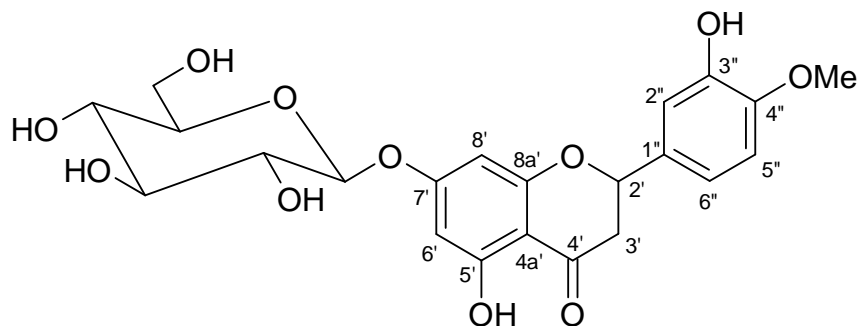


## 9 P ílohy

### 9.1 NMR data derhamnosylovaných produkt

#### Hesperetin-glc



#### NMR spektroskopie:

**P ístroj:** Bruker Avance III 600 MHz (600.23 MHz pro  $^1\text{H}$ , 150.94 MHz pro  $^{13}\text{C}$ ,  $\text{CD}_3\text{OD}$ ,  $30^\circ\text{C}$ )

**Provedená stanovení:**  $^1\text{H}$ ,  $^{13}\text{C}$ , gCOSY, gHSQC, gHMBC.

Tab. 9.1|NMR data hesperetin-glc

Atom	$\delta_{\text{C}}$	m.	$\delta_{\text{H}}$	$n_{\text{H}}$	m.	J[Hz]	HMBC (C to H)
1	101.55, 101.58	D	5.008, 4.998	1	d	7.IV	
2	74.97	D	3.46 <sup>a</sup>	1	m		1 w
3	78.12	D	3.48 <sup>a</sup>	1	m		1
4	71.50	D	3.42 <sup>a</sup>	1	m		6u, 6d
5	78.57	D	3.48 <sup>a</sup>	1	m		1, 6u, 6d w
6	62.66	T	3.903, 3.899	1	dd	12.1, 2.7	
			3.723, 3.715	1	dd	12.1, 5.3	
2÷	80.74, 80.80	D	5.402, 5.396	1	dd	12.4, 3.1	3ød, 2ø, 6ø
3÷	44.32, 44.46	T	3.146	1	dd	17.2, 12.4	
			2.815, 2.804	1	dd	17.2, 3.1	2÷w
4÷	198.68	S	-				2÷ 3øu, 3ød, 6÷w, 8÷
4a÷	105.30, 105.27	S	-				3øu, 6÷; 8÷
5÷	165.20, 165.23	S	-				6÷

<b>6÷</b>	98.36	D	6.215, 6.213	1	d	2.I	8÷
<b>7÷</b>	167.29, 167.36	S	-				1, 6÷, 8÷
<b>8÷</b>	97.32, 97.29	D	6.245, 6.248	1	d	2.I	6÷
<b>8aø</b>	164.77, 164.78	S	-				2÷, 8÷
<b>1ø</b>	133.18, 133.21	S	-				2÷, 3ø, 3ød, 2ø, 5ø, 6ø
<b>2ø</b>	114.93, 114.92	D	6.984	1	d	1.IX	2÷, 5ø, 6ø
<b>3ø</b>	148.12	S	-				2ø, 5ø, 6ø
<b>4ø</b>	149.75	S	-				2ø, 5ø, 6ø, OMe
<b>5ø</b>	112.98	D	6.966	1	d	8.III	2ø, 6ø
<b>6ø</b>	119.41, 119.39	D	6.939	1	dd	8.3, 1.9	2÷, 2ø, 5ø
<b>OMe</b>	56.80	Q	3.888	3	s		

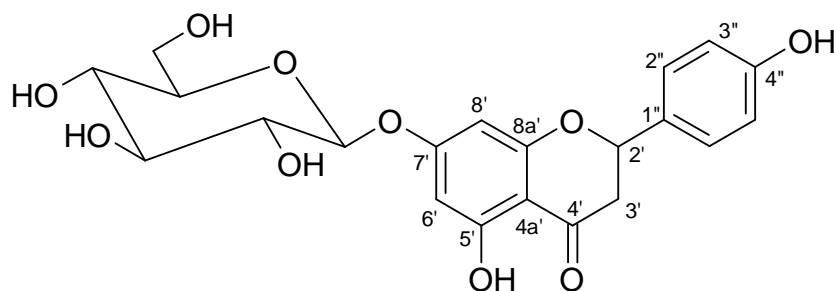
<sup>a</sup> ode et z HSQC

s ó singlet, d ó dublet, dd ó dublet dublet, m ó multiplet, J ó interak ní konstanta

Pom r diastereomer je cca 3:2

V tabulce jsou uvedeny chemické posuny nejprve pro hlavní slofku, potom pro minoritu

## Prunin



### NMR spektroskopie:

**P ístroj:** Bruker Avance III 600 MHz (600.23 MHz pro <sup>1</sup>H, 150.94 MHz pro <sup>13</sup>C, CD<sub>3</sub>OD, 30°C)

**Provedená stanovení:** <sup>1</sup>H, <sup>13</sup>C, gCOSY, gHSQC, gHMBC.

Tab. 9.2|NMR data pruninu

Atom	$\delta_X$	m.	$\delta_H$	$n_H$	m.	J[Hz]	HMBC (C to H)
1	101.55, 101.58	D	4.993, 5.004	1	d	7.II	2
2	74.97, 74.98	D	3.46 <sup>a</sup>	1	m		
3	78.13	D	3.47 <sup>a</sup>	1	m		1, 4
4	71.49, 71.50	D	3.41 <sup>a</sup>	1	m		6u w, 6d
5	78.57, 78.58	D	3.48 <sup>a</sup>	1	m		1, 4, 6u, 6d w
6	62.68	T	3.897, 3.898 3.710	1 1	dd dd	12.2, 2.3 12.2, 5.0	4 w
2÷	80.96, 81.00	D	5.414, 5.419	1	dd	12.8, 3.0	3 $\alpha$ l, 2 $\delta$
3÷	44.29, 44.43	T	3.192, 3.193 2.784, 2.792	1 1	dd dd	17.2, 12.8 17.2, 3.0	
4÷	198.87	S	-	0			2÷, 3 $\alpha$ l, 3 $\alpha$ l, 6÷w
4a÷	105.25, 105.27	S	-	0			3 $\alpha$ l, 6÷, 8÷
5÷	165.23, 165.27	S	-	0			6÷
6÷	98.33, 98.34	D	6.213, 6.216	1	d	2.I	8÷
7÷	167.29, 167.36	S	-	0			1, 6÷, 8÷
8÷	97.25, 97.27	D	6.235, 6.238	1	d	2.I	6÷
8a $\delta$	164.91, 164.92	S	-	0			2÷w, 8÷
1 $\delta$	131.14, 131.18	S	-	0			2÷w, 3 $\alpha$ l, 3 $\alpha$ l, 3 $\delta$
2 $\delta$	129.39, 129.41	D	7.343	2	d	1.IX	2÷, 2 $\delta$
3 $\delta$	116.67, 116.68	D	6.844	2			2 $\delta$ , 3 $\delta$
4 $\delta$	159.39, 159.40	S	-	0			2 $\delta$ , 3 $\delta$

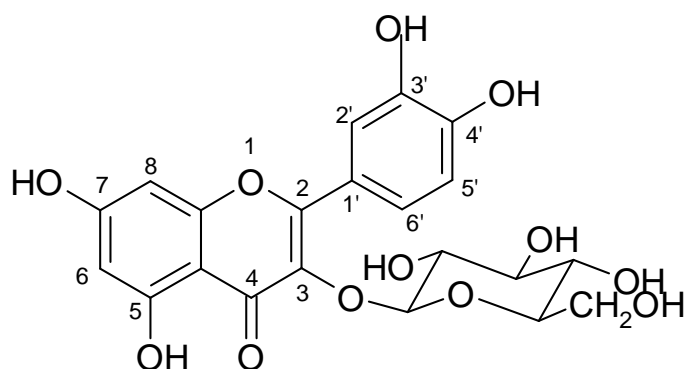
<sup>a</sup> ode et z HSQC

d ó dublet, dd ó dublet dublet , m ó multiplet, J ó interak ní konstanta

Pom r obou diastereomer je cca 1:1

V tabulce jsou uvedeny chemické posuny v po adí up-field, down-field

## Isoquercitrin



### NMR spektroskopie:

**P ístroj:** Varian Mercury-300 (300.07 MHz for  $^1\text{H}$ , 75.45 MHz for  $^{13}\text{C}$ , DMSO- $d_6$ )

**Provedená stanovení:**  $^1\text{H}$ ,  $^{13}\text{C}$ , gCOSY.

Literatura: 1. M. Bouktaib, A. Atmani, Ch. Rolando *Tetrahedron Lett.* **2002**, *43*, 6263-6266

NMR data porovnána (300.07 MHz pro  $^1\text{H}$ , 75.45 MHz pro  $^{13}\text{C}$ ,  $\text{CD}_3\text{OD}$ , pokojová teplota) s literaturou<sup>1</sup>

Tab. 9.3|NMR data isoquercitrinu

Atom	$\delta_{\text{X}}$	$\delta_{\text{X}}^{\alpha}$	m.	$\delta_{\text{H}}$	$\delta_{\text{H}}^{\alpha}$	$n_{\text{H}}$	m.	J[Hz]
2	159.28	159.00	S	-	-	0		
3	135.90	135.65	S	-	-	0		
4	179.73	179.41	S	-	-	0		
5	163.30	162.93	S	-	-	0		
6	100.28	99.98	D	6.376	VI.33	1	d	2.0
7	166.59	165.91	S	-	-	0		
8	95.08	94.75	D	6.188	VI.15	1	d	2.0
9	158.76	158.37	S	-	-	0		
10	105.88	105.67	S	-	-	0		
1÷	123.35	123.04	S	-	-	0		
2÷	117.85	117.62	D	7.710	VII.70	1	d	2.0
3÷	146.19	145.76	S	-	-	0		

<b>4÷</b>	150.15	149.81	S	-	-	0		
<b>5÷</b>	116.30	116.00	D	6.865	VI.75	1	d	8.VIII
<b>6÷</b>	123.49	123.23	D	7.580	VII.57	1	dd	8.8, 2.0
<b>1÷</b>	104.64	104.32	D	5.239	V.23	1	d	7.V
<b>2÷</b>	76.01	75.73	D			1	m	
<b>3÷</b>	78.66	78.34	D	3.20 ó 3.52		1	m	
<b>4÷</b>	71.49	71.19	D		3.18 ó 3.78	1	m	
<b>5÷</b>	78.40	78.10	D			1	m	
<b>6÷</b>	62.83	62.55	T	3.578		1	dd	11.8, 5.4
				3.718		1	dd	11.8, 2.4

<sup>a</sup> lit.<sup>1</sup>

d ó dublet, dd ó dublet dublet , m ó multiplet, J ó interak ní konstanta