catalysts

MDPI

Supplementary Materials

Highly Active and Selective Supported Rhenium Catalysts for Aerobic Oxidation of *n*-Hexane and *n*-Heptane

Gopal S. Mishra [1,2], Elisabete C. B. A. Alegria [1,3,*], Armando J. L. Pombeiro [1] and Luísa M. D. R. S. Martins [1,*]

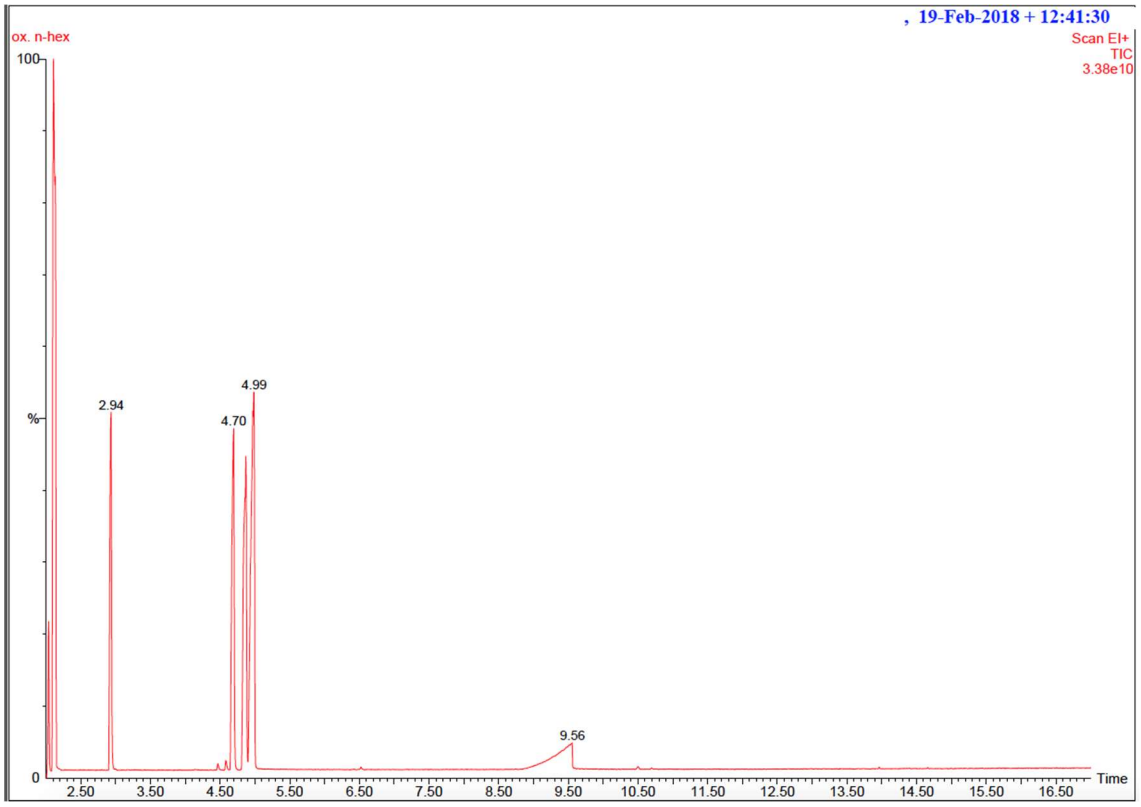
[1] Centro de Química Estrutural, Departamento de Engenharia Química, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa, Portugal; mishrags@gmail.com (G.S.M.); pombeiro@tecnico.ulisboa.pt (A.J.L.P.)

[2] Materials Laboratory, Chemistry Centre, CQ-VR, University of Trás-os-Montes e Alto Douro (UTAD), 5001-801 Vila Real, Portugal

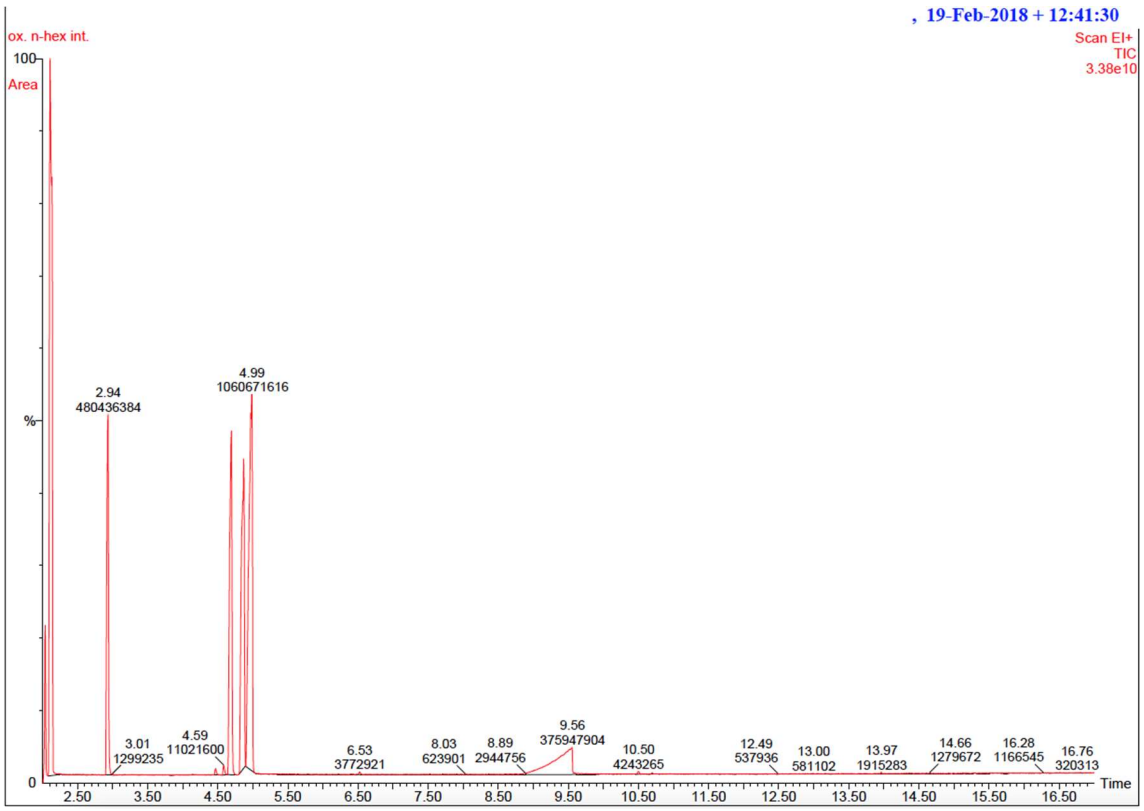
[3] ADEQ, Instituto Superior de Engenharia de Lisboa, Instituto Politécnico de Lisboa, 1959-007 Lisboa, Portugal

* Correspondence: ebastos@deq.isel.ipl.pt (E.C.B.A.A.); luisamargaridamartins@tecnico.ulisboa.pt (L.M.D.R.S.M.); Tel.: +351-218-419-264 (L.M.D.R.S.M.)

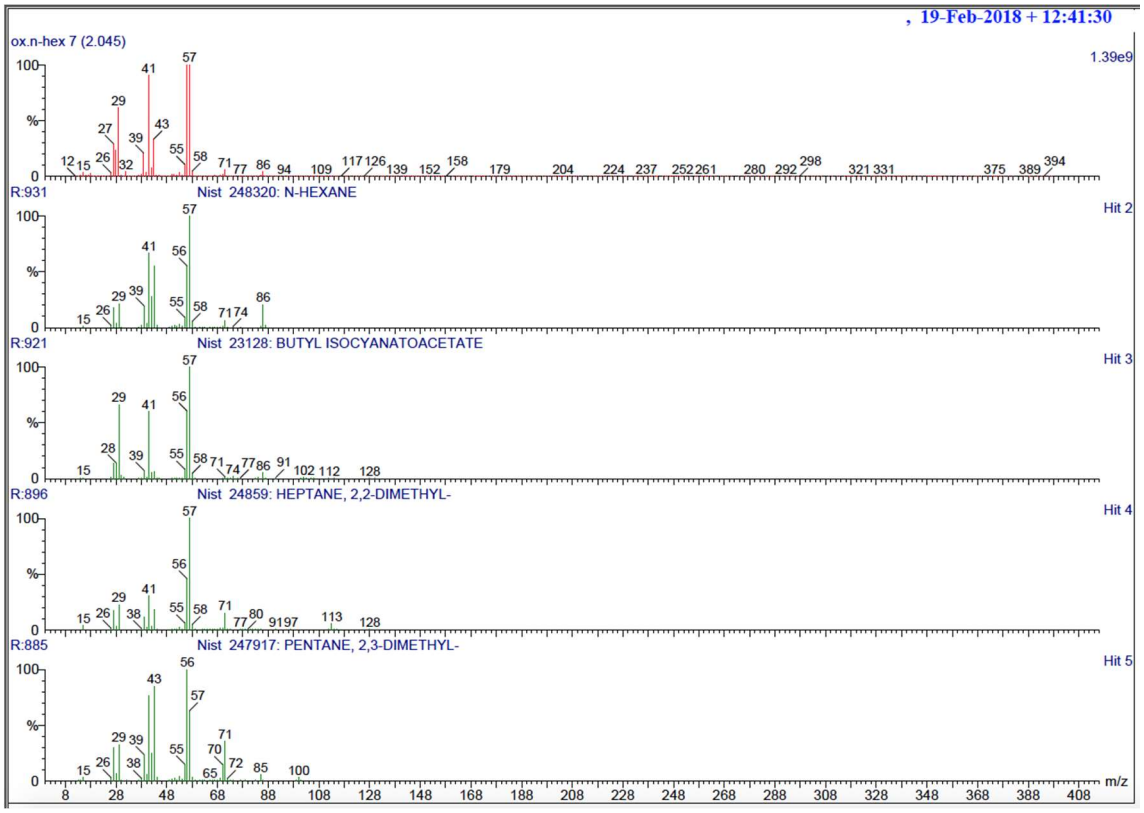
(a1)

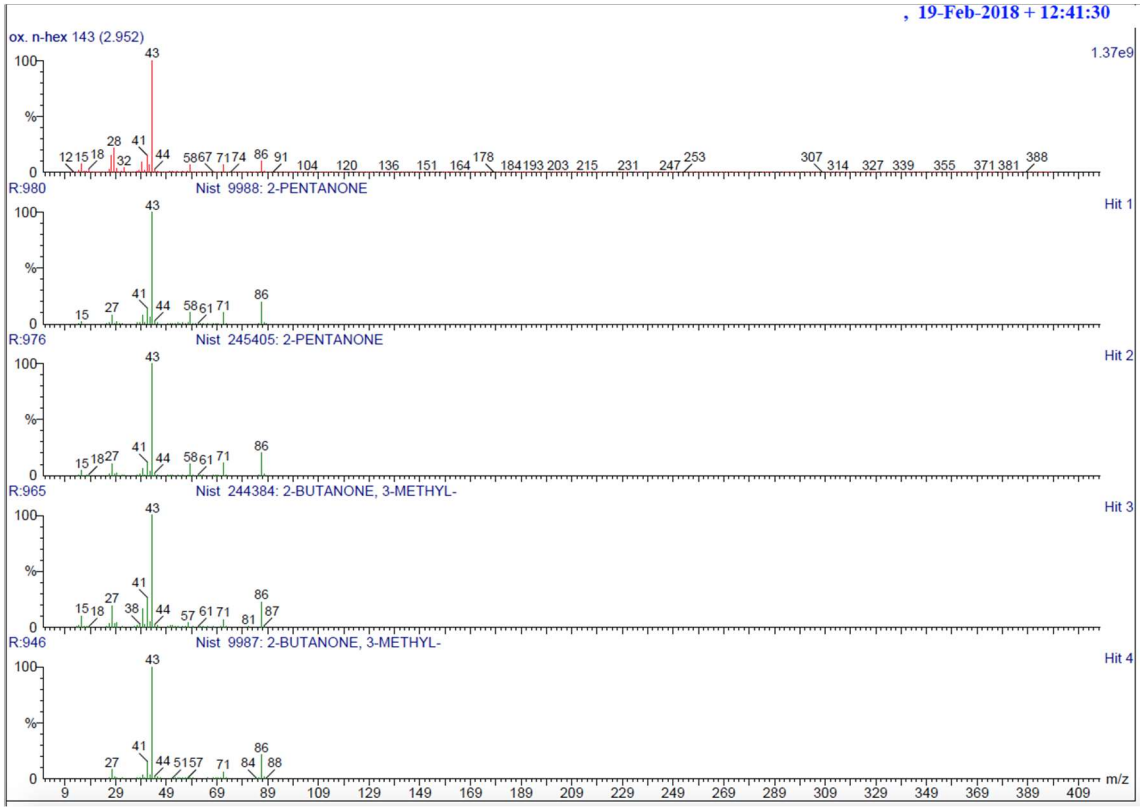

, 19-Feb-2018 + 12:41:30
ox. n-hex
Scan EI+
TIC
3.38e10
100
%
0
2.94
4.70
4.99
9.56
Time
2.50
3.50
4.50
5.50
6.50
7.50
8.50
9.50
10.50
11.50
12.50
13.50
14.50
15.50
16.50

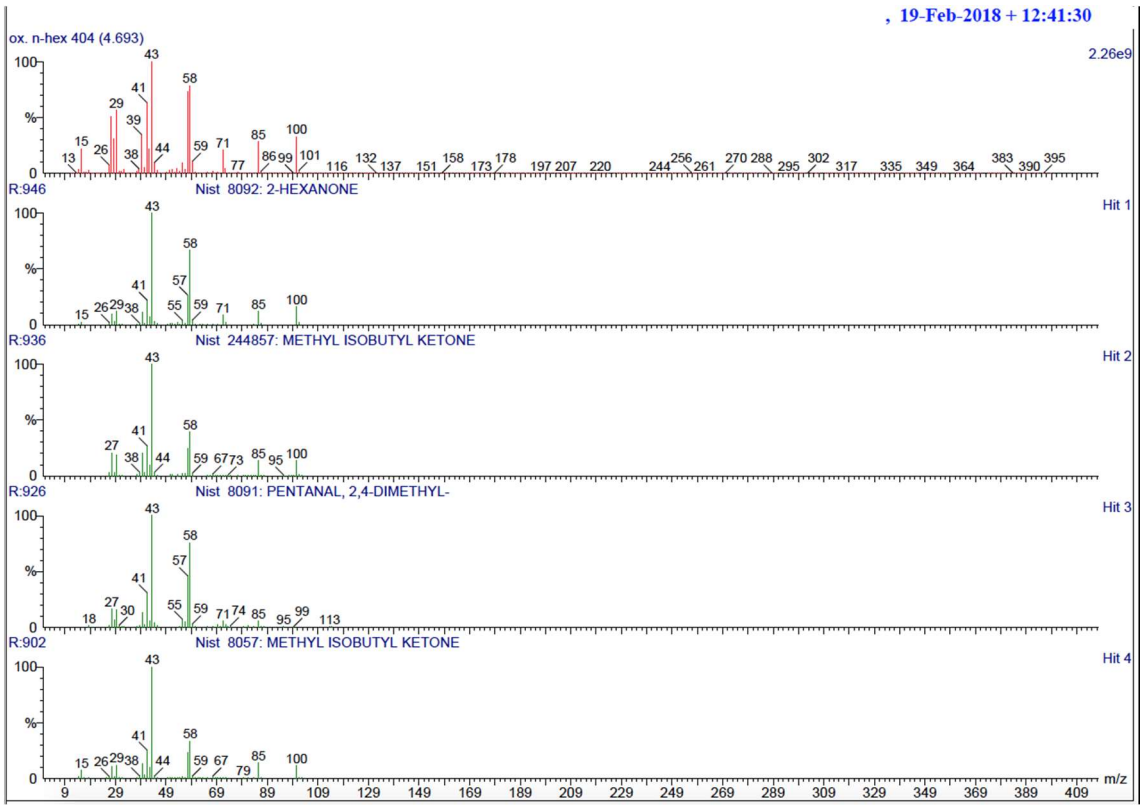
(a2)

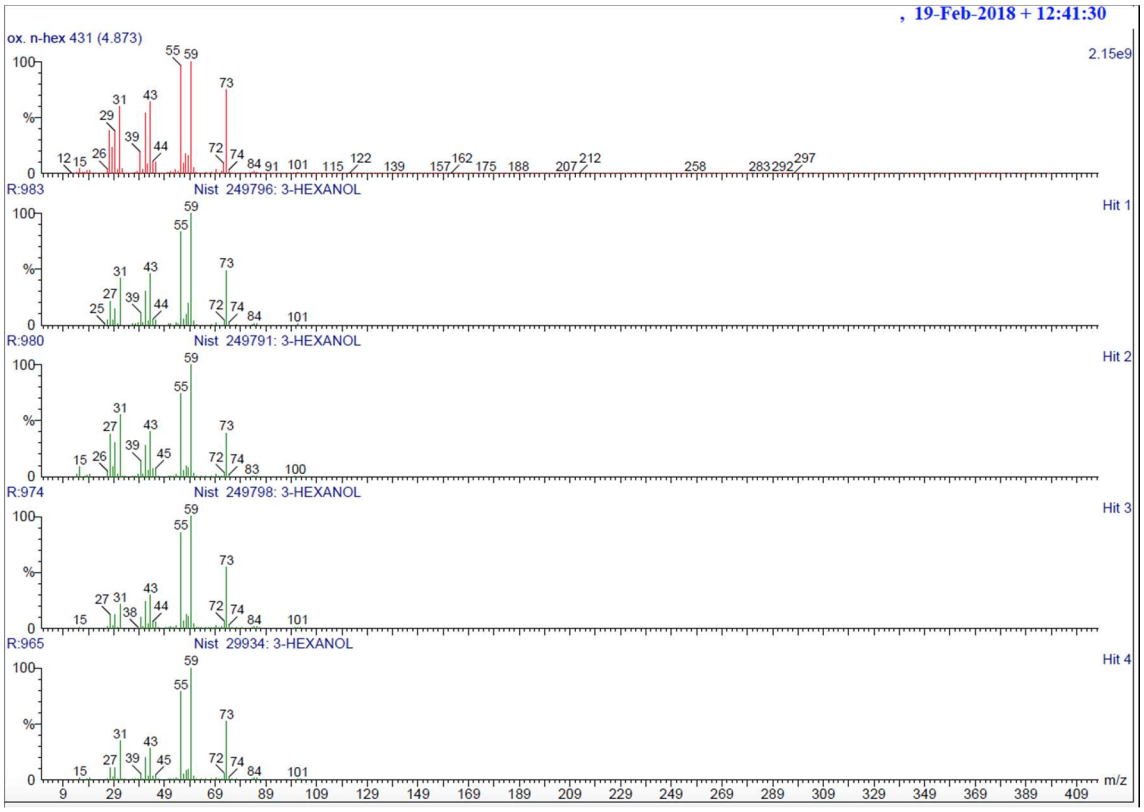

, 19-Feb-2018 + 12:41:30
ox. n-hex int.
Scan EI+
TIC
3.38e10
100
Area
%
0
2.94
480436384
3.01
1299235
4.59
11021600
4.99
1060671616
6.53
3772921
8.03
623901
8.89
2944756
9.56
375947904
10.50
4243265
12.49
537936
13.00
581102
13.97
1915283
14.66
1279672
16.28
1166545
16.76
320313
Time
2.50
3.50
4.50
5.50
6.50
7.50
8.50
9.50
10.50
11.50
12.50
13.50
14.50
15.50
16.50

(b)


, 19-Feb-2018 + 12:41:30
ox.n-hex 7 (2.045)
1.39e9
R:931
Nist 248320: N-HEXANE
Hit 2
R:921
Nist 23128: BUTYL ISOCYANATOACETATE
Hit 3
R:896
Nist 24859: HEPTANE, 2,2-DIMETHYL-
Hit 4
R:885
Nist 247917: PENTANE, 2,3-DIMETHYL-
Hit 5
m/z


, 19-Feb-2018 + 12:41:30
ox. n-hex 143 (2.952)
1.37e9
R:980
Nist 9988: 2-PENTANONE
Hit 1
R:976
Nist 245405: 2-PENTANONE
Hit 2
R:965
Nist 244384: 2-BUTANONE, 3-METHYL-
Hit 3
R:946
Nist 9987: 2-BUTANONE, 3-METHYL-
Hit 4
m/z


, 19-Feb-2018 + 12:41:30
ox. n-hex 404 (4.693)
2.26e9
R:946
Nist 8092: 2-HEXANONE
Hit 1
R:936
Nist 244857: METHYL ISOBUTYL KETONE
Hit 2
R:926
Nist 8091: PENTANAL, 2,4-DIMETHYL-
Hit 3
R:902
Nist 8057: METHYL ISOBUTYL KETONE
Hit 4
m/z


, 19-Feb-2018 + 12:41:30
ox. n-hex 431 (4.873)
2.15e9
R:983
Nist 249796: 3-HEXANOL
Hit 1
R:980
Nist 249791: 3-HEXANOL
Hit 2
R:974
Nist 249798: 3-HEXANOL
Hit 3
R:965
Nist 29934: 3-HEXANOL
Hit 4
m/z

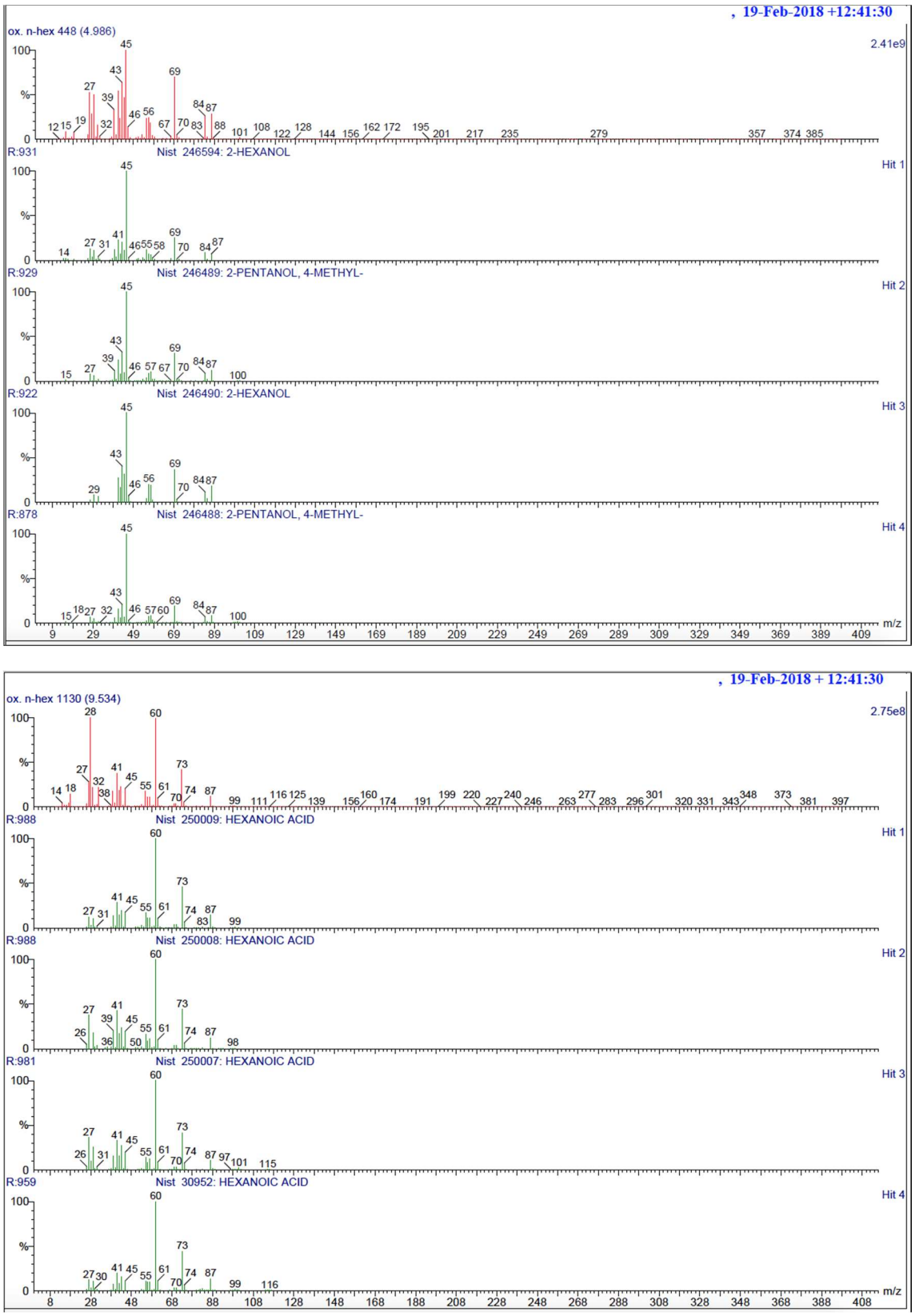
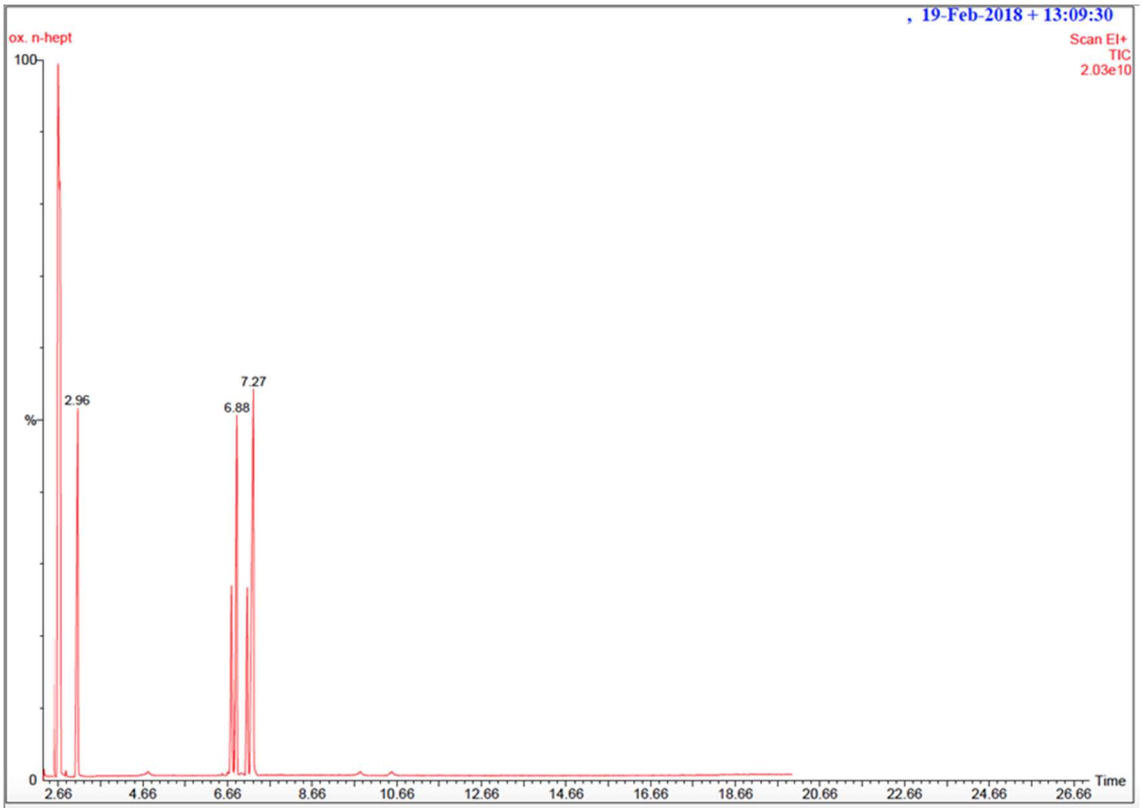
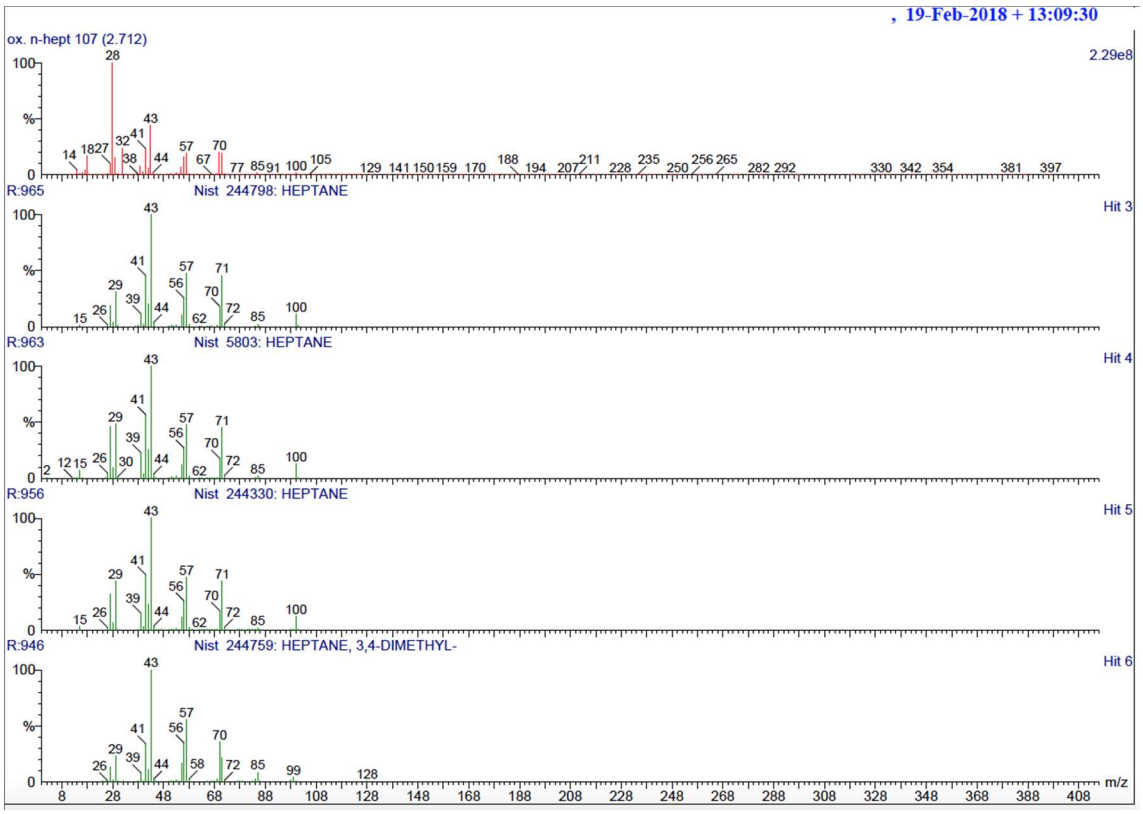


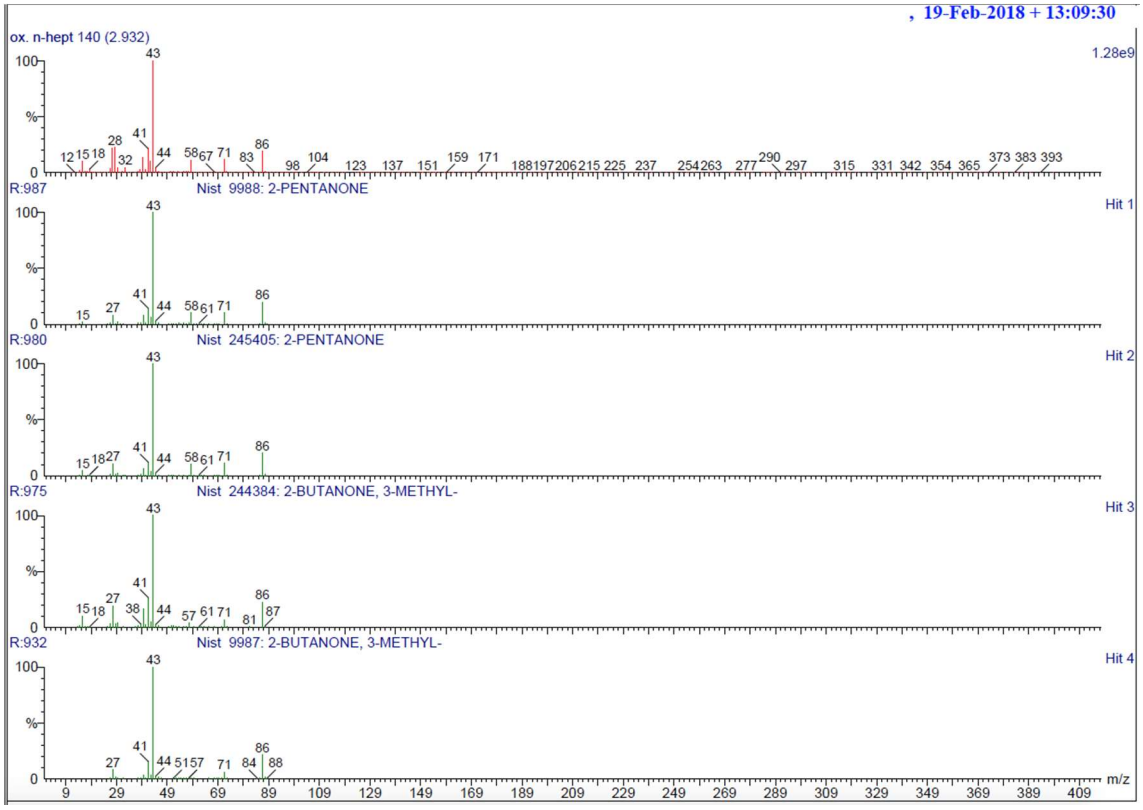
Figure S1. (a1)Exemplary GC-MS chromatogram from the *n*-hexane oxidation with O_2 catalyzed by **C** [$p(O_2)$ = 12 atm, 8 h]; internal standard: 2-pentanone; (a2) integrated chromatogram; (b) fragmentation patterns of selected retention times, obtained from the NIST spectral library stored in the computer software of the mass spectrometer).

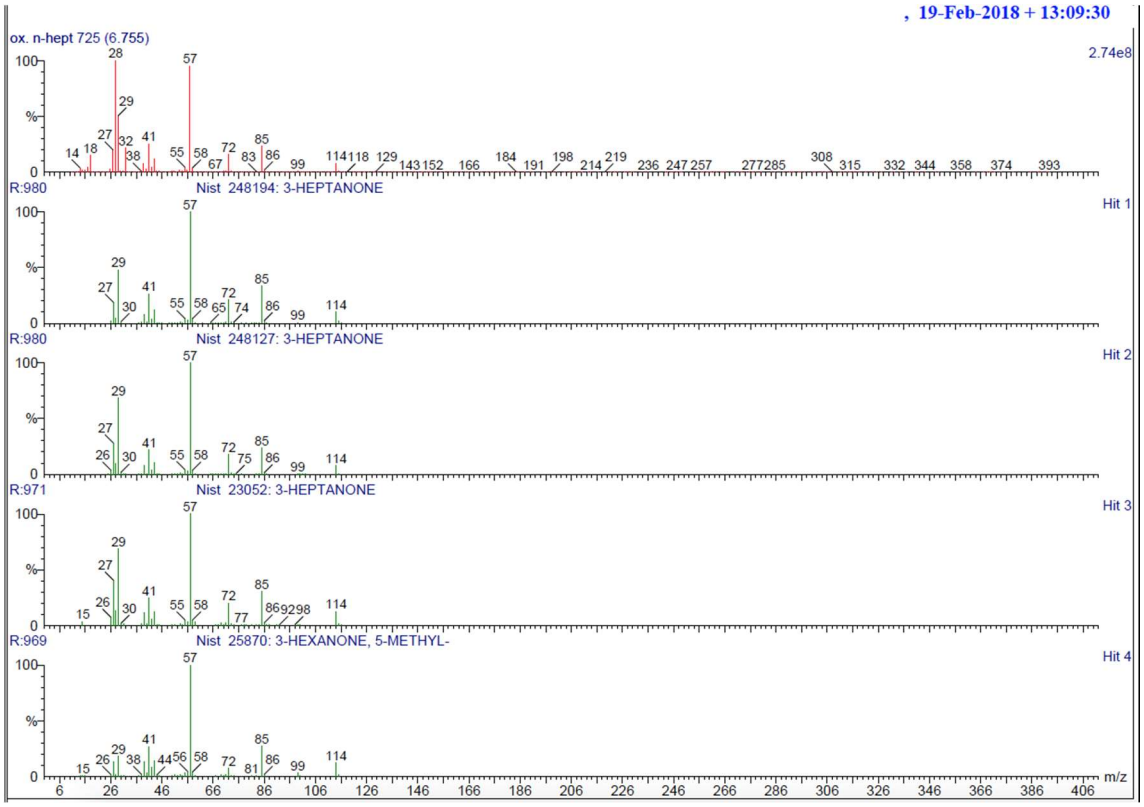
(a)

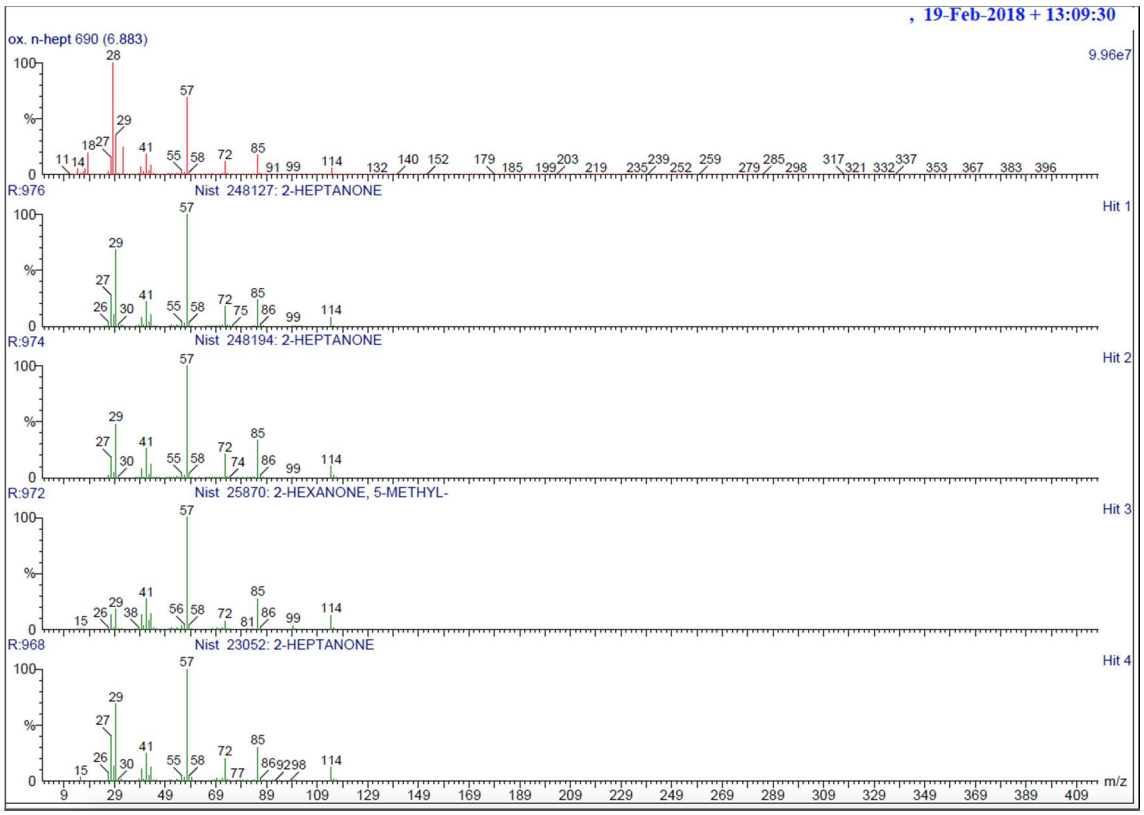

, 19-Feb-2018 + 13:09:30
ox. n-hept
Scan EI+
TIC
2.03e10
100
%
0
2.96
6.88
7.27
Time
2.66
4.66
6.66
8.66
10.66
12.66
14.66
16.66
18.66
20.66
22.66
24.66
26.66

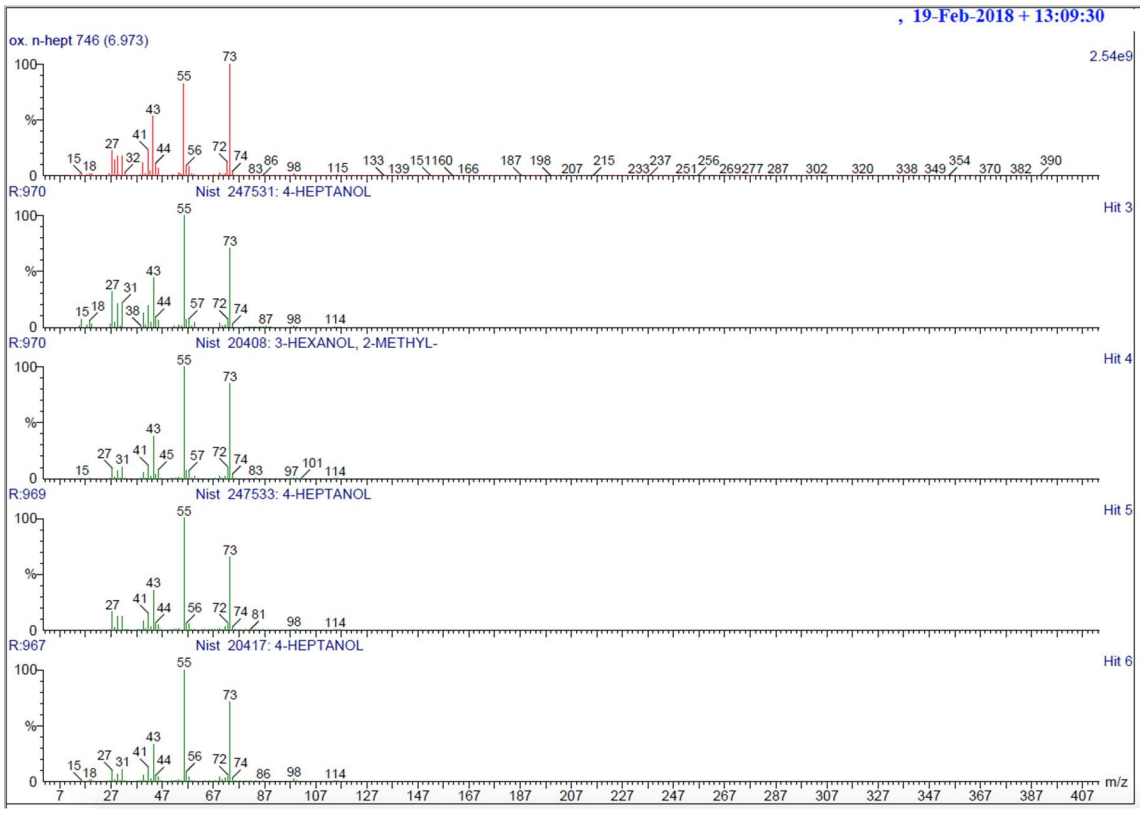
(b)


, 19-Feb-2018 + 13:09:30
ox. n-hept 107 (2.712)
2.29e8
R:965
Nist 244798: HEPTANE
Hit 3
R:963
Nist 5803: HEPTANE
Hit 4
R:956
Nist 244330: HEPTANE
Hit 5
R:946
Nist 244759: HEPTANE, 3,4-DIMETHYL-
Hit 6
m/z


, 19-Feb-2018 + 13:09:30
ox. n-hept 140 (2.932)
1.28e9
R:987
Nist 9988: 2-PENTANONE
Hit 1
R:980
Nist 245405: 2-PENTANONE
Hit 2
R:975
Nist 244384: 2-BUTANONE, 3-METHYL-
Hit 3
R:932
Nist 9987: 2-BUTANONE, 3-METHYL-
Hit 4
m/z


, 19-Feb-2018 + 13:09:30
ox. n-hept 725 (6.755)
2.74e8
R:980
Nist 248194: 3-HEPTANONE
Hit 1
R:980
Nist 248127: 3-HEPTANONE
Hit 2
R:971
Nist 23052: 3-HEPTANONE
Hit 3
R:969
Nist 25870: 3-HEXANONE, 5-METHYL-
Hit 4
m/z


, 19-Feb-2018 + 13:09:30
ox. n-hept 690 (6.883)
9.96e7
R:976
Nist 248127: 2-HEPTANONE
Hit 1
R:974
Nist 248194: 2-HEPTANONE
Hit 2
R:972
Nist 25870: 2-HEXANONE, 5-METHYL-
Hit 3
R:968
Nist 23052: 2-HEPTANONE
Hit 4
m/z


, 19-Feb-2018 + 13:09:30
ox. n-hept 746 (6.973)
2.54e9
R:970
Nist 247531: 4-HEPTANOL
Hit 3
R:970
Nist 20408: 3-HEXANOL, 2-METHYL-
Hit 4
R:969
Nist 247533: 4-HEPTANOL
Hit 5
R:967
Nist 20417: 4-HEPTANOL
Hit 6
m/z

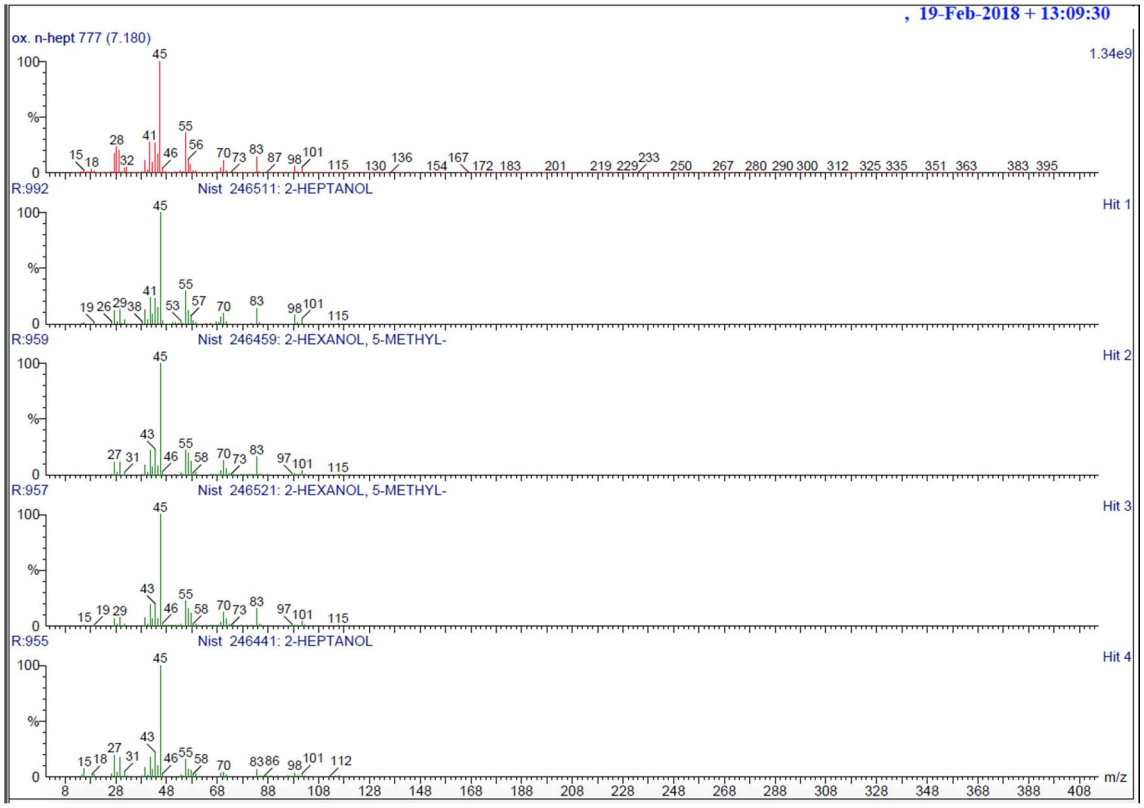


Figure S2. (a)Exemplary GC-MS chromatogram from the *n*-heptane oxidation with O_2 catalyzed by **C** [$p(O_2)$ = 10 atm, 8 h]; internal standard: 2-pentanone; (b) fragmentation patterns of selected retention times, obtained from the NIST spectral library stored in the computer software of the mass spectrometer).