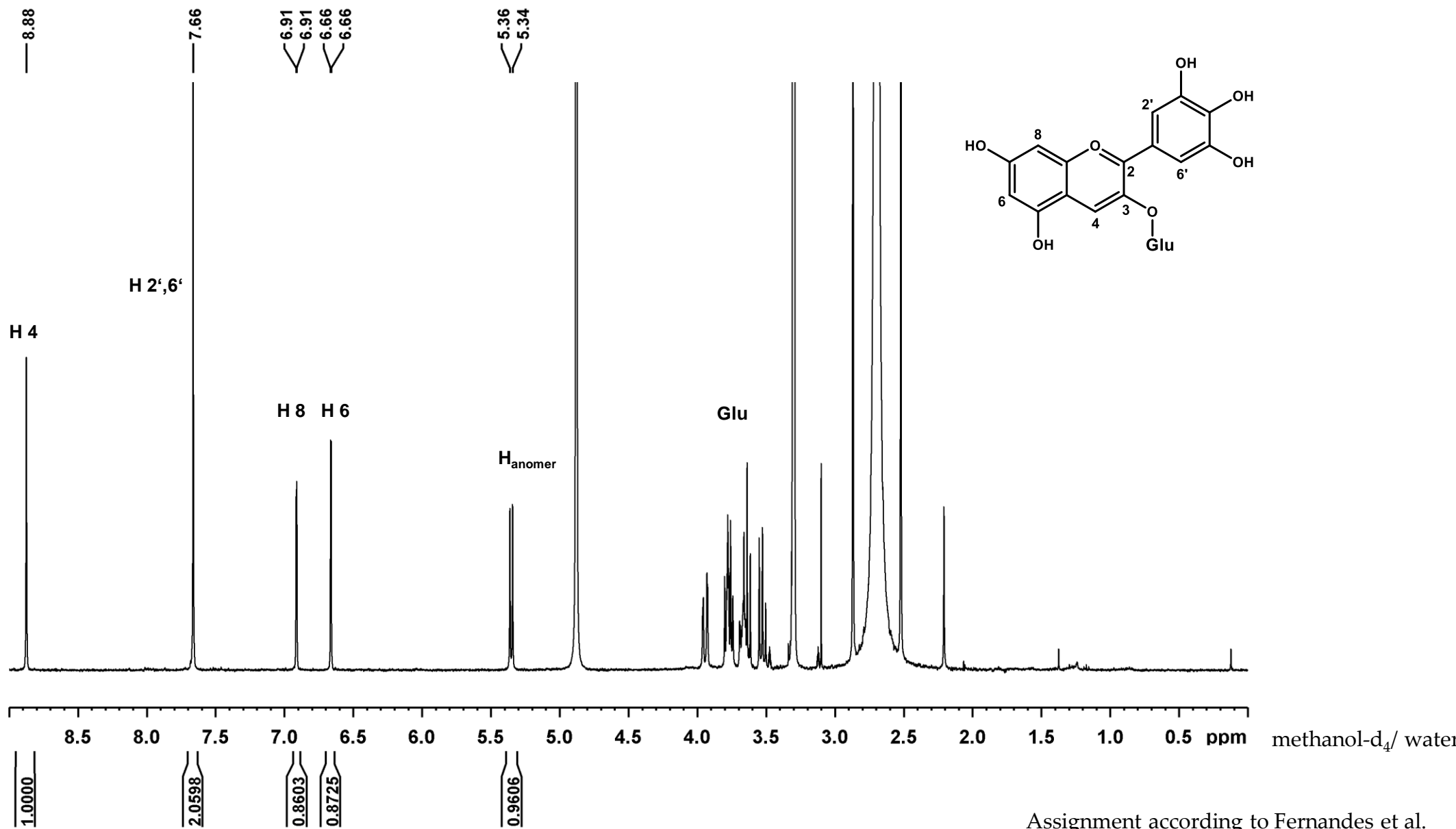


# Supplemental material

**Table S1.** Absorption coefficients of anthocyanidin-3-glucosides calculated by mass concentration  $\gamma$  determined by balance and q-NMR in aqueous buffer at pH 1.

ACY	$\lambda = 520 \text{ nm}$		$\lambda_{\text{max}} \text{ [nm]}$	$\lambda \text{ max}$		Difference of $\epsilon$ between calculation based on q-NMR and balance <sup>[b]</sup> [%]	$\epsilon$ according to [10]
	balance	NMR		balance	NMR		
	$\epsilon /$ ( $\text{L} \cdot \text{mol}^{-1} \cdot \text{cm}^{-1}$ )	$\epsilon /$ ( $\text{L} \cdot \text{mol}^{-1} \cdot \text{cm}^{-1}$ )		$\epsilon /$ ( $\text{L} \cdot \text{mol}^{-1} \cdot \text{cm}^{-1}$ )	$\epsilon /$ ( $\text{L} \cdot \text{mol}^{-1} \cdot \text{cm}^{-1}$ )		
PEL-3-glc	15849 $\pm$ 2070	20317 $\pm$ 423	497	21843 $\pm$ 2825	28006 $\pm$ 774	128	27300
CYD-3-glc	25526 $\pm$ 428	29619 $\pm$ 167	510	26953 $\pm$ 464	31275 $\pm$ 270	116	26900
DPD-3-glc	26935 $\pm$ 680	34070 $\pm$ 580	516	27087 $\pm$ 671	34263 $\pm$ 567	127	
PET-3-glc	26821 $\pm$ 1386	37438 $\pm$ 140	516	26892 $\pm$ 1353	37540 $\pm$ 192	140	
PEO-3-glc	23926 $\pm$ 898	29451 $\pm$ 185	510	25141 $\pm$ 931	30947 $\pm$ 210	123	
MLV-3-glc	27911 $\pm$ 437	33140 $\pm$ 251	518	27923 $\pm$ 443	33154 $\pm$ 257	119	28000

**Figure S1.** Proton spectra recorded at a 400 MHz Spectrometer of delphinidin-3-O-glucoside in buffer pH 1



Assignment according to Fernandes et al. (2015). New Journal of Chemistry, 39, 2602.

# Supplemental material

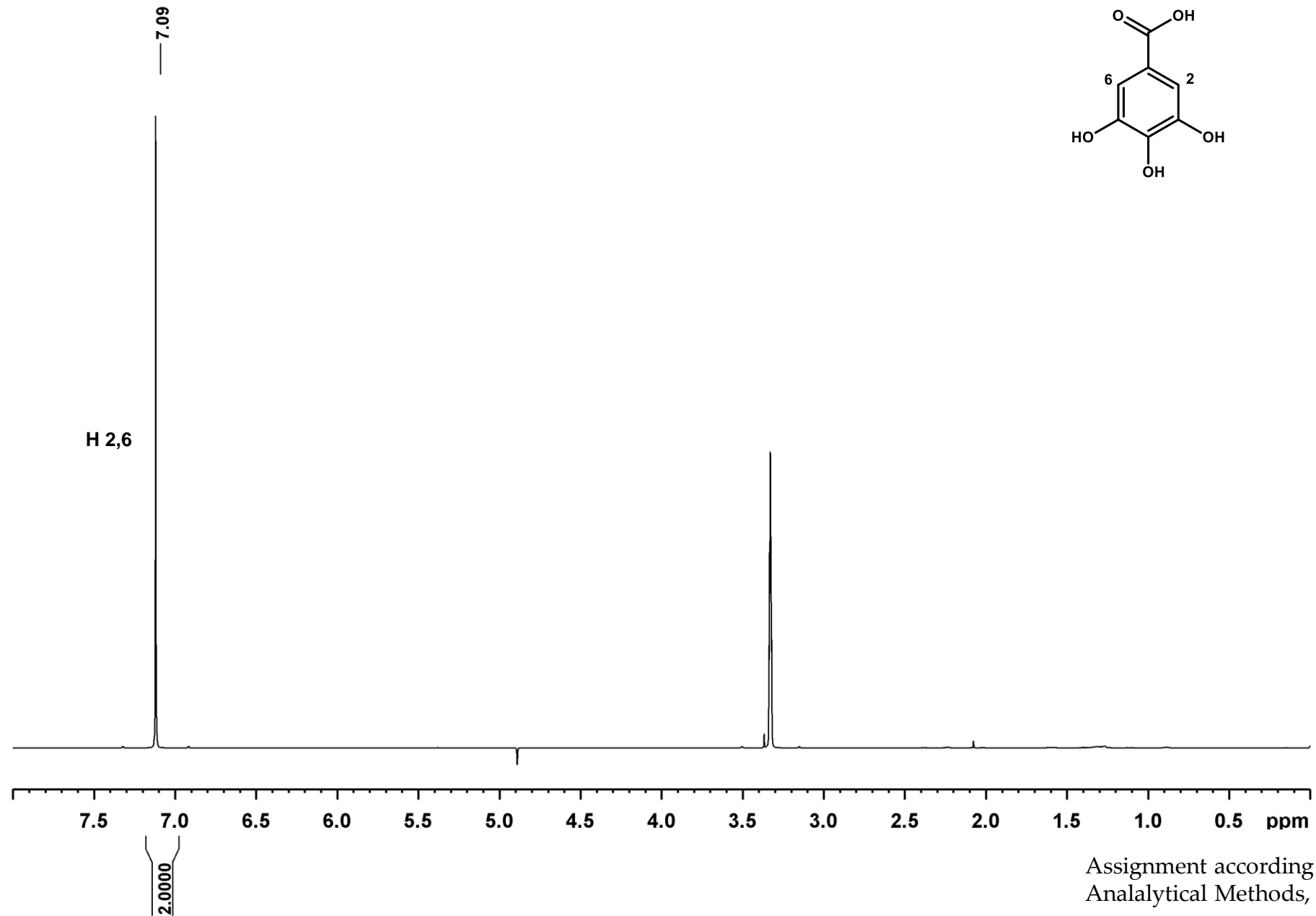
**Table S2.** Mass concentration  $\gamma$  determined by q-NMR in acidic methanol/water (50/50, v/v) and potassium chloride buffer pH 1.

	Quantification					
	by balance		by q-NMR spectroscopy			
	$\gamma$ / (mg/L)	protons for quantification	$\gamma_{\text{methanol/water}}$ /(mg/L)	$\gamma_{\text{buffer}}$ /(mg/L) <sup>[b]</sup>	Difference between balance/NMR [%]	
					methanol/water	buffer
Dpd-3-glc 1	1522	H 4; H 2',6'; H 8; H6; H <sub>anomer</sub>	1408	1120	93	74
Dpd-3-glc 2	979	H 4; H 2',6'; H 8; H6; H <sub>anomer</sub>	885	733	90	75
Dpd-3-glc 1	1522	H 4; H 2',6'	1520	1145	100	75
Dpd-3-glc 2	979	H 4; H 2',6'	937	778	96	79

# Supplemental material

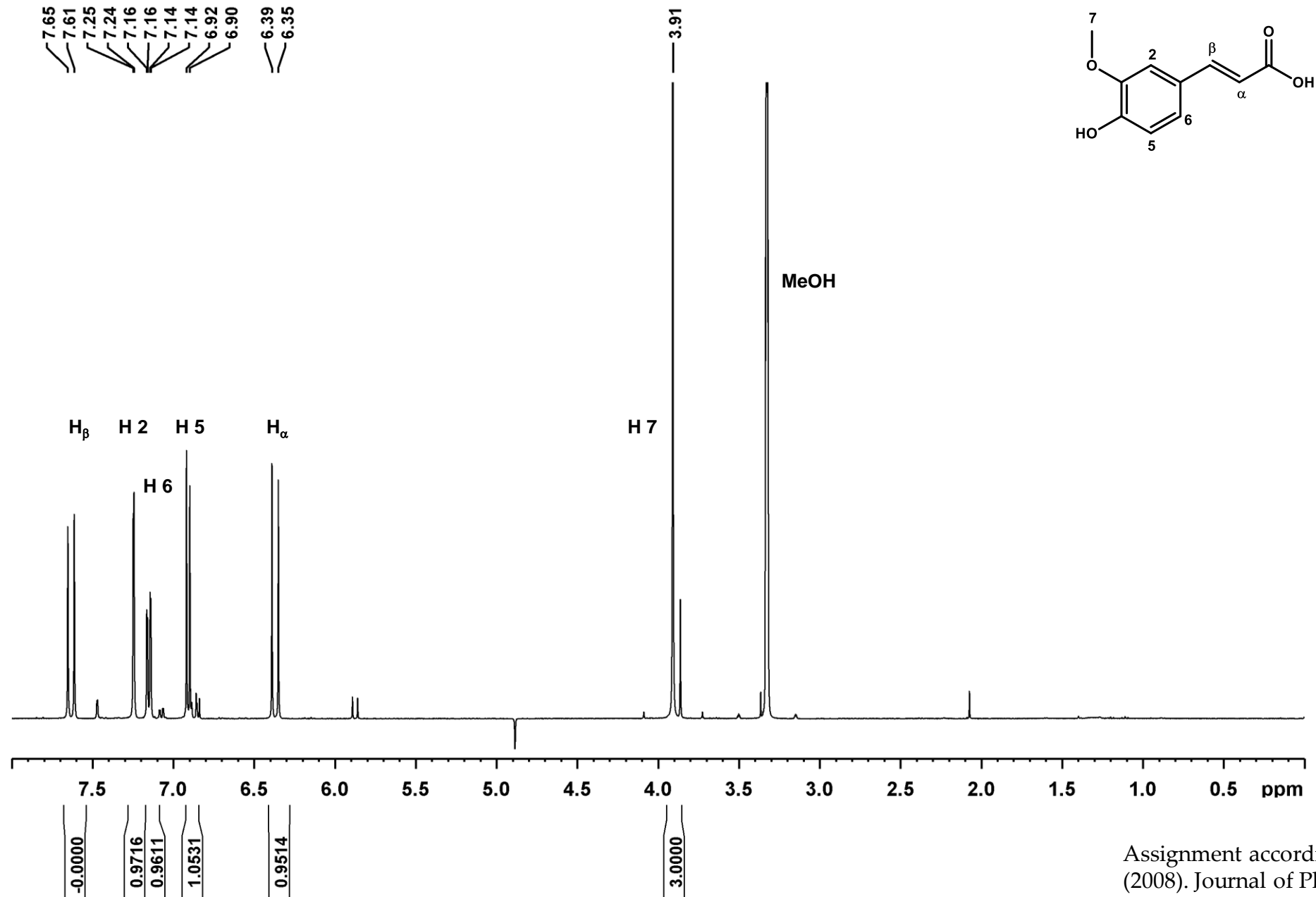
**Figure S2.** Proton spectra recorded at a 400 MHz Spectrometer and used for quantification including signal assignment based on literature and own 2D NMR spectra in methanol-d<sub>4</sub>/ D<sub>2</sub>O

# gallic acid



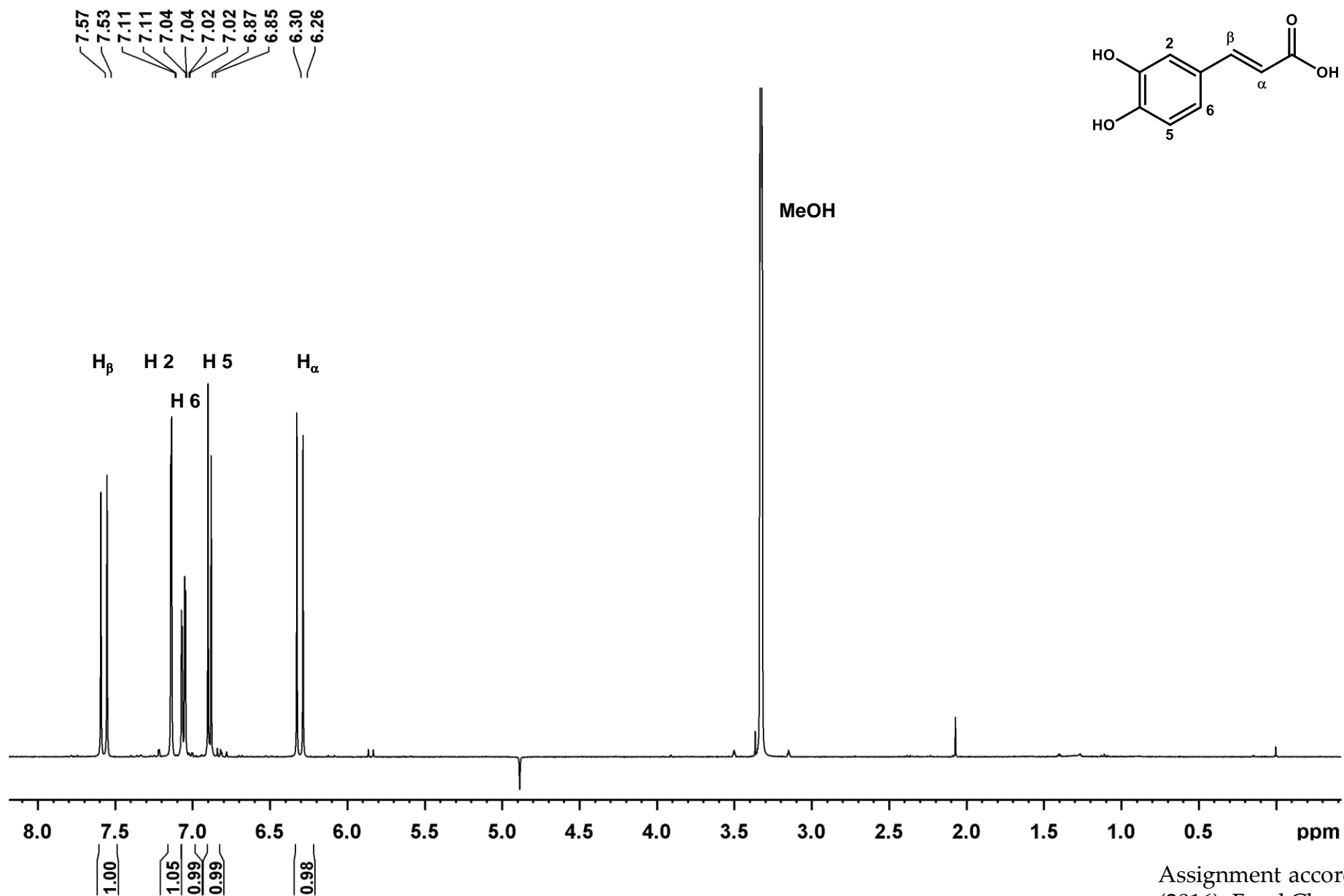
Assignment according to Yuan et al. (2014).  
Analytical Methods, 6, 907-914.

# *trans*-ferulic acid



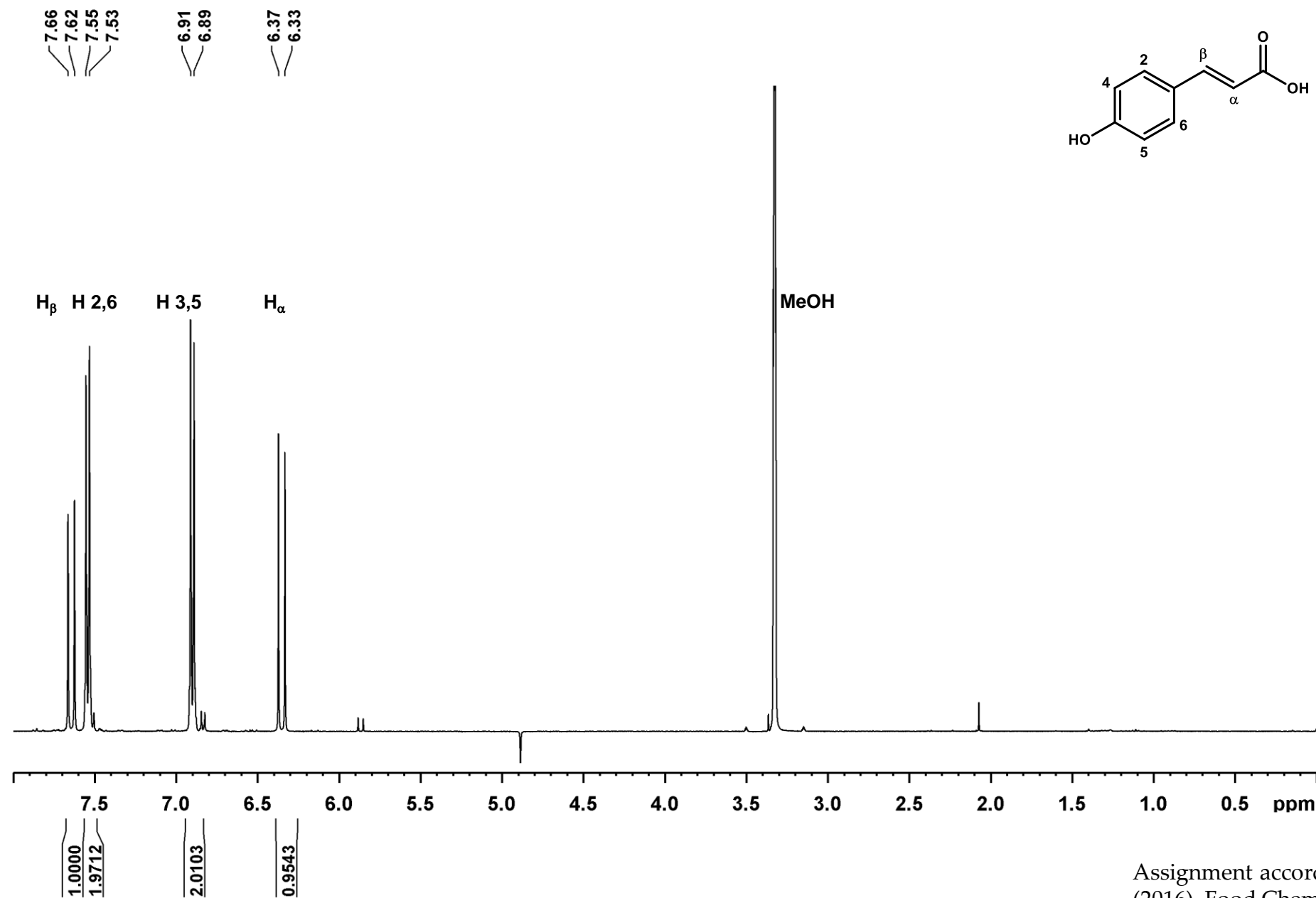
Assignment according to Anselmi et al. (2008). Journal of Pharmaceutical and Biomedical Analysis 46, 4, 645-652.

*trans*-caffeic acid



Assignment according to Forino et al.  
(2016). Food Chemistry, 194, 1254-1259.

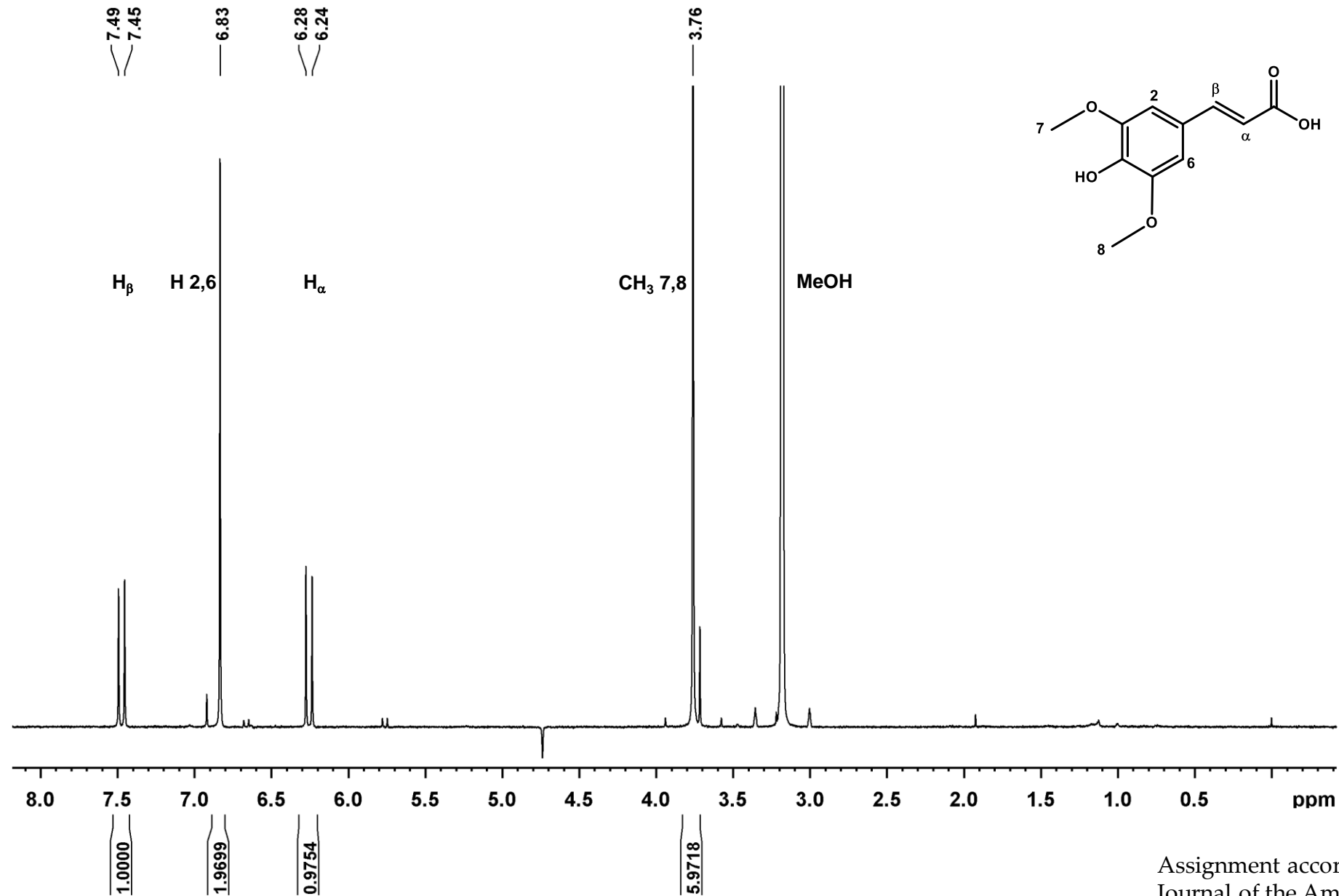
*trans*-coumaric acid



Assignment according to Forino et al.  
(2016). Food Chemistry, 194, 1254-1259.

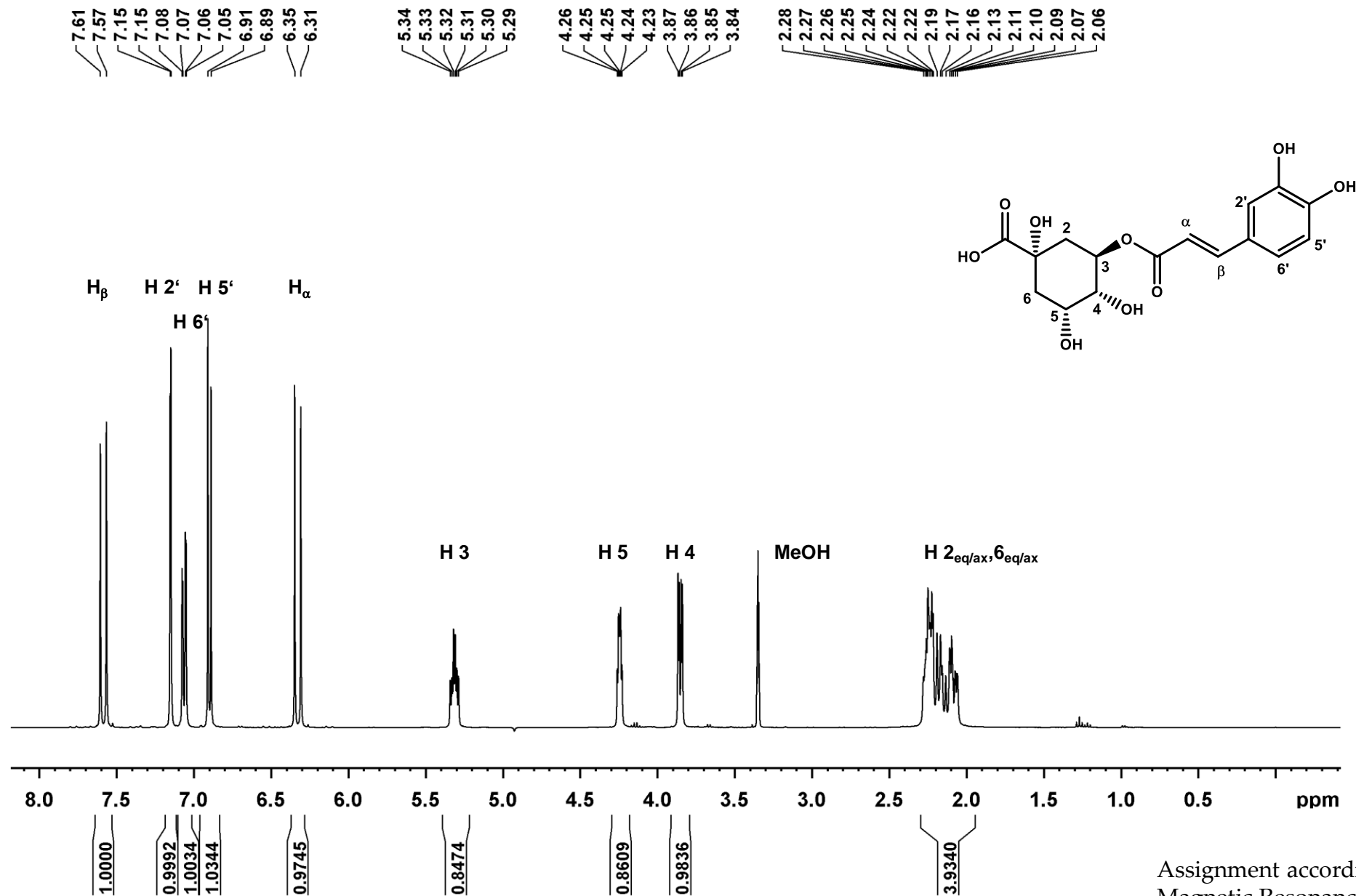


*trans*-sinapinic acid



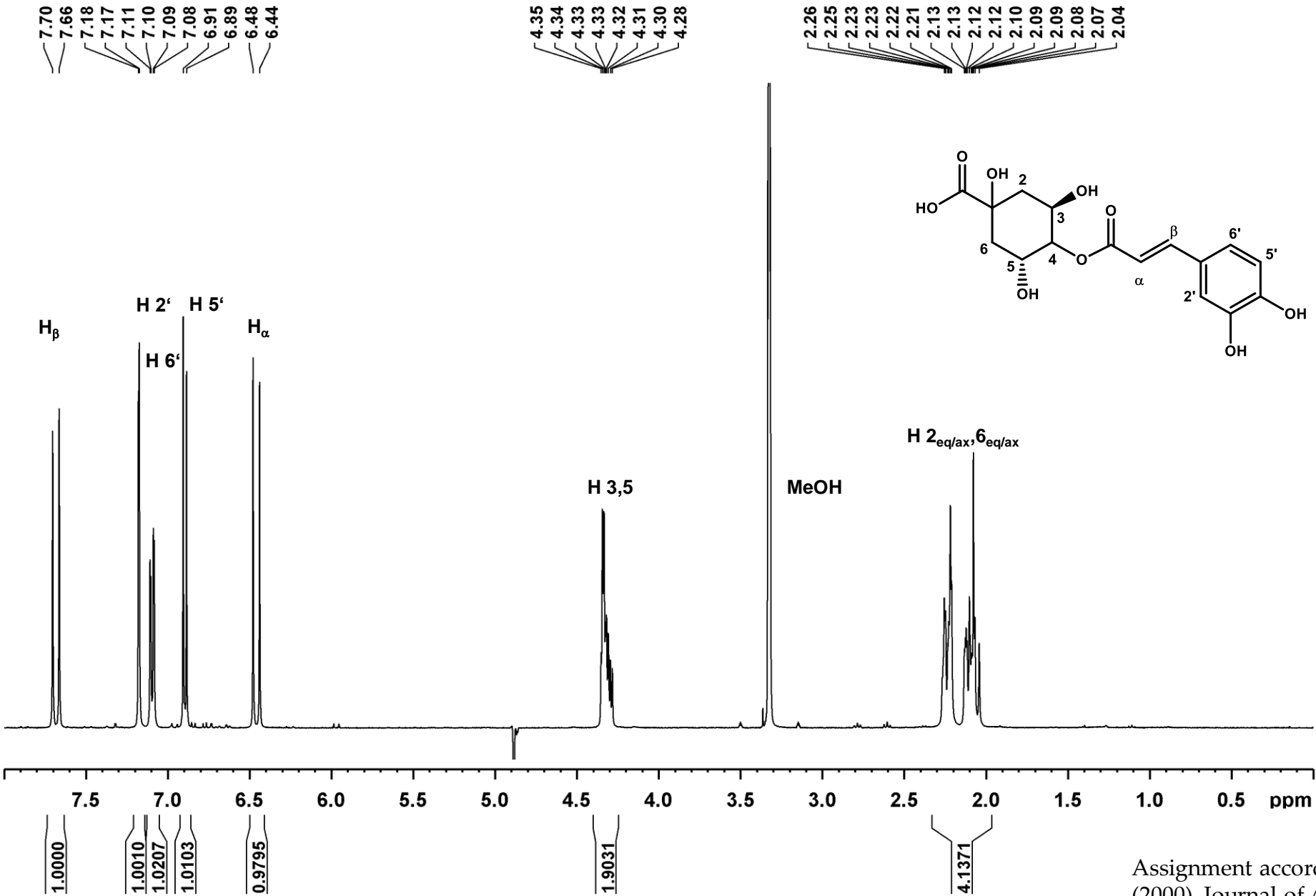
Assignment according to Cai et al. (1999)  
Journal of the American Oil Chemists, 76,  
4, 433-441.

# chlorogenic acid



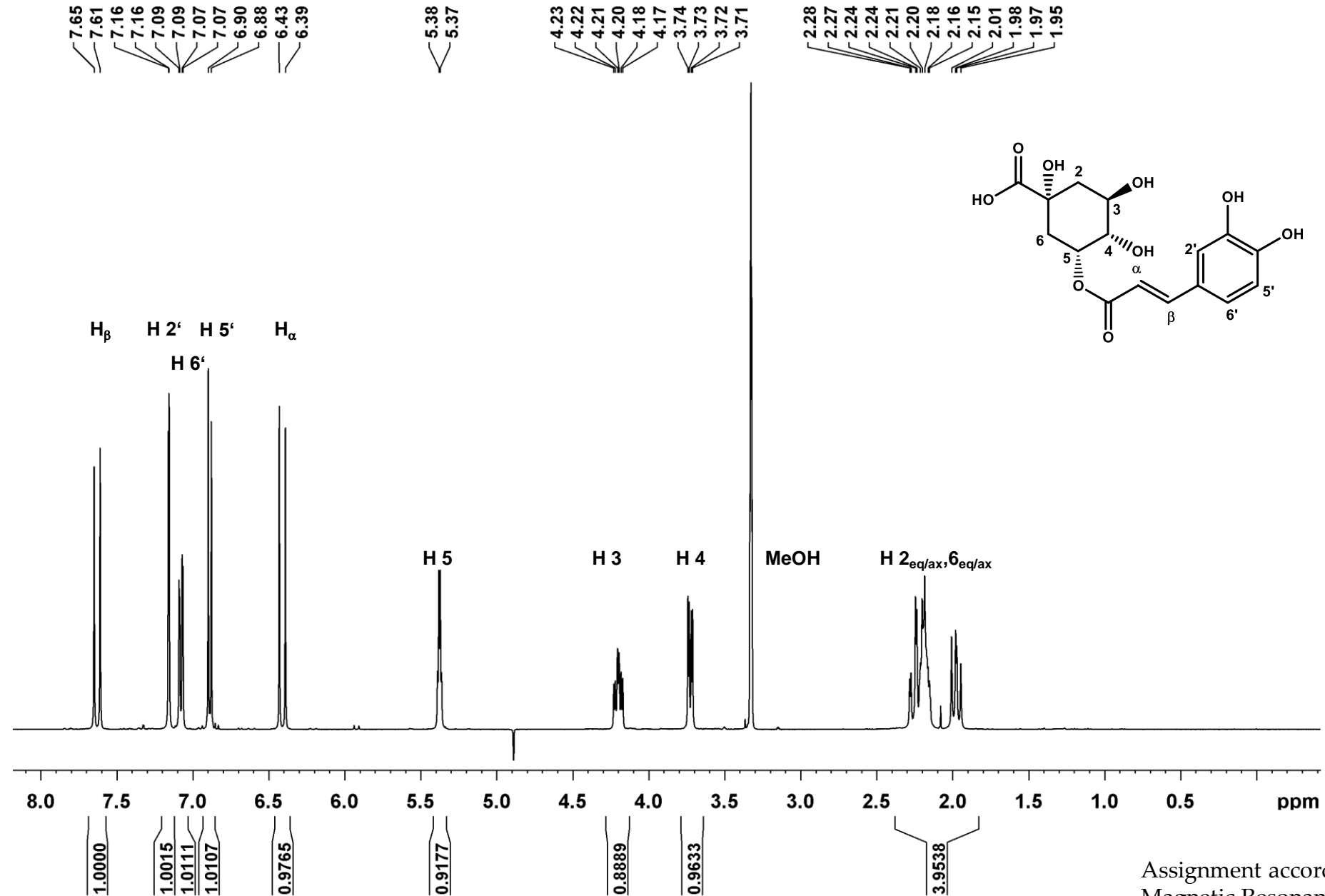
Assignment according to Pauli et al. (1999).  
Magnetic Resonance in Chemistry. Chem.  
37, 11, 827-836.

cryptochlorogenic acid



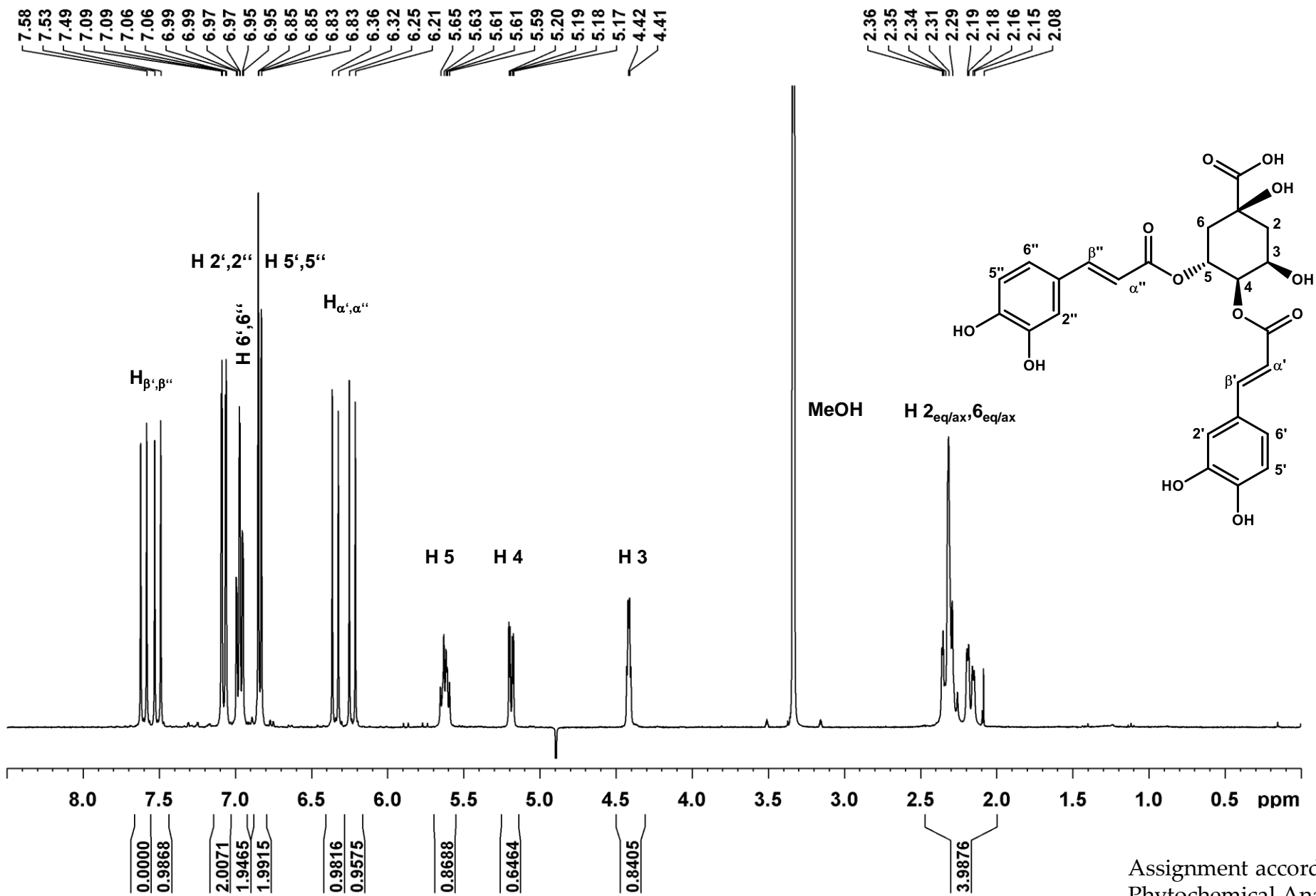
Assignment according to Nakatani et al. (2000). Journal of Agricultural and Food Chemistry, 48, 5512-5516.

# neochlorogenic acid



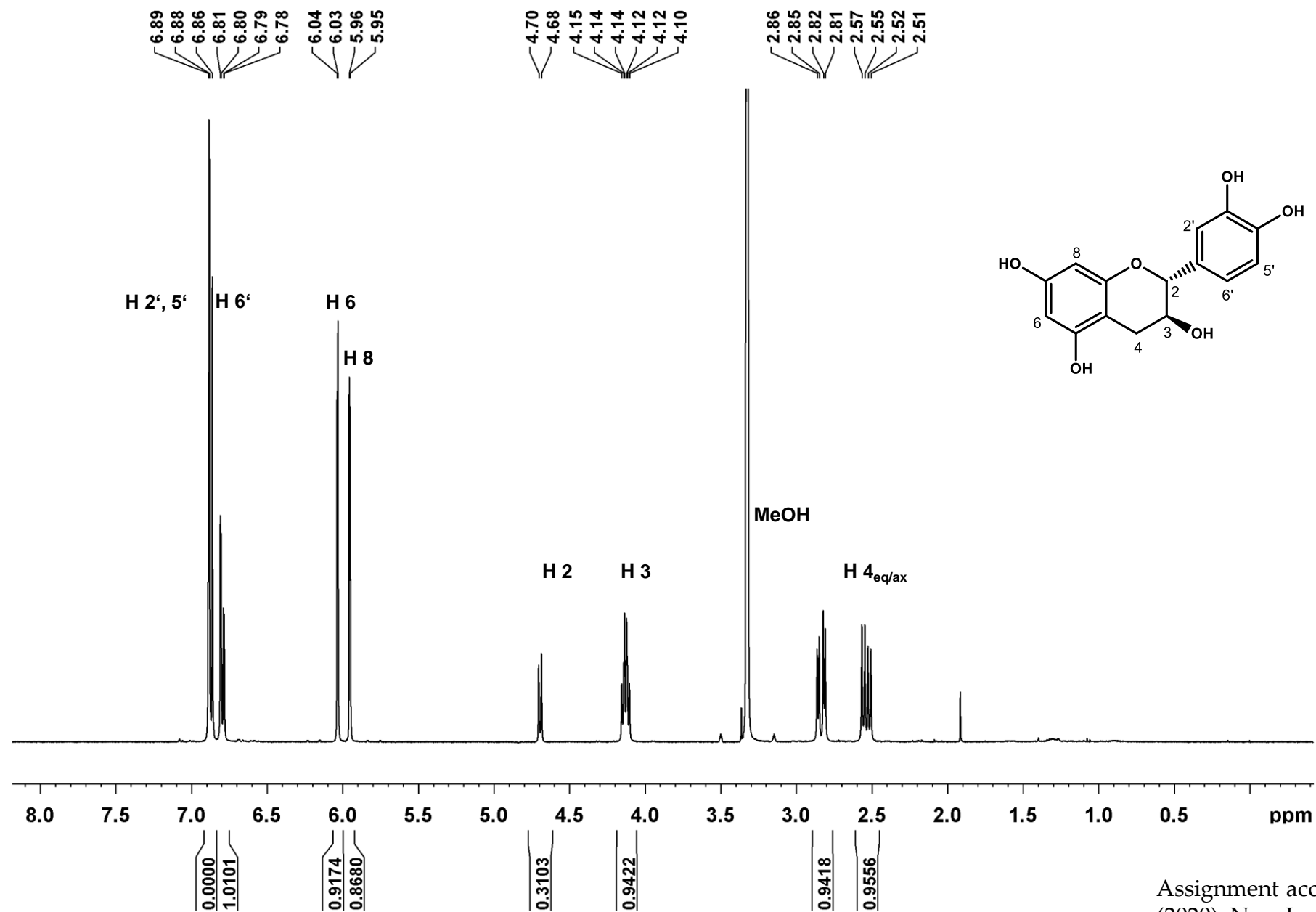
Assignment according to Pauli et al. (1999).  
Magnetic Resonance in Chemistry. Chem.  
37, 11, 827-836.

4,5-dicaffeoylquinic acid



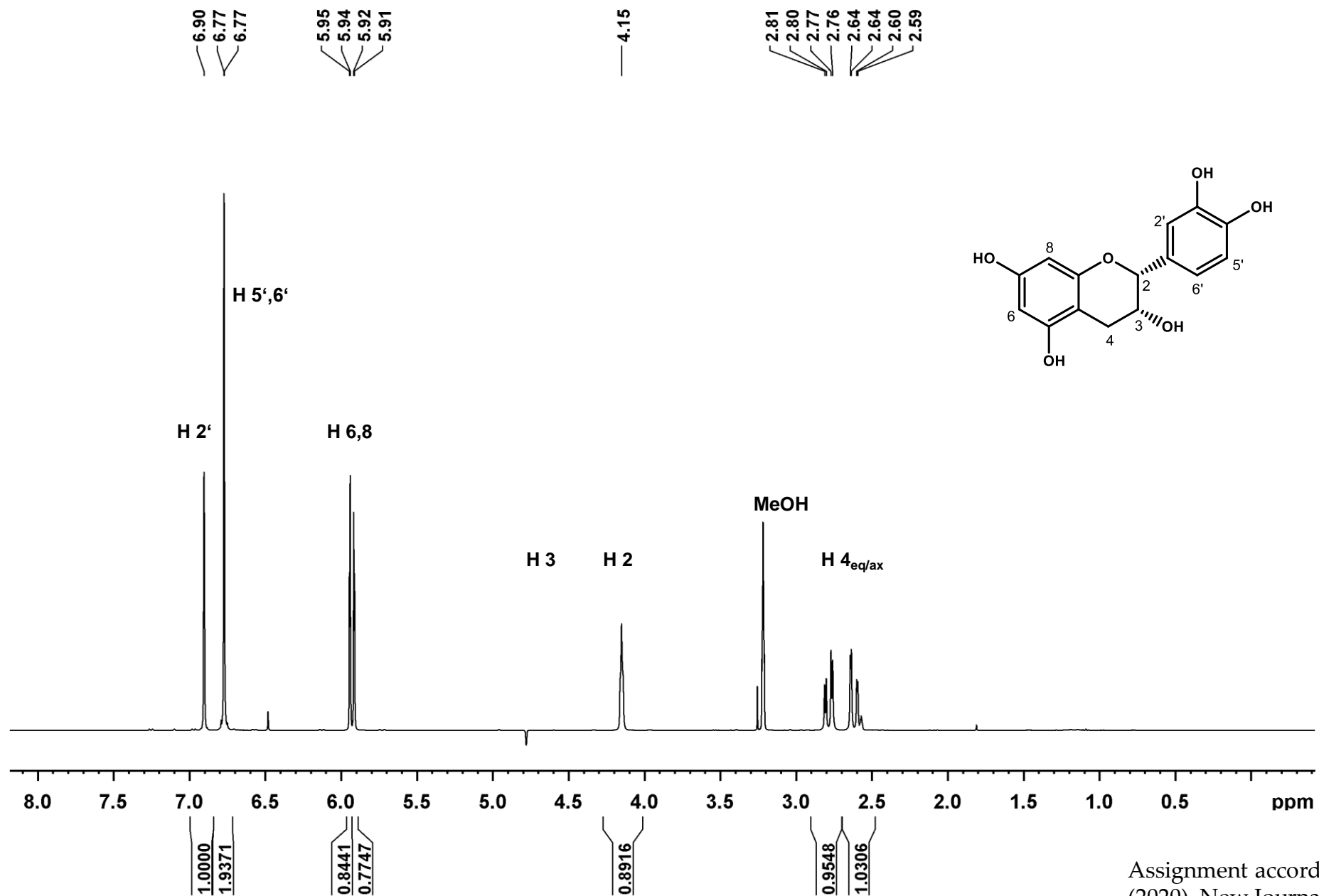
Assignment according to Wu et al. (2007).  
Phytochemical Analysis, 18, 5, 401-410.

# (+)-catechin



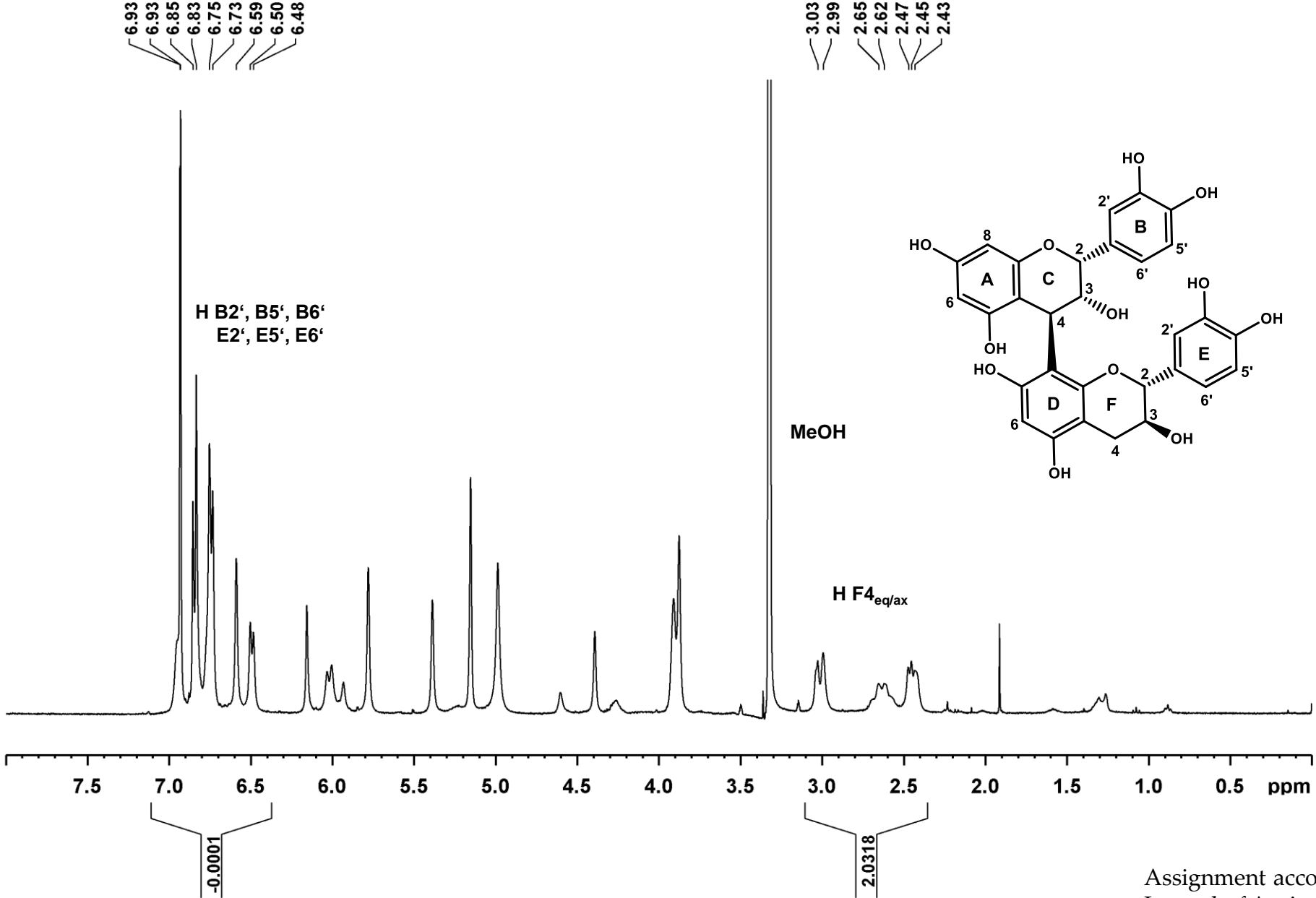
Assignment according to da Silva et al. (2020). New Journal of Chemistry, 44, 17391-17404.

# (-)-epicatechin



Assignment according to da Silva et al. (2020). New Journal of Chemistry, 44, 17391-17404.

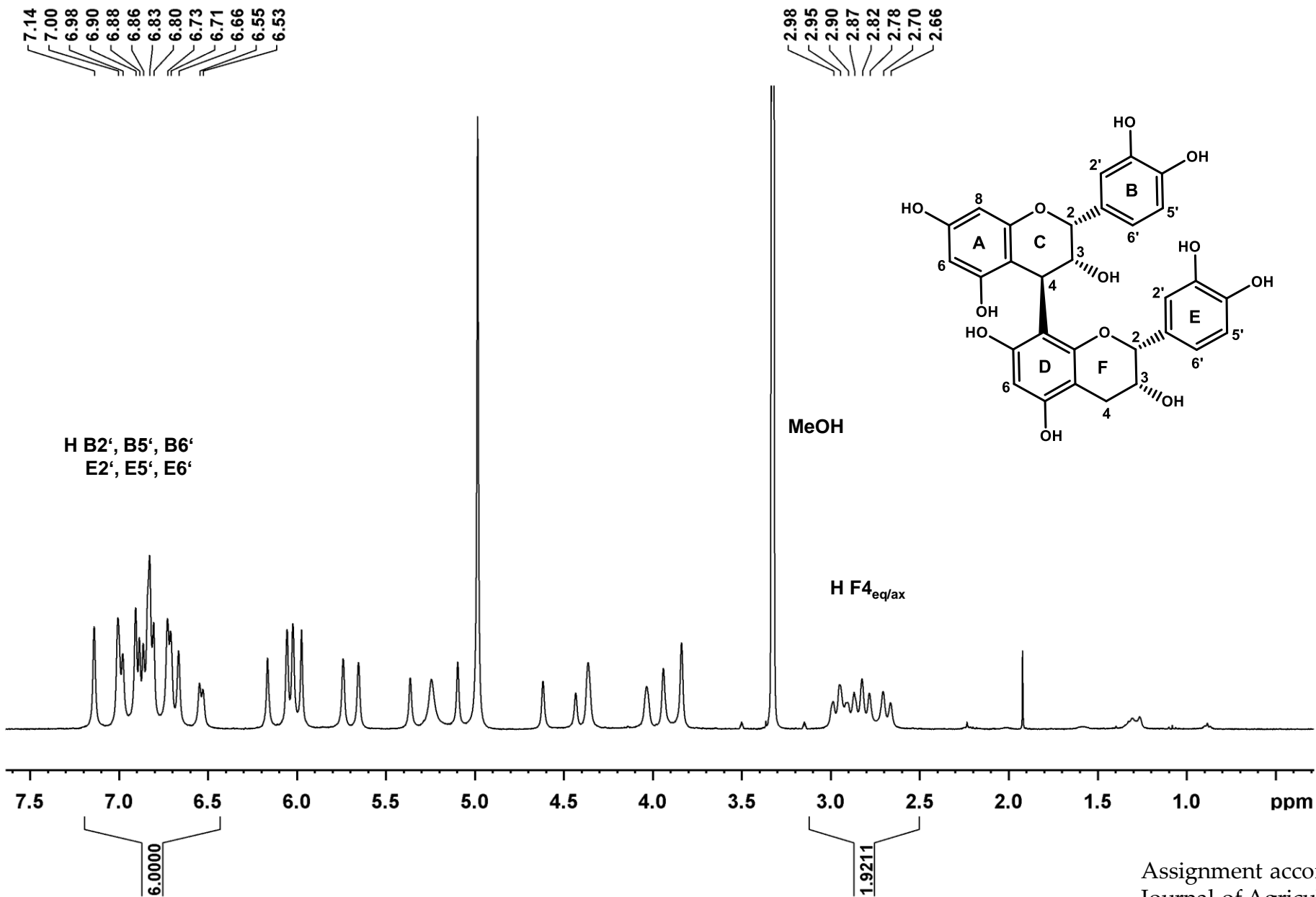
procyanidin B1



Assignment according to Shoji et al. (2003).  
Journal of Agricultural and Food  
Chemistry, 51, 3806-3813.

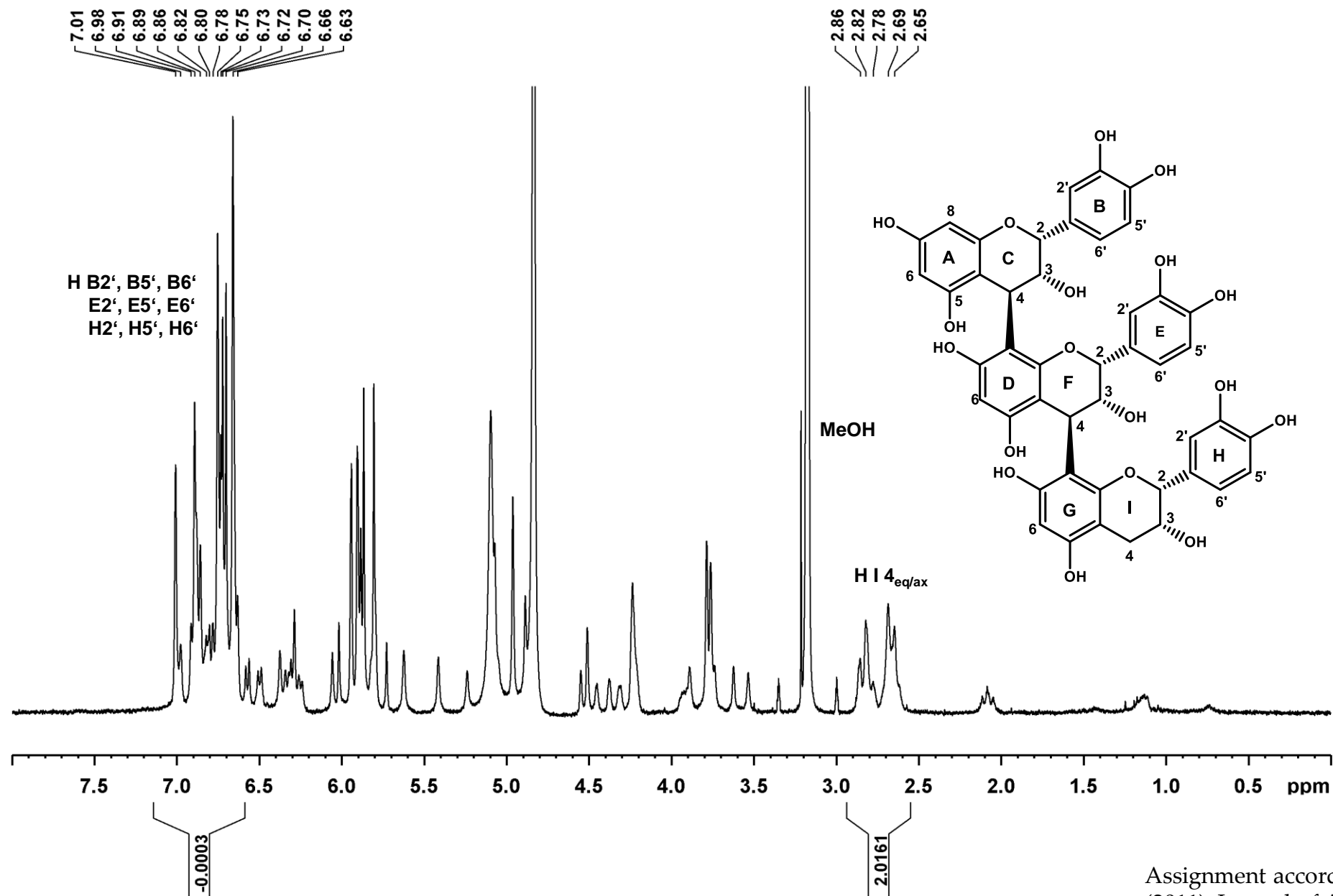


procyanidin B2



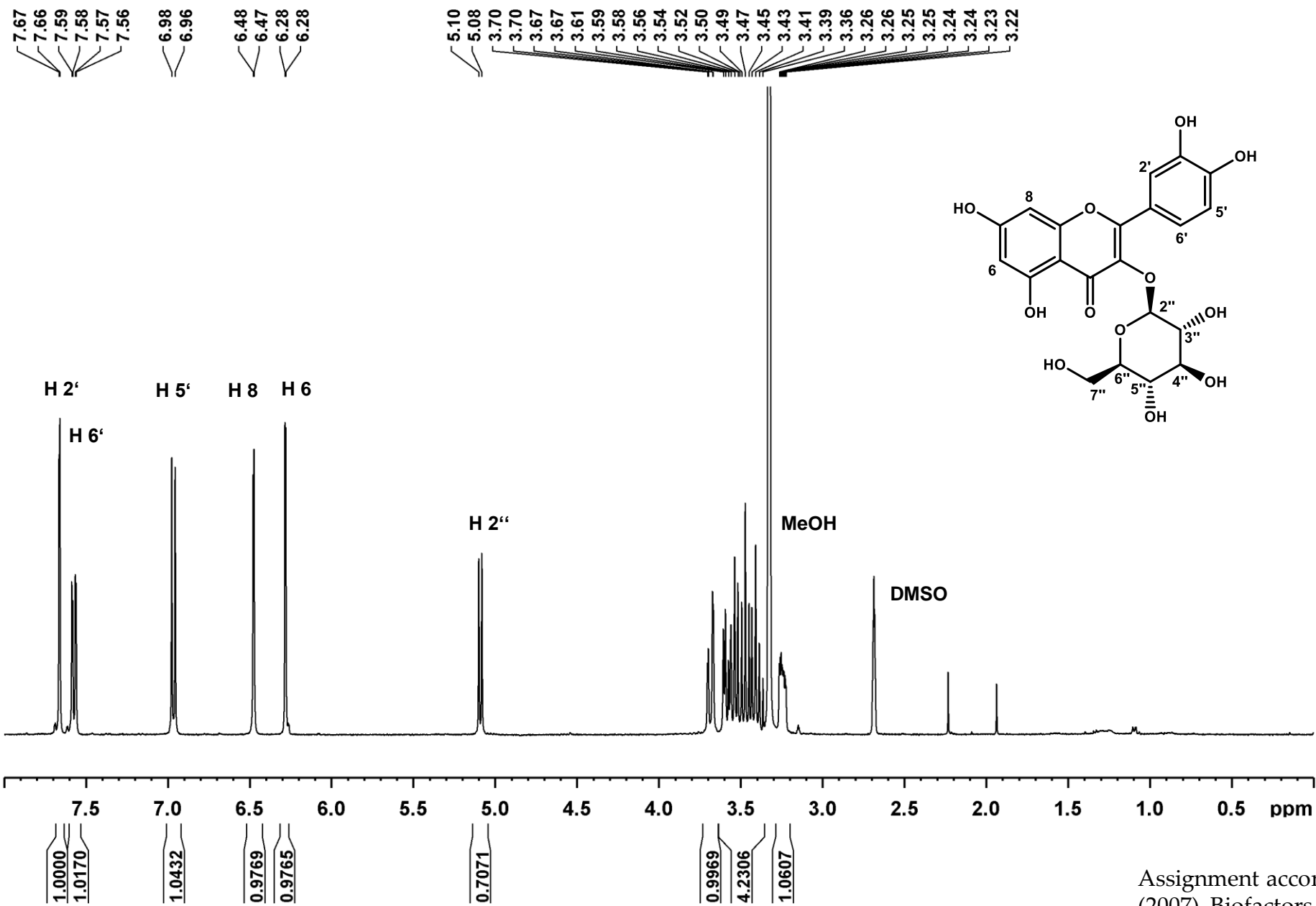
Assignment according to Shoji et al. (2003).  
Journal of Agricultural and Food  
Chemistry, 51, 3806-3813.

# procyanidin C1



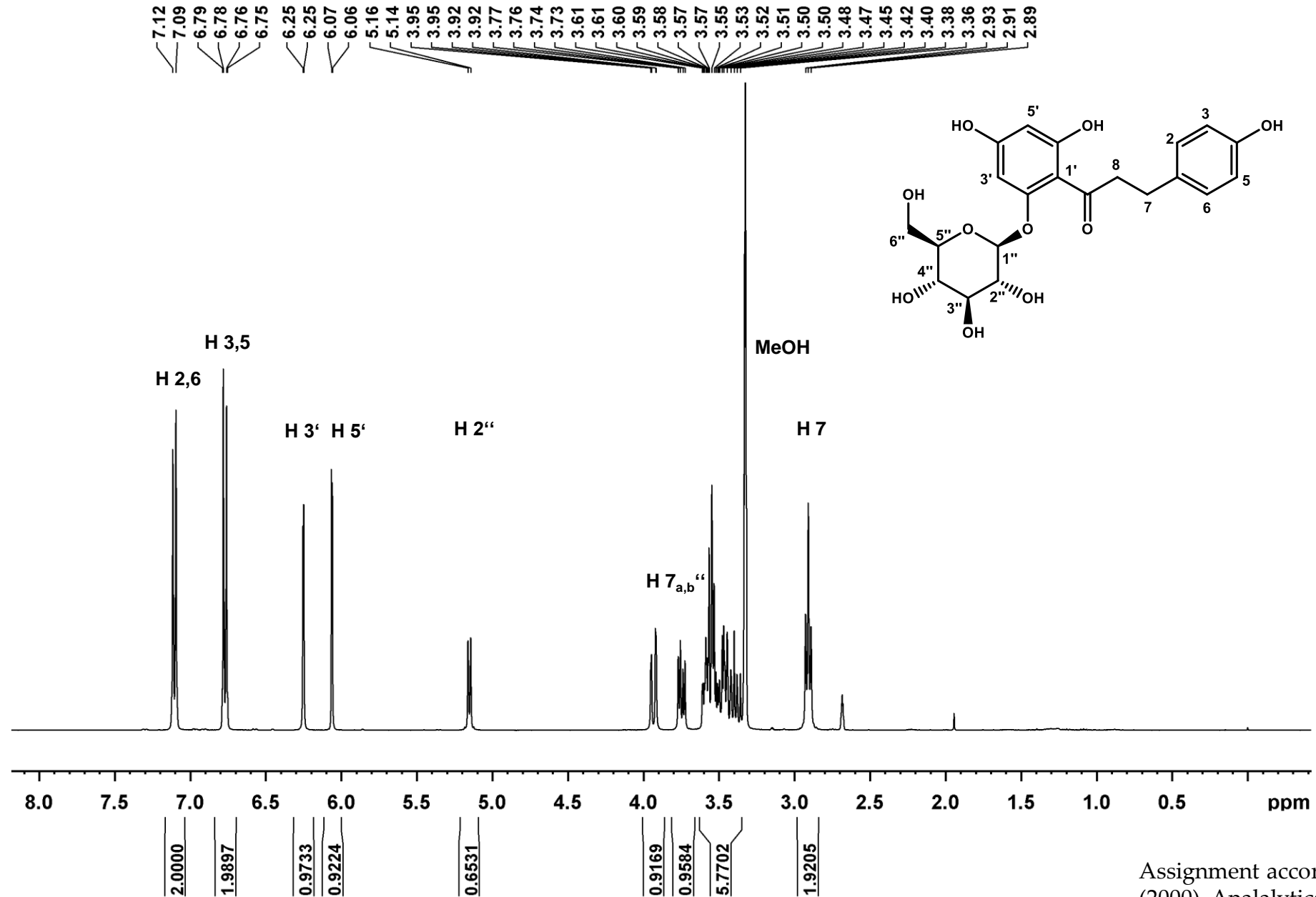
Assignment according to Esatbeyoglu et al. (2011). Journal of Agricultural and Food Chemistry, 59, 62–69.

quercetin-3-O-glucoside



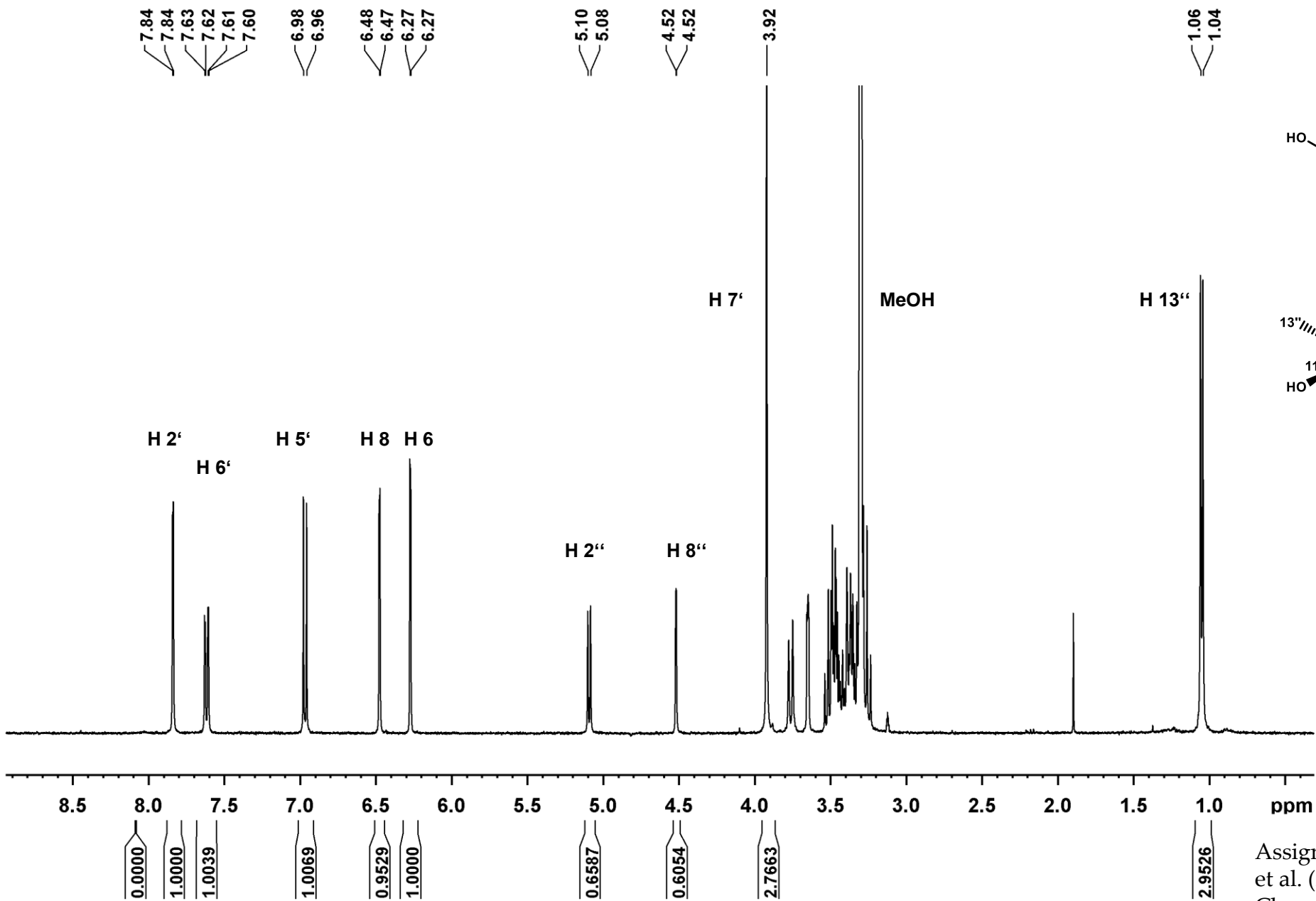
Assignment according to Panda and Kar (2007). Biofactors, 31, 201–210.

# phlorizin



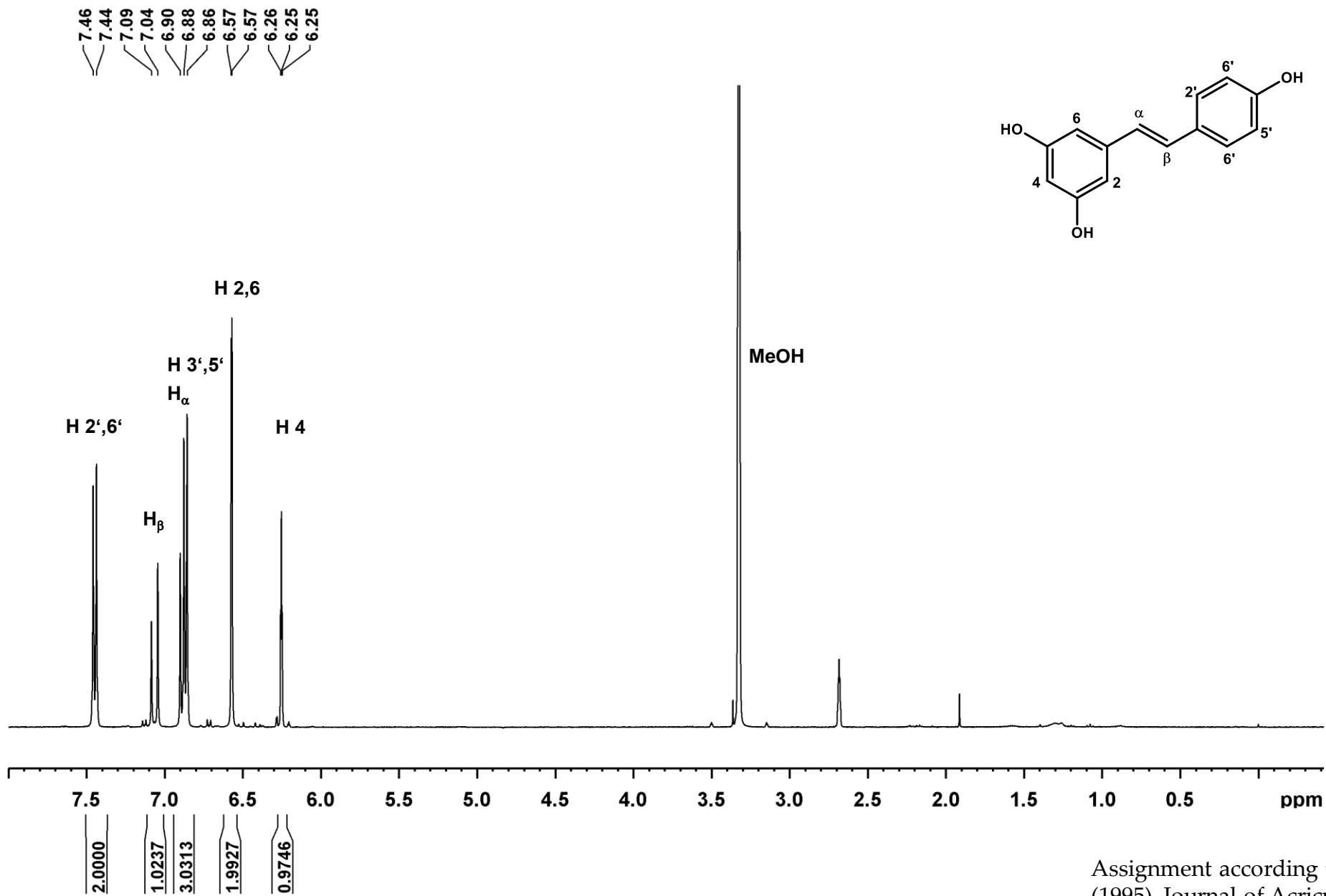
Assignment according to Lommen et al. (2000). Analytical Chemistry, 2000, 72, 1793-1797.

isorhamnetin-3- O-rutinoside



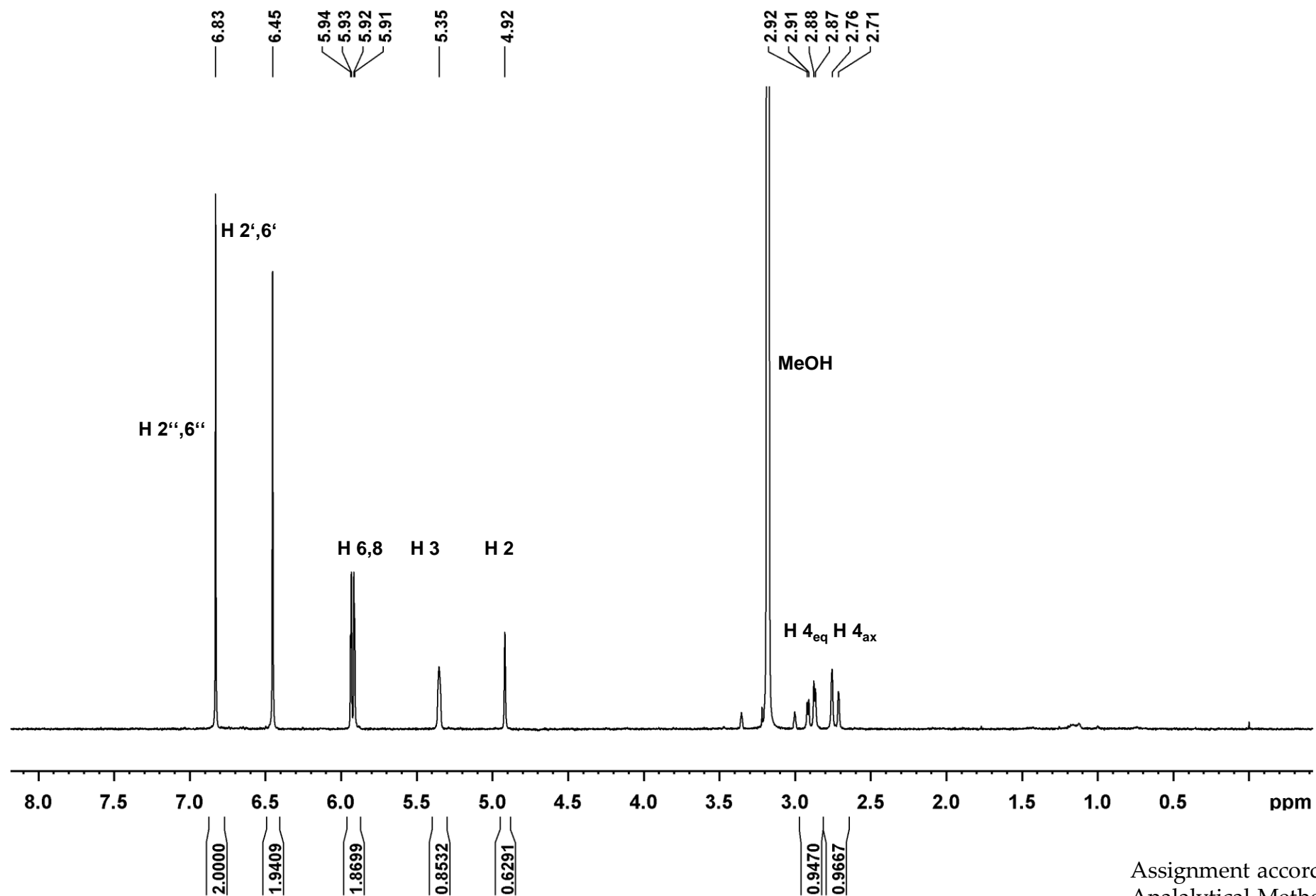
Assignment according to Cao et al. (2009). Journal of Liquid Chromatography & Related Technologies, 32, 273–280.

resveratrol



Assignment according to Mattivi et al. (1995). Journal of Agricultural and Food Chemistry, 43, 1820-1823.

# EGCG



Assignment according to Yuan et al. (2014).  
Analytical Methods, 6, 907-914.