

Supplementary Material

New Insights on the Oxidation of Unsaturated Fatty Acid Methyl Esters Catalyzed by Niobium (V) Oxide. A Study of the Catalyst Surface Reactivity

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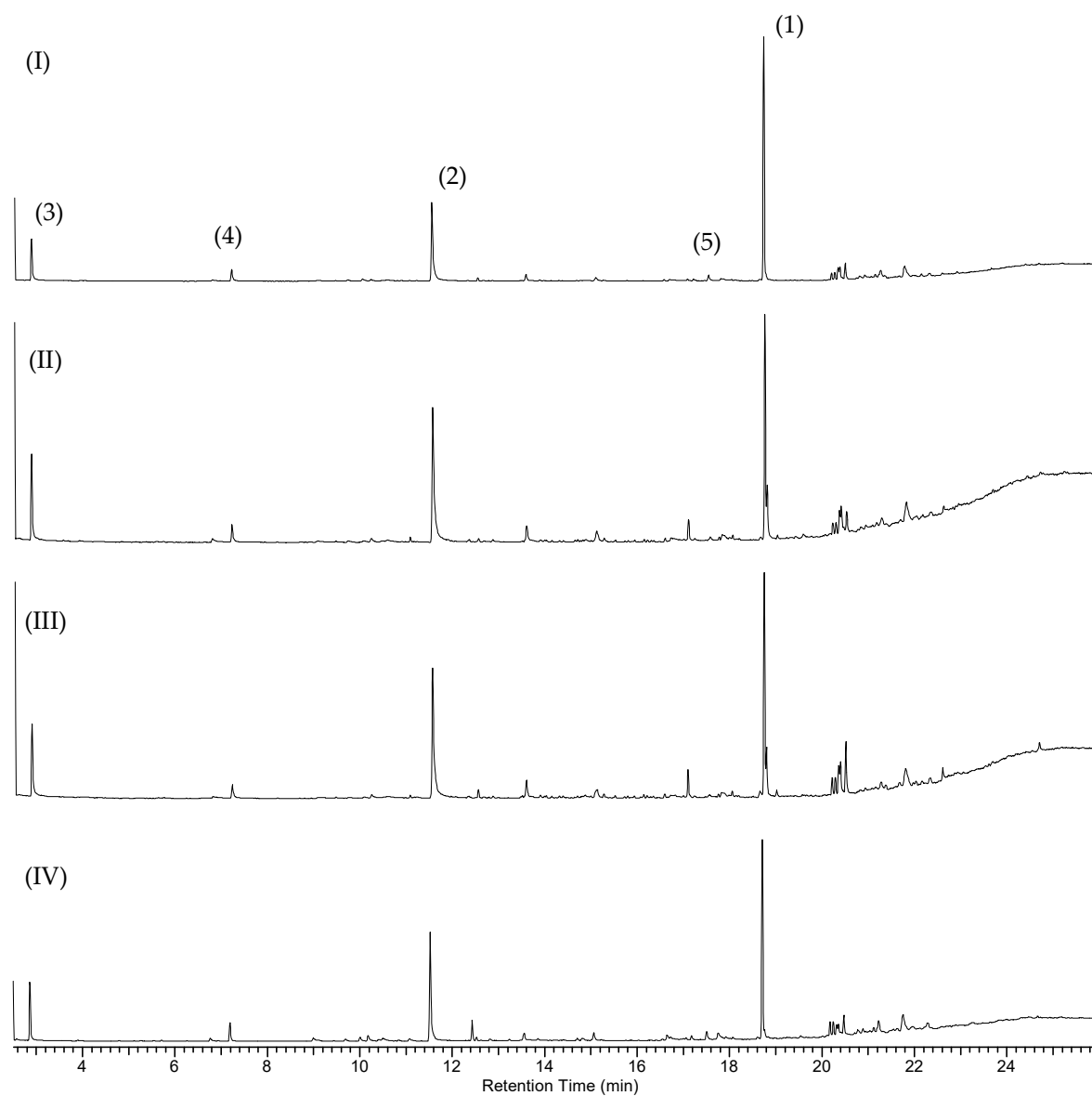


Figure S1. Chromatogram in gas phase (GC) for the oxidation reaction of methyl linoleate in the presence of hydrogen peroxide catalyzed by: (I) HY340; (II) HY340-900; (III) GO and (IV) UP after 60 minutes reaction time.

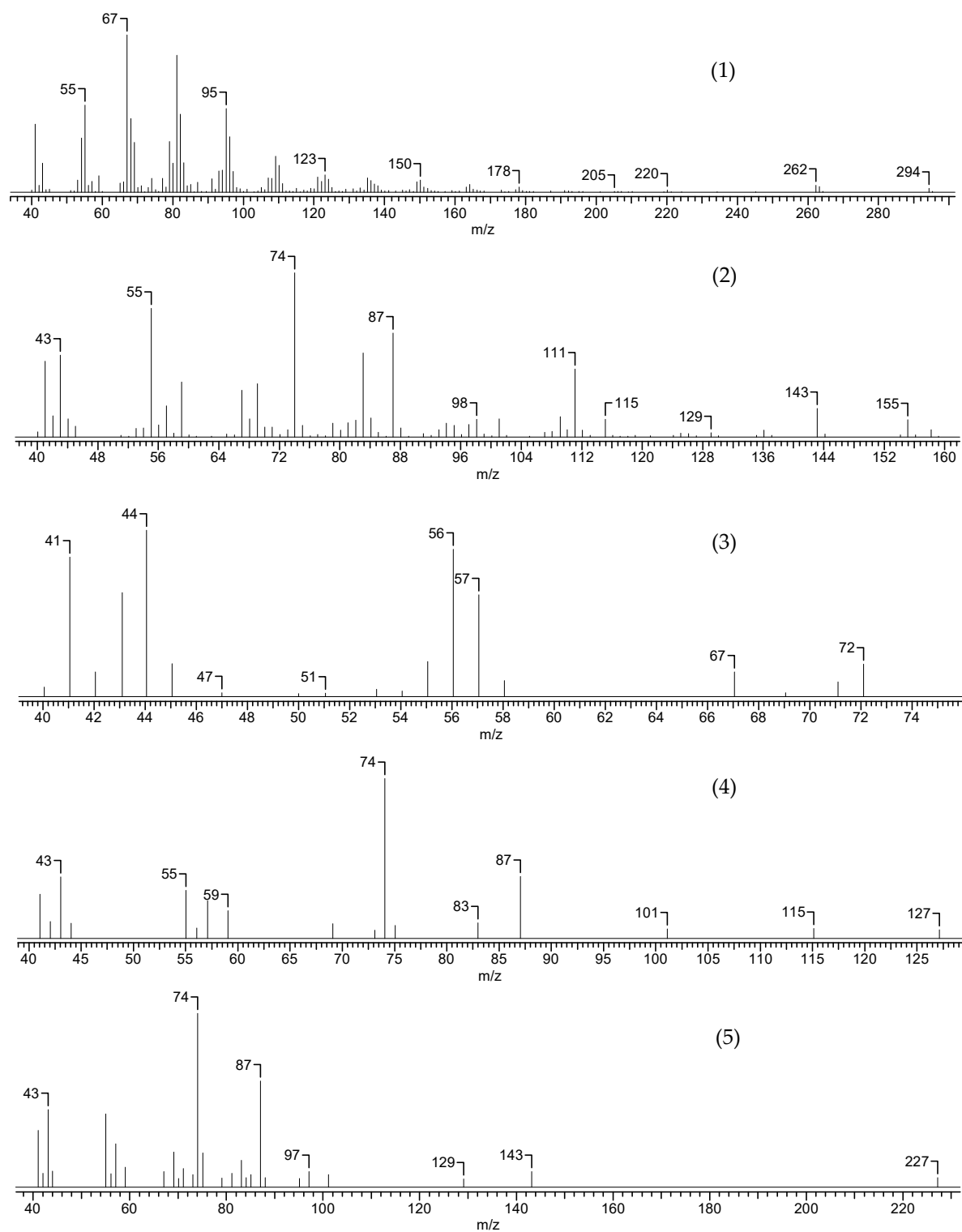


Figure S2. Mass fragments for the oxidation reaction products of methyl linoleate HY340-900 (Figure S1): (1) methyl linoleate; (2) methyl 9-oxo-nonanoate; (3) *n*-hexanal; (4) non-3-enal and (5) methyl 12-oxododec-9-enoate.

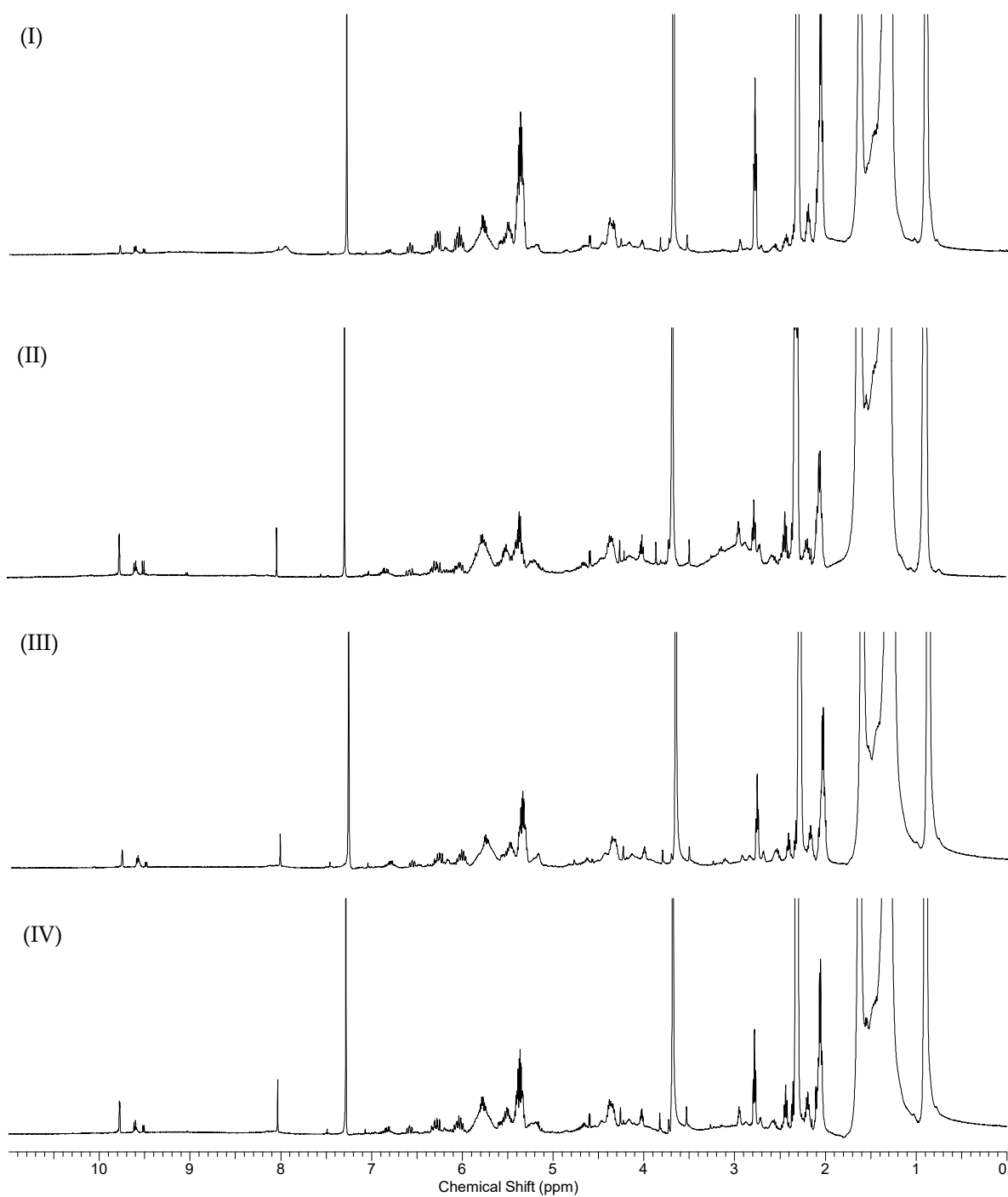


Figure S3. ¹H NMR spectra (500 MHz) for the products of the oxidation reaction of methyl linoleate with hydrogen peroxide catalyzed by: (I) HY340; (II) HY340-900; (III) GO and (IV) UP after 60 minutes reaction time.

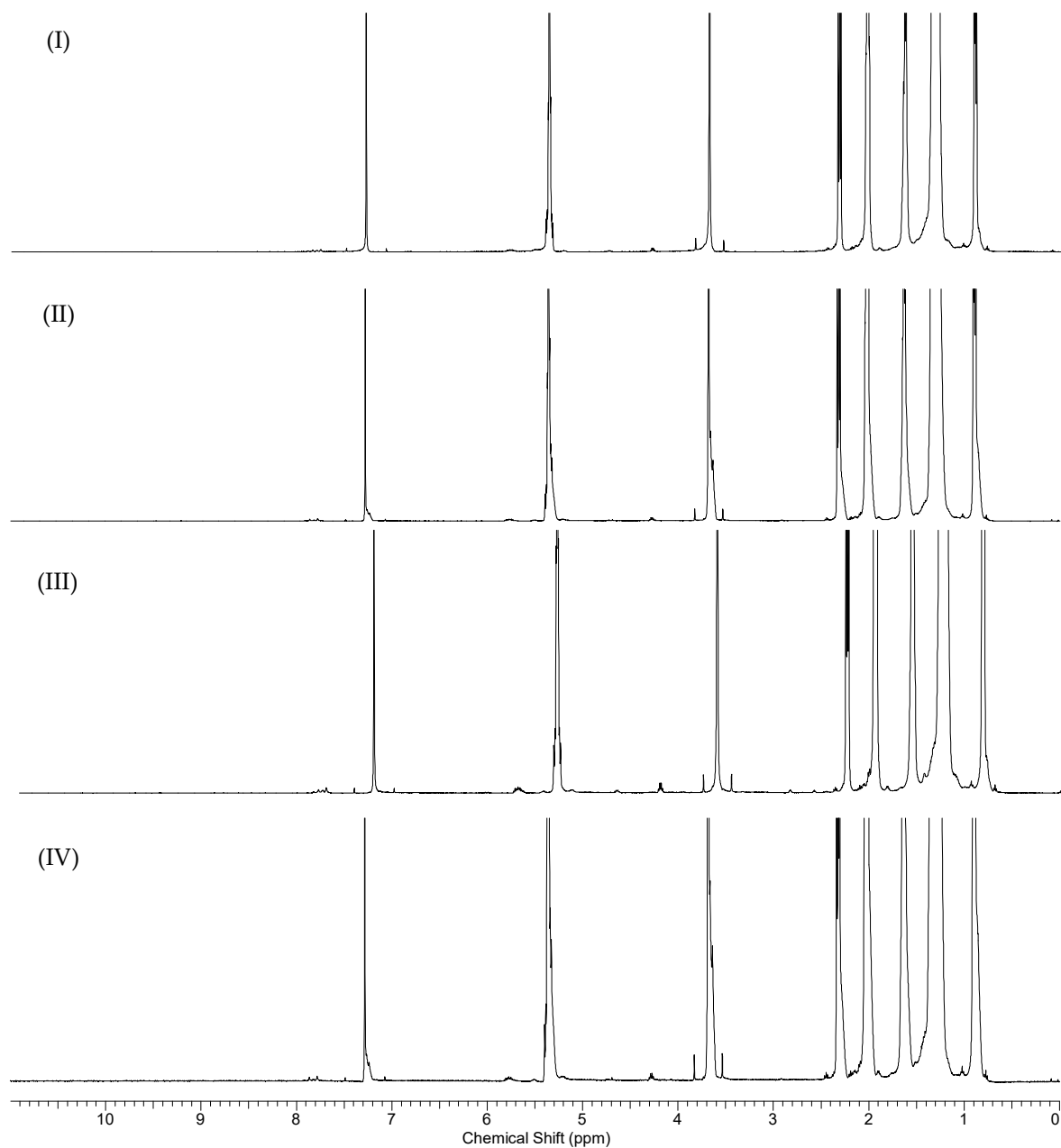


Figure S4. ¹H NMR spectra (500 MHz) for the products of the oxidation reaction of methyl oleate with hydrogen peroxide catalyzed by: (I) HY340; (II) HY340-900; (III) GO and (IV) UP after 60 minutes reaction time.

Table S1. Composition mol percent (mol %) for the oxidation reaction of methyl linoleate with hydrogen peroxide in the presence of catalysts: HY340, HY340-900, GO and UP.

Time (min)	0	10	20	30	40	60	80	100	120
HY340									
n-hexanal	0	0,0	7,4	9,4	12,1	16,9	15,6	21,3	19,3
non-3-enal	0	1,1	0,7	3,4	3,5	4,0	4,6	2,4	4,0
methyl 9-oxo-nonanoate	0	2,7	12,5	21,3	24,8	28,5	33,2	33,7	36,2
methyl 12-oxo-dodec-9-enoate	0	0,0	1,9	2,8	1,9	3,1	3,5	3,2	2,5
methyl linoleate	100	92,2	69,7	48,7	42,3	31,9	27,4	22,2	18,5
others	0	3,9	7,9	14,4	15,4	15,5	15,8	17,2	19,5
HY340-900									
n-hexanal	0	0,0	8,5	14,7	17,8	20,0	20,7	21,6	22,5
non-3-enal	0	1,4	2,4	2,9	3,6	3,9	3,2	3,2	3,5
methyl 9-oxo-nonanoate	0	4,4	16,2	28,4	32,3	35,4	43,2	44,9	45,1
methyl 12-oxo-dodec-9-enoate	0	0,9	1,8	2,1	2,8	3,0	3,2	3,0	3,4
methyl linoleate	100	89,2	62,7	40,4	28,1	16,8	9,4	7,3	4,0
others	0	4,1	8,3	11,4	15,4	21,0	20,3	20,0	21,5
GO									
n-hexanal	0	3,5	9,9	14,4	18,3	21,9	25,7	25,4	24,0
non-3-enal	0	3,9	6,3	5,1	5,1	4,1	5,0	5,4	4,7
methyl 9-oxo-nonanoate	0	7,4	18,2	28,1	35,3	40,4	41,6	41,6	40,2
methyl 12-oxo-dodec-9-enoate	0	3,4	5,2	6,1	5,7	5,0	3,9	4,0	3,8
methyl linoleate	100	75,7	50,0	30,9	19,1	5,2	4,3	2,4	1,0
others	0	6,1	10,5	15,4	16,5	23,3	19,5	21,3	26,3
UP									
n-hexanal	0	4,9	7,5	10,0	10,3	14,9	17,3	19,8	17,0
non-3-enal	0	1,4	1,8	3,4	2,6	7,0	3,1	3,8	3,8
methyl 9-oxo-nonanoate	0	4,9	12,6	16,7	21,3	24,8	28,9	34,6	38,9
methyl 12-oxo-dodec-9-enoate	0	1,9	1,1	0,0	3,2	5,7	0,8	3,2	3,5
methyl linoleate	100	83,1	71,2	61,7	52,0	30,3	22,2	18,3	17,3
others	0	3,8	5,9	8,2	10,6	17,2	27,7	20,3	19,6