

SUPPORTING INFORMATION FOR PUBLICATION

TITLE:

The Effect of Reaction Medium Mixture on The Lipase Catalyzed Synthesis of Diacylglycerol

AUTHORS:

Nurul Nadiah Abd Razak^{1,2}, Yolande Pérès², Lai Ti Gew^{*1}, Patrick Cognet², Mohamed Kheireddine Aroua^{*3,4}.

1. Department of Biological Sciences, School of Science and Technology, Sunway University, No. 5, Jalan Universiti, Bandar Sunway, 47500, Petaling Jaya, Selangor, Malaysia.
2. Laboratoire de Génie Chimique, Université de Toulouse, CNRS, INPT, UPS, Toulouse, France.
3. Centre for Carbon Dioxide Capture and Utilization (CCDCU), School of Science and Technology, Sunway University, No. 5, Jalan Universiti, Bandar Sunway, 47500, Petaling Jaya, Malaysia.
4. Department of Engineering, Lancaster University, Lancaster, LA1 4YW, United Kingdom.

***CORRESPONDING AUTHORS:**

Professor Dr. Mohamed Kheireddine Aroua

Centre for Carbon Dioxide Capture and Utilization (CCDCU), School of Science and Technology, Sunway University, Malaysia.

Email: kheireddinea@sunway.edu.my

Dr. Lai Ti Gew

Department of Biological Sciences, School of Science and Technology, Sunway University, Malaysia.

Email: janeg@sunway.edu.my

Table S1. The definition of symbols and abbreviation used in this study

Symbol & abbreviation	Details description
$[Gly]_{eq}$	Glycerol concentration (mol L ⁻¹) at equilibrium which was calculated from the initial glycerol concentration and minus the total concentration of esters formed at equilibrium.
$[GO]_{max}$	The maximum molar concentration (mol L ⁻¹) of glycerol oleates achieved.
$[GO]_{total}$	The sum of molar concentrations (mol L ⁻¹) of glycerol oleates (GMO, GDO and GTO).
$[GMO]_{eq}$	GMO concentration (mol L ⁻¹) at equilibrium
$[GDO]_{eq}$	GDO concentration (mol L ⁻¹) at equilibrium
$[GTO]_{eq}$	GTO concentration (mol L ⁻¹) at equilibrium
$[H_2O]_{eq}$	water concentration (in mole) at equilibrium which was calculated theoretically from the stoichiometry of glycerol oleates synthesis where 1 mole of water is produced per mole of GMO, 2 mole of water is produced per mole of GDO and 3 mole of water is produced per mole of GTO synthesized
$[OA]_{eq}$	Oleic acid concentration (mol L ⁻¹) at equilibrium
$[OA]_{initial}$	Initial concentration of oleic acid (in mole). A mass balance of oleic acid gives; $[OA]_{initial} = [OA] + [GMO] + 2[GDO] + 3[GTO]$
ΔAbs_{410nm}	absorbance difference at 410 nm at for a specific interval (min ⁻¹)
ΔG	Gibbs free energy change (J mol ⁻¹)
ΔH	enthalpy change (J mol ⁻¹)
ΔS	entropy change (J mol ⁻¹ K ⁻¹)
C_o	initial substrate concentration in bulk organic phase (M)
D	diffusion coefficient (m ² s ⁻¹)
d_{CALB}	enzyme particle size which was taken as 0.005 m
k	consistency coefficient (Pa.s ⁿ)
K_{GMO}	apparent equilibrium constant for GMO which calculated as follows; $K_{GMO} = \frac{[GMO]_{eq} [H_2O]_{eq}}{[Gly]_{eq} [OA]_{eq}}$
K_{GDO}	apparent equilibrium constant for GDO which calculated as follows; $K_{GDO} = \frac{[GDO]_{eq} [H_2O]_{eq}}{[GMO]_{eq} [OA]_{eq}}$
K_{GTO}	apparent equilibrium constant for GTO which calculated as follows; $K_{GMO} = \frac{[GTO]_{eq} [H_2O]_{eq}}{[GDO]_{eq} [OA]_{eq}}$
K_{eq}	apparent equilibrium constant for esterification reaction
k_{SL}	solute–liquid mass transfer coefficient in solvent (m s ⁻¹)
$\log P_{acetone}$	$\log P$ value of acetone
$\log P_{t-BuOH}$	$\log P$ value of <i>tert</i> -butanol
n	dimensionless flow behavior index
ϕ	Association parameter of the liquid
ϕ_{mix}	association parameter of blended liquids

[C]	Initial concentration of reactant (in mole) which referring to [OA] or [Gly]
R	Ideal gas constant (8.3145 J mol ⁻¹ K ⁻¹)
T	absolute temperature (K).
<i>M</i>	molar volume of product at its reaction temperature (m ³ mol ⁻¹)
ϕ	Thiele modulus
U	Activity unit for enzyme reaction (μ mol min ⁻¹)
<i>r</i> _[GO]	Initial esterification rate of glycerol oleates (M h ⁻¹)
<i>Q</i> _{total}	total assay volume (mL)
<i>Q</i> _{<i>p</i>Npp}	volume of <i>p</i> Npp (mL)
<i>W</i>	molecular weight of the solvent (kg mol ⁻¹)
<i>W</i> _{mix}	molecular weight of the blended solvents (kg mol ⁻¹)
<i>X</i> _{acetone}	mole fractions of acetone in reaction mixture
<i>X</i> _{<i>t</i>-BuOH}	mole fractions of t-butanol in reaction mixture
<i>z</i>	stoichiometric coefficients. For each [GO], <i>z</i> is calculated as follows: [GMO], <i>z</i> =1; [GDO], <i>z</i> =2 and [GTO], <i>z</i> =3.
γ	shear rate (s ⁻¹)
Δ [GO]	Changes in the molar concentration (mol L ⁻¹) of glycerol oleates. Each [GO] is designated as follows; [GMO], [GDO] and [GTO] which represent the molar concentration of GMO, GDO and GTO respectively.
ΔG°	Gibbs free energy change at non-standard condition (J mol ⁻¹)
$\Delta t_{[GO]}$	Changes of time for each [GO] (h)
μ	fluid viscosity (kg m ⁻¹ s ⁻¹).
μ_{mix}	mixture of fluid viscosity (kg m ⁻¹ s ⁻¹)
ξ_{410}	extinction coefficient of <i>p</i> -nitrophenol i.e. 1070.43 L mol ⁻¹ min ⁻¹
ρ	density of the liquid (kg m ⁻³)
τ	shear stress (Pa)
τ_0	yield stress (Pa)
GMO	Glycerol monoleates
GDO	Glycerol dioleates
GTO	Glycerol trioleate
1-GMO	1-glycerol monoleates
2-GMO	2-glycerol monoleates
1,2-GDO	1,2-glycerol dioleates
1,3-GDO	1,3-glycerol dioleates
GTO	Glycerol trioleate
MAG	Monoacylglycerol
1(3)-MAG	1(3)- monoacylglycerol
2-MAG	2-monoacylglycerol
DAG	Diacylglycerol
TAG	Triacylglycerol
DGAT	DAG acyltransferase
MGAT	MAG acyltransferase

Details description of the symbols and abbreviation, apparent equilibrium constant for GMO, GDO and GTO, mass balance of oleic acid, water concentration calculation is shown in Table S1. This information is available free of charge via the Internet at <http://pubs.acs.org/>.