Supporting information

SIALIDASE INHIBITORY ACTIVITY OF SYNTHESIZED BIFLAVONOID GLYCOCONJUGATES

Hiroaki Sasaki,[a*] Takayuki Nagai,[b,c,d] Takayuki Nakamura,[a] Yusuke Umezawa,[a] Kazuhiko Miki,[a] Haruki Yamada,[b,c,d] Kiyotaka Koyama,[a] Kunio Takahashi,[a] and Kaoru Kinoshita[a]

[a]Meiji Pharmaceutical University, Noshio 2-522-1, Kiyose-shi, Tokyo 204-8588, Japan; E-Mail: sasaki@my-pharm.ac.jp

[b]Laboratory of Biochemical Pharmacology for Phytomedicines, Ōmura Satoshi Memorial Institute, Kitasato University, 5-9-1 Shirokane, Minato-ku, Tokyo 108-8641, Japan

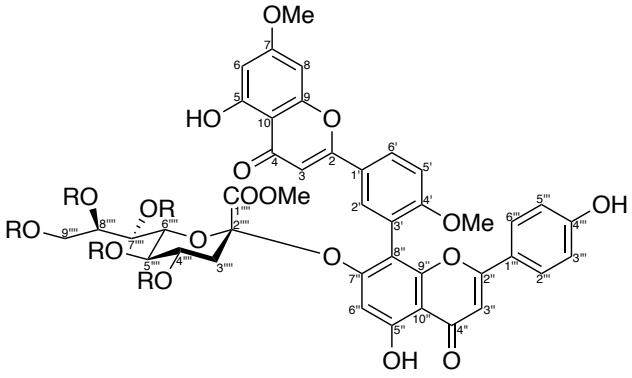
[c]Graduate School of Infection Control Sciences, Kitasato University, 5-9-1 Shirokane, Minato-ku, Tokyo 108-8641, Japan

[d]Oriental Medicine Research Center, Kitasato University, 5-9-1 Shirokane, Minato-ku, Tokyo 108-8642, Japan

Table 1. ^{1}H-NMR spectra of **11R**, **11S**, **12R**, and **12S** (500 MHz)

position	**11R** in DMSO-d_6	**11S** in DMSO-d_6	**12R** in CD_3OD	**12S** in CD_3OD
3	6.98 (s)	6.98 (s)	7.19 (s)	7.14 (s)
6	6.38 (d, 2.4)	6.38 (d 2.4)	6.24 (brs)	6.26 (d 2.0)
8	6.76 (d, 2.4)	6.70 (d, 2.4)	6.76 (brs)	6.78 (d, 2.0)
2'	8.14 (d, 2.4)	8.14 (d, 2.4)	8.06 (d, 2.0)	8.53 (d, 2.1)
5'	7.36 (d, 9.1)	7.40 (d, 9.0)	7.31 (d, 8.4)	7.31 (d, 8.8)
6'	8.25 (dd, 9.1, 2.4)	8.26 (dd, 9.0, 2.4)	8.11 (d, 8.4, 2.0)	8.12 (d, 8.8, 2.1)
3"	6.89 (s)	6.94 (s)	6.75 (s)	6.90 (s)
6"	6.88 (s)	6.88 (s)	6.46 (s)	6.48 (s)
2"', 6"'	7.50 (d, 8.8)	7.55 (d, 8.8)	7.34 (d, 8.9)	7.35 (d, 9.1)
3"', 5"'	6.65 (d, 8.8)	6.74 (d, 8.8)	6.48 (d, 8.9)	6.49 (d, 9.1)
5-OH	12.90 (brs)	12.89 (s)		
5"-OH	13.21 (brs)	13.17 (s)		
7-OCH_3	3.83 (s)	3.83 (s)	3.82 (s)	3.88 (s)
4'-OCH_3	3.79 (s)	3.80 (s)	3.80 (s)	3.80 (s)
3""	2.01 (dd, 13.3, 5.2)	2.00 (m)	1.62 (t, 12.0)	1.62 (t, 12.3)
	2.46 (m)	2.49 (m)	2.71 (dd, 12.0, 3.8)	2.84 (dd, 12.3, 5.0)
4""	4.91 (dt, 9.5, 5.2)	4.93 (dt, 9.6, 5.4)	3.59 (m)	3.63 (m)
5""	4.78 (t, 9.5)	4.81 (t, 9.6)	3.59 (t, 9.3)	3.48 (t, 9.5)
6""	4.36 (dd, 10.2, 1.8)	4.41 (dd, 10.2, 1.6)	4.07 (brd, 9.3)	4.16 (dd, 9.5, 1.3)
7""	5.20 (dd, 7.8, 1.8)	5.21 (dd, 7.5, 1.6)	3.82 (m)*	3.86 (m)*
8""	5.27 (m)	5.29 (m)	3.89 (m)*	3.99 (m)*
9""	4.16 (dd, 12.4, 5.6)	4.18 (dd, 12.4, 5.8)	3.69 (m)	3.73 (dd, 11.3, 5.6)
	4.30 (dd, 12.4, 3.1)	4.32 (dd, 12.4, 2.9)	3.86 (m)*	3.94 (m)*
$COOCH_3$	3.63 (s)	3.68 (s)		
$OCOCH_3$	1.83 (s)	1.79 (s)		
	1.95 (s)	1.96 (s)		
	1.99 (s)	2.00 (s)		
	2.08 (s)×2	2.06 (s)		
		2.09 (s)		

*maybe interchanged

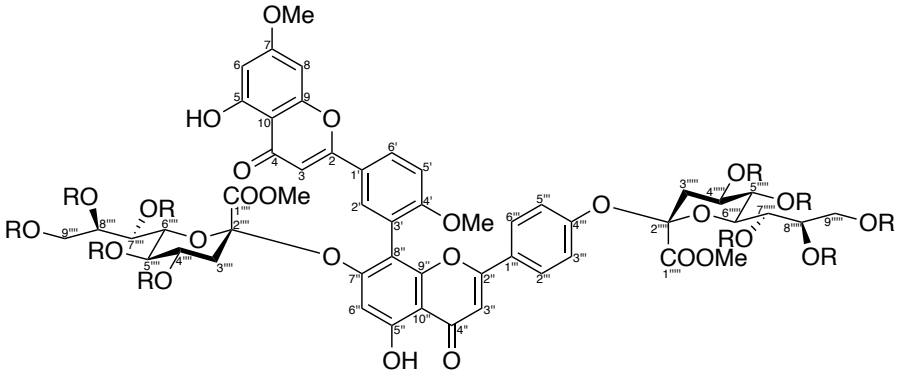


11: R = Ac
12: R = H

Table 2. ^{1}H-NMR spectra of **13R**, **13S**, **14R**, and **14S** (500 MHz)

position	**13R** in DMSO-d_6	**13S** in DMSO-d_6	**14R** in CD_3OD	**14S** in CD_3OD
3	6.96 (s)	6.97 (s)	7.25 (s)	7.15 (s)
6	6.35 (d, 2.1)	6.38 (d, 2.4)	6.27 (d, 2.1)	6.26 (d, 2.0)
8	6.76 (d, 2.1)	6.68 (d, 2.4)	6.78 (d, 2.1)	6.71 (d, 2.0)
2'	8.13 (d, 2.4)	8.11 (d, 2.4)	8.07 (d, 2.2)	8.50 (d, 2.1)
5'	7.36 (d, 9.1)	7.40 (d, 8.9)	7.35 (d, 8.9)	7.33 (d, 8.8)
6'	8.24 (dd, 9.1, 2.4)	8.25 (dd, 8.9, 2.4)	8.12 (d, 8.9, 2.2)	8.10 (d, 8.8, 2.1)
3"	7.08 (s)	7.08 (s)	6.83 (s)	6.84 (s)
6"	6.92 (s)	6.90 (s)	6.71 (s)	6.67 (s)
2"', 6"'	7.63 (d, 9.0)	7.66 (d, 9.1)	7.51 (d, 8.9)	7.51 (d, 9.1)
3"', 5"'	7.03 (d, 9.0)	7.04 (d, 9.1)	7.25 (d, 8.9)	7.24 (d, 9.1)
5-OH	12.89 (s)	12.89 (s)		
5"-OH	13.05 (s)	13.06 (s)		
7-OCH_3	3.84 (s)	3.84 (s)	3.88 (s)	3.87 (s)
4'-OCH_3	3.81 (s)	3.83 (s)	3.78 (s)	3.77 (s)
3""	1.96 (m)	1.98 (m)	1.66 (t, 12.6)	1.62 (t, 12.3)
	2.42 (dd, 13.3, 5.0)	2.48 (m)	2.70 (dd, 12.6, 3.8)	2.82 (dd, 12.3, 4.9)
4""	4.90 (m)	4.92 (m)	3.60 (m)*	3.59 (m)*
5""	4.77 (t, 10.1)	4.80 (t, 10.2)	3.54 (m)*	3.47 (t, 9.4)**
6""	4.35 (dd, 10.1, 1.5)	4.40 (dd, 10.2, 1.7)	3.96 (brd, 9.7)**	4.04 (brd, 9.4)***
7""	5.20 (dd, 7.9, 1.5)	5.21 (m)	3.80 (m)***	3.72 (m)****
8""	5.27 (m)	5.29 (dt, 6.6, 2.8)	3.88 (m)***	3.93 (m)****
9""	4.17 (dd, 12.4, 5.6)	4.17 (m)	3.65 (m)*	3.64 (m)*
	4.30 (dd, 12.4, 2.9)	4.33 (dd, 12.4, 2.9)	3.86 (m)***	3.85 (m)****
3""	2.15 (dd, 13.1, 11.9)	2.18 (dd, 13.2, 11.6)	1.82 (t, 12.3)	1.83 (t, 12.1)
	2.70 (dd, 13.1, 5.0)	2.70 (dd, 13.2, 5.0)	2.87 (dd, 12.3, 4.7)	2.86 (dd, 12.1, 4.7)
4""	4.93 (m)	4.95 (m)	3.62 (m)*	3.63 (m)*
5""	4.79 (t, 10.2)	4.83 (t, 10.2)	3.58 (m)*	3.53 (t, 8.9)**
6""	4.44 (dd, 10.2, 1.8)	4.49 (bd, 10.2)	4.08 (brd, 9.5)**	4.16 (dd, 8.9, 1.6)***
7""	5.18 (dd, 9.0, 1.8)	5.21 (m)	3.85 (m)***	3.78 (m)****
8""	5.09 (m)	5.21 (m)	3.88 (m)***	3.98 (m)****
9""	3.87 (dd, 12.5, 4.3)	4.10 (m)	3.67 (m)*	3.66 (m)*
	4.02 (dd, 12.5, 2.7)	4.19 (m)	3.87 (m)**	3.89 (m)****
$COOCH_3$	3.59 (s)	3.56 (s)		
	3.62 (s)	3.68 (s)		
$OCOCH_3$	1.83 (s)	1.77 (s)		
	1.93 (s)×2	1.84 (s)		
	1.94 (s)	1.95 (s)		
	1.95 (s)×2	1.97 (s)		
	1.99 (s)	1.99 (s)×2		
	2.08 (s)	2.00 (s)		
	2.09 (s)×2	2.05 (s)		
		2.09 (s)×2		

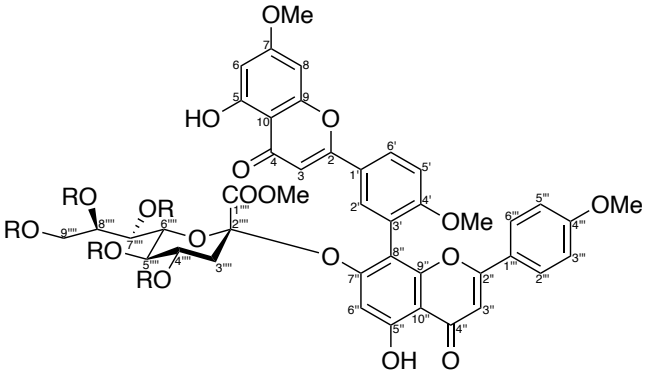
*maybe interchanged



13: R = Ac
14: R = H

Table 3. ^{1}H- NMR spectra of **15R**, **15S**, **16R**, and **16S** (500 MHz)

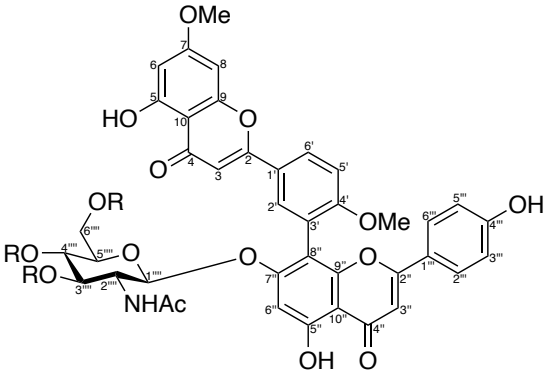
position	**15R** in DMSO-d_6	**15S** in DMSO-d_6	**16R** in CD_3OD	**16S** in CD_3OD
3	6.97 (s)	6.97 (s)	7.26 (s)	7.19 (s)
6	6.37 (d, 2.1)	6.38 (d, 2.2)	6.30 (d, 2.0)	6.30 (d, 2.1)
8	6.73 (d, 2.1)	6.69 (d, 2.2)	6.68 (d, 2.0)	6.76 (d, 2.1)
2'	8.13 (d, 2.4)	8.12 (d, 2.4)	8.07 (brs)	8.52 (d, 2.2)
5'	7.37 (d, 9.0)	7.40 (d, 8.9)	7.31 (d, 9.0)	7.30 (d, 8.7)
6'	8.25 (dd, 9.0, 2.4)	8.26 (dd, 8.9, 2.4)	8.11 (d, 9.0, 2.0)	8.09 (d, 8.7, 2.2)
3"	7.01 (s)	7.03 (s)	6.79 (s)	6.84 (s)
6"	6.91 (s)	6.89 (s)	6.67 (s)	6.69 (s)
2"', 6"'	7.63 (d, 8.8)	7.65 (d, 9.5)	7.57 (d, 8.7)	7.59 (d, 9.0)
3"', 5"'	6.92 (d, 8.8)	6.96 (d, 9.5)	6.90 (d, 8.7)	6.92 (d, 9.0)
5-OH	12.89 (brs)	12.88 (s)		
5"-OH	13.09 (brs)	13.12 (s)		
7-OCH_3	3.82 (s)	3.83 (s)	3.86 (s)	3.87 (s)
4'-OCH_3	3.80 (s)	3.80 (s)	3.79 (s)	3.80 (s)
4"'-OCH_3	3.74 (s)	3.77 (s)	3.78 (s)	3.79 (s)
3""	2.00 (dd, 13.3, 5.1)	1.97 (m)	1.64 (t, 12.0)	1.60 (t, 12.2)
	2.46 (m)	2.50 (m)	2.71 (dd, 12.0, 4.1)	2.83 (dd, 12.2, 4.9)
4""	4.91 (dt, 10.0, 5.1)	4.92 (dd, 9.5, 5.4)	3.55 (m)*	3.62 (dt, 8.8, 4.9)
5""	4.79 (t, 10.0)	4.81 (t, 9.5)	3.53 (m)*	3.47 (t, 8.8)
6""	4.36 (dd, 10.0, 1.6)	4.40 (dd, 9.5, 1.6)	4.07 (brd, 9.0)	4.18 (dd, 8.8, 1.7)
7""	5.21 (dd, 7.6, 1.6)	5.21 (dd, 7.7, 1.6)	3.57 (m)*	3.77 (dd, 7.2, 1.7)
8""	5.27 (m)	5.28 (m)	3.80 (m)*	3.99 (dt, 7.2, 2.8)
9""	4.16 (dd, 12.4, 5.8)	4.18 (dd, 11.2, 5.7)	3.58 (m)*	3.71 (dd, 11.4, 5.7)
	4.30 (dd, 12.4, 2.9)	4.34 (dd, 11.2, 1.6)	3.69 (dd, 11.0, 3.7)	3.92 (dd, 11.4, 2.8)
$COOCH_3$	3.63 (s)	3.68 (s)		
$OCOCH_3$	1.82 (s)	1.78 (s)		
	1.95 (s)	1.95 (s)		
	1.99 (s)	2.00 (s)		
	2.08 (s)	2.05 (s)		
	2.08 (s)	2.09 (s)		



15: R = Ac
16: R = H

Table 4. ^{1}H-NMR spectra of **17R**, **17S**, **18R**, and **18S** in DMSO-d_6 (500 MHz)

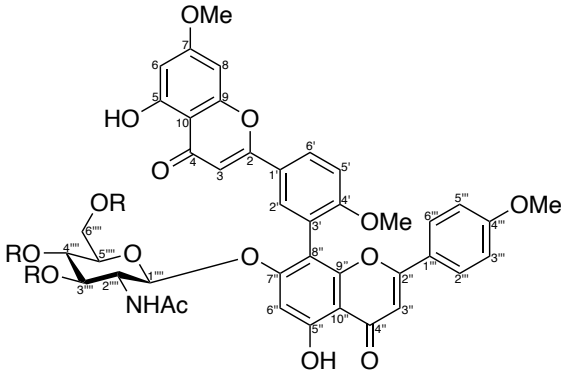
position	**17R** in DMSO-d_6	**17S** in DMSO-d_6	**18R** in DMSO-d_6	**18S** in DMSO-d_6
3	6.95 (s)	6.97 (s)	6.96 (s)	6.96 (s)
6	6.37 (d, 2.4)	6.37 (d, 2.2)	6.35 (d, 2.4)	6.35 (d, 2.2)
8	6.78 (d, 2.4)	6.81 (d, 2.2)	6.78 (d, 2.4)	6.81 (d, 2.2)
2'	7.94 (d, 2.4)	8.03 (d, 2.5)	7.94 (d, 2.5)	7.98 (d, 2.2)
5'	7.36 (d, 9.0)	7.37 (d, 9.1)	7.34 (d, 9.1)	7.34 (d, 8.8)
6'	8.21 (dd, 9.0, 2.4)	8.22 (dd, 9.1, 2.5)	8.20 (dd, 9.1, 2.5)	8.20 (dd, 8.8, 2.2)
3'	6.90 (s)	6.90 (s)	6.87 (s)	6.87 (s)
6'	6.81 (s)	6.84 (s)	6.74 (s)	6.74 (s)
2‴, 6‴	7.50 (d, 8.8)	7.49 (d, 9.2)	7.49 (d, 8.8)	7.48 (d, 9.0)
3‴, 5‴	6.73 (d, 8.8)	6.73 (d, 9.2)	6.73 (d, 8.8)	6.74 (d, 9.0)
5-OH	12.91 (s)	12.93 (s)	12.94 (s)	12.93 (s)
5''-OH	13.19 (s)	13.18 (s)	13.15 (s)	13.14 (s)
4‴-OH	3.83 (s)	3.83 (s)	3.82 (s)	3.84 (s)
7-OCH_3	3.80 (s)	3.73 (s)	3.78 (s)	3.73 (s)
4'-OCH_3				
1''''	5.54 (d, 8.4)	5.48 (d, 8.4)	5.20 (d, 8.4)	5.16 (d, 8.4)
2''''	3.81 (m)	3.78 (m)	3.50 (m)	3.47 (m)
3''''	5.15 (t, 9.8)	5.14 (t, 9.6)	3.38 (m)	3.35 (m)
4''''	4.86 (t, 9.8)	4.84 (t, 9.6)	3.13 (t, 9.2)	3.12 (m)
5''''	4.27 (m)	4.22 (m)	3.40 (m)	3.30 (m)
6''''	4.08 (dd, 12.2, 2.2)	4.06 (dd, 14.7, 5.4)	3.47 (m)	3.50 (m)
	4.18 (dd, 12.2, 6.0)	4.22 (m)	3.74 (m)	3.77 (m)
NH	7.86 (d, 9.2)	7.86 (d, 9.2)	7.59 (d, 9.2)	7.56 (d, 9.2)
$NHCOCH_3$	1.46 (s)	1.58 (s)	1.46 (s)	1.60 (s)
$OCOCH_3$	1.85 (s)	1.86 (s)		
	1.99 (s)	1.97 (s)		
	2.06 (s)	2.00 (s)		



17: R = Ac
18: R = H

Table 5. ^{1}H-NMR spectra of **20R**, **20S**, **21R**, and **21S** in DMSO-d_6 (500 MHz)

position	**20R** in DMSO-d_6	**20S** in DMSO-d_6	**21R** in DMSO-d_6	**21S** in DMSO-d_6
3	6.95 (s)	6.98 (s)	6.97 (s)	6.98 (s)
6	6.36 (d, 2.2)	6.37 (d, 2.2)	6.36 (d, 2.1)	6.36 (d, 2.1)
8	6.77 (d, 2.2)	6.81 (d, 2.2)	6.78 (d, 2.1)	6.80 (d, 2.1)
2'	7.92 (d, 2.4)	8.02 (d, 2.4)	7.94 (d, 2.4)	7.97 (d, 2.3)
5'	7.36 (d, 8.9)	7.35 (d, 8.9)	7.34 (d, 8.9)	7.35 (d, 8.9)
6'	8.22 (dd, 8.9, 2.4)	8.24 (dd, 8.9, 2.4)	8.21 (dd, 8.9, 2.4)	8.23 (dd, 8.9, 2.3)
3"	6.99 (s)	7.00 (s)	6.97 (s)	6.96 (s)
6"	6.83 (s)	6.86 (s)	6.75 (s)	6.78 (s)
2"', 6"'	7.60 (d, 8.9)	7.59 (d, 9.0)	7.59 (d, 9.2)	7.59 (d, 8.9)
3"', 5"'	6.94 (d, 8.9)	6.94 (d, 9.0)	6.94 (d, 9.2)	6.95 (d, 8.9)
5-OH	12.91 (s)	12.93 (s)	12.94 (s)	12.93 (s)
5"-OH	13.15 (s)	13.14 (s)	13.09 (s)	13.09 (s)
4"'-OH	3.82 (s)	3.84 (s)	3.82 (s)	3.84 (s)
7-OCH3	3.80 (s)	3.76 (s)	3.78 (s)	3.74 (s)
4'-OCH3	3.75 (s)	3.74 (s)	3.76 (s)	3.76 (s)
1""	5.54 (d, 8.2)	5.47 (d, 8.5)	5.22 (d, 8.5)	5.15 (d, 8.5)
2""	3.81 (m)	3.79 (m)	3.49 (m)	3.47 (m)
3""	5.15 (t, 9.8)	5.14 (t, 9.6)	3.38 (m)	3.37 (m)
4""	4.86 (t, 9.8)	4.86 (t, 9.6)	3.12 (m)	3.12 (m)
5""	4.27 (m)	4.23 (m)	3.43 (m)	3.38 (m)
6""	4.08 (brd, 10.4)	4.06 (brd, 12.3)	3.46 (m)	3.51 (m)
	4.18 (dd, 12.2, 5.8)	4.23 (dd, 12.3, 5.1)	3.72 (m)	3.75 (m)
NH	7.86 (d, 9.2)	7.85 (d, 9.2)	7.60 (d, 9.2)	7.55 (d, 9.2)
NHCOCH3	1.41 (s)	1.57 (s)	1.46 (s)	1.59 (s)
OCOCH3	1.85 (s)	1.87 (s)		
	1.98 (s)	1.98 (s)		
	2.05 (s)	2.01 (s)		

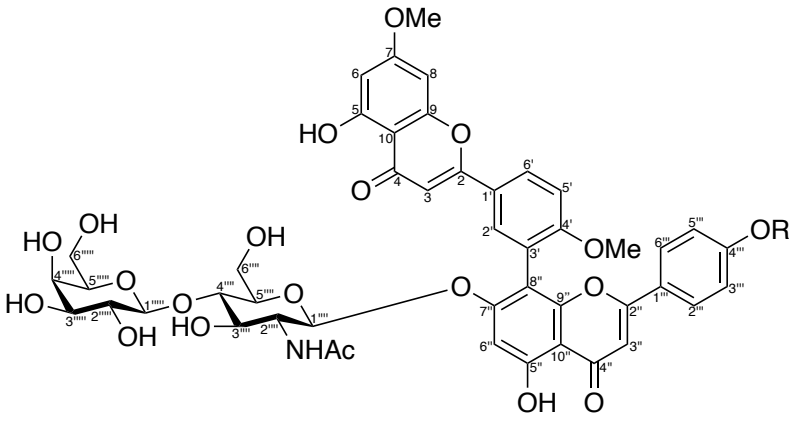


20: R = Ac
21: R = H

Table 6. ^{1}H-NMR spectra of **19R**, **19S**, **22R**, and **22S** in DMSO-d_6 (500 MHz)

position	**19R** in DMSO-d_6	**19S** in DMSO-d_6	**22R** in DMSO-d_6	**22S** in DMSO-d_6
3	6.97 (s)	6.95 (s)	6.96 (s)	6.96 (s)
6	6.36 (d, 2.4)	6.36 (d, 2.2)	6.35 (d, 2.1)	6.36 (d, 2.4)
8	6.79 (d, 2.4)	6.82 (d, 2.2)	6.78 (d, 2.1)	6.81 (d, 2.4)
2'	7.96 (d, 2.4)	7.97 (d, 2.6)	7.96 (d, 2.4)	7.97 (d, 2.3)
5'	7.34 (d, 9.0)	7.34 (d, 9.0)	7.35 (d, 9.0)	7.35 (d, 8.8)
6'	8.20 (dd, 9.0, 2.4)	8.22 (dd, 9.0, 2.6)	8.21 (dd, 9.0, 2.4)	8.23 (dd, 8.8, 2.3)
3"	6.85 (s)	6.86 (s)	6.98 (s)	6.98 (s)
6"	6.77 (s)	6.78 (s)	6.79 (s)	6.80 (s)
2"', 6"'	7.47 (d, 9.0)	7.46 (d, 9.0)	7.59 (d, 9.2)	7.63 (d, 9.2)
3"', 5"'	6.70 (d, 9.0)	6.70 (d, 9.0)	6.93 (d, 9.2)	6.94 (d, 9.2)
5-OH	12.94 (s)	12.93 (s)	12.93 (s)	12.93 (s)
5"-OH	13.18 (s)	13.18 (s)	13.10 (s)	13.10 (s)
4"'-OH	3.82 (s)	3.84 (s)	3.81 (s)	3.84 (s)
7-OCH3	3.78 (s)	3.73 (s)	3.77 (s)	3.74 (s)
4'-OCH3			3.75 (s)	3.76 (s)
1""	5.27 (d, 8.1)	5.27 (d, 7.7)	5.28 (d, 7.9)	5.20 (d, 7.6)
2""	3.55 (m)	3.52 (m)	3.57 (m)*	3.53 (m)
3""	3.57 (m)	3.54 (m)	3.57 (m)*	3.56 (m)
4""	3.37 (m)	3.36 (m)	3.38 (m)	3.37 (m)
5""	3.63 (m)	3.62 (m)	3.64 (m)**	3.61 (m)
6""	3.64 (m)	3.67 (m)	3.64 (m)**	3.75 (m)
	3.84 (m)	3.84 (m)	3.82 (m)	3.85 (m)
NH	7.67 (d, 9.2)	7.64 (d, 8.4)	7.67 (d, 7.9)	7.63 (d, 8.5)
NHCOCH3	1.45 (s)	1.59 (s)	1.46 (s)	1.59 (s)
1"''	4.21 (d, 7.0)	4.20 (d, 7.0)	4.21 (d, 7.0)	4.20 (d, 7.0)
2"''	3.31 (m)	3.30 (m)	3.31 (m)	3.32 (m)
3"''	3.32 (m)	3.29 (m)	3.29 (m)	3.29 (m)
4"''	3.60 (m)	3.60 (m)	3.61 (m)	3.59 (m)
5"''	3.43 (m)	3.43 (m)	3.44 (m)***	3.43 (m)
6"''	3.40 (m)	3.46 (m)	3.44 (m)***	3.47 (m)
	3.48 (m)	3.65 (m)	3.48 (m)	3.66 (m)

*maybe interchanged



19: R = H
22: R = Me

Table 7. ^{1}H-NMR spectra of **11R**, **11S**, **13R**, **13S**, **15R**, and **15S** in DMSO-d_6

position	**11R**	**11S**	**13R**	**13S**	**15R**	**15S**
2	163.6	163.6	163.7	163.8	163.6	163.9
3	103.8	103.8	103.7	103.7	103.8	103.8
4	181.9	181.9	181.9	181.9	181.9	181.7
5	161.1	161.1	161.2	161.1	161.1	161.1
6	98.1	98.1	98.0	98.0	98.0	98.1
7	165.2	165.2	165.2	165.2	165.1	165.2
8	92.7	92.5	92.6	92.4	92.7	92.5
9	157.3	157.3	157.2	157.3	157.3	157.3
10	104.7	104.9	104.7	104.7	104.7	104.7
1'	122.2	122.3	122.3	122.3	122.2	122.3
2'	130.8	130.9	130.7	130.7	130.7	130.8
3'	120.6	120.4	120.5	120.2	120.6	120.4
4'	160.4	160.1	160.3	160.0	160.4	160.1
5'	111.6	111.6	111.6	111.8	111.6	111.6
6'	128.6	128.7	128.6	128.6	128.6	128.7
2"	164.6	164.4	163.4	163.3	163.9	163.5
3"	102.4	103.0	104.7	104.6	103.6	103.6
4"	182.2	182.4	182.5	182.5	182.4	182.4
5"	160.4	160.5	160.3	160.5	160.4	160.3
6"	102.2	101.9	102.7	102.1	102.4	102.0
7"	156.0	156.2	156.5*	156.4	156.1	156.3
8"	108.4	108.1	108.8	108.3	108.6	108.2
9"	153.6	153.6	153.8	153.7	153.7	153.6
10"	106.5	106.4	106.8	106.6	106.6	106.5
1"'	119.7	120.8	125.6	125.4	122.5	122.5
2"', 6"'	128.3	128.3	127.9	127.9	128.0	128.0
3"', 5"'	116.2	115.9	119.2	118.7	114.6	114.6
4"'	163.0	161.4	156.3*	156.5	162.4	162.5
7-OCH_3	56.0	56.0	56.0	55.9	56.0	56.0
4'-OCH_3	55.9	55.9	55.8	55.7	55.9	55.9
4"'-OCH_3					55.5	55.5
1""	166.6	166.9	166.5	166.8	166.5	166.8
2""	99.9	100.1	100.0	100.1	100.0	100.1
3""	35.1	35.0	35.1	35.0	35.1	35.0
4""	68.1	68.2	68.1	68.2	68.1	68.2
5""	66.9	67.0	66.8	67.0	66.9	67.0
6""	71.6	71.7	71.6	71.6	71.6	71.6
7""	66.3	66.3	66.2	66.3	66.3	66.3
8""	68.2	68.3	68.2	68.3	68.2	68.3
9""	61.4	61.5	61.4	61.4	61.4	61.4
1"""			167.3	167.4		
2"""			99.4	99.1		
3"""			37.0	37.0		
4"""			68.1	68.0		
5"""			67.0	67.0		
6"""			71.6	71.6		
7"""			65.5	65.8		
8"""			67.4	67.2		
9"""			61.4	61.4		
$COO\underline{C}H_3$	53.3	53.5	53.4	53.5	53.3	53.5
			53.4	53.3		
$OCO\underline{C}H_3$	20.2	20.2	20.1	20.1	20.2×2	20.1
	20.3	20.3	20.2	20.2	20.3	20.3×2
	20.4×2	20.4	20.3×3	20.3×3	20.4	20.4
	20.6	20.5	20.4×2	20.4×2	20.5	20.5
		20.6	20.5×2	20.5×2		
			20.6	20.6		
$O\underline{C}OCH_3$	169.0	169.0	169.0×2	168.9	169.0	168.8
	169.3×3	168.3×2	169.2	169.0	169.3×3	168.9
	170.0	169.4	169.3×3	169.1	170.0	169.3
		170.0	169.4	169.2		170.0
			169.5	169.3×4		
			169.8	170.0×2		
			170.0			

*maybe interchanged

Table 8. ^{1}H-NMR spectra of **17R−22S** in DMSO-d_6

position	**17R**	**17S**	**18R**	**18S**	**19R**	**19S**	**20R**	**20S**	**21R**	**21S**	**22R**	**22S**
2	163.9	163.8	164.1	164.0	164.0*	163.9	163.7	163.6	164.0	163.9	164.0	164.0
3	104.0	103.9	104.0	103.8	103.9	103.9	104.0	103.8	104.0	103.4	104.0	103.9
4	181.9	181.9	182.0	181.9	182.0	181.9	181.7	181.7	182.0	181.9	182.0	181.9
5	160.9	160.9	160.4	161.1	160.9	161.1	160.9	160.9	160.4	161.1	160.9	160.9*
6	98.0	98.1	98.0*	98.1	98.0	98.1	97.9	98.0	98.0*	98.1	97.9	98.1
7	165.1	165.2	165.1	165.2	165.1	165.2	164.9	165.2	165.1	165.2	165.1	165.2
8	92.8	92.7	92.8	92.7	92.8	92.7	92.7	92.6	92.8	92.7	92.8	92.7
9	157.3	157.3	157.3	157.3	157.3	157.3	157.1	157.1	157.3	157.3	157.3	157.3
10	104.7	104.7	104.7	104.7	104.9	104.7	104.6	104.6	104.7	104.7	105.0	104.8
1'	122.2	122.5	122.6	122.4	122.7	122.4	122.4	122.4	122.6	122.5	122.6*	122.5
2'	130.5	130.9	130.8	131.0	130.8	130.9	130.5	130.7	130.7	130.9	130.8	130.9
3'	120.6	120.5	120.8	120.6	120.7	120.7	120.4	120.3	120.7	120.6	120.7	120.6
4'	160.4	160.2	160.3	160.2	160.3	160.2*	160.1	160.0	160.3	160.2	160.3	160.3
5'	111.9	111.5	111.8	111.4	111.9	111.5	111.7	111.4	111.8	111.5	111.8	111.5
6'	128.5	128.6	128.5	128.5	128.5	128.5	128.5	128.5	128.5	128.5	128.5	128.5
2''	164.2	164.2	164.0	163.9	164.2*	164.2	163.5	163.5	163.6	163.6	163.6	163.9
3''	102.7	102.8	102.7	102.7	102.4	102.4	103.3	103.3	103.3	103.8	103.4	103.4
4''	182.3	182.3	182.2	182.3	182.2	182.2	182.1	182.1	182.3	182.3	182.3	182.3
5''	161.3	161.3	160.9	161.3	161.1	160.9	160.7	160.7	161.1	160.9	161.1	161.1*
6''	98.0	98.7	98.1*	98.6	97.9	98.6	97.9	98.7	97.9	98.7	98.0	98.7
7''	159.2	157.3	160.0	160.3	159.8	160.1*	159.1	159.5	160.0	160.4	159.9	160.2
8''	105.6	106.1	105.4	106.1	105.4	106.1	105.5	106.1	105.4	106.1	105.5	106.2
9''	153.6	153.6	155.5	153.6	153.6	153.6	153.5	153.5	153.6	153.6	153.6	153.6
10''	105.2	105.4	104.9	105.1	104.7	105.1	105.2	105.4	104.9	105.2	104.7	105.2
1'''	120.9	120.9	121.0	120.9	120.8	120.2	122.4	122.4	122.6	122.5	120.6*	122.5
2''', 6'''	128.2	128.1	128.1	128.1	128.1	128.1	127.8	127.8	127.9	127.9	127.9	127.9
3''', 5'''	115.8	115.9	115.9	115.9	116.0	116.1	114.4	114.5	114.6	114.6	114.6	114.6
4'''	161.1	161.1	161.1	161.1	161.9	162.2	162.2	162.2	162.4	162.4	162.4	162.4
7-OCH_3	56.0	56.0	56.0	56.0	56.0	56.0	56.0	56.0	56.0	56.0	56.0	56.0
4'-OCH_3	55.9	55.9	55.9	55.9	55.9	55.9	55.9	55.9	55.9	55.9	55.9	55.9
4'''-OCH_3							55.5	55.5	55.5	55.5	55.5	55.5
1''''	96.8	97.8	97.9*	99.1	97.8	98.8	96.6	97.8	98.0*	99.2	97.7	98.9
2''''	52.8	52.8	55.1	55.0	54.4	54.3	52.8	52.8	55.1	54.9	54.4	54.2
3''''	72.3	72.2	74.1	74.0	72.1	72.0	72.3	72.1	74.0	74.0	72.0	72.0
4''''	68.3	68.3	70.1	70.2	80.7	80.8	68.2	68.2	70.1	70.2	80.6	80.8
5''''	71.0	71.1	77.5	77.6	75.4	75.6	71.0	71.1	77.4	77.6	75.4	75.6**
6''''	61.7	61.7	60.6	60.8	60.1	60.2	61.7	61.6	60.6	60.8	60.1	60.2
$NHCO\underline{C}H_3$	22.1	22.4	22.5	22.7	22.5	22.6	22.1	22.3	22.5	22.7	22.5	22.6
$NH\underline{C}OCH_3$	169.0	168.9	168.8	168.6	168.6	168.4	168.7	168.7	168.8	168.6	168.6	168.4
1'''''					104.0	103.9					103.9	103.9
2'''''					70.6	70.6					70.6	70.6
3'''''					73.2	73.2					73.2	73.2
4'''''					68.2	68.1					68.2	68.1
5'''''					75.6	75.5					75.6	75.5**
6'''''					60.5	60.4					60.5	60.4
$OCO\underline{C}H_3$	20.2	20.2					20.2	20.3				
	20.4	20.3					20.4	20.4				
	20.4	20.4					20.4	20.4				
$O\underline{C}OCH_3$	169.0	169.2					169.1	169.0				
	169.3	169.5					169.4	169.3				
	169.6	170.0					169.8	169.7				

*maybe interchanged