Electronic Supplementary Information (ESI) for

Oxidation of a wood extractive betulin to biologically active oxo-derivatives using supported gold catalysts

Ekaterina N. Kolobova,[a] Ekaterina G. Pakrieva,[a] Sonia A.C. Carabineiro,[b] Nina E. Bogdanchikova,[c] Andrey N. Kharlanov,[d] Sergey O. Kazantsev,[e] Jarl Hemming,[f] Päivi Mäki-Arvela,[f] Alexey N. Pestryakov,[a] Dmitry Yu. Murzin*[f]

[a] Research School of Chemistry & Applied Biomedical Sciences, Tomsk Polytechnic University, Lenin Avenue 30, 634050 Tomsk, Russia

[b] Laboratory of Catalysis and Materials (LCM), Associate Laboratory LSRE-LCM, Department of Chemical Engineering, Faculty of Engineering, University of Porto, Rua Dr Roberto Frias s/n, 4200-465 Porto, Portugal

[c] Centro de Nanociencias y Nanotecnología, UNAM, Post box 14, 22860 Ensenada, México

[d] Department of Chemistry, M.V. Lomonosov Moscow State University, Leninskie Gory, 119991 Moscow, Russia

[e] Institute of Strength Physics and Materials Science of Siberian Branch of Russian Academy of Sciences (ISPMS SB RAS), pr. Akademicheskii 2/4, 634055 Tomsk, Russia

[f] Johan Gadolin Process Chemistry Centre, Abo Akademi University, FI-20500 Turku, Finland

*corresponding author: dmurzin@abo.fi; Fax:+ 358 2 215 4479; Tel: +358 2 215 4985

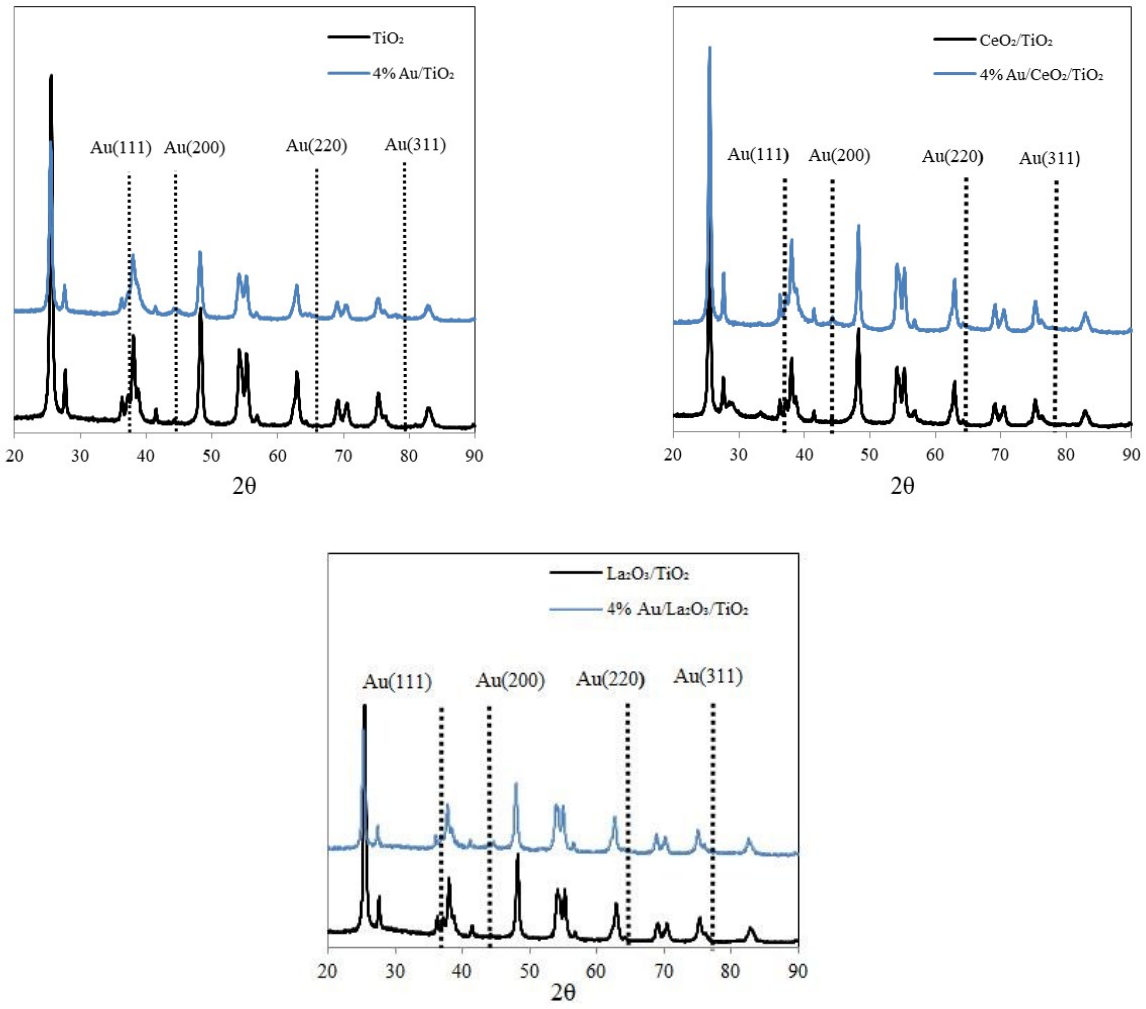


Figure S1. XRD patterns for gold catalysts and the corresponding supports.

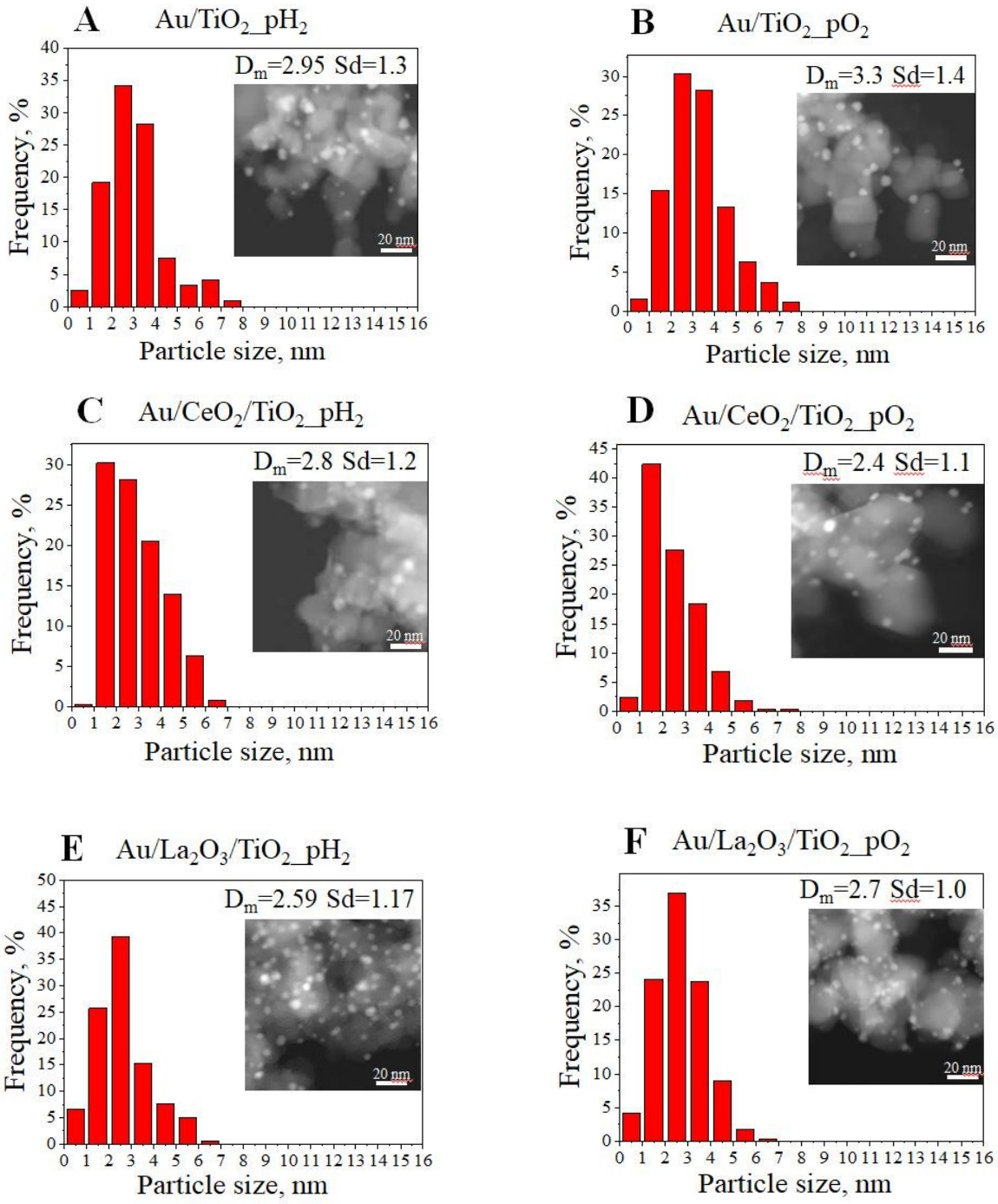
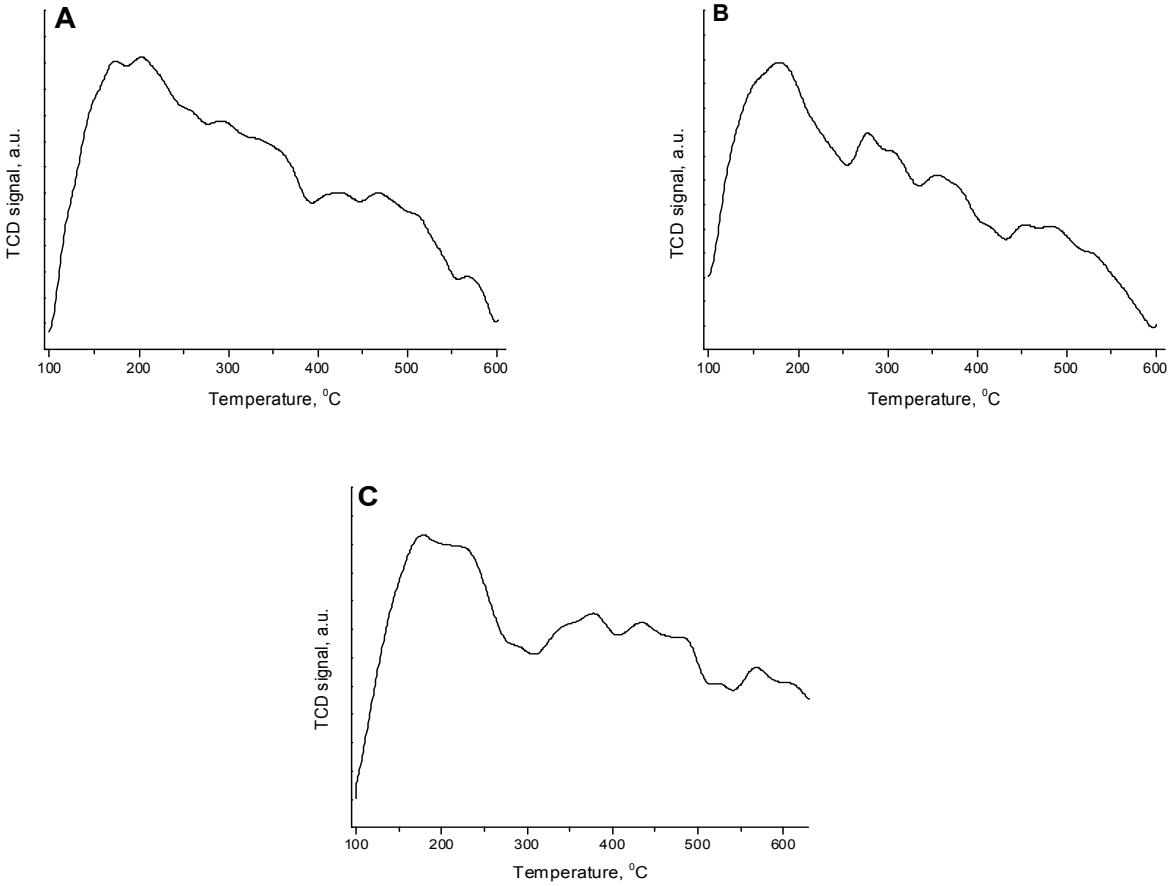
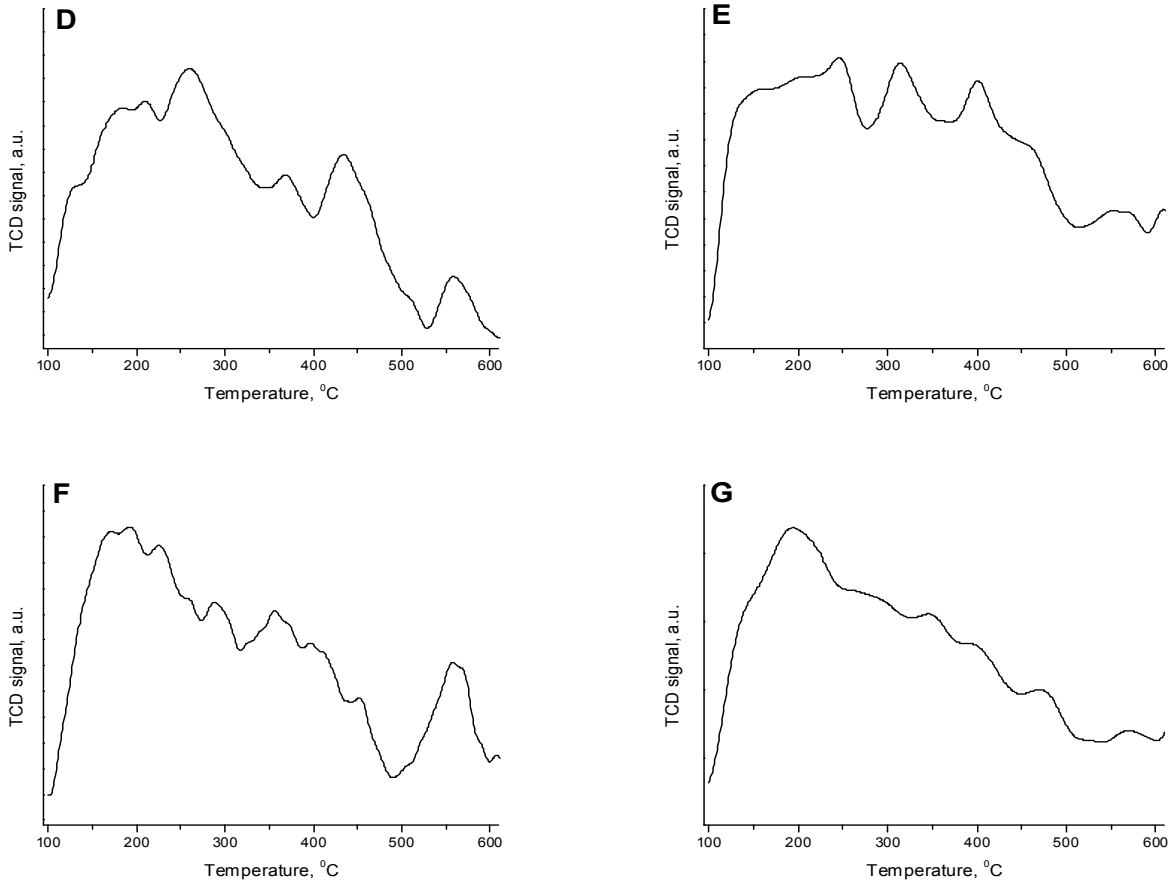


Figure S2. Au particle size distribution and TEM/STEM micrographs of studied catalysts, previously published in[1].


A
B
C
TCD signal, a.u.
100
200
300
400
500
600
Temperature, °C


D
E
F
G
TCD signal, a.u.
100
200
300
400
500
600
Temperature, °C

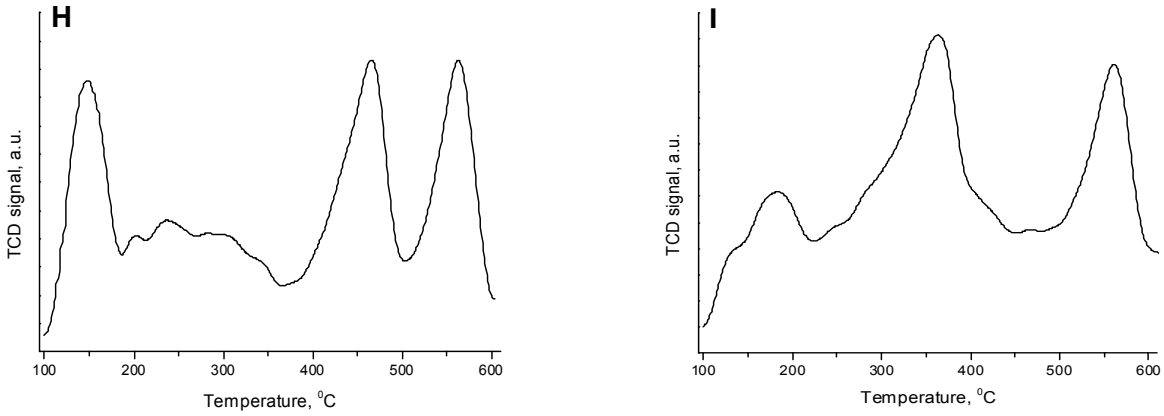
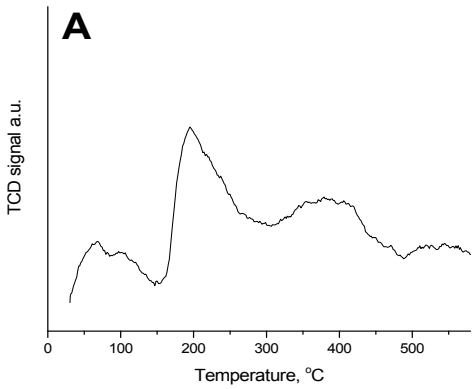
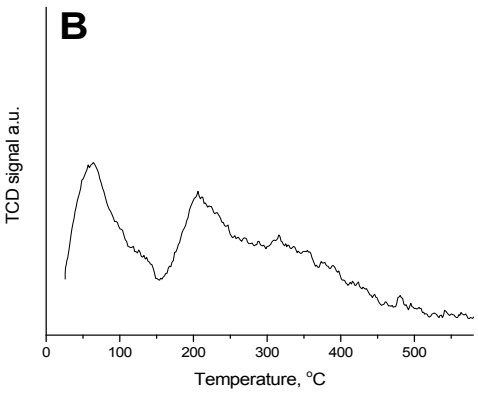
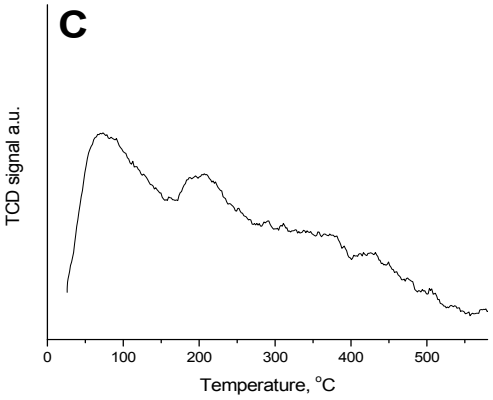
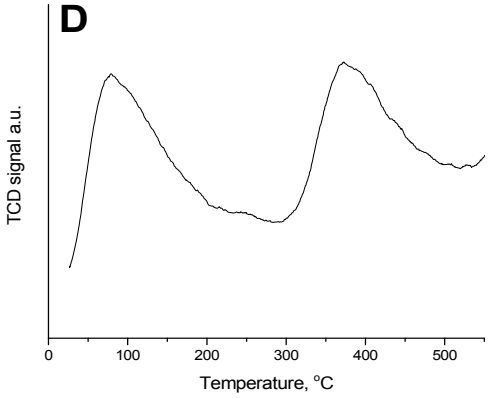


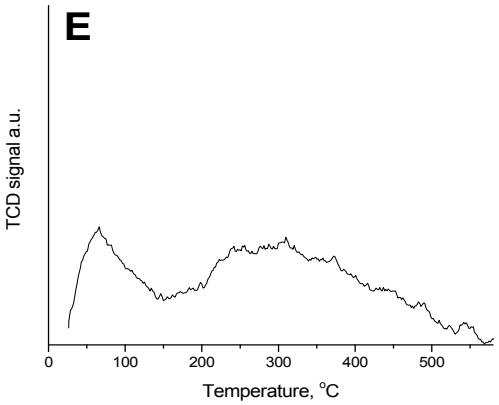
Figure S3. NH_3-TPD profiles of (A) TiO_2, (B) CeO_2/TiO_2, (C) La_2O_3/TiO_2, (D) $Au/TiO_2\_pH_2$, (E) $Au/TiO_2\_pO_2$, (F) $Au/CeO_2/TiO_2\_pH_2$, (G) $Au/CeO_2/TiO_2\_pO_2$, (H) $Au/La_2O_3/TiO_2\_pH_2$, (I) $Au/La_2O_3/TiO_2\_pO_2$

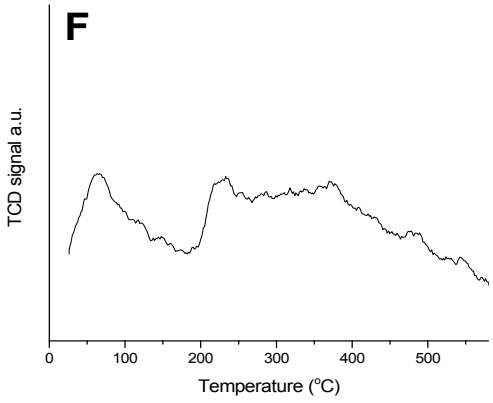

A
TCD signal a.u.
0
100
200
300
400
500
Temperature, °C


B
TCD signal a.u.
0
100
200
300
400
500
Temperature, °C


C
TCD signal a.u.
0
100
200
300
400
500
Temperature, °C


D
TCD signal a.u.
0
100
200
300
400
500
Temperature, °C


E
TCD signal a.u.
0
100
200
300
400
500
Temperature, °C


F
TCD signal a.u.
0
100
200
300
400
500
Temperature (°C)

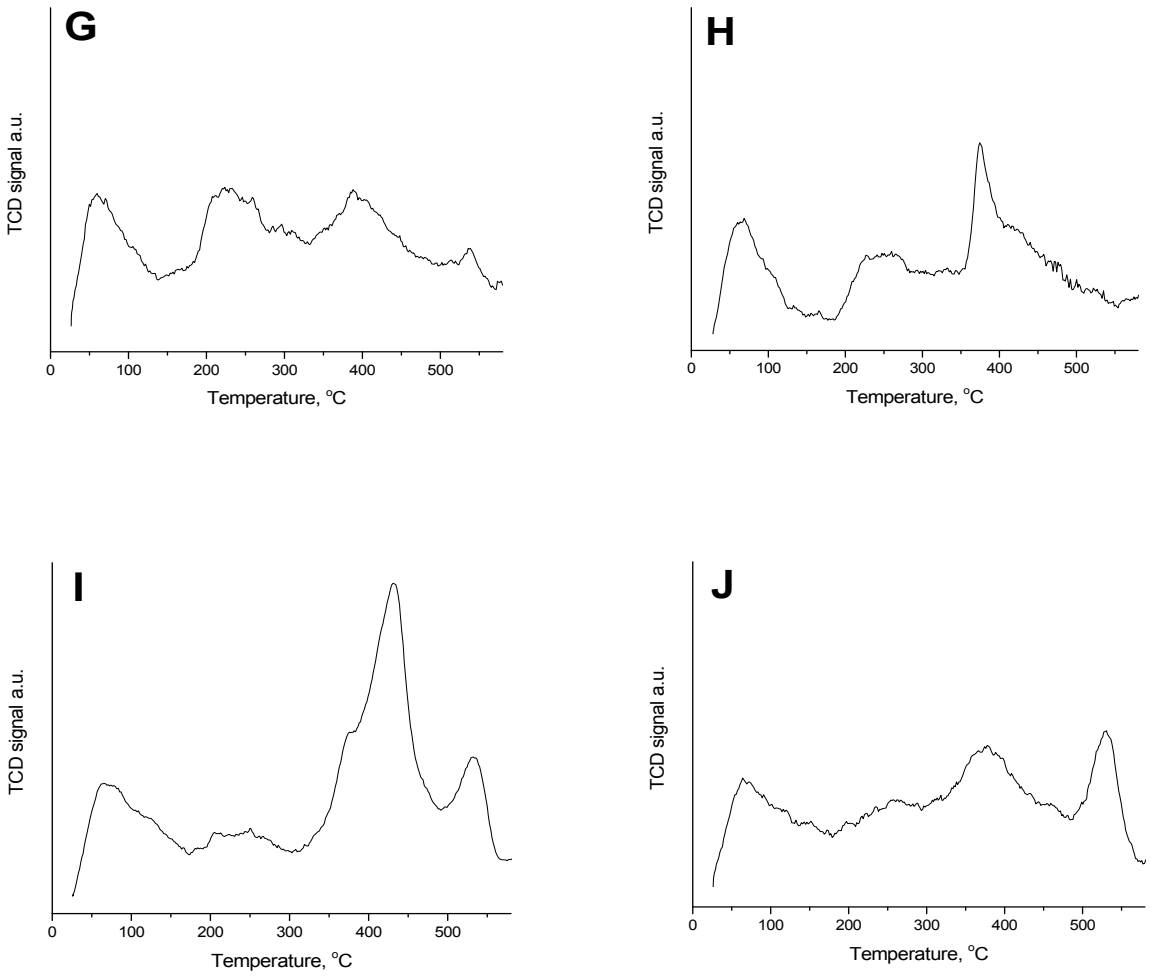


Figure S4. CO_2-TPD profiles of (A) TiO_2, (B) CeO_2/TiO_2, (C) La_2O_3/TiO_2, (D) Hydrotalcite; (E) $Au/TiO_2\_pH_2$, (F) $Au/TiO_2\_pO_2$, (G) $Au/CeO_2/TiO_2\_pH_2$, (H) $Au/CeO_2/TiO_2\_pO_2$, (I) $Au/La_2O_3/TiO_2\_pH_2$, (J) $Au/La_2O_3/TiO_2\_pO_2$

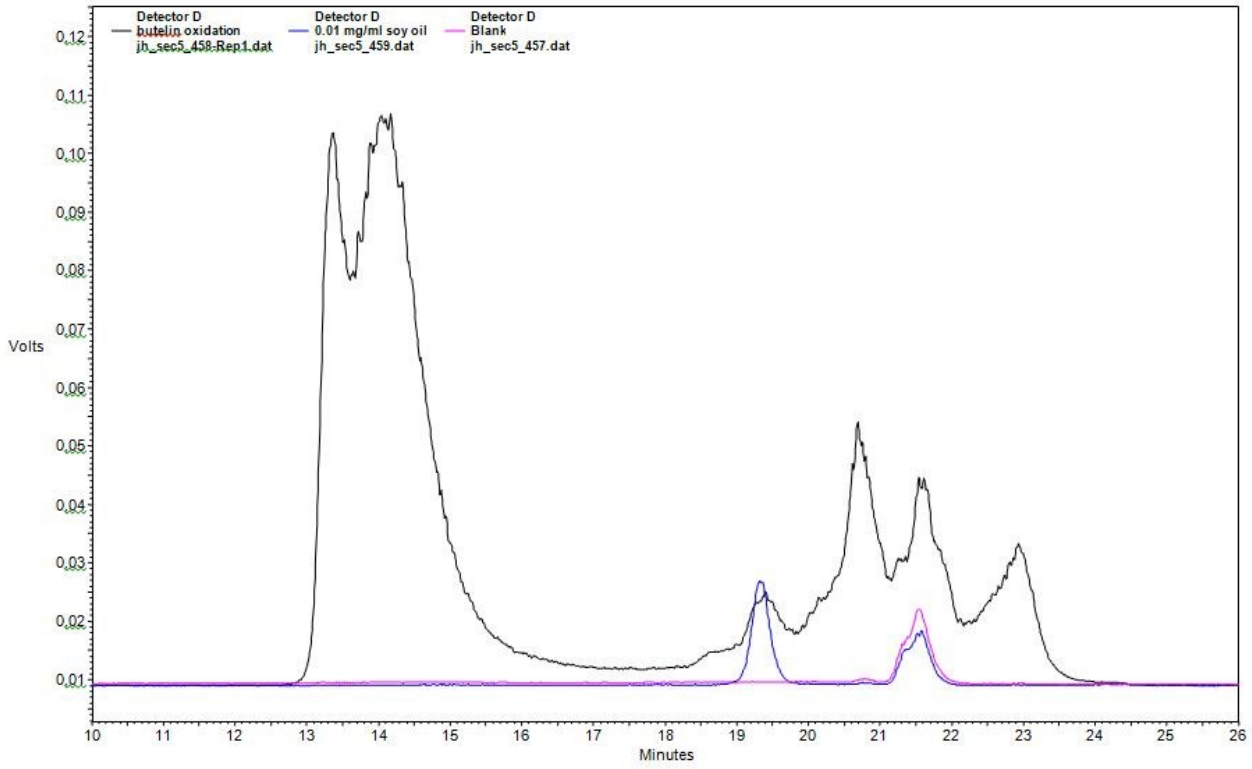


Figure S5. SEC chromatogram of extracted oligomers and polymers from surface of spent catalyst.

Table S1. Calculated rate constants

Constant	Units	Value
ρk_1	s^{-1}	0.016
ρk_2	s^{-1}	0.06
ρk_4	s^{-1}	0.05
ρk_5	s^{-1}	0.22
ρk_{-5}	s^{-1}	1.1
K_D	-	183

Reference

[1] E. Pakrieva, E. Kolobova, G. Mamontov, N. Bogdanchikova, M. H. Farias, L. Pascual, V. Cortés Corberán, S. Martinez Gonzalez, S. A. C. Carabineiro, A. Pestryakov. Green oxidation of n-octanol on supported nanogold catalysts: Formation of gold active sites under combined effect of gold content, additive nature and redox pretreatment, *ChemCatChem* **2019**, 11, 1–11.