Supplementary material.

Table S1. Activity immobilization yield for CALB on anionic exchangers.

Support	Activity immobilization yield (%)*
Amberlite® IRA910	5.35 ± 0.92
Amberlite®IRA958	2.24 ± 1.09
Lewatit® MP 800	11.7 ± 0.5
Nekrolith® RAM 1	19.6 ± 1.4
Purolite® ECR1604	1.20 ± 0.27

* At 25 °C and pH 10 in 10 mM sodium carbonate buffer. The supports were previously equilibrated with this buffer.

Table S2. Composition of the palm olein used in this work.

Fatty acid	Structure	Average composition (%)
Palmitic	16:0	37.63
Oleic	18:1	44.08
Linoleic	18:2	12.66
Stearic	18:0	4.93
Myristic	14:0	0.70

(Average oil MW: 854.41 g/mol)

Figure S1. Chromatogram of palm olein ethyl esters.

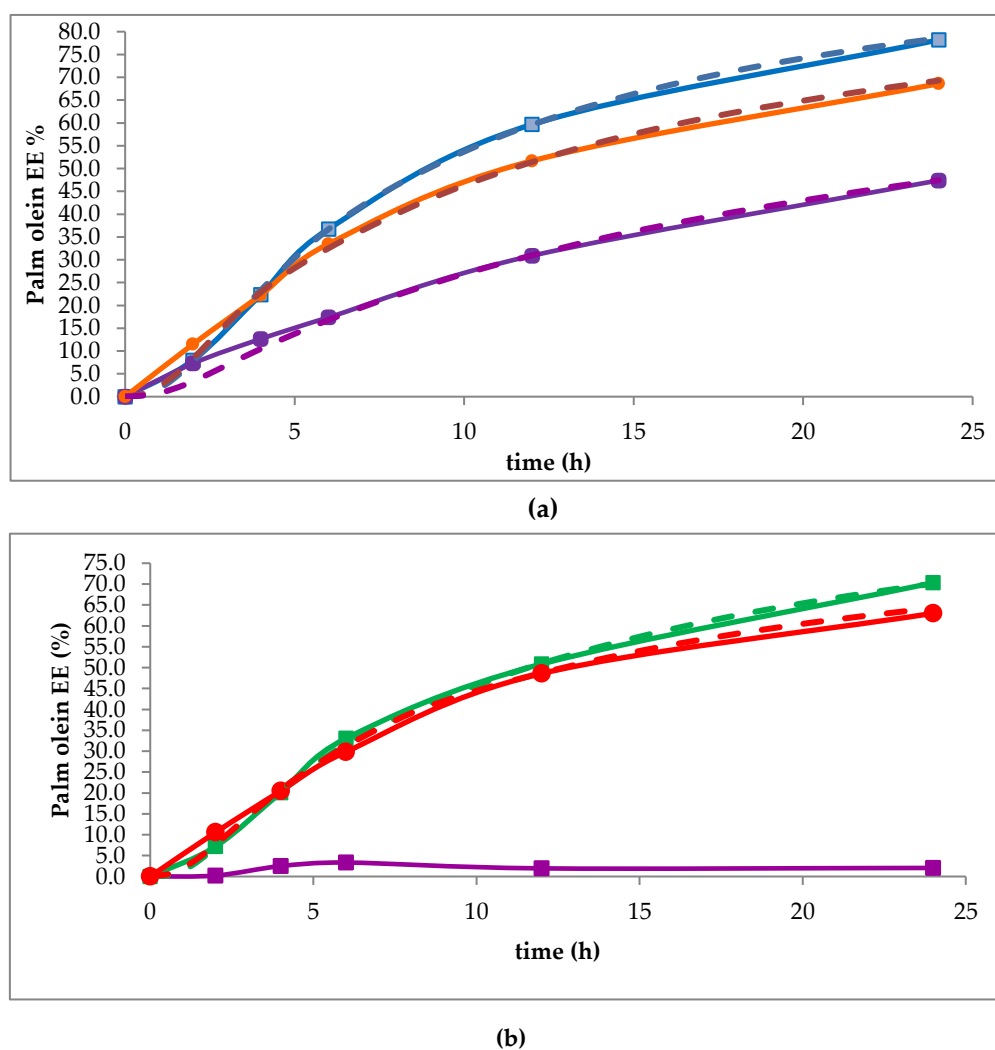| Peak	Fatty acid	Retention time, min	Area
1	Myristic	19,26	1548914
2	Palmitic	22,16	71726084
3	Linoleic	24,41	25058922
4	Oleic	24,48	88851277
5	Stearic	24,78	8719987

Figure S2

(a)

(b)
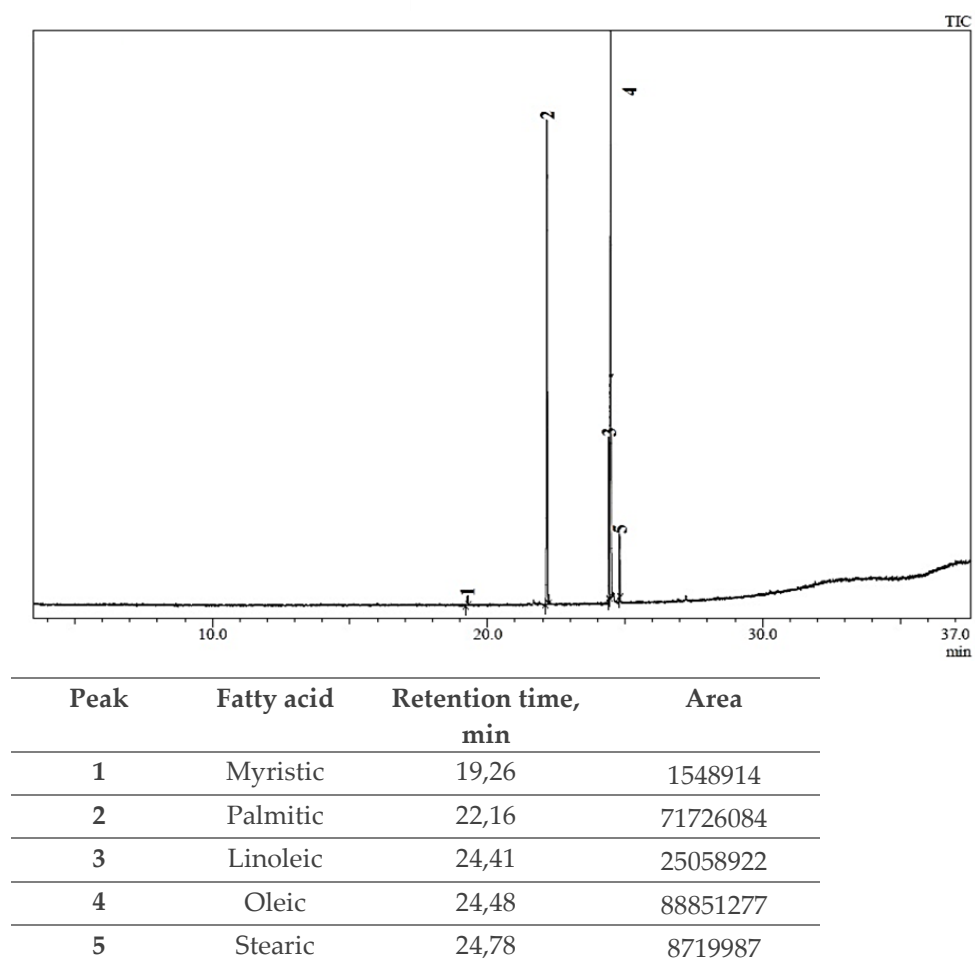
Figure S2. Time-course of EE production for lipase derivatives **(a)** on LW: TLL (blue), RML (orange) and CALB (Purple); **(b)** on PU (lower panel): TLL (green), RML (red) and CALB (orchid). The discontinuous lines represent the results of simulations (Kinetiscope 1.1.8) using the parameters indicated in Table S2 and Table S3 (see below). Error bars not shown for clarity (in all cases, S.D. below 5% units).

Table S3. Values of the adjusted parameters used for the simulation of the reaction course of EE production for the obtained derivatives.

Step [a]	K [b]	Value of $k_{forward}$				
		TLL-LW	CALB-LW	RML-LW	TLL-PU	RML-PU
T + E ↔ D + EX	2.0	700	60	550	500	550
D + E ↔ M + EX	2.0	160	7000	200	350	200
M + E ↔ G + EX	3.2	200	4000	200	350	155
C + EX ↔ B + E	16 [c]	64000	16000	8000	32000	16000
Other processes	K	Other parameters $k_→/k_←$				
T_{bulk} → T [d]	NA	0.00450				
C_{bulk} → C [d]	NA	10				
B → B_{bulk} [d]	NA	0.0270				
M+D+B+G+T_{bulk}+C_{bulk}→ T+C+M+D+G_{bulk}+B_{bulk}[e]	NA	100				
F + E ↔ EF [f]	--	12000/80	NA	NA	12000/80	NA
F + E* ↔ EX [g]	NA	NA	1×10^5/1	1×10^5/1	NA	1×10^5/1
G + E ↔ EG [h]	--	1200/115	1200/50	1200/80	1200/35	1200/50
C + E → EC [i]	NA	5×10^{-5}	5×10^{-5}	1.5×10^{-3}	2×10^{-4}	1×10^{-3}

[a] T (triglyceride), E (enzymatic component), D (diglyceride), EX (acylated enzyme), M (monoglyceride), G (glycerol), C (alcohol), B (Biodiesel), [b] Calculated value according to the kinetic constants and [c] value of the reversible constant when M acts as an effector in the alcoholysis of the acylated enzyme [15]. [d] Transfer of liquid reactants/product to/from the solid reactive biocatalyst surface, [e] M and D as positive effectors in the reactant/product transfer, [f] inhibition by free fatty acids, [g] esterification of free fatty acids, [h] esterification of free fatty acids and [i] inactivation by alcohol [14,15]. NA (Not applicable).

Table S4. Initial reaction conditions for the simulations using Kinetiscope 1.1.8.

Species described in Table S2	Concentration (mol/L)	Calculated initial number of particles
C_{bulk} (ethanol)	2.75	377601
E*	0.00003	4
E2*	0.00003	4
F	0.00435	597
T_{bulk} (oil)	0.887	121793
Total	-	500000
Random number seed		12947

C_{bulk} (initial ethanol concentration); E and E2 (enzyme concentration contributed by C1 and C2 derivatives, respectively, depending on the CL composition); T_{bulk} (initial palm olein concentration). *The values of E and E2 were changed to represent a CL of a desired composition maintaining the total number of active particles (8): in this example, it is represented a CL of a 50% of each mono-lipasic component C1 and C2. Other values were set according to the reaction conditions described in Section 3.3.