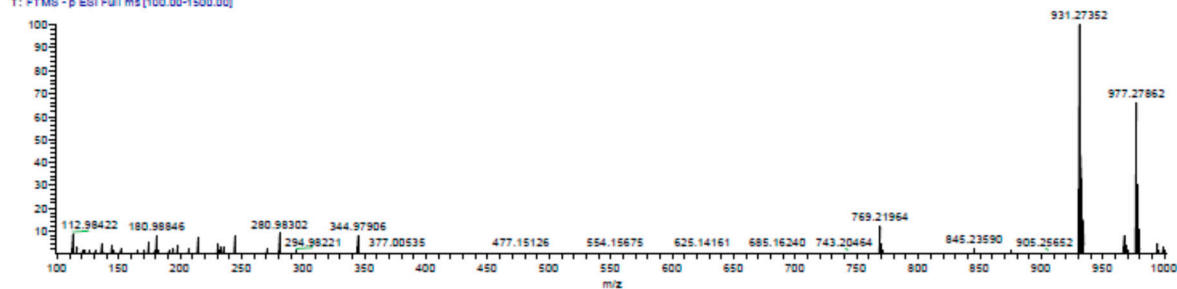
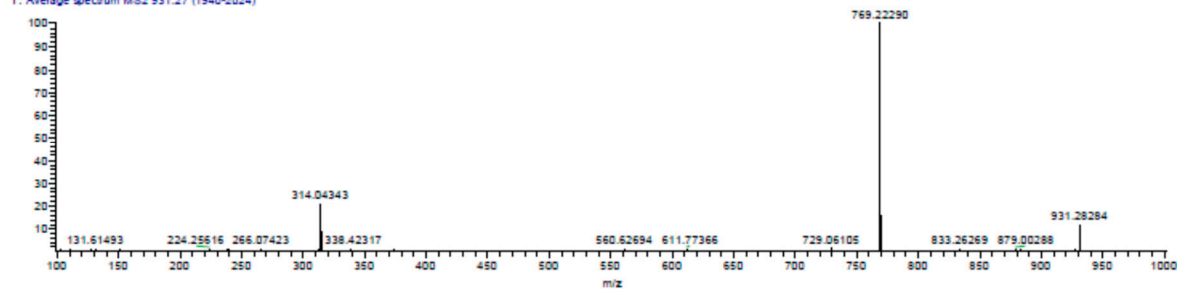


Figure S30: HSQC spectrum of compound 3 (methyl signals of rhamnose moieties)

Histo_07_161219 #1925-2011 RT: 4.53-4.7
T: FTMS - p ESI Full ms [100.00-1500.00]



Histo_07_161219 #1940-2024 RT: 4.56-4.74 AV: 2 NL: 1.17E5
T: Average spectrum MS2 931.27 (1940-2024)



S29: HR-ESI-MS (ESI negative mode) spectrum of the new compound 3

Up: full-scan

Down: MS2 of 931.27352 m/z

Figure S31: HR-ESI-MS (negative mode) of compound 3

Karel_3 B22-32_MRM_Pos_01 #511 RT: 8.83 AV: 1 NL: 2.22E4
T: + c ESI Full ms [60.00-1500.00]

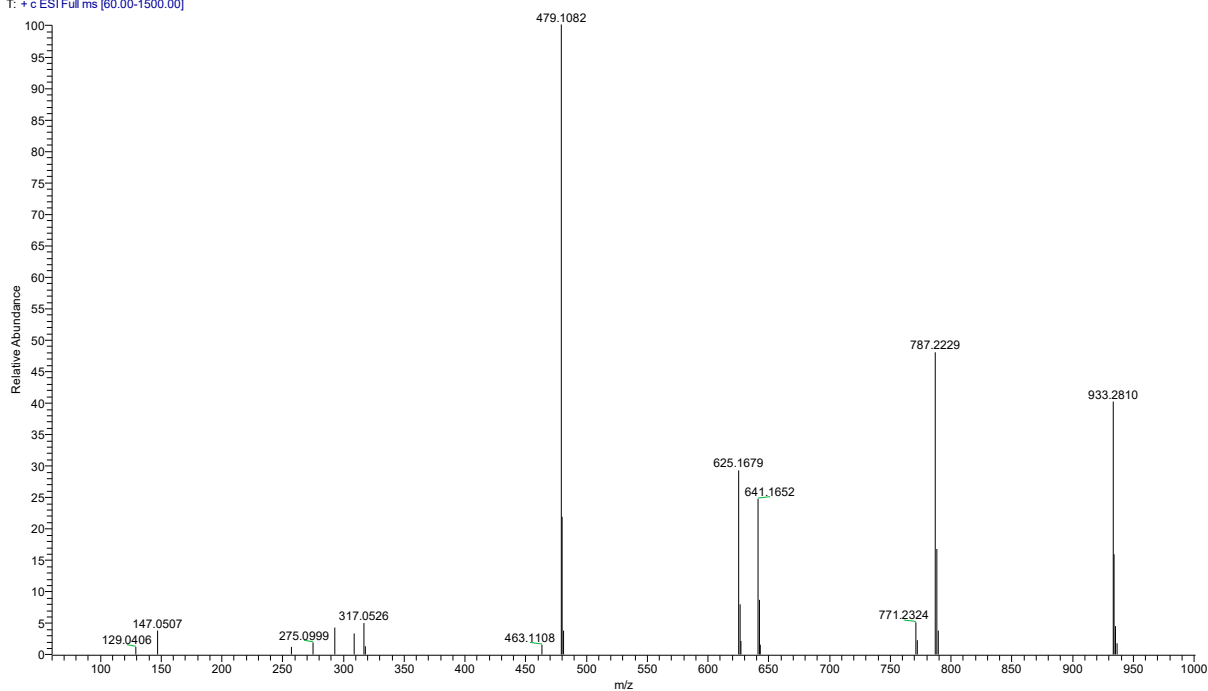


Figure S32: HR-ESI-MS (positive mode) of compound 3

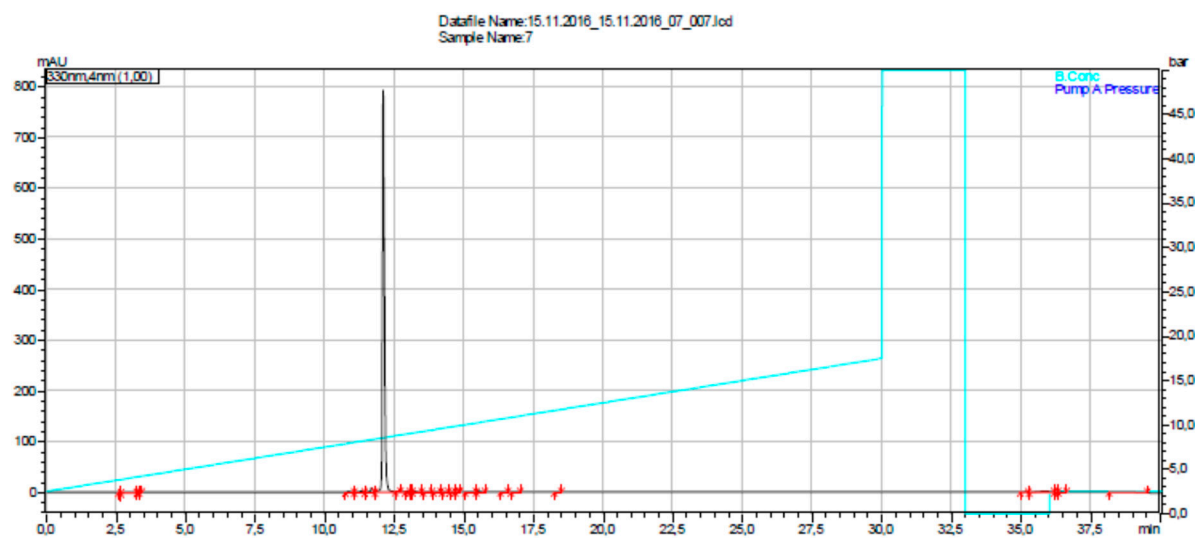


Figure S33: HPLC chromatogram of compound 3

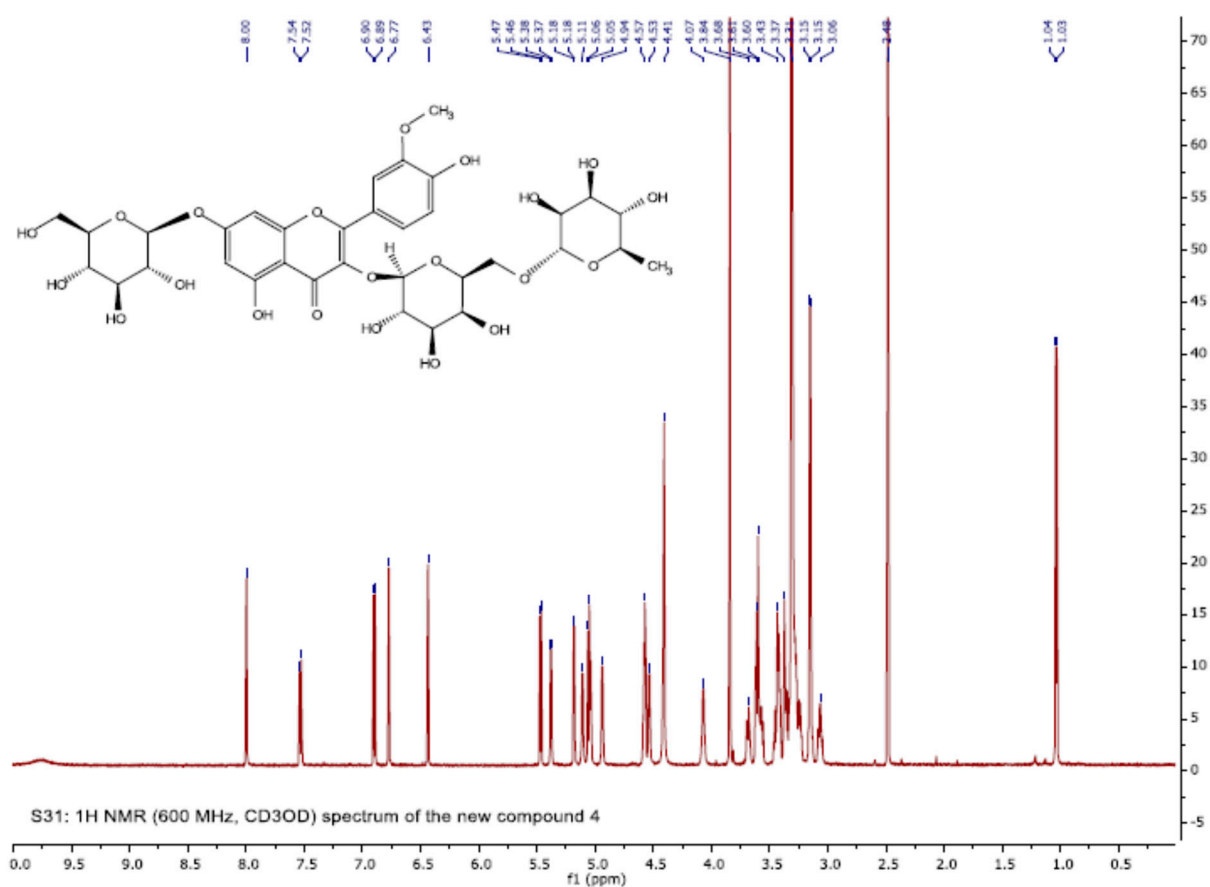


Figure S34: ^1H NMR (600 MHz, CD_3OD) spectrum of compound 4

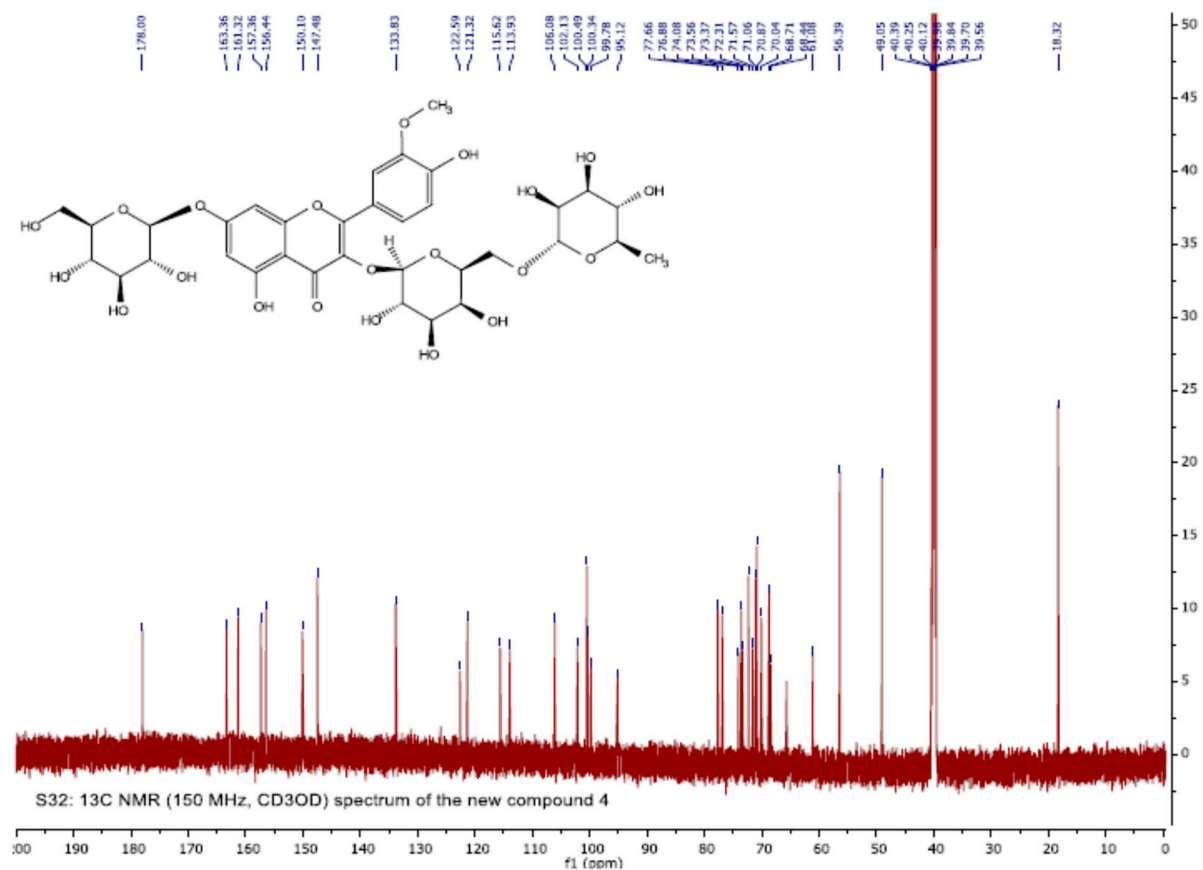


Figure S35: ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound 4

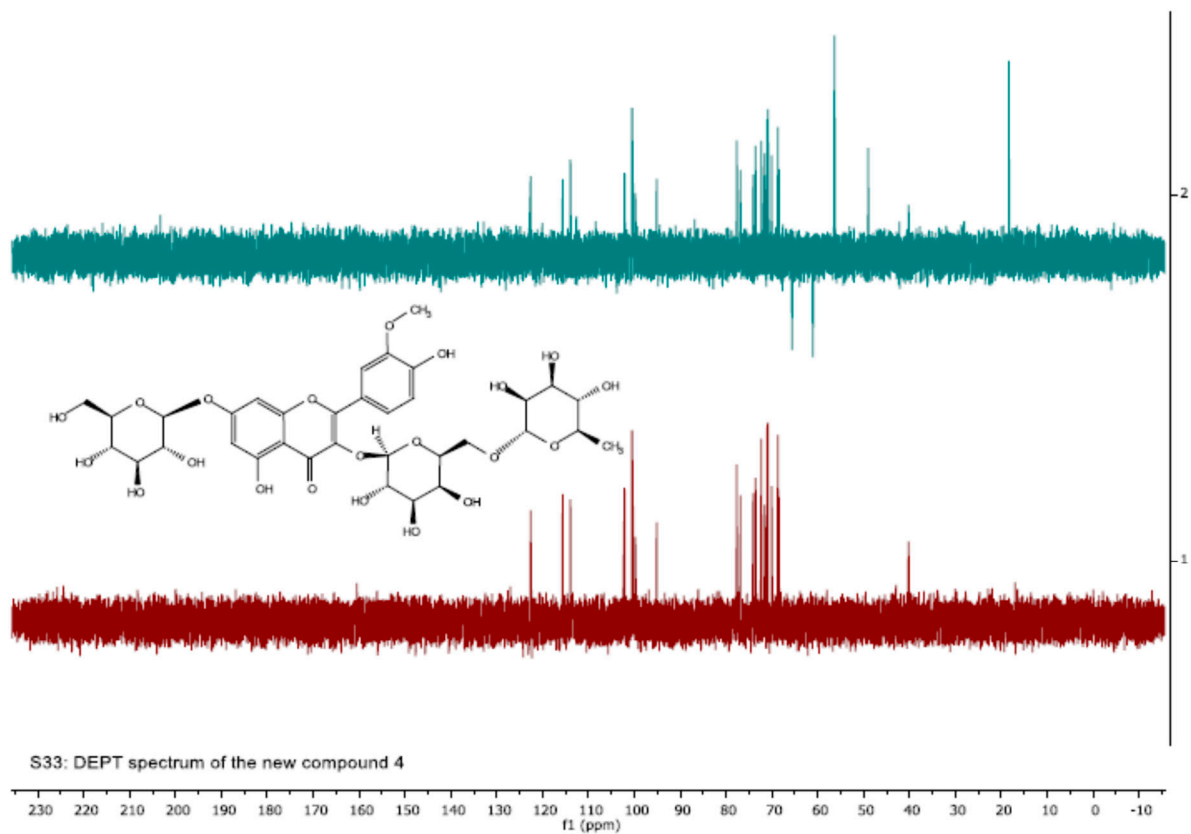


Figure S36: DEPT spectrum of compound 4

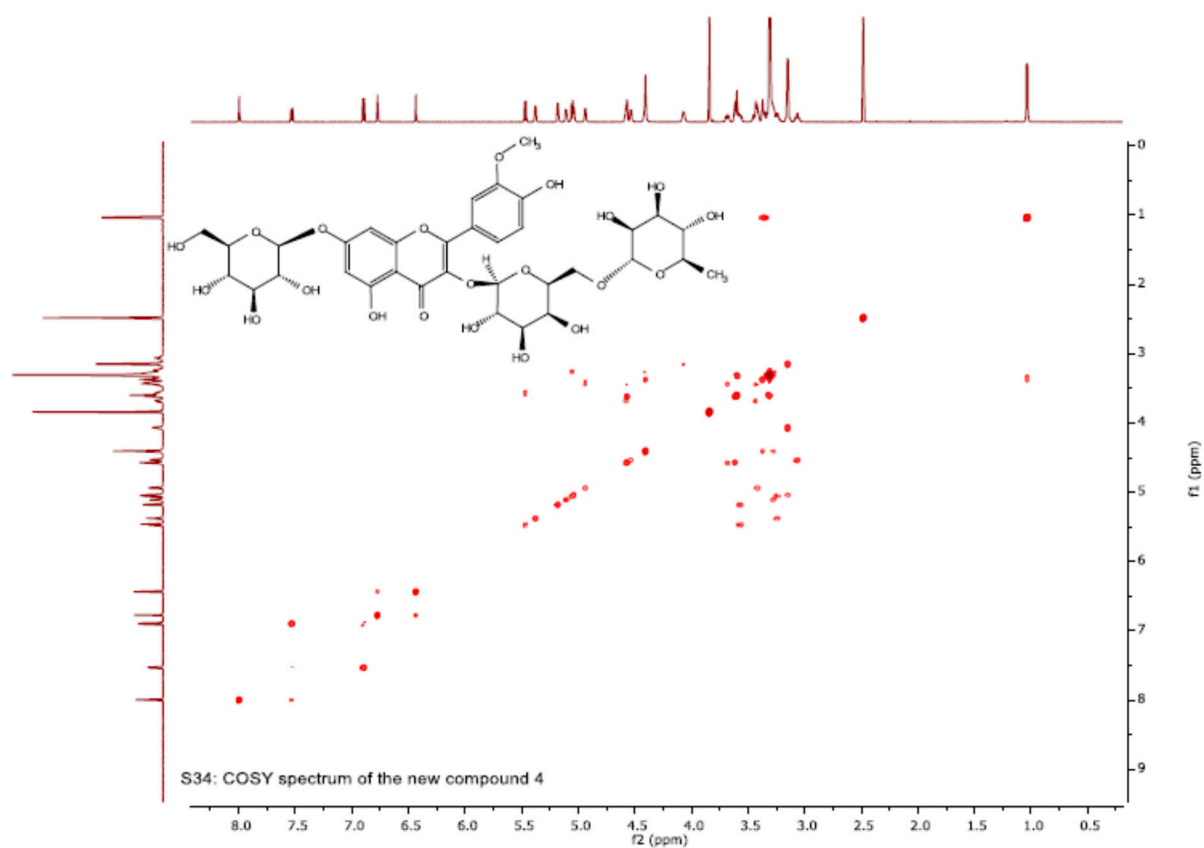


Figure S37: COSY spectrum of compound 4

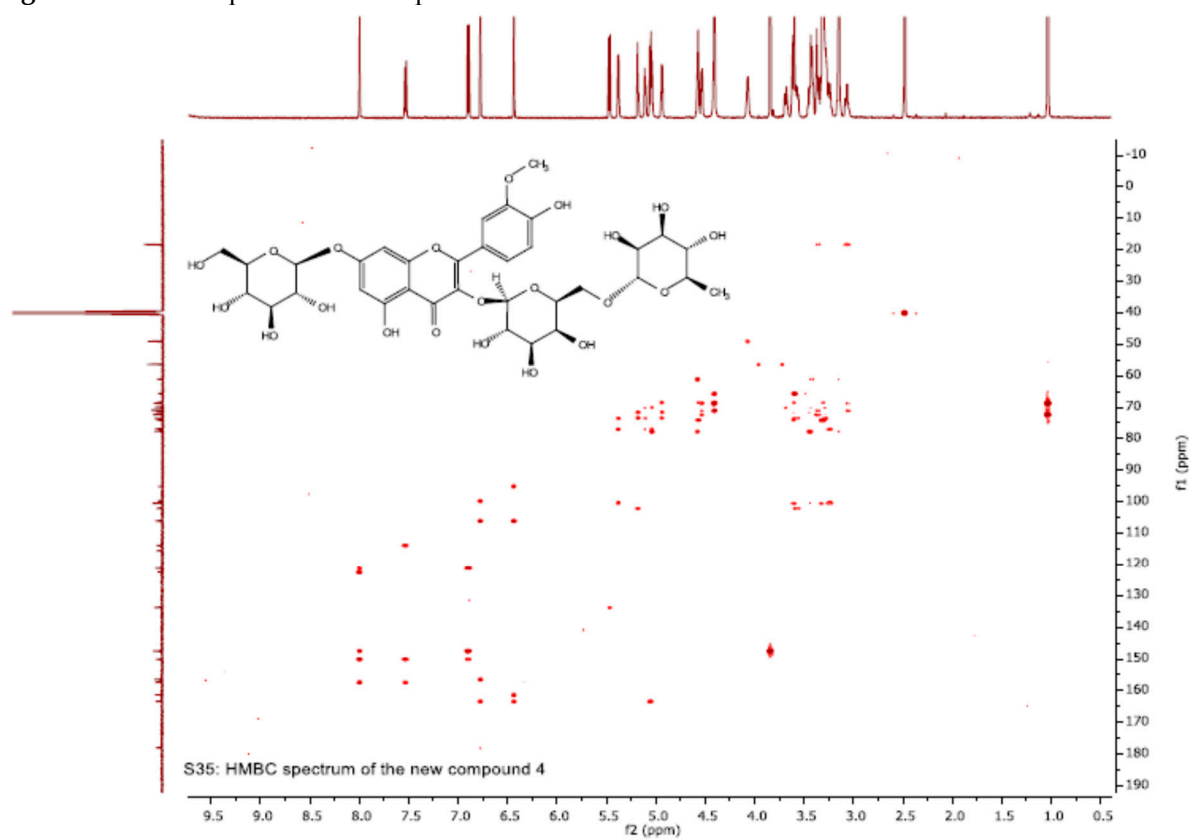


Figure S38: HMBC spectrum of compound 4

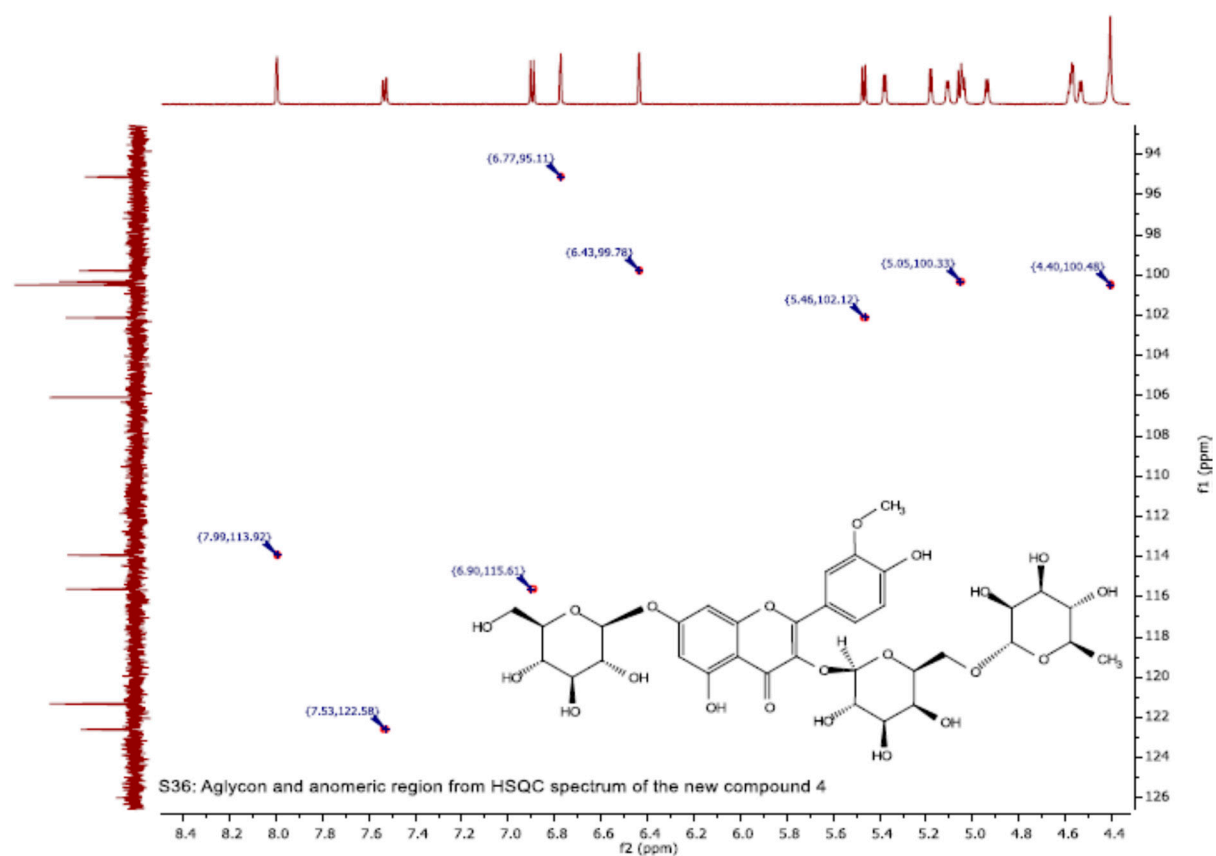


Figure S39: HSQC spectrum of compound 4 (aglycon and anomeric region)

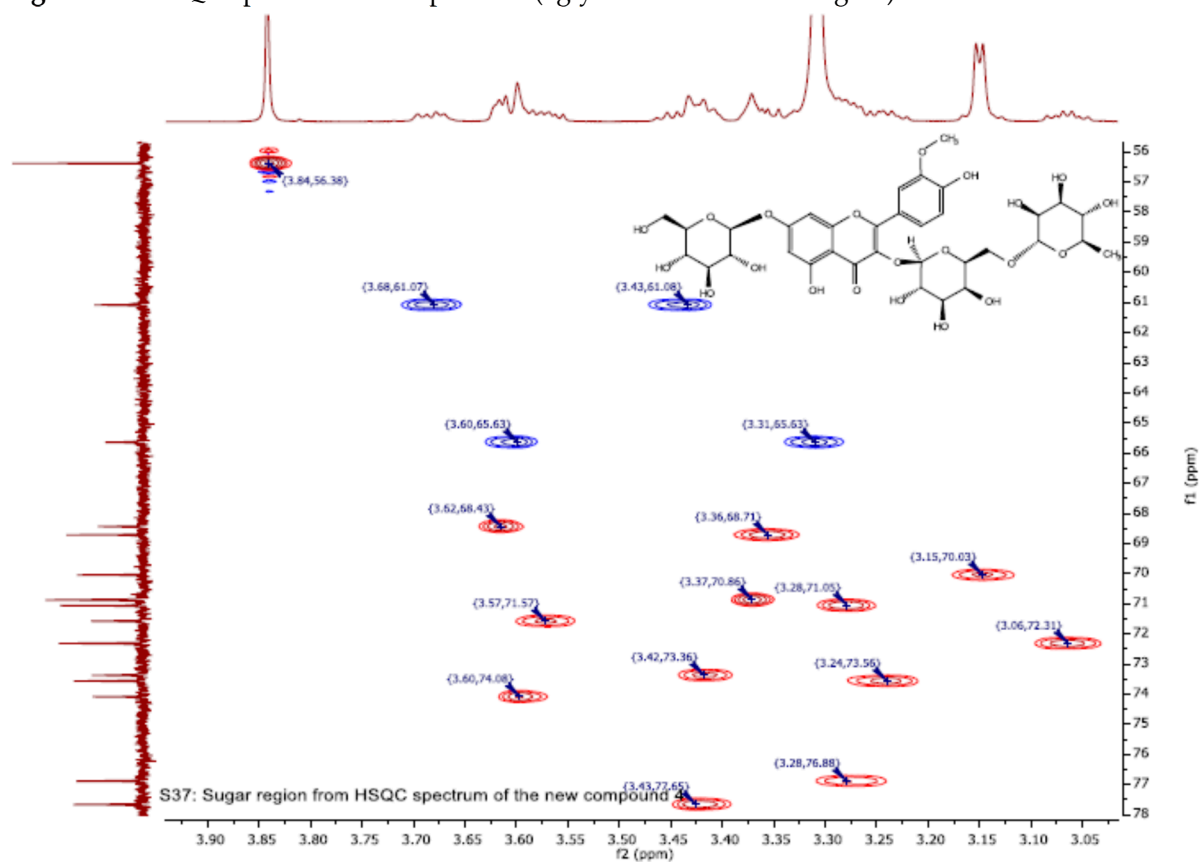


Figure S40: HSQC spectrum of compound 4 (sugar region)

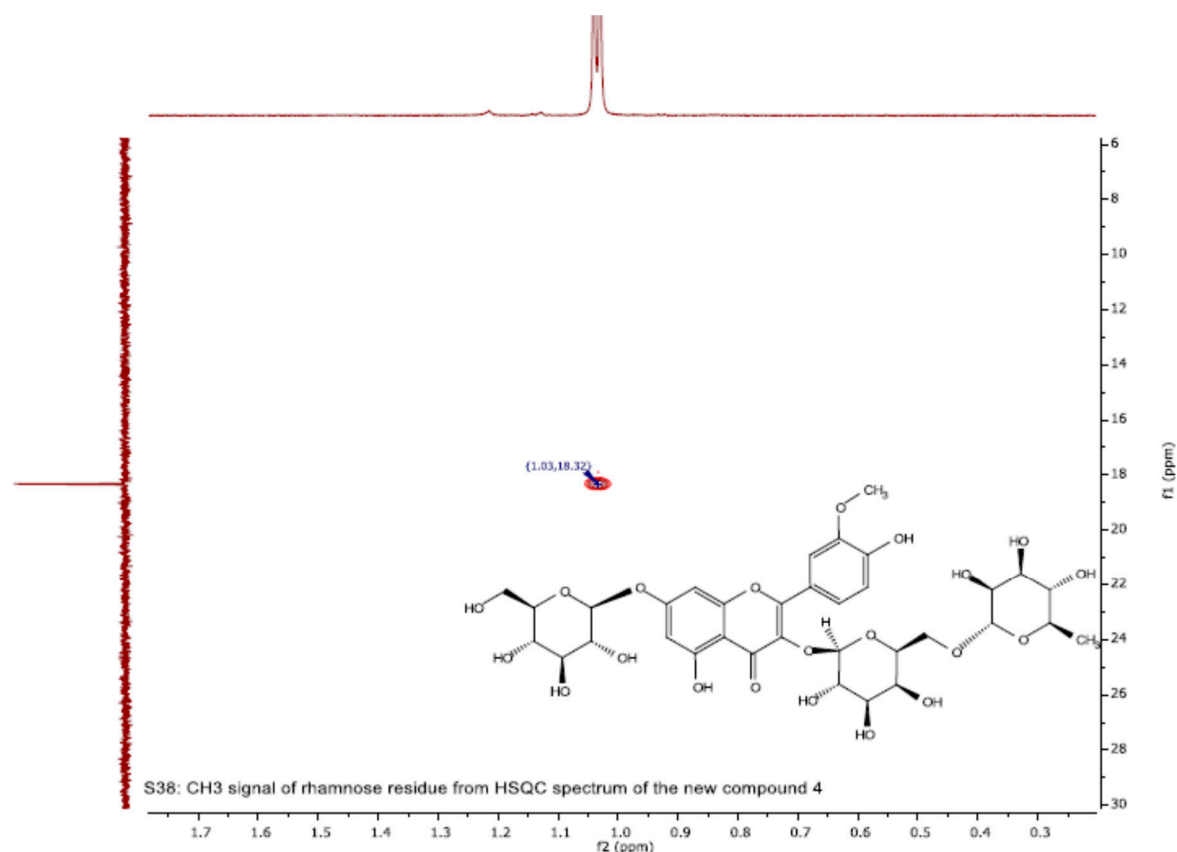
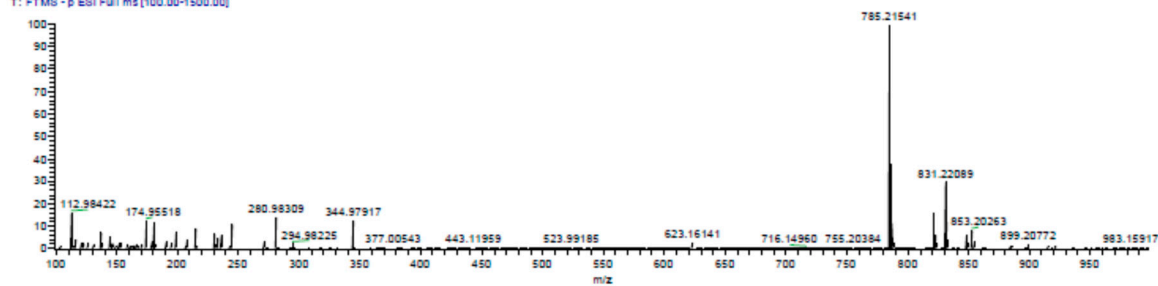


Figure S41: HSQC spectrum of compound 3 (methyl signals of rhamnose moiety)

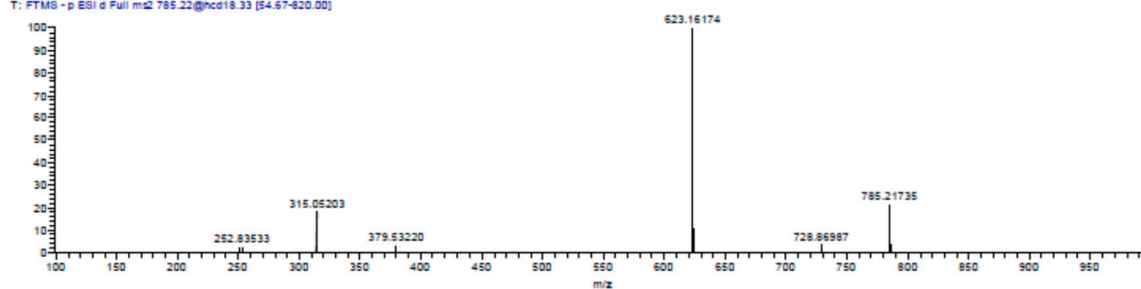
E:\a PhD HR-MS BGL\Histo_10_

12/19/16 20:28:38

Hrldo_10_161219 #2230-2273 RT: 5.35-5.4
T: FTMS - p ESI Full ms [100.00-1500.00]



Hrldo_10_161219 #2236 RT: 5.36 AV: 1 NL: 9.5254
T: FTMS - p ESI d Full ms2 785.22@hcd18.33 [54.67-820.00]



S39: HR-ESI-MS (ESI negative mode) spectrum of the new compound 4

Up: full-scan

Down: MS2 of 785.21541 m/z

Figure S42: HR-ESI-MS (negative mode) of compound 4

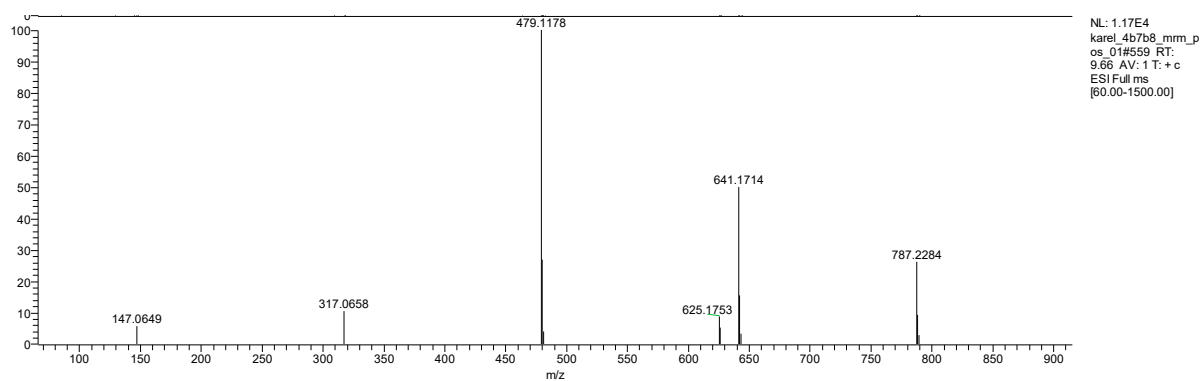


Figure S43: HR-ESI-MS (positive mode) of compound 4

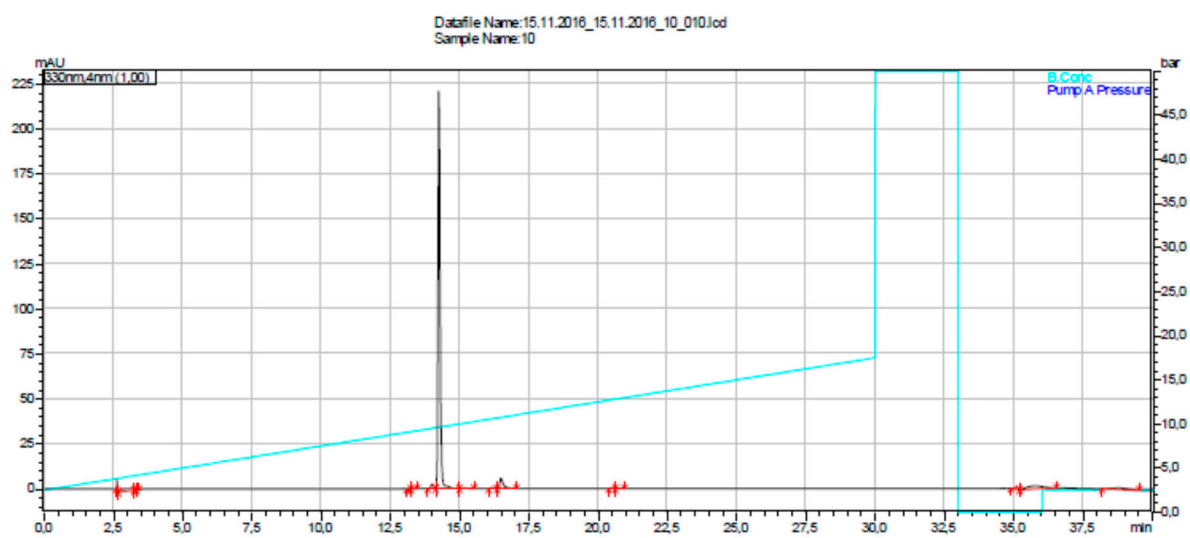


Figure S44: HPLC chromatogram of compound 4

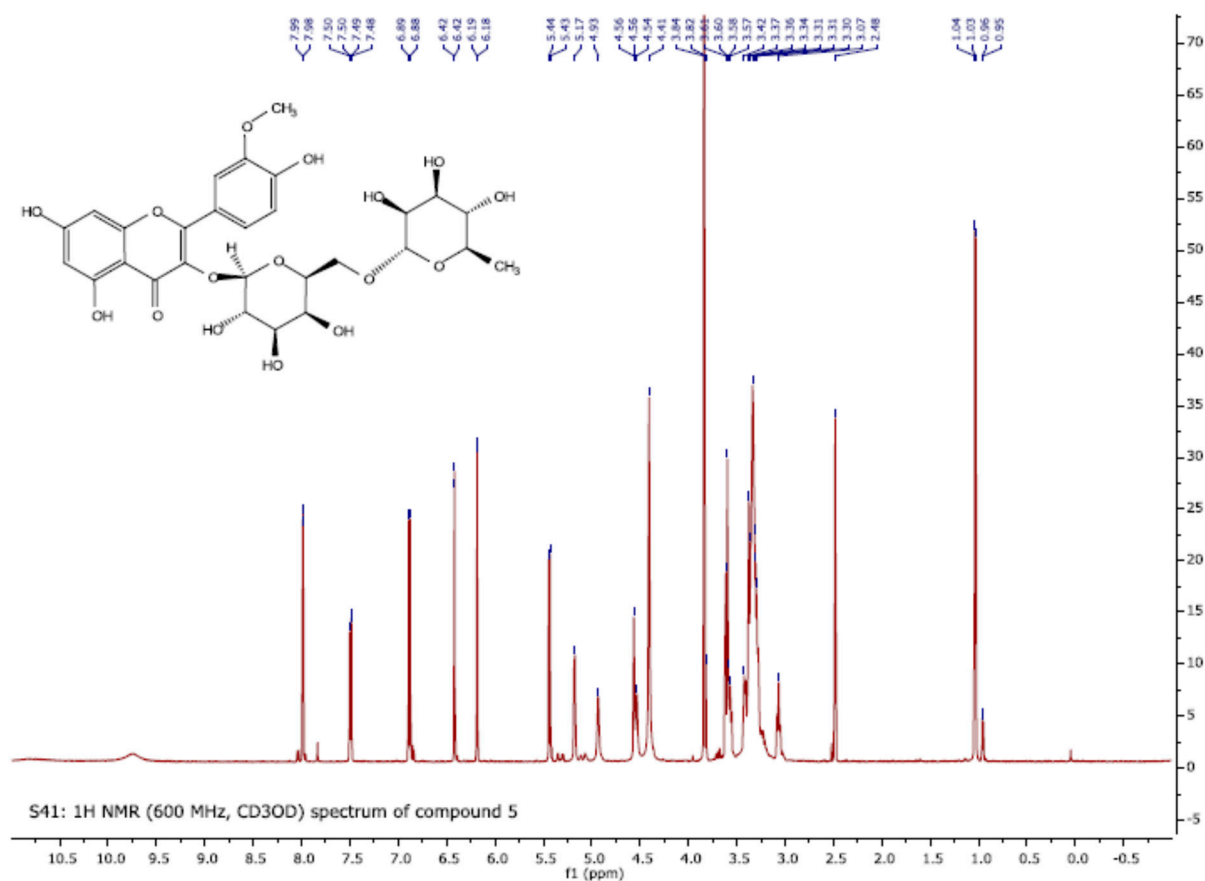


Figure S45: ^1H NMR (600 MHz, CD_3OD) spectrum of compound 5

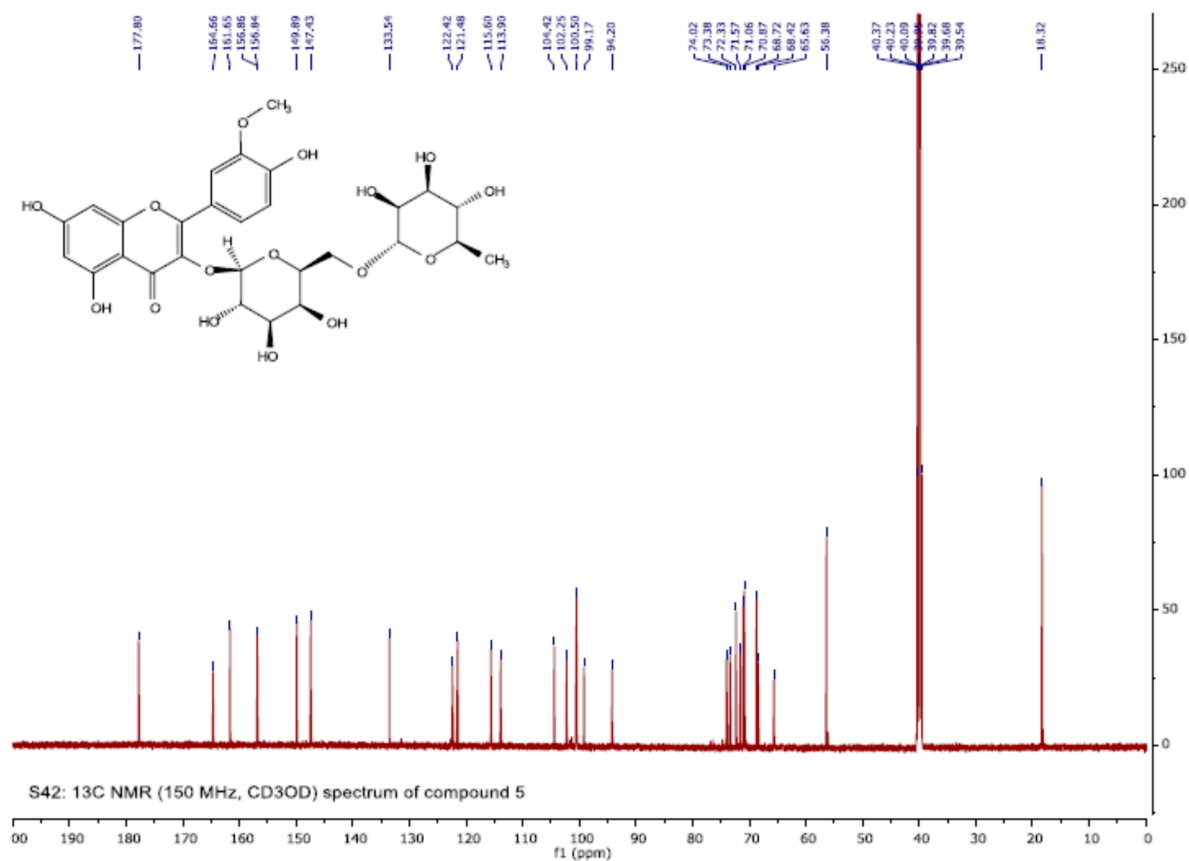


Figure S46: ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound 5

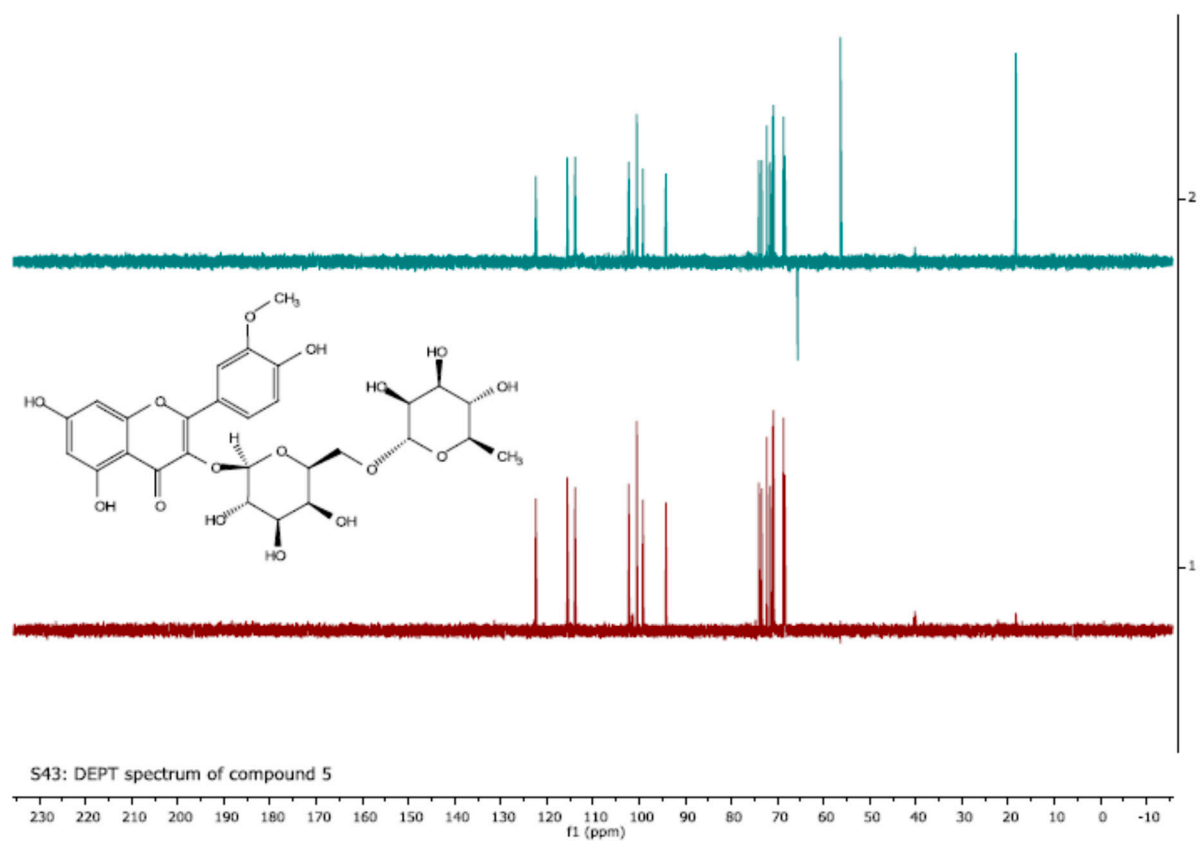


Figure S47: DEPT spectrum of compound 5

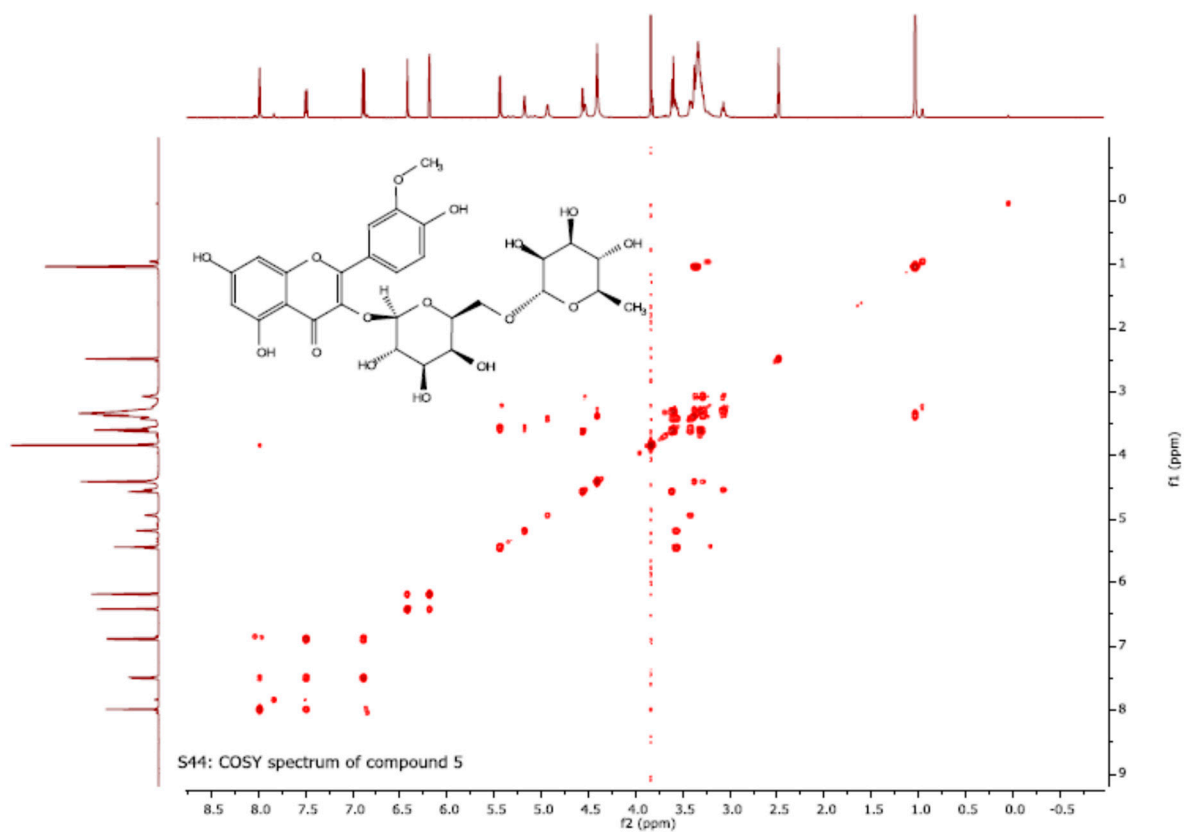


Figure S48: COSY spectrum of compound 5

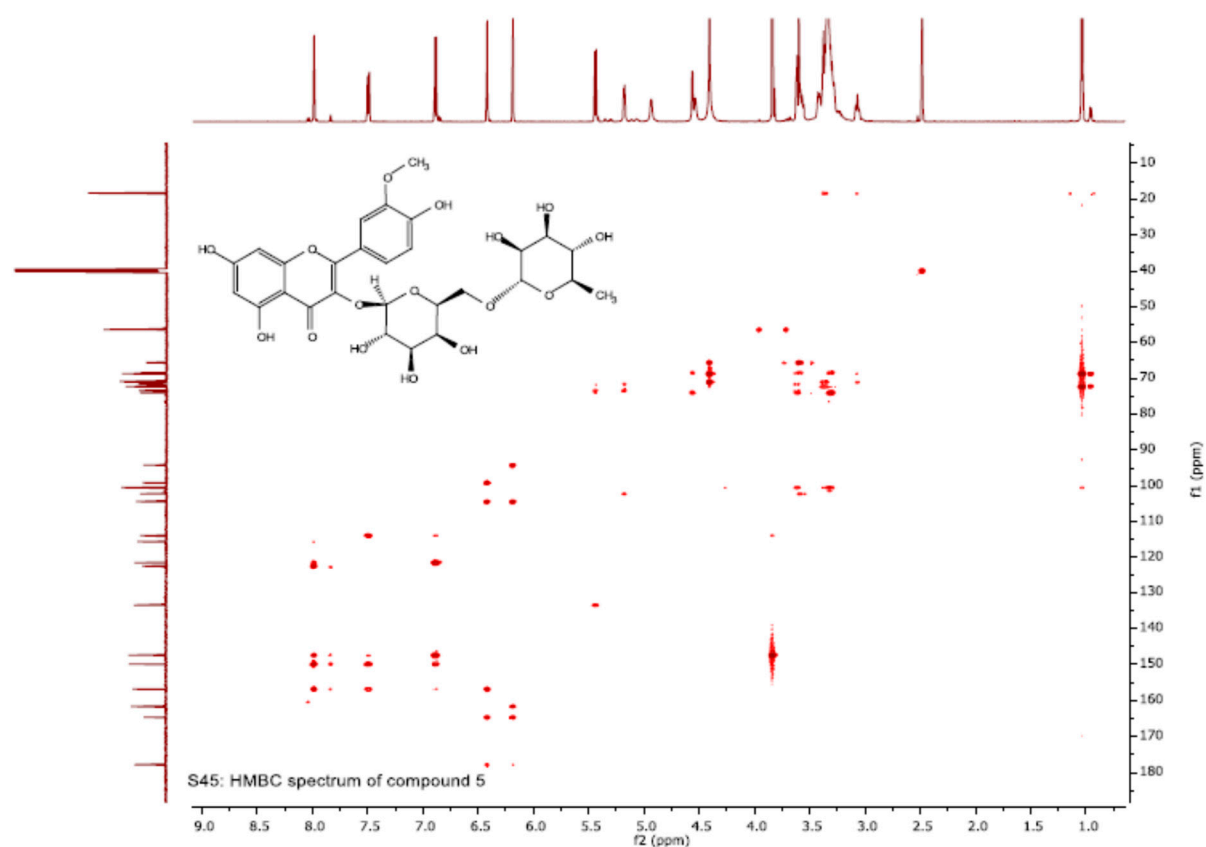


Figure S49: HMBC spectrum of compound 5

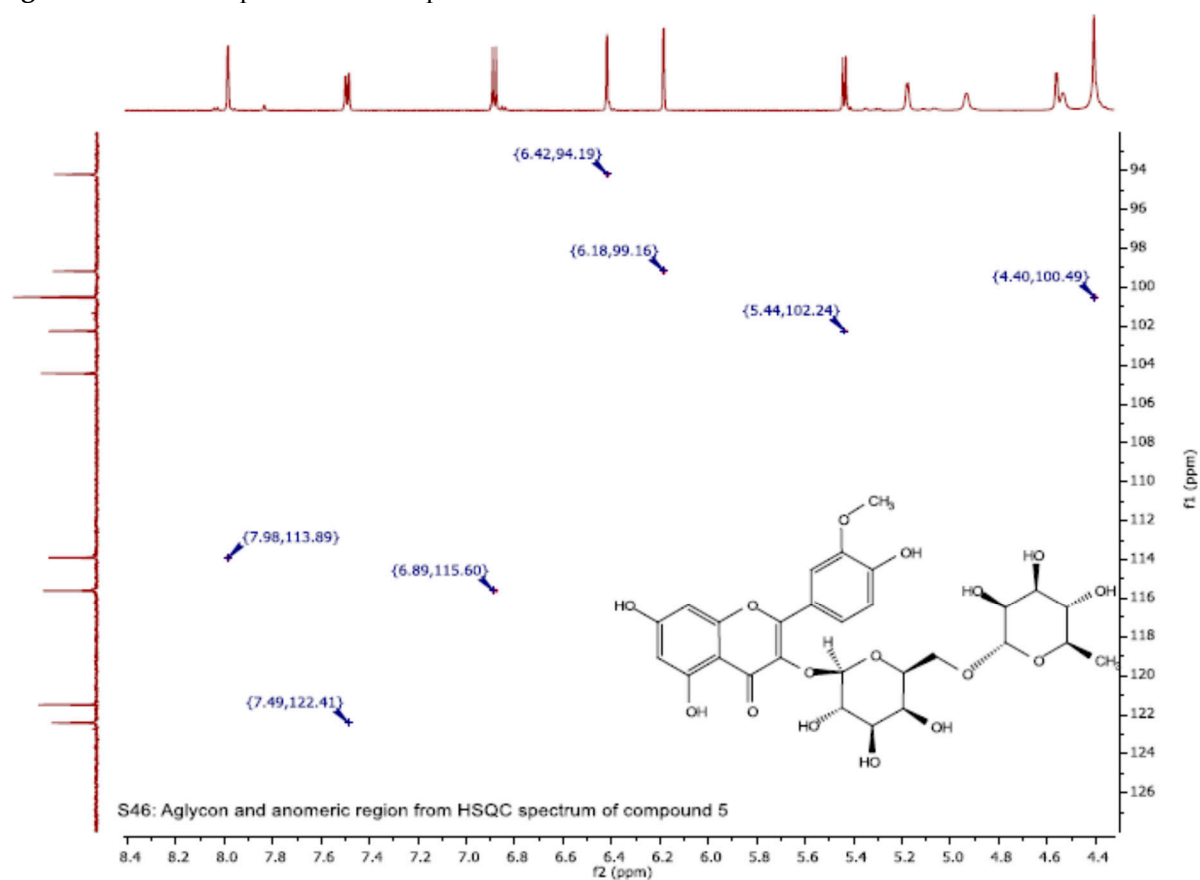


Figure S50: HSQC spectrum of compound 5 (aglycon and anomeric region)

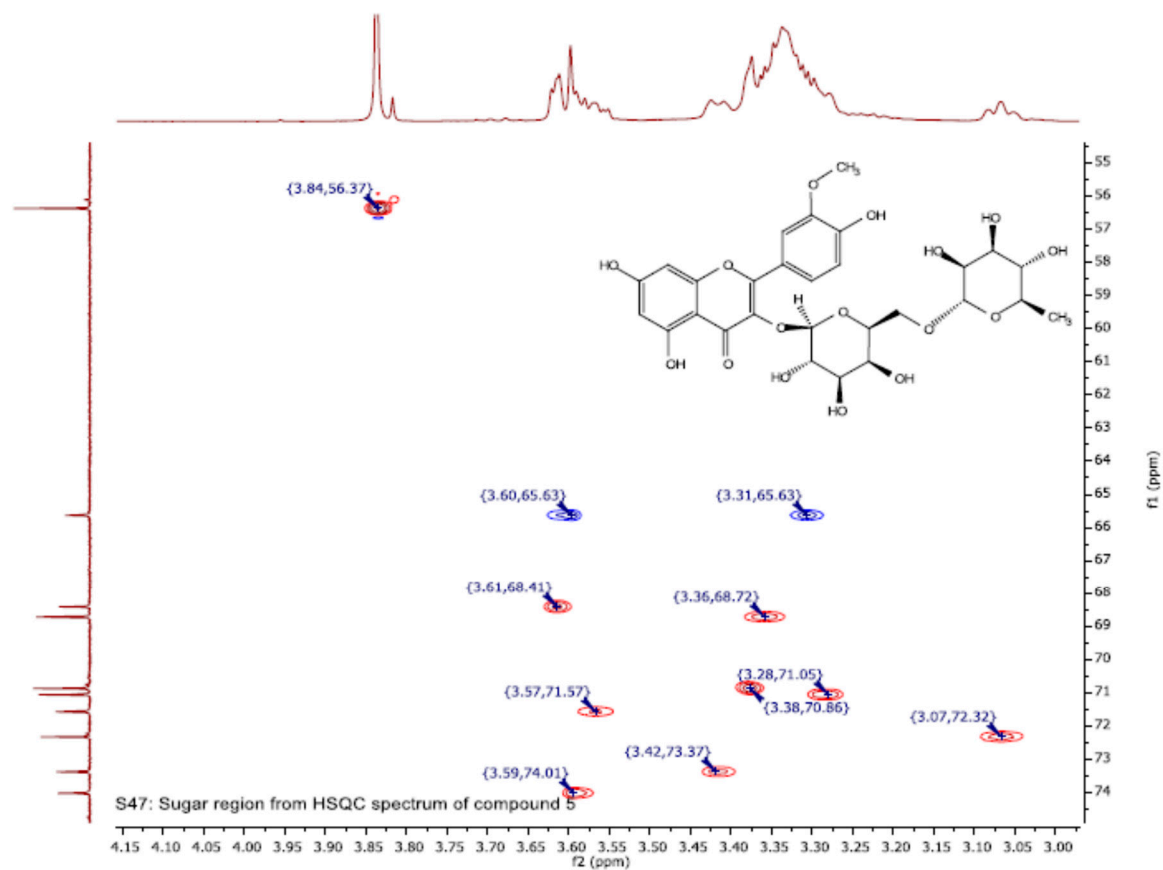


Figure S51: HSQC spectrum of compound 5 (sugar region)

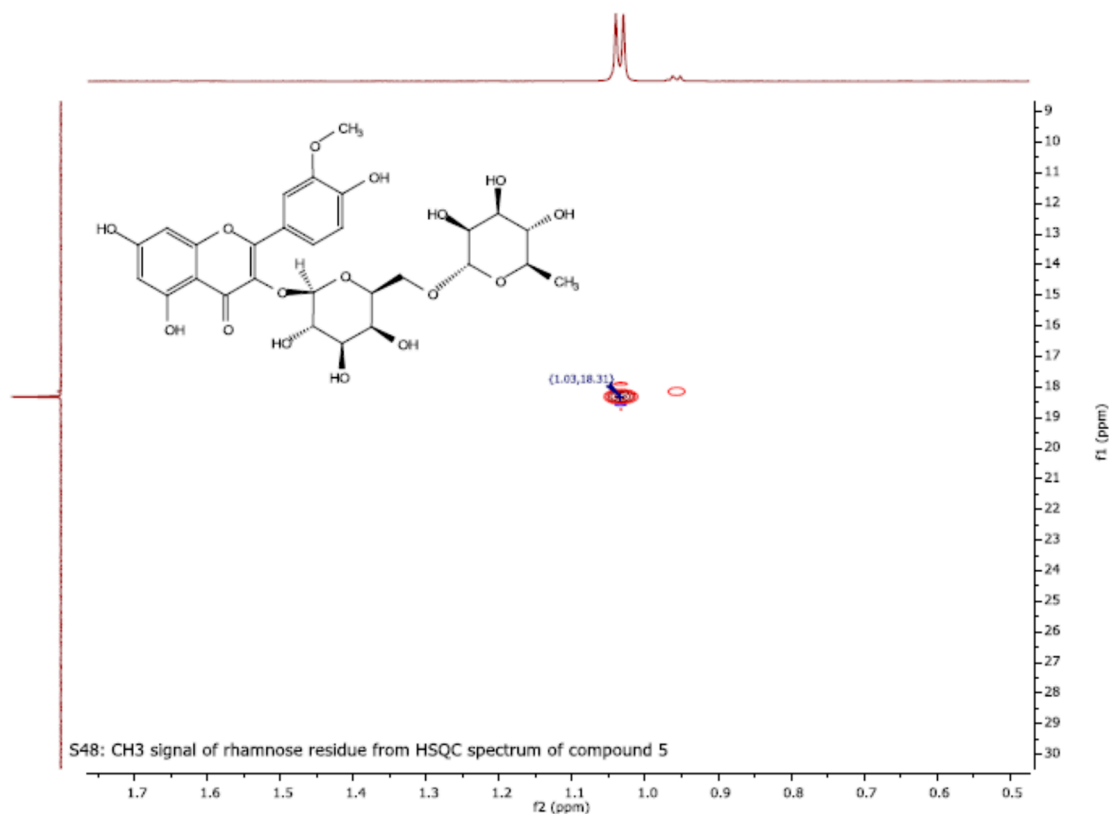
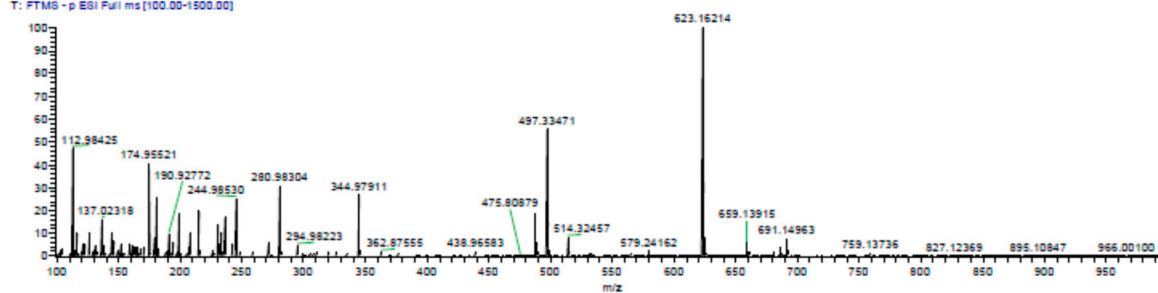


Figure S52: HSQC spectrum of compound 5 (methyl signals of rhamnose moiety)

Histo_11_161219 #3437-3499 RT: 7.94-8.0
T: FTMS - p ESI Full ms (100.00-1500.00)



Histo_11_161219 #3394-3477 RT: 7.85-8.02 AV: 2 NL: 3.31E5
T: Average spectrum MS2 623.16 (3394-3477)

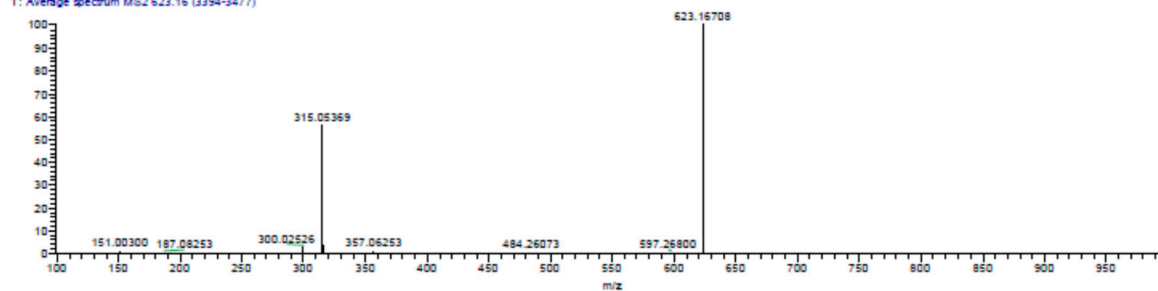


Figure S53: HR-ESI-MS (negative mode) of compound 5

Karel_10F_MRM_Pos_03 #658 RT: 11.37 AV: 1 NL: 4.47E4
T: + c ESI Full ms [60.00-1500.00]

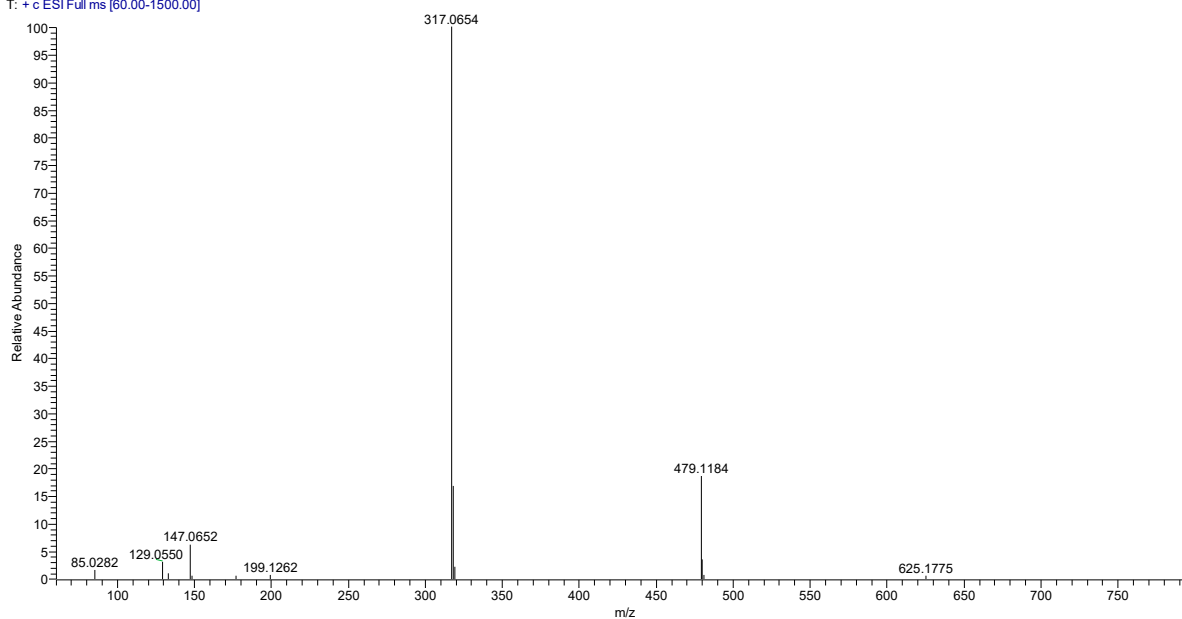


Figure S54: HR-ESI-MS (positive mode) of compound 5

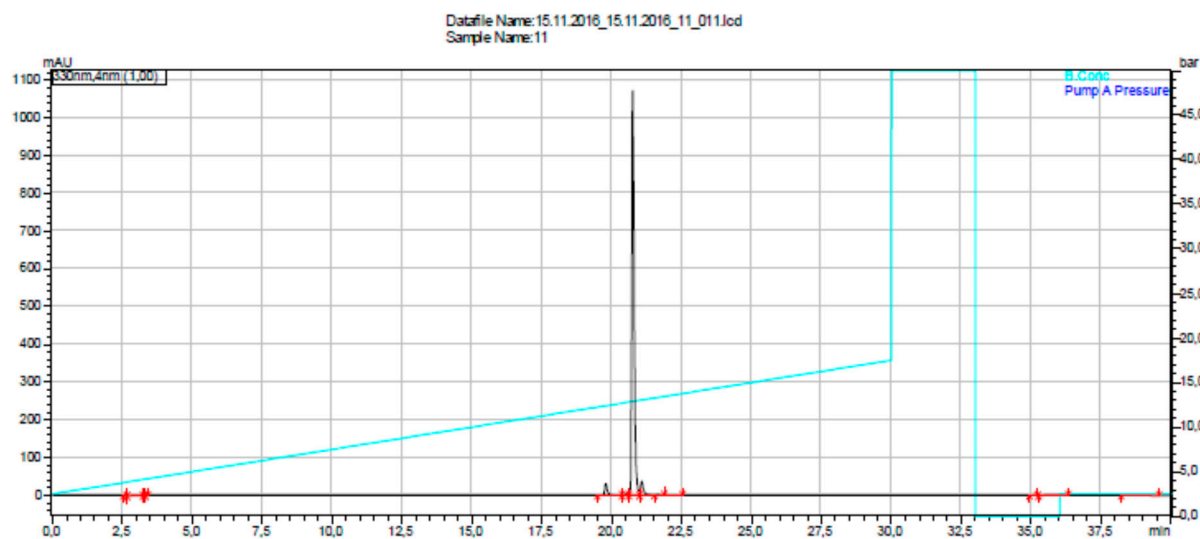


Figure S55: HPLC chromatogram of compound 5

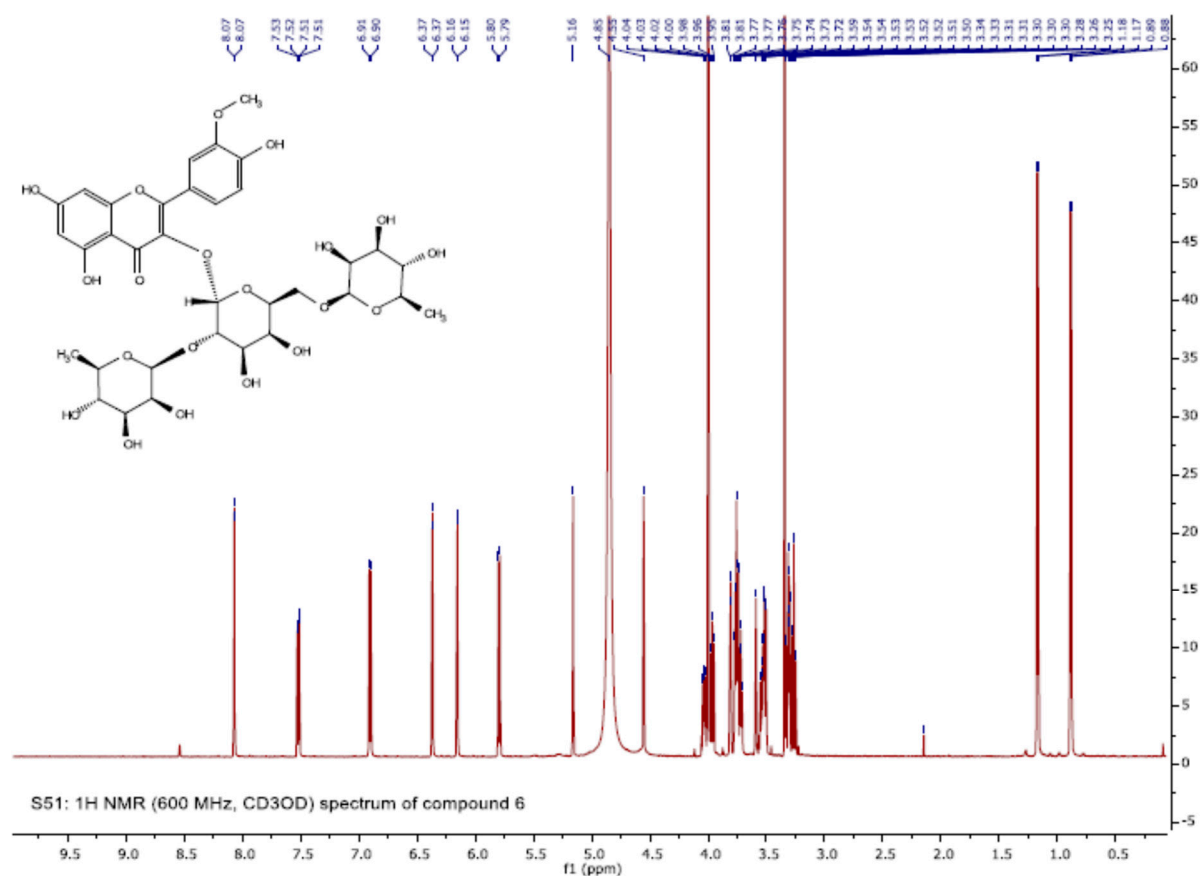


Figure S56: ^1H NMR (600 MHz, CD_3OD) spectrum of compound 6

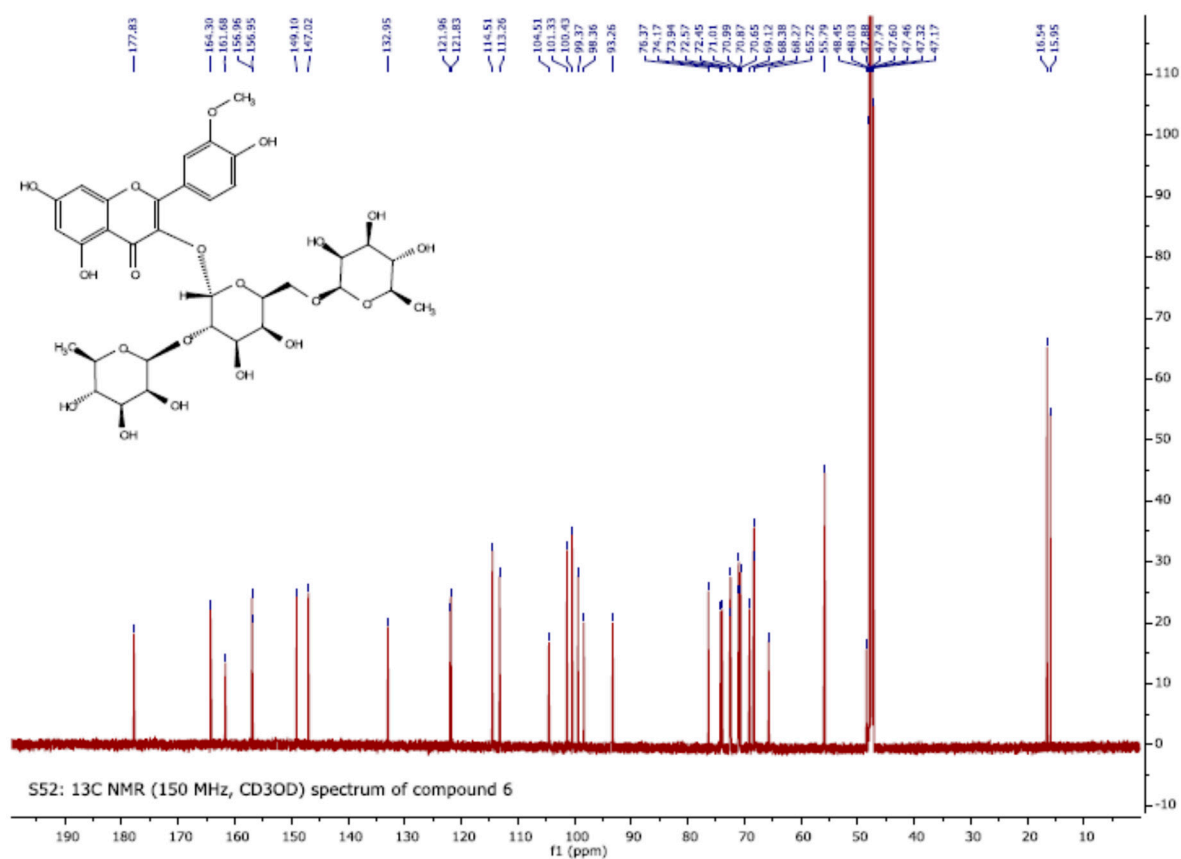


Figure S57: ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound 6

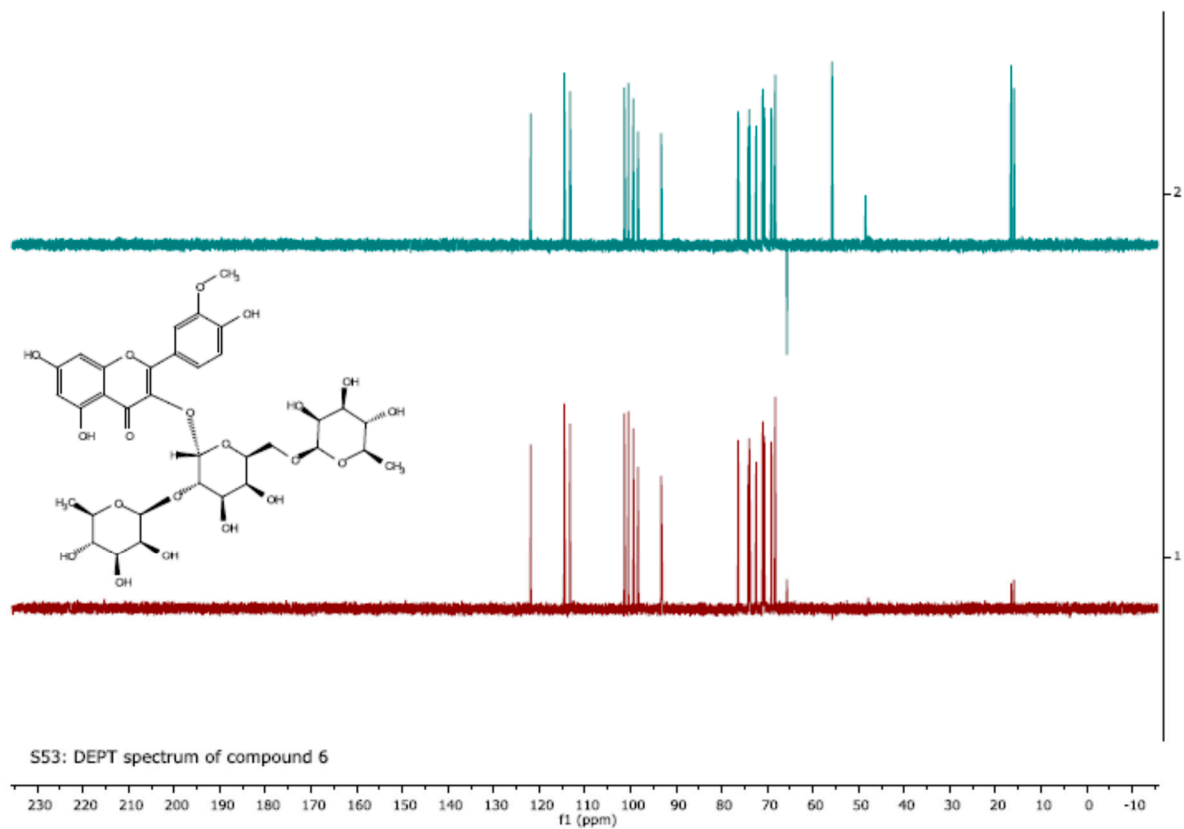


Figure S58: DEPT spectrum of compound 6

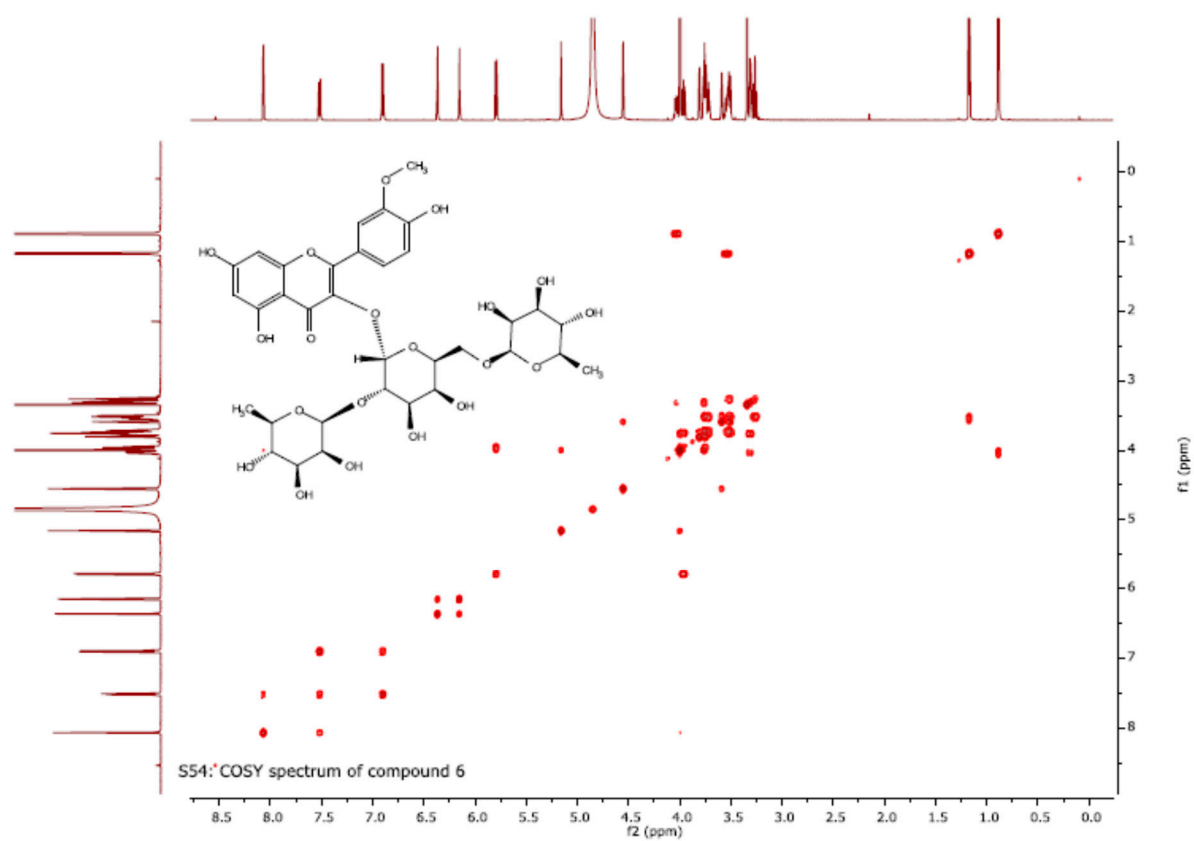


Figure S59: COSY spectrum of compound 6

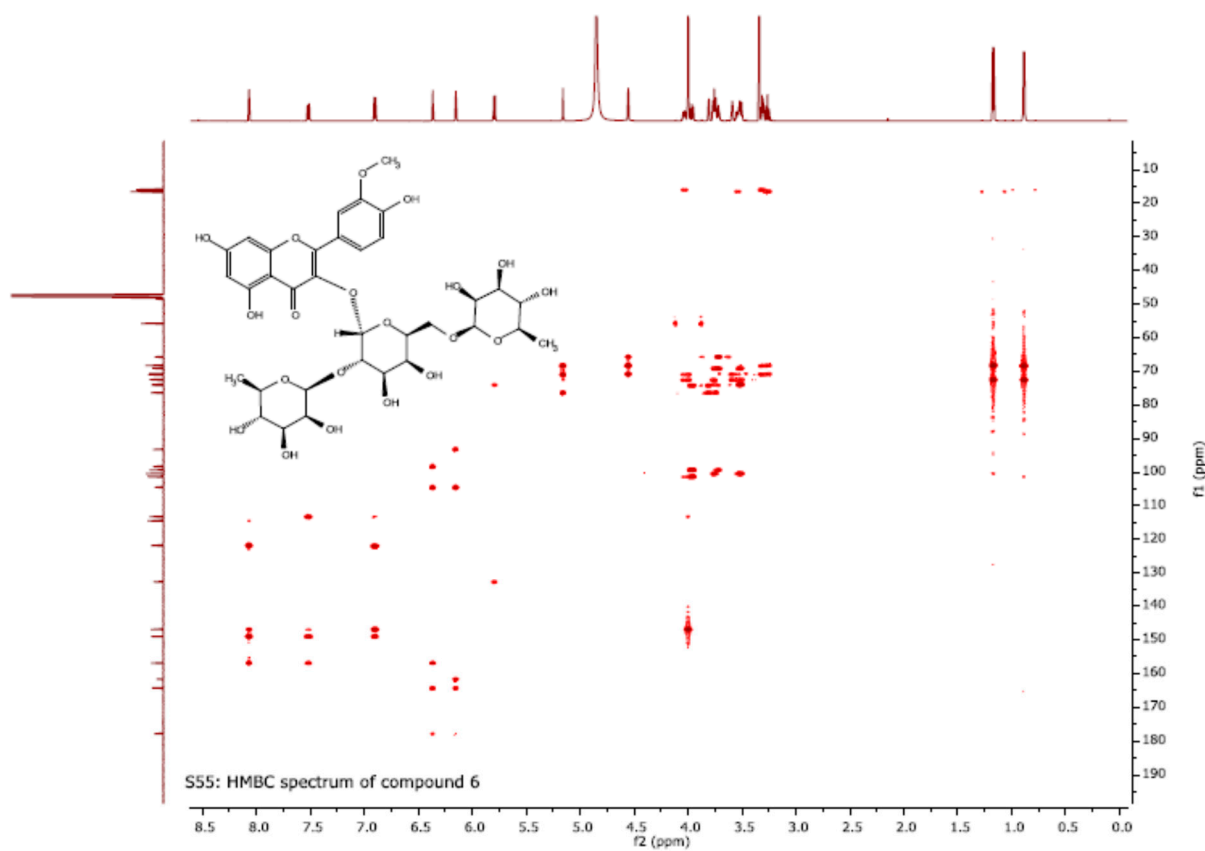


Figure S60: HMBC spectrum of compound 6

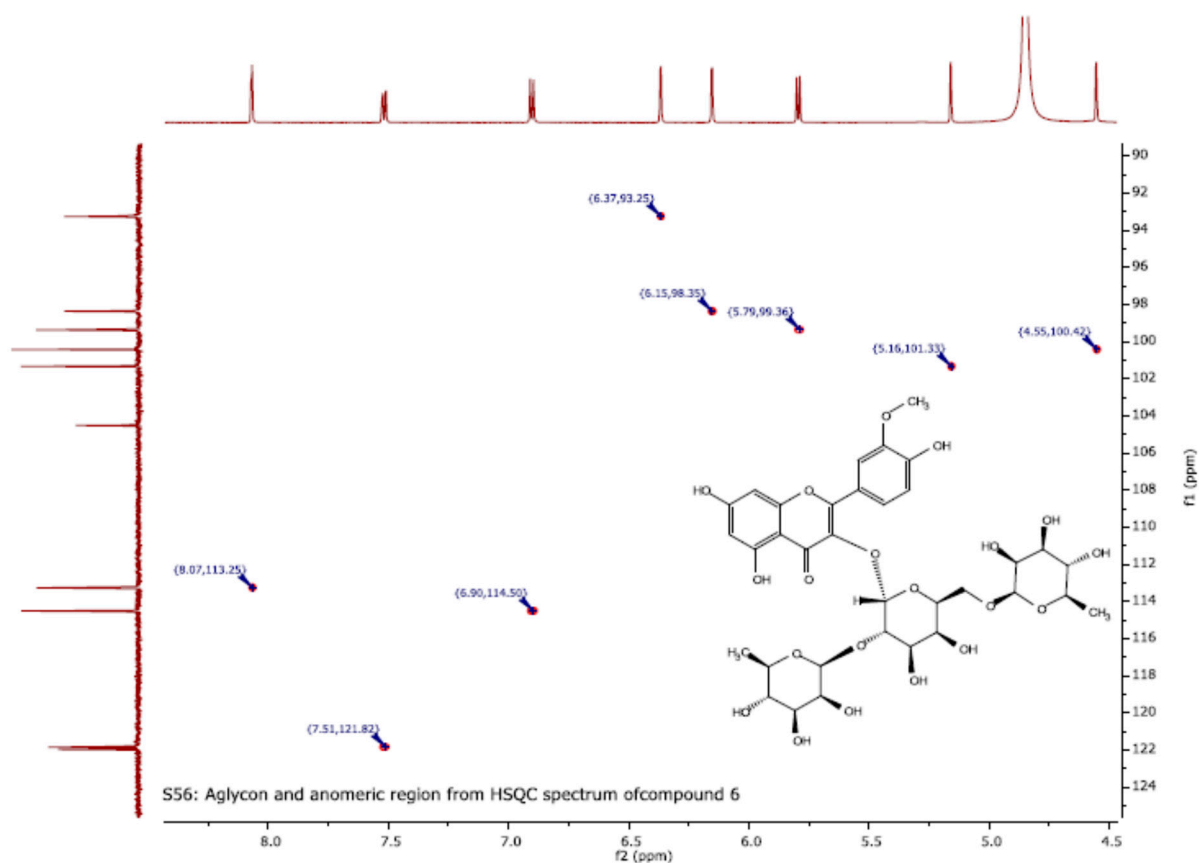


Figure S61: HSQC spectrum of compound 6 (aglycon and anomeric region)

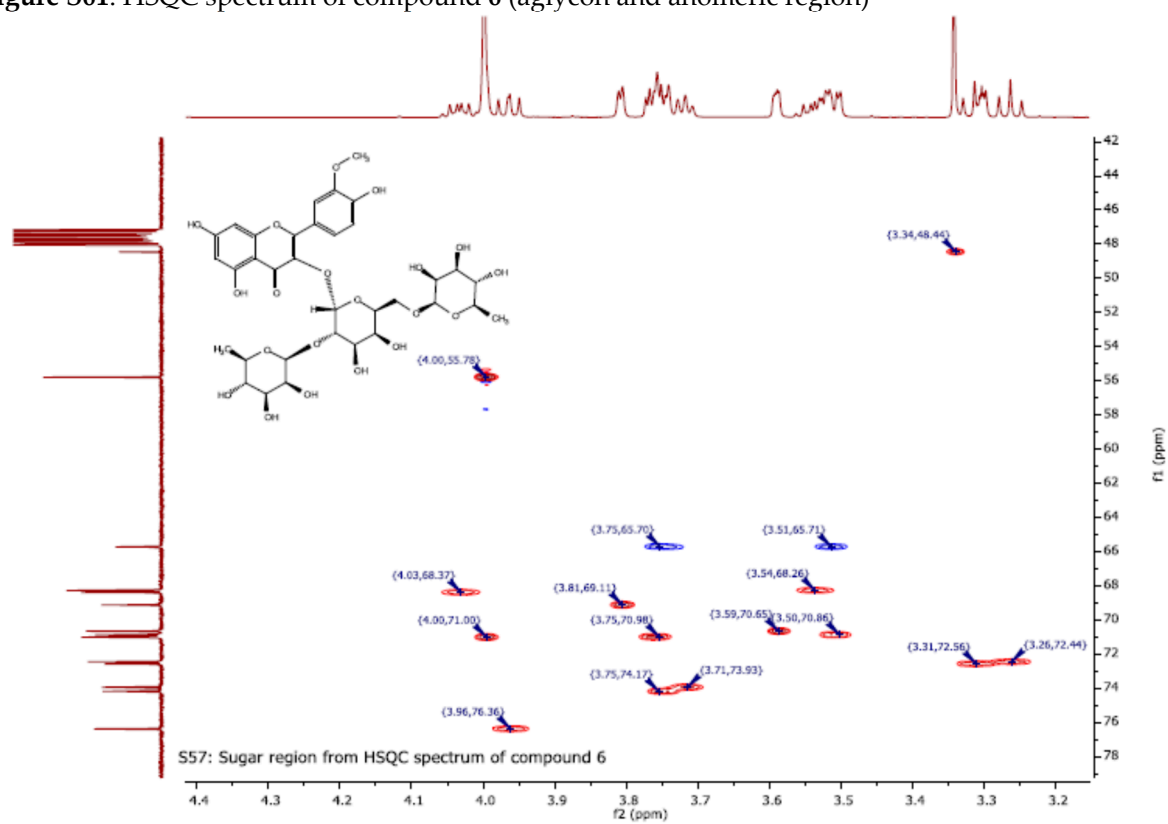


Figure S61: HSQC spectrum of compound 6 (sugar region)

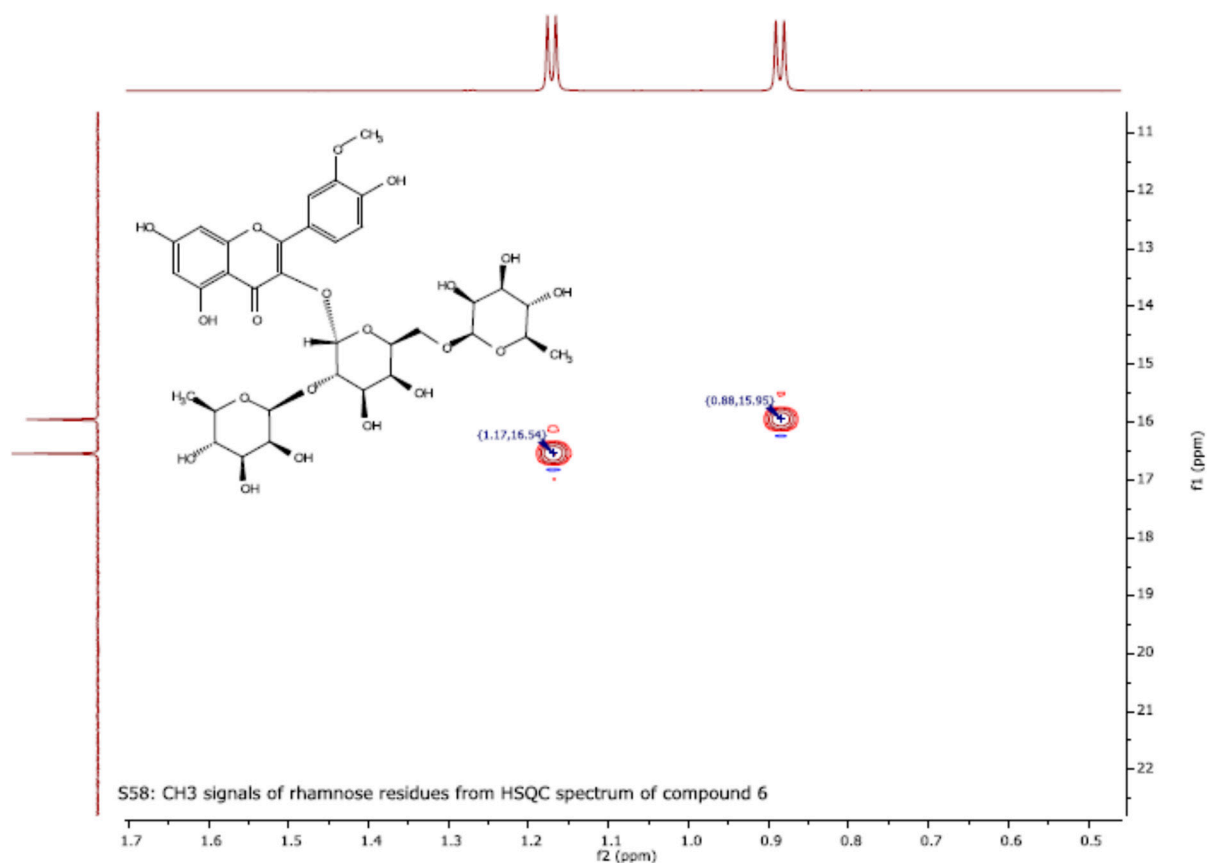


Figure S63: HSQC spectrum of compound 6 (methyl signals of rhamnose moieties)

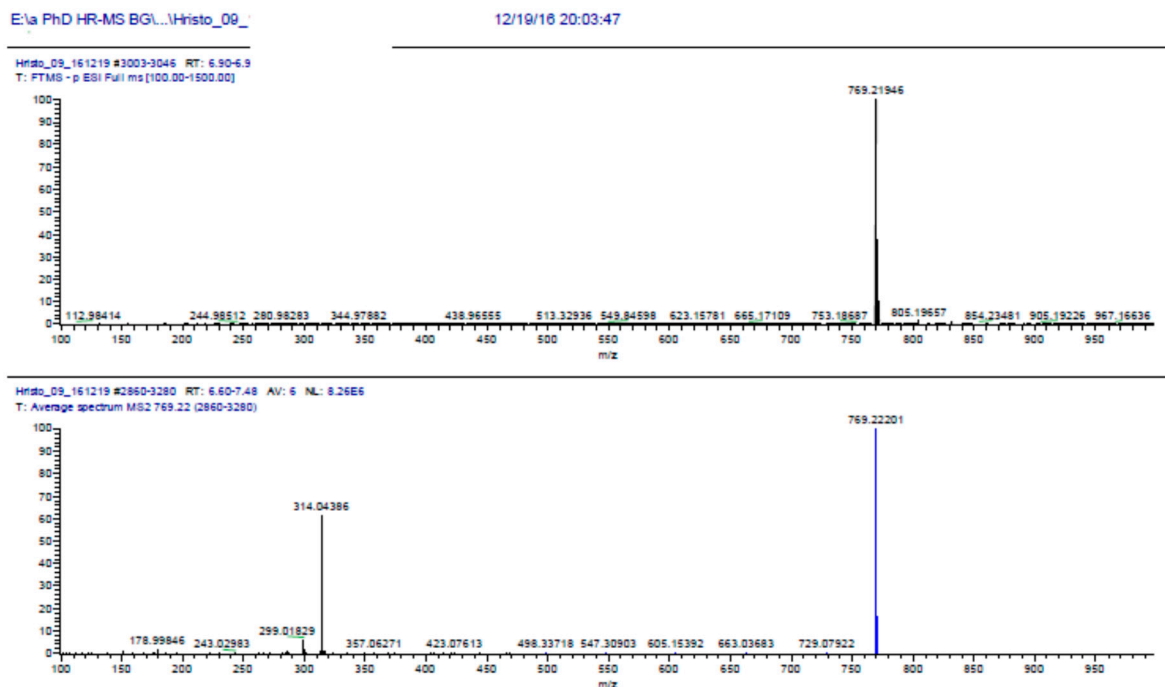


Figure S64: HR-ESI-MS (negative mode) of compound 6

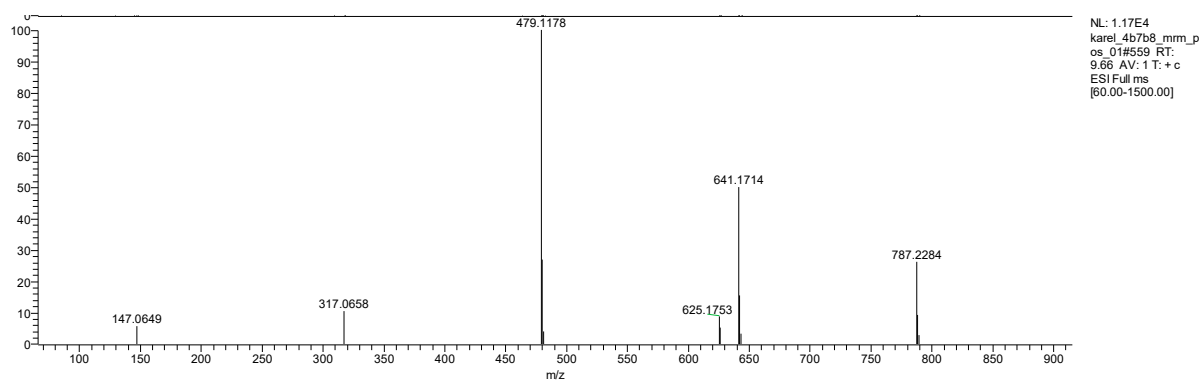


Figure S64: HR-ESI-MS (positive mode) of compound 6

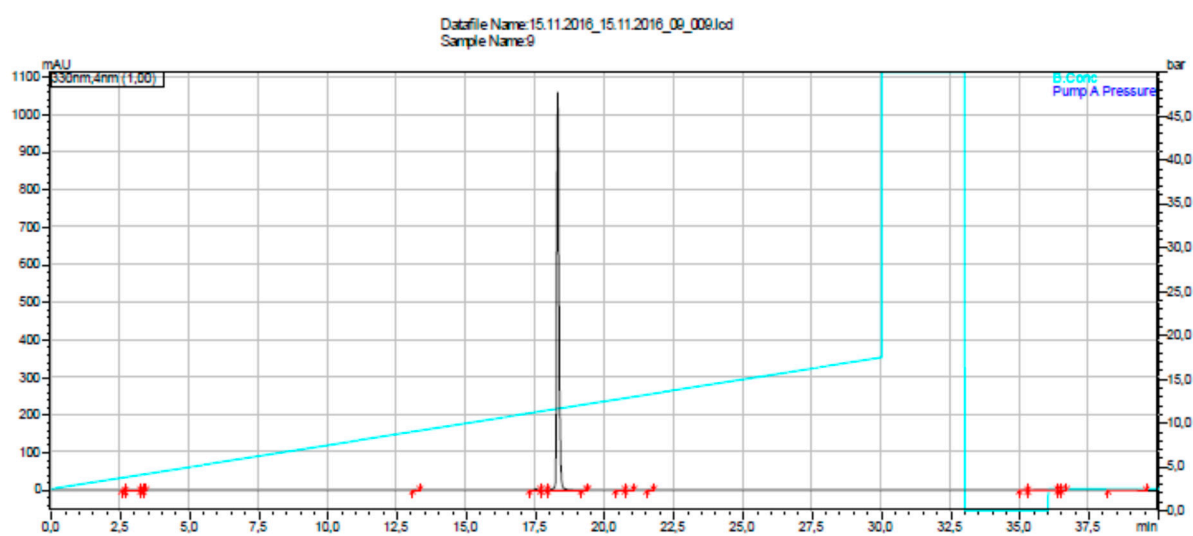


Figure S66: HPLC chromatogram of compound 6

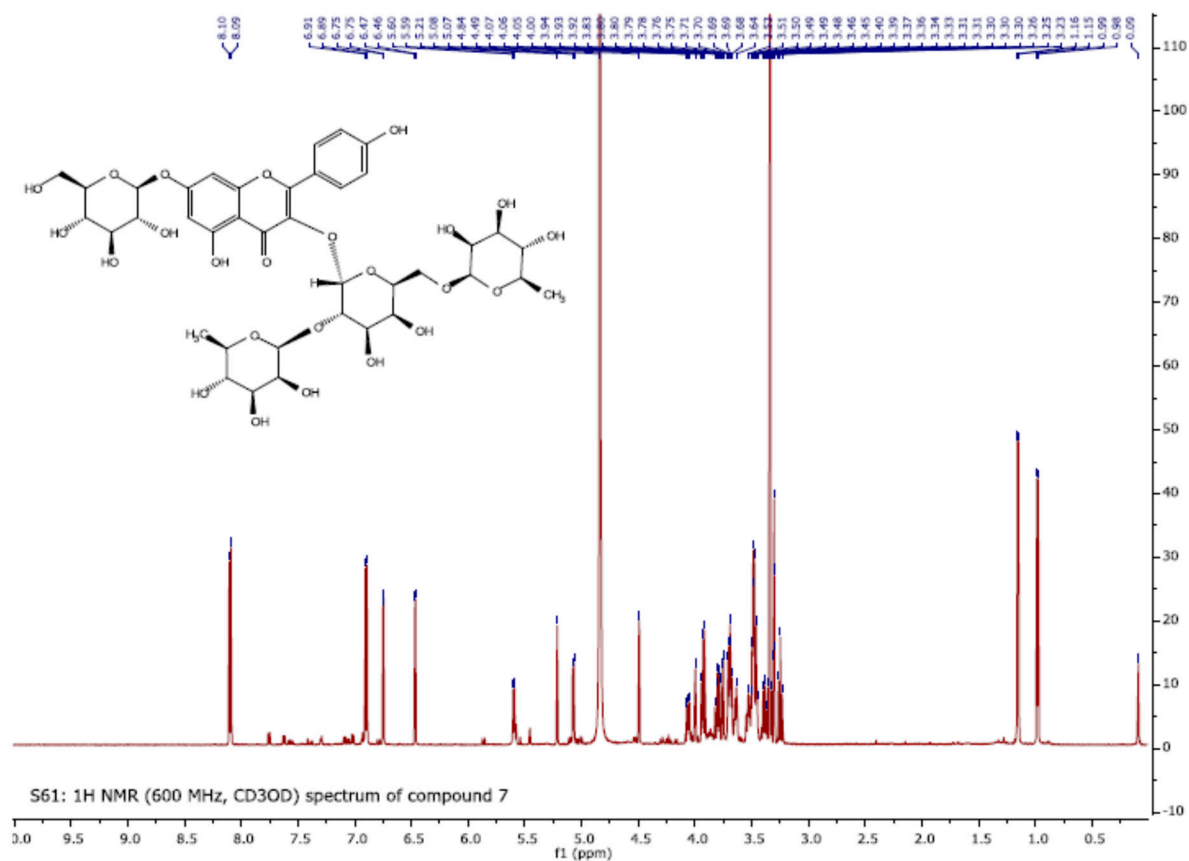


Figure S67: ^1H NMR (600 MHz, CD_3OD) spectrum of compound 7

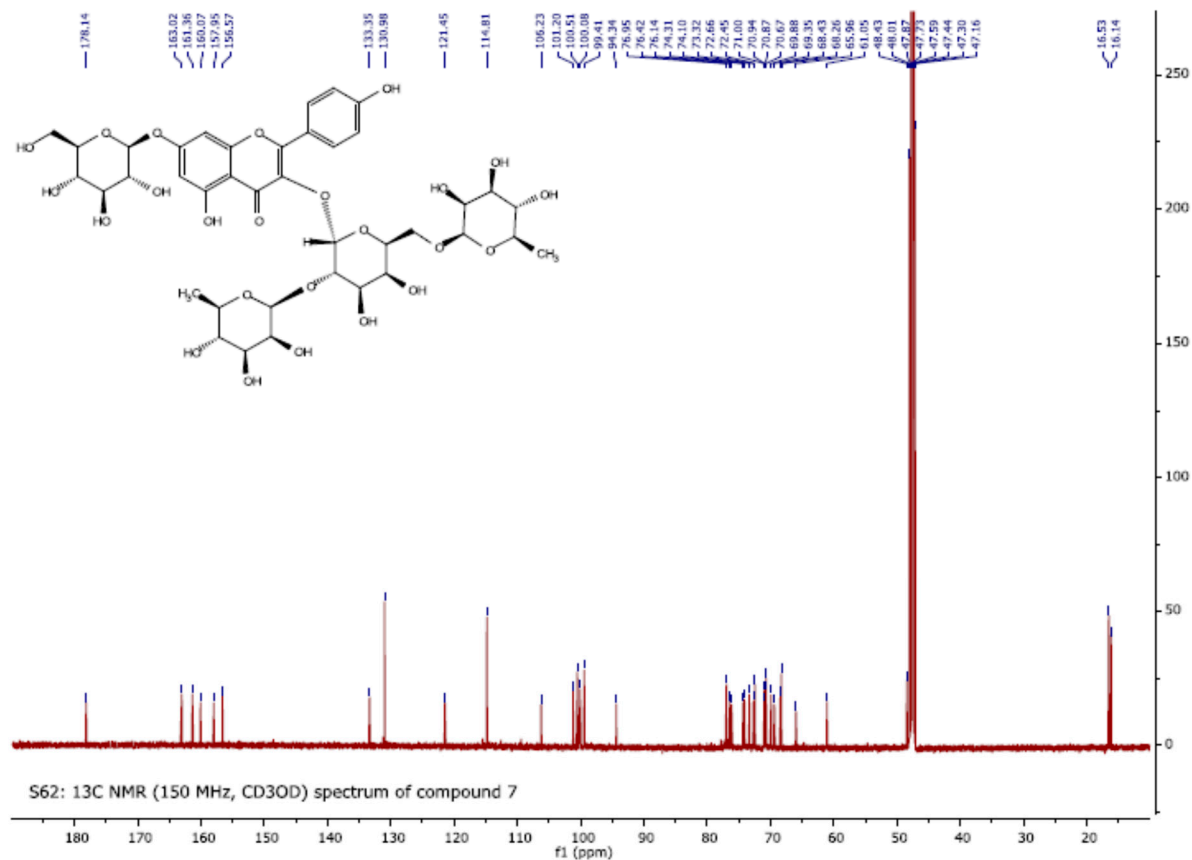


Figure S68: ^{13}C NMR (600 MHz, CD_3OD) spectrum of compound 7

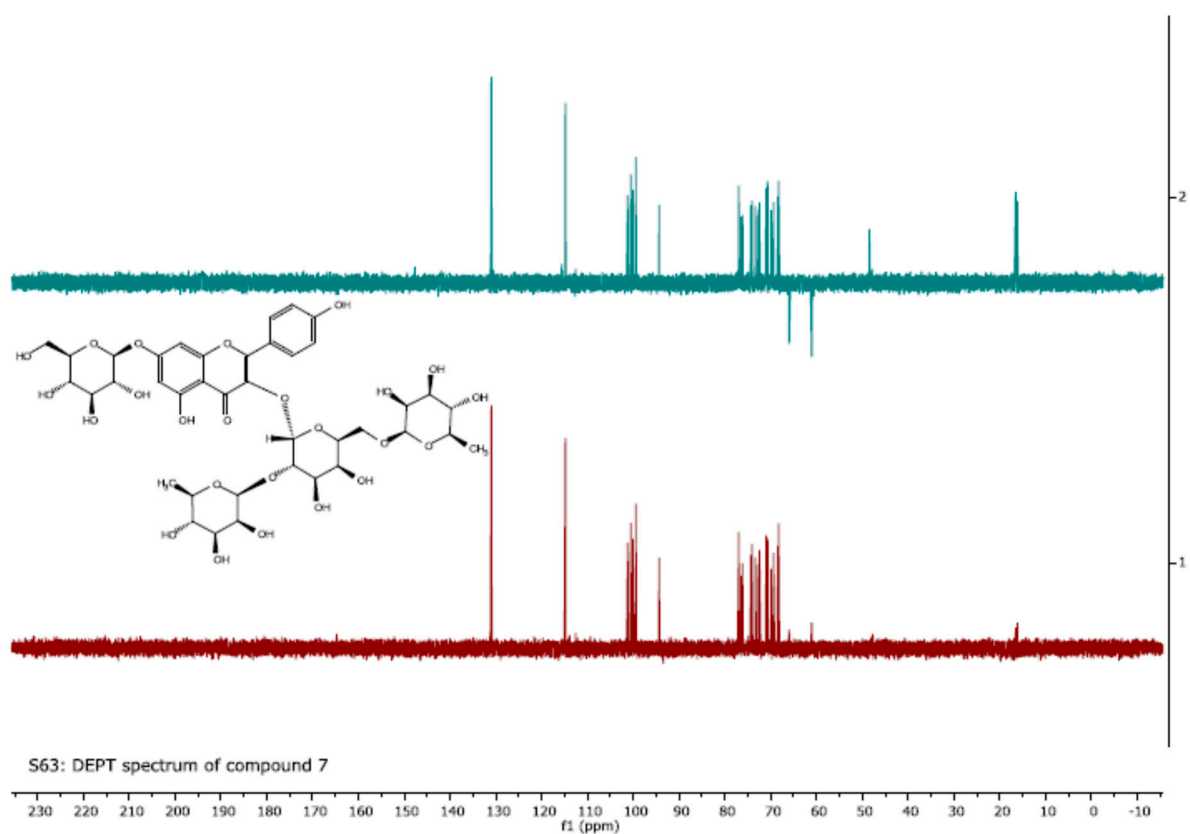


Figure S69: DEPT spectrum of compound 7

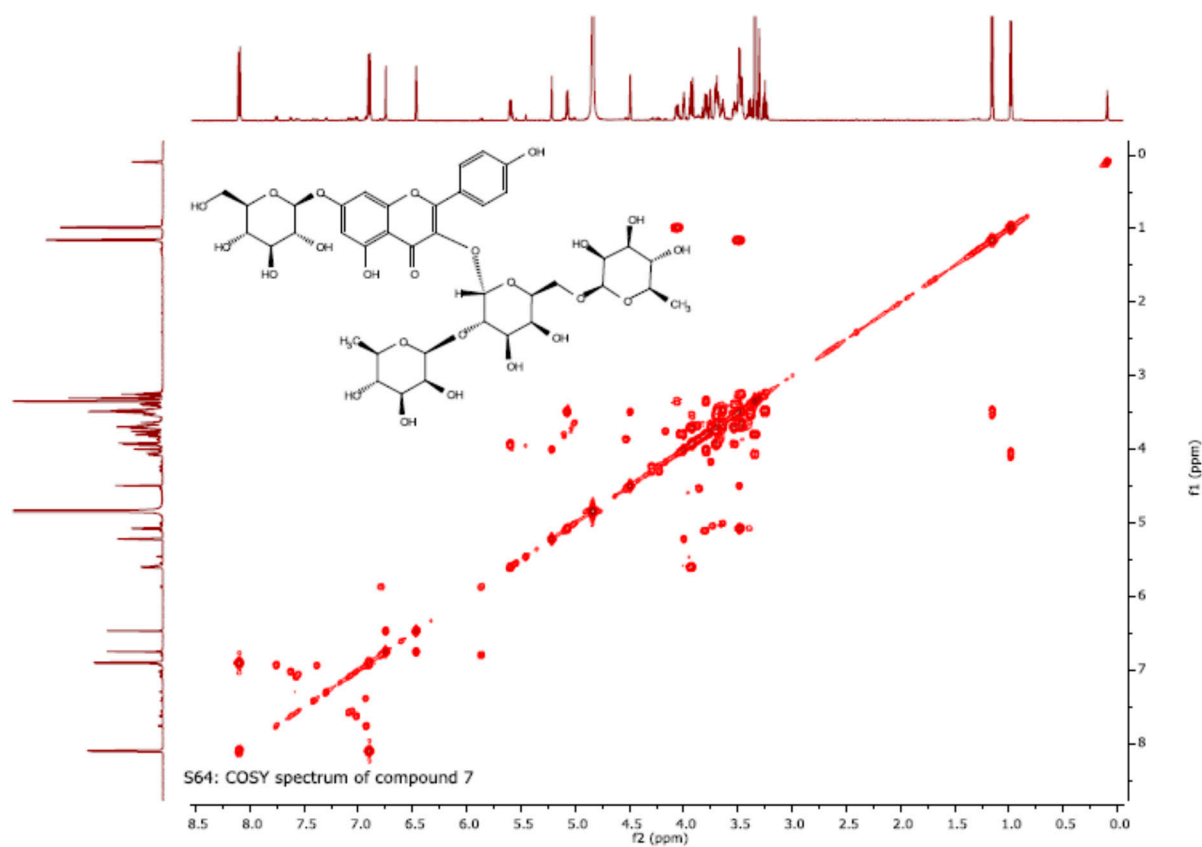


Figure S70: COSY spectrum of compound 7

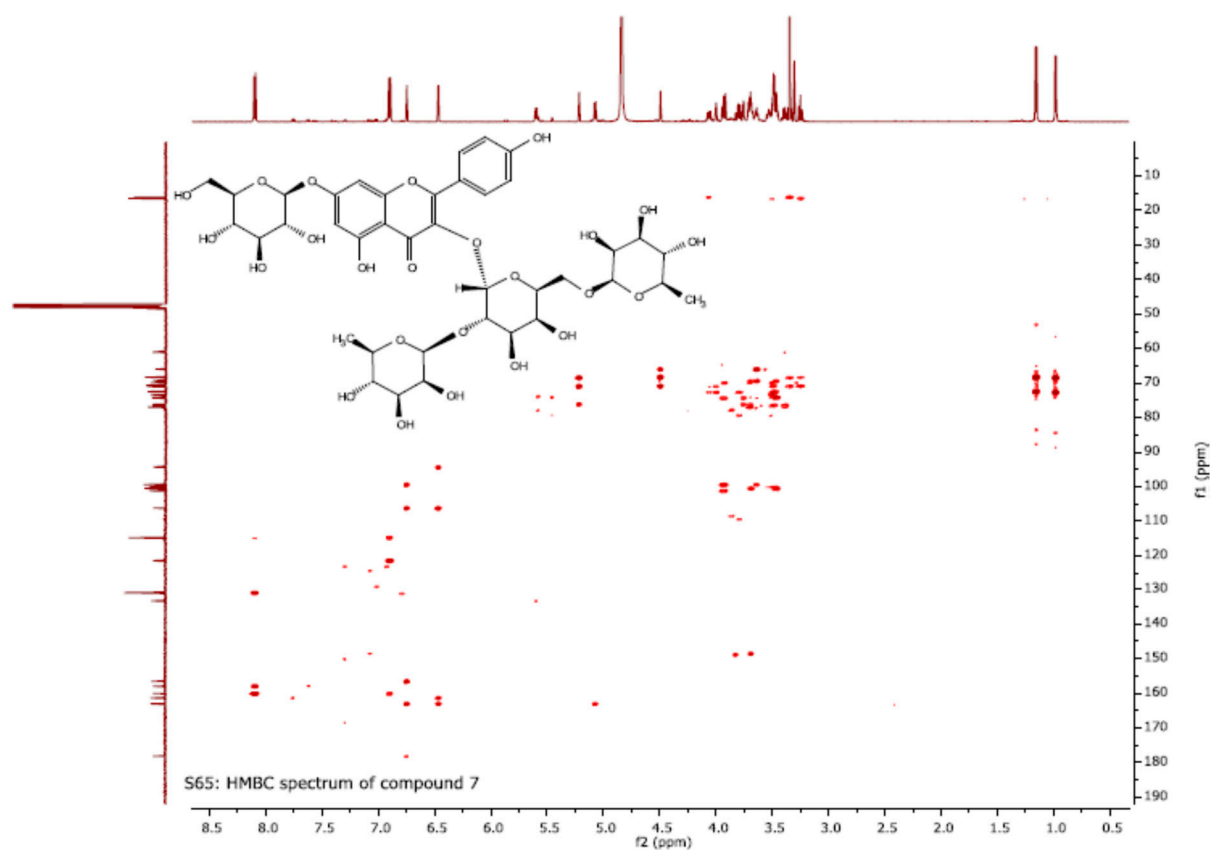


Figure S71: HMBC spectrum of compound 7

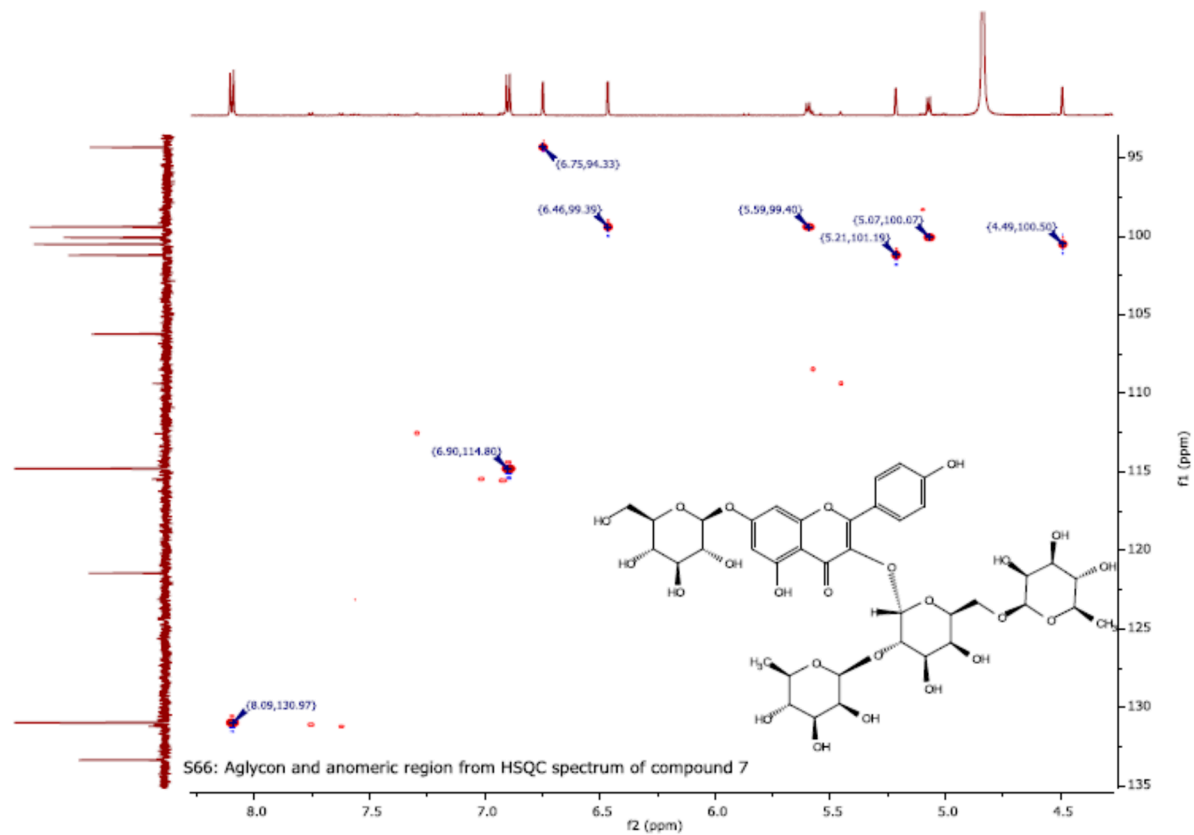


Figure S72: HSQC spectrum of compound 6 (aglycon and anomeric region)

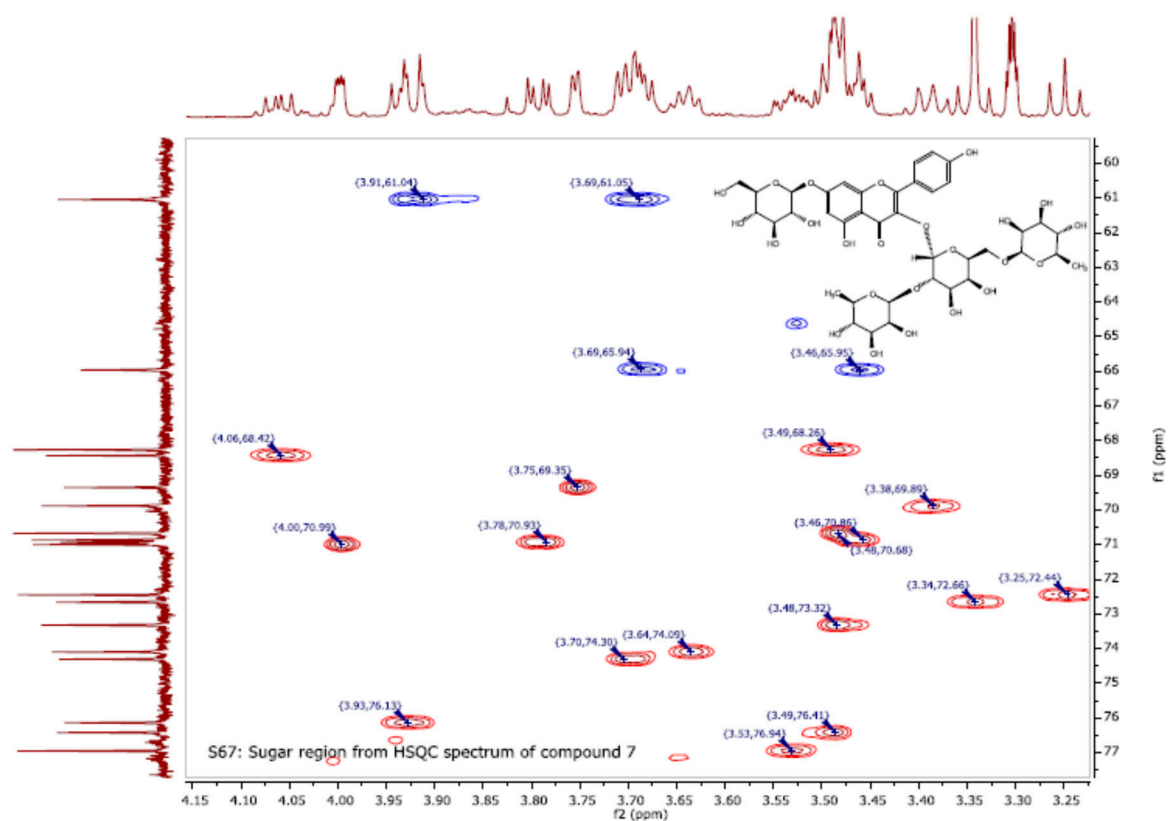


Figure S73: HSQC spectrum of compound 7 (sugar region)

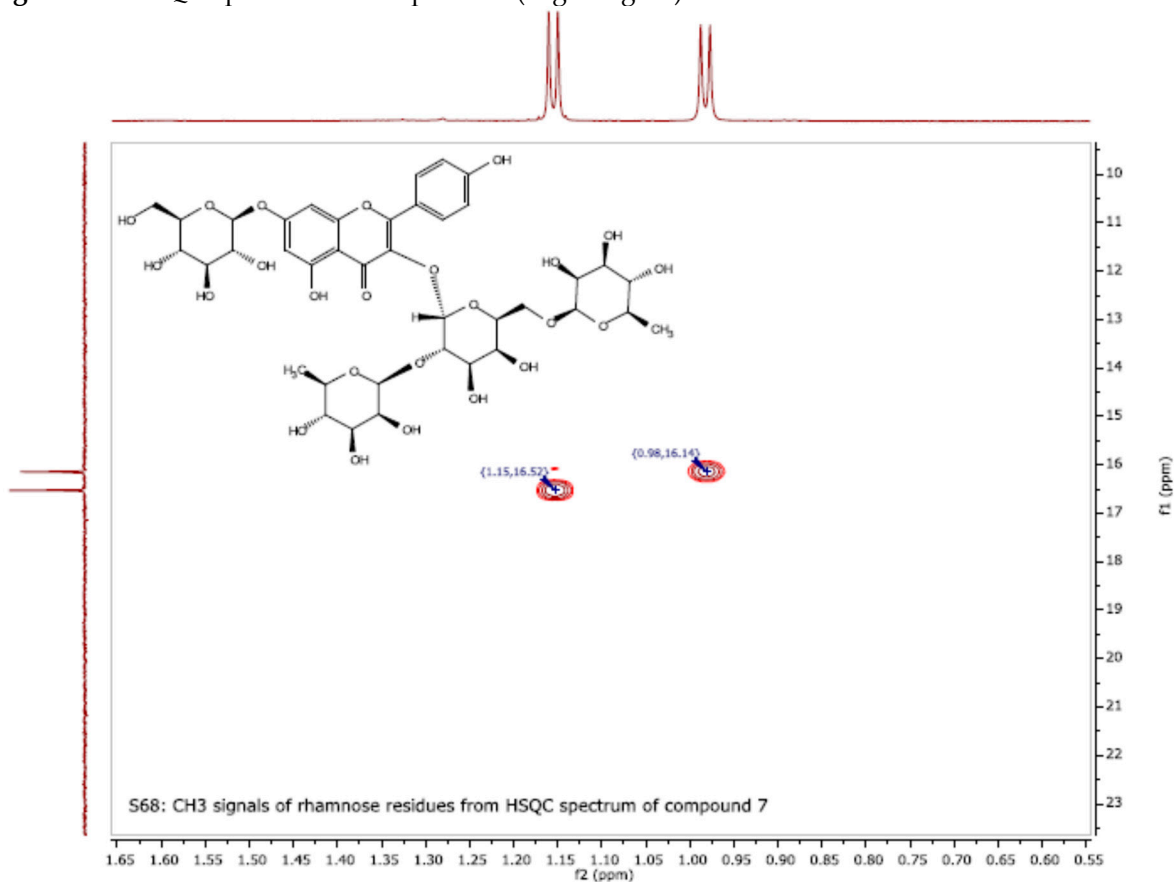


Figure S74: HSQC spectrum of compound 7 (methyl signals of rhamnose moieties)

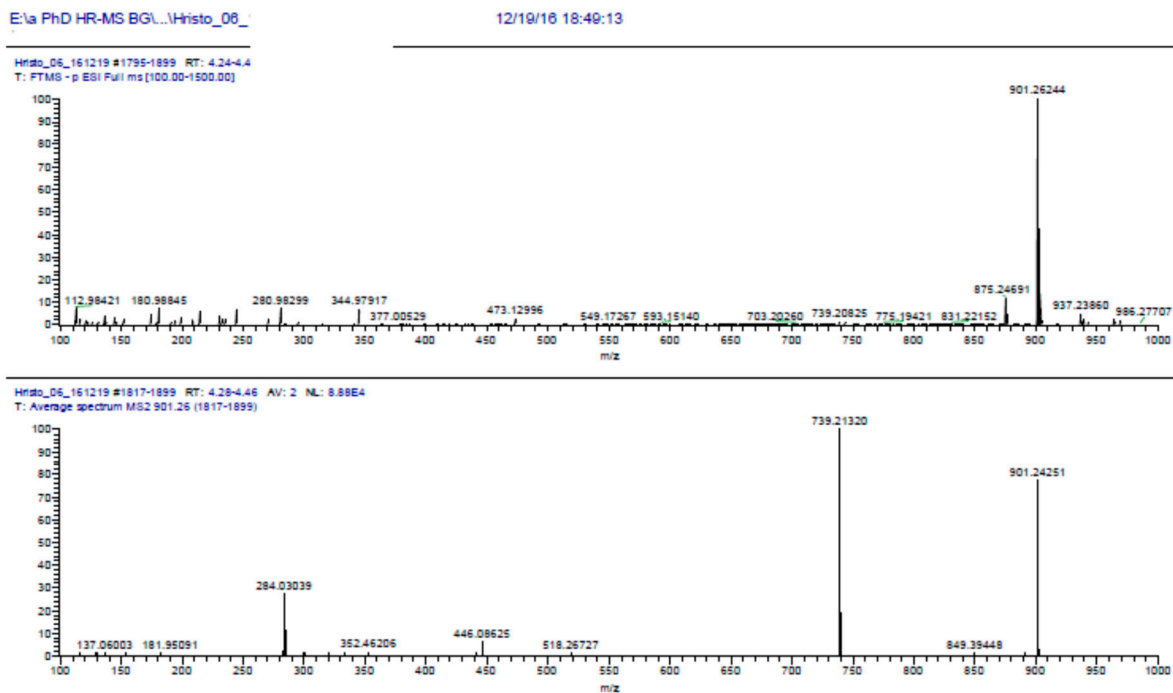


Figure S75: HR-ESI-MS (negative mode) of compound **7**

Karel_2 B22-32_MRM_Pos_01 #499 RT: 8.62 AV: 1 NL: 5.45E4
T: + c ESI Full ms [60.00-1500.00]

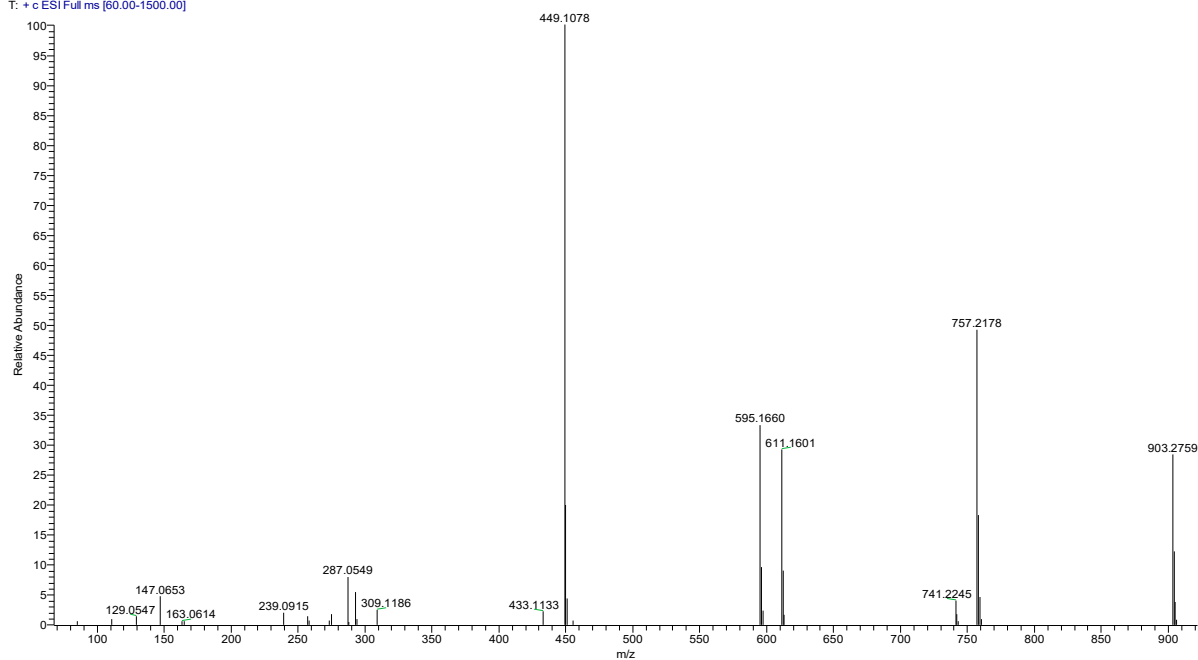


Figure S76: HR-ESI-MS (positive mode) of compound **7**

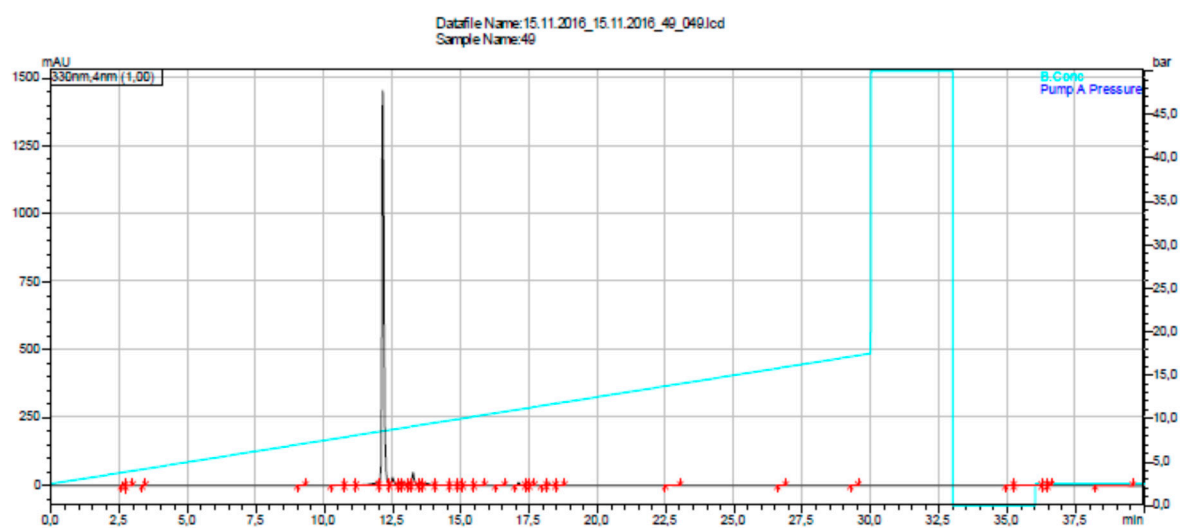


Figure S77: HPLC chromatogram of compound 7