Supplementary material

Spectroscopic Evidence, Evaluation of Biological Activity and Prediction of Safety Profile of Fatty Hydroxamic Acids Derived from Olive Oil Triacylglycerides

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Table S1. The list of vibrational frequencies and their assignments in FTIR (KBr) and Raman spectra of recorded FHAs.

FHAs (KBr pellet)		Assignment
IR/cm^{-1}	Raman/cm^{-1}	
3600 – 2500		ν O-H in CONHOH
3285 m [1]		ν [2] N-H
3001 w [3]	3001 m	ν_{as} =C-H
2952 m	2957 w	ν_{as} CH_3
2918 vs [4]	2932 m	$\nu_{as}CH_2$
2872 vw [5]	2900 w	$\nu_{sym}CH_3$
	2881 vs	
2849 vs	2847 vs	ν_{sym} CH_2
	2728 w	
	2719 w	
1664 s [6]	1659 m	ν C=O (NH) (Amide I)
1624 s	1622 vw	ν C=O (NH) (Amide II)
1464 s		δ [7] C-H
1441 m	1441 s, b	δ C-H
1427 w		δ C-H
1406 vw	1406 vw	
1381 w	1380 vw	δ O-H
	1295 s	*ν* C-N
1275 vw	1270 m	
1117 m	1121 w	*ν* C-O
1096 m	1095 m	*ν* -C-C-
1069 w	1062 m	*ν* -C-C-
968 m	969 w	*γ* [8] CH_2
893 vw	890 w	
725 m		*ν* -CH_2-CH_2-CH_2-CH_2-
650 w		
542 w		

[1] medium

[2] stretching (in index as for antisymmetric and sym for symmetric)

[3] weak

[4] very strong

[5] very weak

[6] strong

[7] bending

[8] rocking/wagging/twisting

Table S2. ^{13}C- and ^{1}H-NMR spectroscopic data (data (recorded at 175 and 700 MHz, respectively; $CDCl_3$))of fatty hydoxamic acids mixture (FHAs) consisted of oleoyl (OHA) and linoleyl hydroxamic acid (LHA*) and theoretical[2,3] spectral data of OHA and LHA* and literature spectral data of LHA.

Position	FHAs	OHA		LHA			FHAs
	δ_C[1] Type	δ_C[2]	δ_C[3]	δ_C[2]	δ_C[3]	δ_C[4]	δ_H (J in Hz)
1	171.73, C	169.14	169.90	169.14	169.9	172.08	NHOH, 8.674, bs[5]
1*	‘’	‘’	‘’	‘’	‘’	‘’	
2	31.80, CH_2	32.26	32.50				2.135, t[6], $^3J_{HH}$ = 7.05 Hz
2*	31.41, CH_2			32.26	32.50	32.61	‘’
3	25.27, CH_2	25.08	25.60				1.621, m[7]
3*	25.52, CH_2			25.08	25.60	25.34	‘’
4	29.42, CH_2	29.27	28.60				1.272, m
4*	29.25, CH_2			29.27	28.60	28.99	‘’
5	29.66, CH_2	29.51	29.00				1.272, m
5*	29.49, CH_2			29.51	29.00	29.07	‘’
6	29.00, CH_2	29.11	29.70				1.272, m
6*	29.19, CH_2			29.11	29.70	29.13	‘’
7	29.08, CH_2	29.23	29.90				1.272, m
7*	29.52, CH_2			29.60	29.90	29.54	
8	27.12, CH_2	27.77	27.70				2.009, dt[8], $^3J_{HH}$ = 12.7 Hz, $^3J_{HH}$ = 6.5 Hz
8*	27.06, CH_2			27.20	27.80	26.97	‘’
9	129.56, CH	130.04	130.60				5.339, m
9*	129.86, CH			130.40	130.30	129.66	‘’
10	129.94, CH	130.04	130.60				5.339, m
10*	127.78, CH			128.70	127.30	127.85	‘’
11	27.12, CH_2	27.77	27.70	26.20	25.60	25.61	2.009, dt, $^3J_{HH}$ = 12.7 Hz, $^3J_{HH}$ = 6.5 Hz
11*	25.52, CH_2						2.766, m
12	29.22, CH_2	29.23	29.90	128.70	127.30	127.91	1.272, m
12*	130.14, CH						5.339, m
13	29.59, CH_2	29.40	29.70				1.272, m
13*	127.99, CH			131.00	130.30	129.74	5.339, m
14	29.59, CH_2	29.38	29.70				1.272, m
14*	27.06, CH_2			27.70	27.80	26.99	
15	29.25, CH_2	29.24	29.30	30.00	29.60	29.30	1.272, m
15*	29.55, CH_2						‘’
16	31.80, CH_2	31.80	31.90				1.272, m
16*	31.41, CH_2			31.75	31.90	31.48	‘’
17	22.57, CH_2	22.67	22.70				1.272, m
17*	22.35, CH_2			22.97	22.80	22.45	‘’
18	13.99, CH_3	14.08	14.10				0.880, t, $^3J_{HH}$ = 6.91 Hz

18*	,''		14.05	14.10	13.26	''

[1] $CDCl_3$

[2] Chemical shifts predicted by nmrshiftdb software package at http://nmrshiftdb.nmr.uni-koeln.de

[3] Chemical shifts predicted by ChemDraw Ultra 11 software package

[4] Chemical shifts of LHA recorded in CD_3OD [24]

[5] broad signal

[6] triplet

[7] multiplet

[8] quartet

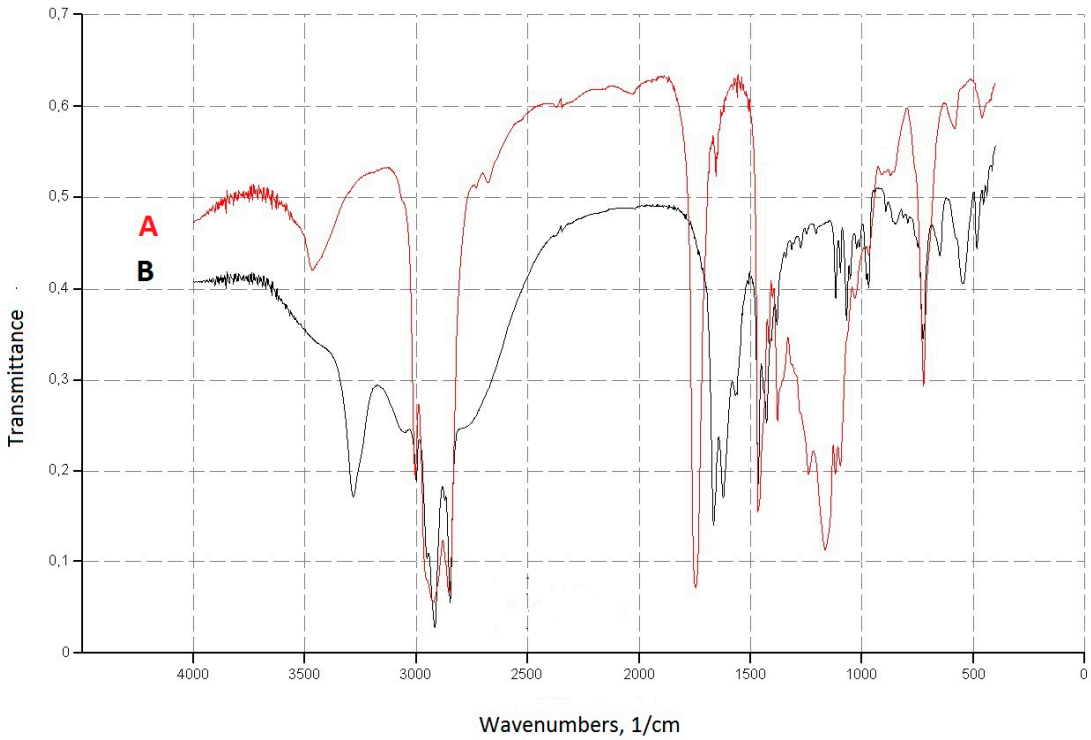

Figure S1. A parallel display of FTIR spectra of olive oil recorded as liquid on potassium bromide (KBr) pellet (**A**) and fatty hydroxamic acids (FHAs) recorded in potassium bromide (KBr) pellet (**B**).

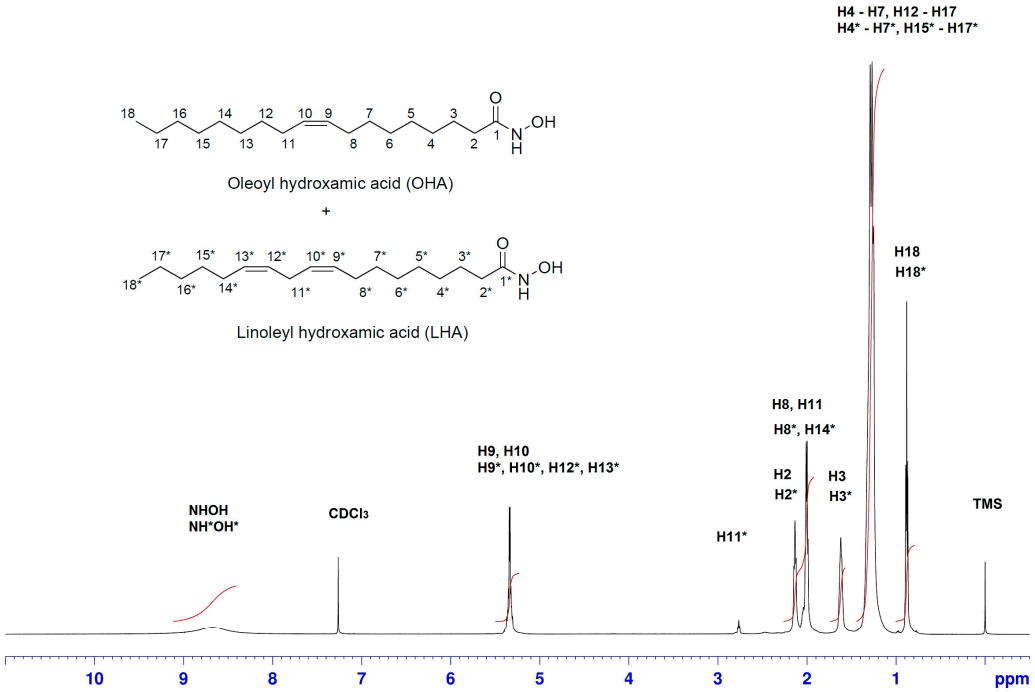

Figure S2. The ^{1}H-NMR spectrum of FHAs mixture recorded in $CDCl_3$ and chemical structures of its main components, *i.e.,* OHA and LHA with indicated signals for each proton groups.

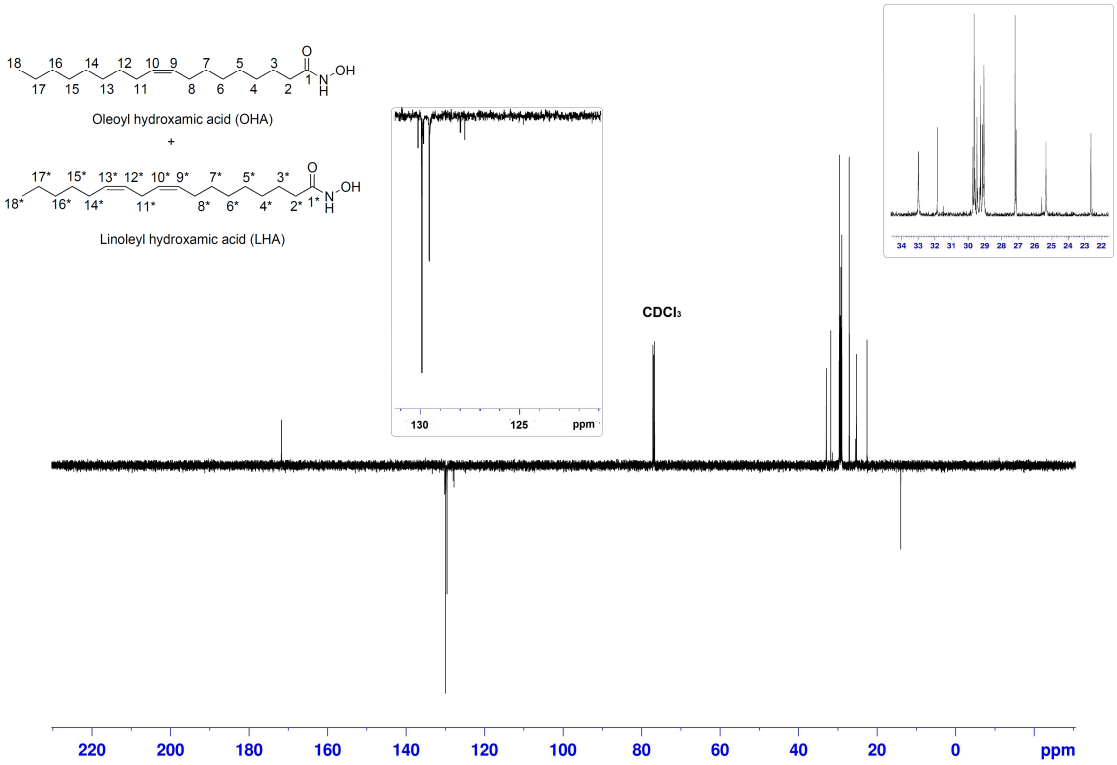

Figure S3. ^{13}C-NMR spectrum of fatty hydroxamic acid (FHAs) mixture and chemical structures of its main components, *i.e.,* oleoyl and linoleyl hydroxamic acid (OHA and LHA, respectively) with labeled C-atoms.

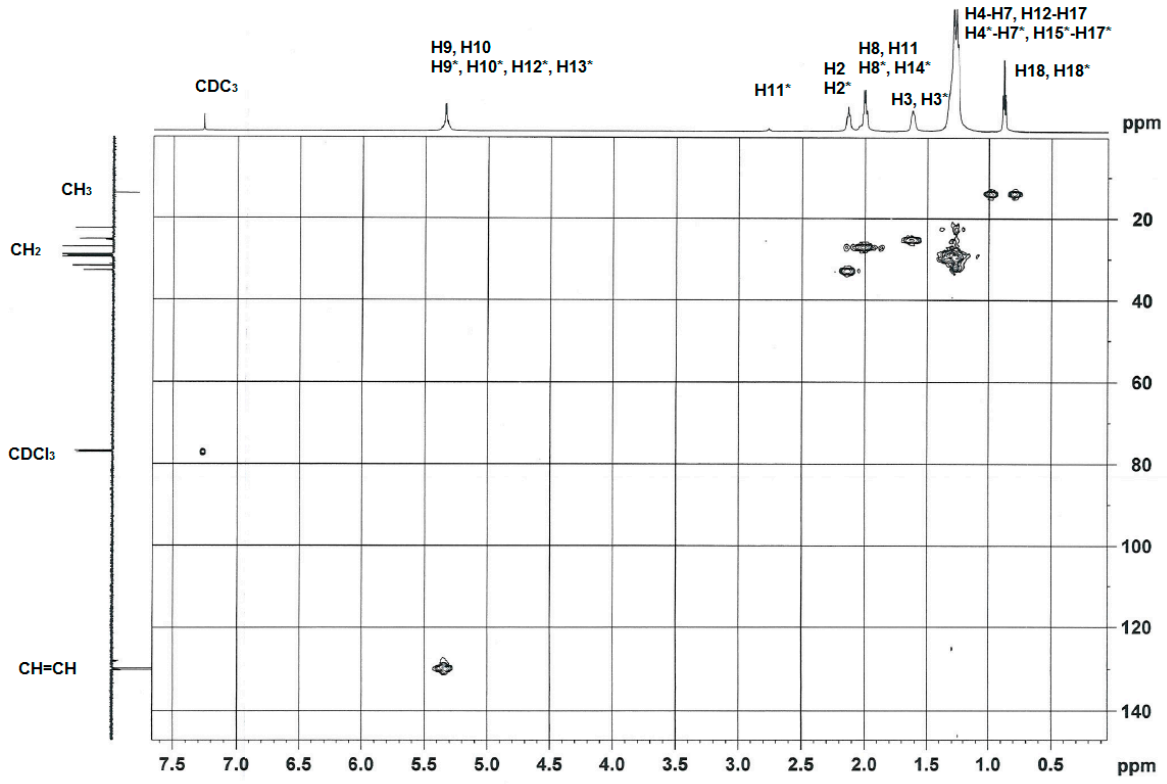

Figure S4. The 2D NMR HMQC (Heteronuclear Multiple Quantum Coherence) spectrum of FHAs in the region of aliphatic and olefinic protons displaying correlations through one bond. (The signal at 77.0 ppm (13C-NMR) and 7.24 ppm (1H-NMR) belong to CDCl3 solvent).

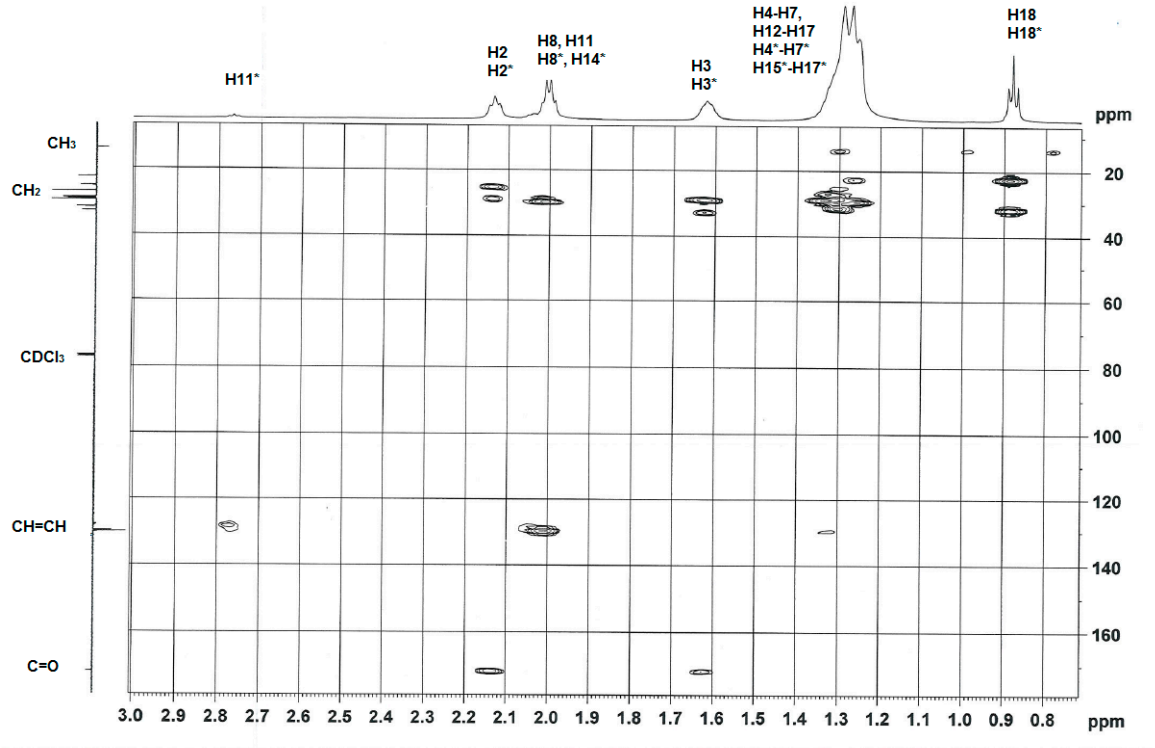

Figure S5. A part of 2D NMR HMBC (Heteronuclear Multiple Bond Coherence) spectrum of FHAs displaying correlations through multiple bonds in the region of aliphatic and olefinic protons

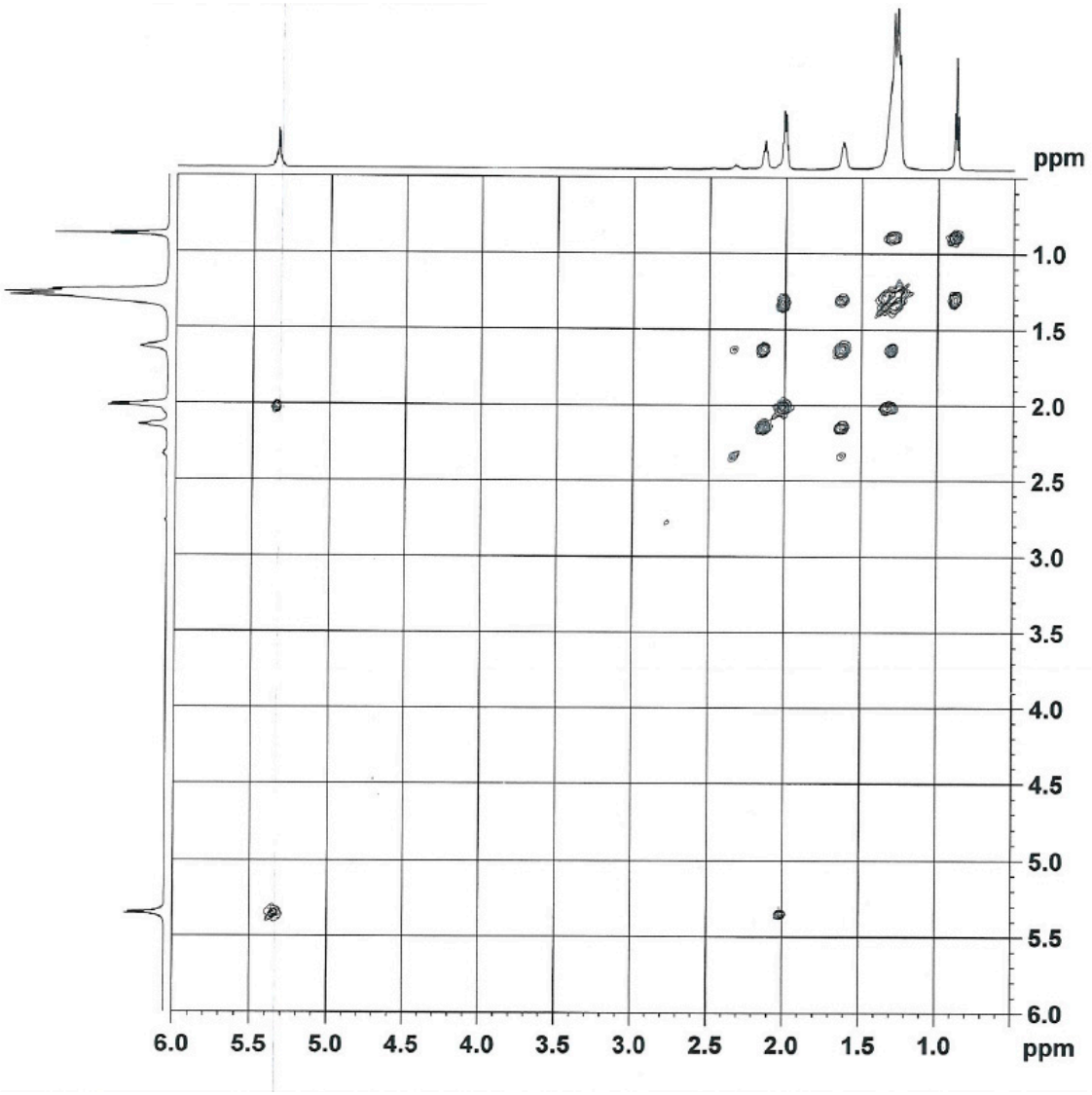

Figure S6. A part of ^{1}H-^{1}H- COSY spectrum of FHAs in the region of aliphatic and olefinic protons.

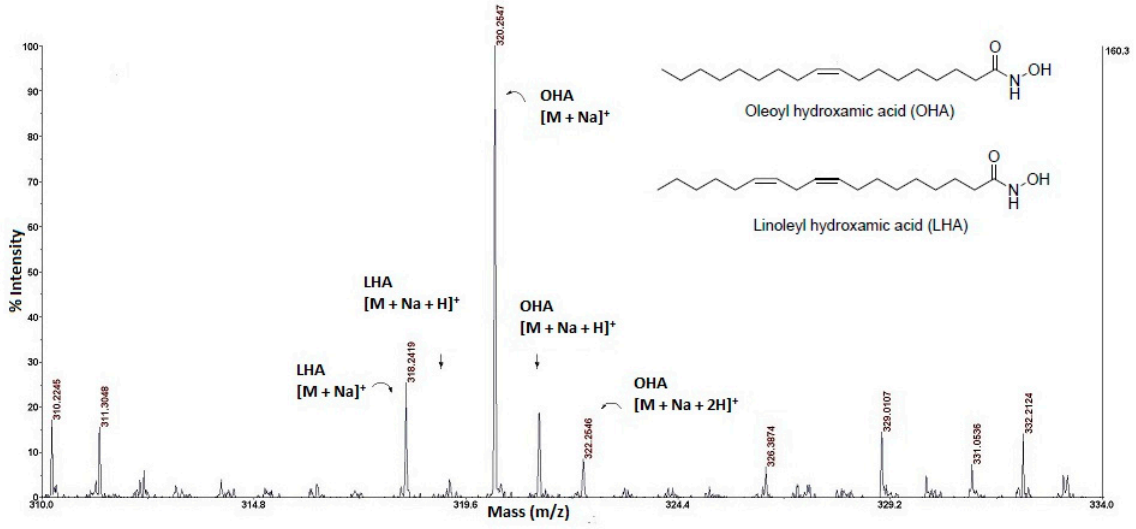

Figure S7. A MALDI-TOF/TOF tandem mass spectrum of FHAs mixture representing the region of unsaturated fatty hydroxamic acids, *i.e.*, m/z 310 – 323 with molecular ions of OHA and LHA as their sodium alkali adducts $[M + Na]^+$, $[M + Na + H]^+$ and $[M + Na + 2H]^+$.