Figure S1

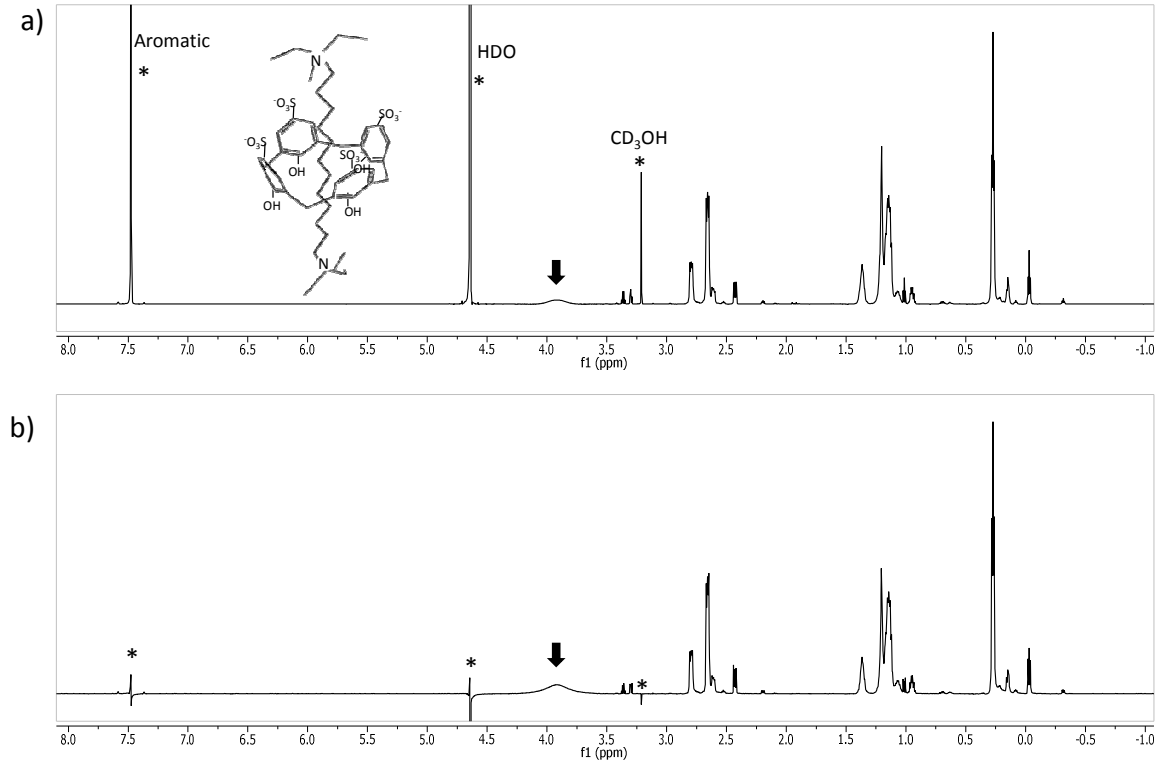

Figure S1. Spectra of sulfo(4)calixarene and dodecane 1,12-bis (triethylammonium bromide) surfactant 1:1 dissolved in a mixture of solvents D_2O/CD_3OD. a) 1D ^1H spectrum and b) 1D s-filter^{rev} with a mixing time of 75 ms. The position of the singlets peaks is indicated with an asterisk. The signal indicated with an arrow corresponds to a broad multiplet peak with relatively much shorter T_2 relaxation time than the other signals.

Figure S2

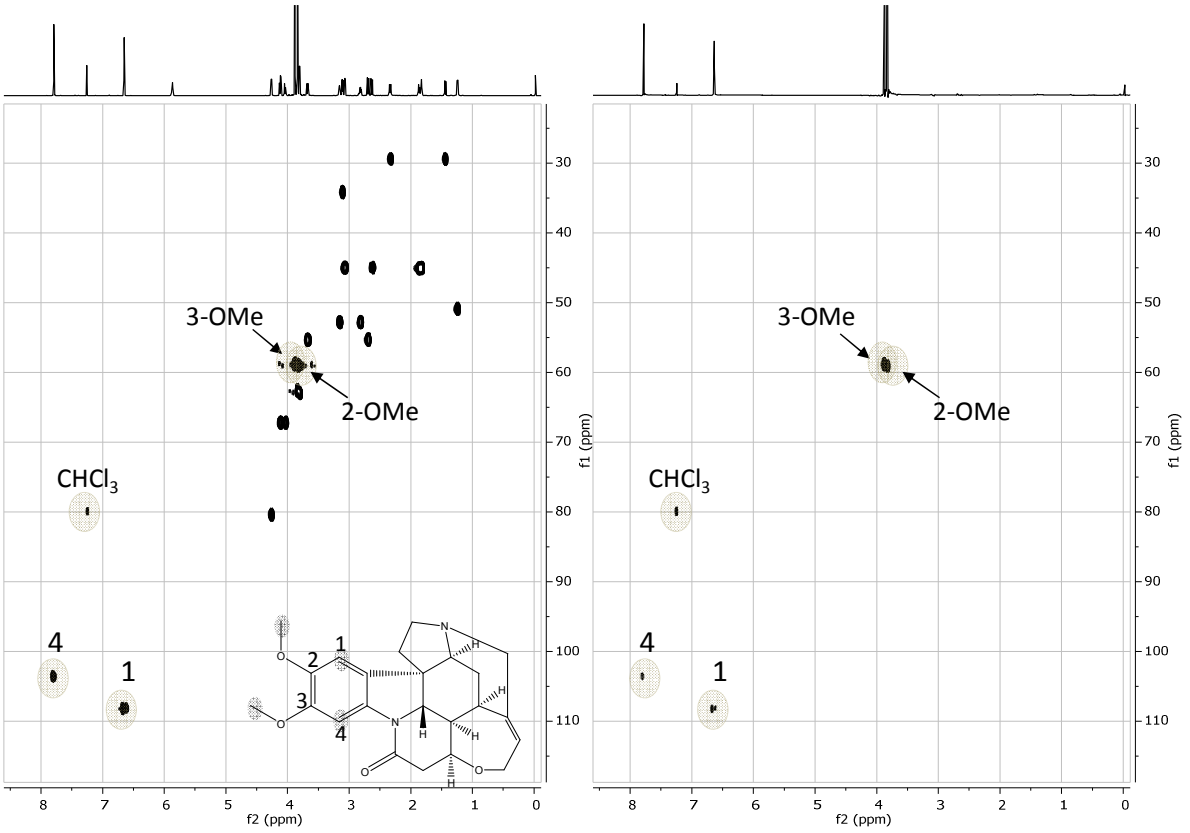

Figure S2. Spectra of brucine in $CDCl_3$. a) 2D ^{1}H-^{13}C HSQC, b) 2D s-filter[3] ^{1}H-^{13}C HSQC using the parameters of Table 1 for a number of cycles n=3. The shaded signals correspond to the singlet peaks.

Figure S3

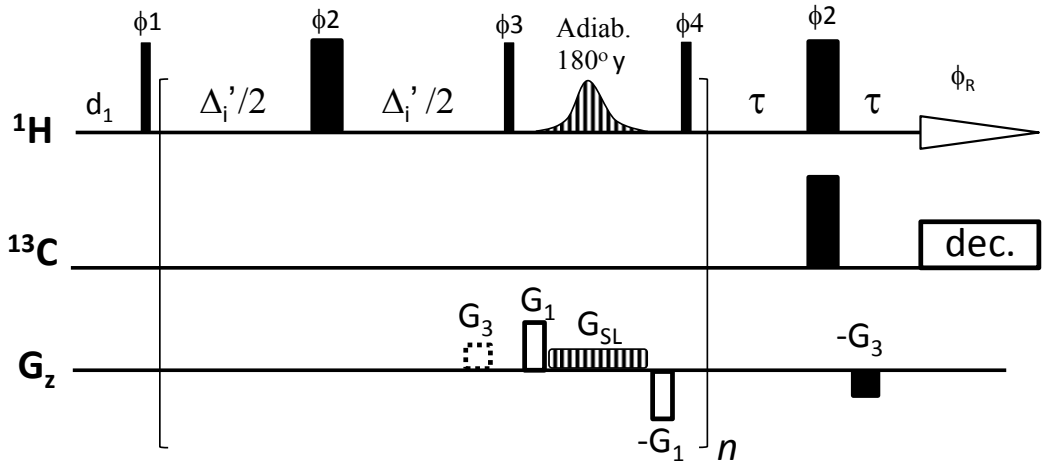

Figure S3. Pulse sequence 1D ^{1}H s-filter experiment with inversion of proton signals attached to ^{13}C (e.g. ^{13}C satellites). Narrow and wide lines correspond to hard pulses of 90^{o} and 180^{o}, respectively. Other experimental details are identical to those described for the pulse sequence of Fig. 1b.

Figure S4

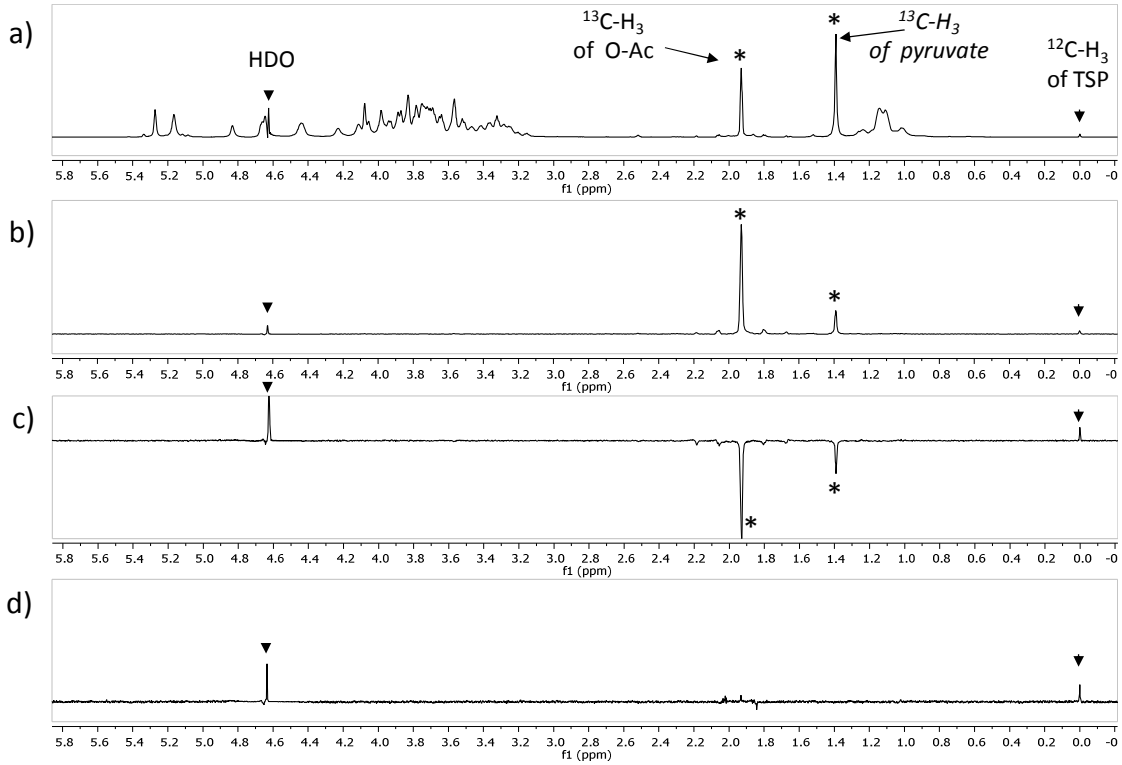

Figure S4. ^{1}H s-filter experiments for the edition or suppression of the responses of proton singlet peaks bound to ^{13}C respect to proton singlets bound to other type of nuclei (e.g. ^{12}C). The spectra were obtained for a sample of uniformly ^{13}C labelled exo-polysaccharide colanic acid in D_2O containing 0.03% of TSP. a) ^{1}H {^{13}C} decoupled experiment, b) ^{1}H s-filter^{4} {^{13}C} decoupled experiment (pulse sequence of Fig. 1a). c) ^{1}H s-filter^{4} {^{13}C} decoupled experiment with inversion of protons bound to ^{13}C (pulse sequence of Fig. S3). d) ^{1}H s-filter^{4} {^{13}C} decoupled experiment with suppression of protons bound to ^{13}C (pulse sequence of Fig. 1b). In these spectra the signals of four singlet peaks are indicated. The signals labelled with asterisks correspond to the methyl protons of acetyl and di-substituted pyruvate groups of U-^{13}C colanic acid. These methyl protons are bound to ^{13}C and uncoupled to other protons. The two singlet peaks labelled with arrows are protons that are not bound to ^{13}C, they correspond to HDO and to methyl protons of TSP bound to ^{12}C (i.e. natural abundance). The four spectra were obtained with 128 using soft presaturation of HDO signal and with broad-band *Garp* ^{13}C decoupling during acquisition. The ^{1}H-sfilter spectra b) to d) used the conditions described in Fig. 1 and Table 1 for a number of cycles n=4 and a nominal value of J_{CH} of 130 Hz. The signal assignment of colanic acid can be found in the following reference: Meredith C. T.; Mamat, U.; Kaczynski, Z.; Lindner, B.; Holst, O.; Woodard, R.W.

Modification of Lipopolysaccharide with Colanic Acid (M-antigen) Repeats in Escherichia coli. *J. Biol. Chem.*, **2007**, 282, 7790-7798.

Table S1. Metabolites described for wine samples that generate singlets or small $^{n}J_{HH}$ scalar couplings (J ≤ 3 Hz) in the 1D proton spectrum. These signals can be edited in the ^{1}H s-filter spectrum of the sample.

Compound	$\delta^{1}H$ in ppm (number of protons, multiplicity, J in Hz, assignment,)[a]	Ref.	HMDB code[(a)]
formic acid	8.32 (1, s, H-2)	(c)	HMDB00142
Quercetin	7.74 (1, d,H-12, J=2.02), 6.40 (1, d, H-7, J≤ 3), 6.19 (1, d, H-9, J≤ 3)	(d)	HMDB05794
syringic acid	7.32 (2, s,H-5, H-3), 3.87 (3+3, s, H-9, H-13)	(d)	HMDB02085
gallic acid	7.08 (2, s, H-3, H-5)	(d)	HMDB05807
(-)epicatechin	6.97 (1, d,H-12, J=1.24), 5.94 (1, d, H-7, J=2.1),5.92 (1, d, H-9, J=1.97), 4.81 (1, d,H-2, J≤ 3)	(d)	HMDB01871
(+)catechin	6.84 (1, d, H-12, J=1.98), 5.93 (1, d, H-7, J=2.26), 5.85 (1, d, H-9, J=2.26)	(d)	HMDB02780
kaempferol	6.41 (1, d, H-19, J=2.09), 6.18 (1, d, H-17, J=2.09)	(d)	HMDB05801
tartaric acid[(b)]	4.41 (2, s, CH-4, CH-6)	(c)	HMDB00956
ferulic acid	3.90 (3, s, H-8)	(d)	HMDB00954
Methanol	3.35 (3, s, H-2)	(c)	HMDB01875
succinic acid	2.62 (2+2, s, H-4, H-5)	(c)	HMDB00254
pyruvic acid[(b)]	2.35 (3, s, H-6)	(c)	HMDB00243
acetone	2.2 (3+3, s, H-3, H-4)	(c)	HMDB01659
acetic acid/acetates	2.06 (3, s, H-4)	(c)	HMDB00042

(a) Coupling constants (J) and signal assignments corresponds to the ^{1}H NMR data of the compound in the Human Metabolome Database (HMDB): http://www.hmdb.ca .

(b) Tentative identification.

(c) Chemical shifts extracted from Table 1 of ref. 5.

(d) Chemical shifts extracted from Table 2 of ref. 4.

Table S2. Metabolites described for olive oil samples that generate singlets or small $^{n}J_{HH}$ scalar couplings (J ≤ 3 Hz) in the 1D proton spectrum. These signals can be edited in the ^{1}H s-filter spectrum of the sample.

Compound	**δ ^{1}H in ppm[(a)]** (number of protons, multiplicity, J in Hz)
-Ph-*H* (phenolic ring)	6.970 (1, s)
Terpene	4.699 (1, s)
Terpene	4.648 (1, s)
squalene	1.662 (3, s)
stigmasterol	0.687 (3, s)
β-sitosterol	0.669 (3, s)

(a) Chemical shifts and coupling pattern extracted from Table 1 of ref. 12.